



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 10:05 PM EST

PDB ID : 4V9A
Title : Crystal Structure of the 70S ribosome with tetracycline.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

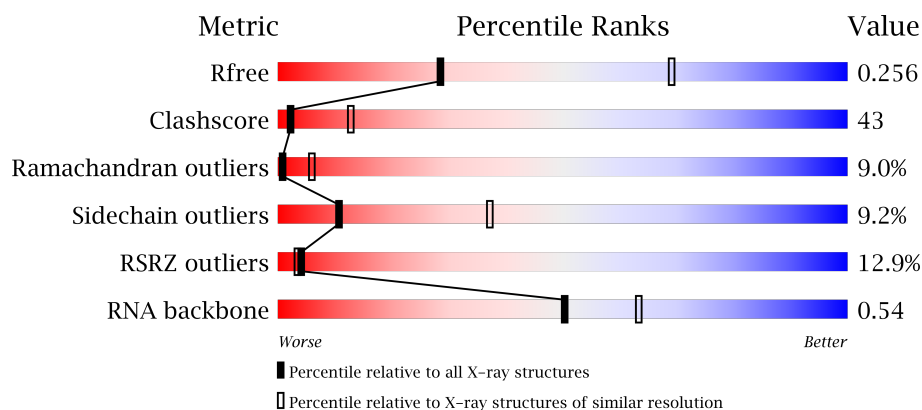
1 Overall quality at a glance

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}	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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>34%</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	

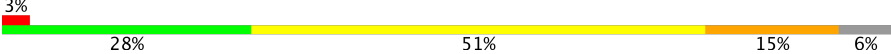
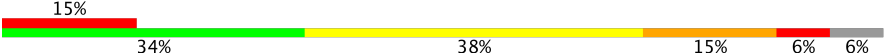
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Mol	Chain	Length	Quality of chain
40	D2	101	
41	BS	113	
41	DS	113	
42	BT	96	
42	DT	96	
43	BU	110	
43	DU	110	
44	BV	206	
44	DV	206	
45	B3	85	
45	D3	85	
46	BZ	98	
46	DZ	98	
47	BW	72	
47	DW	72	
48	BX	60	
48	DX	60	
49	B4	71	
49	D4	71	
50	B5	60	
50	D5	60	
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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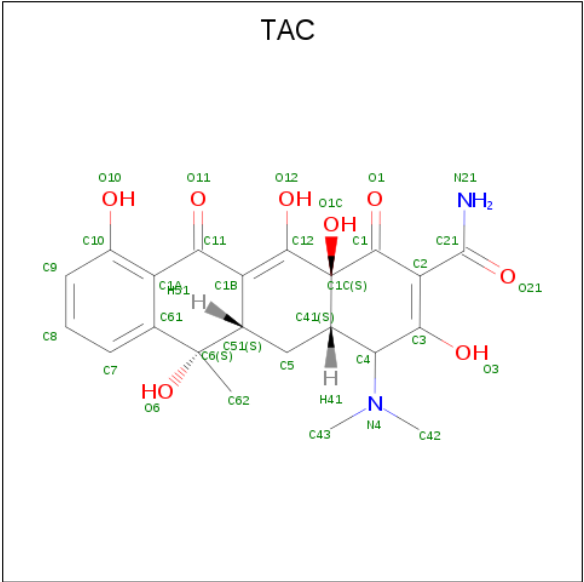
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CH	1	Total 1	Mg 1	0	0
54	DZ	2	Total 2	Mg 2	0	0
54	B8	1	Total 1	Mg 1	0	0
54	BE	5	Total 5	Mg 5	0	0
54	DU	1	Total 1	Mg 1	0	0
54	B1	2	Total 2	Mg 2	0	0
54	BP	1	Total 1	Mg 1	0	0
54	AS	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	17	Total 17	Mg 17	0	0
54	AJ	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: C₂₂H₂₄N₂O₈).



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			

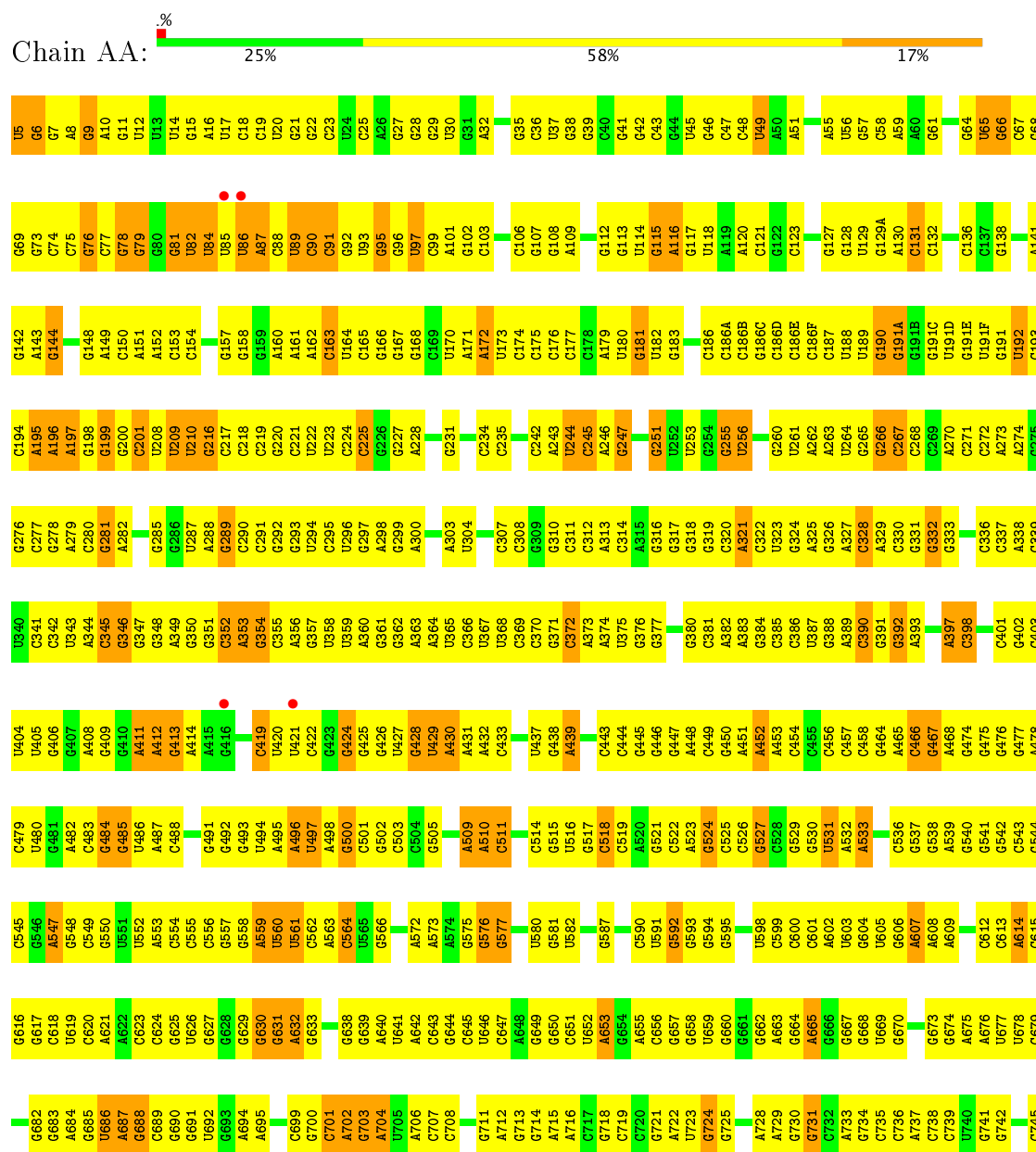
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

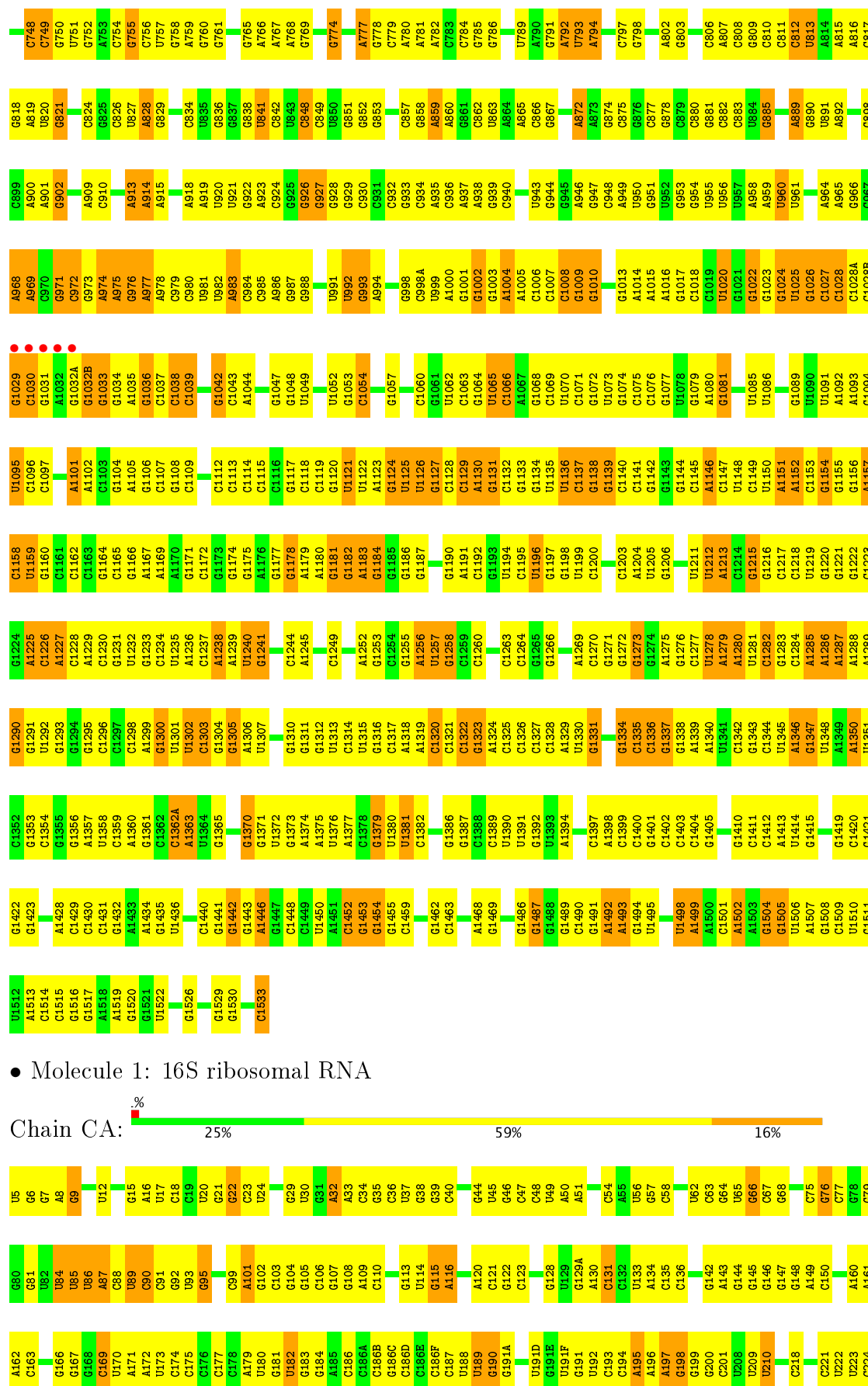
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total	Zn	0	0
			1	1		
56	AQ	1	Total	Zn	0	0
			1	1		
56	CQ	1	Total	Zn	0	0
			1	1		
56	CG	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

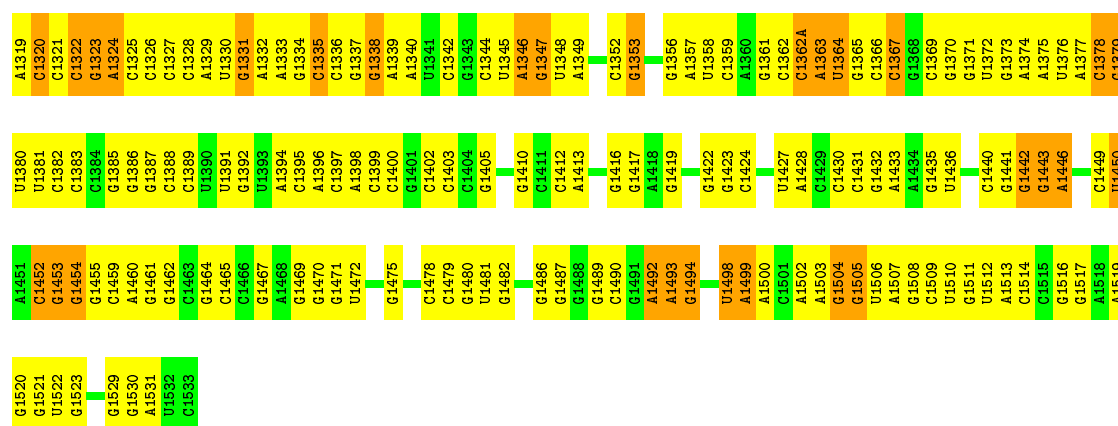
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S ribosomal RNA

