



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:06 PM GMT

PDB ID : 4V8C
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex with paromomycin).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-07
Resolution : 3.30 Å(reported)

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

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

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

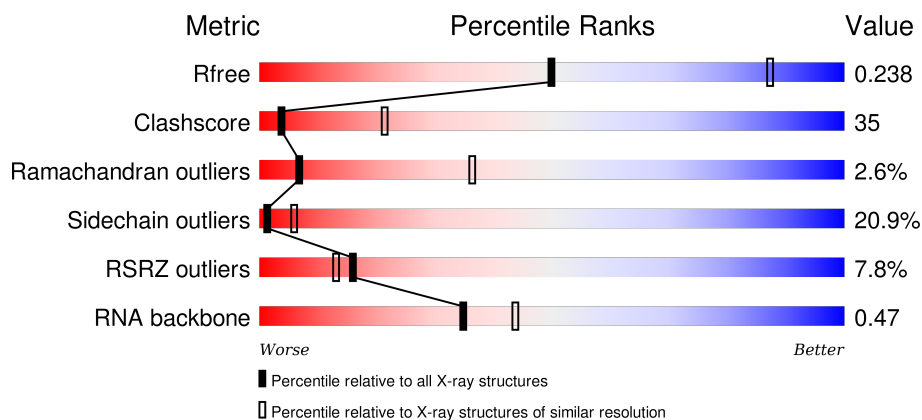
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	2912	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 28% 50% 20% </div> </div>
1	BA	2912	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 27% 51% 20% </div> </div>
2	AB	122	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 32% 48% 18% </div> </div>
2	BB	122	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 25% 56% 19% </div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	276	
3	BD	276	
4	AE	206	
4	BE	206	
5	AF	210	
5	BF	210	
6	AG	182	
6	BG	182	
7	AH	180	
7	BH	180	
8	AK	148	
8	BK	148	
9	AM	140	
9	BM	140	
10	AN	122	
10	BN	122	
11	AO	150	
11	BO	150	
12	AP	141	
12	BP	141	
13	A0	118	
13	B0	118	
14	AQ	112	
14	BQ	112	
15	AR	146	




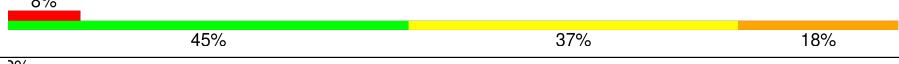
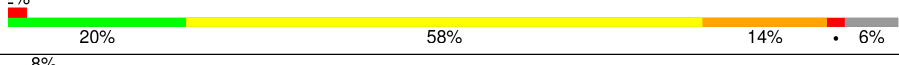
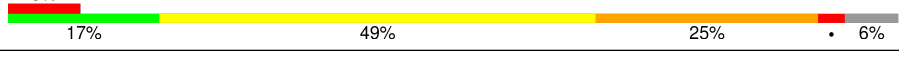
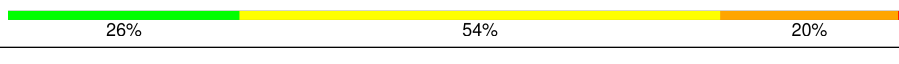
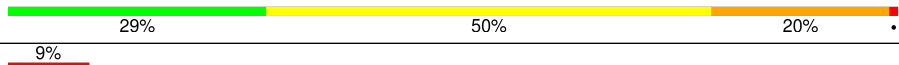
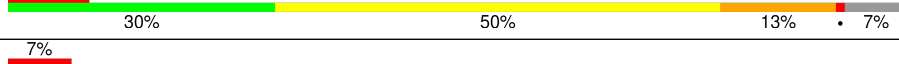
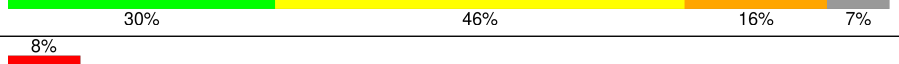

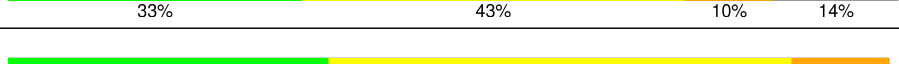
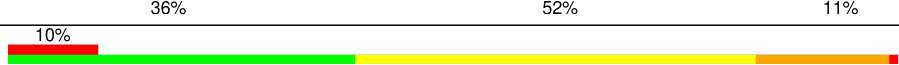
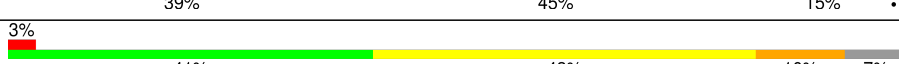
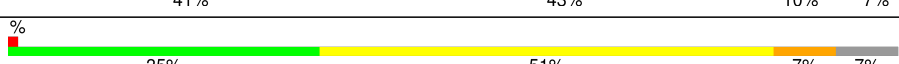
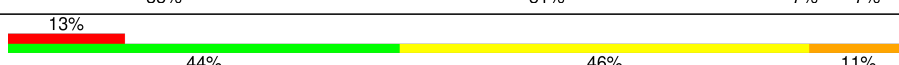


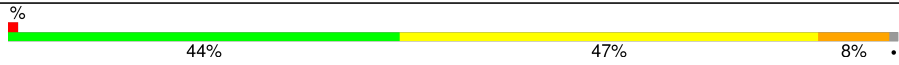


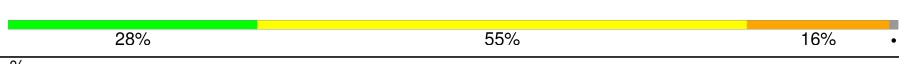

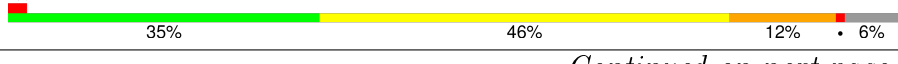

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Mol	Chain	Length	Quality of chain
15	BR	146	
16	A1	118	
16	B1	118	
17	A2	101	
17	B2	101	
18	AS	113	
18	BS	113	
19	AT	96	
19	BT	96	
20	AU	110	
20	BU	110	
21	AV	206	
21	BV	206	
22	A3	85	
22	B3	85	
23	AZ	98	
23	BZ	98	
24	AW	72	
24	BW	72	
25	AX	60	
25	BX	60	
26	A4	71	
26	B4	71	
27	A5	60	
27	B5	60	

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Mol	Chain	Length	Quality of chain
28	A6	54	
28	B6	54	
29	A7	49	
29	B7	49	
30	A8	65	
30	B8	65	
31	CA	1506	
31	DA	1506	
32	CE	256	
32	DE	256	
33	CF	239	
33	DF	239	
34	CG	208	
34	DG	208	
35	CH	162	
35	DH	162	
36	CI	101	
36	DI	101	
37	CJ	156	
37	DJ	156	
38	CK	138	
38	DK	138	
39	CL	128	
39	DL	128	
40	CM	105	

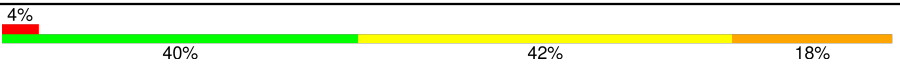


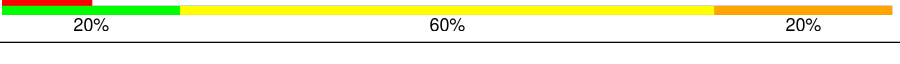
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Mol	Chain	Length	Quality of chain
40	DM	105	
41	CN	129	
41	DN	129	
42	CO	132	
42	DO	132	
43	CP	126	
43	DP	126	
44	CQ	61	
44	DQ	61	
45	CR	89	
45	DR	89	
46	CS	88	
46	DS	88	
47	CT	105	
47	DT	105	
48	CU	88	
48	DU	88	
49	CV	93	
49	DV	93	
50	CW	106	
50	DW	106	
51	CX	27	
51	DX	27	
52	CB	87	
52	DB	87	

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Mol	Chain	Length	Quality of chain
53	CC	77	
53	CD	77	
53	DC	77	
53	DD	77	
54	C1	10	
54	D1	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	A1	201	-	-	-	X
55	MG	A6	101	-	-	-	X
55	MG	AA	3001	-	-	-	X
55	MG	AA	3002	-	-	-	X
55	MG	AA	3004	-	-	-	X
55	MG	AA	3006	-	-	-	X
55	MG	AA	3010	-	-	-	X
55	MG	AA	3012	-	-	-	X
55	MG	AA	3016	-	-	-	X
55	MG	AA	3021	-	-	-	X
55	MG	AA	3024	-	-	-	X
55	MG	AA	3027	-	-	-	X
55	MG	AA	3031	-	-	-	X
55	MG	AA	3034	-	-	-	X
55	MG	AA	3037	-	-	-	X
55	MG	AA	3040	-	-	-	X
55	MG	AA	3044	-	-	-	X
55	MG	AA	3045	-	-	-	X
55	MG	AA	3047	-	-	-	X
55	MG	AA	3051	-	-	-	X
55	MG	AA	3052	-	-	-	X
55	MG	AA	3053	-	-	-	X
55	MG	AA	3054	-	-	-	X
55	MG	AA	3055	-	-	-	X
55	MG	AA	3057	-	-	-	X
55	MG	AA	3058	-	-	-	X
55	MG	AA	3068	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3074	-	-	-	X
55	MG	AA	3081	-	-	-	X
55	MG	AA	3082	-	-	-	X
55	MG	AA	3083	-	-	-	X
55	MG	AA	3085	-	-	-	X
55	MG	AA	3086	-	-	-	X
55	MG	AA	3092	-	-	-	X
55	MG	AA	3093	-	-	-	X
55	MG	AA	3094	-	-	-	X
55	MG	AA	3098	-	-	-	X
55	MG	AA	3106	-	-	-	X
55	MG	AA	3112	-	-	-	X
55	MG	AA	3113	-	-	-	X
55	MG	AA	3116	-	-	-	X
55	MG	AA	3119	-	-	-	X
55	MG	AA	3123	-	-	-	X
55	MG	AA	3124	-	-	-	X
55	MG	AA	3125	-	-	-	X
55	MG	AA	3128	-	-	-	X
55	MG	AA	3135	-	-	-	X
55	MG	AA	3138	-	-	-	X
55	MG	AA	3139	-	-	-	X
55	MG	AA	3141	-	-	-	X
55	MG	AA	3144	-	-	-	X
55	MG	AA	3150	-	-	-	X
55	MG	AA	3153	-	-	-	X
55	MG	AA	3154	-	-	-	X
55	MG	AA	3160	-	-	-	X
55	MG	AA	3162	-	-	-	X
55	MG	AA	3165	-	-	-	X
55	MG	AA	3168	-	-	-	X
55	MG	AA	3174	-	-	-	X
55	MG	AA	3177	-	-	-	X
55	MG	AA	3186	-	-	-	X
55	MG	AA	3195	-	-	-	X
55	MG	AA	3212	-	-	-	X
55	MG	AA	3214	-	-	-	X
55	MG	AA	3222	-	-	-	X
55	MG	AA	3223	-	-	-	X
55	MG	AA	3228	-	-	-	X
55	MG	AA	3233	-	-	-	X
55	MG	AA	3245	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3247	-	-	-	X
55	MG	AA	3249	-	-	-	X
55	MG	AA	3253	-	-	-	X
55	MG	AA	3262	-	-	-	X
55	MG	AA	3263	-	-	-	X
55	MG	AA	3266	-	-	-	X
55	MG	AA	3267	-	-	-	X
55	MG	AA	3269	-	-	-	X
55	MG	AA	3272	-	-	-	X
55	MG	AA	3277	-	-	-	X
55	MG	AA	3307	-	-	-	X
55	MG	AA	3310	-	-	-	X
55	MG	AA	3315	-	-	-	X
55	MG	AA	3322	-	-	-	X
55	MG	AA	3323	-	-	-	X
55	MG	AA	3328	-	-	-	X
55	MG	AA	3336	-	-	-	X
55	MG	AA	3343	-	-	-	X
55	MG	AA	3351	-	-	-	X
55	MG	AA	3355	-	-	-	X
55	MG	AA	3356	-	-	-	X
55	MG	AA	3379	-	-	-	X
55	MG	AA	3400	-	-	-	X
55	MG	AA	3408	-	-	-	X
55	MG	AA	3428	-	-	-	X
55	MG	AA	3448	-	-	-	X
55	MG	AA	3459	-	-	-	X
55	MG	AA	3462	-	-	-	X
55	MG	AA	3464	-	-	-	X
55	MG	AA	3489	-	-	-	X
55	MG	AA	3497	-	-	-	X
55	MG	AA	3513	-	-	-	X
55	MG	AA	3521	-	-	-	X
55	MG	AA	3530	-	-	-	X
55	MG	AA	3538	-	-	-	X
55	MG	AA	3540	-	-	-	X
55	MG	AA	3541	-	-	-	X
55	MG	AA	3548	-	-	-	X
55	MG	AA	3549	-	-	-	X
55	MG	AA	3550	-	-	-	X
55	MG	AA	3551	-	-	-	X
55	MG	AA	3565	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3567	-	-	-	X
55	MG	AA	3568	-	-	-	X
55	MG	AA	3570	-	-	-	X
55	MG	AA	3574	-	-	-	X
55	MG	AA	3578	-	-	-	X
55	MG	AA	3588	-	-	-	X
55	MG	AA	3590	-	-	-	X
55	MG	AA	3592	-	-	-	X
55	MG	AA	3599	-	-	-	X
55	MG	AA	3603	-	-	-	X
55	MG	AA	3609	-	-	-	X
55	MG	AA	3623	-	-	-	X
55	MG	AA	3625	-	-	-	X
55	MG	AB	202	-	-	-	X
55	MG	AB	215	-	-	-	X
55	MG	AB	217	-	-	-	X
55	MG	AE	303	-	-	-	X
55	MG	AF	303	-	-	-	X
55	MG	AO	201	-	-	-	X
55	MG	AO	203	-	-	-	X
55	MG	BA	3009	-	-	-	X
55	MG	BA	3010	-	-	-	X
55	MG	BA	3012	-	-	-	X
55	MG	BA	3023	-	-	-	X
55	MG	BA	3037	-	-	-	X
55	MG	BA	3058	-	-	-	X
55	MG	BA	3067	-	-	-	X
55	MG	BA	3081	-	-	-	X
55	MG	BA	3086	-	-	-	X
55	MG	BA	3094	-	-	-	X
55	MG	BA	3100	-	-	-	X
55	MG	BA	3107	-	-	-	X
55	MG	BA	3118	-	-	-	X
55	MG	BA	3125	-	-	-	X
55	MG	BA	3127	-	-	-	X
55	MG	BA	3129	-	-	-	X
55	MG	BA	3135	-	-	-	X
55	MG	BA	3136	-	-	-	X
55	MG	BA	3140	-	-	-	X
55	MG	BA	3144	-	-	-	X
55	MG	BA	3145	-	-	-	X
55	MG	BA	3152	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3155	-	-	-	X
55	MG	BA	3156	-	-	-	X
55	MG	BA	3157	-	-	-	X
55	MG	BA	3158	-	-	-	X
55	MG	BA	3163	-	-	-	X
55	MG	BA	3167	-	-	-	X
55	MG	BA	3169	-	-	-	X
55	MG	BA	3174	-	-	-	X
55	MG	BA	3178	-	-	-	X
55	MG	BA	3179	-	-	-	X
55	MG	BA	3180	-	-	-	X
55	MG	BA	3187	-	-	-	X
55	MG	BA	3189	-	-	-	X
55	MG	BA	3203	-	-	-	X
55	MG	BA	3208	-	-	-	X
55	MG	BA	3211	-	-	-	X
55	MG	BA	3217	-	-	-	X
55	MG	BA	3218	-	-	-	X
55	MG	BA	3219	-	-	-	X
55	MG	BA	3220	-	-	-	X
55	MG	BA	3224	-	-	-	X
55	MG	BA	3227	-	-	-	X
55	MG	BA	3228	-	-	-	X
55	MG	BA	3229	-	-	-	X
55	MG	BA	3231	-	-	-	X
55	MG	BA	3233	-	-	-	X
55	MG	BA	3236	-	-	-	X
55	MG	BA	3237	-	-	-	X
55	MG	BA	3238	-	-	-	X
55	MG	BA	3239	-	-	-	X
55	MG	BA	3242	-	-	-	X
55	MG	BA	3254	-	-	-	X
55	MG	BA	3266	-	-	-	X
55	MG	BA	3278	-	-	-	X
55	MG	BA	3279	-	-	-	X
55	MG	BA	3283	-	-	-	X
55	MG	BA	3288	-	-	-	X
55	MG	BA	3309	-	-	-	X
55	MG	BA	3317	-	-	-	X
55	MG	BA	3324	-	-	-	X
55	MG	BA	3325	-	-	-	X
55	MG	BA	3329	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3331	-	-	-	X
55	MG	BA	3350	-	-	-	X
55	MG	BA	3355	-	-	-	X
55	MG	BA	3363	-	-	-	X
55	MG	BA	3366	-	-	-	X
55	MG	BA	3367	-	-	-	X
55	MG	BA	3369	-	-	-	X
55	MG	BA	3376	-	-	-	X
55	MG	BA	3384	-	-	-	X
55	MG	BA	3396	-	-	-	X
55	MG	BA	3404	-	-	-	X
55	MG	BA	3412	-	-	-	X
55	MG	BA	3446	-	-	-	X
55	MG	BA	3447	-	-	-	X
55	MG	BA	3481	-	-	-	X
55	MG	BA	3484	-	-	-	X
55	MG	BA	3489	-	-	-	X
55	MG	BA	3490	-	-	-	X
55	MG	BA	3492	-	-	-	X
55	MG	BA	3494	-	-	-	X
55	MG	BA	3496	-	-	-	X
55	MG	BA	3512	-	-	-	X
55	MG	BA	3514	-	-	-	X
55	MG	BB	207	-	-	-	X
55	MG	BR	202	-	-	-	X
55	MG	CA	1610	-	-	-	X
55	MG	CA	1620	-	-	-	X
55	MG	CA	1628	-	-	-	X
55	MG	CA	1632	-	-	-	X
55	MG	CA	1636	-	-	-	X
55	MG	CA	1639	-	-	-	X
55	MG	CA	1645	-	-	-	X
55	MG	CA	1651	-	-	-	X
55	MG	CA	1658	-	-	-	X
55	MG	CA	1663	-	-	-	X
55	MG	CA	1667	-	-	-	X
55	MG	CA	1678	-	-	-	X
55	MG	CA	1679	-	-	-	X
55	MG	CA	1691	-	-	-	X
55	MG	CA	1711	-	-	-	X
55	MG	CA	1712	-	-	-	X
55	MG	CA	1715	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	1717	-	-	-	X
55	MG	CA	1722	-	-	-	X
55	MG	CA	1760	-	-	-	X
55	MG	CA	1767	-	-	-	X
55	MG	CA	1780	-	-	-	X
55	MG	CA	1792	-	-	-	X
55	MG	CA	1819	-	-	-	X
55	MG	CA	1836	-	-	-	X
55	MG	DA	1604	-	-	-	X
55	MG	DA	1606	-	-	-	X
55	MG	DA	1610	-	-	-	X
55	MG	DA	1616	-	-	-	X
55	MG	DA	1617	-	-	-	X
55	MG	DA	1621	-	-	-	X
55	MG	DA	1638	-	-	-	X
55	MG	DA	1644	-	-	-	X
55	MG	DA	1645	-	-	-	X
55	MG	DA	1646	-	-	-	X
55	MG	DA	1649	-	-	-	X
55	MG	DA	1653	-	-	-	X
55	MG	DA	1656	-	-	-	X
55	MG	DA	1664	-	-	-	X
55	MG	DA	1667	-	-	-	X
55	MG	DA	1670	-	-	-	X
55	MG	DA	1675	-	-	-	X
55	MG	DA	1677	-	-	-	X
55	MG	DA	1684	-	-	-	X
55	MG	DA	1685	-	-	-	X
55	MG	DA	1689	-	-	-	X
55	MG	DA	1690	-	-	-	X
55	MG	DA	1710	-	-	-	X
55	MG	DA	1715	-	-	-	X
55	MG	DA	1721	-	-	-	X
55	MG	DA	1722	-	-	-	X
55	MG	DA	1728	-	-	-	X
55	MG	DA	1737	-	-	-	X
55	MG	DA	1747	-	-	-	X
55	MG	DA	1748	-	-	-	X
55	MG	DA	1752	-	-	-	X
55	MG	DA	1753	-	-	-	X
55	MG	DA	1755	-	-	-	X
55	MG	DA	1756	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	1763	-	-	-	X
55	MG	DA	1782	-	-	-	X
55	MG	DA	1795	-	-	-	X
55	MG	DA	1799	-	-	-	X
55	MG	DA	1801	-	-	-	X
56	PAR	CA	1841	-	-	-	X
56	PAR	DA	1805	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299682 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	BA	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
AA	161	U	-	EXPRESSION TAG	GB AP008226.1
AA	654A	A	G	CONFLICT	GB AP008226.1
AA	654E	C	G	CONFLICT	GB AP008226.1
AA	654P	G	C	CONFLICT	GB AP008226.1
AA	654T	A	C	CONFLICT	GB AP008226.1
AA	1058	U	G	CONFLICT	GB AP008226.1
AA	1080	A	C	CONFLICT	GB AP008226.1
BA	158	U	-	EXPRESSION TAG	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

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	B0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	B3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	B4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
28	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
29	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
30	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
49	DV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 52 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CB	87	Total	C	N	O	P	9	0	0
			1861	829	333	612	87			
52	DB	87	Total	C	N	O	P	8	0	0
			1861	829	333	612	87			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	DD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	18	C	U	CONFLICT	GB AP012306.1
CD	18	C	U	CONFLICT	GB AP012306.1
DC	18	C	U	CONFLICT	GB AP012306.1
DD	18	C	U	CONFLICT	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
54	D1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

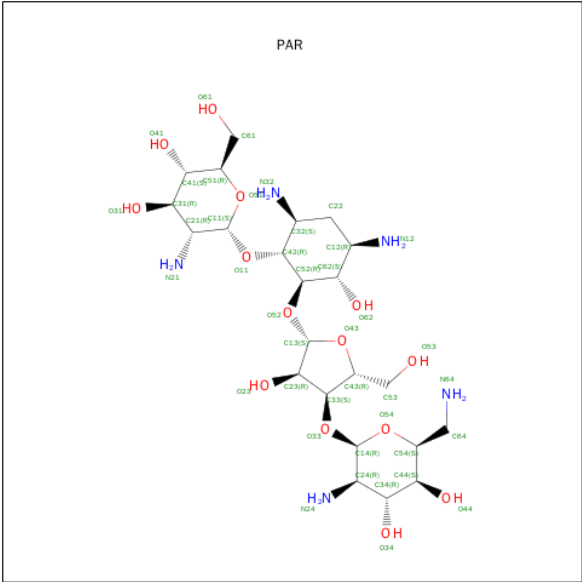
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	528	Total Mg 528 528	0	0
55	CA	240	Total Mg 240 240	0	0
55	AB	17	Total Mg 17 17	0	0
55	A6	1	Total Mg 1 1	0	0
55	BE	3	Total Mg 3 3	0	0
55	B1	1	Total Mg 1 1	0	0
55	C1	1	Total Mg 1 1	0	0
55	CD	1	Total Mg 1 1	0	0
55	BP	1	Total Mg 1 1	0	0
55	CN	2	Total Mg 2 2	0	0
55	A2	1	Total Mg 1 1	0	0
55	DC	8	Total Mg 8 8	0	0
55	B5	1	Total Mg 1 1	0	0
55	BB	15	Total Mg 15 15	0	0
55	AE	4	Total Mg 4 4	0	0
55	DG	2	Total Mg 2 2	0	0
55	AA	626	Total Mg 626 626	0	0
55	CQ	2	Total Mg 2 2	0	0
55	A5	2	Total Mg 2 2	0	0
55	CG	2	Total Mg 2 2	0	0
55	A1	1	Total Mg 1 1	0	0
55	AD	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	CT	1	Total 1	Mg 1	0	0
55	DH	1	Total 1	Mg 1	0	0
55	CC	7	Total 7	Mg 7	0	0
55	DS	1	Total 1	Mg 1	0	0
55	B3	1	Total 1	Mg 1	0	0
55	BR	2	Total 2	Mg 2	0	0
55	AZ	1	Total 1	Mg 1	0	0
55	DA	204	Total 204	Mg 204	0	0
55	AU	1	Total 1	Mg 1	0	0
55	A0	1	Total 1	Mg 1	0	0
55	CB	5	Total 5	Mg 5	0	0
55	A7	2	Total 2	Mg 2	0	0
55	BD	1	Total 1	Mg 1	0	0
55	AO	3	Total 3	Mg 3	0	0
55	A3	1	Total 1	Mg 1	0	0
55	AF	3	Total 3	Mg 3	0	0
55	DB	2	Total 2	Mg 2	0	0

- Molecule 56 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	CA	1	Total	C	N	O	0	0
			42	23	5	14		
56	DA	1	Total	C	N	O	0	0
			42	23	5	14		

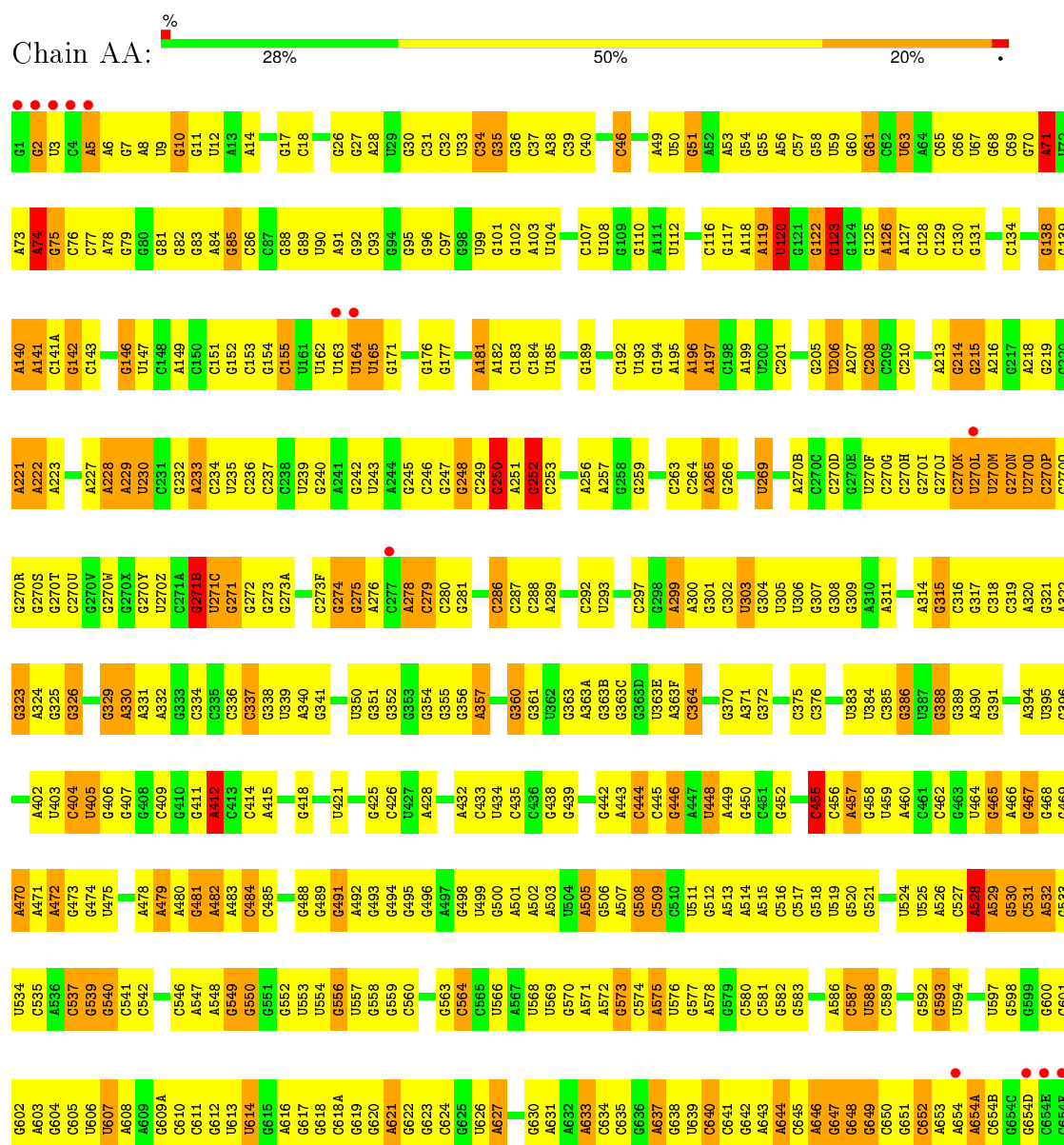
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DG	1	Total	Zn	0	0
			1	1		
57	CQ	1	Total	Zn	0	0
			1	1		
57	DQ	1	Total	Zn	0	0
			1	1		
57	CG	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

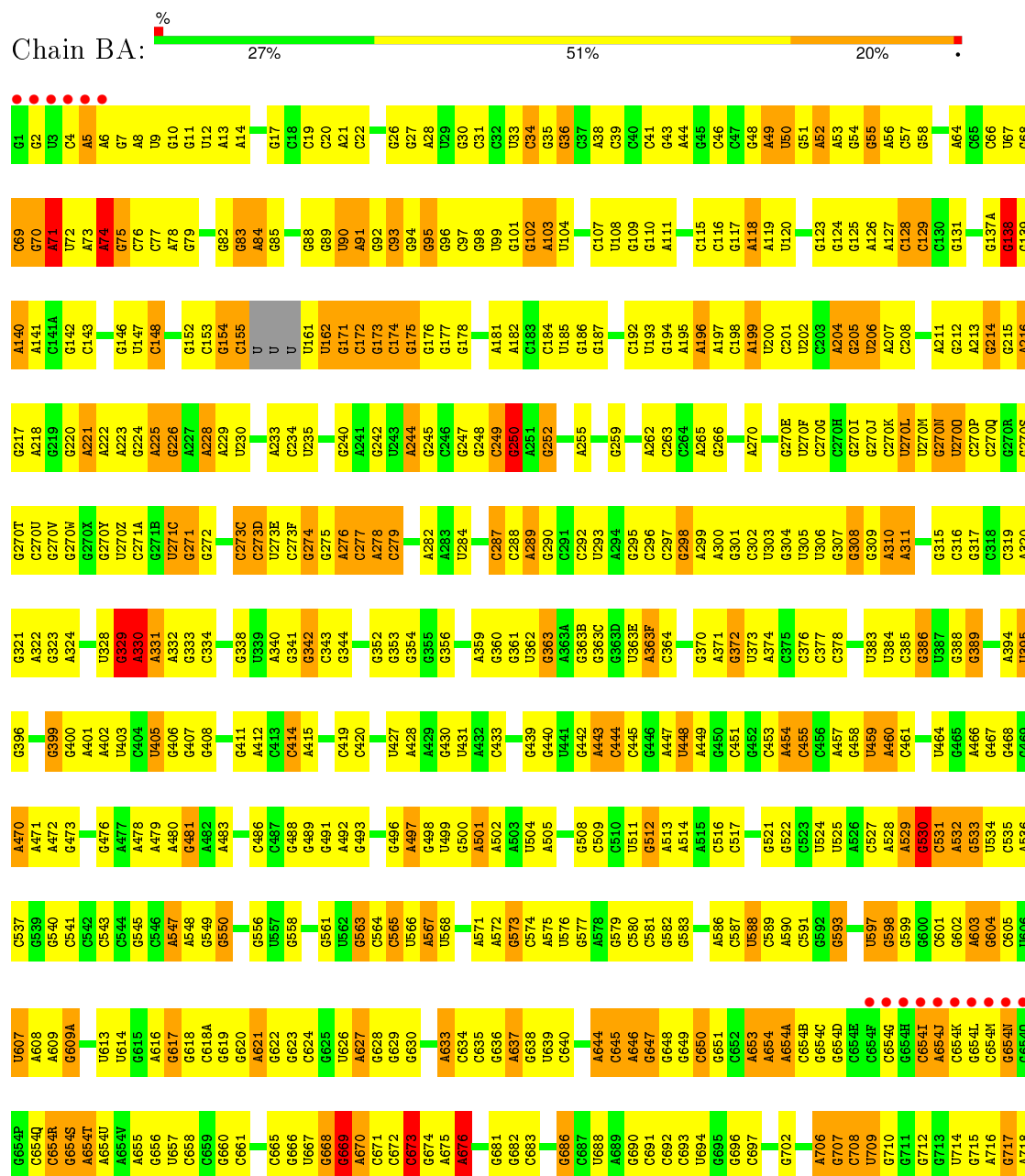
• Molecule 1: RNA (2912-MER)



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G1525	G1526	G1527	G1528	A1529	G1530	G1531	G1532	G1533	G1534	A1535	A1536	G1537	G1538	G1539	G1540	G1541	G1542	A1543	G1544	G1545	A1546	G1547	G1548	G1549	G1550	A1553	A1554	G1555	G1556	A1557	G1558	A1559	G1560	G1561	A1562	G1563	G1564	A1565	A1566	A1567	G1568	A1569	A1570	A1571	A1572	G1575	A1576	A1577	A1578	A1579	A1580	A1581	G1582	A1583	G1584	G1585																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
A1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	A1469	G1470	A1471	G1474	G1475	G1476	A1477	G1478	G1479	G1480	G1482	G1483	G1484	G1487	G1488	A1489	A1490	G1491	G1492	G1493	A1494	A1495	A1496	A1497	G1498	G1499	G1500	G1501	G1502	A1503	G1504	A1505	G1506	A1507	A1508	G1509	A1510	A1511	G1512	G1513	G1514	G1515	G1516	G1517	A1579	A1580	G1581	G1582	A1583	G1584	G1585																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A1395	A1396	A1397	C1398	C1399	G1400	G1401	G1402	C1403	A1404	G1405	A1406	C1407	C1408	C1409	G1410	C1411	A1412	G1413	G1416	C1417	G1418	A1419	A1420	G1421	G1424	G1425	G1426	A1427	G1428	G1429	A1430	A1431	C1432	G1433	A1434	G1435	G1436	C1437	A1438	A1439	G1440	G1441	G1442	G1443	G1444	A1444A	G1448	A1449	G1449A	G1453	A1454	G1455	G1458	A1459	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770	G1771	G1772	G1773	G1774	G1775	G1776	G1777	G1778	G1779	G1780	G1781	G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850	G1851	G1852	G1853	G1854	G1855	G1856	G1857	G1858	G1859	G1860	G1861	G1862	G1863	G1864	G1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	G1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892	G1893	G1894	G1895	G1896	G1897	G1898	G1899	G1900	G1901	G1902	G1903	G1904	G1905	G1906	G1907	G1908	G1909	G1910	G1911	G1912	G1913	G1914	G1915	G1916	G1917	G1918	G1919	G1920	G1921	G1922	G1923	G1924	G1925	G1926	G1927	G1928	G1929	G1930	G1931	G1932	G1933	G1934	G1935	G1936	G1937	G1938	G1939	G1940	G1941	G1942	G1943	G1944	G1945	G1946	G1947	G1948	G1949	G1950	G1951	G1952	G1953	G1954	G1955	G1956	G1957	G1958	G1959	G1960	G1961	G1962	G1963	G1964	G1965	G1966	G1967	G1968	G1969	G1970	G1971	G1972	G1973	G1974	G1975	G1976	G1977	G1978	G1979	G1980	G1981	G1982	G1983	G1984	G1985	G1986	G1987	G1988	G1989	G1990	G1991	G1992	G1993	G1994	G1995	G1996	G1997	G1998	G1999	G2000	G2001	G2002	G2003	G2004	G2005	G2006	G2007	G2008	G2009	G2010	G2011	G2012	G2013	G2014	G2015	G2016	G2017	G2018	G2019	G2020	G2021	G2022	G2023	G2024	G2025	G2026	G2027	G2028	G2029	G2030	G2031	G2032	G2033	G2034	G2035	G2036	G2037	G2038	G2039	G2040	G2041	G2042	G2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058	G2059	G2060	G2061	G2062	G2063	G2064	G2065	G2066	G2067	G2068	G2069	G2070	G2071	G2072	G2073	G2074	G2075	G2076	G2077	G2078	G2079	G2080	G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	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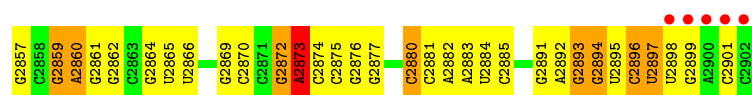
WORLDWIDE
PDB
PROTEIN DATA BANK