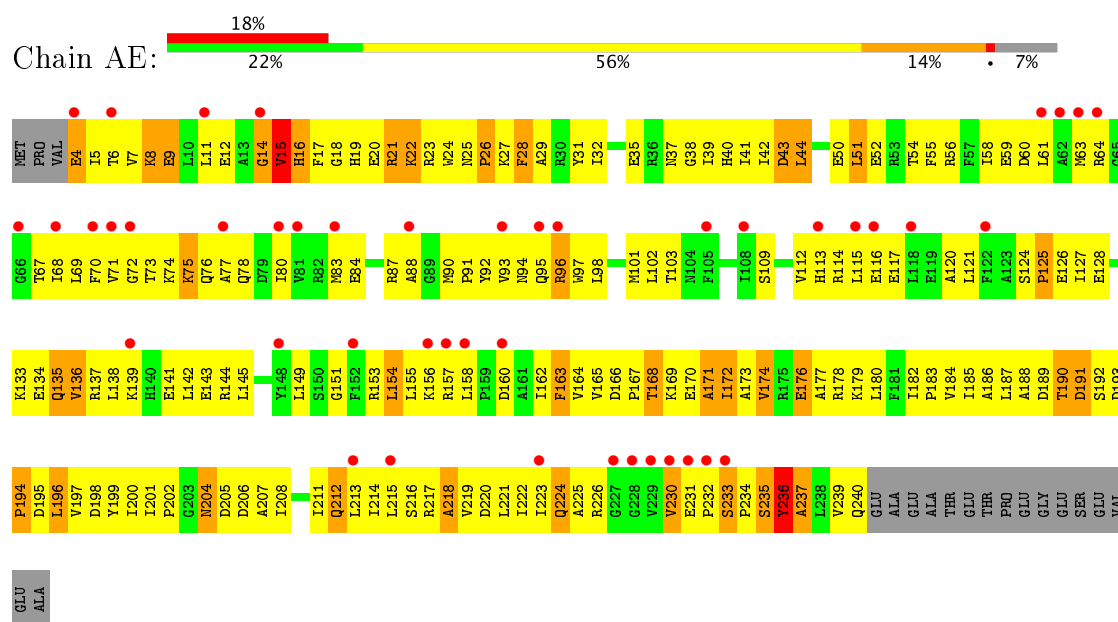




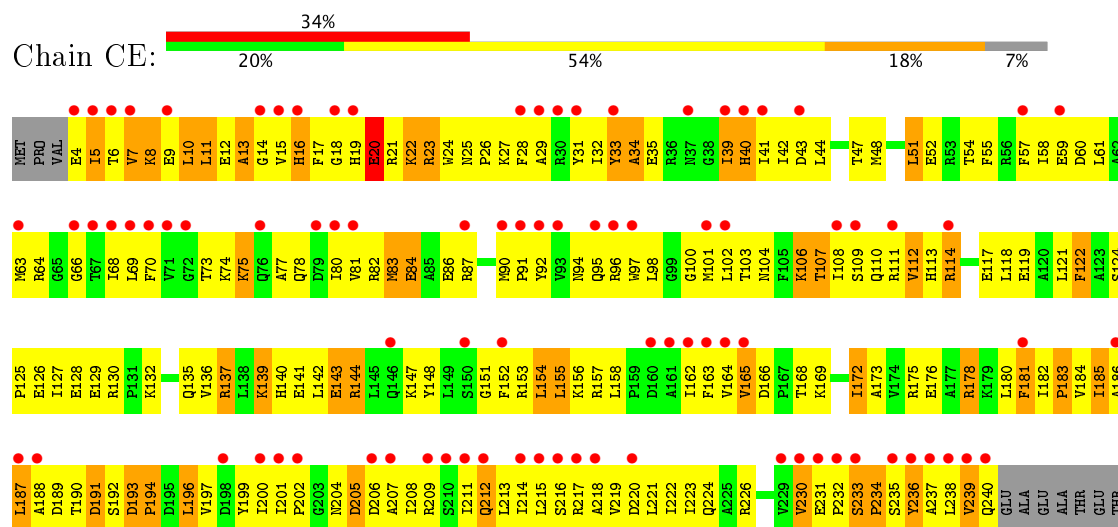
G1255	G1195	C1128	A1067	G1009	U950	G380	U801	G730	G661	G594	C528	A452	C386	G316	C225
A1256	U1196	C1129	G1068	G1010	G951	G881	A802	G731	G662	G595	G529	A453	U387	G346	G226
A1257	G1197	A1130	C1069	G1011	U952	C882	G803	U732	A663	C596	G530	C454	G388	A321	U229
G1258	G1198	G1131	U1070	U1012	G953	C883	U1012	G734	G664	G597	U531	G457	A389	C322	G230
C1259	U1199	G1132	C1071	G1013	G954	U894	C811	C735	A665	U598	A532	C458	C390	U323	G231
C1260	G1200	G1133	G1072	G1014	U955	G895	G812	C736	G666	C600	A533	C459	C392	U324	C241
A1201	A1201	A1015	U1073	A1015	U956	U896	U813	A737	U671	C601	U534	C464	A393	G324	C242
G1202	G1203	U1135	G1074	A1016	U957	A899	A814	C738	G672	A602	A535	C465	A394	G325	C243
C1203	C1203	U1136	C1075	A958	A958	G890	A815	C739	U673	G402	C536	C466	G394	A326	C244
A1204	A1204	G1137	U959	A959	A959	U891	A816	U740	G674	U605	G537	C467	C395	A327	U244
G1205	G1138	G1077	A892	C817	A892	G892	C817	G741	G675	G606	G538	A468	G396	C328	C245
G1206	G1139	U1078	G1079	G1021	U961	C893	G818	G742	A675	A607	G539	G474	A397	A329	A246
G1207	C1140	G1073	A1080	G1022	C962	G894	G819	U743	U676	G476	G540	G475	C398	G247	
C1208	C1141	U1074	G1081	G1023	G963	G895	U820	C745	U677	A608	G541	G476			
C1209	G1142	G1075	G1082	U1025	A964	C896	G821	U748	U678	A611	G542	G477	G402	G332	A250
G1210	G1143	U1076	C897	C897	A965	C897		C749	G682	C612	C543	A478	C403	G333	G251
U1211	U1144	U1083	G1084	G1026	G966	G966	C826	G749	G683	G613	G544	C479	U404	C337	U252
U1212	C1145	C967	U927	G900	A968	A901	U827	G750	G682	C613	C545	U480	U405	A338	U253
C1213	A1146	U1085	A828	A901	A968	A901	A828	U751	A684	A614	C546	G481	G406	C339	G254
C1214	C1147	U1086	G829	G902	A969	G902	G829	C752	G685	C615	A547	A482	G407	U340	G255
G1215	U1148	G1087	C970	G903	C970	U833	U833	G753	U686	G616	U550	C483	A408	C341	U256
G1216	C1149	U1088	G971	G906	C971	G906	U834	C754	A687	G617	U551	G484	G409		
C1217	U1150	G1089	C972	A907	C972	A907	G835	G755	G688	C618	U552	G485	G410	A344	U261
C1218	A1151	U1090	G973	A907	C973	A907	U836	C756	U689	U619	U553	U486	A411	G345	A262
G1283	U1152	U1091	A974	A974	C974	A974	G837	U757	G690	C620	A553	U487	A412	G346	A263
C1284	C1153	A1092	G1032A	G1032A	A975	C912	G837	U757	G691	A621	C554	G490	A413	G347	U264
A1285	U1154	A1093	G1032B	G1032B	G976	A913	G838	C758	U692	A622		G491	A414	C418	G266
A1286	G1155	G1094	G1033	G1033	G977	A914	U841	C759	G693	C623	U558	A495	C419	G349	G267
A1287	G1156	U1095	G1034	A915	A978	A915	G842	G760	A694	C624	U559	A496	C418	A348	G268
A1288	A1157	C1096	A1035	G979	C979	G916	U843	A766	G625	G625	U560	U497	G351	C352	C269
A1289	U1158	C1097	G1036	C980	C980	G917	C848	A767	A696	U626	U561	A498	G352	C353	C270
C1226	U1159	U1098	G1037	U981	U981	A918	C849	A768	U697	G627	U562	U498	G353	A353	A270
A1227	G1160	C1099	C1038	U982	U982	A919	U850	C769	G628	G628	C562	G500	C422	G354	C271
C1228	C1161	U1100	C1039	A983	C983	U920	G851	C770	G629	C501	U563	C502	G423	C355	C272
G1293	C1162	A1101	U1040	C984	C984	U921	G852	G771	G630	G502	C564	G503	G424	A356	A273
G1294	U1102	A1041	C985	G922	C985	G922	G853	U772	G631	G503	U565	C504	G425	G357	A274
G1295	G1231	G1042	A986	A923	A986	A923	G854	G773	A704	A632	U566	C505	G426	U358	G275
C1296	U1232	C1043	G987	G987	G987	G987	G855	U773	U705	G633	U567	G506	U427	U359	G276
C1297	G1233	A1044	G988	G926	G988	G926	C856	A777	A706	C634	U571	G507	G428	A360	C277
C1298	C1234	C1045	C989	G927	C989	G927	C857	G778	C707	G635	A572	C507	U429	G361	G278
A1299	U1235	G1173	C990	G927	C990	G927	C858	C708	U636	A573	A574	A509	A430	U365	A279
G1300	A1236	G1107	U991	C930	U991	C930	A859	A782	G709	G637	A574	A509	A431	U366	C280
C1301	C1237	C1108	U992	C931	U992	C931	A860	C783	G710	G638	G575	A510	A432	C366	G281
U1302	A1238	G1177	G993	G932	G993	G932	G861	C784	G711	G639	G576	C511	C433	U367	A282
C1303	A1239	G1178	A994	G933	A994	G933	C862	G785	A712	C643	G577	U512	U434		C283
G1304	U1240	A1179	C995	G934	C995	G934	U863	G786	G713	C644	U580	C513	C435	C370	G286
G1305	G1241	A1180	U996	A935	C996	A935	A864	A787	G714	G644	G581	C514	C436	G371	U287
A1306	C1242	G1181	U997	C936	U997	C936	A865	U788	G715	C645	U582	G515	U437	C372	A288
C1307	C1243	G1182	G998	A937	G998	A937	A866	C789	A716	G646	U583	U516	G438	A373	G289
U1308	G1244	A1183	C998A	A938	C998A	A938	G867	A790	C717	A648	G584	G517	A439	U374	
G1309	A1245	G1184	U999	G939	U999	G939	C868	G791	G718	G649	G584	C518	A440	U375	C295
C1310	C1246	C1119	U1000	C940	A1000	C940	G869	A792	C719	G650	G585	C519	C442	G376	G296
G1311	U1247	G1185	G1059	G941	G1001	G941	U870	U793	C720	C651	C586	A520	C443	C377	U296
G1312	A1248	U1121	C1060	G1002	G1002	G1002	U871	A794	G721	G652	G587	G521	C444	G378	G297
U1313	C1249	A1188	G1061	G1003	G1003	G1003	A872	C795	A722	C522	G588	C522	C444	C379	A298
C1314	A1250	A1123	U1062	A1004	A1004	A1004	A873	C796	U723	G589	C590	A523	C447	A382	G299
U1315	A1251	A1123	C1063	A1005	A1005	A1005	G874	C797	G724	G657	C591	G524	G448	A448	A300
G1316	A1252	A1191	G1064	C1006	C1006	C1006	G874	C798	G725	G658	U591	C525	C449	A383	G301
C1317	G1253	U1126	U1065	C1007	C1007	C1007	G878	G799	C726	G659	U592	C526	G450	G384	
A1318	C1254	G1127	G1127	C1066	C1008	A949	C879	G800		G660	G593	G527	A451	C385	C312

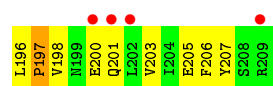


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

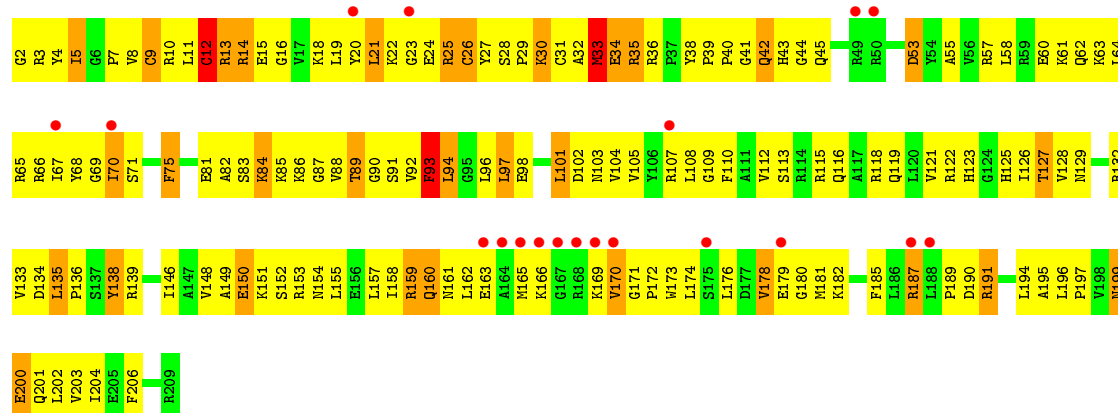


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

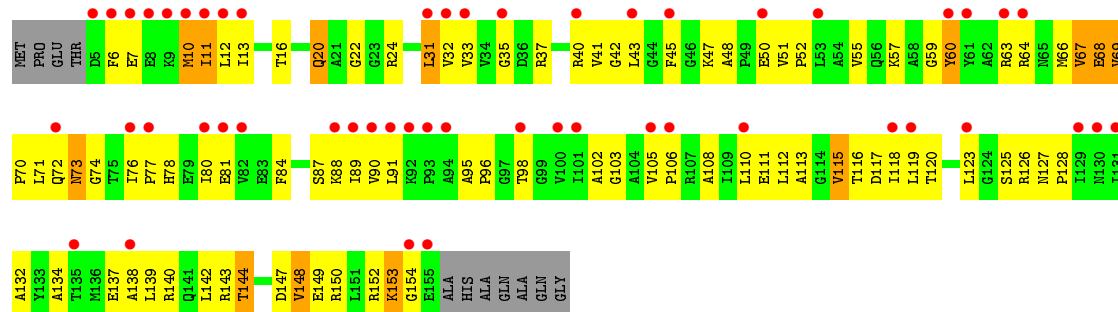




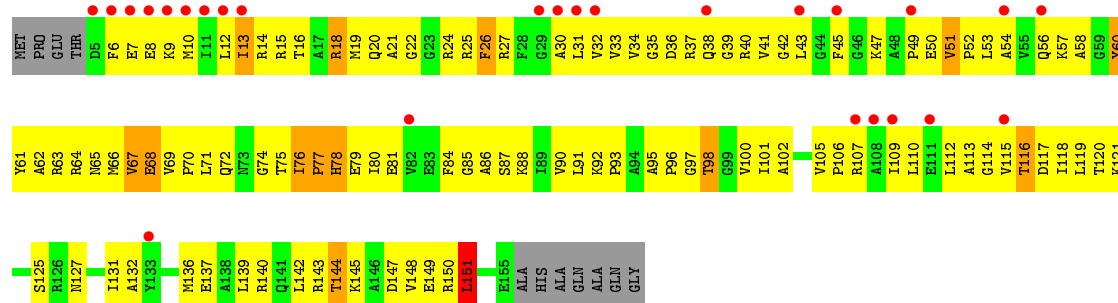
● Molecule 4: 30S RIBOSOMAL PROTEIN S4



● Molecule 5: 30S RIBOSOMAL PROTEIN S5

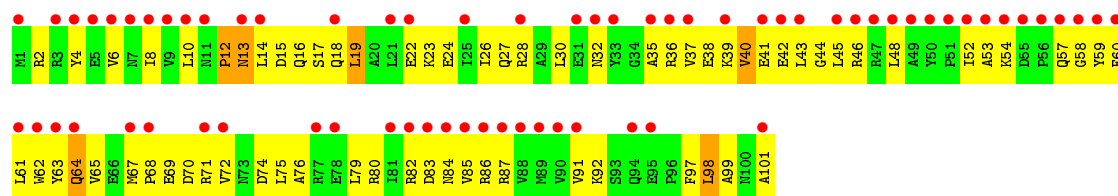


● Molecule 5: 30S RIBOSOMAL PROTEIN S5

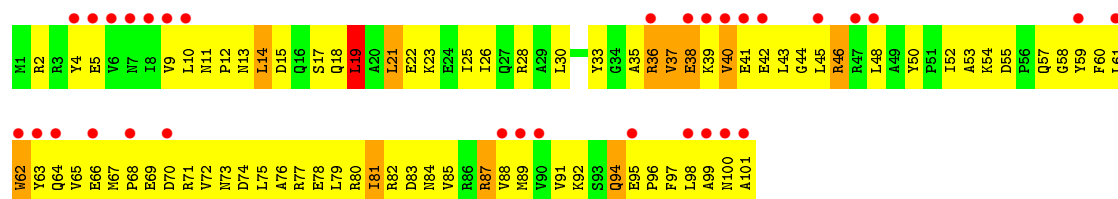


● Molecule 6: 30S RIBOSOMAL PROTEIN S6

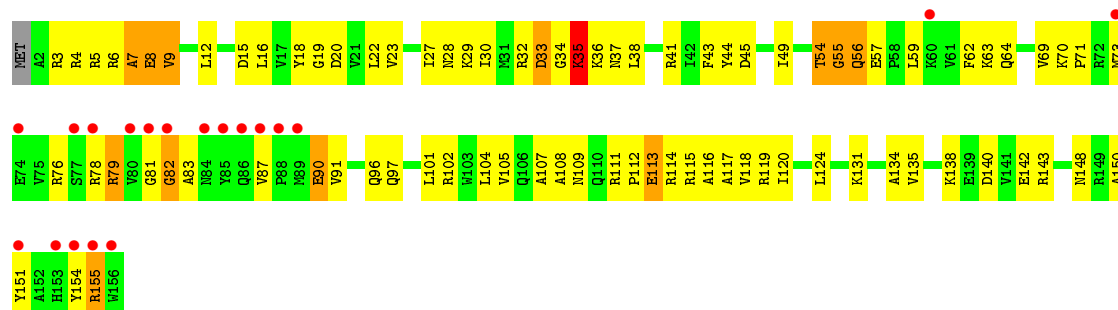




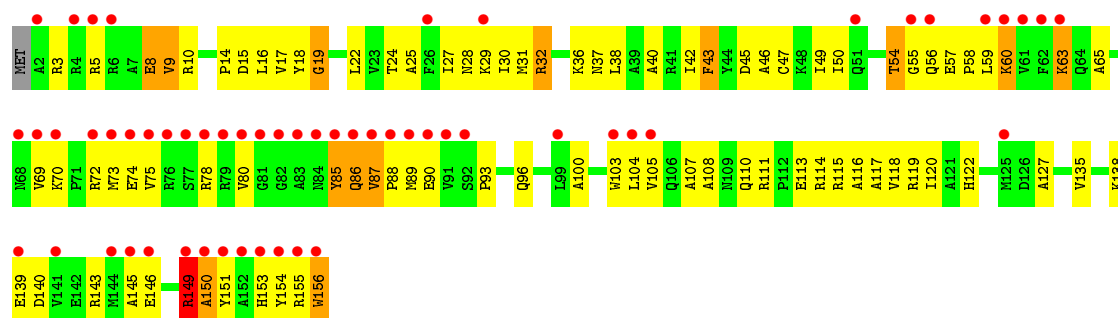
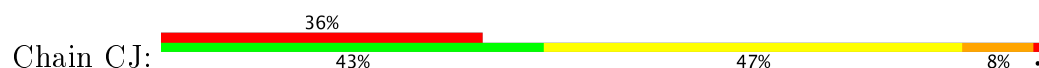
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



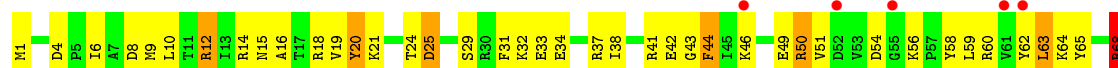
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

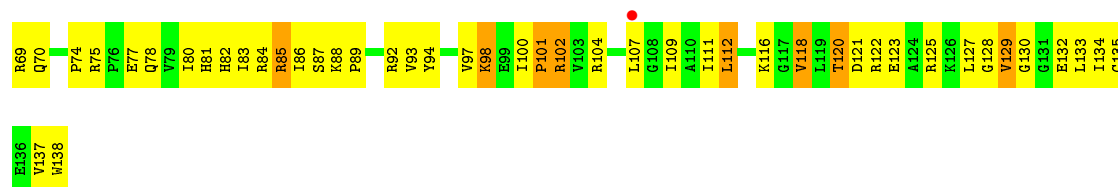


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

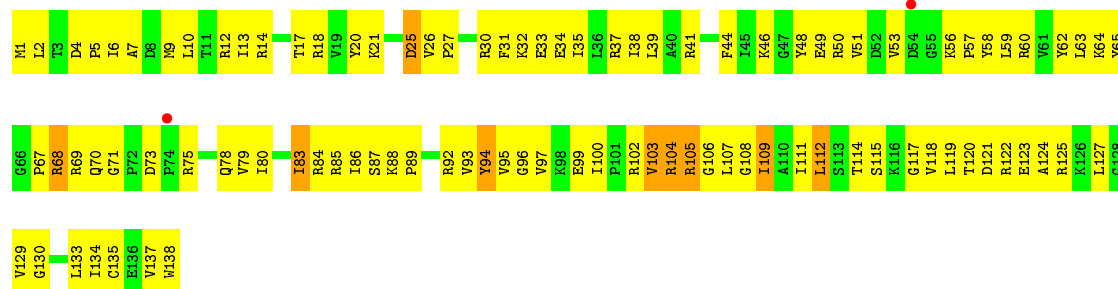


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

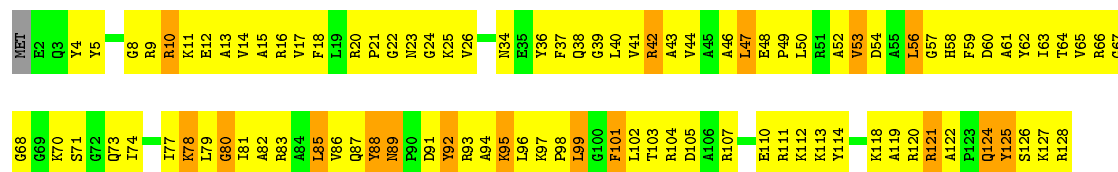




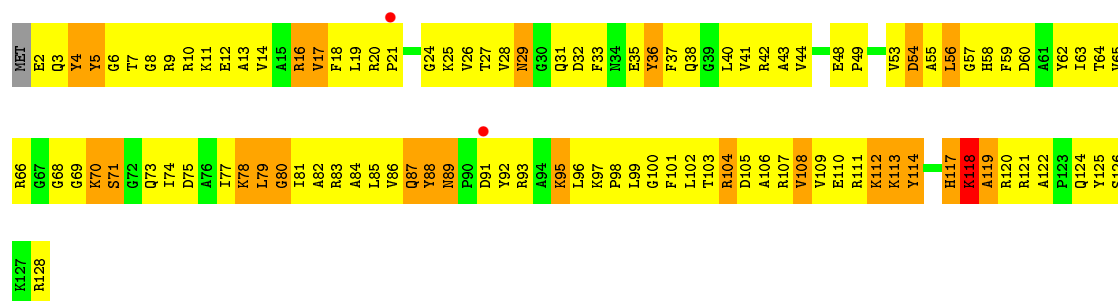
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



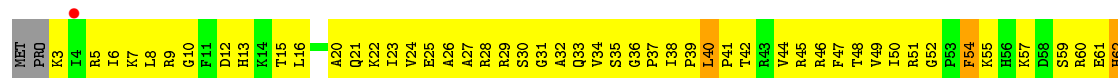
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

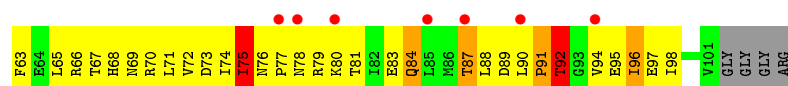


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

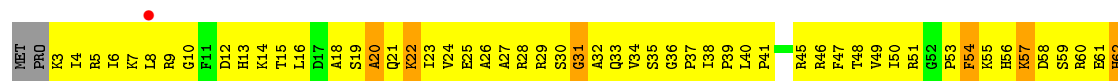


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

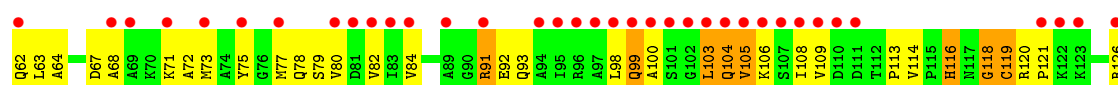
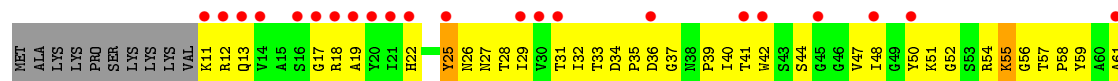




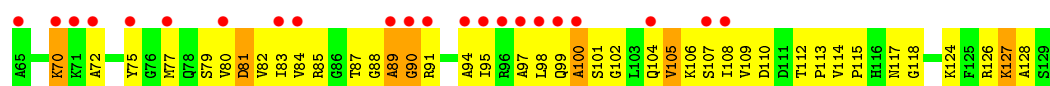
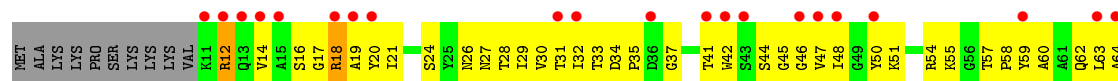
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



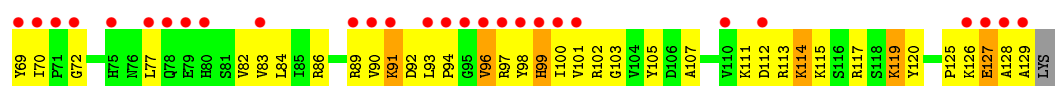
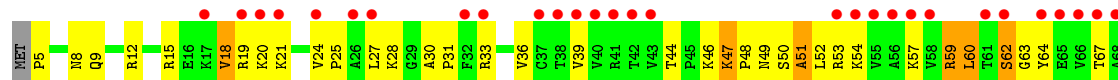
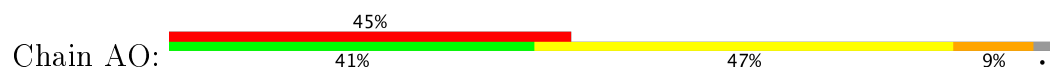
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



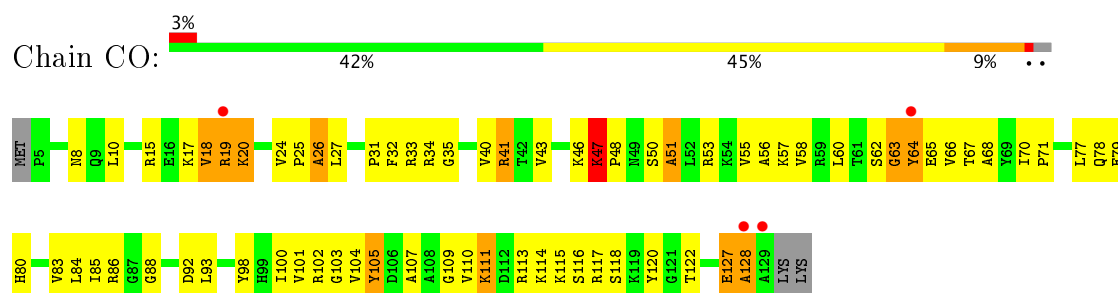
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



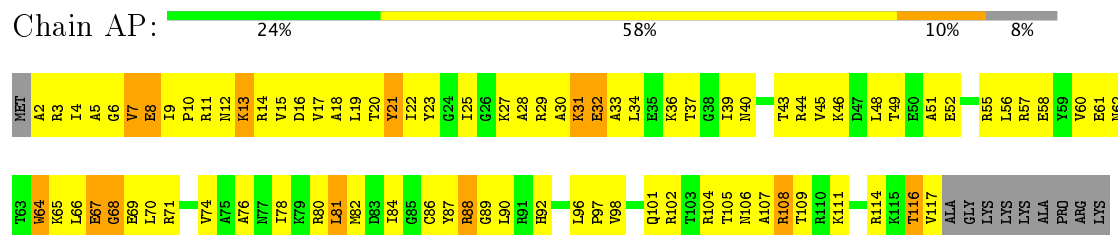
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



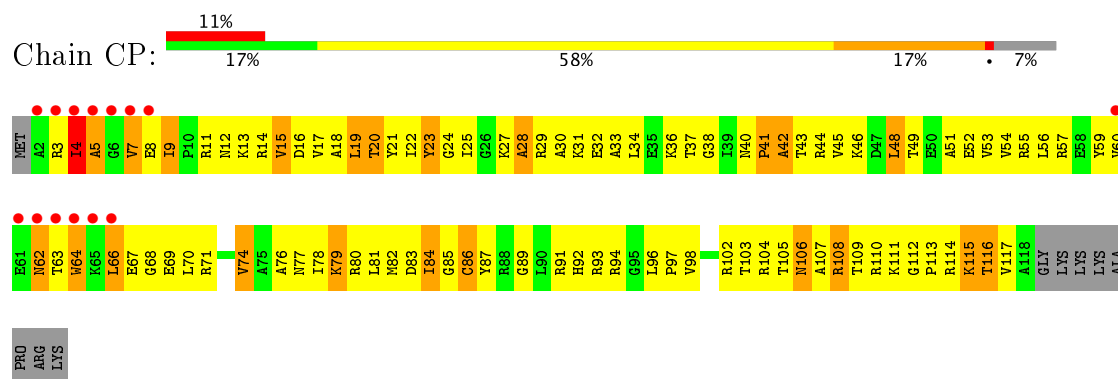
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



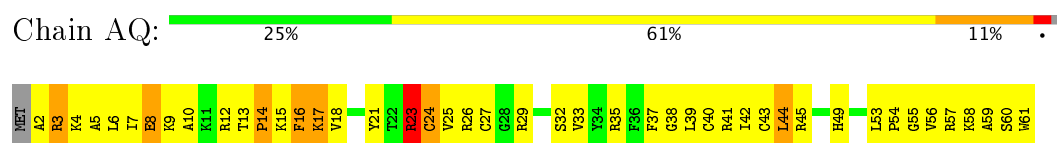
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



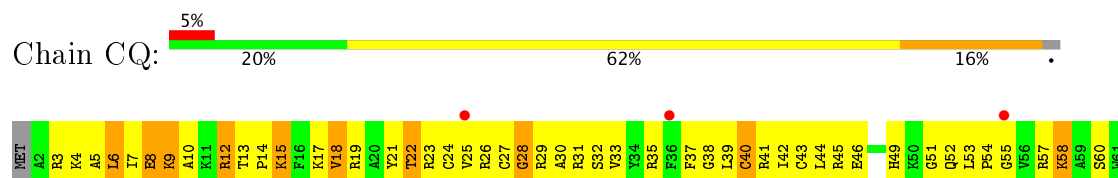
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



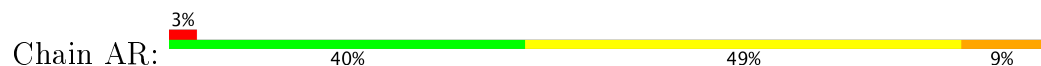
• Molecule 14: 30S RIBOSOMAL PROTEIN S14

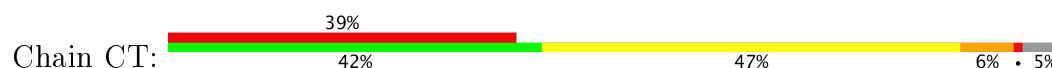


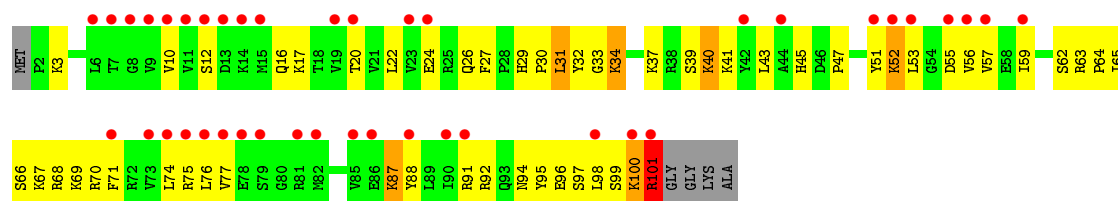
• Molecule 14: 30S RIBOSOMAL PROTEIN S14



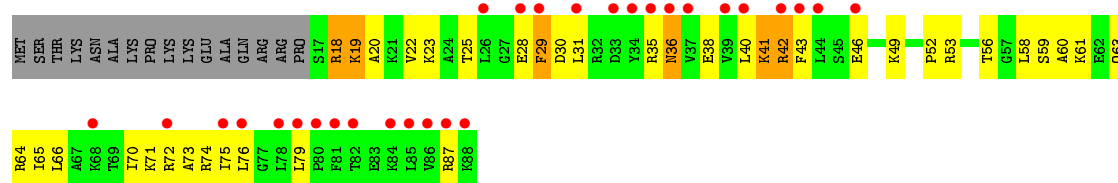
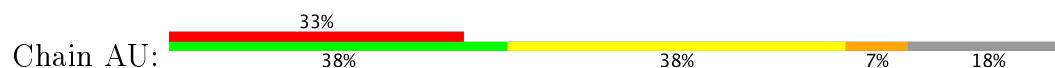
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



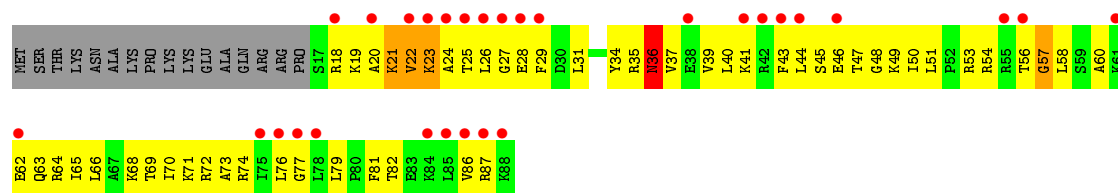




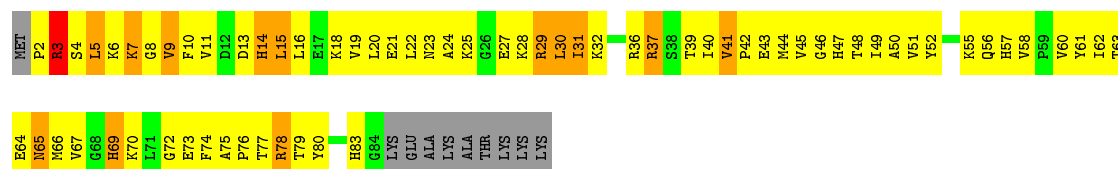
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



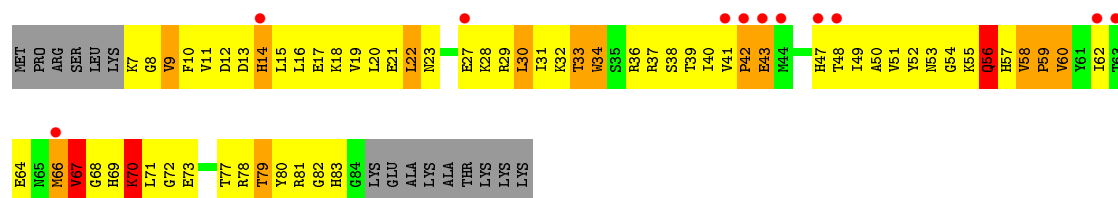
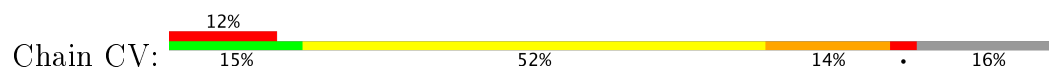
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

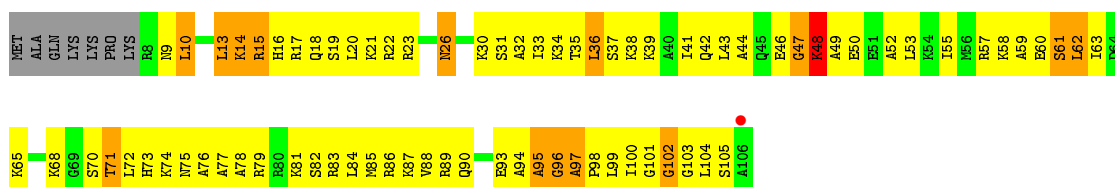


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

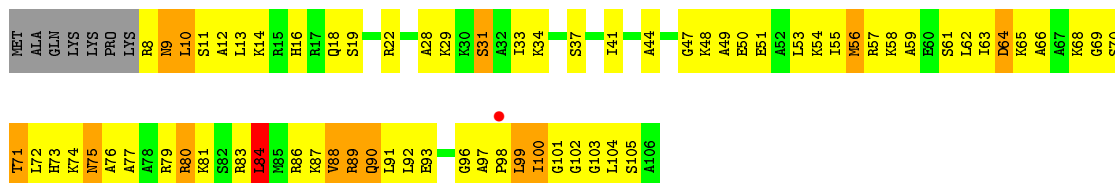


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

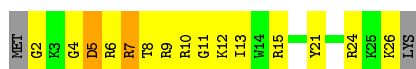




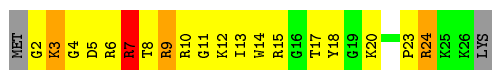
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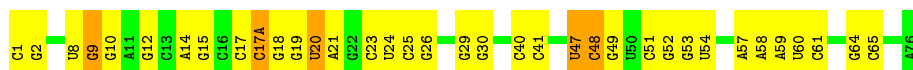
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



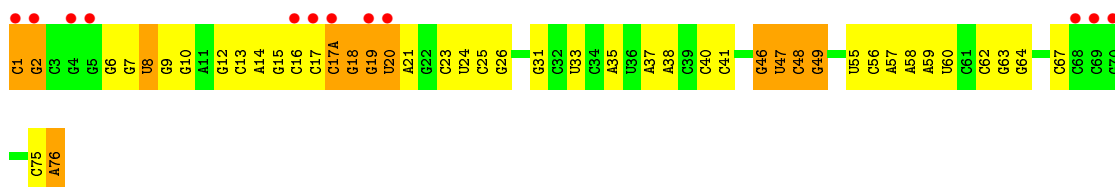
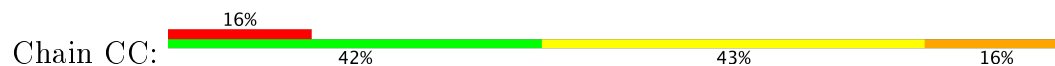
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: TRNA-FMET