- Molecule 1: RNA (2912-MER)

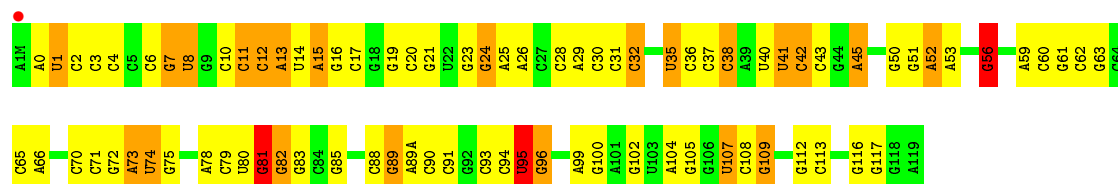




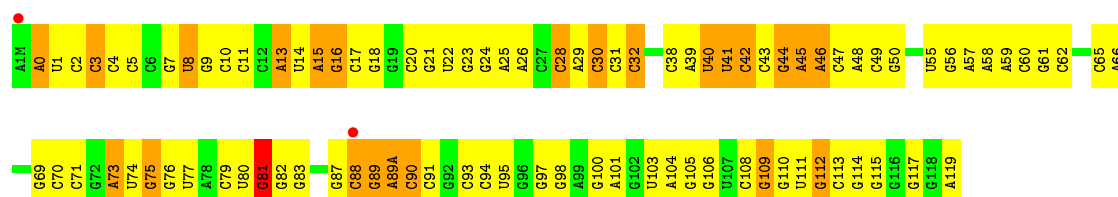
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C2788	A2721	U2649	A2577	U2512	A2435	G2368	A2305	G2237	C2161	G2100	C1965	A1889	C1734	C1734
C2789	C2722	U2650	G2578	G2513	G2436	G2371	G2306	G2238	G2162	C2103	A1966	U1805	C1735	C1735
A2790	C2723	U2651	C2579	G2514	U2437	G2372	G2307	G2239	C2163	G2104	C1967	A1810	C1741	C1741
C2791	C2724	U2652	U2580	G2515	U2438	G2373	G2308	C2240	C2164	C2105	C1968	A1811	C1742	C1742
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G2805	G2735	C2663	A2450	C2527	A2450	G2385	A2320	G2252	C2175	G2115	G1984	G1906	A1821	A1821
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A2809	U2738	C2666	A2453	U2530	C2453	U2388	A2323	G2255	U2180	A2118	G1989	C1909	G1758	G1758
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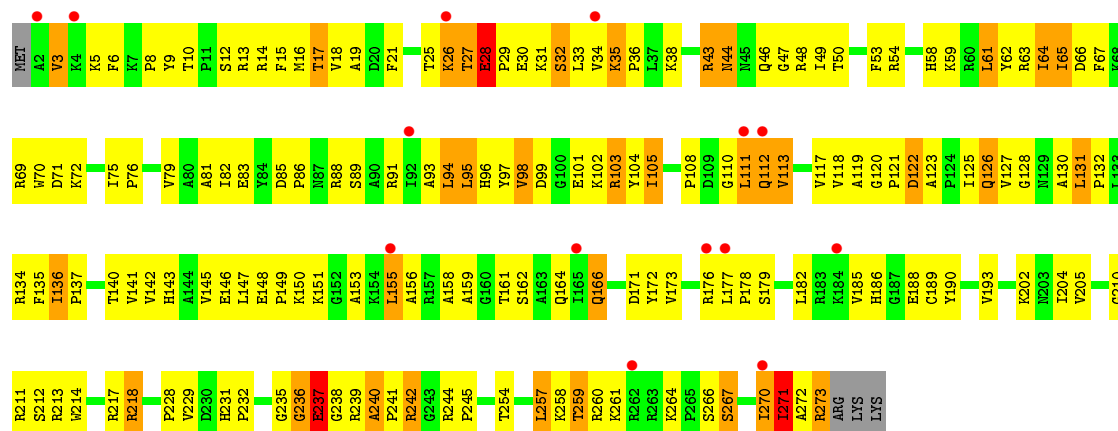
• Molecule 2: 5S RIBOSOMAL RNA



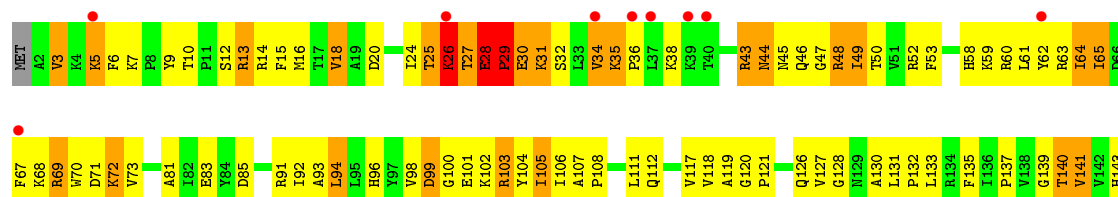
• Molecule 2: 5S RIBOSOMAL RNA

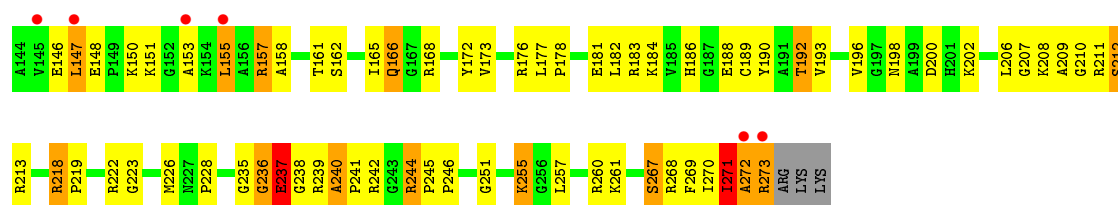


• Molecule 3: 50S ribosomal protein L2

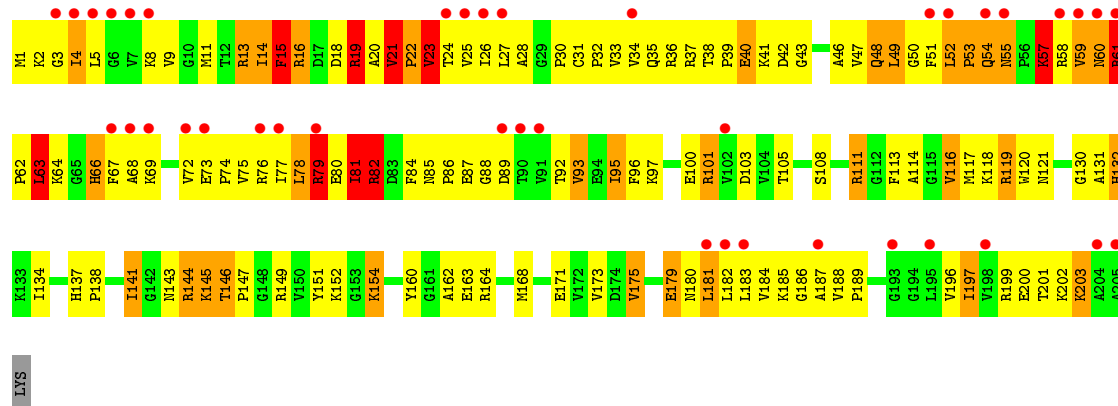


• Molecule 3: 50S ribosomal protein L2

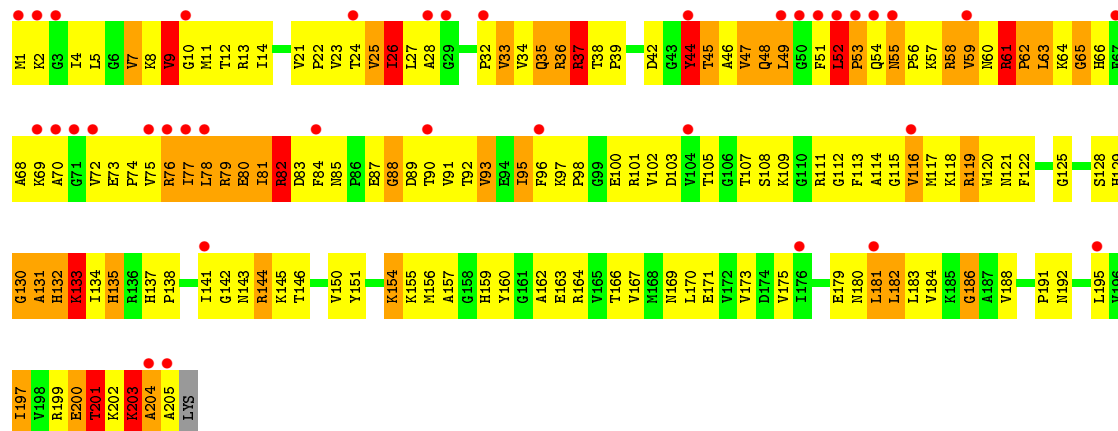




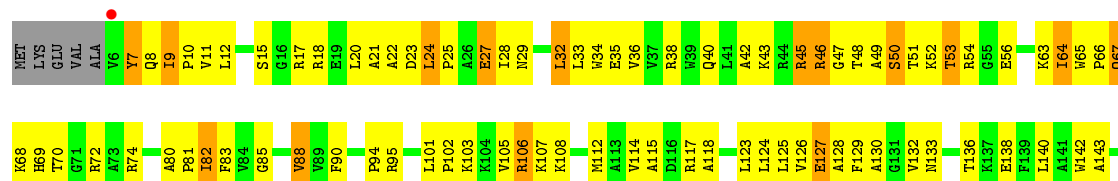
• Molecule 4: 50S ribosomal protein L3

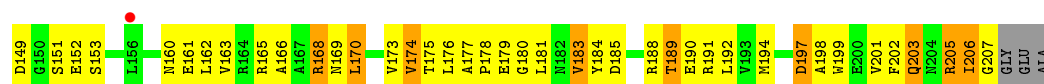


• Molecule 4: 50S ribosomal protein L3

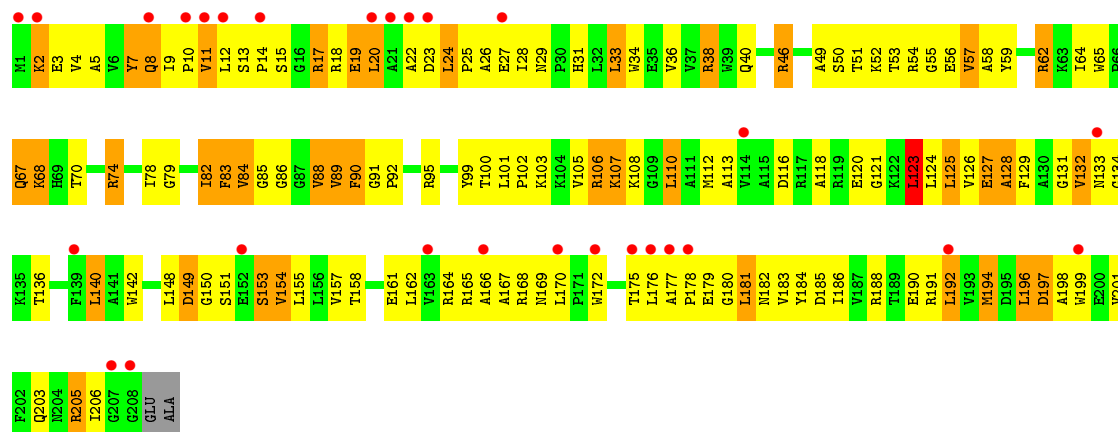


• Molecule 5: 50S ribosomal protein L4

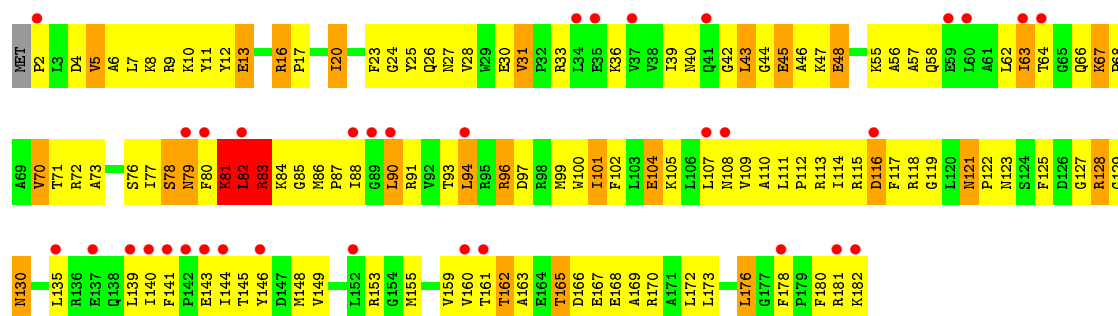




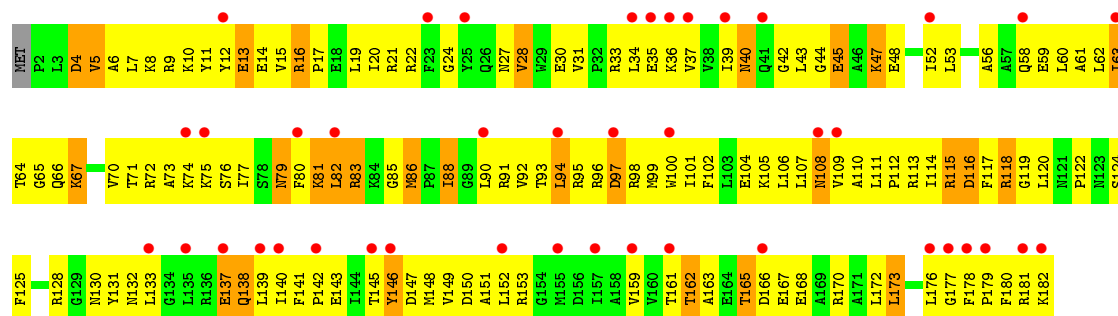
• Molecule 5: 50S ribosomal protein L4



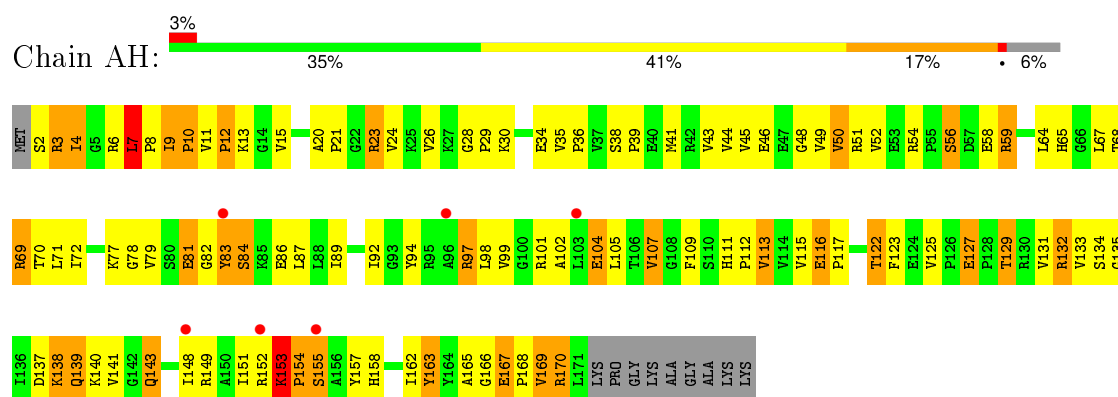
• Molecule 6: 50S ribosomal protein L5



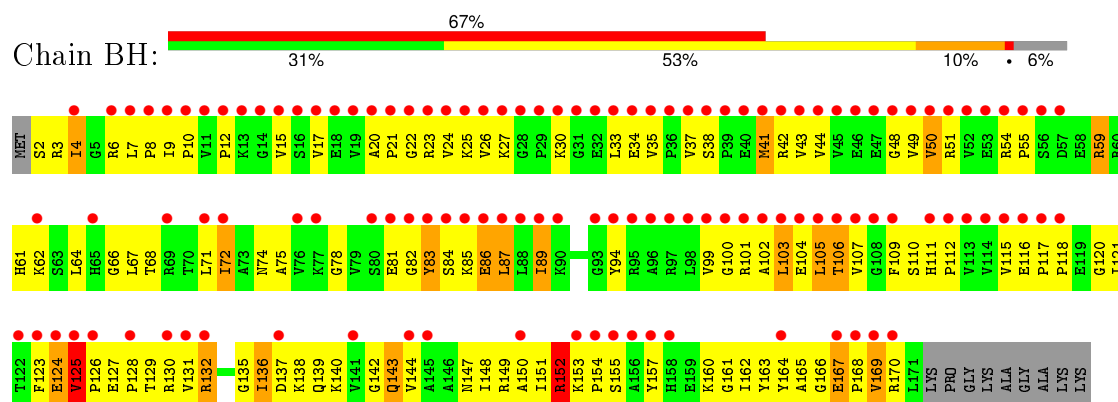
• Molecule 6: 50S ribosomal protein L5



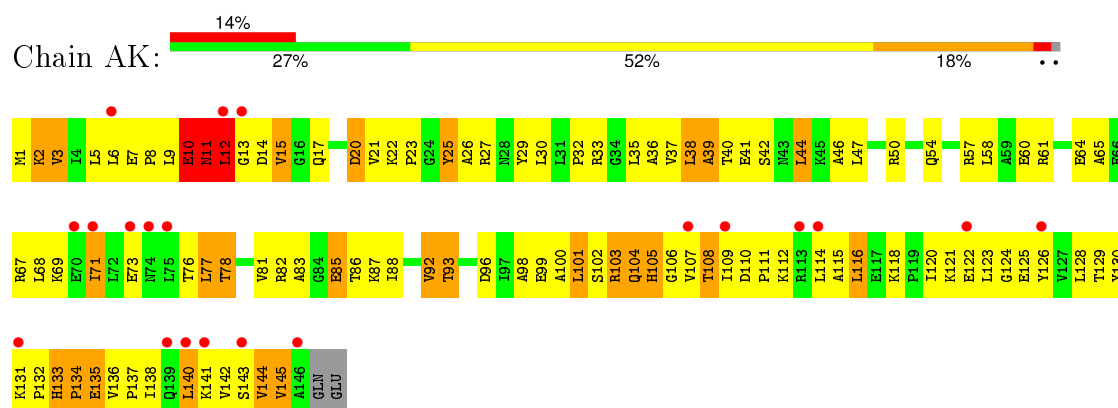
• Molecule 7: 50S ribosomal protein L6



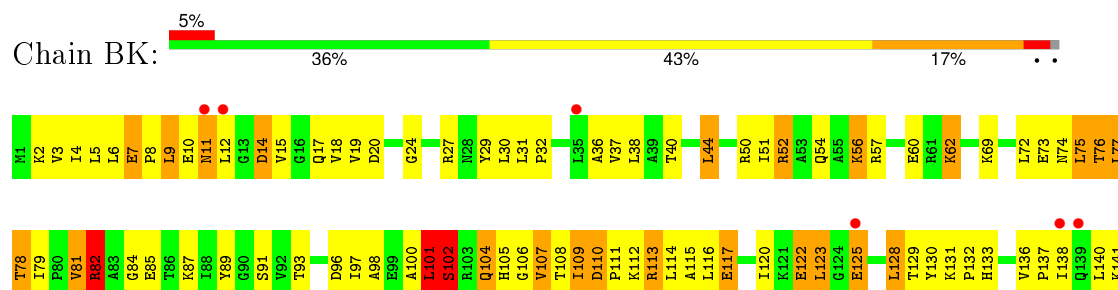
• Molecule 7: 50S ribosomal protein L6

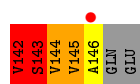


• Molecule 8: 50S ribosomal protein L9

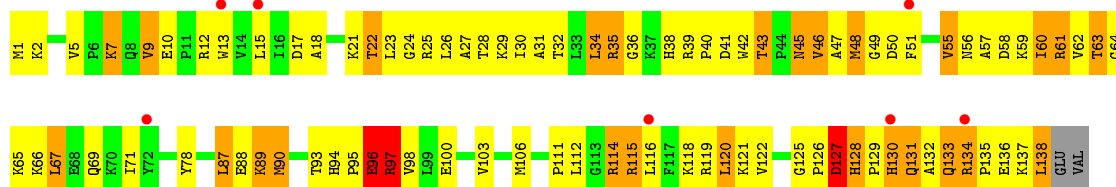


• Molecule 8: 50S ribosomal protein L9

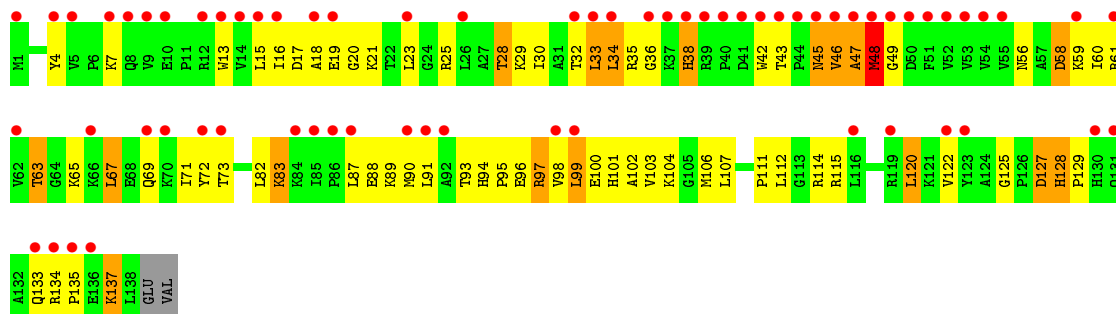




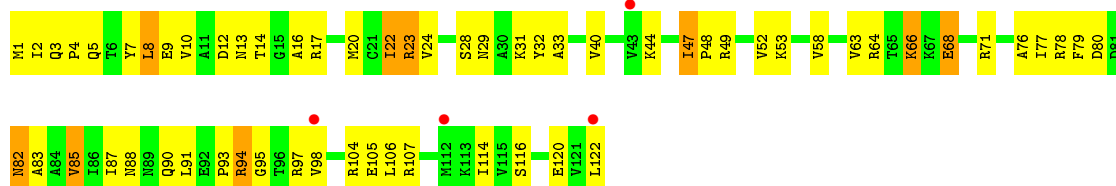
• Molecule 9: 50S ribosomal protein L13



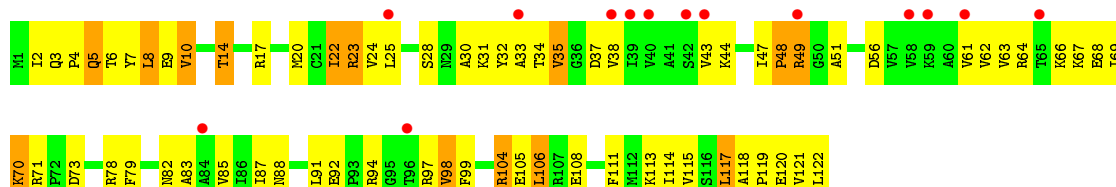
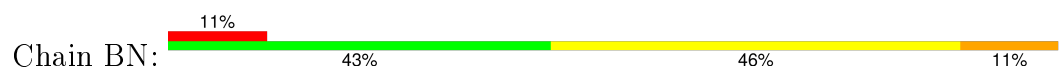
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



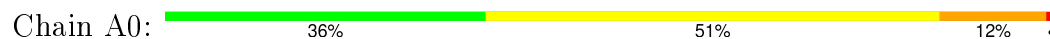
• Molecule 10: 50S ribosomal protein L14



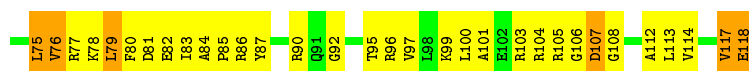
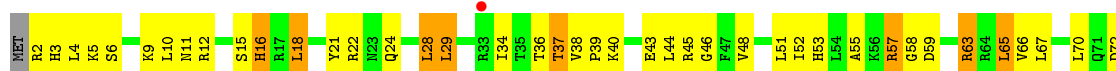
• Molecule 11: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L17



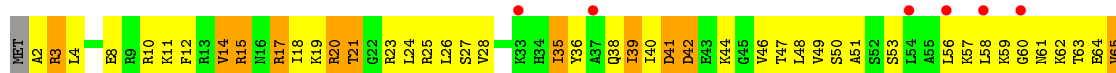
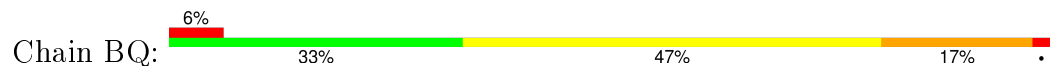
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

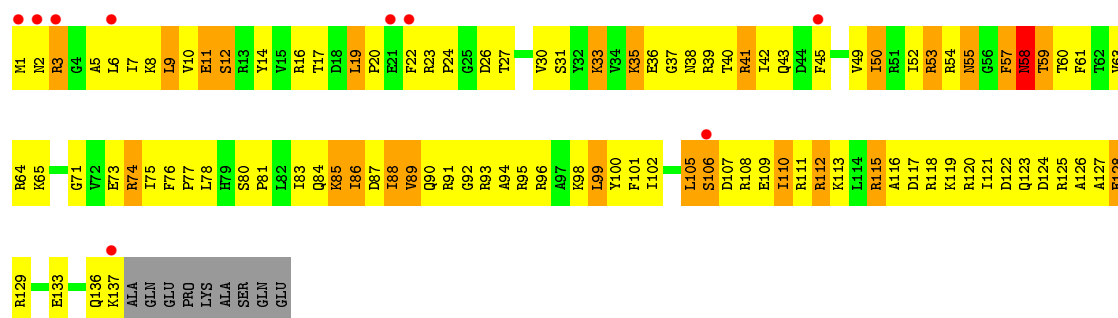


- Molecule 14: 50S ribosomal protein L18

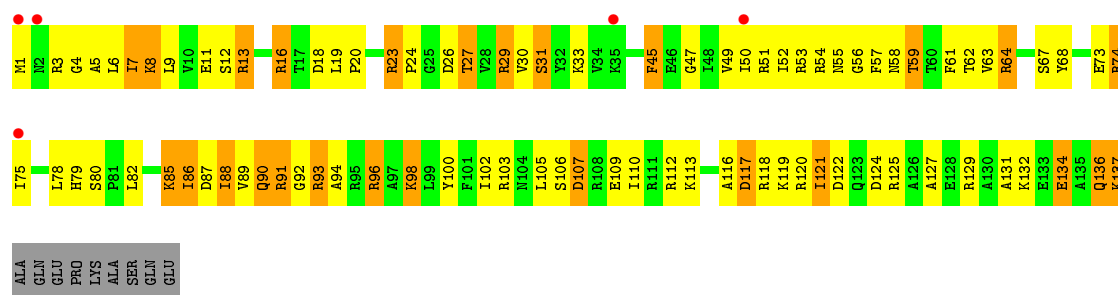


- Molecule 15: 50S ribosomal protein L19

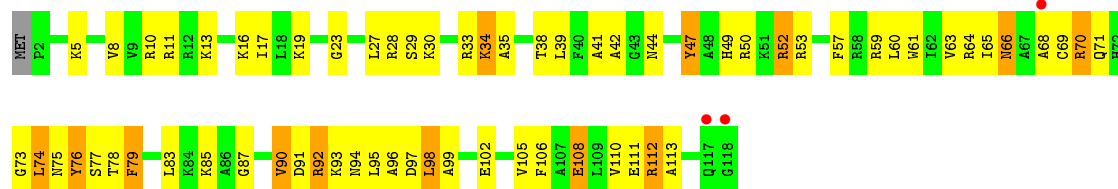
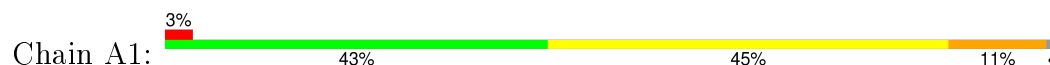




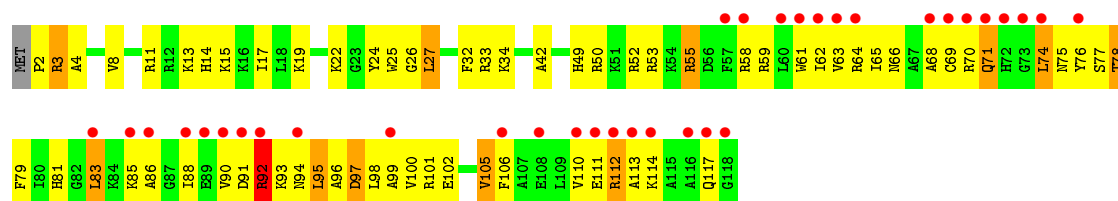
- Molecule 15: 50S ribosomal protein L19



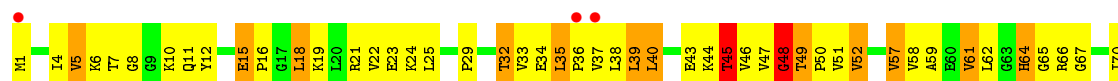
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20

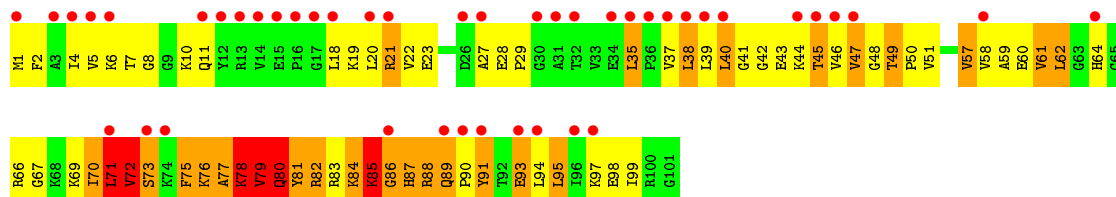
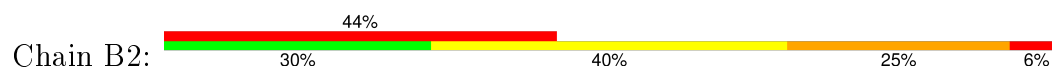


- Molecule 17: 50S ribosomal protein L21

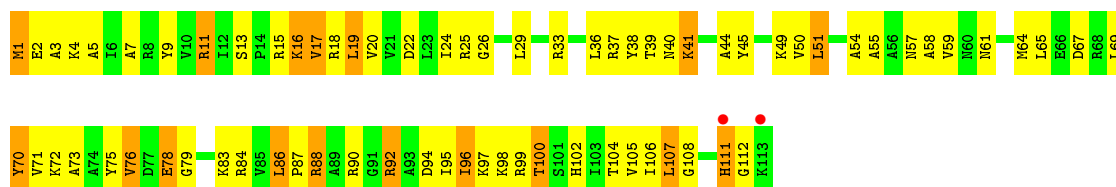




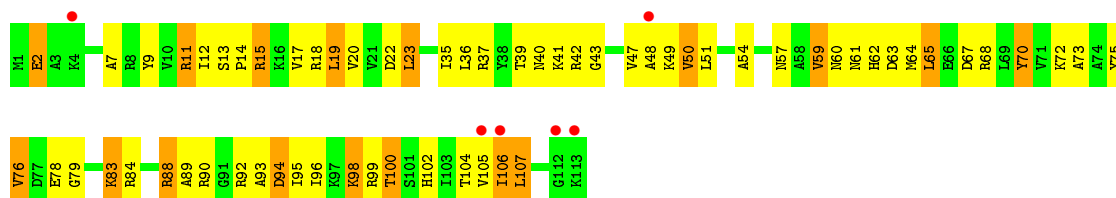
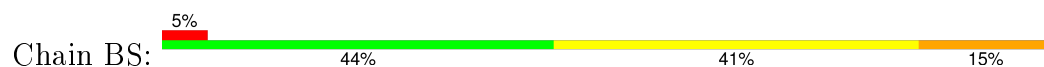
• Molecule 17: 50S ribosomal protein L21



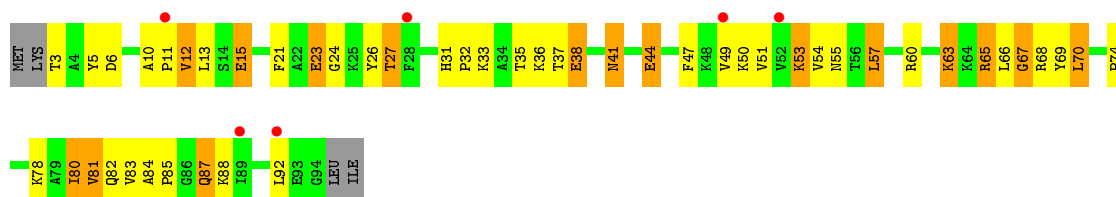
• Molecule 18: 50S ribosomal protein L22



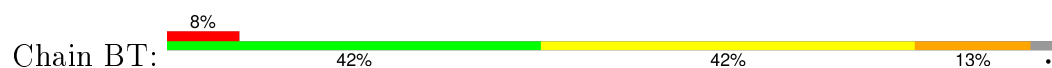
• Molecule 18: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L23