• Molecule 22: TRNA-FMET



• Molecule 23: MRNA



A16
U17
G18
U19

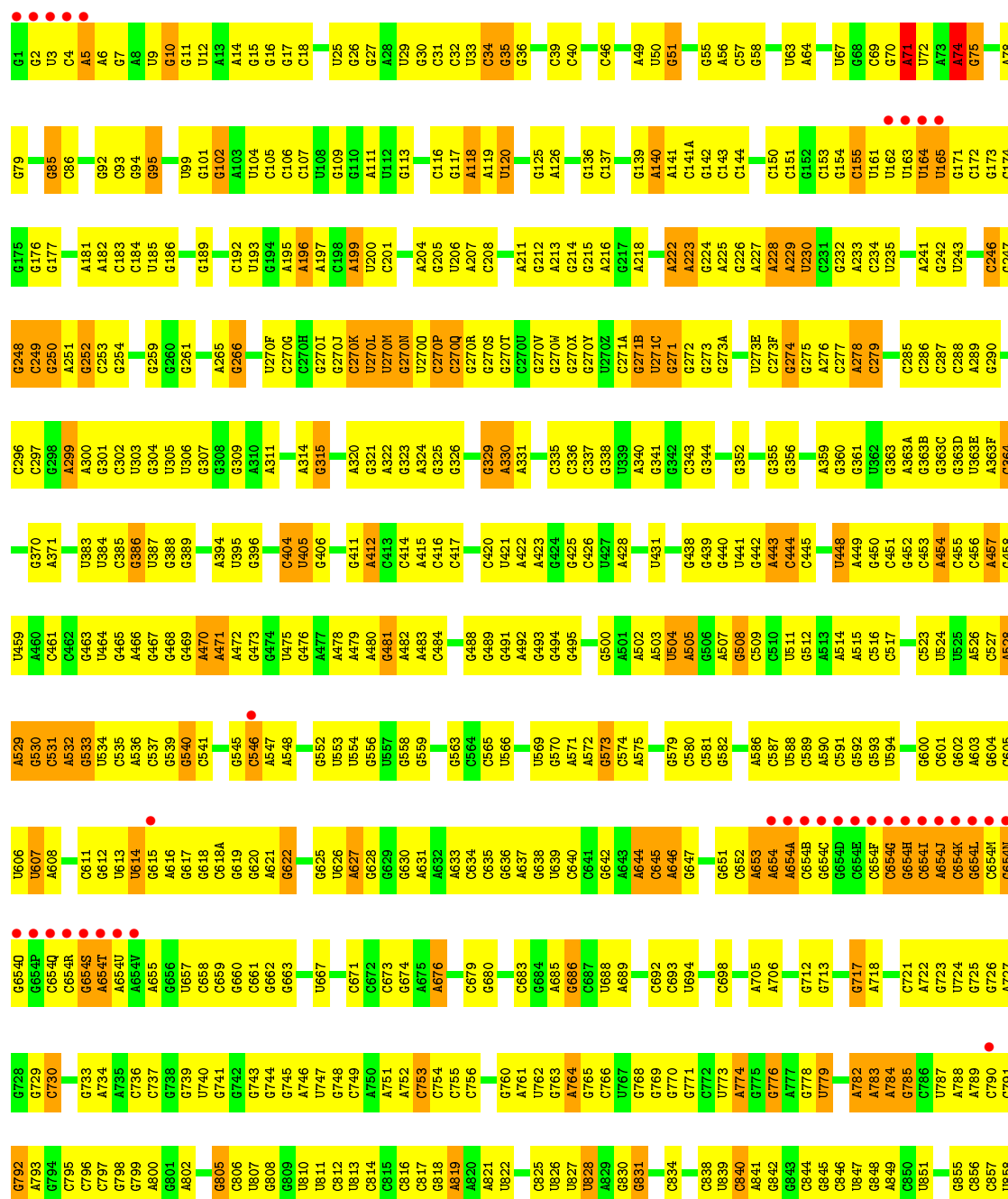
• Molecule 23: MRNA

Chain C1: 50% 50%

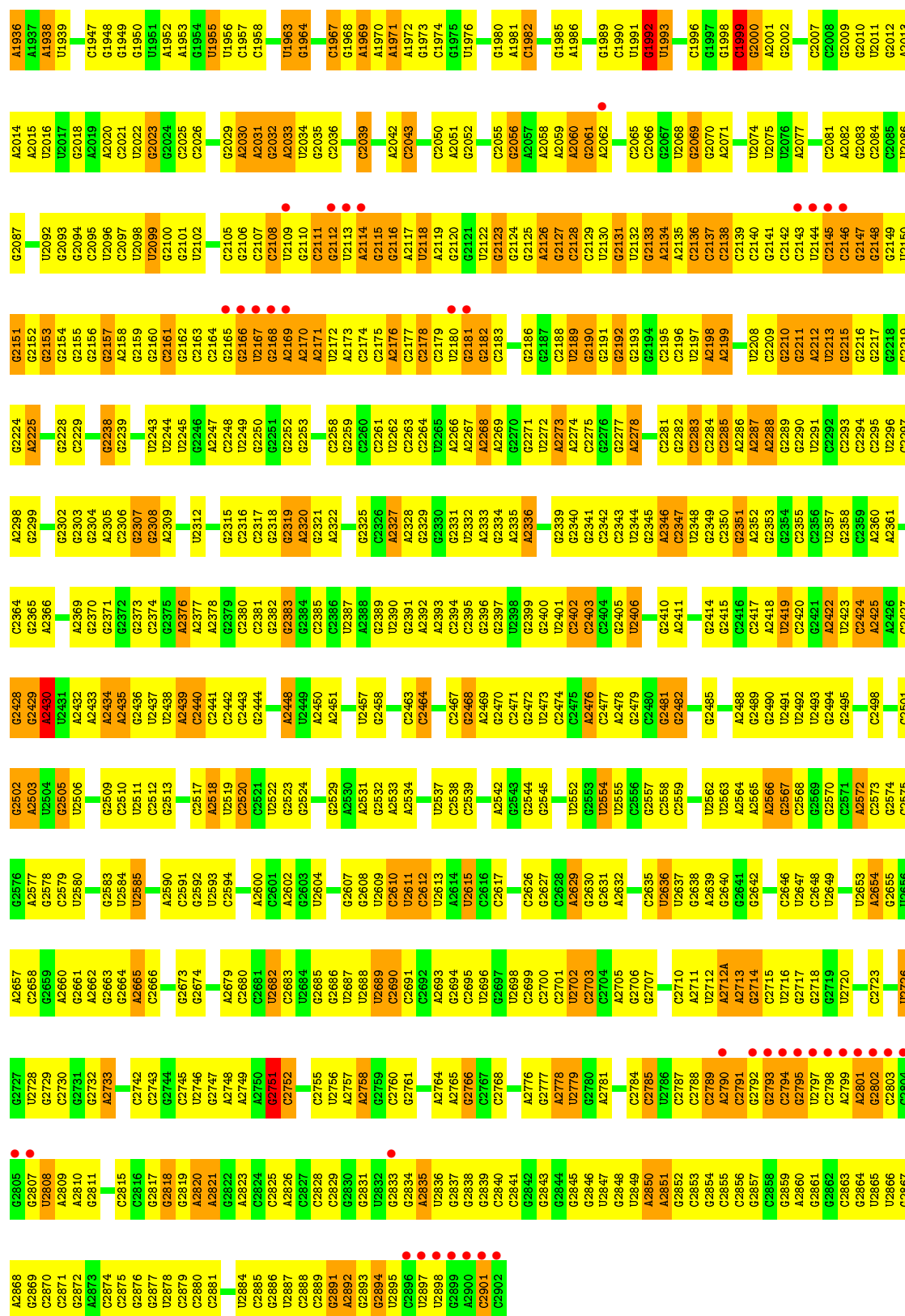
A16
U17
G18
U19

• Molecule 24: 23S ribosomal RNA

Chain BA: 3% 33% 52% 15%



A1854	A1855	A1858	A1859	G1869	A1791	A1792	A1793	A1794	G1878	A1879	C1880	C1881	C1882	A1883	A1884	A1885	G1888	A1889	A1890	G1891	G1899	A1900	A1901	G1902	G1903	G1904	G1905	G1824	G1825	G1826	G1827	G1828	A1829	A1830	G1831	A1832	A1833	A1834	G1835	G1836	C1837	C1838	C1924	C1925	G1926	G1929	G1930	G1931	C1934	G1935							
G1782	A1783	A1784	A1785	A1786	G1790	A1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	A1802	A1803	C1804	A1805	A1808	A1809	A1812	A1813	G1814	A1815	G1816	A1817	A1818	A1819	U1820	G1824	A1825	G1826	G1827	G1828	A1829	A1830	G1831	A1832	A1833	A1834	G1835	G1836	C1837	C1838	C1924	C1925	G1926	G1929	G1930	G1931	C1934	G1935			
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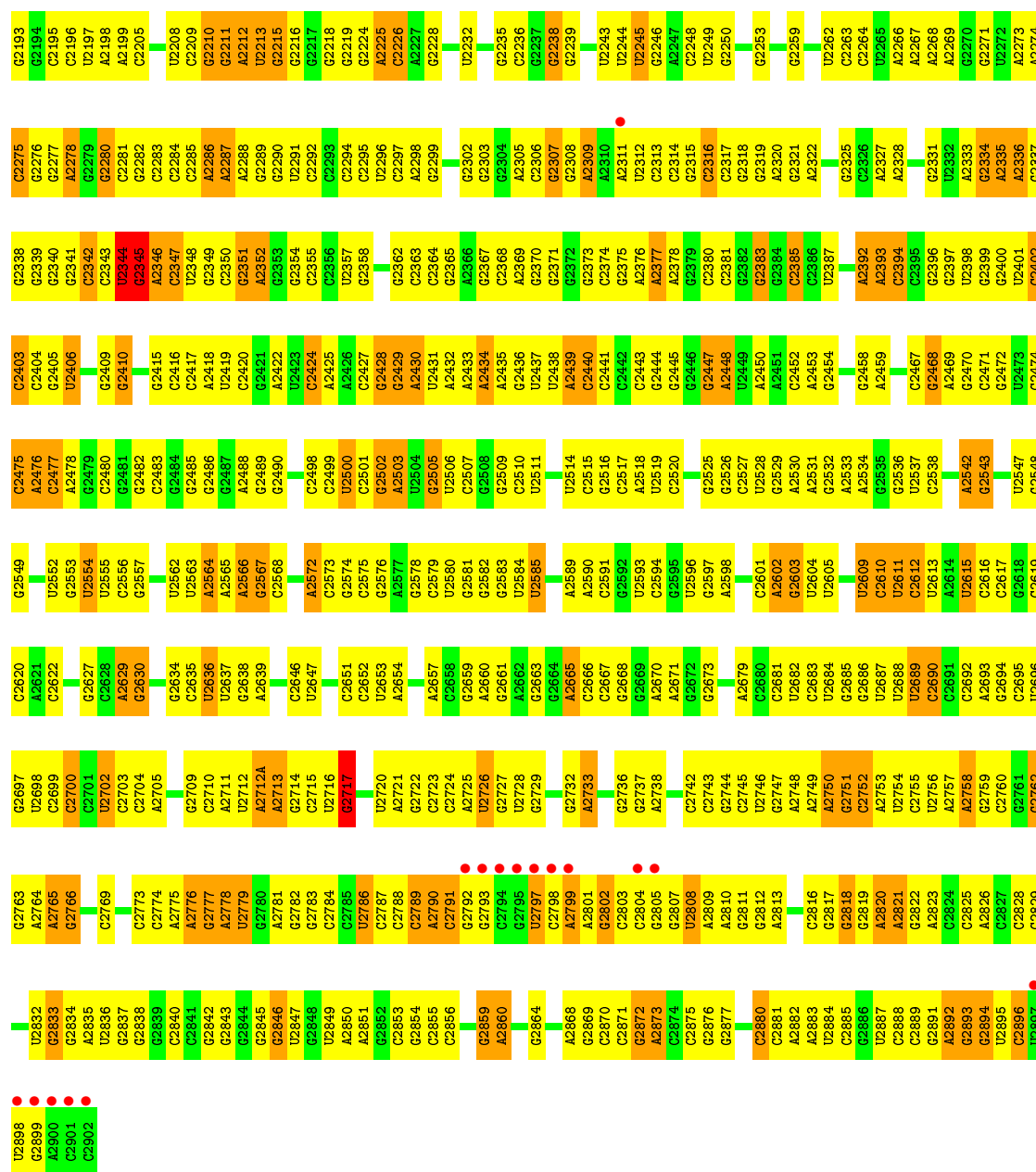


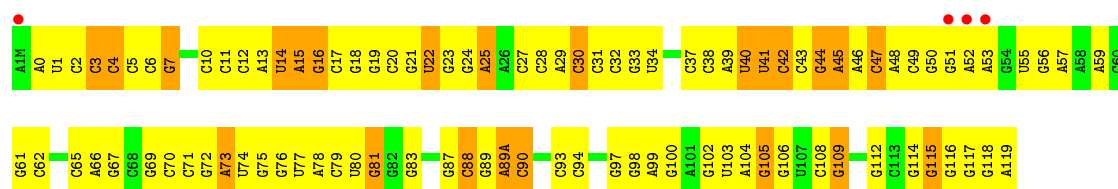
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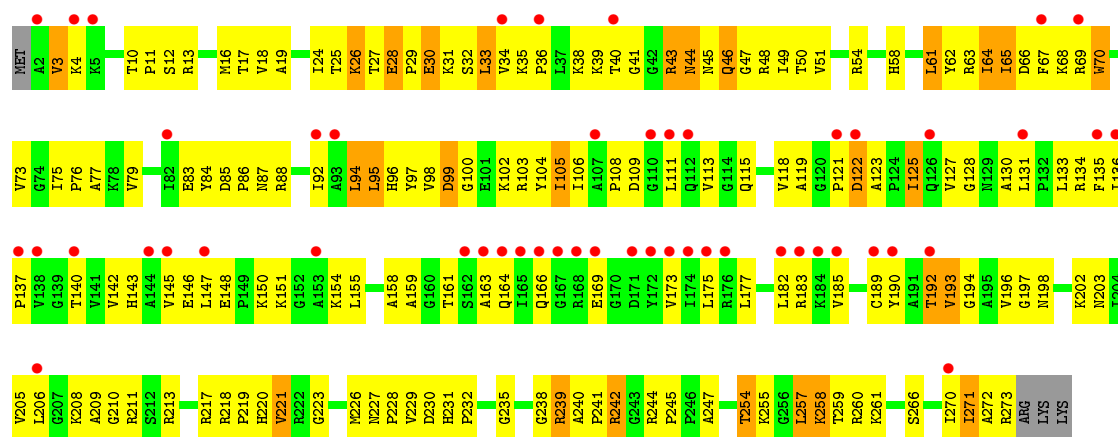
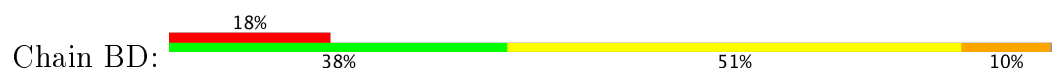
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G1036	A973	A901	A841	A774	G696	A643	C574	U504	U431	C343	A278	C246	C174	G82	U3
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C1038	C975	C903	G842	G776	C698	A645	U577	A507	G442	G352	C280	G248	G176	A84	A6
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G1042	G978	U907	C846	G780	G701	G649	C590	U511	C446	A357	C285	C253	A182	G92	G10
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G1049	G987	A917	G854	A788	G710	C654B	U588	G518	C456	U363F	C295	G266	A190	G101	U25
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U1081	G1016	G884	C884	C755	C755	C755	G626	U555	C487	G411	G327	U270Z	A225	C144	G61
G1082	C953	A824	C885	C825	C756	C756	U626	U557	C488	A412	U328	C271B	G226	G145	C66
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A1084	C955	U827	C887	U827	C758	C758	G628	U559	C490	C414	A330	U271D	A230	G150	G68
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G1087	C958	A829	C889	A829	C671	C671	A631	U562	C493	C417	A333	C273	A232	C153	A71
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WORLDWIDE
PDB
PROTEIN DATA BANK

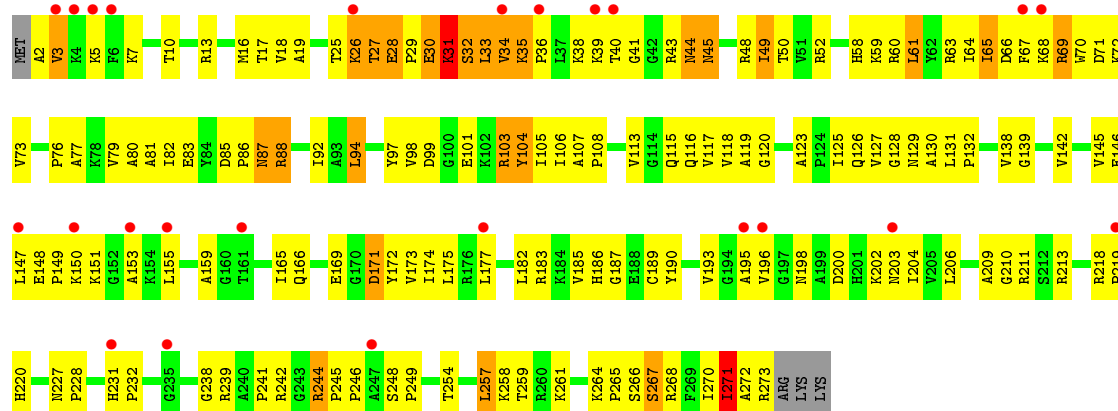
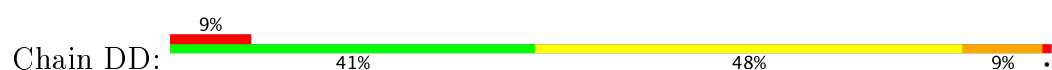




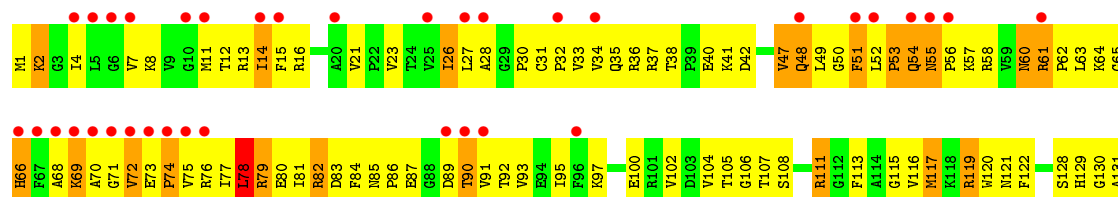
• Molecule 26: 50S ribosomal protein L2

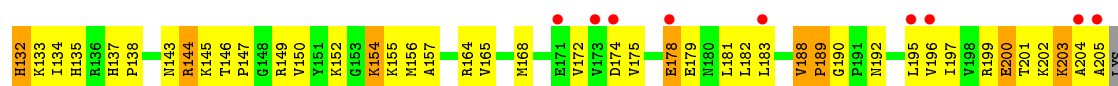


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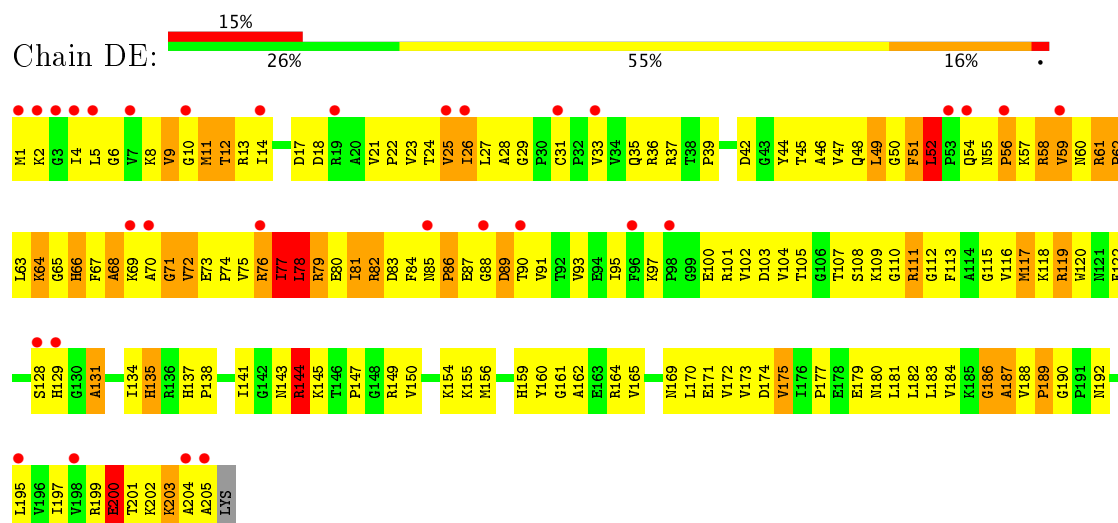


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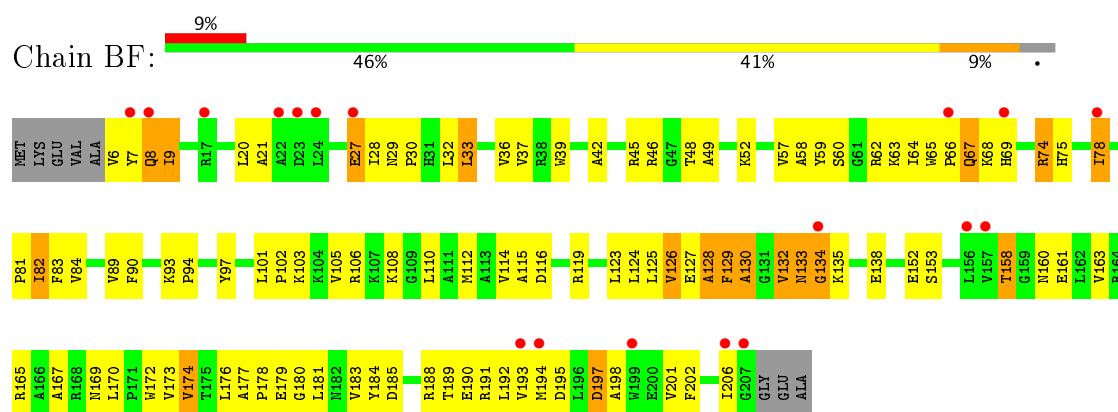




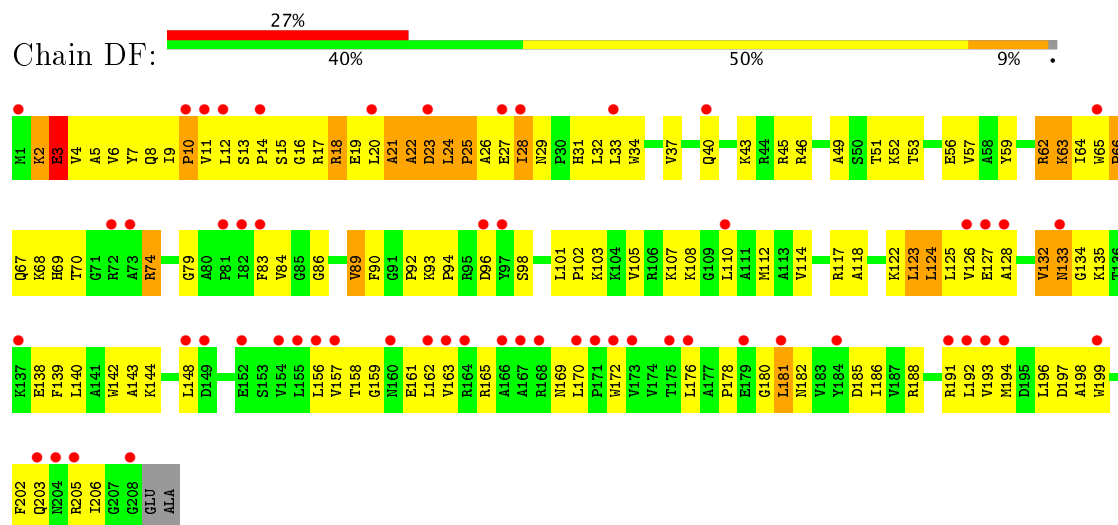
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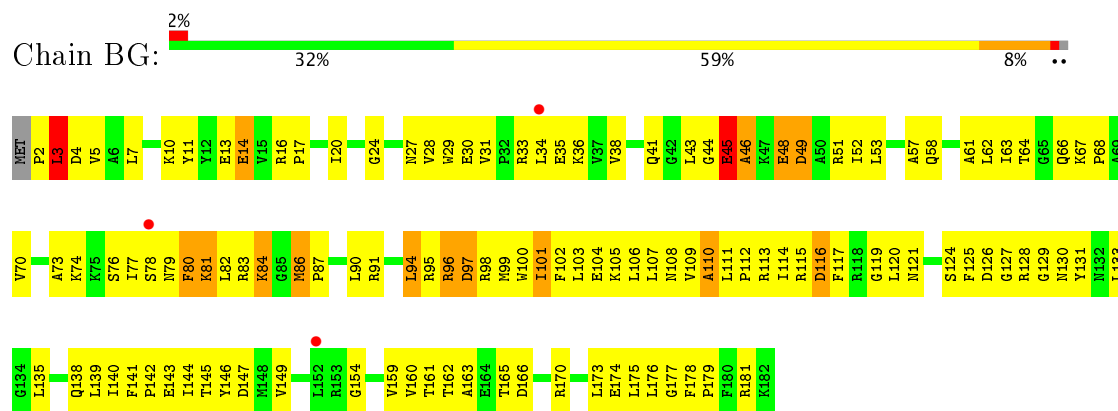
• Molecule 28: 50S ribosomal protein L4



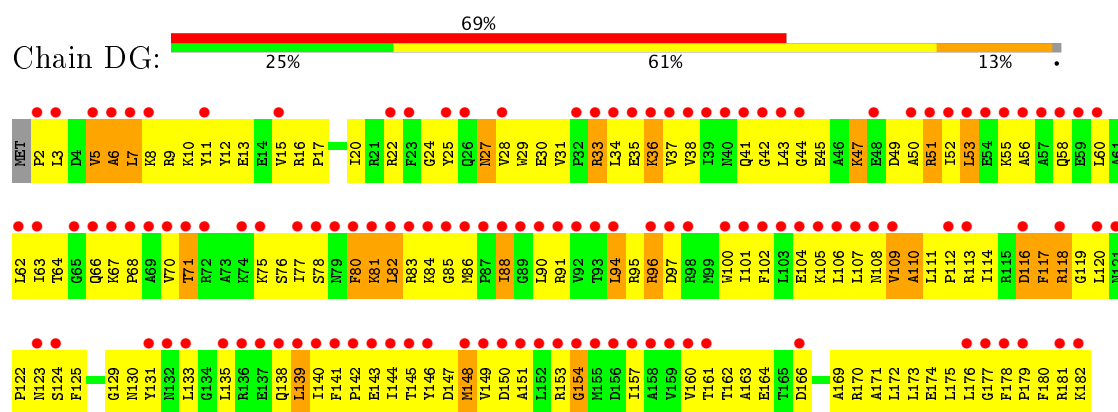
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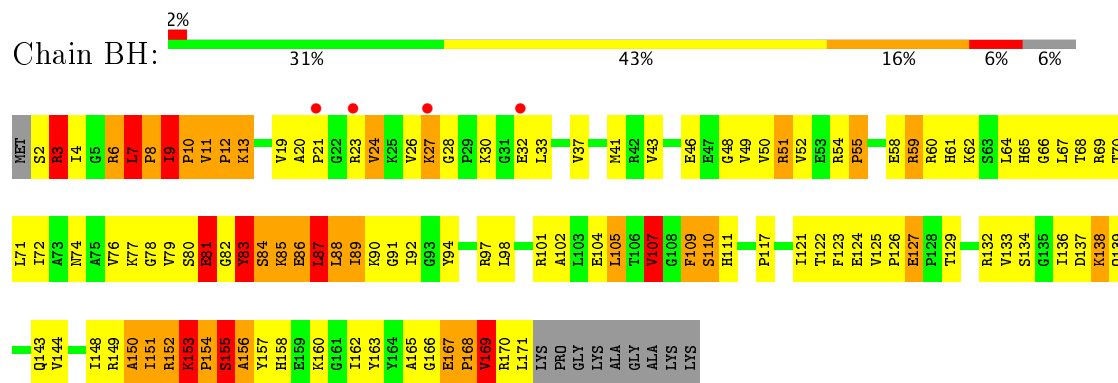
- Molecule 29: 50S ribosomal protein L5



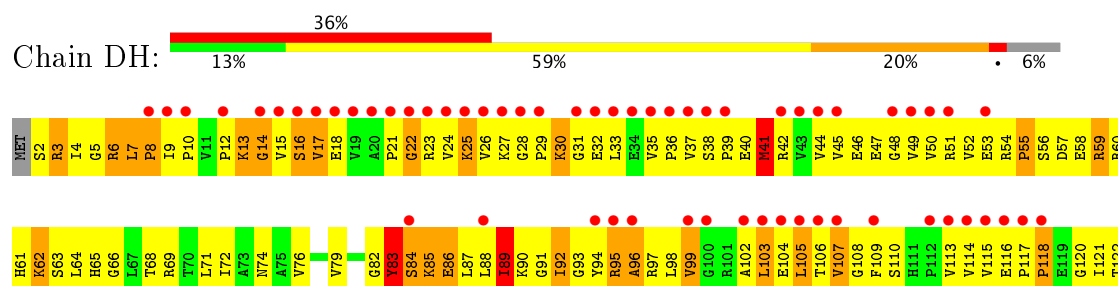
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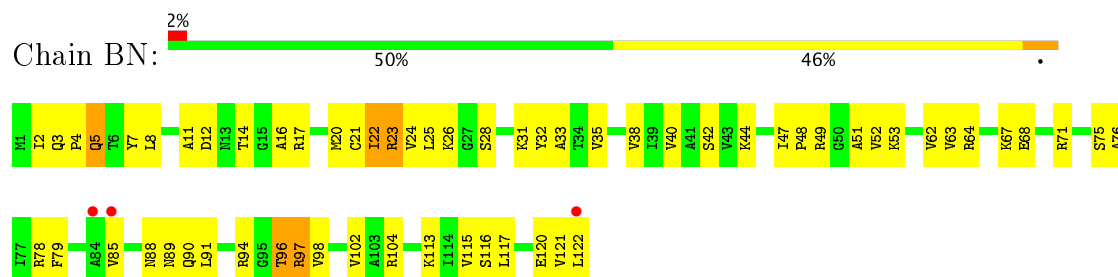
- Molecule 30: 50S ribosomal protein L6



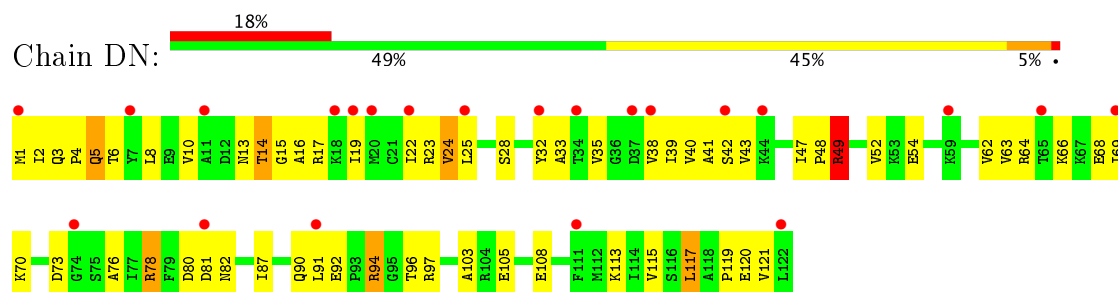
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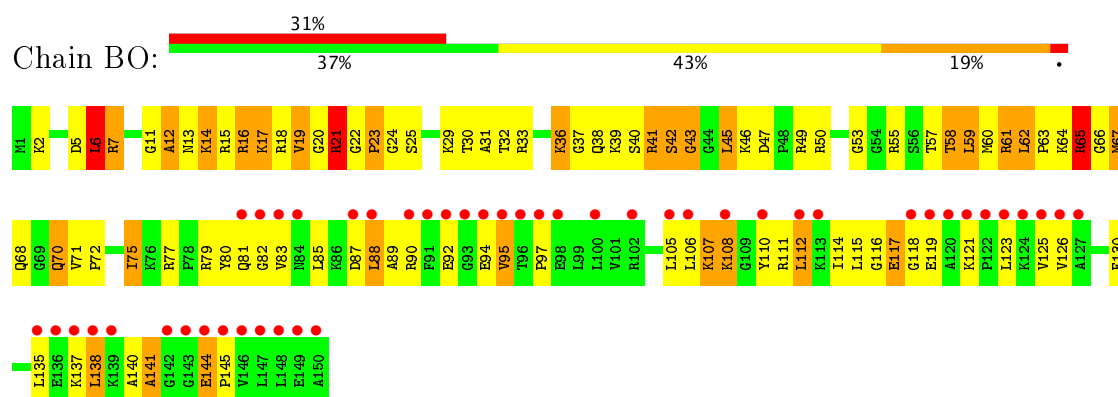
- Molecule 33: 50S ribosomal protein L14



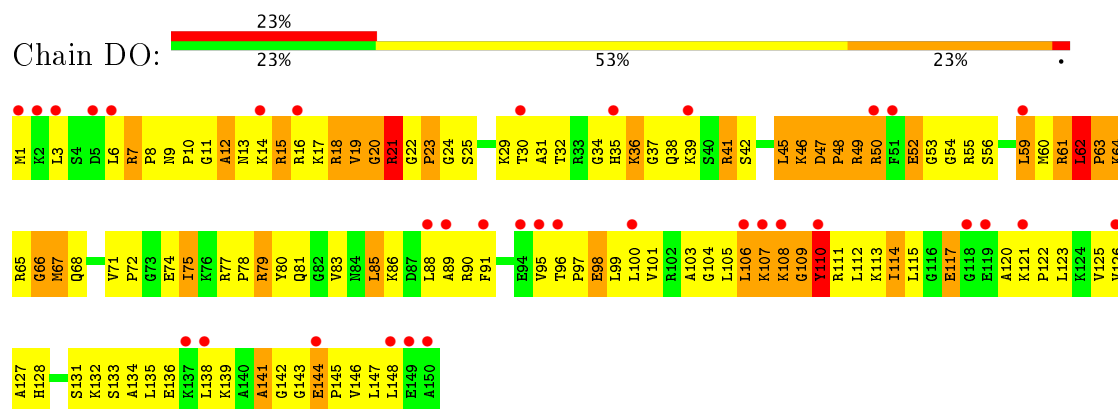
- Molecule 33: 50S ribosomal protein L14