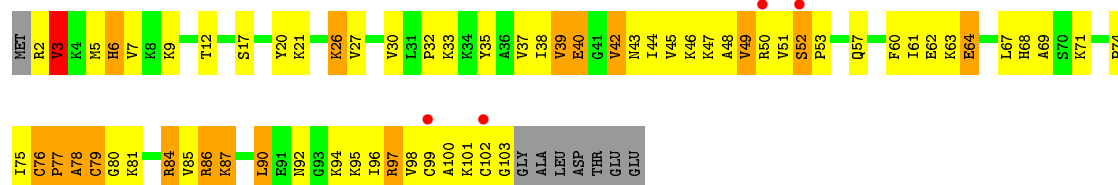


• Molecule 19: 50S ribosomal protein L23

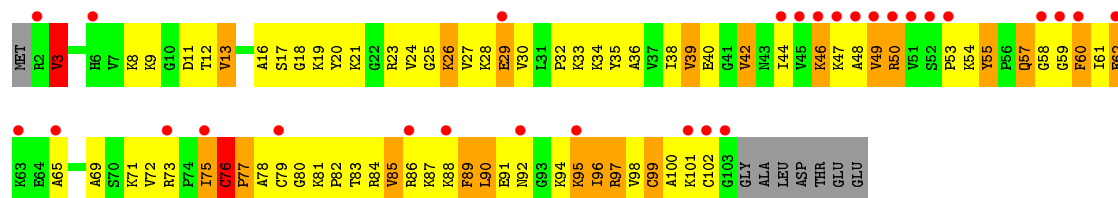




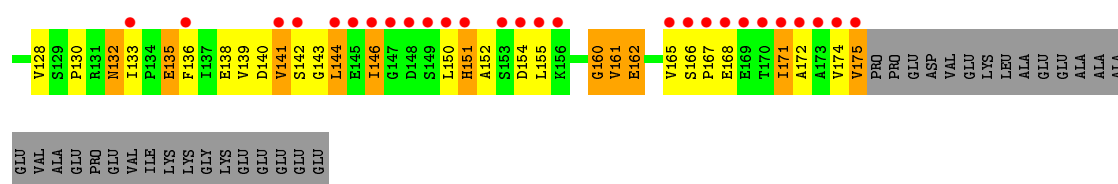
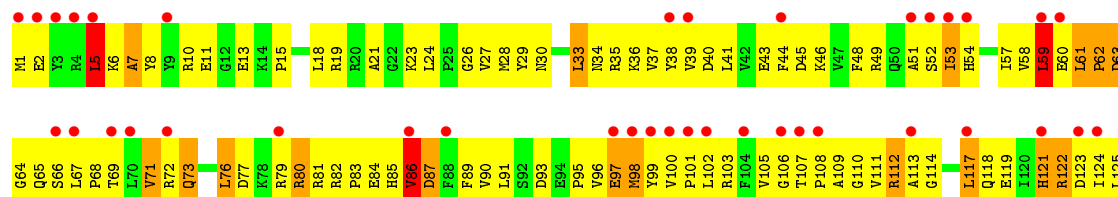
• Molecule 20: 50S ribosomal protein L24



• Molecule 20: 50S ribosomal protein L24

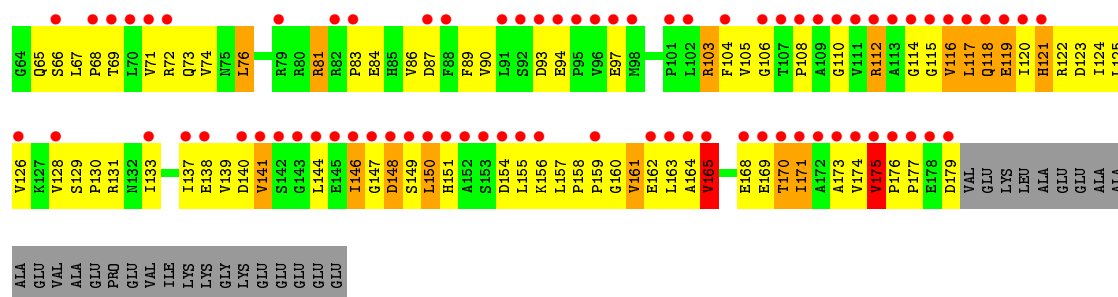


• Molecule 21: 50S ribosomal protein L25

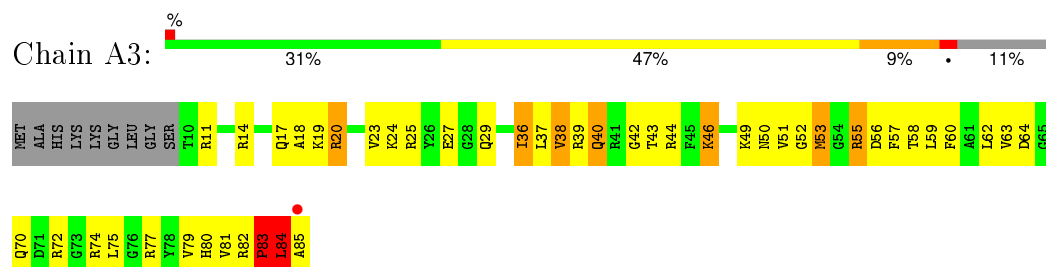


• Molecule 21: 50S ribosomal protein L25

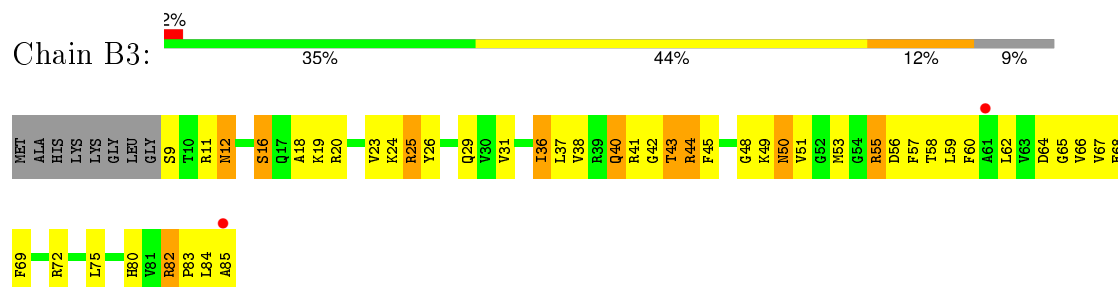




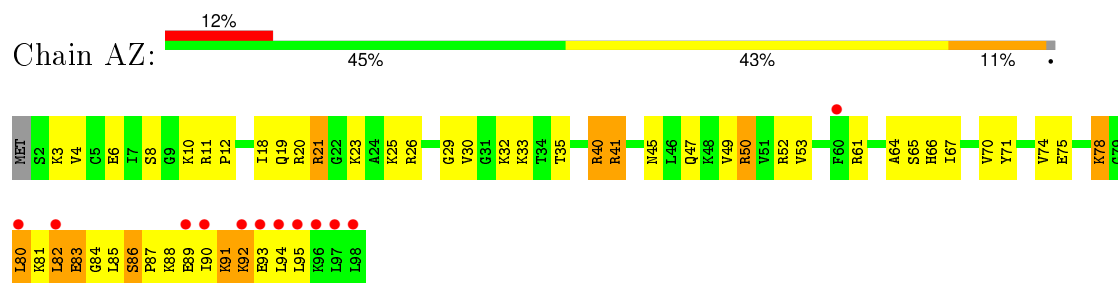
• Molecule 22: 50S ribosomal protein L27



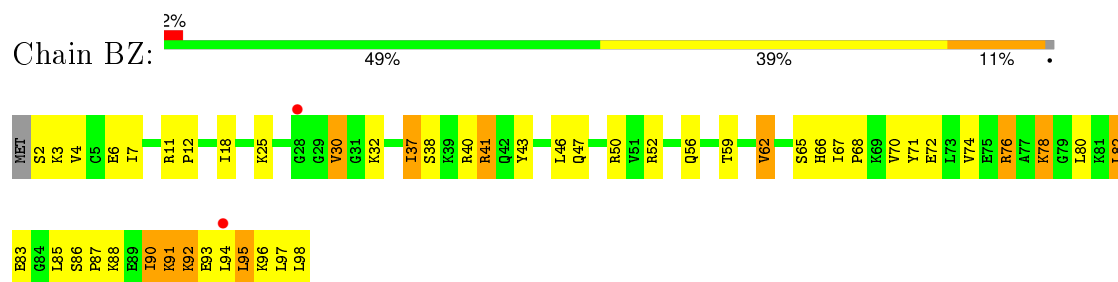
• Molecule 22: 50S ribosomal protein L27



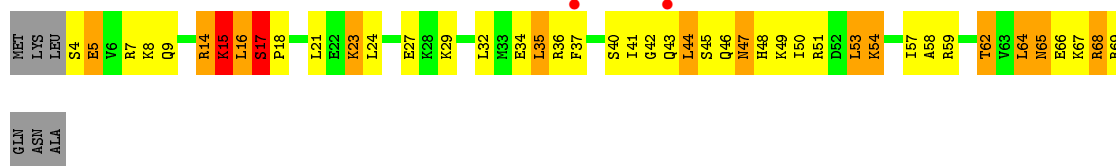
• Molecule 23: 50S ribosomal protein L28



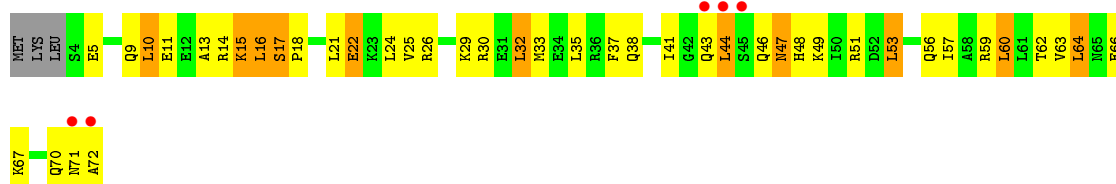
• Molecule 23: 50S ribosomal protein L28




• Molecule 24: 50S ribosomal protein L29

Chain AW: 


• Molecule 24: 50S ribosomal protein L29

Chain BW: 

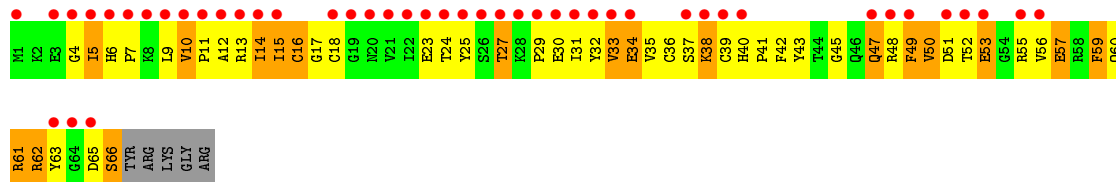

• Molecule 25: 50S ribosomal protein L30

Chain AX: 


• Molecule 25: 50S ribosomal protein L30

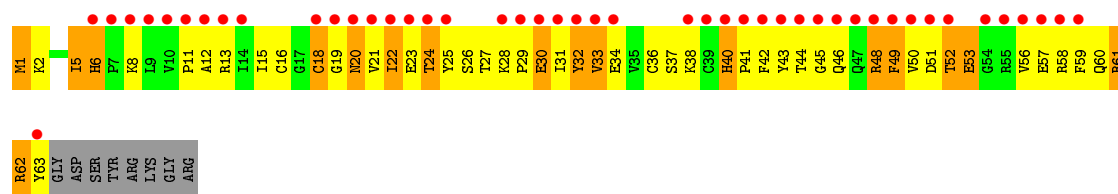
Chain BX: 

• Molecule 26: 50S ribosomal protein L31

Chain A4: 

• Molecule 26: 50S ribosomal protein L31

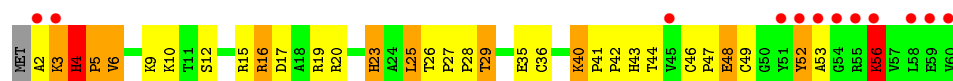
Chain B4: 



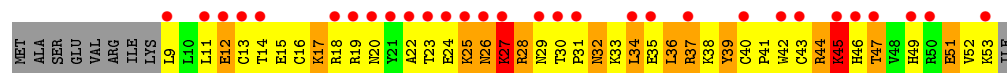
- Molecule 27: 50S ribosomal protein L32



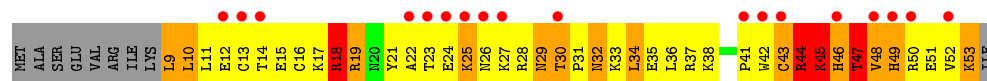
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



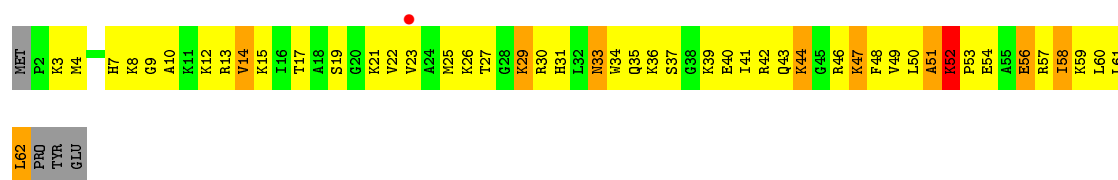
- Molecule 29: 50S ribosomal protein L34



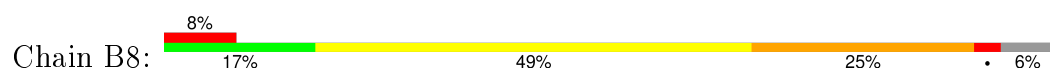
- Molecule 29: 50S ribosomal protein L34



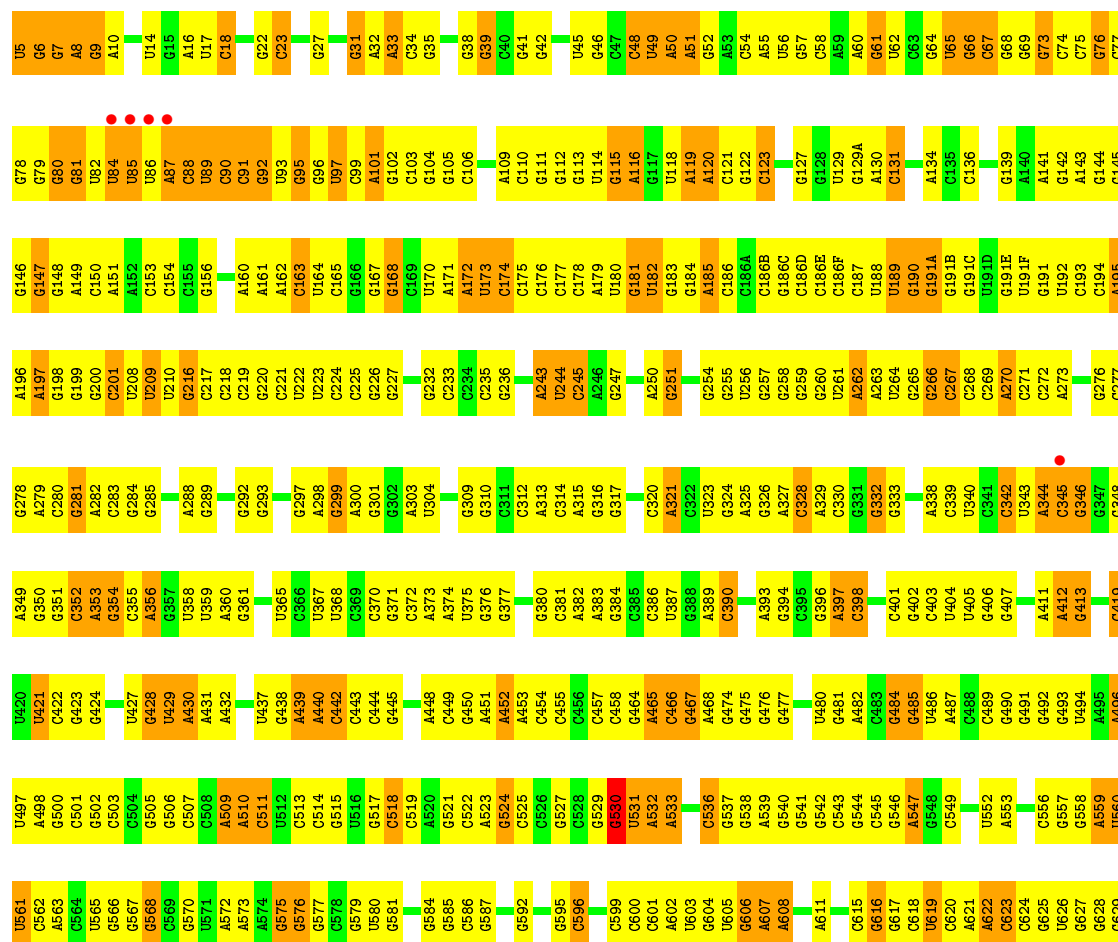
- Molecule 30: 50S ribosomal protein L35

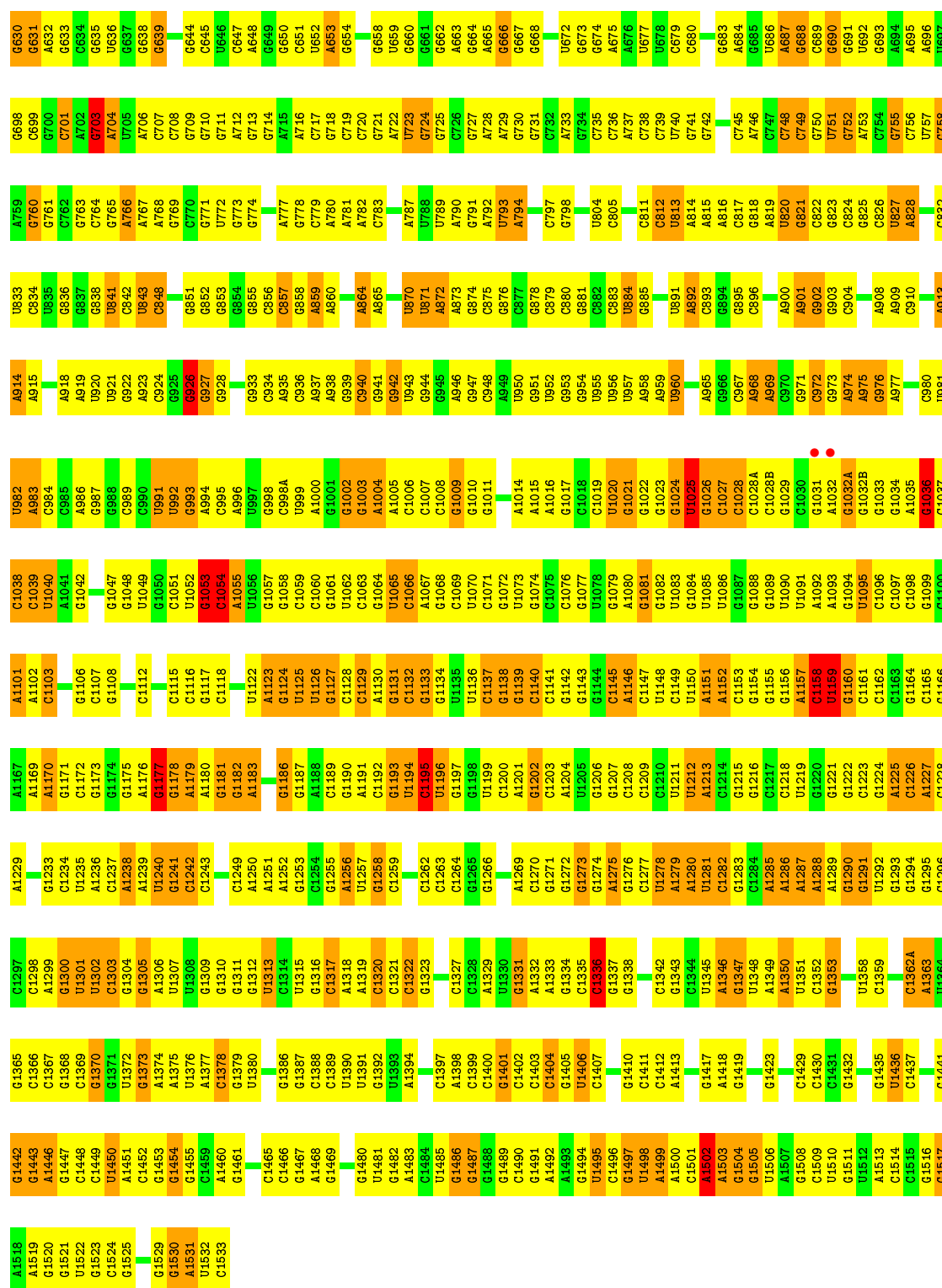


- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 16S ribosomal RNA

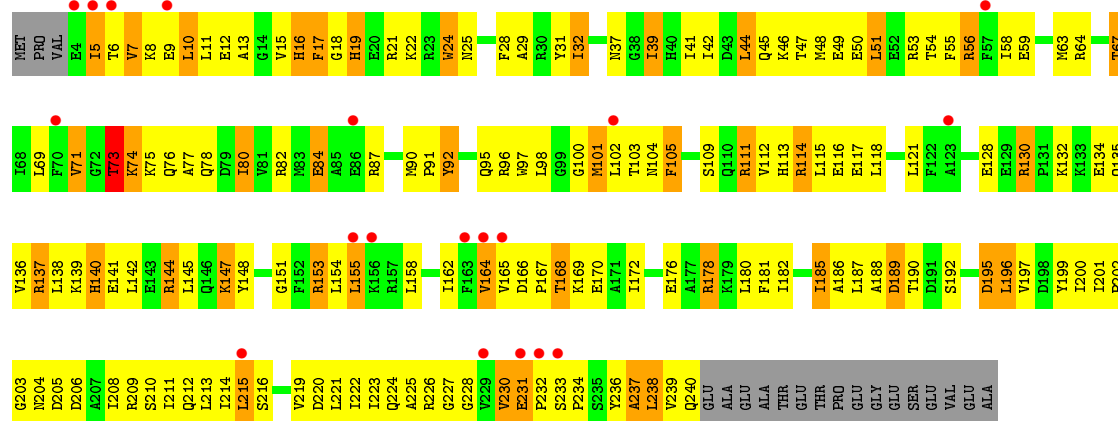




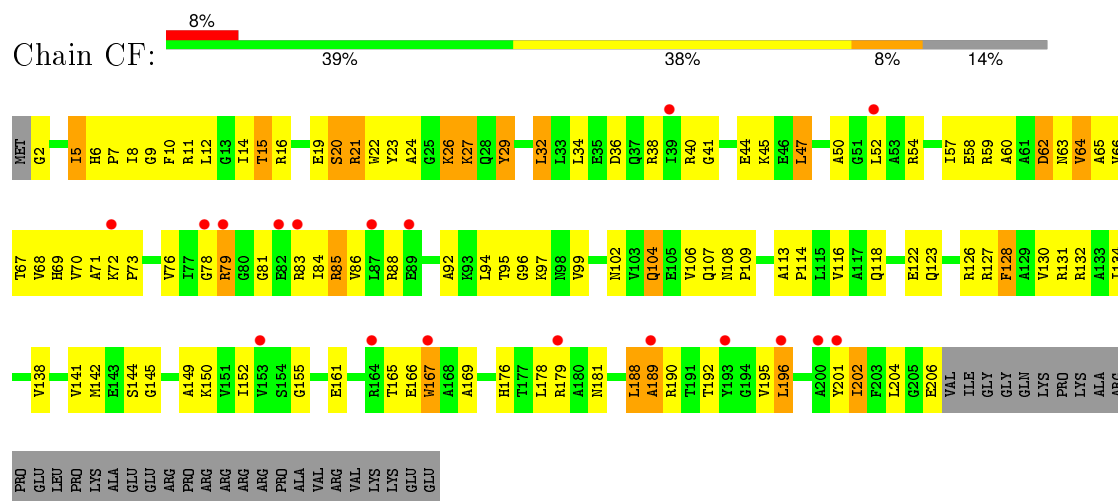
- Molecule 31: 16S ribosomal RNA



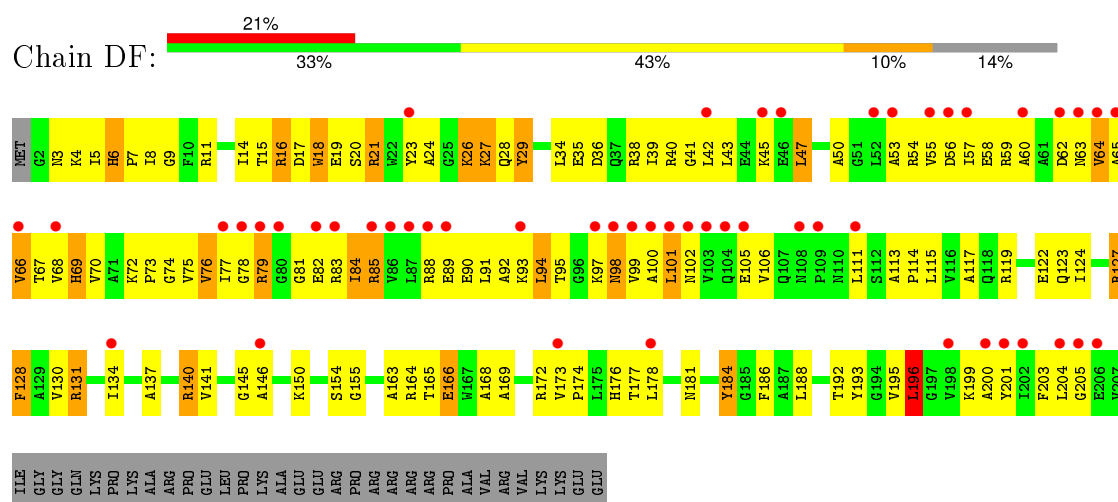
G1139	G1018	A959	A892	U813	G741	G666	U591	G521	C443	C372	A298	G220	C153	G78
C1140	C1019	U960	C893	A814	G742	G667	G592	G527	C444	A373	G299	C221	C154	G79
G1141	U1020	A815	G894	A816	G745	G668	G593	C528	G445	A374	A300	U222	C155	G80
G1142	G1021	C962	G895	C817	G746	U669	C596	C529	A448	U375	G301	U223	C156	G81
G1143	G1022	G963	C896	G818	A747	G673	G597	G530	C449	G376	G302	C224	C157	U82
G1144	G1023	A964	C897	G819	G748	G674	G600	U531	C450	C379	G309	C225	U84	U85
G1145	U1024	A965	C898	U820	G749	G675	G601	A532	C451	U387	U86	U229	U86	U87
G1146	U1025	G966	C899	G822	G750	U677	G604	A533	A452	A382	C312	G230	A161	A162
C1147	G1026	G821	A900	C823	G751	U678	G605	U534	A453	G384	A313	G231	A163	C98
U1148	C1027	A968	A901	G824	G752	G680	G606	A535	C457	G385	G316	C235	U164	C90
G1149	C1028	A969	G902	C825	G753	U686	G607	C536	C458	C386	U87	U230	G165	C91
U1150	G1028A	G970	A907	G826	G754	U687	A608	A539	G464	U387	C320	C241	G167	G92
U1151	C1028B	C972	A908	C827	G755	A687	A609	U540	A465	C390	A321	C242	G168	U93
A1152	G1029	G973	A909	U827	G756	G688	U609	G541	A466	G391	A322	C243	C169	G95
C1153	C1030	A974	C910	G829	G757	C689	U612	G542	C467	A397	G326	U244	U170	A101
G1154	G1031	A975	G903	G830	G758	G690	C613	G543	A468	G403	C327	C245	U171	G105
G1155	A1032	A976	A913	U831	A759	G691	C614	G544	G474	U404	A328	C246	U172	G106
G1156	G1032A	A977	A914	C832	G760	U692	C615	G545	G475	C403	A329	G247	C174	G107
A1157	G1032B	A978	A915	U833	G761	G693	C616	G546	G476	G407	G332	G248	C175	G108
C1158	G1033	C979	U920	G836	G762	G694	C617	G547	G477	U404	A333	G249	C176	G109
U1159	G1034	U921	U921	G837	G763	A695	G618	U550	G478	U404	A334	G250	C177	G110
G1160	A1035	U981	G922	G838	G764	A703	C620	U551	C479	U404	A335	G251	C178	G111
C1161	G1036	U982	G923	U841	A704	A704	A621	U552	G481	U404	A336	G252	C179	G112
C1162	C1037	A983	G924	G842	A766	G707	A622	U553	A482	C403	A337	G253	C180	G113
C1163	C1038	C984	G925	U843	A767	C707	C623	U554	G483	G409	A338	G254	C181	G114
A1170	A1105	C985	G926	U844	A768	G708	C624	C555	C484	G410	A339	G255	C182	G115
G1171	G1106	A986	G927	C948	G769	G709	C625	C556	G485	C411	U340	G256	C183	G116
C1172	C1107	G987	G928	C949	C770	G710	C626	C557	G486	C342	U341	G257	C184	G117
G1173	G1108	G988	G929	U850	C771	G711	C627	G558	A487	C343	U342	G258	C185	G118
G1174	C1109	C989	C930	G851	G772	G712	G627	G559	C488	C344	U343	G259	C186	G119
G1175	A1110	C990	C931	G852	G773	A712	G628	U560	C489	C345	U344	G260	C187	G120
A1176	A1111	U991	C932	G853	G774	G713	G629	U561	C490	C346	U345	G261	C188	G121
G1177	C1112	G992	G933	G854	G775	G714	G630	C562	G491	C347	U346	G262	C189	G122
A1179	G1113	G993	C934	G855	A777	A715	G631	C563	G492	C348	U347	G263	C190	G123
C1180	C1114	A994	C935	C856	G778	A716	A632	C564	G493	C417	U348	G264	C191	G124
G1181	G1115	C995	A936	C857	G779	C719	A633	C565	U494	C418	G350	G265	C192	G125
G1182	U1052	A996	C936	C858	A780	G720	C634	C566	A495	C419	C351	G266	C193	G126
A1183	G1053	U997	A937	G859	A781	G721	G635	C567	A496	U420	C352	G267	C194	G127
G1184	C1054	G998	A938	A860	A782	A722	U636	C568	A497	U421	C353	G268	C195	G128
G1185	A1055	C998A	G939	G861	G783	G723	C647	C569	A498	G422	A354	G269	C196	G129
G1186	U1056	U999	C940	G862	A784	U724	C648	C570	G501	G423	A355	G270	C197	G130
G1187	G1057	A1000	G941	C863	U785	G725	A649	U571	C502	G424	C356	G271	C198	G131
A1188	C1058	G1001	G942	U863	U786	G726	G649	C572	G503	U425	A357	G272	C199	G132
C1189	G1059	G1002	U943	G869	U787	G727	A649	C573	C504	G426	A358	G273	C200	G133
G1190	C1060	G1003	G944	U870	A790	C728	G650	A574	G505	U427	U359	G274	C201	G134
A1191	G1061	A1004	G945	U871	G791	G729	C651	C575	C506	G428	U360	G275	C202	G135
C1192	U1062	A1005	A946	U872	A792	A730	U652	G576	G507	U429	A360	G276	C203	G136
G1193	C1063	C1006	G947	A872	A793	G731	A653	G577	A509	U430	A361	G277	C204	G137
G1194	G1064	C1007	C948	A873	A794	G732	G654	C578	A510	C433	G362	G278	C205	G138
U1195	U1065	G1008	A949	G874	G795	G733	A655	C579	C511	C434	A363	G279	C206	G139
C1196	C1066	C1009	U950	C877	G800	A734	G656	U580	C512	C435	A364	G280	C207	G140
G1197	A1067	G1010	G951	G878	U801	G735	G657	U581	C513	C436	U365	G281	C208	G141
G1198	G1068	G1011	U952	C879	A802	C736	G660	U582	U516	C437	U366	G282	C209	G142
G1199	C1069	U1012	G953	C879	G803	A737	G661	C584	G517	G438	U367	G283	C210	G143
U1199	G1134	G1013	G954	C883	U804	C738	G662	C585	C518	G439	U368	G284	C211	G144
C1200	C1071	A1014	U955	U884	A739	C739	A663	C586	C519	A440	U369	G285	C212	G145
A1201	U1072	A1015	U956	G885	C811	U740	A664	C587	C520	C442	G371	G286	C213	G146
G1202	G1073	C1137	U957	U886	C812	U741	A665	C590	A520			G287	C214	G147
C1203	G1138											G288	C215	G148
												G289	C216	G149
												G290	C217	G150
												G291	C218	G151
												G292	C219	G152



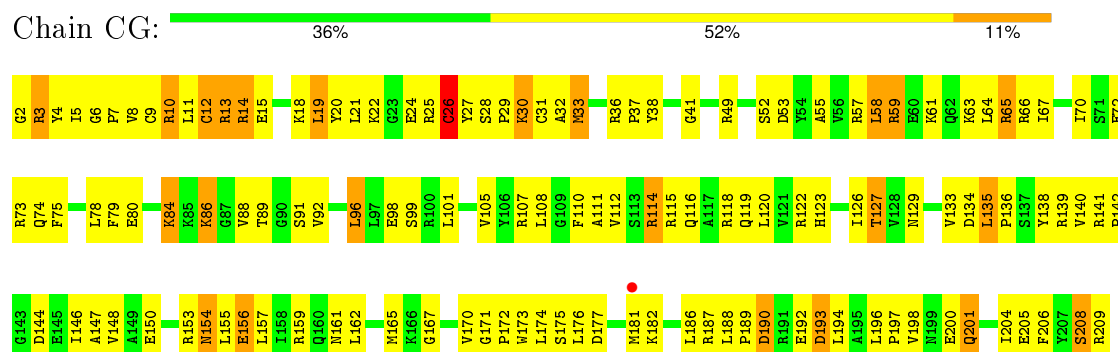
• Molecule 33: 30S RIBOSOMAL PROTEIN S3



• Molecule 33: 30S RIBOSOMAL PROTEIN S3

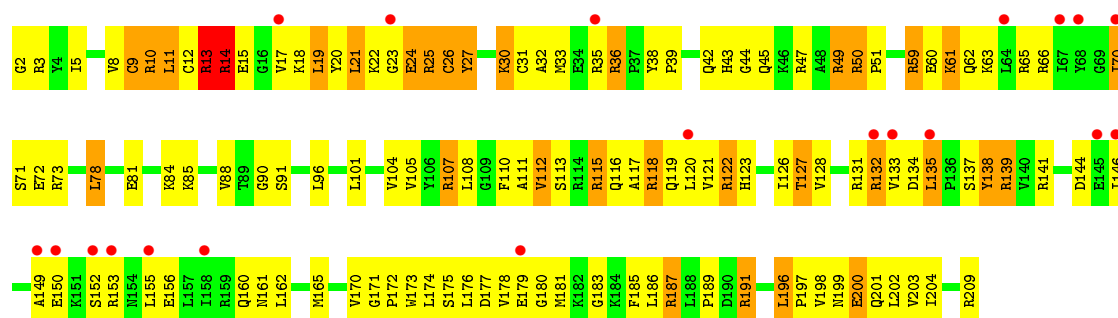


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

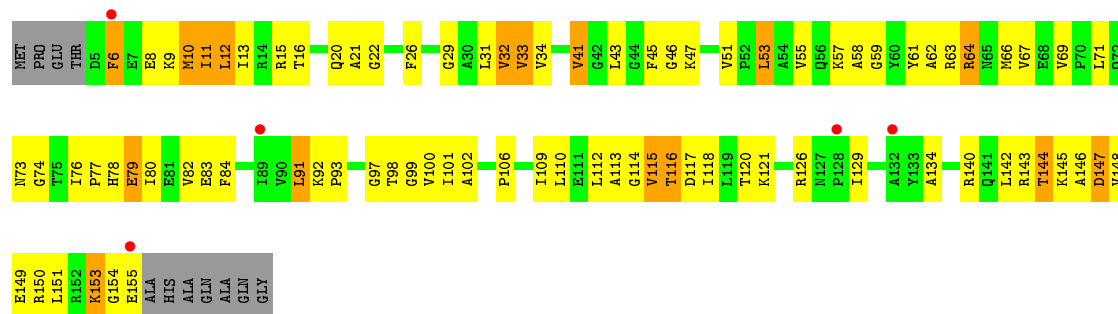
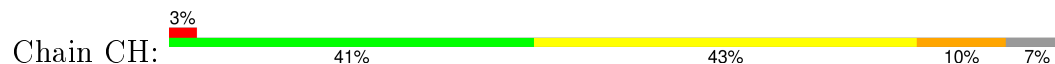