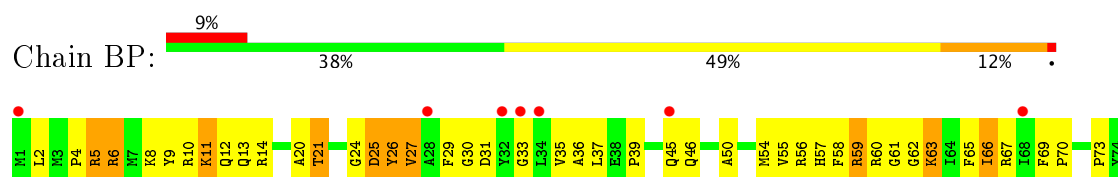
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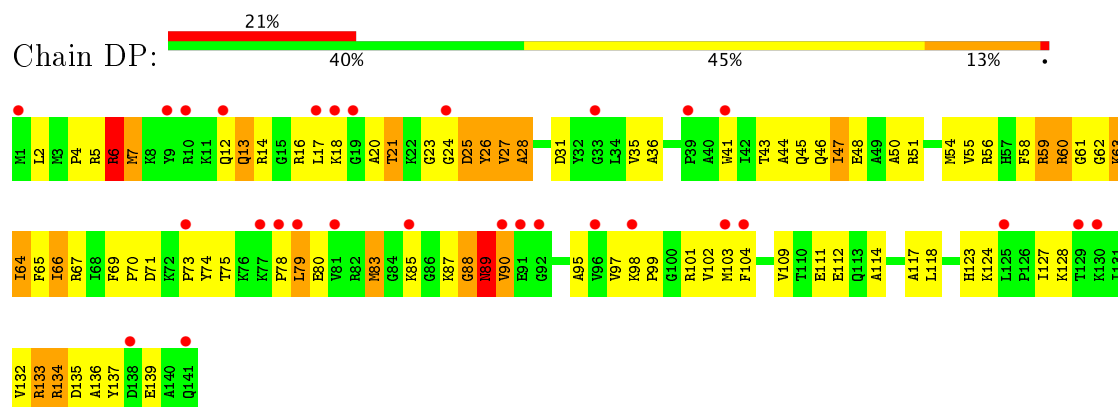
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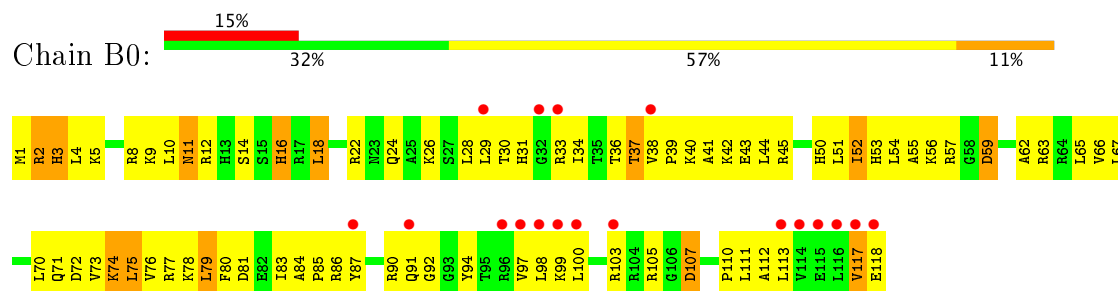
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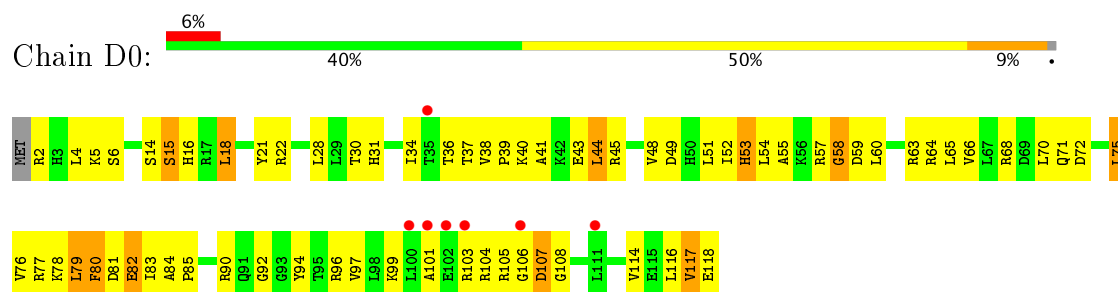
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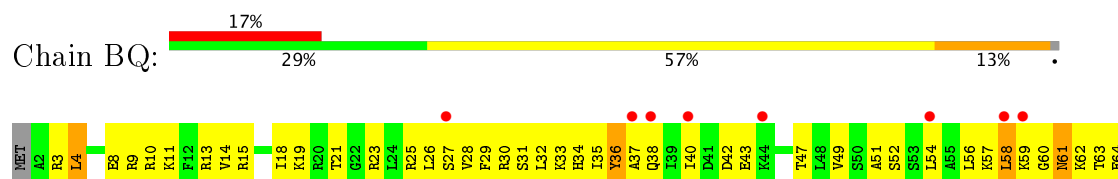
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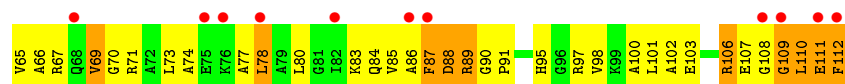


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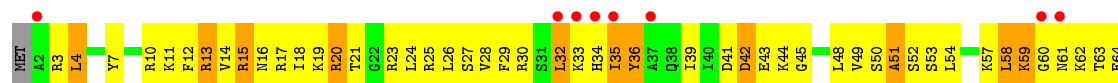


• Molecule 37: 50S ribosomal protein L18

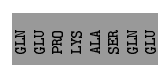
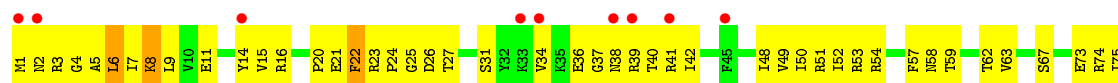




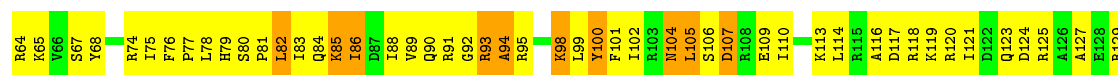
• Molecule 37: 50S ribosomal protein L18



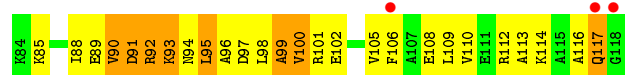
• Molecule 38: 50S ribosomal protein L19



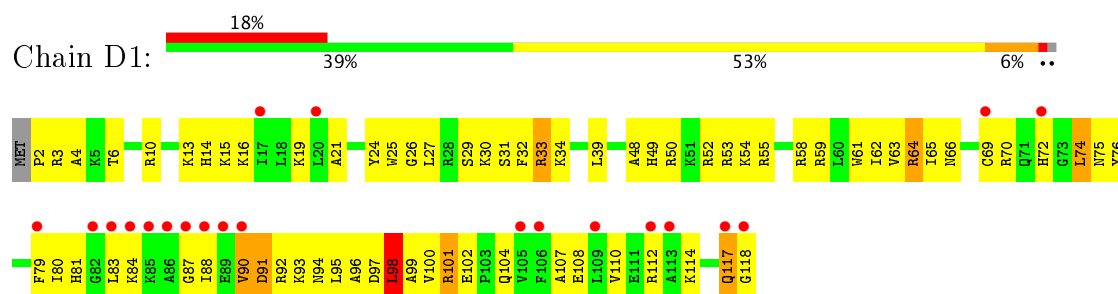
• Molecule 38: 50S ribosomal protein L19



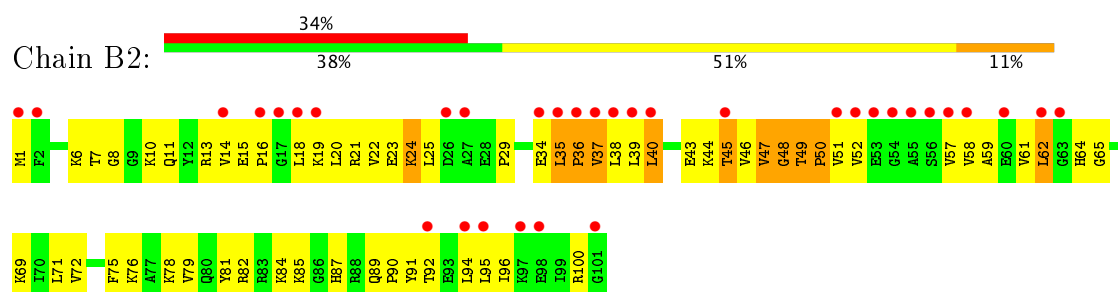
• Molecule 39: 50S ribosomal protein L20



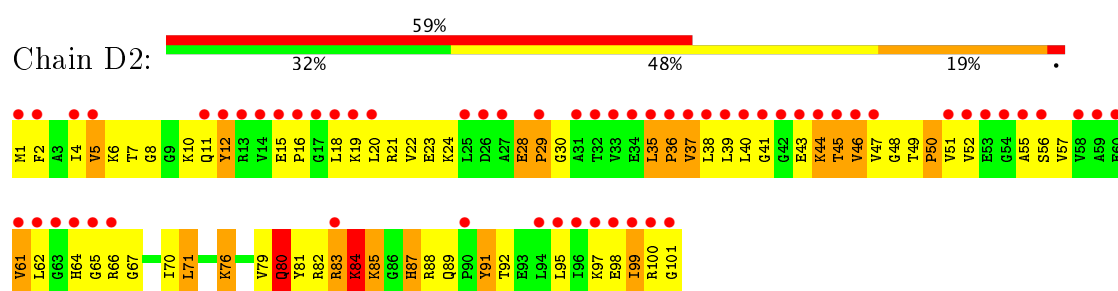
- Molecule 39: 50S ribosomal protein L20



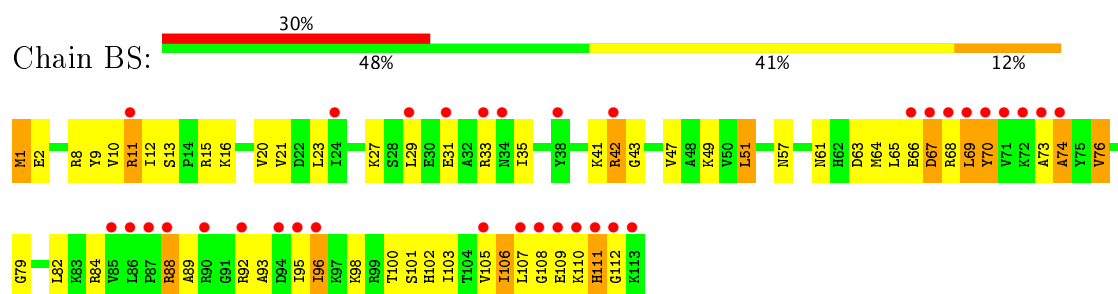
- Molecule 40: 50S ribosomal protein L21



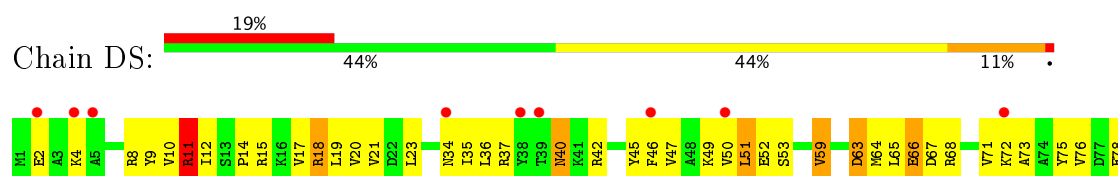
- Molecule 40: 50S ribosomal protein L21

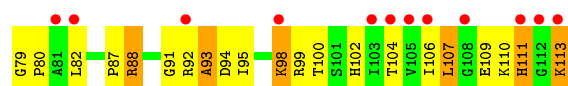


- Molecule 41: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L22

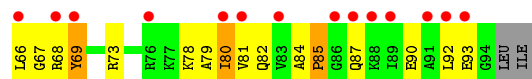
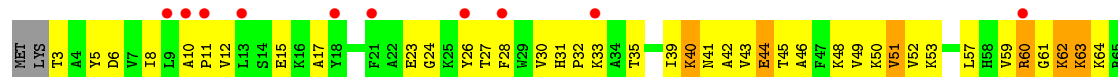
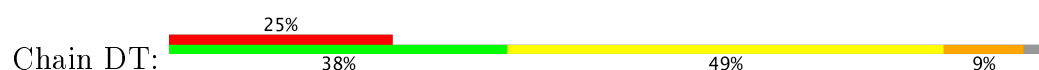




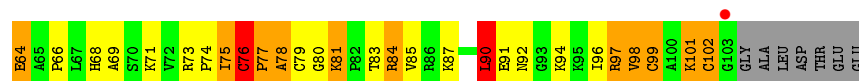
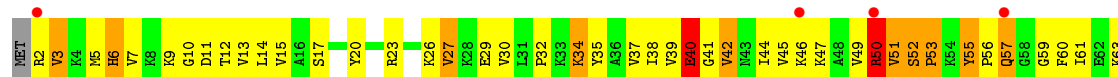
• Molecule 42: 50S ribosomal protein L23



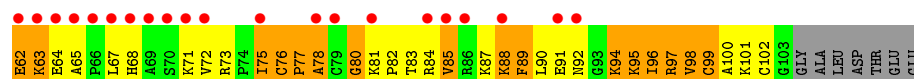
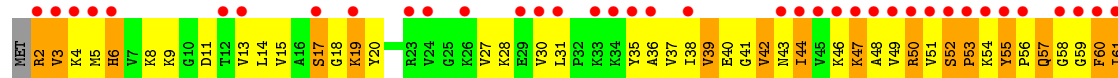
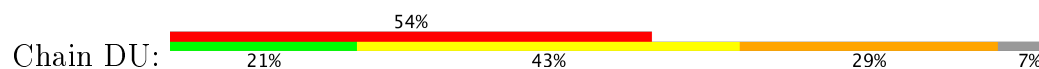
• Molecule 42: 50S ribosomal protein L23



• Molecule 43: 50S ribosomal protein L24

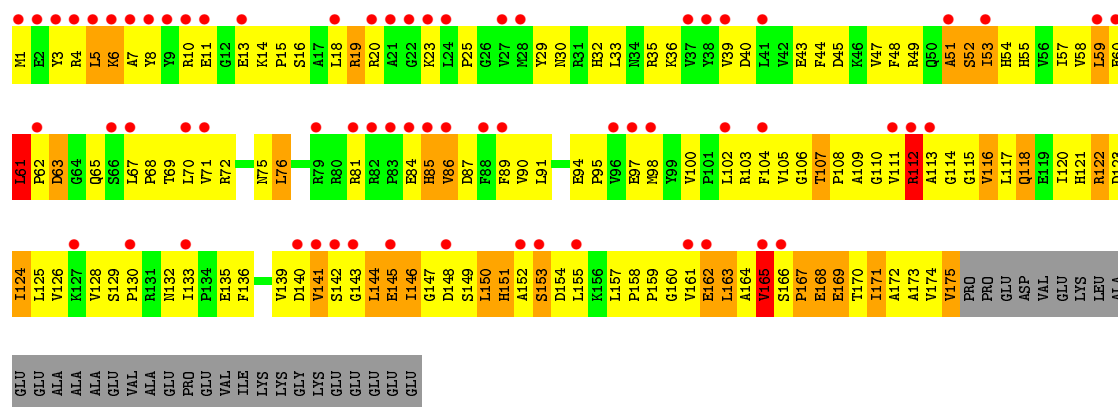


• Molecule 43: 50S ribosomal protein L24

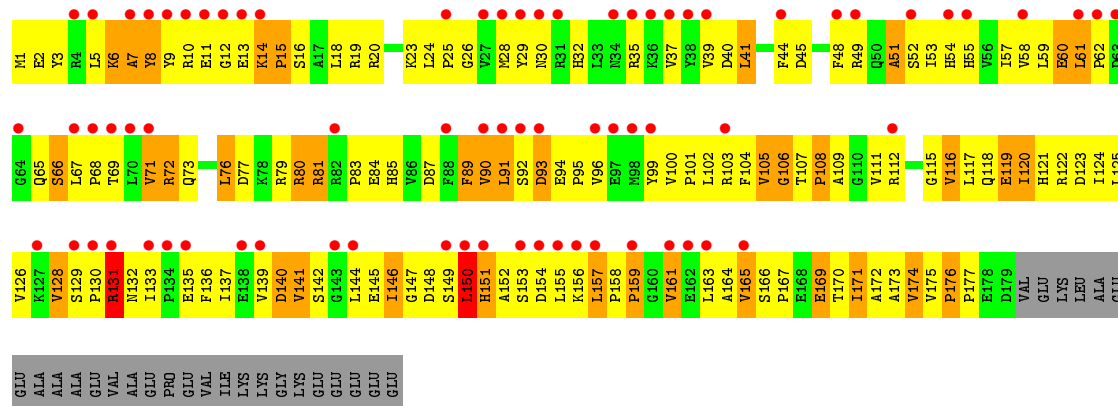
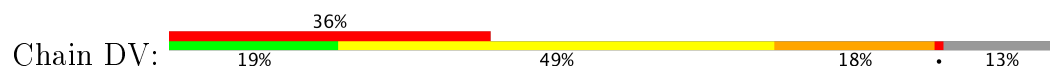