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

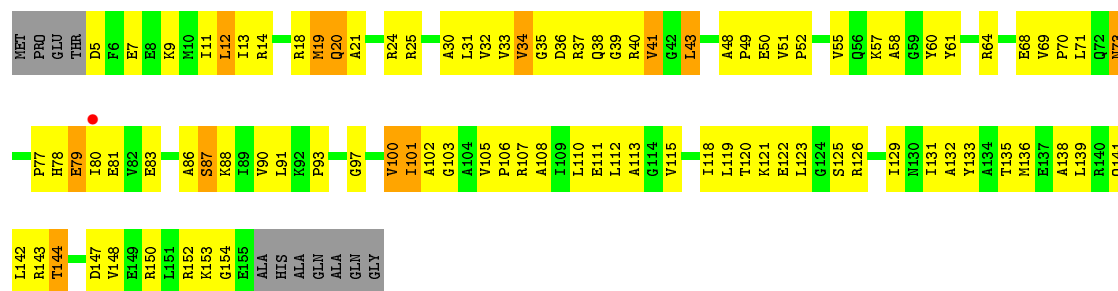




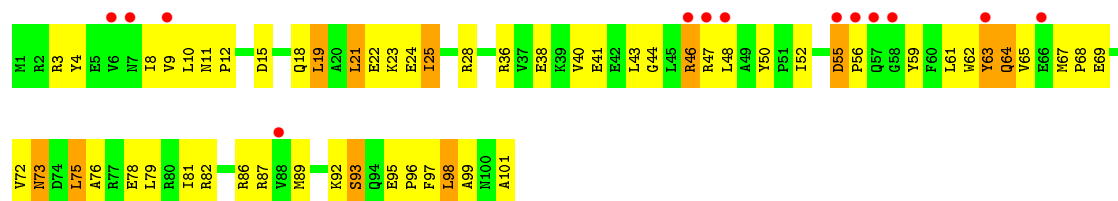
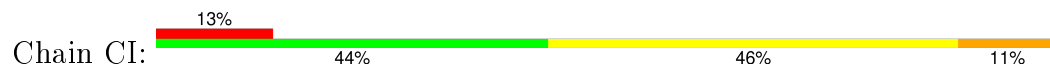
• Molecule 35: 30S RIBOSOMAL PROTEIN S5



• Molecule 35: 30S RIBOSOMAL PROTEIN S5

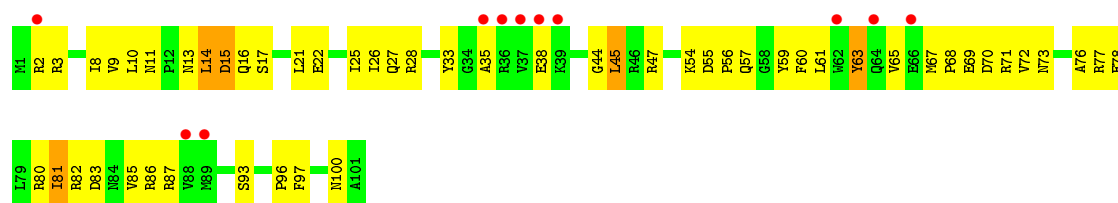


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

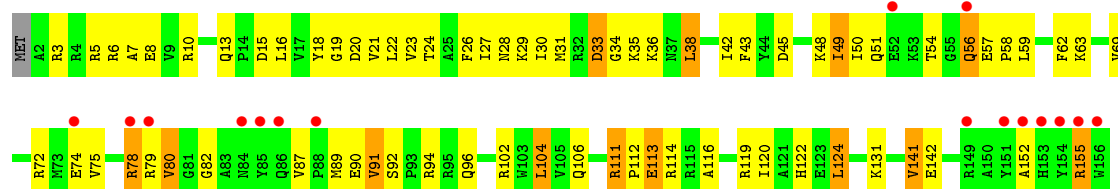


• Molecule 36: 30S RIBOSOMAL PROTEIN S6

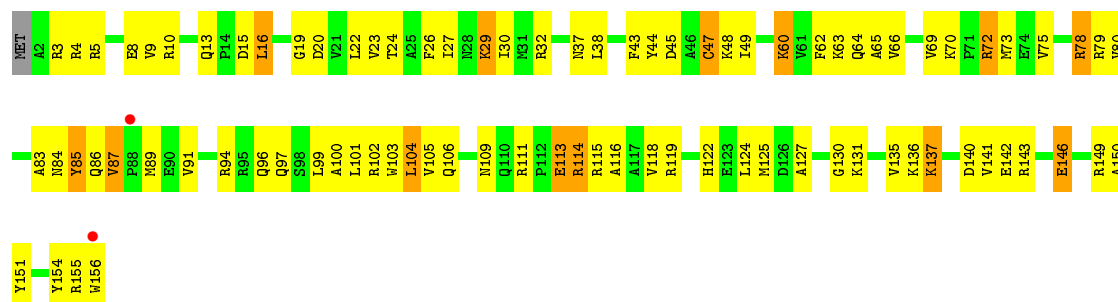
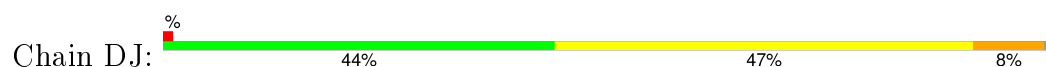




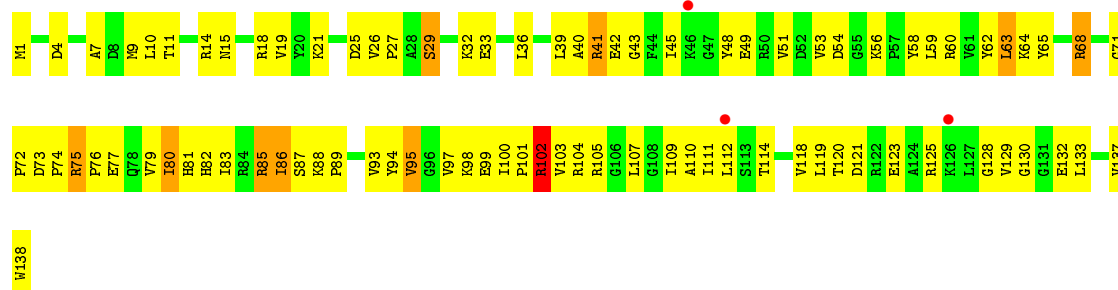
• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 37: 30S RIBOSOMAL PROTEIN S7



• Molecule 38: 30S RIBOSOMAL PROTEIN S8

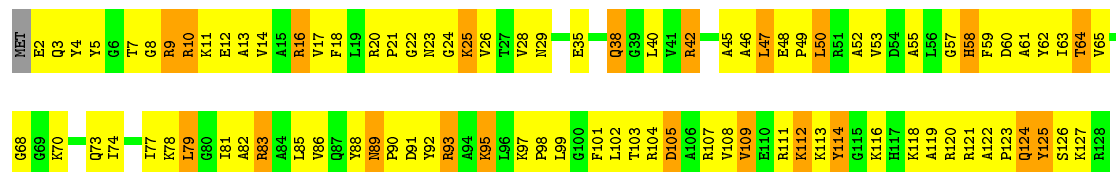


• Molecule 38: 30S RIBOSOMAL PROTEIN S8

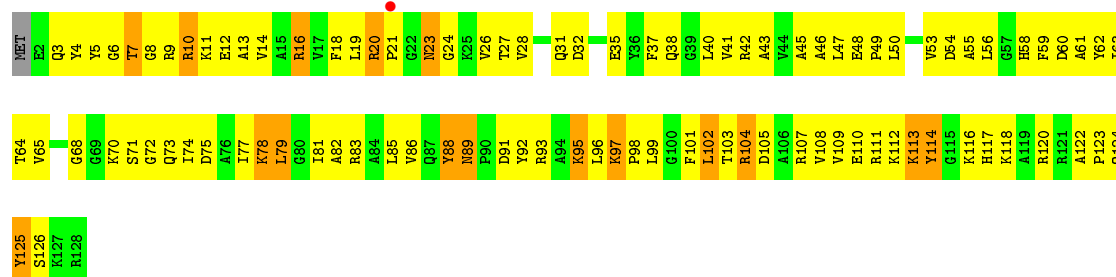




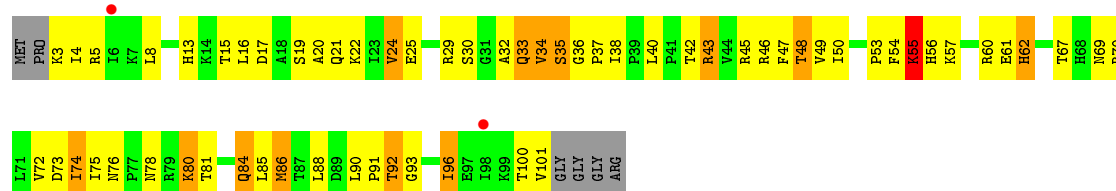
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



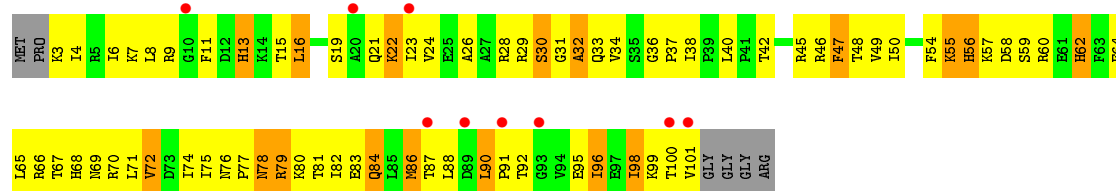
• Molecule 39: 30S RIBOSOMAL PROTEIN S9



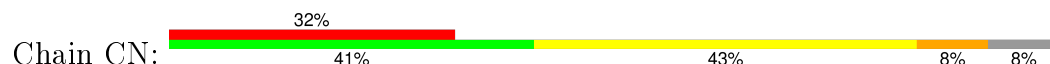
• Molecule 40: 30S RIBOSOMAL PROTEIN S10

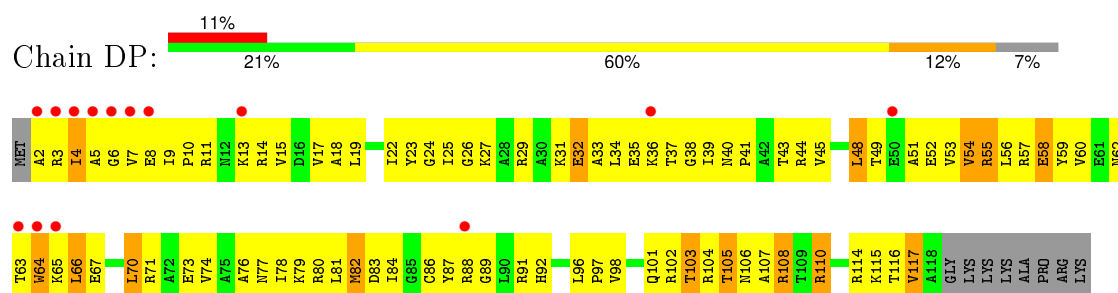


• Molecule 40: 30S RIBOSOMAL PROTEIN S10

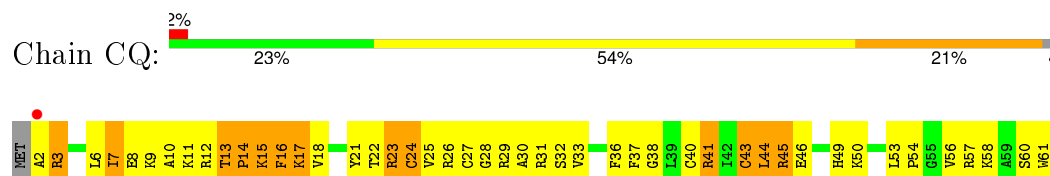


• Molecule 41: 30S RIBOSOMAL PROTEIN S11

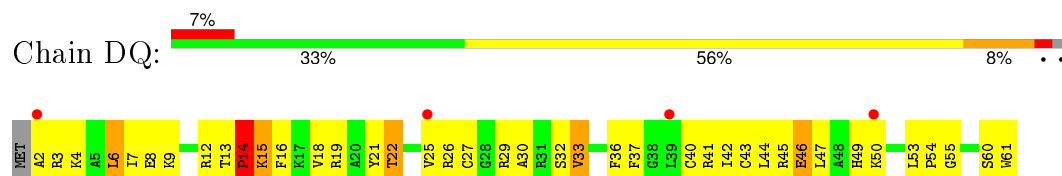




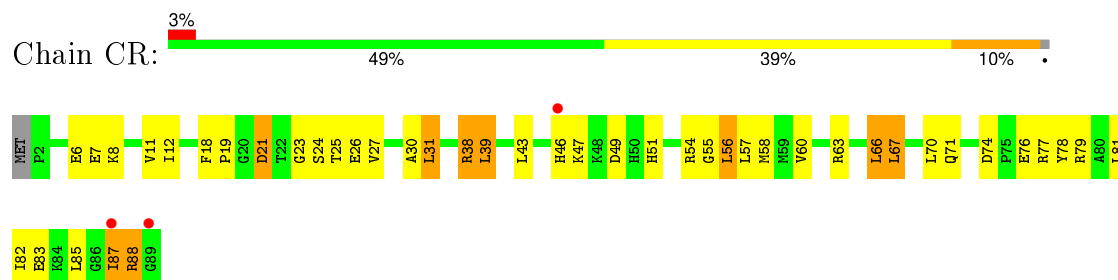
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



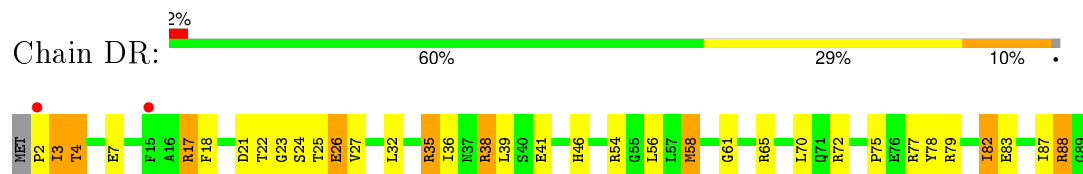
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



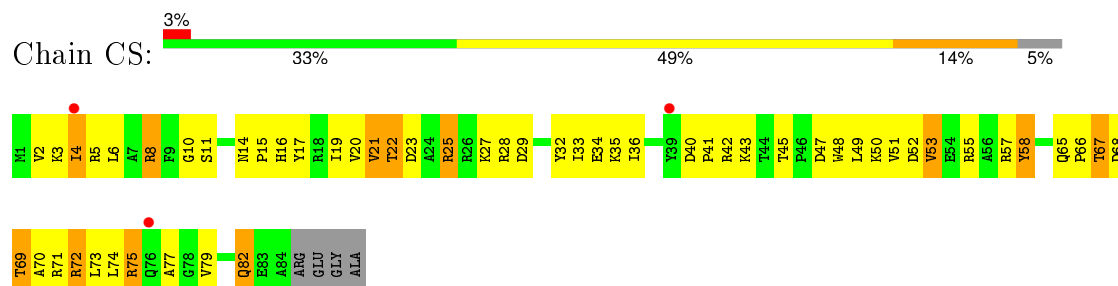
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



• Molecule 45: 30S RIBOSOMAL PROTEIN S15



• Molecule 46: 30S RIBOSOMAL PROTEIN S16



[illegible]

Chain CT:

Amino Acid	CT
Met	1
P2	1
K3	1
T7	1
G8	1
V9	1
V10	1
S11	1
S12	1
D13	1
Q16	1
K17	1
T18	1
V19	1
T20	1
V21	1
L22	1
Q26	1
F27	1
P28	1
H29	1
Y32	1
G33	1
K34	1
V35	1
I36	1
K37	1
R38	1
S39	1
K40	1
K41	1
L42	1
L43	1
A44	1
H45	1
D46	1
P47	1
E48	1
P49	1
K50	1
V51	1
S52	1
D55	1
E58	1
D61	1
S62	1
R63	1
P64	1
L65	1
S66	1
K67	1
R68	1
V69	1
R70	1
F71	1
R72	1
V73	1
L74	1
R75	1
L76	1
V77	1
E78	1
S79	1
G80	1
R81	1
S82	1
D83	1
L84	1
V85	1
L89	1
L98	1
S99	1
K100	1
R101	1
GLY	1
GLY	1
LYS	1
ALA	1

Chain DT:

Category	Percentage
58%	58%
35%	35%
5%	5%

Chain CU:

13% 38% 36% 7% 18%

CU	Category
MET	Grey
SER	Grey
THR	Grey
LYS	Grey
ASN	Grey
ALA	Grey
LYS	Grey
PRO	Grey
LYS	Grey
GLU	Grey
ALA	Grey
GLN	Grey
ARG	Grey
ARG	Grey
PRO	Grey
S17	Green
A18	Green
K19	Green
A20	Green
F29	Green
D30	Green
L31	Green
R32	Green
R35	Green
N36	Green
V37	Green
E38	Green
K41	Yellow
K42	Yellow
F43	Yellow
L44	Yellow
S45	Yellow
E46	Yellow
T47	Yellow
G48	Yellow
K49	Yellow
I50	Yellow
L51	Yellow
P52	Yellow
R53	Yellow
G57	Yellow
L58	Yellow
S59	Yellow
A60	Yellow
K61	Yellow
E62	Yellow
L65	Yellow
I66	Yellow
A67	Yellow
K68	Yellow
T69	Yellow
I70	Yellow
A73	Yellow
R74	Yellow
I75	Yellow
L76	Yellow
G77	Yellow
L78	Yellow
L79	Yellow
P80	Yellow
F81	Yellow
T82	Yellow
E83	Yellow
K84	Yellow
L85	Yellow
R86	Yellow
R87	Yellow
K88	Yellow

Chain DU:

Category	Value
36%	Green
40%	Yellow
6%	Orange
18%	Grey

8%

Category	Value
8%	Red

36%

40%

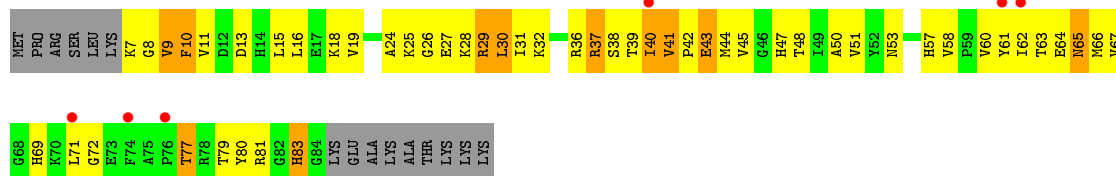
6%

18%

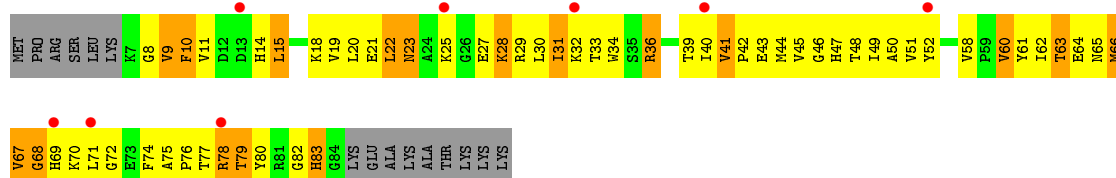
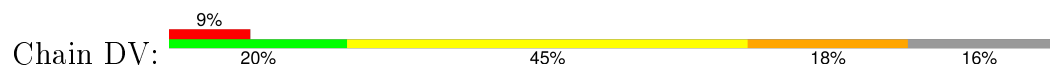
MET
SER
THR
LYS
ASN
ALA
LYS
PRO
PRO
LYS
LYS
GLU
ALA
GLN
ARG
ARG
PRO
S17
R18
K19
A20
K21
V22
K23
A24
T25
L26
G27
E28
F29
D30
L31
R32
V37
F38
V39
R42
F43
L44
S45
E46
L47
G48
K49
L50
L51
P52
R53
R54
R55
T56
G57
L58
S59
A60
Q63
R64
T65

L66
I70
R74
L78
L79
F80
T82
E83
R84
L85
V86
R87
R88

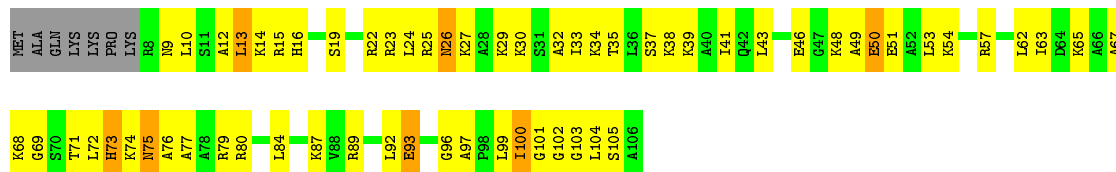
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



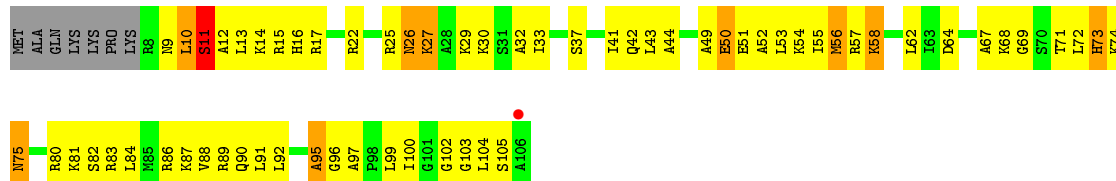
- Molecule 49: 30S RIBOSOMAL PROTEIN S19



- Molecule 50: 30S RIBOSOMAL PROTEIN S20



- Molecule 50: 30S RIBOSOMAL PROTEIN S20



- Molecule 51: 30S RIBOSOMAL PROTEIN THX

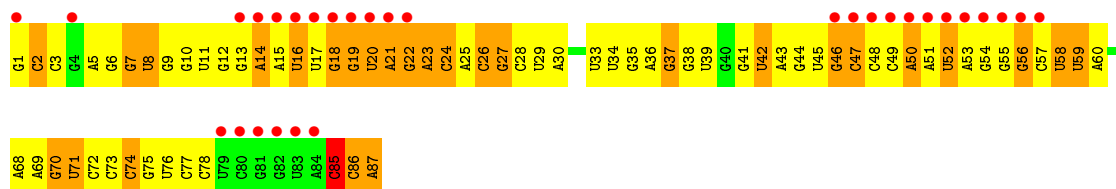
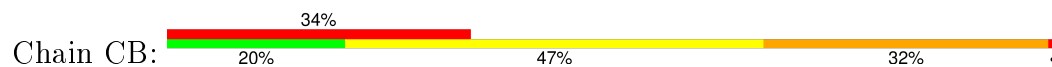


- Molecule 51: 30S RIBOSOMAL PROTEIN THX

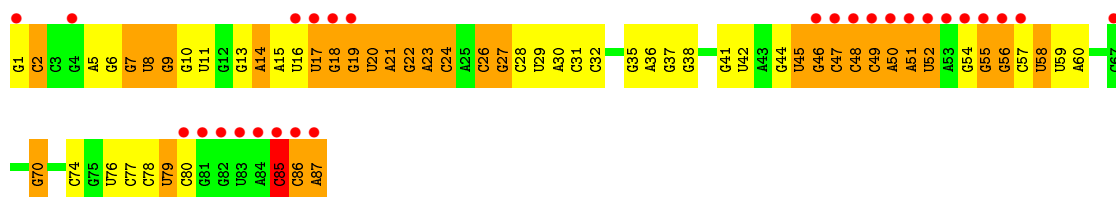




• Molecule 52: TRNA-LEU



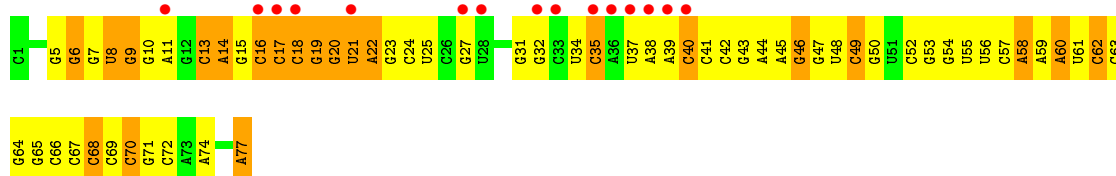
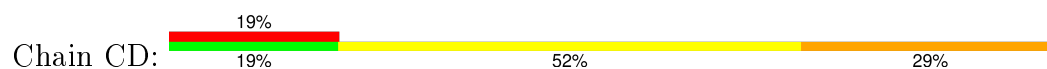
• Molecule 52: TRNA-LEU



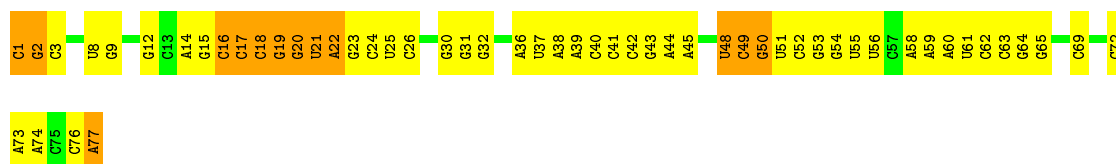
• Molecule 53: TRNA-FMET



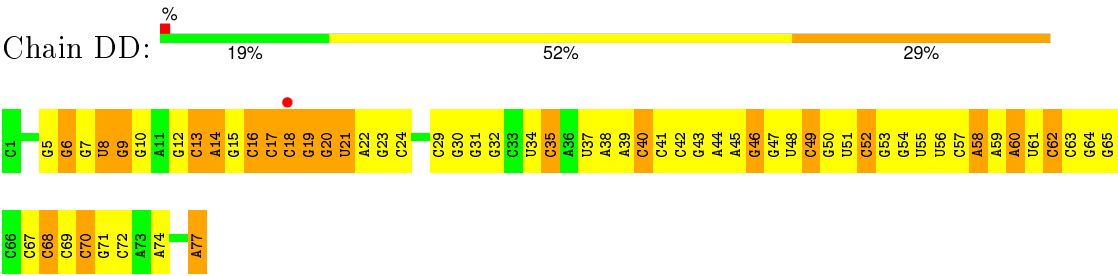
• Molecule 53: TRNA-FMET



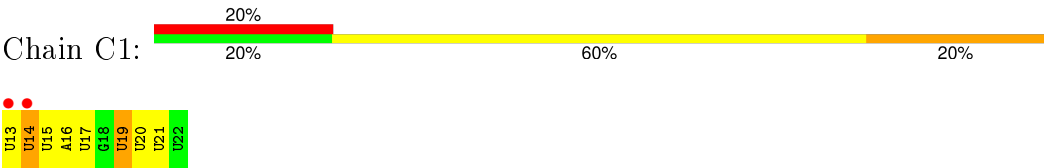
• Molecule 53: TRNA-FMET



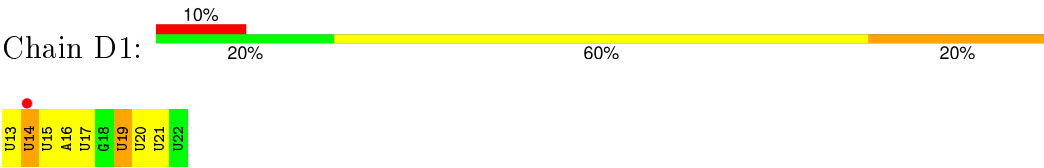
• Molecule 53: TRNA-FMET



• Molecule 54: MRNA



• Molecule 54: MRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.43Å 448.15Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.73 – 3.30 224.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (189.73-3.30) 95.4 (224.07-3.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.199 , 0.237 0.198 , 0.238	Depositor DCC
R_{free} test set	2000 reflections (0.24%)	DCC
Wilson B-factor (Å ²)	101.9	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 864978 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	299682	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR

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	0.62	12/70233 (0.0%)	1.11	353/109643 (0.3%)
1	BA	0.56	6/70167 (0.0%)	1.03	240/109541 (0.2%)
2	AB	0.53	0/2928	1.07	13/4568 (0.3%)
2	BB	0.45	0/2928	0.93	6/4568 (0.1%)
3	AD	0.55	0/2165	0.81	3/2919 (0.1%)
3	BD	0.47	0/2165	0.73	1/2919 (0.0%)
4	AE	0.44	0/1601	0.73	1/2160 (0.0%)
4	BE	0.41	0/1601	0.72	1/2160 (0.0%)
5	AF	0.45	0/1620	0.72	0/2194
5	BF	0.38	0/1662	0.67	0/2249
6	AG	0.36	0/1499	0.60	0/2016
6	BG	0.30	0/1499	0.55	0/2016
7	AH	0.41	0/1332	0.71	0/1802
7	BH	0.29	0/1332	0.58	0/1802
8	AK	0.38	0/1151	0.72	1/1558 (0.1%)
8	BK	0.36	0/1151	0.66	1/1558 (0.1%)
9	AM	0.45	0/1131	0.71	0/1525
9	BM	0.32	0/1131	0.58	0/1525
10	AN	0.41	0/943	0.66	0/1269
10	BN	0.40	0/943	0.61	0/1269
11	AO	0.39	0/1162	0.71	1/1544 (0.1%)
11	BO	0.33	0/1162	0.64	1/1544 (0.1%)
12	AP	0.41	0/1143	0.59	0/1527
12	BP	0.33	0/1143	0.52	0/1527
13	A0	0.41	0/982	0.71	1/1312 (0.1%)
13	B0	0.40	0/974	0.67	0/1302
14	AQ	0.40	0/892	0.69	1/1187 (0.1%)
14	BQ	0.34	0/892	0.62	1/1187 (0.1%)
15	AR	0.45	0/1155	0.70	0/1542
15	BR	0.41	0/1155	0.63	0/1542
16	A1	0.46	0/982	0.67	0/1306
16	B1	0.38	0/982	0.59	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.44	0/790	0.71	0/1057
17	B2	0.33	0/790	0.59	0/1057
18	AS	0.43	0/911	0.69	0/1220
18	BS	0.42	0/911	0.65	0/1220
19	AT	0.52	0/739	0.69	0/993
19	BT	0.48	0/739	0.66	0/993
20	AU	0.48	0/798	0.72	0/1064
20	BU	0.43	0/798	0.72	0/1064
21	AV	0.35	0/1427	0.67	2/1935 (0.1%)
21	BV	0.28	0/1460	0.56	0/1982
22	A3	0.46	0/615	0.69	0/819
22	B3	0.40	0/621	0.64	0/827
23	AZ	0.46	0/770	0.78	0/1022
23	BZ	0.43	0/770	0.75	0/1022
24	AW	0.51	0/560	0.75	0/741
24	BW	0.40	0/583	0.62	0/771
25	AX	0.35	0/474	0.61	0/635
25	BX	0.33	0/474	0.54	0/635
26	A4	0.39	0/545	0.73	1/733 (0.1%)
26	B4	0.34	0/527	0.65	0/709
27	A5	0.45	0/473	0.67	0/639
27	B5	0.40	0/473	0.73	0/639
28	A6	0.47	0/396	0.68	0/529
28	B6	0.36	0/396	0.60	0/529
29	A7	0.50	0/438	0.71	0/575
29	B7	0.40	0/438	0.62	0/575
30	A8	0.56	0/494	0.87	0/649
30	B8	0.40	0/494	0.58	0/649
31	CA	0.49	1/36234 (0.0%)	0.94	68/56554 (0.1%)
31	DA	0.46	0/36237	0.90	64/56558 (0.1%)
32	CE	0.31	0/1959	0.55	0/2642
32	DE	0.30	0/1959	0.54	0/2642
33	CF	0.34	0/1629	0.54	0/2195
33	DF	0.32	0/1636	0.57	1/2205 (0.0%)
34	CG	0.42	1/1733 (0.1%)	0.62	0/2318
34	DG	0.38	0/1733	0.63	0/2318
35	CH	0.38	0/1171	0.58	0/1576
35	DH	0.34	0/1171	0.58	0/1576
36	CI	0.38	0/856	0.58	0/1154
36	DI	0.36	0/856	0.55	0/1154
37	CJ	0.31	0/1276	0.48	0/1709
37	DJ	0.32	0/1276	0.48	0/1709
38	CK	0.36	0/1136	0.64	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DK	0.31	0/1136	0.54	0/1527
39	CL	0.30	0/1029	0.52	0/1379
39	DL	0.29	0/1029	0.53	0/1379
40	CM	0.32	0/814	0.61	1/1095 (0.1%)
40	DM	0.31	0/814	0.59	0/1095
41	CN	0.37	0/900	0.61	0/1213
41	DN	0.36	0/900	0.59	0/1213
42	CO	0.45	0/991	0.75	1/1327 (0.1%)
42	DO	0.41	0/991	0.65	0/1327
43	CP	0.33	0/938	0.59	0/1258
43	DP	0.29	0/943	0.53	0/1265
44	CQ	0.42	1/501 (0.2%)	0.68	1/664 (0.2%)
44	DQ	0.32	0/501	0.57	0/664
45	CR	0.38	0/745	0.64	0/992
45	DR	0.35	0/745	0.53	0/992
46	CS	0.31	0/721	0.55	0/970
46	DS	0.38	0/721	0.60	0/970
47	CT	0.36	0/847	0.56	0/1131
47	DT	0.34	0/847	0.55	0/1131
48	CU	0.35	0/596	0.62	0/790
48	DU	0.36	0/596	0.57	0/790
49	CV	0.34	0/638	0.57	0/860
49	DV	0.29	0/638	0.63	0/860
50	CW	0.32	0/765	0.55	0/1007
50	DW	0.35	0/765	0.63	0/1007
51	CX	0.29	0/221	0.49	0/288
51	DX	0.27	0/221	0.48	0/288
52	CB	0.44	0/2080	0.80	1/3242 (0.0%)
52	DB	0.46	0/2080	0.80	3/3242 (0.1%)
53	CC	0.46	0/1835	0.85	0/2859
53	CD	0.28	0/1835	0.66	2/2859 (0.1%)
53	DC	0.44	0/1835	0.83	0/2859
53	DD	0.27	0/1835	0.63	1/2859 (0.0%)
54	C1	0.69	0/226	0.84	0/348
54	D1	0.58	0/226	0.81	0/348
All	All	0.51	21/324077 (0.0%)	0.93	771/485305 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AD	0	6
3	BD	0	3
4	AE	0	1
4	BE	0	6
5	BF	0	2
6	AG	0	1
6	BG	0	1
7	AH	0	2
7	BH	0	4
8	AK	0	5
8	BK	0	5
9	AM	0	1
11	AO	0	3
11	BO	0	3
13	B0	0	1
14	AQ	0	2
14	BQ	0	3
15	AR	0	2
16	A1	0	2
17	A2	0	1
20	BU	0	2
21	AV	0	3
21	BV	0	3
22	A3	0	2
24	AW	0	2
24	BW	0	1
26	A4	0	3
26	B4	0	1
27	A5	0	3
27	B5	0	1
28	A6	0	1
28	B6	0	1
30	A8	0	2
32	CE	0	3
32	DE	0	4
33	CF	0	1
33	DF	0	1
34	DG	0	1
38	CK	0	1
40	CM	0	1
40	DM	0	1
42	CO	0	2
44	CQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	DQ	0	1
45	CR	0	1
50	DW	0	1
All	All	0	98

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1143	A	N7-C5	-9.76	1.33	1.39
1	BA	1342	A	N7-C5	-8.93	1.33	1.39
1	BA	2873	A	N7-C5	-8.51	1.34	1.39
1	BA	2287	A	N9-C4	-8.15	1.32	1.37
1	AA	1021	A	N9-C4	-8.08	1.32	1.37

The worst 5 of 771 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	1025	U	C5-C4-O4	-13.19	117.99	125.90
1	BA	933	A	C6-C5-N7	-12.57	123.50	132.30
1	AA	1899	G	N3-C4-N9	-12.39	118.57	126.00
1	BA	1899	G	N3-C4-N9	-12.35	118.59	126.00
1	BA	2720	U	C2-N3-C4	-11.91	119.85	127.00

There are no chirality outliers.