• Molecule 44: 50S ribosomal protein L25

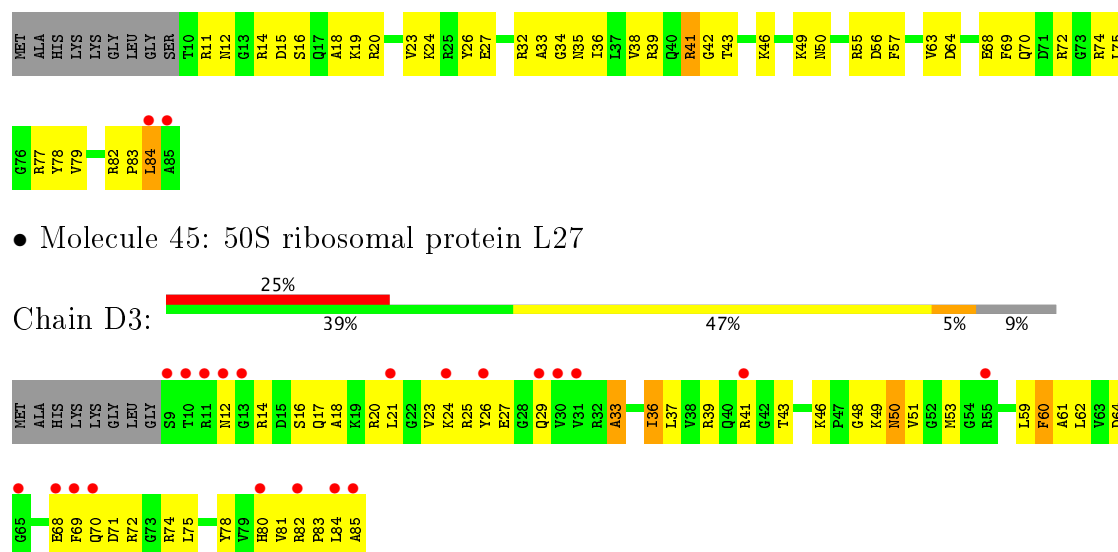
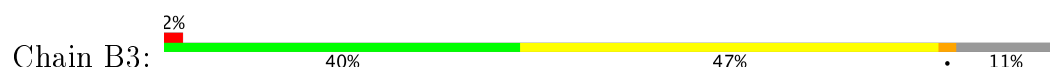




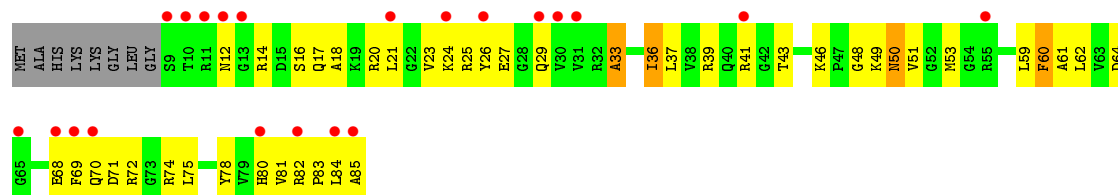
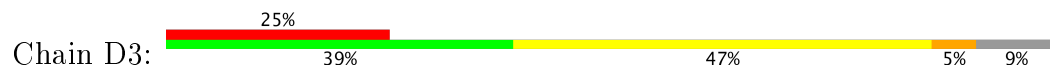
• Molecule 44: 50S ribosomal protein L25



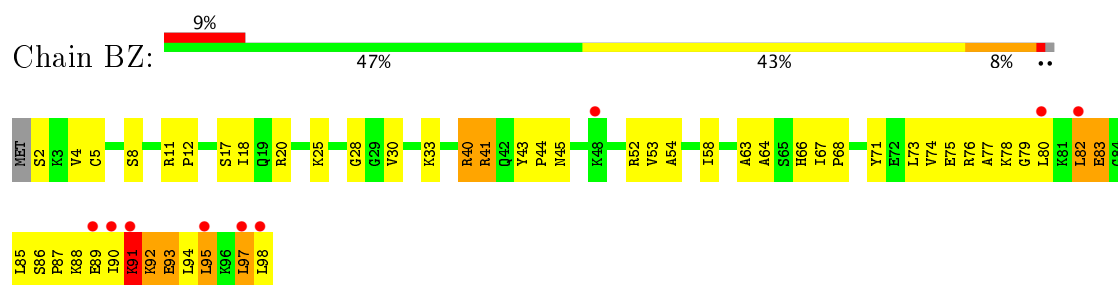
• Molecule 45: 50S ribosomal protein L27



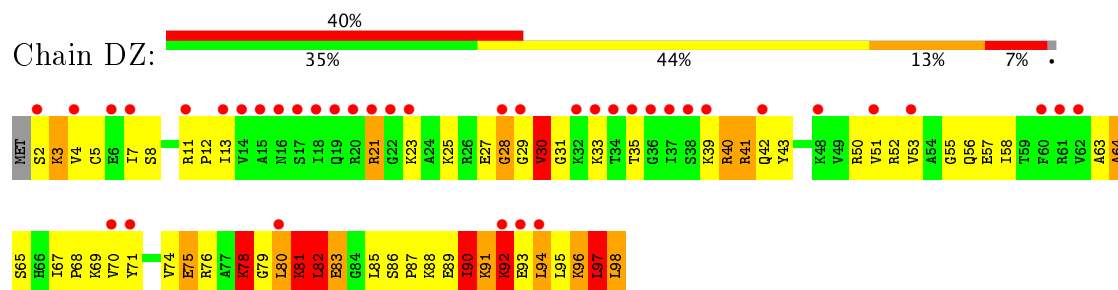
• Molecule 45: 50S ribosomal protein L27



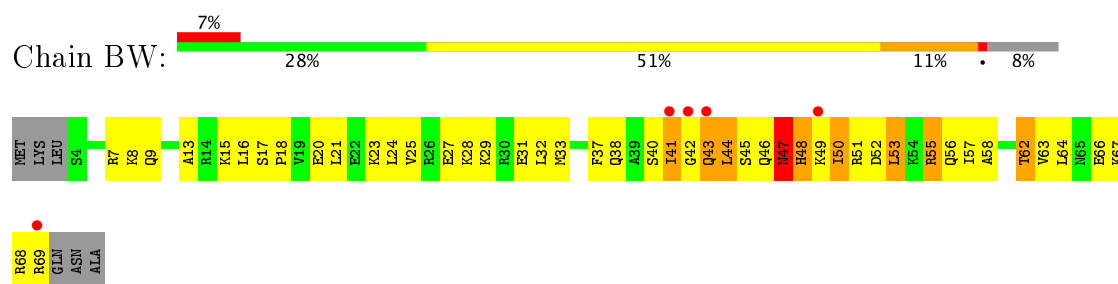
• Molecule 46: 50S ribosomal protein L28



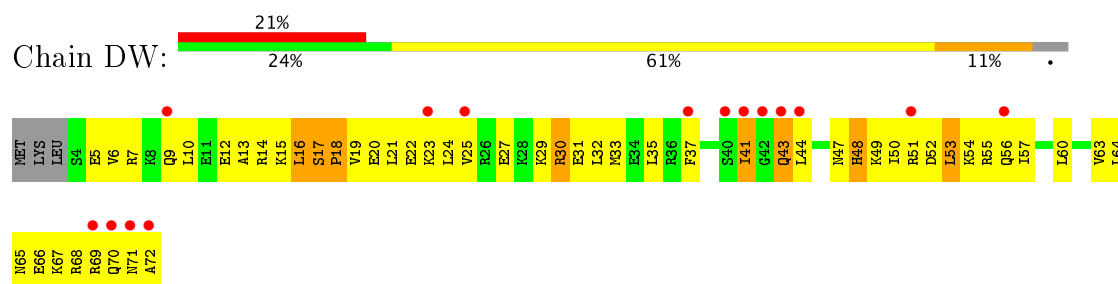
- Molecule 46: 50S ribosomal protein L28



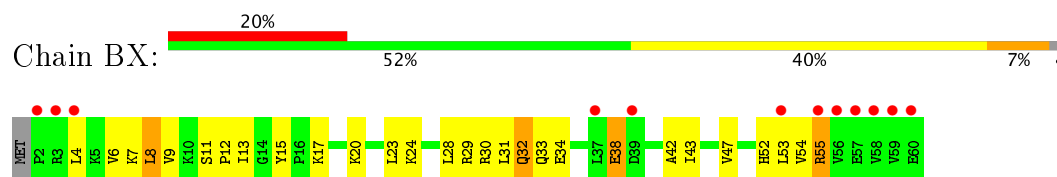
- Molecule 47: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L29

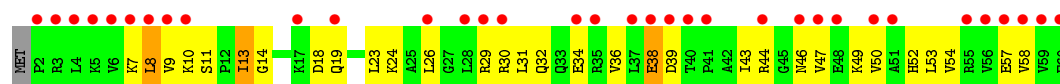


- Molecule 48: 50S ribosomal protein L30

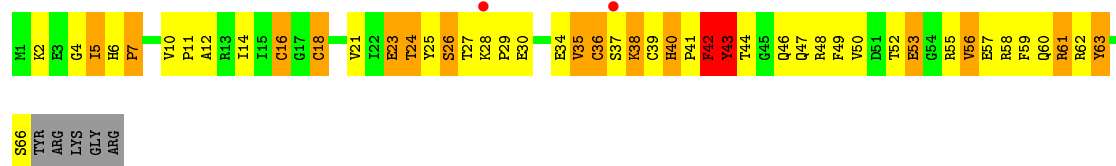


- Molecule 48: 50S ribosomal protein L30

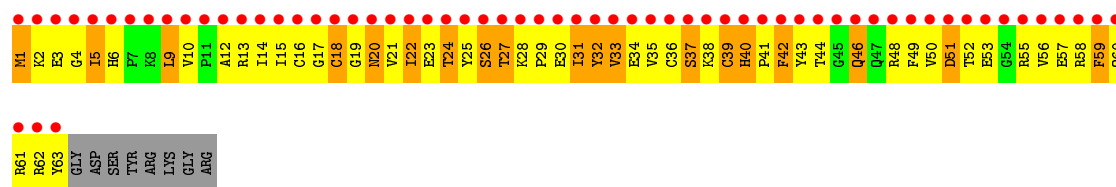
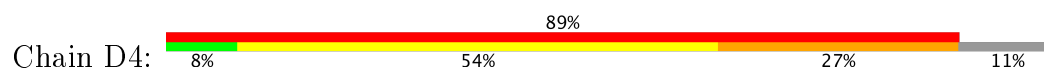




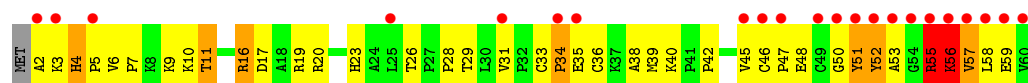
- Molecule 49: 50S ribosomal protein L31



- Molecule 49: 50S ribosomal protein L31



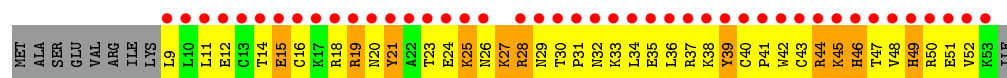
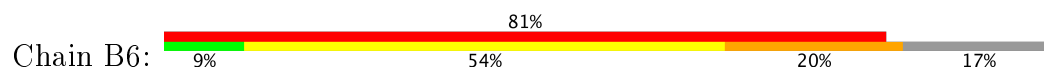
- Molecule 50: 50S ribosomal protein L32



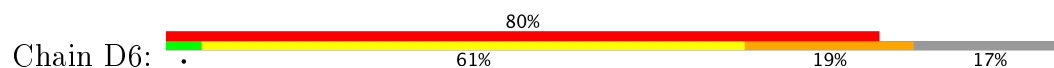
- Molecule 50: 50S ribosomal protein L32

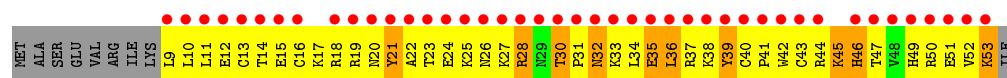


- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33

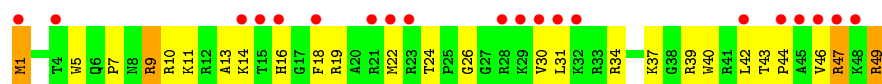
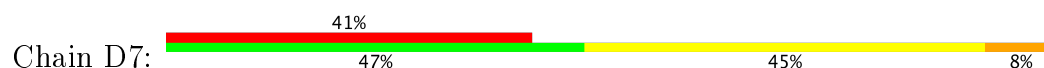




- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34

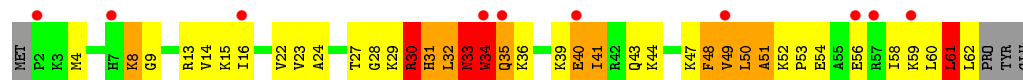


- Molecule 53: 50S ribosomal protein L35



GLU

- 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 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
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	9
4	AG	206/208 (99%)	157 (76%)	35 (17%)	14 (7%)	1	10
4	CG	206/208 (99%)	140 (68%)	44 (21%)	22 (11%)	0	4
5	AH	149/162 (92%)	127 (85%)	17 (11%)	5 (3%)	4	27
5	CH	149/162 (92%)	112 (75%)	31 (21%)	6 (4%)	3	23
6	AI	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	3	23
6	CI	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	13
7	AJ	153/156 (98%)	126 (82%)	17 (11%)	10 (6%)	1	12
7	CJ	153/156 (98%)	112 (73%)	33 (22%)	8 (5%)	2	16
8	AK	136/138 (99%)	103 (76%)	27 (20%)	6 (4%)	3	20
8	CK	136/138 (99%)	114 (84%)	15 (11%)	7 (5%)	2	17
9	AL	125/128 (98%)	93 (74%)	26 (21%)	6 (5%)	2	18
9	CL	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1	6
10	AM	97/105 (92%)	75 (77%)	17 (18%)	5 (5%)	2	16
10	CM	97/105 (92%)	69 (71%)	23 (24%)	5 (5%)	2	16
11	AN	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	8
11	CN	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	2	17
12	AO	123/128 (96%)	96 (78%)	17 (14%)	10 (8%)	1	7
12	CO	123/128 (96%)	91 (74%)	23 (19%)	9 (7%)	1	9
13	AP	114/126 (90%)	87 (76%)	15 (13%)	12 (10%)	0	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	10
14	CQ	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	0	4
15	AR	86/89 (97%)	71 (83%)	9 (10%)	6 (7%)	1	10
15	CR	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	15	50
16	AS	82/88 (93%)	61 (74%)	18 (22%)	3 (4%)	4	25
16	CS	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	9
17	AT	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	22
17	CT	98/105 (93%)	76 (78%)	15 (15%)	7 (7%)	1	10
18	AU	70/88 (80%)	58 (83%)	7 (10%)	5 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	2	14
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	2
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	6
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	20
26	DD	270/276 (98%)	223 (83%)	35 (13%)	12 (4%)	3	20
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%)	3	23
28	DF	206/210 (98%)	155 (75%)	33 (16%)	18 (9%)	1	6
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	0
31	BK	144/148 (97%)	102 (71%)	28 (19%)	14 (10%)	1	5
31	DK	144/148 (97%)	98 (68%)	31 (22%)	15 (10%)	0	4
32	BM	136/140 (97%)	101 (74%)	24 (18%)	11 (8%)	1	7
32	DM	136/140 (97%)	103 (76%)	22 (16%)	11 (8%)	1	7
33	BN	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	11	42
33	DN	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	6	34
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	4
35	DP	139/141 (99%)	100 (72%)	24 (17%)	15 (11%)	0	3
36	B0	116/118 (98%)	91 (78%)	14 (12%)	11 (10%)	1	5
36	D0	115/118 (98%)	85 (74%)	21 (18%)	9 (8%)	1	8
37	BQ	109/112 (97%)	82 (75%)	15 (14%)	12 (11%)	0	3
37	DQ	109/112 (97%)	74 (68%)	22 (20%)	13 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	135/146 (92%)	101 (75%)	25 (18%)	9 (7%)	1	11
38	DR	135/146 (92%)	105 (78%)	19 (14%)	11 (8%)	1	7
39	B1	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	2	16
39	D1	115/118 (98%)	89 (77%)	20 (17%)	6 (5%)	2	16
40	B2	99/101 (98%)	74 (75%)	17 (17%)	8 (8%)	1	7
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	15
41	DS	111/113 (98%)	86 (78%)	17 (15%)	8 (7%)	1	10
42	BT	90/96 (94%)	75 (83%)	13 (14%)	2 (2%)	8	37
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	2
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	32
45	D3	75/85 (88%)	63 (84%)	9 (12%)	3 (4%)	3	23
46	BZ	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	1	12
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	8
47	DW	67/72 (93%)	51 (76%)	9 (13%)	7 (10%)	0	4
48	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	10	42
48	DX	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	4	26
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	6
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	1
52	B7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	8	38
52	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
53	B8	59/65 (91%)	44 (75%)	10 (17%)	5 (8%)	1	6