5 of 98 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AD	122	ASP	Peptide
3	AD	236	GLY	Peptide
3	AD	27	THR	Peptide
3	AD	28	GLU	Peptide
3	AD	47	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	62707	0	31613	2746	0
1	BA	62647	0	31583	2774	1
2	AB	2617	0	1328	105	0
2	BB	2617	0	1328	133	0
3	AD	2115	0	2195	263	0
3	BD	2115	0	2195	244	0
4	AE	1568	0	1634	288	0
4	BE	1568	0	1634	286	0
5	AF	1585	0	1632	143	0
5	BF	1627	0	1680	208	0
6	AG	1474	0	1535	200	0
6	BG	1474	0	1535	164	0
7	AH	1307	0	1382	158	0
7	BH	1307	0	1382	148	2
8	AK	1136	0	1223	128	0
8	BK	1136	0	1223	102	0
9	AM	1104	0	1180	139	0
9	BM	1104	0	1180	102	0
10	AN	933	0	996	53	0
10	BN	933	0	996	68	0
11	AO	1145	0	1228	245	0
11	BO	1145	0	1228	306	0
12	AP	1122	0	1179	208	0
12	BP	1122	0	1179	250	0
13	A0	968	0	1033	81	0
13	B0	960	0	1021	82	0
14	AQ	882	0	943	101	0
14	BQ	882	0	943	104	0
15	AR	1141	0	1202	128	0
15	BR	1141	0	1202	132	0
16	A1	964	0	1022	109	0
16	B1	964	0	1022	108	0
17	A2	779	0	852	98	1
17	B2	779	0	852	182	0
18	AS	900	0	964	86	0
18	BS	900	0	964	56	0
19	AT	725	0	778	60	0
19	BT	725	0	778	60	0
20	AU	785	0	878	95	0
20	BU	785	0	878	113	0
21	AV	1397	0	1430	140	0
21	BV	1428	0	1454	142	0
22	A3	607	0	628	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B3	613	0	633	59	0
23	AZ	763	0	848	61	0
23	BZ	763	0	848	59	0
24	AW	558	0	610	47	0
24	BW	581	0	629	63	0
25	AX	469	0	518	36	0
25	BX	469	0	518	33	0
26	A4	533	0	522	78	0
26	B4	515	0	510	109	0
27	A5	459	0	480	78	1
27	B5	459	0	480	72	0
28	A6	389	0	404	90	0
28	B6	389	0	404	110	0
29	A7	430	0	480	28	0
29	B7	430	0	480	32	0
30	A8	488	0	560	105	0
30	B8	488	0	560	153	0
31	CA	32369	0	16339	1550	2
31	DA	32372	0	16338	1515	1
32	CE	1924	0	1975	186	0
32	DE	1924	0	1975	206	0
33	CF	1605	0	1668	123	0
33	DF	1612	0	1677	160	0
34	CG	1703	0	1764	180	0
34	DG	1703	0	1763	158	1
35	CH	1155	0	1213	81	0
35	DH	1155	0	1213	91	0
36	CI	843	0	857	59	1
36	DI	843	0	857	48	0
37	CJ	1257	0	1296	72	0
37	DJ	1257	0	1296	90	0
38	CK	1116	0	1177	100	0
38	DK	1116	0	1177	62	0
39	CL	1010	0	1037	111	0
39	DL	1010	0	1037	130	0
40	CM	801	0	849	86	0
40	DM	801	0	849	95	0
41	CN	885	0	904	76	0
41	DN	885	0	904	45	0
42	CO	975	0	1062	63	0
42	DO	975	0	1062	89	0
43	CP	928	0	987	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DP	933	0	992	108	0
44	CQ	492	0	529	55	0
44	DQ	492	0	529	56	0
45	CR	734	0	771	55	0
45	DR	734	0	771	44	0
46	CS	705	0	725	63	0
46	DS	705	0	725	45	0
47	CT	834	0	904	79	0
47	DT	834	0	904	44	0
48	CU	591	0	662	31	0
48	DU	591	0	662	43	0
49	CV	624	0	636	74	0
49	DV	624	0	636	100	0
50	CW	763	0	861	76	0
50	DW	763	0	861	71	0
51	CX	217	0	234	20	0
51	DX	217	0	234	28	0
52	CB	1861	0	938	84	0
52	DB	1861	0	938	82	0
53	CC	1643	0	837	69	0
53	CD	1643	0	837	98	0
53	DC	1643	0	837	78	0
53	DD	1643	0	837	111	0
54	C1	205	0	103	9	0
54	D1	205	0	103	9	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A2	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	2	0	0	0	0
55	A6	1	0	0	0	0
55	A7	2	0	0	0	0
55	AA	626	0	0	0	0
55	AB	17	0	0	0	0
55	AD	1	0	0	0	0
55	AE	4	0	0	0	0
55	AF	3	0	0	0	0
55	AO	3	0	0	0	0
55	AU	1	0	0	0	0
55	AZ	1	0	0	0	0
55	B1	1	0	0	0	0
55	B3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B5	1	0	0	0	0
55	BA	528	0	0	0	0
55	BB	15	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BP	1	0	0	0	0
55	BR	2	0	0	0	0
55	C1	1	0	0	0	0
55	CA	240	0	0	0	0
55	CB	5	0	0	0	0
55	CC	7	0	0	0	0
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CN	2	0	0	0	0
55	CQ	2	0	0	0	0
55	CT	1	0	0	0	0
55	DA	204	0	0	0	0
55	DB	2	0	0	0	0
55	DC	8	0	0	0	0
55	DG	2	0	0	0	0
55	DH	1	0	0	0	0
55	DS	1	0	0	0	0
56	CA	42	0	45	4	0
56	DA	42	0	45	5	0
57	CG	1	0	0	0	0
57	CQ	1	0	0	0	0
57	DG	1	0	0	0	0
57	DQ	1	0	0	0	0
All	All	299682	0	201028	17558	5

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 35.

The worst 5 of 17558 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)
11:BO:62:LEU:CD1	30:B8:30:ARG:HH11	1.03	1.63
11:BO:71:VAL:CG1	11:BO:72:PRO:HD3	1.32	1.59
4:AE:23:VAL:HG12	4:AE:185:LYS:CA	1.33	1.59
1:BA:2015:A:C1'	27:B5:2:ALA:HA	1.42	1.48
4:BE:51:PHE:CG	4:BE:52:LEU:HB3	1.45	1.47

All (5) 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)
1:BA:276:A:OP2	31:DA:86:U:O2'[3_555]	1.96	0.24
7:BH:100:GLY:O	31:CA:85:U:O2'[3_545]	2.02	0.18
36:CI:15:ASP:OD2	34:DG:27:TYR:OH[4_555]	2.06	0.14
7:BH:132:ARG:O	31:CA:84:U:N3[3_545]	2.18	0.02
17:A2:51:VAL:N	27:A5:60:VAL:O[4_465]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	270/276 (98%)	244 (90%)	20 (7%)	6 (2%)	8	41
3	BD	270/276 (98%)	246 (91%)	15 (6%)	9 (3%)	5	30
4	AE	203/206 (98%)	149 (73%)	37 (18%)	17 (8%)	1	7
4	BE	203/206 (98%)	149 (73%)	34 (17%)	20 (10%)	1	5
5	AF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
5	BF	206/210 (98%)	172 (84%)	29 (14%)	5 (2%)	7	38
6	AG	179/182 (98%)	155 (87%)	17 (10%)	7 (4%)	4	25
6	BG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	30	68
7	AH	168/180 (93%)	135 (80%)	25 (15%)	8 (5%)	3	20
7	BH	168/180 (93%)	129 (77%)	37 (22%)	2 (1%)	16	54
8	AK	144/148 (97%)	108 (75%)	28 (19%)	8 (6%)	2	16
8	BK	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	9	42
9	AM	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	3	22
9	BM	136/140 (97%)	120 (88%)	12 (9%)	4 (3%)	6	34
10	AN	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	BN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	24	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AO	148/150 (99%)	101 (68%)	31 (21%)	16 (11%)	0	4
11	BO	148/150 (99%)	95 (64%)	32 (22%)	21 (14%)	0	1
12	AP	139/141 (99%)	101 (73%)	19 (14%)	19 (14%)	0	2
12	BP	139/141 (99%)	88 (63%)	34 (24%)	17 (12%)	0	2
13	A0	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	21	60
13	B0	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
14	AQ	109/112 (97%)	87 (80%)	20 (18%)	2 (2%)	11	46
14	BQ	109/112 (97%)	87 (80%)	18 (16%)	4 (4%)	4	27
15	AR	135/146 (92%)	111 (82%)	22 (16%)	2 (2%)	13	49
15	BR	135/146 (92%)	124 (92%)	11 (8%)	0	100	100
16	A1	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	21	60
16	B1	115/118 (98%)	102 (89%)	12 (10%)	1 (1%)	21	60
17	A2	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	5	33
17	B2	99/101 (98%)	73 (74%)	13 (13%)	13 (13%)	0	2
18	AS	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	21	60
18	BS	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
19	AT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	8	41
19	BT	90/96 (94%)	81 (90%)	8 (9%)	1 (1%)	17	57
20	AU	100/110 (91%)	84 (84%)	10 (10%)	6 (6%)	2	15
20	BU	100/110 (91%)	67 (67%)	27 (27%)	6 (6%)	2	15
21	AV	173/206 (84%)	131 (76%)	35 (20%)	7 (4%)	4	24
21	BV	177/206 (86%)	139 (78%)	30 (17%)	8 (4%)	3	21
22	A3	74/85 (87%)	68 (92%)	4 (5%)	2 (3%)	6	35
22	B3	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	AZ	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	5	31
23	BZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	17	57
24	AW	64/72 (89%)	60 (94%)	1 (2%)	3 (5%)	3	20
24	BW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	13	49
25	AX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
25	BX	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	A4	64/71 (90%)	42 (66%)	20 (31%)	2 (3%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B4	61/71 (86%)	32 (52%)	27 (44%)	2 (3%)	5	30
27	A5	57/60 (95%)	48 (84%)	8 (14%)	1 (2%)	11	46
27	B5	57/60 (95%)	48 (84%)	6 (10%)	3 (5%)	2	17
28	A6	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	3	20
28	B6	43/54 (80%)	26 (60%)	11 (26%)	6 (14%)	0	2
29	A7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	B7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	A8	59/65 (91%)	54 (92%)	4 (7%)	1 (2%)	11	47
30	B8	59/65 (91%)	42 (71%)	10 (17%)	7 (12%)	0	3
32	CE	235/256 (92%)	190 (81%)	44 (19%)	1 (0%)	39	76
32	DE	235/256 (92%)	186 (79%)	45 (19%)	4 (2%)	11	47
33	CF	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
33	DF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	19	58
34	CG	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	34	71
34	DG	206/208 (99%)	177 (86%)	28 (14%)	1 (0%)	34	71
35	CH	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	26	66
35	DH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
36	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
36	DI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
37	CJ	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
37	DJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
38	CK	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	26	66
38	DK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
39	CL	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
39	DL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	CM	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
40	DM	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	9	42
41	CN	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
41	DN	117/129 (91%)	105 (90%)	12 (10%)	0	100	100
42	CO	123/132 (93%)	108 (88%)	13 (11%)	2 (2%)	12	48
42	DO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	CP	114/126 (90%)	90 (79%)	24 (21%)	0	100	100
43	DP	115/126 (91%)	97 (84%)	17 (15%)	1 (1%)	21	60
44	CQ	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	5	29
44	DQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	47
45	CR	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
45	DR	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
46	CS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
46	DS	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
47	CT	98/105 (93%)	89 (91%)	7 (7%)	2 (2%)	9	43
47	DT	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
48	CU	70/88 (80%)	63 (90%)	6 (9%)	1 (1%)	14	50
48	DU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	CV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	7	36
49	DV	76/93 (82%)	58 (76%)	13 (17%)	5 (7%)	1	12
50	CW	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	19	58
50	DW	97/106 (92%)	81 (84%)	15 (16%)	1 (1%)	19	58
51	CX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
51	DX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
All	All	11336/12052 (94%)	9645 (85%)	1396 (12%)	295 (3%)	7	36

5 of 295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	237	GLU
3	AD	271	ILE
4	AE	15	PHE
4	AE	19	ARG
4	AE	23	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	214/218 (98%)	176 (82%)	38 (18%)	2	10
3	BD	214/218 (98%)	163 (76%)	51 (24%)	1	3
4	AE	165/166 (99%)	119 (72%)	46 (28%)	0	2
4	BE	165/166 (99%)	127 (77%)	38 (23%)	1	4
5	AF	161/166 (97%)	125 (78%)	36 (22%)	1	4
5	BF	165/166 (99%)	124 (75%)	41 (25%)	1	3
6	AG	155/156 (99%)	121 (78%)	34 (22%)	1	5
6	BG	155/156 (99%)	116 (75%)	39 (25%)	1	2
7	AH	142/148 (96%)	110 (78%)	32 (22%)	1	4
7	BH	142/148 (96%)	118 (83%)	24 (17%)	2	12
8	AK	122/124 (98%)	99 (81%)	23 (19%)	2	8
8	BK	122/124 (98%)	89 (73%)	33 (27%)	0	2
9	AM	117/119 (98%)	88 (75%)	29 (25%)	1	3
9	BM	117/119 (98%)	95 (81%)	22 (19%)	2	8
10	AN	100/100 (100%)	86 (86%)	14 (14%)	4	20
10	BN	100/100 (100%)	80 (80%)	20 (20%)	1	6
11	AO	116/116 (100%)	81 (70%)	35 (30%)	0	1
11	BO	116/116 (100%)	76 (66%)	40 (34%)	0	1
12	AP	111/111 (100%)	86 (78%)	25 (22%)	1	4
12	BP	111/111 (100%)	86 (78%)	25 (22%)	1	4
13	A0	101/101 (100%)	80 (79%)	21 (21%)	1	6
13	B0	100/101 (99%)	81 (81%)	19 (19%)	2	8
14	AQ	87/88 (99%)	69 (79%)	18 (21%)	1	6
14	BQ	87/88 (99%)	66 (76%)	21 (24%)	1	3
15	AR	120/127 (94%)	91 (76%)	29 (24%)	1	3
15	BR	120/127 (94%)	84 (70%)	36 (30%)	0	1
16	A1	93/94 (99%)	77 (83%)	16 (17%)	2	12
16	B1	93/94 (99%)	80 (86%)	13 (14%)	4	20
17	A2	82/82 (100%)	59 (72%)	23 (28%)	0	2
17	B2	82/82 (100%)	54 (66%)	28 (34%)	0	1
18	AS	92/92 (100%)	72 (78%)	20 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	BS	92/92 (100%)	66 (72%)	26 (28%)	0	2
19	AT	74/78 (95%)	58 (78%)	16 (22%)	1	5
19	BT	74/78 (95%)	60 (81%)	14 (19%)	2	8
20	AU	85/91 (93%)	68 (80%)	17 (20%)	1	6
20	BU	85/91 (93%)	61 (72%)	24 (28%)	0	2
21	AV	154/179 (86%)	123 (80%)	31 (20%)	1	6
21	BV	158/179 (88%)	130 (82%)	28 (18%)	2	10
22	A3	61/67 (91%)	52 (85%)	9 (15%)	4	17
22	B3	62/67 (92%)	50 (81%)	12 (19%)	2	7
23	AZ	82/83 (99%)	70 (85%)	12 (15%)	4	18
23	BZ	82/83 (99%)	66 (80%)	16 (20%)	2	7
24	AW	62/67 (92%)	46 (74%)	16 (26%)	0	2
24	BW	64/67 (96%)	51 (80%)	13 (20%)	1	6
25	AX	51/52 (98%)	47 (92%)	4 (8%)	16	50
25	BX	51/52 (98%)	38 (74%)	13 (26%)	1	2
26	A4	59/63 (94%)	42 (71%)	17 (29%)	0	1
26	B4	57/63 (90%)	41 (72%)	16 (28%)	0	2
27	A5	51/52 (98%)	37 (72%)	14 (28%)	0	2
27	B5	51/52 (98%)	38 (74%)	13 (26%)	1	2
28	A6	44/52 (85%)	28 (64%)	16 (36%)	0	1
28	B6	44/52 (85%)	29 (66%)	15 (34%)	0	1
29	A7	42/42 (100%)	35 (83%)	7 (17%)	3	13
29	B7	42/42 (100%)	30 (71%)	12 (29%)	0	1
30	A8	51/55 (93%)	41 (80%)	10 (20%)	1	7
30	B8	51/55 (93%)	37 (72%)	14 (28%)	0	2
32	CE	205/220 (93%)	164 (80%)	41 (20%)	1	6
32	DE	205/220 (93%)	168 (82%)	37 (18%)	2	10
33	CF	159/188 (85%)	132 (83%)	27 (17%)	2	12
33	DF	160/188 (85%)	129 (81%)	31 (19%)	2	7
34	CG	180/180 (100%)	150 (83%)	30 (17%)	3	13
34	DG	180/180 (100%)	141 (78%)	39 (22%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	CH	116/123 (94%)	94 (81%)	22 (19%)	2	8
35	DH	116/123 (94%)	97 (84%)	19 (16%)	3	14
36	CI	90/90 (100%)	78 (87%)	12 (13%)	5	21
36	DI	90/90 (100%)	78 (87%)	12 (13%)	5	21
37	CJ	126/127 (99%)	105 (83%)	21 (17%)	3	13
37	DJ	126/127 (99%)	100 (79%)	26 (21%)	1	6
38	CK	119/119 (100%)	106 (89%)	13 (11%)	8	32
38	DK	119/119 (100%)	102 (86%)	17 (14%)	4	19
39	CL	98/99 (99%)	69 (70%)	29 (30%)	0	1
39	DL	98/99 (99%)	72 (74%)	26 (26%)	0	2
40	CM	89/92 (97%)	69 (78%)	20 (22%)	1	4
40	DM	89/92 (97%)	65 (73%)	24 (27%)	0	2
41	CN	90/99 (91%)	77 (86%)	13 (14%)	4	19
41	DN	90/99 (91%)	79 (88%)	11 (12%)	6	26
42	CO	104/109 (95%)	88 (85%)	16 (15%)	3	16
42	DO	104/109 (95%)	85 (82%)	19 (18%)	2	9
43	CP	94/101 (93%)	76 (81%)	18 (19%)	2	8
43	DP	94/101 (93%)	77 (82%)	17 (18%)	2	9
44	CQ	49/50 (98%)	34 (69%)	15 (31%)	0	1
44	DQ	49/50 (98%)	37 (76%)	12 (24%)	1	3
45	CR	79/80 (99%)	69 (87%)	10 (13%)	5	24
45	DR	79/80 (99%)	68 (86%)	11 (14%)	4	20
46	CS	72/74 (97%)	58 (81%)	14 (19%)	2	7
46	DS	72/74 (97%)	58 (81%)	14 (19%)	2	7
47	CT	95/97 (98%)	83 (87%)	12 (13%)	5	24
47	DT	95/97 (98%)	88 (93%)	7 (7%)	17	52
48	CU	63/77 (82%)	51 (81%)	12 (19%)	2	8
48	DU	63/77 (82%)	50 (79%)	13 (21%)	1	6
49	CV	67/80 (84%)	50 (75%)	17 (25%)	1	2
49	DV	67/80 (84%)	53 (79%)	14 (21%)	1	6
50	CW	76/82 (93%)	64 (84%)	12 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	DW	76/82 (93%)	62 (82%)	14 (18%)	2	9
51	CX	20/22 (91%)	15 (75%)	5 (25%)	1	3
51	DX	20/22 (91%)	18 (90%)	2 (10%)	9	36
All	All	9579/9996 (96%)	7581 (79%)	1998 (21%)	1	6

5 of 1998 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	BO	101	VAL
20	BU	96	ILE
40	DM	30	SER
12	BP	83	MET
15	BR	134	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 265 such sidechains are listed below:

Mol	Chain	Res	Type
16	B1	49	HIS
23	BZ	66	HIS
40	DM	13	HIS
17	B2	64	HIS
19	BT	82	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	700 (24%)	52 (1%)
1	BA	2908/2912 (99%)	711 (24%)	53 (1%)
2	AB	121/122 (99%)	29 (23%)	0
2	BB	121/122 (99%)	29 (23%)	0
31	CA	1506/1506 (100%)	346 (22%)	35 (2%)
31	DA	1505/1506 (99%)	353 (23%)	49 (3%)
52	CB	86/87 (98%)	37 (43%)	4 (4%)
52	DB	86/87 (98%)	33 (38%)	3 (3%)
53	CC	77/77 (100%)	17 (22%)	4 (5%)
53	CD	76/77 (98%)	27 (35%)	1 (1%)
53	DC	77/77 (100%)	17 (22%)	4 (5%)
53	DD	76/77 (98%)	26 (34%)	1 (1%)
54	C1	9/10 (90%)	2 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	D1	9/10 (90%)	2 (22%)	0
All	All	9568/9582 (99%)	2329 (24%)	206 (2%)

5 of 2329 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	G
1	AA	5	A
1	AA	10	G
1	AA	34	C
1	AA	35	G

5 of 206 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	2282	G
31	CA	428	G
31	DA	1305	G
1	BA	2422	A
1	BA	2893	G

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 1703 ligands modelled in this entry, 1701 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
56	PAR	CA	1841	-	45,45,45	0.54	0	59,67,67	1.34	9 (15%)
56	PAR	DA	1805	-	45,45,45	0.57	0	59,67,67	1.64	16 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PAR	CA	1841	-	-	0/18/94/94	0/4/4/4
56	PAR	DA	1805	-	-	0/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	1805	PAR	C13-O52-C52	-4.10	107.28	118.01
56	DA	1805	PAR	C11-O11-C42	-3.23	109.58	118.01
56	DA	1805	PAR	C14-O33-C33	-2.95	110.29	118.01
56	DA	1805	PAR	O34-C34-C44	-2.77	104.09	110.34
56	CA	1841	PAR	C11-O11-C42	-2.64	111.10	118.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	CA	1841	PAR	4	0
56	DA	1805	PAR	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	2912/2912 (100%)	-0.03	43 (1%) 76 71	50, 81, 215, 247	0
1	BA	2909/2912 (99%)	-0.14	42 (1%) 78 73	60, 95, 235, 249	0
2	AB	122/122 (100%)	-0.26	1 (0%) 87 84	81, 105, 124, 182	0
2	BB	122/122 (100%)	-0.34	2 (1%) 74 69	98, 133, 156, 203	0
3	AD	272/276 (98%)	0.78	14 (5%) 32 25	47, 72, 94, 112	0
3	BD	272/276 (98%)	0.57	15 (5%) 29 23	56, 82, 103, 138	0
4	AE	205/206 (99%)	0.91	40 (19%) 1 1	55, 91, 137, 149	0
4	BE	205/206 (99%)	1.06	37 (18%) 2 1	66, 104, 153, 172	0
5	AF	202/210 (96%)	0.08	2 (0%) 84 80	52, 84, 123, 137	0
5	BF	208/210 (99%)	0.82	28 (13%) 4 3	64, 108, 166, 191	0
6	AG	181/182 (99%)	1.20	34 (18%) 2 1	95, 115, 143, 157	0
6	BG	181/182 (99%)	1.23	42 (23%) 1 1	125, 148, 169, 176	0
7	AH	170/180 (94%)	0.28	6 (3%) 48 40	89, 119, 138, 160	0
7	BH	170/180 (94%)	3.56	121 (71%) 0 0	161, 203, 224, 232	0
8	AK	146/148 (98%)	0.72	20 (13%) 4 3	85, 134, 151, 157	0
8	BK	146/148 (98%)	0.38	7 (4%) 34 28	91, 134, 158, 167	0
9	AM	138/140 (98%)	0.33	7 (5%) 32 25	70, 95, 131, 144	0
9	BM	138/140 (98%)	1.95	66 (47%) 0 0	86, 118, 148, 158	0
10	AN	122/122 (100%)	0.65	4 (3%) 50 43	63, 82, 98, 111	0
10	BN	122/122 (100%)	0.93	14 (11%) 6 5	76, 98, 117, 133	0
11	AO	150/150 (100%)	0.28	5 (3%) 50 43	45, 90, 122, 167	0
11	BO	150/150 (100%)	0.62	13 (8%) 13 10	44, 101, 149, 186	0
12	AP	141/141 (100%)	0.75	13 (9%) 11 9	58, 91, 116, 142	0
12	BP	141/141 (100%)	1.63	45 (31%) 1 1	58, 107, 142, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	0.10	0 100 100	64, 90, 109, 123	0
13	B0	117/118 (99%)	0.15	1 (0%) 85 82	68, 90, 113, 128	0
14	AQ	111/112 (99%)	0.80	13 (11%) 6 5	83, 103, 126, 142	0
14	BQ	111/112 (99%)	0.41	7 (6%) 23 19	95, 132, 156, 175	0
15	AR	137/146 (93%)	0.68	9 (6%) 22 17	75, 97, 147, 178	0
15	BR	137/146 (93%)	0.40	5 (3%) 46 39	86, 107, 167, 187	0
16	A1	117/118 (99%)	-0.13	3 (2%) 59 53	61, 84, 116, 145	0
16	B1	117/118 (99%)	1.49	35 (29%) 1 1	71, 106, 146, 165	0
17	A2	101/101 (100%)	0.20	3 (2%) 54 47	61, 105, 126, 145	0
17	B2	101/101 (100%)	2.09	44 (43%) 0 0	73, 131, 148, 158	0
18	AS	113/113 (100%)	-0.07	2 (1%) 71 65	55, 80, 111, 163	0
18	BS	113/113 (100%)	0.58	6 (5%) 30 24	69, 84, 121, 162	0
19	AT	92/96 (95%)	0.62	6 (6%) 22 18	63, 78, 102, 118	0
19	BT	92/96 (95%)	0.78	8 (8%) 13 10	78, 96, 119, 134	0
20	AU	102/110 (92%)	0.23	4 (3%) 43 36	82, 107, 157, 172	0
20	BU	102/110 (92%)	1.56	29 (28%) 1 1	97, 123, 176, 191	0
21	AV	175/206 (84%)	1.58	65 (37%) 0 1	93, 133, 193, 198	0
21	BV	179/206 (86%)	3.04	109 (60%) 0 0	128, 166, 212, 218	0
22	A3	76/85 (89%)	0.25	1 (1%) 79 74	65, 84, 98, 137	0
22	B3	77/85 (90%)	0.39	2 (2%) 59 53	79, 101, 122, 155	0
23	AZ	97/98 (98%)	0.83	12 (12%) 5 4	61, 81, 137, 165	0
23	BZ	97/98 (98%)	0.34	2 (2%) 67 60	69, 91, 141, 162	0
24	AW	66/72 (91%)	0.12	2 (3%) 54 47	69, 87, 106, 137	0
24	BW	69/72 (95%)	0.70	5 (7%) 18 15	90, 114, 148, 183	0
25	AX	59/60 (98%)	-0.02	2 (3%) 49 42	73, 90, 120, 135	0
25	BX	59/60 (98%)	1.42	13 (22%) 1 1	86, 114, 146, 166	0
26	A4	66/71 (92%)	3.46	46 (69%) 0 0	127, 161, 179, 187	0
26	B4	63/71 (88%)	3.70	46 (73%) 0 0	154, 190, 200, 207	0
27	A5	59/60 (98%)	0.52	7 (11%) 6 5	55, 95, 180, 185	0
27	B5	59/60 (98%)	1.14	12 (20%) 1 1	65, 94, 181, 192	0
28	A6	45/54 (83%)	3.36	30 (66%) 0 0	122, 152, 173, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	45/54 (83%)	1.91	18 (40%) 0 0	141, 173, 188, 192	0
29	A7	49/49 (100%)	0.08	2 (4%) 41 34	50, 60, 106, 137	0
29	B7	49/49 (100%)	0.46	4 (8%) 14 11	60, 69, 129, 148	0
30	A8	61/65 (93%)	0.41	1 (1%) 74 69	64, 78, 95, 120	0
30	B8	61/65 (93%)	0.96	5 (8%) 14 11	78, 95, 110, 142	0
31	CA	1506/1506 (100%)	-0.34	7 (0%) 91 90	64, 112, 193, 248	0
31	DA	1506/1506 (100%)	-0.38	7 (0%) 91 90	76, 122, 195, 248	0
32	CE	237/256 (92%)	0.56	22 (9%) 11 9	115, 149, 188, 198	0
32	DE	237/256 (92%)	0.27	19 (8%) 15 12	127, 165, 200, 215	0
33	CF	205/239 (85%)	0.67	18 (8%) 12 10	98, 124, 158, 166	0
33	DF	206/239 (86%)	1.16	51 (24%) 1 1	128, 151, 180, 188	0
34	CG	208/208 (100%)	-0.08	1 (0%) 91 90	95, 119, 143, 154	0
34	DG	208/208 (100%)	0.75	20 (9%) 10 9	91, 116, 137, 151	0
35	CH	151/162 (93%)	0.42	5 (3%) 50 43	87, 109, 132, 166	0
35	DH	151/162 (93%)	-0.02	1 (0%) 89 86	104, 125, 148, 169	0
36	CI	101/101 (100%)	0.91	13 (12%) 5 3	89, 112, 130, 153	0
36	DI	101/101 (100%)	0.69	11 (10%) 7 6	87, 109, 130, 156	0
37	CJ	155/156 (99%)	0.69	16 (10%) 9 7	111, 128, 158, 167	0
37	DJ	155/156 (99%)	-0.12	2 (1%) 79 74	116, 136, 164, 170	0
38	CK	138/138 (100%)	0.14	3 (2%) 65 59	95, 116, 130, 137	0
38	DK	138/138 (100%)	-0.23	0 100 100	109, 129, 143, 151	0
39	CL	127/128 (99%)	-0.25	0 100 100	99, 147, 167, 173	0
39	DL	127/128 (99%)	-0.49	1 (0%) 87 84	120, 158, 174, 178	0
40	CM	99/105 (94%)	-0.10	2 (2%) 68 62	93, 146, 176, 179	0
40	DM	99/105 (94%)	0.40	9 (9%) 11 9	127, 164, 180, 185	0
41	CN	119/129 (92%)	1.85	41 (34%) 0 1	79, 110, 142, 169	0
41	DN	119/129 (92%)	0.60	9 (7%) 17 14	90, 116, 148, 172	0
42	CO	125/132 (94%)	1.10	26 (20%) 1 1	76, 87, 119, 164	0
42	DO	125/132 (94%)	1.32	32 (25%) 1 1	88, 112, 137, 175	0
43	CP	116/126 (92%)	0.63	11 (9%) 10 9	98, 132, 151, 160	0
43	DP	117/126 (92%)	0.85	14 (11%) 6 5	117, 160, 174, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CQ	60/61 (98%)	0.06	1 (1%) 73 67	95, 115, 129, 139	0
44	DQ	60/61 (98%)	0.38	4 (6%) 21 17	129, 146, 159, 166	0
45	CR	88/89 (98%)	0.22	3 (3%) 49 42	86, 108, 129, 133	0
45	DR	88/89 (98%)	0.21	2 (2%) 64 57	85, 118, 142, 148	0
46	CS	84/88 (95%)	0.19	3 (3%) 46 39	104, 121, 148, 179	0
46	DS	84/88 (95%)	0.15	0 100 100	94, 111, 134, 166	0
47	CT	100/105 (95%)	0.18	5 (5%) 32 26	94, 115, 132, 146	0
47	DT	100/105 (95%)	0.23	4 (4%) 42 34	95, 117, 141, 155	0
48	CU	72/88 (81%)	0.97	11 (15%) 3 2	91, 112, 146, 173	0
48	DU	72/88 (81%)	0.65	7 (9%) 10 9	97, 120, 156, 173	0
49	CV	78/93 (83%)	0.65	6 (7%) 16 13	112, 136, 151, 158	0
49	DV	78/93 (83%)	0.83	8 (10%) 9 7	150, 167, 187, 191	0
50	CW	99/106 (93%)	-0.15	0 100 100	106, 130, 158, 169	0
50	DW	99/106 (93%)	-0.16	1 (1%) 84 80	97, 124, 158, 172	0
51	CX	25/27 (92%)	-0.21	0 100 100	101, 124, 142, 160	0
51	DX	25/27 (92%)	-0.08	1 (4%) 42 34	126, 149, 163, 175	0
52	CB	87/87 (100%)	1.63	30 (34%) 0 1	91, 155, 201, 213	2 (2%)
52	DB	87/87 (100%)	1.52	27 (31%) 1 1	97, 156, 203, 216	2 (2%)
53	CC	77/77 (100%)	0.35	3 (3%) 43 36	82, 118, 149, 164	0
53	CD	77/77 (100%)	0.77	15 (19%) 1 1	86, 232, 246, 248	0
53	DC	77/77 (100%)	-0.29	0 100 100	87, 120, 153, 167	0
53	DD	77/77 (100%)	-0.46	1 (1%) 79 74	91, 234, 245, 249	0
54	C1	10/10 (100%)	1.33	2 (20%) 1 1	85, 102, 117, 131	0
54	D1	10/10 (100%)	-0.12	1 (10%) 9 8	88, 109, 119, 137	0
All	All	21107/21634 (97%)	0.33	1656 (7%) 16 13	44, 110, 191, 249	4 (0%)

The worst 5 of 1656 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	654(J)	A	14.2
21	BV	179	ASP	13.9
1	AA	654(K)	C	12.0
41	CN	11	LYS	12.0
7	BH	29	PRO	11.7

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(\AA^2)	Q<0.9
55	MG	AA	3489	1/1	0.81	0.66	45.39	86,86,86,86	0
55	MG	AA	3550	1/1	0.95	0.53	37.01	39,39,39,39	0
55	MG	AA	3307	1/1	0.70	0.45	33.71	76,76,76,76	0
55	MG	AA	3058	1/1	0.94	0.28	30.68	64,64,64,64	0
55	MG	AA	3228	1/1	0.93	0.46	30.27	79,79,79,79	0
55	MG	AA	3086	1/1	0.93	0.57	29.33	62,62,62,62	0
55	MG	DA	1690	1/1	0.95	0.41	28.53	92,92,92,92	0
55	MG	AA	3074	1/1	0.96	0.51	27.90	68,68,68,68	0
55	MG	DA	1748	1/1	0.73	0.50	27.53	91,91,91,91	0
55	MG	AA	3356	1/1	0.78	0.55	27.47	86,86,86,86	0
55	MG	DA	1753	1/1	0.86	0.51	27.41	87,87,87,87	0
55	MG	BA	3156	1/1	0.98	0.40	26.77	87,87,87,87	0
55	MG	AA	3530	1/1	0.93	0.39	26.43	79,79,79,79	0
55	MG	DA	1752	1/1	0.91	0.37	26.12	89,89,89,89	0
55	MG	AA	3010	1/1	0.96	0.39	26.07	47,47,47,47	0
55	MG	AA	3123	1/1	0.95	0.42	25.41	52,52,52,52	0
55	MG	BA	3350	1/1	0.73	0.51	25.33	77,77,77,77	0
55	MG	AA	3267	1/1	0.96	0.36	24.68	62,62,62,62	0
55	MG	AA	3497	1/1	0.70	0.61	24.45	95,95,95,95	0
55	MG	AA	3214	1/1	0.91	0.44	24.38	47,47,47,47	0
55	MG	A1	201	1/1	0.95	0.37	24.28	64,64,64,64	0
55	MG	BA	3412	1/1	0.98	0.41	24.19	50,50,50,50	0
55	MG	AA	3549	1/1	0.98	0.54	24.09	50,50,50,50	0
55	MG	AA	3540	1/1	0.91	0.41	23.63	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3112	1/1	0.98	0.59	23.49	45,45,45,45	0
55	MG	AA	3150	1/1	0.93	0.54	23.25	59,59,59,59	0
55	MG	AA	3154	1/1	0.98	0.44	23.05	52,52,52,52	0
55	MG	AA	3053	1/1	0.70	0.58	23.04	67,67,67,67	0
55	MG	CA	1722	1/1	0.69	0.41	23.02	74,74,74,74	0
55	MG	DA	1710	1/1	0.60	0.49	22.80	100,100,100,100	0
55	MG	AA	3177	1/1	0.96	0.46	22.46	46,46,46,46	0
55	MG	AA	3588	1/1	0.84	0.47	22.42	68,68,68,68	0
55	MG	AB	215	1/1	0.93	0.39	22.10	93,93,93,93	0
55	MG	AA	3521	1/1	0.88	0.45	21.50	75,75,75,75	0
55	MG	DA	1616	1/1	0.92	0.35	21.13	100,100,100,100	0
55	MG	AA	3057	1/1	0.96	0.41	21.03	66,66,66,66	0
55	MG	AA	3094	1/1	0.77	0.35	20.87	62,62,62,62	0
55	MG	AA	3125	1/1	0.98	0.42	20.35	55,55,55,55	0
55	MG	AA	3093	1/1	0.74	0.52	20.05	65,65,65,65	0
55	MG	DA	1728	1/1	0.88	0.32	20.03	112,112,112,112	0
55	MG	BA	3174	1/1	0.58	0.32	19.80	82,82,82,82	0
55	MG	AA	3315	1/1	0.89	0.48	19.49	70,70,70,70	0
55	MG	BA	3396	1/1	0.86	0.35	19.39	91,91,91,91	0
55	MG	AA	3119	1/1	0.93	0.38	19.26	75,75,75,75	0
55	MG	AA	3322	1/1	0.87	0.53	18.89	68,68,68,68	0
55	MG	DA	1689	1/1	0.98	0.33	18.86	72,72,72,72	0
55	MG	DA	1675	1/1	0.94	0.39	18.28	60,60,60,60	0
55	MG	AA	3004	1/1	0.98	0.39	18.24	40,40,40,40	0
55	MG	BA	3157	1/1	0.95	0.42	18.21	93,93,93,93	0
55	MG	AA	3027	1/1	0.99	0.36	18.01	45,45,45,45	0
55	MG	BA	3496	1/1	0.92	0.35	17.99	96,96,96,96	0
55	MG	BA	3187	1/1	0.91	0.37	17.84	65,65,65,65	0
55	MG	AA	3245	1/1	0.87	0.41	17.73	75,75,75,75	0
55	MG	CA	1639	1/1	0.79	0.42	17.64	86,86,86,86	0
55	MG	DA	1795	1/1	0.49	0.32	17.57	101,101,101,101	0
55	MG	AA	3006	1/1	0.96	0.54	17.40	46,46,46,46	0
55	MG	AA	3002	1/1	0.95	0.43	16.92	41,41,41,41	0
55	MG	AA	3138	1/1	0.92	0.42	16.50	45,45,45,45	0
55	MG	AA	3144	1/1	0.95	0.47	16.39	45,45,45,45	0
55	MG	AA	3106	1/1	0.95	0.35	16.31	69,69,69,69	0
55	MG	AA	3031	1/1	0.90	0.43	16.29	52,52,52,52	0
55	MG	AA	3113	1/1	0.97	0.50	16.05	49,49,49,49	0
55	MG	BA	3278	1/1	0.74	0.32	15.93	92,92,92,92	0
55	MG	CA	1715	1/1	0.70	0.26	15.68	115,115,115,115	0
55	MG	AA	3343	1/1	0.95	0.35	15.67	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3448	1/1	0.84	0.38	15.59	106,106,106,106	0
55	MG	AA	3400	1/1	0.97	0.47	15.56	39,39,39,39	0
55	MG	DA	1670	1/1	0.95	0.36	15.34	49,49,49,49	0
55	MG	BA	3254	1/1	0.91	0.46	15.30	69,69,69,69	0
55	MG	AA	3081	1/1	0.92	0.56	15.22	51,51,51,51	0
55	MG	BA	3236	1/1	0.96	0.43	15.05	41,41,41,41	0
55	MG	AA	3085	1/1	0.95	0.41	14.92	34,34,34,34	0
55	MG	DA	1737	1/1	0.92	0.35	14.84	74,74,74,74	0
55	MG	DA	1756	1/1	0.86	0.46	14.79	106,106,106,106	0
55	MG	AA	3408	1/1	0.83	0.38	14.67	83,83,83,83	0
55	MG	CA	1792	1/1	0.94	0.31	14.43	81,81,81,81	0
55	MG	BA	3145	1/1	0.98	0.36	14.28	53,53,53,53	0
55	MG	AA	3045	1/1	0.93	0.49	14.08	54,54,54,54	0
55	MG	AA	3212	1/1	0.92	0.34	13.96	52,52,52,52	0
55	MG	AA	3128	1/1	0.92	0.38	13.94	56,56,56,56	0
55	MG	AA	3141	1/1	0.98	0.35	13.88	50,50,50,50	0
55	MG	AA	3574	1/1	0.96	0.34	13.48	54,54,54,54	0
55	MG	CA	1679	1/1	0.45	0.35	13.42	101,101,101,101	0
55	MG	AA	3165	1/1	0.91	0.45	13.33	82,82,82,82	0
55	MG	AA	3570	1/1	0.94	0.39	13.32	41,41,41,41	0
55	MG	BA	3489	1/1	0.97	0.40	13.23	68,68,68,68	0
55	MG	AA	3044	1/1	0.95	0.42	13.04	52,52,52,52	0
55	MG	DA	1782	1/1	0.90	0.36	12.99	94,94,94,94	0
55	MG	AA	3578	1/1	0.95	0.39	12.98	50,50,50,50	0
55	MG	AA	3098	1/1	0.97	0.39	12.95	81,81,81,81	0
55	MG	AA	3609	1/1	0.89	0.28	12.94	62,62,62,62	0
55	MG	AA	3001	1/1	0.96	0.45	12.67	44,44,44,44	0
55	MG	AA	3174	1/1	0.97	0.41	12.66	40,40,40,40	0
55	MG	AA	3037	1/1	0.95	0.35	12.65	69,69,69,69	0
55	MG	AA	3034	1/1	0.96	0.40	12.29	52,52,52,52	0
55	MG	AA	3538	1/1	0.98	0.32	12.22	36,36,36,36	0
55	MG	DA	1685	1/1	0.86	0.43	12.17	72,72,72,72	0
55	MG	BA	3446	1/1	0.81	0.32	12.16	98,98,98,98	0
55	MG	AA	3047	1/1	0.94	0.26	12.14	60,60,60,60	0
55	MG	AA	3351	1/1	0.89	0.37	12.10	82,82,82,82	0
55	MG	DA	1801	1/1	0.48	0.32	12.06	90,90,90,90	0
55	MG	AA	3565	1/1	0.98	0.37	12.03	53,53,53,53	0
55	MG	AA	3021	1/1	0.97	0.30	11.98	42,42,42,42	0
55	MG	BA	3180	1/1	0.92	0.29	11.90	57,57,57,57	0
55	MG	BA	3155	1/1	0.92	0.30	11.76	87,87,87,87	0
55	MG	AA	3328	1/1	0.81	0.39	11.73	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3124	1/1	0.96	0.51	11.69	47,47,47,47	0
55	MG	BA	3203	1/1	0.87	0.39	11.60	53,53,53,53	0
55	MG	DA	1646	1/1	0.95	0.27	11.52	65,65,65,65	0
55	MG	AA	3551	1/1	0.95	0.31	11.37	69,69,69,69	0
55	MG	AA	3083	1/1	0.97	0.39	11.25	34,34,34,34	0
55	MG	BA	3135	1/1	0.97	0.33	11.21	52,52,52,52	0
55	MG	BA	3144	1/1	0.93	0.49	11.05	95,95,95,95	0
55	MG	CA	1645	1/1	0.96	0.42	11.05	60,60,60,60	0
55	MG	AA	3116	1/1	0.97	0.47	10.99	37,37,37,37	0
55	MG	AA	3379	1/1	0.91	0.31	10.99	66,66,66,66	0
55	MG	DA	1621	1/1	0.84	0.46	10.97	99,99,99,99	0
55	MG	BA	3324	1/1	0.96	0.38	10.96	75,75,75,75	0
55	MG	AA	3247	1/1	0.96	0.42	10.83	74,74,74,74	0
55	MG	AO	201	1/1	0.91	0.43	10.68	65,65,65,65	0
55	MG	AA	3269	1/1	0.92	0.50	10.66	55,55,55,55	0
55	MG	DA	1721	1/1	0.96	0.36	10.64	71,71,71,71	0
55	MG	BA	3367	1/1	0.48	0.39	10.56	91,91,91,91	0
55	MG	DA	1645	1/1	0.91	0.34	10.48	51,51,51,51	0
55	MG	DA	1667	1/1	0.92	0.27	10.41	82,82,82,82	0
55	MG	AA	3513	1/1	0.72	0.36	10.08	83,83,83,83	0
55	MG	BA	3224	1/1	0.94	0.26	10.05	51,51,51,51	0
55	MG	BA	3355	1/1	0.74	0.43	10.00	87,87,87,87	0
55	MG	AA	3262	1/1	0.90	0.29	9.98	33,33,33,33	0
55	MG	BA	3125	1/1	0.79	1.05	9.96	104,104,104,104	0
55	MG	BA	3279	1/1	0.93	0.34	9.87	73,73,73,73	0
55	MG	CA	1658	1/1	0.97	0.43	9.78	50,50,50,50	0
55	MG	AA	3625	1/1	0.84	0.29	9.76	89,89,89,89	0
55	MG	AA	3603	1/1	0.92	0.43	9.70	41,41,41,41	0
55	MG	AA	3623	1/1	0.91	0.29	9.70	74,74,74,74	0
55	MG	CA	1678	1/1	0.94	0.29	9.66	69,69,69,69	0
55	MG	BA	3238	1/1	0.93	0.26	9.58	66,66,66,66	0
55	MG	AA	3016	1/1	0.98	0.32	9.55	48,48,48,48	0
55	MG	AA	3249	1/1	0.69	0.41	9.54	76,76,76,76	0
55	MG	BA	3233	1/1	0.89	0.36	9.53	74,74,74,74	0
55	MG	DA	1644	1/1	0.95	0.31	9.48	82,82,82,82	0
55	MG	AA	3139	1/1	0.98	0.29	9.38	54,54,54,54	0
55	MG	DA	1722	1/1	0.73	0.28	9.35	106,106,106,106	0
55	MG	AA	3012	1/1	0.99	0.38	9.21	40,40,40,40	0
55	MG	BA	3384	1/1	0.65	0.35	8.99	92,92,92,92	0
55	MG	BA	3229	1/1	0.96	0.33	8.91	50,50,50,50	0
55	MG	AA	3272	1/1	0.84	0.37	8.75	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3253	1/1	0.63	0.30	8.66	81,81,81,81	0
55	MG	DA	1604	1/1	0.89	0.27	8.42	92,92,92,92	0
55	MG	BA	3512	1/1	0.89	0.27	8.36	75,75,75,75	0
55	MG	AA	3153	1/1	0.97	0.26	8.28	48,48,48,48	0
55	MG	AA	3040	1/1	0.95	0.31	8.25	68,68,68,68	0
55	MG	AA	3266	1/1	0.96	0.47	8.21	49,49,49,49	0
55	MG	DA	1763	1/1	0.63	0.28	8.18	89,89,89,89	0
55	MG	BA	3129	1/1	0.95	0.24	8.16	41,41,41,41	0
55	MG	BA	3266	1/1	0.76	0.48	8.16	91,91,91,91	0
55	MG	AA	3548	1/1	0.90	0.30	8.13	54,54,54,54	0
55	MG	CA	1819	1/1	0.63	0.21	8.12	109,109,109,109	0
55	MG	DA	1656	1/1	0.95	0.37	8.10	99,99,99,99	0
55	MG	BA	3242	1/1	0.95	0.35	8.06	62,62,62,62	0
55	MG	BB	207	1/1	0.57	0.34	8.06	116,116,116,116	0
55	MG	AA	3068	1/1	0.96	0.36	7.83	72,72,72,72	0
55	MG	AA	3233	1/1	0.97	0.30	7.78	55,55,55,55	0
55	MG	BA	3058	1/1	0.81	0.35	7.74	89,89,89,89	0
55	MG	BA	3481	1/1	0.96	0.26	7.67	49,49,49,49	0
55	MG	CA	1628	1/1	0.64	0.40	7.67	85,85,85,85	0
55	MG	AA	3263	1/1	0.85	0.28	7.65	51,51,51,51	0
55	MG	BA	3227	1/1	0.97	0.37	7.64	50,50,50,50	0
55	MG	DA	1799	1/1	0.88	0.37	7.64	68,68,68,68	0
55	MG	BA	3376	1/1	0.81	0.33	7.50	65,65,65,65	0
55	MG	DA	1606	1/1	0.73	0.30	7.49	95,95,95,95	0
55	MG	DA	1715	1/1	0.94	0.31	7.39	92,92,92,92	0
55	MG	AA	3355	1/1	0.91	0.37	7.31	94,94,94,94	0
55	MG	CA	1651	1/1	0.94	0.38	7.27	75,75,75,75	0
55	MG	BA	3118	1/1	0.83	0.26	7.25	110,110,110,110	0
55	MG	CA	1760	1/1	0.61	0.20	7.21	91,91,91,91	0
55	MG	AA	3459	1/1	0.93	0.28	7.18	81,81,81,81	0
55	MG	AA	3223	1/1	0.85	0.30	7.17	71,71,71,71	0
55	MG	AA	3024	1/1	0.98	0.39	7.10	45,45,45,45	0
55	MG	AB	217	1/1	0.88	0.40	7.07	110,110,110,110	0
55	MG	BA	3211	1/1	0.98	0.25	7.02	57,57,57,57	0
55	MG	BA	3218	1/1	0.97	0.35	7.00	51,51,51,51	0
55	MG	AA	3055	1/1	0.81	0.35	6.98	67,67,67,67	0
55	MG	AA	3082	1/1	0.97	0.38	6.97	50,50,50,50	0
55	MG	AA	3222	1/1	0.89	0.46	6.95	54,54,54,54	0
55	MG	BR	202	1/1	0.63	0.82	6.91	105,105,105,105	0
55	MG	AO	203	1/1	0.84	0.34	6.88	43,43,43,43	0
55	MG	CA	1636	1/1	0.92	0.29	6.85	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3092	1/1	0.91	0.31	6.85	71,71,71,71	0
55	MG	BA	3492	1/1	0.96	0.28	6.81	47,47,47,47	0
55	MG	BA	3167	1/1	0.97	0.29	6.78	59,59,59,59	0
55	MG	BA	3514	1/1	0.94	0.34	6.67	51,51,51,51	0
55	MG	DA	1649	1/1	0.99	0.29	6.63	93,93,93,93	0
55	MG	AA	3462	1/1	0.97	0.33	6.58	85,85,85,85	0
55	MG	CA	1711	1/1	0.64	0.30	6.58	98,98,98,98	0
55	MG	DA	1755	1/1	0.92	0.47	6.44	79,79,79,79	0
55	MG	CA	1836	1/1	0.96	0.26	6.40	71,71,71,71	0
55	MG	CA	1691	1/1	0.90	0.34	6.35	56,56,56,56	0
55	MG	AA	3277	1/1	0.59	0.32	6.31	82,82,82,82	0
55	MG	BA	3317	1/1	0.93	0.32	6.30	91,91,91,91	0
55	MG	DA	1638	1/1	0.97	0.25	6.18	74,74,74,74	0
55	MG	BA	3023	1/1	0.88	0.39	6.17	70,70,70,70	0
55	MG	CA	1610	1/1	0.95	0.32	6.15	54,54,54,54	0
55	MG	BA	3447	1/1	0.59	0.30	6.12	100,100,100,100	0
55	MG	BA	3179	1/1	0.97	0.34	6.06	61,61,61,61	0
55	MG	CA	1667	1/1	0.97	0.27	6.03	77,77,77,77	0
55	MG	DA	1617	1/1	0.97	0.28	5.89	102,102,102,102	0
55	MG	AA	3592	1/1	0.89	0.35	5.80	76,76,76,76	0
55	MG	BA	3325	1/1	0.95	0.42	5.66	50,50,50,50	0
55	MG	BA	3100	1/1	0.96	0.24	5.66	66,66,66,66	0
55	MG	AA	3052	1/1	0.95	0.29	5.64	73,73,73,73	0
55	MG	DA	1747	1/1	0.68	0.30	5.60	105,105,105,105	0
55	MG	AA	3428	1/1	0.82	0.23	5.57	120,120,120,120	0
55	MG	AA	3541	1/1	0.97	0.24	5.34	48,48,48,48	0
55	MG	BA	3189	1/1	0.87	0.32	5.32	61,61,61,61	0
55	MG	BA	3404	1/1	0.63	0.21	5.32	101,101,101,101	0
55	MG	BA	3094	1/1	0.78	0.23	5.25	79,79,79,79	0
55	MG	BA	3012	1/1	0.97	0.32	5.08	63,63,63,63	0
55	MG	DA	1610	1/1	0.94	0.24	5.06	97,97,97,97	0
55	MG	AE	303	1/1	0.64	0.37	5.04	91,91,91,91	0
55	MG	CA	1712	1/1	0.87	0.28	4.94	92,92,92,92	0
55	MG	BA	3369	1/1	0.85	0.35	4.92	69,69,69,69	0
55	MG	DA	1677	1/1	0.85	0.24	4.92	82,82,82,82	0
55	MG	BA	3363	1/1	0.62	0.23	4.91	88,88,88,88	0
55	MG	DA	1664	1/1	0.50	0.20	4.84	97,97,97,97	0
55	MG	BA	3107	1/1	0.77	0.23	4.82	89,89,89,89	0
55	MG	AA	3599	1/1	0.85	0.32	4.79	87,87,87,87	0
55	MG	BA	3239	1/1	0.97	0.24	4.77	80,80,80,80	0
55	MG	BA	3208	1/1	0.96	0.24	4.76	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3127	1/1	0.98	0.38	4.74	55,55,55,55	0
55	MG	AA	3054	1/1	0.94	0.29	4.69	62,62,62,62	0
55	MG	BA	3220	1/1	0.93	0.32	4.65	40,40,40,40	0
56	PAR	CA	1841	42/42	0.95	0.30	4.59	40,56,74,83	0
55	MG	BA	3067	1/1	0.62	0.42	4.57	74,74,74,74	0
55	MG	BA	3237	1/1	0.98	0.21	4.55	47,47,47,47	0
55	MG	AA	3464	1/1	0.72	0.32	4.49	83,83,83,83	0
55	MG	BA	3010	1/1	0.98	0.24	4.36	68,68,68,68	0
55	MG	BA	3331	1/1	0.68	0.21	4.34	101,101,101,101	0
55	MG	BA	3163	1/1	0.76	0.21	4.24	84,84,84,84	0
55	MG	BA	3152	1/1	0.94	0.19	4.16	73,73,73,73	0
55	MG	CA	1780	1/1	0.93	0.34	4.07	55,55,55,55	0
55	MG	AA	3135	1/1	0.88	0.30	3.92	66,66,66,66	0
55	MG	BA	3086	1/1	0.86	0.38	3.88	82,82,82,82	0
55	MG	DA	1653	1/1	0.97	0.24	3.84	96,96,96,96	0
55	MG	AA	3590	1/1	0.95	0.31	3.78	81,81,81,81	0
55	MG	BA	3009	1/1	0.98	0.25	3.75	48,48,48,48	0
55	MG	AA	3310	1/1	0.79	0.26	3.74	65,65,65,65	0
55	MG	CA	1717	1/1	0.85	0.22	3.71	69,69,69,69	0
55	MG	AA	3336	1/1	0.83	0.25	3.70	82,82,82,82	0
55	MG	BA	3366	1/1	0.83	0.25	3.65	76,76,76,76	0
55	MG	BA	3169	1/1	0.98	0.25	3.65	56,56,56,56	0
55	MG	AA	3323	1/1	0.82	0.26	3.61	71,71,71,71	0
55	MG	AA	3051	1/1	0.94	0.33	3.56	71,71,71,71	0
55	MG	AA	3160	1/1	0.98	0.30	3.50	32,32,32,32	0
55	MG	BA	3037	1/1	0.63	0.26	3.42	75,75,75,75	0
55	MG	BA	3217	1/1	0.96	0.30	3.33	39,39,39,39	0
55	MG	DA	1684	1/1	0.79	0.25	3.21	92,92,92,92	0
55	MG	BA	3231	1/1	0.96	0.25	3.15	47,47,47,47	0
55	MG	BA	3140	1/1	0.97	0.26	3.10	42,42,42,42	0
55	MG	BA	3228	1/1	0.92	0.35	3.09	74,74,74,74	0
55	MG	AA	3162	1/1	0.93	0.30	3.06	45,45,45,45	0
55	MG	BA	3136	1/1	0.95	0.23	3.01	43,43,43,43	0
55	MG	AA	3568	1/1	0.97	0.24	2.84	49,49,49,49	0
55	MG	BA	3219	1/1	0.96	0.25	2.84	48,48,48,48	0
55	MG	AB	202	1/1	0.70	0.23	2.82	92,92,92,92	0
55	MG	BA	3484	1/1	0.96	0.25	2.80	65,65,65,65	0
55	MG	BA	3158	1/1	0.96	0.21	2.79	70,70,70,70	0
55	MG	CA	1663	1/1	0.89	0.24	2.78	52,52,52,52	0
55	MG	CA	1620	1/1	0.96	0.19	2.76	74,74,74,74	0
55	MG	CA	1632	1/1	0.94	0.21	2.75	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3288	1/1	0.96	0.22	2.74	98,98,98,98	0
55	MG	BA	3494	1/1	0.88	0.33	2.70	88,88,88,88	0
55	MG	AF	303	1/1	0.90	0.33	2.67	69,69,69,69	0
55	MG	AA	3195	1/1	0.92	0.21	2.67	62,62,62,62	0
55	MG	BA	3329	1/1	0.29	0.18	2.67	66,66,66,66	0
55	MG	AA	3168	1/1	0.94	0.31	2.63	68,68,68,68	0
55	MG	BA	3178	1/1	0.93	0.27	2.38	62,62,62,62	0
55	MG	BA	3081	1/1	0.63	0.21	2.36	91,91,91,91	0
55	MG	BA	3283	1/1	0.96	0.23	2.35	43,43,43,43	0
55	MG	AA	3186	1/1	0.90	0.21	2.34	58,58,58,58	0
55	MG	BA	3490	1/1	0.97	0.25	2.30	52,52,52,52	0
55	MG	CA	1767	1/1	0.53	0.27	2.20	120,120,120,120	0
55	MG	BA	3309	1/1	0.88	0.30	2.19	80,80,80,80	0
55	MG	AA	3567	1/1	0.96	0.25	2.08	39,39,39,39	0
56	PAR	DA	1805	42/42	0.94	0.21	2.07	46,59,73,84	0
55	MG	AA	3042	1/1	0.81	0.18	1.89	77,77,77,77	0
55	MG	AA	3088	1/1	0.90	0.22	1.88	42,42,42,42	0
55	MG	AA	3547	1/1	0.86	0.20	1.87	45,45,45,45	0
55	MG	CA	1752	1/1	0.70	0.15	1.85	96,96,96,96	0
57	ZN	CG	303	1/1	0.98	0.34	1.82	95,95,95,95	0
55	MG	BA	3385	1/1	0.93	0.18	1.82	97,97,97,97	0
55	MG	AA	3014	1/1	0.92	0.29	1.77	38,38,38,38	0
55	MG	BA	3097	1/1	0.96	0.25	1.74	60,60,60,60	0
55	MG	DA	1609	1/1	0.98	0.23	1.71	116,116,116,116	0
55	MG	BA	3133	1/1	0.97	0.22	1.69	50,50,50,50	0
55	MG	DA	1624	1/1	0.55	0.25	1.69	95,95,95,95	0
55	MG	BA	3517	1/1	0.97	0.21	1.68	61,61,61,61	0
55	MG	BA	3168	1/1	0.98	0.21	1.67	60,60,60,60	0
55	MG	DA	1629	1/1	0.61	0.20	1.63	92,92,92,92	0
55	MG	AA	3018	1/1	0.97	0.36	1.63	43,43,43,43	0
55	MG	BA	3482	1/1	0.98	0.19	1.61	65,65,65,65	0
55	MG	BA	3186	1/1	0.94	0.28	1.59	52,52,52,52	0
55	MG	BA	3142	1/1	0.92	0.23	1.49	70,70,70,70	0
55	MG	AA	3386	1/1	0.85	0.17	1.40	74,74,74,74	0
55	MG	AA	3084	1/1	0.97	0.26	1.38	43,43,43,43	0
55	MG	CA	1608	1/1	0.91	0.22	1.29	68,68,68,68	0
55	MG	CA	1635	1/1	0.58	0.28	1.29	100,100,100,100	0
55	MG	BA	3248	1/1	0.97	0.22	1.27	54,54,54,54	0
55	MG	BA	3267	1/1	0.90	0.23	1.14	62,62,62,62	0
55	MG	CA	1619	1/1	0.98	0.26	1.09	59,59,59,59	0
55	MG	BA	3315	1/1	0.92	0.18	1.08	91,91,91,91	0
55	MG	CA	1823	1/1	0.47	0.14	1.07	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1661	1/1	0.73	0.17	1.04	52,52,52,52	0
55	MG	DA	1632	1/1	0.93	0.17	1.02	84,84,84,84	0
55	MG	BA	3080	1/1	0.95	0.20	1.01	72,72,72,72	0
55	MG	CA	1812	1/1	0.84	0.20	0.99	84,84,84,84	0
55	MG	AZ	101	1/1	0.80	0.30	0.98	77,77,77,77	0
55	MG	BA	3486	1/1	0.95	0.24	0.96	30,30,30,30	0
55	MG	CC	105	1/1	0.97	0.23	0.96	105,105,105,105	0
55	MG	BA	3509	1/1	0.90	0.34	0.95	73,73,73,73	0
55	MG	AA	3020	1/1	0.96	0.25	0.85	39,39,39,39	0
55	MG	CA	1743	1/1	0.79	0.16	0.82	112,112,112,112	0
55	MG	B1	201	1/1	0.93	0.24	0.74	82,82,82,82	0
55	MG	DA	1668	1/1	0.92	0.16	0.65	73,73,73,73	0
55	MG	AA	3026	1/1	0.98	0.24	0.59	40,40,40,40	0
55	MG	CA	1682	1/1	0.95	0.16	0.48	106,106,106,106	0
55	MG	BA	3322	1/1	0.86	0.22	0.44	79,79,79,79	0
55	MG	AA	3305	1/1	0.86	0.36	0.40	80,80,80,80	0
55	MG	BE	303	1/1	0.95	0.23	0.36	57,57,57,57	0
55	MG	DA	1740	1/1	0.64	0.17	0.33	113,113,113,113	0
55	MG	BA	3190	1/1	0.91	0.23	0.32	73,73,73,73	0
55	MG	AA	3423	1/1	0.76	0.20	0.31	74,74,74,74	0
55	MG	BA	3109	1/1	0.81	0.16	0.29	75,75,75,75	0
55	MG	AA	3175	1/1	0.96	0.20	0.23	45,45,45,45	0
55	MG	AA	3308	1/1	0.58	0.23	0.18	96,96,96,96	0
55	MG	A6	101	1/1	0.66	0.50	0.17	111,111,111,111	0
55	MG	BA	3054	1/1	0.91	0.17	0.11	81,81,81,81	0
55	MG	DA	1652	1/1	0.97	0.17	0.08	85,85,85,85	0
55	MG	AA	3610	1/1	0.99	0.19	0.06	46,46,46,46	0
55	MG	BA	3230	1/1	0.95	0.19	0.06	68,68,68,68	0
55	MG	A0	201	1/1	0.95	0.21	0.06	62,62,62,62	0
55	MG	CA	1601	1/1	0.96	0.19	0.06	56,56,56,56	0
55	MG	CG	302	1/1	0.72	0.17	0.04	122,122,122,122	0
55	MG	DA	1622	1/1	0.95	0.13	-0.01	98,98,98,98	0
55	MG	CA	1822	1/1	0.83	0.14	-0.06	105,105,105,105	0
55	MG	BA	3042	1/1	0.90	0.16	-0.09	86,86,86,86	0
55	MG	DA	1697	1/1	0.89	0.17	-0.13	111,111,111,111	0
57	ZN	DG	303	1/1	0.99	0.29	-0.16	134,134,134,134	0
55	MG	AA	3577	1/1	0.96	0.19	-0.18	52,52,52,52	0
55	MG	AA	3164	1/1	0.92	0.25	-0.25	95,95,95,95	0
55	MG	AA	3332	1/1	0.73	0.15	-0.30	62,62,62,62	0
55	MG	AA	3484	1/1	0.96	0.21	-0.31	44,44,44,44	0
55	MG	BA	3466	1/1	0.77	0.14	-0.32	73,73,73,73	0
55	MG	BD	301	1/1	0.97	0.21	-0.33	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3295	1/1	0.97	0.17	-0.34	58,58,58,58	0
55	MG	AA	3517	1/1	0.94	0.20	-0.36	66,66,66,66	0
55	MG	BA	3069	1/1	0.88	0.14	-0.40	70,70,70,70	0
55	MG	DA	1627	1/1	0.77	0.13	-0.48	105,105,105,105	0
55	MG	BA	3429	1/1	0.66	0.16	-0.49	95,95,95,95	0
55	MG	CA	1602	1/1	0.94	0.17	-0.50	74,74,74,74	0
55	MG	AA	3433	1/1	0.28	0.12	-0.52	152,152,152,152	0
55	MG	AF	301	1/1	0.79	0.20	-0.53	80,80,80,80	0
55	MG	AA	3525	1/1	0.69	0.17	-0.53	73,73,73,73	0
55	MG	BA	3461	1/1	0.63	0.19	-0.57	83,83,83,83	0
57	ZN	DQ	101	1/1	0.97	0.17	-0.58	118,118,118,118	0
55	MG	BE	302	1/1	0.82	0.15	-0.63	76,76,76,76	0
55	MG	BA	3434	1/1	0.83	0.16	-0.78	90,90,90,90	0
55	MG	BA	3501	1/1	0.94	0.16	-0.79	88,88,88,88	0
55	MG	CA	1835	1/1	0.94	0.16	-0.80	87,87,87,87	0
55	MG	BA	3342	1/1	0.87	0.17	-0.81	80,80,80,80	0
55	MG	AA	3217	1/1	0.78	0.17	-0.82	64,64,64,64	0
55	MG	BA	3407	1/1	0.49	0.14	-1.00	96,96,96,96	0
55	MG	AA	3571	1/1	0.96	0.19	-1.01	52,52,52,52	0
55	MG	AA	3178	1/1	0.97	0.17	-1.03	54,54,54,54	0
55	MG	BA	3181	1/1	0.95	0.15	-1.12	49,49,49,49	0
57	ZN	CQ	103	1/1	0.99	0.13	-1.12	144,144,144,144	0
55	MG	AA	3591	1/1	0.95	0.18	-1.14	74,74,74,74	0
55	MG	AE	304	1/1	0.67	0.13	-1.16	87,87,87,87	0
55	MG	BB	202	1/1	0.92	0.14	-1.17	103,103,103,103	0
55	MG	DA	1781	1/1	0.85	0.13	-1.22	87,87,87,87	0
55	MG	CA	1762	1/1	0.82	0.14	-1.32	89,89,89,89	0
55	MG	BA	3361	1/1	0.79	0.15	-1.34	88,88,88,88	0
55	MG	AA	3072	1/1	0.89	0.12	-1.40	101,101,101,101	0
55	MG	DA	1648	1/1	0.96	0.10	-1.44	69,69,69,69	0
55	MG	BA	3182	1/1	0.96	0.17	-1.56	47,47,47,47	0