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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	29
2	CE	205/220 (93%)	176 (86%)	29 (14%)	4	19
3	AF	159/188 (85%)	147 (92%)	12 (8%)	16	48
3	CF	160/188 (85%)	146 (91%)	14 (9%)	12	40
4	AG	180/180 (100%)	166 (92%)	14 (8%)	15	46
4	CG	180/180 (100%)	161 (89%)	19 (11%)	8	31
5	AH	116/123 (94%)	105 (90%)	11 (10%)	10	35
5	CH	116/123 (94%)	104 (90%)	12 (10%)	8	32
6	AI	90/90 (100%)	85 (94%)	5 (6%)	25	60
6	CI	90/90 (100%)	81 (90%)	9 (10%)	9	33
7	AJ	126/127 (99%)	118 (94%)	8 (6%)	21	56
7	CJ	126/127 (99%)	116 (92%)	10 (8%)	14	45
8	AK	119/119 (100%)	108 (91%)	11 (9%)	11	37
8	CK	119/119 (100%)	108 (91%)	11 (9%)	11	37
9	AL	98/99 (99%)	86 (88%)	12 (12%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CL	98/99 (99%)	79 (81%)	19 (19%)	1	7
10	AM	89/92 (97%)	82 (92%)	7 (8%)	14	45
10	CM	89/92 (97%)	82 (92%)	7 (8%)	14	45
11	AN	90/99 (91%)	86 (96%)	4 (4%)	33	67
11	CN	90/99 (91%)	85 (94%)	5 (6%)	25	60
12	AO	104/107 (97%)	97 (93%)	7 (7%)	19	53
12	CO	104/107 (97%)	97 (93%)	7 (7%)	19	53
13	AP	94/101 (93%)	89 (95%)	5 (5%)	26	62
13	CP	94/101 (93%)	78 (83%)	16 (17%)	2	11
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	8	32
14	CQ	49/50 (98%)	45 (92%)	4 (8%)	13	44
15	AR	79/80 (99%)	73 (92%)	6 (8%)	15	47
15	CR	79/80 (99%)	76 (96%)	3 (4%)	38	70
16	AS	72/74 (97%)	62 (86%)	10 (14%)	4	20
16	CS	72/74 (97%)	68 (94%)	4 (6%)	25	60
17	AT	95/97 (98%)	90 (95%)	5 (5%)	26	62
17	CT	95/97 (98%)	92 (97%)	3 (3%)	44	74
18	AU	63/77 (82%)	60 (95%)	3 (5%)	30	65
18	CU	63/77 (82%)	59 (94%)	4 (6%)	21	56
19	AV	72/80 (90%)	63 (88%)	9 (12%)	5	24
19	CV	67/80 (84%)	56 (84%)	11 (16%)	2	13
20	AW	76/82 (93%)	70 (92%)	6 (8%)	14	45
20	CW	76/82 (93%)	69 (91%)	7 (9%)	11	37
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	18 (90%)	2 (10%)	9	33
26	BD	214/218 (98%)	192 (90%)	22 (10%)	8	32
26	DD	214/218 (98%)	197 (92%)	17 (8%)	14	45
27	BE	165/166 (99%)	149 (90%)	16 (10%)	9	35
27	DE	165/166 (99%)	150 (91%)	15 (9%)	11	38
28	BF	161/166 (97%)	150 (93%)	11 (7%)	18	53
28	DF	165/166 (99%)	156 (94%)	9 (6%)	25	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BG	155/156 (99%)	145 (94%)	10 (6%)	20	55
29	DG	155/156 (99%)	141 (91%)	14 (9%)	11	39
30	BH	142/148 (96%)	119 (84%)	23 (16%)	3	13
30	DH	142/148 (96%)	128 (90%)	14 (10%)	9	34
31	BK	122/124 (98%)	110 (90%)	12 (10%)	9	34
31	DK	122/124 (98%)	109 (89%)	13 (11%)	8	30
32	BM	117/119 (98%)	113 (97%)	4 (3%)	42	73
32	DM	117/119 (98%)	109 (93%)	8 (7%)	18	53
33	BN	100/100 (100%)	95 (95%)	5 (5%)	28	64
33	DN	100/100 (100%)	95 (95%)	5 (5%)	28	64
34	BO	116/116 (100%)	101 (87%)	15 (13%)	5	22
34	DO	116/116 (100%)	102 (88%)	14 (12%)	6	25
35	BP	111/111 (100%)	102 (92%)	9 (8%)	14	44
35	DP	111/111 (100%)	102 (92%)	9 (8%)	14	44
36	B0	101/101 (100%)	94 (93%)	7 (7%)	18	53
36	D0	100/101 (99%)	95 (95%)	5 (5%)	28	64
37	BQ	87/88 (99%)	82 (94%)	5 (6%)	24	60
37	DQ	87/88 (99%)	78 (90%)	9 (10%)	8	32
38	BR	120/127 (94%)	111 (92%)	9 (8%)	16	48
38	DR	120/127 (94%)	107 (89%)	13 (11%)	7	30
39	B1	93/94 (99%)	87 (94%)	6 (6%)	20	55
39	D1	93/94 (99%)	88 (95%)	5 (5%)	26	62
40	B2	82/82 (100%)	75 (92%)	7 (8%)	12	42
40	D2	82/82 (100%)	71 (87%)	11 (13%)	4	21
41	BS	92/92 (100%)	82 (89%)	10 (11%)	7	30
41	DS	92/92 (100%)	82 (89%)	10 (11%)	7	30
42	BT	74/78 (95%)	69 (93%)	5 (7%)	18	53
42	DT	74/78 (95%)	69 (93%)	5 (7%)	18	53
43	BU	85/91 (93%)	70 (82%)	15 (18%)	2	10
43	DU	85/91 (93%)	73 (86%)	12 (14%)	4	19
44	BV	154/179 (86%)	135 (88%)	19 (12%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DV	158/179 (88%)	144 (91%)	14 (9%)	11	39
45	B3	61/67 (91%)	58 (95%)	3 (5%)	29	65
45	D3	62/67 (92%)	57 (92%)	5 (8%)	14	44
46	BZ	82/83 (99%)	77 (94%)	5 (6%)	22	57
46	DZ	82/83 (99%)	65 (79%)	17 (21%)	1	6
47	BW	62/67 (92%)	55 (89%)	7 (11%)	7	28
47	DW	64/67 (96%)	62 (97%)	2 (3%)	45	75
48	BX	51/52 (98%)	47 (92%)	4 (8%)	15	46
48	DX	51/52 (98%)	48 (94%)	3 (6%)	23	58
49	B4	59/63 (94%)	51 (86%)	8 (14%)	4	20
49	D4	57/63 (90%)	51 (90%)	6 (10%)	8	31
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%)	11	38
51	D6	44/52 (85%)	38 (86%)	6 (14%)	4	20
52	B7	42/42 (100%)	38 (90%)	4 (10%)	10	35
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	26
All	All	9584/9992 (96%)	8705 (91%)	879 (9%)	11	37

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	1.49	5 (15%)	41,58,58	1.73	6 (14%)
55	TAC	CA	1805	54	33,35,35	1.45	5 (15%)	41,58,58	1.74	7 (17%)

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 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1805	TAC	C6-C61	-3.73	1.50	1.53
55	AA	1833	TAC	C1C-C1	-3.14	1.50	1.55
55	AA	1833	TAC	C6-C61	-3.13	1.50	1.53
55	CA	1805	TAC	C1C-C1	-2.82	1.51	1.55
55	AA	1833	TAC	C2-C3	-2.32	1.34	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
55	AA	1833	TAC	O12-C12-C1B	-5.81	118.37	123.86
55	CA	1805	TAC	O12-C12-C1B	-5.51	118.66	123.86
55	AA	1833	TAC	C41-C1C-C1	-5.06	105.24	111.05
55	CA	1805	TAC	C41-C1C-C1	-4.84	105.49	111.05
55	CA	1805	TAC	C43-N4-C4	-2.37	108.58	114.09

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%)	-0.53	9 (0%) 89 88	89, 141, 216, 277	0
1	CA	1506/1506 (100%)	-0.65	9 (0%) 89 88	103, 152, 218, 275	0
2	AE	237/256 (92%)	0.74	45 (18%) 1 1	139, 172, 204, 216	0
2	CE	237/256 (92%)	1.61	88 (37%) 0 1	160, 191, 219, 228	0
3	AF	205/239 (85%)	2.26	118 (57%) 0 0	116, 151, 183, 201	0
3	CF	206/239 (86%)	1.75	75 (36%) 0 1	148, 179, 201, 211	0
4	AG	208/208 (100%)	1.39	64 (30%) 0 1	112, 149, 172, 183	0
4	CG	208/208 (100%)	0.35	19 (9%) 10 10	128, 153, 171, 180	0
5	AH	151/162 (93%)	1.69	51 (33%) 0 1	111, 139, 161, 195	0
5	CH	151/162 (93%)	0.80	26 (17%) 2 1	129, 154, 177, 196	0
6	AI	101/101 (100%)	2.95	67 (66%) 0 0	116, 141, 162, 167	0
6	CI	101/101 (100%)	1.27	32 (31%) 0 1	128, 149, 163, 178	0
7	AJ	155/156 (99%)	0.21	19 (12%) 5 4	129, 151, 187, 211	0
7	CJ	155/156 (99%)	1.69	56 (36%) 0 1	146, 167, 195, 204	0
8	AK	138/138 (100%)	0.15	6 (4%) 36 34	118, 148, 162, 170	0
8	CK	138/138 (100%)	0.12	2 (1%) 75 73	131, 159, 174, 180	0
9	AL	127/128 (99%)	-0.72	0 100 100	119, 169, 186, 192	0
9	CL	127/128 (99%)	-0.45	2 (1%) 72 69	133, 185, 199, 208	0
10	AM	99/105 (94%)	0.33	8 (8%) 13 12	119, 170, 197, 210	0
10	CM	99/105 (94%)	-0.22	3 (3%) 51 49	149, 191, 204, 209	0
11	AN	119/129 (92%)	2.60	61 (51%) 0 0	115, 137, 170, 198	0
11	CN	119/129 (92%)	1.68	43 (36%) 0 1	124, 149, 178, 196	0
12	AO	125/128 (97%)	2.07	57 (45%) 0 0	106, 128, 150, 192	0
12	CO	125/128 (97%)	0.27	4 (3%) 48 46	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%)	-0.70	0 100 100	103, 153, 174, 184	0
13	CP	117/126 (92%)	0.04	14 (11%) 5 4	143, 179, 196, 205	0
14	AQ	60/61 (98%)	-0.19	0 100 100	123, 143, 159, 161	0
14	CQ	60/61 (98%)	-0.37	3 (5%) 30 27	148, 176, 188, 191	0
15	AR	88/89 (98%)	0.02	3 (3%) 46 42	109, 136, 155, 162	0
15	CR	88/89 (98%)	0.98	16 (18%) 1 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%)	-0.64	0 100 100	121, 143, 167, 203	0
17	AT	100/105 (95%)	0.13	4 (4%) 39 36	123, 147, 162, 173	0
17	CT	100/105 (95%)	1.53	41 (41%) 0 0	122, 145, 159, 182	0
18	AU	72/88 (81%)	1.60	29 (40%) 0 0	118, 142, 168, 195	0
18	CU	72/88 (81%)	1.77	29 (40%) 0 0	134, 157, 181, 199	0
19	AV	83/93 (89%)	-0.38	0 100 100	133, 158, 180, 191	0
19	CV	78/93 (83%)	0.50	11 (14%) 3 3	169, 195, 210, 221	0
20	AW	99/106 (93%)	-0.42	1 (1%) 82 81	137, 159, 187, 196	0
20	CW	99/106 (93%)	-0.20	1 (1%) 82 81	112, 142, 177, 194	0
21	AX	25/27 (92%)	-0.65	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%)	-0.26	0 100 100	102, 125, 153, 175	0
22	CC	77/77 (100%)	0.52	12 (15%) 2 2	106, 145, 175, 205	0
23	A1	4/4 (100%)	-0.36	0 100 100	106, 109, 114, 165	0
23	C1	4/4 (100%)	-0.27	0 100 100	127, 131, 143, 184	0
24	BA	2912/2912 (100%)	-0.15	75 (2%) 56 53	68, 102, 240, 278	0
24	DA	2909/2912 (99%)	-0.24	100 (3%) 46 42	79, 114, 258, 279	0
25	BB	122/122 (100%)	-0.56	1 (0%) 86 85	92, 122, 145, 211	0
25	DB	122/122 (100%)	-0.37	4 (3%) 47 44	115, 152, 178, 226	0
26	BD	272/276 (98%)	0.93	51 (18%) 1 1	69, 96, 117, 140	0
26	DD	272/276 (98%)	0.73	24 (8%) 11 10	72, 106, 130, 155	0
27	BE	205/206 (99%)	1.11	45 (21%) 1 1	73, 117, 163, 177	0
27	DE	205/206 (99%)	0.84	31 (15%) 3 2	79, 122, 168, 196	0
28	BF	202/210 (96%)	0.38	18 (8%) 10 10	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%)	1.50	57 (27%) 1 1	82, 125, 187, 213	0
29	BG	181/182 (99%)	-0.22	3 (1%) 70 67	105, 127, 167, 186	0
29	DG	181/182 (99%)	3.22	125 (69%) 0 0	136, 166, 194, 204	0
30	BH	170/180 (94%)	-0.19	4 (2%) 59 56	103, 135, 159, 175	0
30	DH	170/180 (94%)	2.01	65 (38%) 0 0	154, 222, 249, 262	0
31	BK	146/148 (98%)	-0.11	8 (5%) 26 24	103, 151, 170, 179	0
31	DK	146/148 (98%)	-0.12	9 (6%) 21 21	111, 159, 178, 185	0
32	BM	138/140 (98%)	0.63	12 (8%) 11 10	90, 115, 153, 183	0
32	DM	138/140 (98%)	0.79	23 (16%) 2 2	93, 129, 168, 189	0
33	BN	122/122 (100%)	0.09	3 (2%) 58 54	83, 111, 132, 139	0
33	DN	122/122 (100%)	1.04	22 (18%) 2 1	86, 116, 130, 140	0
34	BO	150/150 (100%)	1.13	47 (31%) 0 1	70, 113, 143, 207	0
34	DO	150/150 (100%)	1.22	34 (22%) 1 1	85, 129, 167, 206	0
35	BP	141/141 (100%)	0.48	12 (8%) 11 11	85, 107, 132, 163	0
35	DP	141/141 (100%)	0.95	29 (20%) 1 1	95, 126, 152, 177	0
36	B0	118/118 (100%)	0.88	18 (15%) 2 2	90, 110, 131, 148	0
36	D0	117/118 (99%)	0.27	7 (5%) 23 21	88, 111, 135, 146	0
37	BQ	111/112 (99%)	0.70	19 (17%) 2 1	90, 119, 148, 164	0
37	DQ	111/112 (99%)	0.46	9 (8%) 13 12	114, 146, 168, 190	0
38	BR	137/146 (93%)	0.51	16 (11%) 5 4	104, 125, 173, 202	0
38	DR	137/146 (93%)	0.59	13 (9%) 9 8	103, 121, 177, 212	0
39	B1	117/118 (99%)	0.03	4 (3%) 46 42	77, 106, 141, 168	0
39	D1	117/118 (99%)	0.87	21 (17%) 2 1	90, 122, 155, 178	0
40	B2	101/101 (100%)	1.28	34 (33%) 0 1	79, 122, 154, 181	0
40	D2	101/101 (100%)	2.91	60 (59%) 0 0	95, 149, 165, 181	0
41	BS	113/113 (100%)	1.51	34 (30%) 1 1	81, 102, 141, 191	0
41	DS	113/113 (100%)	1.14	21 (18%) 1 1	83, 107, 140, 194	0
42	BT	92/96 (95%)	0.62	8 (8%) 11 10	81, 98, 126, 145	0
42	DT	92/96 (95%)	1.18	24 (26%) 1 1	96, 117, 140, 159	0
43	BU	102/110 (92%)	0.05	5 (4%) 30 28	95, 123, 171, 190	0
43	DU	102/110 (92%)	2.77	59 (57%) 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%)	1.86	66 (37%) 0 1	104, 142, 218, 229	0
44	DV	179/206 (86%)	1.78	74 (41%) 0 0	132, 174, 237, 251	0
45	B3	76/85 (89%)	0.13	2 (2%) 56 53	85, 101, 121, 163	0
45	D3	77/85 (90%)	1.75	21 (27%) 1 1	98, 117, 141, 175	0
46	BZ	97/98 (98%)	0.51	9 (9%) 9 9	83, 106, 149, 195	0
46	DZ	97/98 (98%)	1.83	39 (40%) 0 0	87, 116, 159, 191	0
47	BW	66/72 (91%)	0.62	5 (7%) 15 14	80, 108, 133, 171	0
47	DW	69/72 (95%)	1.11	15 (21%) 1 1	106, 138, 163, 196	0
48	BX	59/60 (98%)	1.19	12 (20%) 1 1	85, 106, 148, 160	0
48	DX	59/60 (98%)	2.56	34 (57%) 0 0	97, 126, 159, 194	0
49	B4	66/71 (92%)	-0.06	2 (3%) 51 49	127, 176, 209, 219	0
49	D4	63/71 (88%)	7.46	63 (100%) 0 0	181, 212, 226, 235	0
50	B5	59/60 (98%)	2.45	22 (37%) 0 1	78, 115, 194, 210	0
50	D5	59/60 (98%)	1.38	12 (20%) 1 1	87, 114, 191, 218	0
51	B6	45/54 (83%)	8.23	44 (97%) 0 0	149, 184, 197, 201	0
51	D6	45/54 (83%)	11.08	43 (95%) 0 0	158, 195, 212, 215	0
52	B7	49/49 (100%)	0.72	7 (14%) 3 3	73, 83, 124, 154	0
52	D7	49/49 (100%)	2.29	20 (40%) 0 0	78, 91, 134, 156	0
53	B8	61/65 (93%)	0.17	2 (3%) 47 44	81, 96, 116, 145	0
53	D8	61/65 (93%)	1.17	10 (16%) 2 2	94, 109, 131, 161	0
All	All	20772/21286 (97%)	0.41	2684 (12%) 4 3	68, 133, 207, 279	0

The worst 5 of 2684 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	D6	13	CYS	25.6
50	D5	59	GLU	23.2
51	D6	22	ALA	22.8
24	BA	654(K)	C	22.6
24	BA	1	G	21.9

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

There are no such residues in this entry.