55	MG	AE	301	1/1	0.88	0.15	-1.60	65,65,65,65	0
55	MG	BA	3499	1/1	0.82	0.15	-1.61	78,78,78,78	0
55	MG	BA	3246	1/1	0.89	0.14	-1.70	99,99,99,99	0
55	MG	AA	3512	1/1	0.83	0.14	-1.71	97,97,97,97	0
55	MG	DC	102	1/1	0.97	0.16	-1.73	74,74,74,74	0
55	MG	CA	1824	1/1	0.86	0.14	-1.73	94,94,94,94	0
55	MG	BA	3184	1/1	0.94	0.14	-1.81	76,76,76,76	0
55	MG	DA	1768	1/1	0.58	0.13	-1.89	82,82,82,82	0
55	MG	CN	201	1/1	0.87	0.09	-1.94	78,78,78,78	0
55	MG	AA	3206	1/1	0.81	0.16	-1.97	51,51,51,51	0
55	MG	AA	3064	1/1	0.79	0.12	-2.28	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1794	1/1	0.83	0.13	-2.29	106,106,106,106	0
55	MG	AA	3046	1/1	0.98	0.14	-2.30	57,57,57,57	0
55	MG	CA	1703	1/1	0.84	0.15	-2.30	103,103,103,103	0
55	MG	BA	3131	1/1	0.98	0.17	-2.32	49,49,49,49	0
55	MG	CA	1701	1/1	0.65	0.15	-2.33	105,105,105,105	0
55	MG	DG	302	1/1	0.76	0.08	-2.35	112,112,112,112	0
55	MG	AA	3170	1/1	0.89	0.17	-2.37	41,41,41,41	0
55	MG	BA	3112	1/1	0.74	0.12	-2.46	69,69,69,69	0
55	MG	BA	3488	1/1	0.98	0.15	-2.47	59,59,59,59	0
55	MG	BA	3491	1/1	0.94	0.10	-2.99	49,49,49,49	0
55	MG	CA	1789	1/1	0.93	0.07	-3.07	71,71,71,71	0
55	MG	AA	3584	1/1	0.94	0.15	-3.21	63,63,63,63	0
55	MG	CA	1700	1/1	0.93	0.09	-3.43	72,72,72,72	0
55	MG	BA	3006	1/1	0.95	0.09	-3.49	47,47,47,47	0
55	MG	BA	3016	1/1	0.97	0.07	-3.65	56,56,56,56	0
55	MG	BA	3516	1/1	0.90	0.14	-3.85	73,73,73,73	0
55	MG	CA	1786	1/1	0.95	0.08	-3.89	74,74,74,74	0
55	MG	BA	3284	1/1	0.93	0.12	-3.98	61,61,61,61	0
55	MG	BA	3297	1/1	0.72	0.12	-4.30	63,63,63,63	0
55	MG	BA	3321	1/1	0.87	0.11	-5.04	59,59,59,59	0
55	MG	CA	1702	1/1	0.96	0.09	-5.15	71,71,71,71	0
55	MG	CA	1606	1/1	0.94	0.07	-5.26	94,94,94,94	0
55	MG	AA	3137	1/1	0.95	0.12	-5.52	51,51,51,51	0
55	MG	DA	1673	1/1	0.97	0.13	-6.69	88,88,88,88	0
55	MG	BA	3106	1/1	0.85	0.06	-6.75	85,85,85,85	0
55	MG	BA	3430	1/1	0.96	0.08	-6.79	89,89,89,89	0
55	MG	AA	3487	1/1	0.90	0.08	-7.41	77,77,77,77	0
55	MG	BA	3113	1/1	0.82	0.12	-7.71	84,84,84,84	0
55	MG	AA	3159	1/1	0.93	0.07	-7.75	28,28,28,28	0
55	MG	BA	3007	1/1	0.89	0.07	-8.11	83,83,83,83	0
55	MG	AA	3581	1/1	0.95	0.12	-10.77	36,36,36,36	0
55	MG	AA	3242	1/1	0.76	0.23	-	93,93,93,93	0
55	MG	BA	3345	1/1	0.69	0.19	-	87,87,87,87	0
55	MG	AA	3455	1/1	0.98	0.46	-	49,49,49,49	0
55	MG	CA	1611	1/1	0.58	0.21	-	97,97,97,97	0
55	MG	CD	101	1/1	0.78	0.19	-	105,105,105,105	0
55	MG	AA	3406	1/1	0.91	0.41	-	83,83,83,83	0
55	MG	BA	3046	1/1	0.76	0.34	-	83,83,83,83	0
55	MG	DA	1718	1/1	0.70	0.21	-	132,132,132,132	0
55	MG	DA	1636	1/1	0.76	0.24	-	103,103,103,103	0
55	MG	BB	201	1/1	0.85	0.24	-	90,90,90,90	0
55	MG	AA	3172	1/1	0.74	0.30	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3298	1/1	0.80	0.15	-	61,61,61,61	0
55	MG	CA	1833	1/1	0.79	0.13	-	95,95,95,95	0
55	MG	BA	3518	1/1	0.92	0.42	-	74,74,74,74	0
55	MG	BA	3282	1/1	0.66	0.30	-	93,93,93,93	0
55	MG	BA	3452	1/1	0.92	0.14	-	96,96,96,96	0
55	MG	CA	1649	1/1	0.82	0.29	-	86,86,86,86	0
55	MG	CA	1654	1/1	0.93	0.38	-	75,75,75,75	0
55	MG	BA	3346	1/1	0.81	0.41	-	99,99,99,99	0
55	MG	DA	1723	1/1	0.97	0.32	-	83,83,83,83	0
55	MG	DA	1708	1/1	0.72	0.59	-	102,102,102,102	0
55	MG	DA	1658	1/1	0.95	0.21	-	113,113,113,113	0
55	MG	DA	1628	1/1	0.86	0.42	-	97,97,97,97	0
55	MG	BA	3310	1/1	0.87	0.24	-	74,74,74,74	0
55	MG	AA	3107	1/1	0.56	0.31	-	69,69,69,69	0
55	MG	BA	3422	1/1	0.38	0.36	-	102,102,102,102	0
55	MG	AA	3056	1/1	0.87	0.65	-	98,98,98,98	0
55	MG	BA	3269	1/1	0.86	0.30	-	58,58,58,58	0
55	MG	CA	1714	1/1	0.25	0.47	-	118,118,118,118	0
55	MG	BA	3449	1/1	0.61	0.29	-	109,109,109,109	0
55	MG	AA	3564	1/1	0.40	0.34	-	76,76,76,76	0
55	MG	AA	3259	1/1	0.67	0.30	-	81,81,81,81	0
55	MG	DA	1655	1/1	0.76	0.33	-	96,96,96,96	0
55	MG	DG	301	1/1	0.84	0.35	-	94,94,94,94	0
55	MG	AA	3558	1/1	0.89	0.33	-	89,89,89,89	0
55	MG	DC	105	1/1	0.96	0.39	-	75,75,75,75	0
55	MG	AA	3099	1/1	0.80	0.46	-	64,64,64,64	0
55	MG	DA	1640	1/1	0.85	0.17	-	101,101,101,101	0
55	MG	AA	3190	1/1	0.87	0.24	-	58,58,58,58	0
55	MG	BA	3250	1/1	0.93	0.24	-	58,58,58,58	0
55	MG	CA	1623	1/1	0.77	0.30	-	73,73,73,73	0
55	MG	DA	1686	1/1	0.78	0.34	-	97,97,97,97	0
55	MG	AA	3167	1/1	0.94	0.38	-	50,50,50,50	0
55	MG	AA	3352	1/1	0.97	0.35	-	52,52,52,52	0
55	MG	AA	3192	1/1	0.97	0.35	-	63,63,63,63	0
55	MG	DA	1635	1/1	0.80	0.29	-	79,79,79,79	0
55	MG	CA	1626	1/1	0.84	0.33	-	88,88,88,88	0
55	MG	CA	1817	1/1	0.78	0.27	-	85,85,85,85	0
55	MG	AA	3450	1/1	0.96	0.46	-	72,72,72,72	0
55	MG	BA	3241	1/1	0.98	0.36	-	52,52,52,52	0
55	MG	AA	3229	1/1	0.93	0.20	-	89,89,89,89	0
55	MG	BB	214	1/1	0.57	0.34	-	99,99,99,99	0
55	MG	AA	3466	1/1	0.37	0.48	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1731	1/1	0.84	0.35	-	98,98,98,98	0
55	MG	DA	1788	1/1	0.79	0.39	-	90,90,90,90	0
55	MG	AA	3482	1/1	0.36	0.32	-	96,96,96,96	0
55	MG	AA	3071	1/1	0.91	0.48	-	56,56,56,56	0
55	MG	BA	3318	1/1	0.62	0.33	-	89,89,89,89	0
55	MG	AA	3585	1/1	0.89	0.61	-	91,91,91,91	0
55	MG	CA	1708	1/1	0.95	0.43	-	45,45,45,45	0
55	MG	CA	1839	1/1	0.90	0.21	-	68,68,68,68	0
55	MG	DA	1726	1/1	0.90	0.50	-	79,79,79,79	0
55	MG	BA	3445	1/1	0.80	0.23	-	95,95,95,95	0
55	MG	AA	3268	1/1	0.78	0.49	-	85,85,85,85	0
55	MG	CB	102	1/1	0.32	0.33	-	106,106,106,106	0
55	MG	DC	107	1/1	0.55	0.42	-	105,105,105,105	0
55	MG	CA	1759	1/1	0.65	0.36	-	117,117,117,117	0
55	MG	AA	3393	1/1	0.35	0.58	-	98,98,98,98	0
55	MG	DA	1626	1/1	0.80	0.34	-	104,104,104,104	0
55	MG	AA	3473	1/1	0.80	0.46	-	77,77,77,77	0
55	MG	AA	3598	1/1	0.90	0.29	-	87,87,87,87	0
55	MG	AA	3449	1/1	0.87	0.26	-	63,63,63,63	0
55	MG	AA	3375	1/1	0.76	0.43	-	88,88,88,88	0
55	MG	AA	3197	1/1	0.87	0.40	-	74,74,74,74	0
55	MG	BA	3207	1/1	0.88	0.29	-	46,46,46,46	0
55	MG	CA	1725	1/1	0.62	0.31	-	98,98,98,98	0
55	MG	DA	1776	1/1	0.83	0.27	-	70,70,70,70	0
55	MG	AA	3243	1/1	0.95	0.39	-	51,51,51,51	0
55	MG	BA	3316	1/1	0.88	0.26	-	67,67,67,67	0
55	MG	AA	3595	1/1	0.75	0.36	-	79,79,79,79	0
55	MG	AA	3420	1/1	0.64	0.31	-	88,88,88,88	0
55	MG	AA	3600	1/1	0.96	0.45	-	74,74,74,74	0
55	MG	AA	3009	1/1	0.89	0.33	-	63,63,63,63	0
55	MG	AA	3426	1/1	0.71	0.44	-	80,80,80,80	0
55	MG	AA	3285	1/1	0.95	0.52	-	80,80,80,80	0
55	MG	BA	3510	1/1	0.85	0.26	-	67,67,67,67	0
55	MG	A7	102	1/1	0.93	0.46	-	68,68,68,68	0
55	MG	CA	1659	1/1	0.83	0.30	-	71,71,71,71	0
55	MG	AA	3508	1/1	0.90	0.37	-	101,101,101,101	0
55	MG	BA	3381	1/1	0.87	0.36	-	80,80,80,80	0
55	MG	AA	3209	1/1	0.96	0.37	-	81,81,81,81	0
55	MG	AA	3514	1/1	0.94	0.37	-	67,67,67,67	0
55	MG	BA	3264	1/1	0.98	0.25	-	59,59,59,59	0
55	MG	AA	3145	1/1	0.91	0.63	-	91,91,91,91	0
55	MG	AA	3019	1/1	0.97	0.29	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1749	1/1	0.65	0.25	-	101,101,101,101	0
55	MG	AA	3412	1/1	0.84	0.37	-	110,110,110,110	0
55	MG	BA	3427	1/1	0.78	0.33	-	100,100,100,100	0
55	MG	DA	1731	1/1	0.90	0.43	-	70,70,70,70	0
55	MG	AA	3100	1/1	0.91	0.52	-	67,67,67,67	0
55	MG	BB	211	1/1	0.95	0.31	-	71,71,71,71	0
55	MG	BA	3515	1/1	0.97	0.21	-	59,59,59,59	0
55	MG	DA	1741	1/1	0.90	0.37	-	93,93,93,93	0
55	MG	BA	3249	1/1	0.88	0.21	-	40,40,40,40	0
55	MG	AA	3583	1/1	0.72	0.56	-	103,103,103,103	0
55	MG	CA	1669	1/1	0.93	0.23	-	70,70,70,70	0
55	MG	BA	3457	1/1	0.67	0.24	-	99,99,99,99	0
55	MG	DA	1732	1/1	0.92	0.39	-	94,94,94,94	0
55	MG	BA	3386	1/1	0.84	0.23	-	81,81,81,81	0
55	MG	AA	3280	1/1	0.73	0.34	-	94,94,94,94	0
55	MG	AA	3536	1/1	0.79	0.47	-	92,92,92,92	0
55	MG	BA	3338	1/1	0.85	0.38	-	71,71,71,71	0
55	MG	AA	3121	1/1	0.75	0.71	-	90,90,90,90	0
55	MG	DA	1794	1/1	0.48	0.43	-	91,91,91,91	0
55	MG	AA	3102	1/1	0.88	0.33	-	90,90,90,90	0
55	MG	DA	1725	1/1	0.77	0.39	-	96,96,96,96	0
55	MG	AA	3552	1/1	0.87	0.34	-	83,83,83,83	0
55	MG	BA	3495	1/1	0.82	0.29	-	81,81,81,81	0
55	MG	DA	1660	1/1	0.77	0.24	-	102,102,102,102	0
55	MG	CA	1733	1/1	0.88	0.18	-	107,107,107,107	0
55	MG	CA	1644	1/1	0.80	0.21	-	84,84,84,84	0
55	MG	BA	3075	1/1	0.85	0.17	-	99,99,99,99	0
55	MG	AA	3325	1/1	0.49	0.37	-	100,100,100,100	0
55	MG	CA	1642	1/1	0.98	0.32	-	69,69,69,69	0
55	MG	BA	3030	1/1	0.83	0.20	-	99,99,99,99	0
55	MG	AA	3069	1/1	0.91	0.28	-	64,64,64,64	0
55	MG	BA	3195	1/1	0.81	0.40	-	94,94,94,94	0
55	MG	AA	3445	1/1	0.66	0.30	-	95,95,95,95	0
55	MG	AA	3008	1/1	0.97	0.37	-	44,44,44,44	0
55	MG	AA	3292	1/1	0.82	0.39	-	76,76,76,76	0
55	MG	CB	103	1/1	0.85	0.21	-	110,110,110,110	0
55	MG	BA	3021	1/1	0.82	0.35	-	105,105,105,105	0
55	MG	BA	3149	1/1	0.95	0.23	-	72,72,72,72	0
55	MG	DA	1733	1/1	0.92	0.35	-	98,98,98,98	0
55	MG	AA	3033	1/1	0.94	0.33	-	49,49,49,49	0
55	MG	AA	3156	1/1	0.53	0.46	-	94,94,94,94	0
55	MG	BA	3421	1/1	0.71	0.14	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CC	104	1/1	0.90	0.18	-	97,97,97,97	0
55	MG	BA	3399	1/1	0.44	0.27	-	104,104,104,104	0
55	MG	AA	3199	1/1	0.92	0.48	-	46,46,46,46	0
55	MG	BA	3359	1/1	0.85	0.46	-	98,98,98,98	0
55	MG	AA	3110	1/1	0.99	0.16	-	40,40,40,40	0
55	MG	AA	3362	1/1	0.65	0.36	-	89,89,89,89	0
55	MG	BA	3204	1/1	0.75	0.30	-	74,74,74,74	0
55	MG	DA	1712	1/1	0.73	0.43	-	100,100,100,100	0
55	MG	AD	301	1/1	0.83	0.29	-	99,99,99,99	0
55	MG	DA	1688	1/1	0.67	0.27	-	99,99,99,99	0
55	MG	BA	3004	1/1	0.63	0.27	-	105,105,105,105	0
55	MG	BA	3326	1/1	0.81	0.23	-	84,84,84,84	0
55	MG	AA	3500	1/1	0.81	0.40	-	103,103,103,103	0
55	MG	CA	1769	1/1	0.90	0.09	-	79,79,79,79	0
55	MG	CA	1716	1/1	0.57	0.30	-	117,117,117,117	0
55	MG	AA	3200	1/1	0.89	0.35	-	71,71,71,71	0
55	MG	AA	3240	1/1	0.91	0.32	-	80,80,80,80	0
55	MG	BA	3162	1/1	0.83	0.15	-	92,92,92,92	0
55	MG	CA	1813	1/1	0.69	0.59	-	94,94,94,94	0
55	MG	CA	1830	1/1	0.90	0.33	-	94,94,94,94	0
55	MG	DA	1651	1/1	0.89	0.27	-	72,72,72,72	0
55	MG	DA	1716	1/1	0.88	0.42	-	105,105,105,105	0
55	MG	DA	1691	1/1	0.93	0.49	-	82,82,82,82	0
55	MG	BA	3188	1/1	0.81	0.30	-	85,85,85,85	0
55	MG	AA	3105	1/1	0.90	0.43	-	61,61,61,61	0
55	MG	BA	3374	1/1	0.75	0.52	-	86,86,86,86	0
55	MG	AA	3029	1/1	0.96	0.20	-	46,46,46,46	0
55	MG	AA	3309	1/1	0.71	0.70	-	90,90,90,90	0
55	MG	AA	3563	1/1	0.93	0.40	-	52,52,52,52	0
55	MG	BA	3471	1/1	0.21	0.38	-	96,96,96,96	0
55	MG	BA	3119	1/1	0.78	0.20	-	79,79,79,79	0
55	MG	BA	3336	1/1	0.50	0.34	-	97,97,97,97	0
55	MG	BA	3171	1/1	0.94	0.24	-	63,63,63,63	0
55	MG	BA	3071	1/1	0.94	0.29	-	78,78,78,78	0
55	MG	BB	210	1/1	0.59	0.38	-	96,96,96,96	0
55	MG	AA	3579	1/1	0.98	0.29	-	39,39,39,39	0
55	MG	AA	3077	1/1	0.70	0.49	-	103,103,103,103	0
55	MG	CQ	102	1/1	0.72	0.25	-	97,97,97,97	0
55	MG	AA	3526	1/1	0.90	0.42	-	90,90,90,90	0
55	MG	DA	1772	1/1	0.83	0.32	-	68,68,68,68	0
55	MG	AA	3516	1/1	0.97	0.32	-	76,76,76,76	0
55	MG	AA	3278	1/1	0.60	0.71	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3533	1/1	0.91	0.20	-	67,67,67,67	0
55	MG	BA	3159	1/1	0.96	0.23	-	83,83,83,83	0
55	MG	DA	1631	1/1	0.79	0.20	-	102,102,102,102	0
55	MG	BA	3031	1/1	0.83	0.32	-	60,60,60,60	0
55	MG	DB	102	1/1	0.88	0.11	-	107,107,107,107	0
55	MG	BA	3507	1/1	0.45	0.34	-	102,102,102,102	0
55	MG	BA	3258	1/1	0.79	0.34	-	64,64,64,64	0
55	MG	AA	3048	1/1	0.83	0.31	-	86,86,86,86	0
55	MG	AA	3221	1/1	0.87	0.41	-	47,47,47,47	0
55	MG	BA	3493	1/1	0.94	0.27	-	39,39,39,39	0
55	MG	BA	3013	1/1	0.92	0.26	-	74,74,74,74	0
55	MG	AA	3612	1/1	0.47	0.69	-	92,92,92,92	0
55	MG	AA	3049	1/1	0.96	0.36	-	80,80,80,80	0
55	MG	CA	1805	1/1	0.78	0.37	-	75,75,75,75	0
55	MG	AA	3003	1/1	0.98	0.48	-	64,64,64,64	0
55	MG	BA	3008	1/1	0.64	0.32	-	89,89,89,89	0
55	MG	CA	1638	1/1	0.93	0.42	-	108,108,108,108	0
55	MG	CA	1749	1/1	0.95	0.32	-	62,62,62,62	0
55	MG	AA	3605	1/1	0.84	0.58	-	72,72,72,72	0
55	MG	AA	3346	1/1	0.82	0.43	-	88,88,88,88	0
55	MG	BA	3270	1/1	0.78	0.28	-	81,81,81,81	0
55	MG	BA	3373	1/1	0.86	0.40	-	88,88,88,88	0
55	MG	AA	3374	1/1	0.69	0.41	-	74,74,74,74	0
55	MG	CA	1739	1/1	0.81	0.56	-	86,86,86,86	0
55	MG	CA	1828	1/1	0.61	0.23	-	98,98,98,98	0
55	MG	BA	3213	1/1	0.90	0.26	-	75,75,75,75	0
55	MG	BA	3470	1/1	0.88	0.28	-	81,81,81,81	0
55	MG	BA	3199	1/1	0.91	0.37	-	76,76,76,76	0
55	MG	AA	3198	1/1	0.83	0.65	-	74,74,74,74	0
55	MG	BA	3173	1/1	0.94	0.39	-	50,50,50,50	0
55	MG	BA	3048	1/1	0.89	0.17	-	74,74,74,74	0
55	MG	BA	3243	1/1	0.90	0.26	-	65,65,65,65	0
55	MG	DA	1641	1/1	0.30	0.31	-	95,95,95,95	0
55	MG	BA	3214	1/1	0.93	0.27	-	77,77,77,77	0
55	MG	CA	1811	1/1	0.93	0.33	-	95,95,95,95	0
55	MG	AA	3114	1/1	0.94	0.50	-	56,56,56,56	0
55	MG	BA	3409	1/1	0.96	0.30	-	71,71,71,71	0
55	MG	AA	3546	1/1	0.94	0.25	-	74,74,74,74	0
55	MG	DA	1681	1/1	0.91	0.22	-	106,106,106,106	0
55	MG	AA	3483	1/1	0.88	0.17	-	87,87,87,87	0
55	MG	BA	3521	1/1	0.52	0.33	-	79,79,79,79	0
55	MG	CA	1802	1/1	0.89	0.23	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3528	1/1	0.85	0.20	-	98,98,98,98	0
55	MG	AA	3443	1/1	0.66	0.34	-	90,90,90,90	0
55	MG	AB	211	1/1	0.81	0.53	-	100,100,100,100	0
55	MG	DC	108	1/1	0.81	0.17	-	102,102,102,102	0
55	MG	DA	1774	1/1	0.51	0.33	-	103,103,103,103	0
55	MG	CA	1793	1/1	0.86	0.15	-	96,96,96,96	0
55	MG	AA	3566	1/1	0.97	0.29	-	27,27,27,27	0
55	MG	BA	3467	1/1	0.67	0.40	-	93,93,93,93	0
55	MG	BA	3104	1/1	0.52	0.35	-	115,115,115,115	0
55	MG	AA	3452	1/1	0.79	0.43	-	76,76,76,76	0
55	MG	AA	3189	1/1	0.85	0.38	-	90,90,90,90	0
55	MG	BA	3064	1/1	0.72	0.24	-	103,103,103,103	0
55	MG	AA	3401	1/1	0.94	0.49	-	93,93,93,93	0
55	MG	AA	3505	1/1	0.89	0.57	-	85,85,85,85	0
55	MG	BA	3307	1/1	0.92	0.35	-	106,106,106,106	0
55	MG	BA	3206	1/1	0.93	0.26	-	98,98,98,98	0
55	MG	CA	1668	1/1	0.82	0.53	-	79,79,79,79	0
55	MG	BA	3424	1/1	0.60	0.63	-	86,86,86,86	0
55	MG	AA	3252	1/1	0.86	0.49	-	94,94,94,94	0
55	MG	AA	3498	1/1	0.52	0.50	-	95,95,95,95	0
55	MG	BA	3273	1/1	0.81	0.34	-	102,102,102,102	0
55	MG	AA	3364	1/1	0.78	0.34	-	69,69,69,69	0
55	MG	CA	1721	1/1	0.89	0.28	-	89,89,89,89	0
55	MG	AA	3520	1/1	0.94	0.27	-	68,68,68,68	0
55	MG	CA	1837	1/1	0.90	0.25	-	88,88,88,88	0
55	MG	DA	1647	1/1	0.99	0.18	-	71,71,71,71	0
55	MG	CA	1829	1/1	0.84	0.22	-	102,102,102,102	0
55	MG	BA	3268	1/1	0.99	0.15	-	59,59,59,59	0
55	MG	BA	3352	1/1	0.96	0.42	-	102,102,102,102	0
55	MG	CA	1647	1/1	0.69	0.21	-	92,92,92,92	0
55	MG	CA	1698	1/1	0.84	0.26	-	89,89,89,89	0
55	MG	CA	1614	1/1	0.92	0.32	-	101,101,101,101	0
55	MG	AA	3250	1/1	0.81	0.33	-	99,99,99,99	0
55	MG	AA	3115	1/1	0.96	0.55	-	70,70,70,70	0
55	MG	AA	3224	1/1	-0.03	0.45	-	93,93,93,93	0
55	MG	CC	103	1/1	0.91	0.39	-	104,104,104,104	0
55	MG	AA	3279	1/1	0.32	0.32	-	89,89,89,89	0
55	MG	CA	1624	1/1	0.91	0.19	-	97,97,97,97	0
55	MG	C1	101	1/1	0.62	0.49	-	98,98,98,98	0
55	MG	CA	1808	1/1	0.78	0.26	-	67,67,67,67	0
55	MG	BA	3339	1/1	0.66	0.20	-	90,90,90,90	0
55	MG	BA	3172	1/1	0.82	0.31	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3486	1/1	0.66	0.35	-	90,90,90,90	0
55	MG	BA	3443	1/1	0.85	0.23	-	92,92,92,92	0
55	MG	DA	1698	1/1	0.77	0.48	-	103,103,103,103	0
55	MG	AA	3465	1/1	0.84	0.32	-	71,71,71,71	0
55	MG	B3	101	1/1	0.86	0.21	-	76,76,76,76	0
55	MG	AA	3357	1/1	0.63	0.58	-	99,99,99,99	0
55	MG	AA	3065	1/1	0.89	0.42	-	88,88,88,88	0
55	MG	AA	3447	1/1	0.91	0.59	-	75,75,75,75	0
55	MG	AA	3103	1/1	0.91	0.39	-	97,97,97,97	0
55	MG	AA	3299	1/1	0.90	0.34	-	79,79,79,79	0
55	MG	AA	3490	1/1	0.71	0.58	-	97,97,97,97	0
55	MG	CA	1800	1/1	0.62	0.17	-	104,104,104,104	0
55	MG	CA	1818	1/1	0.89	0.25	-	89,89,89,89	0
55	MG	AA	3411	1/1	0.83	0.50	-	85,85,85,85	0
55	MG	DA	1778	1/1	0.72	0.25	-	118,118,118,118	0
55	MG	BA	3027	1/1	0.36	0.24	-	107,107,107,107	0
55	MG	DA	1634	1/1	0.91	0.24	-	77,77,77,77	0
55	MG	CA	1630	1/1	0.81	0.28	-	112,112,112,112	0
55	MG	DA	1630	1/1	0.87	0.26	-	102,102,102,102	0
55	MG	AA	3290	1/1	0.87	0.42	-	72,72,72,72	0
55	MG	CA	1755	1/1	0.84	0.26	-	81,81,81,81	0
55	MG	AA	3237	1/1	0.81	0.45	-	83,83,83,83	0
55	MG	BA	3425	1/1	0.94	0.49	-	85,85,85,85	0
55	MG	DA	1706	1/1	0.96	0.61	-	90,90,90,90	0
55	MG	CA	1771	1/1	0.82	0.22	-	102,102,102,102	0
55	MG	AA	3615	1/1	0.83	0.32	-	102,102,102,102	0
55	MG	AA	3365	1/1	0.77	0.38	-	74,74,74,74	0
55	MG	DA	1665	1/1	0.92	0.37	-	82,82,82,82	0
55	MG	BA	3117	1/1	0.76	0.39	-	91,91,91,91	0
55	MG	AA	3311	1/1	0.91	0.57	-	68,68,68,68	0
55	MG	AA	3256	1/1	0.75	0.39	-	66,66,66,66	0
55	MG	BA	3511	1/1	0.95	0.21	-	68,68,68,68	0
55	MG	AA	3479	1/1	0.72	0.21	-	94,94,94,94	0
55	MG	AA	3453	1/1	0.86	0.30	-	95,95,95,95	0
55	MG	AA	3618	1/1	0.84	0.54	-	97,97,97,97	0
55	MG	AA	3560	1/1	0.67	0.35	-	87,87,87,87	0
55	MG	DA	1783	1/1	0.88	0.33	-	86,86,86,86	0
55	MG	BA	3479	1/1	0.82	0.35	-	95,95,95,95	0
55	MG	AA	3297	1/1	0.88	0.39	-	69,69,69,69	0
55	MG	AA	3502	1/1	0.79	0.66	-	96,96,96,96	0
55	MG	AA	3522	1/1	0.50	0.55	-	97,97,97,97	0
55	MG	CA	1660	1/1	0.98	0.38	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3293	1/1	0.69	0.22	-	96,96,96,96	0
55	MG	AA	3013	1/1	0.94	0.34	-	44,44,44,44	0
55	MG	BA	3205	1/1	0.86	0.24	-	70,70,70,70	0
55	MG	BA	3402	1/1	0.75	0.32	-	95,95,95,95	0
55	MG	DA	1659	1/1	0.89	0.12	-	80,80,80,80	0
55	MG	BA	3455	1/1	0.83	0.18	-	92,92,92,92	0
55	MG	AA	3097	1/1	0.66	0.59	-	106,106,106,106	0
55	MG	DS	101	1/1	0.76	0.48	-	87,87,87,87	0
55	MG	BA	3111	1/1	0.77	0.20	-	82,82,82,82	0
55	MG	AA	3418	1/1	0.76	0.30	-	91,91,91,91	0
55	MG	BA	3418	1/1	0.94	0.17	-	73,73,73,73	0
55	MG	DA	1614	1/1	0.81	0.54	-	93,93,93,93	0
55	MG	CB	104	1/1	0.54	0.36	-	101,101,101,101	0
55	MG	DA	1669	1/1	0.87	0.46	-	68,68,68,68	0
55	MG	AA	3385	1/1	0.23	0.54	-	88,88,88,88	0
55	MG	AA	3143	1/1	0.95	0.38	-	35,35,35,35	0
55	MG	BA	3240	1/1	0.90	0.33	-	72,72,72,72	0
55	MG	A5	101	1/1	0.92	0.22	-	51,51,51,51	0
55	MG	BA	3049	1/1	0.89	0.23	-	86,86,86,86	0
55	MG	AE	302	1/1	0.97	0.41	-	45,45,45,45	0
55	MG	DA	1707	1/1	0.86	0.25	-	95,95,95,95	0
55	MG	AA	3604	1/1	0.56	0.46	-	93,93,93,93	0
55	MG	AA	3127	1/1	0.97	0.38	-	53,53,53,53	0
55	MG	BA	3485	1/1	0.97	0.28	-	46,46,46,46	0
55	MG	CC	101	1/1	0.72	0.30	-	108,108,108,108	0
55	MG	CA	1689	1/1	0.66	0.22	-	115,115,115,115	0
55	MG	AA	3495	1/1	0.85	0.60	-	90,90,90,90	0
55	MG	BA	3057	1/1	0.73	0.20	-	97,97,97,97	0
55	MG	AA	3493	1/1	0.77	0.33	-	92,92,92,92	0
55	MG	AA	3067	1/1	0.71	0.52	-	108,108,108,108	0
55	MG	AA	3238	1/1	0.83	0.52	-	82,82,82,82	0
55	MG	AA	3507	1/1	0.83	0.49	-	99,99,99,99	0
55	MG	AA	3166	1/1	0.95	0.38	-	53,53,53,53	0
55	MG	DA	1742	1/1	0.96	0.26	-	82,82,82,82	0
55	MG	AA	3230	1/1	0.97	0.10	-	34,34,34,34	0
55	MG	BA	3126	1/1	0.95	0.21	-	51,51,51,51	0
55	MG	CA	1816	1/1	0.71	0.20	-	95,95,95,95	0
55	MG	AA	3383	1/1	0.92	0.30	-	85,85,85,85	0
55	MG	CA	1748	1/1	0.78	0.38	-	87,87,87,87	0
55	MG	AA	3210	1/1	0.91	0.43	-	72,72,72,72	0
55	MG	BA	3442	1/1	0.75	0.37	-	91,91,91,91	0
55	MG	AA	3244	1/1	0.94	0.44	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3184	1/1	0.81	0.39	-	94,94,94,94	0
55	MG	BA	3011	1/1	0.97	0.29	-	65,65,65,65	0
55	MG	AA	3339	1/1	0.95	0.35	-	85,85,85,85	0
55	MG	BA	3405	1/1	0.81	0.23	-	87,87,87,87	0
55	MG	BA	3289	1/1	0.77	0.44	-	70,70,70,70	0
55	MG	CA	1693	1/1	0.17	0.37	-	102,102,102,102	0
55	MG	CA	1807	1/1	0.93	0.38	-	64,64,64,64	0
55	MG	CG	301	1/1	0.50	0.49	-	94,94,94,94	0
55	MG	AA	3515	1/1	0.81	0.37	-	77,77,77,77	0
55	MG	AA	3005	1/1	0.96	0.30	-	25,25,25,25	0
55	MG	BA	3462	1/1	0.89	0.11	-	123,123,123,123	0
55	MG	CA	1652	1/1	0.75	0.30	-	93,93,93,93	0
55	MG	CA	1758	1/1	0.50	0.40	-	97,97,97,97	0
55	MG	AA	3441	1/1	0.53	0.60	-	101,101,101,101	0
55	MG	AA	3422	1/1	0.90	0.47	-	106,106,106,106	0
55	MG	AA	3028	1/1	0.96	0.38	-	54,54,54,54	0
55	MG	DA	1797	1/1	0.86	0.34	-	85,85,85,85	0
55	MG	CA	1745	1/1	0.51	0.37	-	95,95,95,95	0
55	MG	AA	3023	1/1	0.98	0.55	-	56,56,56,56	0
55	MG	BA	3193	1/1	0.53	0.34	-	102,102,102,102	0
55	MG	AA	3621	1/1	0.94	0.46	-	91,91,91,91	0
55	MG	BA	3395	1/1	0.41	0.21	-	89,89,89,89	0
55	MG	BA	3340	1/1	0.89	0.16	-	84,84,84,84	0
55	MG	CA	1685	1/1	0.74	0.27	-	103,103,103,103	0
55	MG	CA	1643	1/1	0.93	0.39	-	91,91,91,91	0
55	MG	AA	3414	1/1	0.88	0.48	-	94,94,94,94	0
55	MG	AA	3063	1/1	0.87	0.30	-	85,85,85,85	0
55	MG	BA	3039	1/1	0.72	0.32	-	85,85,85,85	0
55	MG	BA	3084	1/1	0.85	0.15	-	99,99,99,99	0
55	MG	AA	3317	1/1	0.84	0.41	-	85,85,85,85	0
55	MG	AB	208	1/1	0.69	0.33	-	92,92,92,92	0
55	MG	CA	1694	1/1	0.12	0.60	-	104,104,104,104	0
55	MG	AA	3573	1/1	0.96	0.34	-	31,31,31,31	0
55	MG	DA	1602	1/1	0.76	0.33	-	85,85,85,85	0
55	MG	BA	3025	1/1	0.87	0.13	-	80,80,80,80	0
55	MG	AA	3542	1/1	0.80	0.37	-	93,93,93,93	0
55	MG	AA	3050	1/1	0.90	0.76	-	108,108,108,108	0
55	MG	CA	1740	1/1	0.93	0.38	-	72,72,72,72	0
55	MG	BA	3392	1/1	0.66	0.21	-	85,85,85,85	0
55	MG	CA	1757	1/1	0.55	0.43	-	92,92,92,92	0
55	MG	BA	3441	1/1	0.68	0.34	-	93,93,93,93	0
55	MG	CA	1688	1/1	0.85	0.23	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3043	1/1	0.78	0.22	-	108,108,108,108	0
55	MG	BA	3305	1/1	0.76	0.33	-	76,76,76,76	0
55	MG	BA	3343	1/1	0.84	0.24	-	75,75,75,75	0
55	MG	DA	1757	1/1	0.59	0.32	-	104,104,104,104	0
55	MG	AA	3371	1/1	0.79	0.43	-	89,89,89,89	0
55	MG	CA	1776	1/1	0.52	0.49	-	79,79,79,79	0
55	MG	AA	3035	1/1	0.99	0.30	-	45,45,45,45	0
55	MG	BA	3437	1/1	0.94	0.35	-	73,73,73,73	0
55	MG	BA	3065	1/1	0.73	0.44	-	101,101,101,101	0
55	MG	AA	3161	1/1	0.96	0.33	-	42,42,42,42	0
55	MG	BA	3478	1/1	0.57	0.39	-	92,92,92,92	0
55	MG	AA	3122	1/1	0.89	0.20	-	84,84,84,84	0
55	MG	DA	1694	1/1	0.90	0.60	-	84,84,84,84	0
55	MG	AB	209	1/1	0.79	0.50	-	108,108,108,108	0
55	MG	AA	3327	1/1	0.98	0.52	-	84,84,84,84	0
55	MG	BA	3450	1/1	0.87	0.31	-	99,99,99,99	0
55	MG	DA	1692	1/1	0.93	0.40	-	81,81,81,81	0
55	MG	AA	3416	1/1	0.41	0.45	-	95,95,95,95	0
55	MG	DA	1612	1/1	0.95	0.14	-	73,73,73,73	0
55	MG	BB	204	1/1	0.86	0.33	-	90,90,90,90	0
55	MG	BA	3060	1/1	0.95	0.17	-	51,51,51,51	0
55	MG	AA	3334	1/1	0.76	0.70	-	76,76,76,76	0
55	MG	AA	3597	1/1	0.96	0.17	-	91,91,91,91	0
55	MG	AA	3434	1/1	0.96	0.50	-	44,44,44,44	0
55	MG	BA	3096	1/1	0.88	0.19	-	89,89,89,89	0
55	MG	AA	3503	1/1	0.81	0.47	-	81,81,81,81	0
55	MG	BA	3319	1/1	0.95	0.43	-	68,68,68,68	0
55	MG	BA	3165	1/1	0.77	0.34	-	42,42,42,42	0
55	MG	AA	3446	1/1	0.55	0.40	-	93,93,93,93	0
55	MG	CA	1705	1/1	0.91	0.16	-	95,95,95,95	0
55	MG	BA	3382	1/1	0.73	0.24	-	89,89,89,89	0
55	MG	AA	3555	1/1	0.89	0.19	-	67,67,67,67	0
55	MG	AA	3091	1/1	0.88	0.43	-	78,78,78,78	0
55	MG	CA	1781	1/1	0.94	0.38	-	62,62,62,62	0
55	MG	AA	3348	1/1	0.86	0.25	-	94,94,94,94	0
55	MG	BA	3299	1/1	0.64	0.21	-	82,82,82,82	0
55	MG	CA	1699	1/1	0.94	0.11	-	63,63,63,63	0
55	MG	BA	3314	1/1	0.95	0.29	-	71,71,71,71	0
55	MG	AA	3373	1/1	0.72	0.44	-	106,106,106,106	0
55	MG	BA	3348	1/1	0.80	0.32	-	98,98,98,98	0
55	MG	AA	3436	1/1	0.98	0.46	-	66,66,66,66	0
55	MG	BA	3463	1/1	0.37	0.29	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1605	1/1	0.91	0.43	-	82,82,82,82	0
55	MG	CQ	101	1/1	0.89	0.18	-	102,102,102,102	0
55	MG	CA	1787	1/1	0.71	0.29	-	100,100,100,100	0
55	MG	DA	1730	1/1	0.83	0.42	-	102,102,102,102	0
55	MG	AA	3358	1/1	0.77	0.68	-	89,89,89,89	0
55	MG	AA	3270	1/1	0.68	0.30	-	69,69,69,69	0
55	MG	BA	3397	1/1	0.62	0.32	-	96,96,96,96	0
55	MG	DA	1711	1/1	0.68	0.41	-	89,89,89,89	0
55	MG	AA	3458	1/1	0.88	0.26	-	70,70,70,70	0
55	MG	BA	3391	1/1	0.76	0.29	-	95,95,95,95	0
55	MG	CA	1713	1/1	0.92	0.29	-	83,83,83,83	0
55	MG	DA	1717	1/1	0.71	0.19	-	103,103,103,103	0
55	MG	BA	3201	1/1	0.86	0.22	-	94,94,94,94	0
55	MG	AA	3011	1/1	0.95	0.37	-	37,37,37,37	0
55	MG	BA	3302	1/1	0.86	0.36	-	75,75,75,75	0
55	MG	CA	1683	1/1	0.76	0.32	-	104,104,104,104	0
55	MG	DA	1745	1/1	0.72	0.24	-	106,106,106,106	0
55	MG	BA	3093	1/1	0.79	0.17	-	78,78,78,78	0
55	MG	BA	3210	1/1	0.98	0.37	-	55,55,55,55	0
55	MG	AA	3129	1/1	0.92	0.45	-	73,73,73,73	0
55	MG	CA	1687	1/1	0.80	0.29	-	78,78,78,78	0
55	MG	A2	201	1/1	0.82	0.50	-	101,101,101,101	0
55	MG	AA	3456	1/1	0.48	0.42	-	91,91,91,91	0
55	MG	AA	3366	1/1	0.50	0.55	-	92,92,92,92	0
55	MG	AA	3251	1/1	0.82	0.34	-	68,68,68,68	0
55	MG	AA	3118	1/1	0.64	0.41	-	87,87,87,87	0
55	MG	AA	3131	1/1	0.83	0.20	-	90,90,90,90	0
55	MG	DA	1687	1/1	0.91	0.39	-	72,72,72,72	0
55	MG	AA	3543	1/1	0.90	0.45	-	46,46,46,46	0
55	MG	AA	3090	1/1	0.95	0.30	-	45,45,45,45	0
55	MG	AB	205	1/1	0.91	0.38	-	83,83,83,83	0
55	MG	CA	1770	1/1	0.54	0.32	-	90,90,90,90	0
55	MG	AA	3496	1/1	0.85	0.49	-	87,87,87,87	0
55	MG	A7	101	1/1	0.87	0.38	-	60,60,60,60	0
55	MG	BA	3101	1/1	0.65	0.25	-	94,94,94,94	0
55	MG	CA	1664	1/1	0.97	0.13	-	47,47,47,47	0
55	MG	AA	3227	1/1	0.80	0.63	-	90,90,90,90	0
55	MG	AA	3073	1/1	0.52	0.57	-	97,97,97,97	0
55	MG	BA	3257	1/1	0.89	0.56	-	86,86,86,86	0
55	MG	BA	3459	1/1	0.60	0.22	-	115,115,115,115	0
55	MG	AA	3504	1/1	0.92	0.41	-	80,80,80,80	0
55	MG	BA	3073	1/1	0.67	0.41	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1625	1/1	0.87	0.18	-	71,71,71,71	0
55	MG	CA	1695	1/1	0.87	0.36	-	90,90,90,90	0
55	MG	DA	1695	1/1	0.86	0.43	-	88,88,88,88	0
55	MG	BB	213	1/1	0.77	0.45	-	97,97,97,97	0
55	MG	AA	3501	1/1	0.54	0.44	-	99,99,99,99	0
55	MG	AA	3470	1/1	0.84	0.52	-	96,96,96,96	0
55	MG	AA	3424	1/1	0.85	0.48	-	54,54,54,54	0
55	MG	CA	1613	1/1	0.53	0.17	-	94,94,94,94	0
55	MG	A3	101	1/1	0.71	0.42	-	74,74,74,74	0
55	MG	DA	1775	1/1	0.85	0.41	-	102,102,102,102	0
55	MG	BA	3005	1/1	0.87	0.29	-	70,70,70,70	0
55	MG	DA	1671	1/1	0.84	0.41	-	77,77,77,77	0
55	MG	AA	3171	1/1	0.76	0.33	-	84,84,84,84	0
55	MG	BA	3371	1/1	0.23	0.16	-	129,129,129,129	0
55	MG	BA	3088	1/1	0.78	0.20	-	94,94,94,94	0
55	MG	BA	3079	1/1	0.84	0.18	-	82,82,82,82	0
55	MG	BA	3351	1/1	0.87	0.47	-	81,81,81,81	0
55	MG	CA	1838	1/1	0.89	0.14	-	103,103,103,103	0
55	MG	CA	1727	1/1	0.54	0.27	-	103,103,103,103	0
55	MG	BA	3130	1/1	0.93	0.25	-	44,44,44,44	0
55	MG	AA	3376	1/1	0.75	0.62	-	85,85,85,85	0
55	MG	BA	3341	1/1	0.81	0.43	-	82,82,82,82	0
55	MG	BA	3308	1/1	0.86	0.22	-	108,108,108,108	0
55	MG	DA	1618	1/1	0.68	0.31	-	104,104,104,104	0
55	MG	AA	3607	1/1	0.97	0.36	-	44,44,44,44	0
55	MG	BA	3028	1/1	0.95	0.50	-	85,85,85,85	0
55	MG	BA	3502	1/1	0.83	0.19	-	91,91,91,91	0
55	MG	DA	1800	1/1	0.65	0.33	-	99,99,99,99	0
55	MG	AA	3380	1/1	0.91	0.20	-	96,96,96,96	0
55	MG	AA	3300	1/1	0.91	0.44	-	81,81,81,81	0
55	MG	AA	3289	1/1	0.83	0.55	-	84,84,84,84	0
55	MG	AA	3152	1/1	0.94	0.54	-	58,58,58,58	0
55	MG	AA	3208	1/1	0.90	0.23	-	44,44,44,44	0
55	MG	DA	1666	1/1	0.92	0.35	-	115,115,115,115	0
55	MG	AA	3596	1/1	0.90	0.49	-	93,93,93,93	0
55	MG	AA	3587	1/1	0.85	0.55	-	77,77,77,77	0
55	MG	CA	1726	1/1	0.79	0.26	-	103,103,103,103	0
55	MG	BA	3074	1/1	0.80	0.20	-	83,83,83,83	0
55	MG	DA	1603	1/1	0.84	0.44	-	89,89,89,89	0
55	MG	DA	1714	1/1	0.65	0.29	-	105,105,105,105	0
55	MG	AB	216	1/1	0.82	0.35	-	106,106,106,106	0
55	MG	BB	208	1/1	0.31	0.42	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3326	1/1	0.92	0.31	-	64,64,64,64	0
55	MG	AA	3582	1/1	0.88	0.31	-	44,44,44,44	0
55	MG	BA	3022	1/1	0.94	0.23	-	75,75,75,75	0
55	MG	CA	1788	1/1	0.61	0.15	-	105,105,105,105	0
55	MG	CA	1707	1/1	0.85	0.38	-	78,78,78,78	0
55	MG	CA	1681	1/1	0.68	0.35	-	80,80,80,80	0
55	MG	BA	3330	1/1	0.84	0.39	-	91,91,91,91	0
55	MG	BA	3251	1/1	0.93	0.24	-	81,81,81,81	0
55	MG	AA	3539	1/1	0.98	0.30	-	49,49,49,49	0
55	MG	DA	1633	1/1	0.80	0.32	-	88,88,88,88	0
55	MG	AA	3372	1/1	0.65	0.28	-	87,87,87,87	0
55	MG	AA	3060	1/1	0.67	0.43	-	84,84,84,84	0
55	MG	DA	1623	1/1	0.73	0.38	-	96,96,96,96	0
55	MG	AA	3474	1/1	0.91	0.34	-	65,65,65,65	0
55	MG	BA	3047	1/1	0.79	0.18	-	80,80,80,80	0
55	MG	CC	102	1/1	0.83	0.29	-	69,69,69,69	0
55	MG	AA	3340	1/1	0.68	0.38	-	83,83,83,83	0
55	MG	AA	3147	1/1	0.93	0.54	-	89,89,89,89	0
55	MG	AA	3075	1/1	0.59	0.61	-	85,85,85,85	0
55	MG	BA	3477	1/1	0.72	0.25	-	94,94,94,94	0
55	MG	AA	3477	1/1	0.95	0.60	-	86,86,86,86	0
55	MG	AA	3157	1/1	0.94	0.45	-	39,39,39,39	0
55	MG	DA	1601	1/1	0.83	0.16	-	107,107,107,107	0
55	MG	BA	3089	1/1	0.74	0.27	-	83,83,83,83	0
55	MG	AA	3562	1/1	0.86	0.30	-	82,82,82,82	0
55	MG	BA	3175	1/1	0.63	0.22	-	100,100,100,100	0
55	MG	AA	3148	1/1	0.54	0.59	-	83,83,83,83	0
55	MG	BA	3072	1/1	0.87	0.26	-	104,104,104,104	0
55	MG	AA	3389	1/1	0.94	0.56	-	72,72,72,72	0
55	MG	AA	3601	1/1	0.72	0.23	-	86,86,86,86	0
55	MG	CA	1814	1/1	0.84	0.28	-	86,86,86,86	0
55	MG	DA	1764	1/1	0.65	0.41	-	85,85,85,85	0
55	MG	CB	105	1/1	0.78	0.12	-	113,113,113,113	0
55	MG	AA	3312	1/1	0.95	0.46	-	76,76,76,76	0
55	MG	AA	3294	1/1	0.78	0.77	-	93,93,93,93	0
55	MG	CB	101	1/1	0.71	0.32	-	108,108,108,108	0
55	MG	BA	3456	1/1	0.94	0.23	-	88,88,88,88	0
55	MG	DA	1729	1/1	0.94	0.46	-	84,84,84,84	0
55	MG	BA	3292	1/1	0.94	0.36	-	51,51,51,51	0
55	MG	CA	1603	1/1	0.98	0.20	-	73,73,73,73	0
55	MG	BA	3300	1/1	0.95	0.38	-	56,56,56,56	0
55	MG	AA	3142	1/1	0.96	0.22	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3354	1/1	0.57	0.38	-	84,84,84,84	0
55	MG	CA	1799	1/1	0.77	0.38	-	95,95,95,95	0
55	MG	CA	1673	1/1	0.94	0.40	-	76,76,76,76	0
55	MG	CA	1686	1/1	0.89	0.37	-	86,86,86,86	0
55	MG	AA	3337	1/1	0.88	0.45	-	99,99,99,99	0
55	MG	CA	1615	1/1	0.65	0.32	-	104,104,104,104	0
55	MG	AA	3286	1/1	0.57	0.46	-	86,86,86,86	0
55	MG	AA	3025	1/1	0.97	0.39	-	40,40,40,40	0
55	MG	BA	3394	1/1	0.68	0.43	-	88,88,88,88	0
55	MG	BA	3475	1/1	0.60	0.32	-	90,90,90,90	0
55	MG	BA	3099	1/1	0.74	0.20	-	98,98,98,98	0
55	MG	AA	3130	1/1	0.98	0.22	-	67,67,67,67	0
55	MG	AA	3066	1/1	0.95	0.53	-	48,48,48,48	0
55	MG	BA	3003	1/1	0.54	0.50	-	99,99,99,99	0
55	MG	CA	1796	1/1	0.97	0.44	-	82,82,82,82	0
55	MG	DA	1613	1/1	0.67	0.42	-	88,88,88,88	0
55	MG	AA	3478	1/1	0.90	0.31	-	75,75,75,75	0
55	MG	AA	3080	1/1	0.50	0.57	-	104,104,104,104	0
55	MG	BB	215	1/1	0.69	0.17	-	101,101,101,101	0
55	MG	BA	3108	1/1	0.78	0.40	-	99,99,99,99	0
55	MG	AA	3454	1/1	0.89	0.56	-	94,94,94,94	0
55	MG	AA	3158	1/1	0.83	0.35	-	68,68,68,68	0
55	MG	AA	3611	1/1	0.87	0.26	-	100,100,100,100	0
55	MG	BA	3414	1/1	0.87	0.18	-	92,92,92,92	0
55	MG	BA	3194	1/1	0.94	0.38	-	70,70,70,70	0
55	MG	AA	3492	1/1	0.66	0.32	-	94,94,94,94	0
55	MG	AA	3163	1/1	0.80	0.31	-	55,55,55,55	0
55	MG	AA	3353	1/1	0.77	0.52	-	86,86,86,86	0
55	MG	BA	3472	1/1	0.36	0.44	-	83,83,83,83	0
55	MG	AA	3231	1/1	0.76	0.54	-	106,106,106,106	0
55	MG	BA	3244	1/1	0.95	0.34	-	54,54,54,54	0
55	MG	BA	3438	1/1	0.84	0.23	-	88,88,88,88	0
55	MG	AA	3225	1/1	0.79	0.44	-	95,95,95,95	0
55	MG	AA	3553	1/1	0.89	0.35	-	87,87,87,87	0
55	MG	BA	3078	1/1	0.28	0.23	-	95,95,95,95	0
55	MG	AA	3140	1/1	0.89	0.39	-	67,67,67,67	0
55	MG	CA	1825	1/1	0.96	0.07	-	114,114,114,114	0
55	MG	AA	3180	1/1	0.93	0.52	-	64,64,64,64	0
55	MG	BA	3132	1/1	0.99	0.25	-	54,54,54,54	0
55	MG	DA	1785	1/1	0.60	0.30	-	93,93,93,93	0
55	MG	AA	3321	1/1	0.94	0.33	-	65,65,65,65	0
55	MG	AA	3437	1/1	0.63	0.47	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1765	1/1	0.73	0.25	-	109,109,109,109	0
55	MG	BA	3513	1/1	0.67	0.23	-	104,104,104,104	0
55	MG	CA	1612	1/1	0.75	0.23	-	102,102,102,102	0
55	MG	AA	3149	1/1	0.93	0.37	-	57,57,57,57	0
55	MG	BA	3401	1/1	0.66	0.21	-	100,100,100,100	0
55	MG	BA	3261	1/1	0.95	0.38	-	65,65,65,65	0
55	MG	DA	1661	1/1	0.75	0.50	-	98,98,98,98	0
55	MG	AA	3476	1/1	0.97	0.63	-	79,79,79,79	0
55	MG	BA	3313	1/1	0.71	0.20	-	106,106,106,106	0
55	MG	AA	3318	1/1	0.96	0.30	-	92,92,92,92	0
55	MG	AA	3442	1/1	0.74	0.37	-	78,78,78,78	0
55	MG	BA	3085	1/1	0.85	0.34	-	74,74,74,74	0
55	MG	CA	1662	1/1	0.68	0.43	-	81,81,81,81	0
55	MG	CA	1751	1/1	0.92	0.23	-	78,78,78,78	0
55	MG	AA	3207	1/1	0.81	0.21	-	50,50,50,50	0
55	MG	CA	1696	1/1	0.93	0.39	-	90,90,90,90	0
55	MG	BA	3423	1/1	0.56	0.42	-	91,91,91,91	0
55	MG	DA	1704	1/1	0.95	0.48	-	87,87,87,87	0
55	MG	AA	3319	1/1	0.57	0.33	-	94,94,94,94	0
55	MG	BA	3040	1/1	0.78	0.20	-	94,94,94,94	0
55	MG	AA	3457	1/1	0.93	0.56	-	64,64,64,64	0
55	MG	CA	1734	1/1	0.80	0.51	-	86,86,86,86	0
55	MG	BB	205	1/1	0.90	0.21	-	86,86,86,86	0
55	MG	AA	3215	1/1	0.81	0.32	-	79,79,79,79	0
55	MG	AA	3202	1/1	0.96	0.29	-	46,46,46,46	0
55	MG	BA	3439	1/1	0.86	0.23	-	103,103,103,103	0
55	MG	BA	3105	1/1	0.69	0.24	-	81,81,81,81	0
55	MG	DA	1724	1/1	0.97	0.45	-	72,72,72,72	0
55	MG	AA	3463	1/1	0.77	0.42	-	90,90,90,90	0
55	MG	BA	3253	1/1	0.93	0.42	-	66,66,66,66	0
55	MG	AA	3043	1/1	0.91	0.37	-	108,108,108,108	0
55	MG	DA	1771	1/1	0.82	0.29	-	114,114,114,114	0
55	MG	CA	1671	1/1	0.89	0.27	-	72,72,72,72	0
55	MG	AA	3589	1/1	0.82	0.38	-	60,60,60,60	0
55	MG	BA	3411	1/1	0.82	0.35	-	83,83,83,83	0
55	MG	AA	3472	1/1	0.93	0.67	-	80,80,80,80	0
55	MG	AA	3108	1/1	0.72	0.49	-	66,66,66,66	0
55	MG	BA	3212	1/1	0.84	0.49	-	70,70,70,70	0
55	MG	AA	3468	1/1	0.82	0.29	-	95,95,95,95	0
55	MG	CA	1795	1/1	0.88	0.30	-	68,68,68,68	0
55	MG	AA	3260	1/1	0.77	0.54	-	91,91,91,91	0
55	MG	AA	3451	1/1	0.82	0.38	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3520	1/1	0.58	0.32	-	101,101,101,101	0
55	MG	DA	1619	1/1	0.89	0.33	-	77,77,77,77	0
55	MG	AA	3185	1/1	0.68	0.60	-	88,88,88,88	0
55	MG	CT	201	1/1	0.84	0.32	-	102,102,102,102	0
55	MG	AA	3397	1/1	0.57	0.46	-	95,95,95,95	0
55	MG	BP	201	1/1	0.92	0.18	-	65,65,65,65	0
55	MG	AA	3387	1/1	0.93	0.64	-	80,80,80,80	0
55	MG	CA	1834	1/1	0.77	0.33	-	90,90,90,90	0
55	MG	AA	3036	1/1	0.95	0.21	-	39,39,39,39	0
55	MG	BA	3226	1/1	0.64	0.45	-	82,82,82,82	0
55	MG	AO	202	1/1	0.89	0.60	-	80,80,80,80	0
55	MG	BA	3051	1/1	0.47	0.33	-	90,90,90,90	0
55	MG	BA	3235	1/1	0.68	0.44	-	74,74,74,74	0
55	MG	AA	3491	1/1	0.88	0.45	-	85,85,85,85	0
55	MG	BA	3192	1/1	0.90	0.35	-	72,72,72,72	0
55	MG	BA	3306	1/1	0.89	0.25	-	86,86,86,86	0
55	MG	AA	3173	1/1	0.78	0.34	-	67,67,67,67	0
55	MG	DA	1639	1/1	0.79	0.34	-	78,78,78,78	0
55	MG	DA	1615	1/1	0.70	0.32	-	96,96,96,96	0
55	MG	AA	3511	1/1	0.82	0.70	-	98,98,98,98	0
55	MG	DA	1746	1/1	0.71	0.25	-	104,104,104,104	0
55	MG	AA	3427	1/1	0.97	0.38	-	82,82,82,82	0
55	MG	BA	3083	1/1	0.88	0.21	-	92,92,92,92	0
55	MG	BA	3161	1/1	0.89	0.30	-	89,89,89,89	0
55	MG	BA	3098	1/1	0.53	0.25	-	106,106,106,106	0
55	MG	AA	3101	1/1	0.97	0.32	-	79,79,79,79	0
55	MG	BA	3379	1/1	0.61	0.32	-	84,84,84,84	0
55	MG	BA	3063	1/1	0.68	0.30	-	89,89,89,89	0
55	MG	BA	3216	1/1	0.99	0.28	-	56,56,56,56	0
55	MG	BA	3087	1/1	0.92	0.41	-	80,80,80,80	0
55	MG	CA	1791	1/1	0.86	0.17	-	97,97,97,97	0
55	MG	CA	1737	1/1	0.79	0.26	-	92,92,92,92	0
55	MG	AA	3425	1/1	0.55	0.33	-	94,94,94,94	0
55	MG	BA	3056	1/1	0.67	0.25	-	96,96,96,96	0
55	MG	AA	3390	1/1	0.70	0.40	-	109,109,109,109	0
55	MG	BA	3413	1/1	0.56	0.53	-	94,94,94,94	0
55	MG	DA	1679	1/1	0.92	0.33	-	64,64,64,64	0
55	MG	BA	3335	1/1	0.84	0.12	-	100,100,100,100	0
55	MG	DA	1637	1/1	0.82	0.30	-	97,97,97,97	0
55	MG	AB	206	1/1	0.86	0.48	-	93,93,93,93	0
55	MG	AA	3271	1/1	0.87	0.36	-	92,92,92,92	0
55	MG	DH	201	1/1	0.80	0.18	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1672	1/1	0.96	0.32	-	63,63,63,63	0
55	MG	AA	3287	1/1	0.91	0.28	-	69,69,69,69	0
55	MG	AA	3439	1/1	0.75	0.40	-	97,97,97,97	0
55	MG	AA	3089	1/1	0.89	0.54	-	64,64,64,64	0
55	MG	AA	3528	1/1	0.95	0.49	-	76,76,76,76	0
55	MG	BA	3337	1/1	0.77	0.34	-	100,100,100,100	0
55	MG	AA	3188	1/1	0.91	0.51	-	57,57,57,57	0
55	MG	AA	3444	1/1	0.83	0.33	-	58,58,58,58	0
55	MG	DA	1802	1/1	0.29	0.47	-	102,102,102,102	0
55	MG	AA	3419	1/1	0.71	0.57	-	89,89,89,89	0
55	MG	DA	1754	1/1	0.64	0.25	-	98,98,98,98	0
55	MG	AA	3485	1/1	0.88	0.52	-	71,71,71,71	0
55	MG	AA	3126	1/1	0.77	0.24	-	83,83,83,83	0
55	MG	BA	3364	1/1	0.87	0.22	-	76,76,76,76	0
55	MG	BA	3114	1/1	0.71	0.29	-	103,103,103,103	0
55	MG	AA	3438	1/1	0.78	0.45	-	90,90,90,90	0
55	MG	CA	1674	1/1	0.92	0.33	-	102,102,102,102	0
55	MG	BA	3153	1/1	0.81	0.39	-	77,77,77,77	0
55	MG	CA	1797	1/1	0.64	0.20	-	93,93,93,93	0
55	MG	BA	3383	1/1	0.32	0.49	-	95,95,95,95	0
55	MG	AA	3007	1/1	0.99	0.29	-	42,42,42,42	0
55	MG	CA	1738	1/1	0.78	0.31	-	103,103,103,103	0
55	MG	AA	3518	1/1	0.79	0.36	-	90,90,90,90	0
55	MG	BA	3256	1/1	0.78	0.35	-	102,102,102,102	0
55	MG	AA	3396	1/1	0.75	0.55	-	104,104,104,104	0
55	MG	AA	3440	1/1	0.82	0.42	-	87,87,87,87	0
55	MG	BA	3323	1/1	0.87	0.55	-	74,74,74,74	0
55	MG	DA	1798	1/1	0.73	0.22	-	92,92,92,92	0
55	MG	CA	1718	1/1	0.46	0.39	-	93,93,93,93	0
55	MG	BA	3415	1/1	0.77	0.30	-	109,109,109,109	0
55	MG	AA	3391	1/1	0.59	0.43	-	106,106,106,106	0
55	MG	BA	3055	1/1	0.82	0.30	-	99,99,99,99	0
55	MG	AA	3576	1/1	0.98	0.47	-	46,46,46,46	0
55	MG	CA	1720	1/1	0.25	0.27	-	102,102,102,102	0
55	MG	BA	3191	1/1	0.71	0.43	-	77,77,77,77	0
55	MG	AA	3281	1/1	0.93	0.45	-	74,74,74,74	0
55	MG	CA	1801	1/1	0.94	0.24	-	84,84,84,84	0
55	MG	BA	3497	1/1	0.96	0.23	-	63,63,63,63	0
55	MG	AA	3363	1/1	0.71	0.43	-	95,95,95,95	0
55	MG	AB	213	1/1	0.87	0.54	-	73,73,73,73	0
55	MG	AA	3324	1/1	0.94	0.24	-	92,92,92,92	0
55	MG	DA	1759	1/1	0.64	0.42	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3191	1/1	0.91	0.17	-	95,95,95,95	0
55	MG	BA	3272	1/1	0.94	0.39	-	81,81,81,81	0
55	MG	BA	3092	1/1	0.79	0.25	-	95,95,95,95	0
55	MG	BA	3426	1/1	0.77	0.39	-	87,87,87,87	0
55	MG	AA	3608	1/1	0.97	0.27	-	41,41,41,41	0
55	MG	DA	1743	1/1	0.81	0.24	-	94,94,94,94	0
55	MG	BE	301	1/1	0.90	0.26	-	54,54,54,54	0
55	MG	AA	3155	1/1	0.87	0.46	-	71,71,71,71	0
55	MG	BA	3234	1/1	0.88	0.30	-	67,67,67,67	0
55	MG	AA	3432	1/1	0.89	0.42	-	87,87,87,87	0
55	MG	AA	3523	1/1	0.80	0.22	-	91,91,91,91	0
55	MG	AA	3265	1/1	0.60	0.23	-	95,95,95,95	0
55	MG	AA	3176	1/1	0.87	0.22	-	74,74,74,74	0
55	MG	BA	3474	1/1	0.67	0.41	-	88,88,88,88	0
55	MG	DA	1739	1/1	0.86	0.15	-	113,113,113,113	0
55	MG	DA	1678	1/1	0.79	0.46	-	86,86,86,86	0
55	MG	CA	1646	1/1	0.82	0.37	-	75,75,75,75	0
55	MG	DA	1709	1/1	0.83	0.29	-	109,109,109,109	0
55	MG	BA	3505	1/1	0.81	0.29	-	94,94,94,94	0
55	MG	AA	3213	1/1	0.95	0.46	-	59,59,59,59	0
55	MG	DA	1683	1/1	0.72	0.56	-	80,80,80,80	0
55	MG	BA	3393	1/1	0.60	0.10	-	84,84,84,84	0
55	MG	BA	3147	1/1	0.92	0.23	-	63,63,63,63	0
55	MG	CA	1706	1/1	0.59	0.34	-	91,91,91,91	0
55	MG	AA	3274	1/1	0.84	0.42	-	72,72,72,72	0
55	MG	AA	3407	1/1	0.38	0.48	-	110,110,110,110	0
55	MG	BA	3277	1/1	0.45	0.30	-	109,109,109,109	0
55	MG	AA	3430	1/1	0.54	0.28	-	105,105,105,105	0
55	MG	AA	3405	1/1	0.88	0.72	-	90,90,90,90	0
55	MG	BA	3500	1/1	0.58	0.20	-	104,104,104,104	0
55	MG	BA	3312	1/1	0.60	0.33	-	98,98,98,98	0
55	MG	BA	3128	1/1	0.92	0.23	-	56,56,56,56	0
55	MG	DA	1701	1/1	0.93	0.52	-	80,80,80,80	0
55	MG	BA	3469	1/1	0.67	0.35	-	92,92,92,92	0
55	MG	BA	3139	1/1	0.95	0.19	-	58,58,58,58	0
55	MG	DA	1789	1/1	0.72	0.22	-	77,77,77,77	0
55	MG	BA	3050	1/1	0.68	0.24	-	103,103,103,103	0
55	MG	CA	1680	1/1	0.93	0.31	-	79,79,79,79	0
55	MG	BA	3435	1/1	0.74	0.16	-	108,108,108,108	0
55	MG	AA	3534	1/1	0.96	0.43	-	49,49,49,49	0
55	MG	CA	1704	1/1	-0.20	0.42	-	113,113,113,113	0
55	MG	CA	1735	1/1	0.71	0.46	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3078	1/1	0.78	0.64	-	88,88,88,88	0
55	MG	CA	1746	1/1	0.94	0.25	-	98,98,98,98	0
55	MG	BA	3290	1/1	0.59	0.21	-	82,82,82,82	0
55	MG	BA	3294	1/1	0.63	0.28	-	98,98,98,98	0
55	MG	BA	3408	1/1	0.87	0.42	-	88,88,88,88	0
55	MG	BA	3002	1/1	0.97	0.22	-	66,66,66,66	0
55	MG	CA	1804	1/1	0.63	0.39	-	107,107,107,107	0
55	MG	AA	3194	1/1	0.86	0.49	-	102,102,102,102	0
55	MG	AA	3291	1/1	0.76	0.45	-	68,68,68,68	0
55	MG	BA	3380	1/1	0.70	0.23	-	78,78,78,78	0
55	MG	BA	3170	1/1	0.65	0.24	-	96,96,96,96	0
55	MG	BA	3304	1/1	0.76	0.33	-	91,91,91,91	0
55	MG	CA	1810	1/1	0.83	0.35	-	108,108,108,108	0
55	MG	DB	101	1/1	0.91	0.21	-	103,103,103,103	0
55	MG	BA	3358	1/1	0.87	0.51	-	85,85,85,85	0
55	MG	AA	3342	1/1	0.88	0.49	-	70,70,70,70	0
55	MG	AA	3399	1/1	0.91	0.30	-	60,60,60,60	0
55	MG	AA	3572	1/1	0.88	0.49	-	54,54,54,54	0
55	MG	BA	3523	1/1	0.89	0.43	-	84,84,84,84	0
55	MG	AA	3276	1/1	0.81	0.53	-	78,78,78,78	0
55	MG	DA	1735	1/1	0.90	0.39	-	106,106,106,106	0
55	MG	BA	3453	1/1	0.68	0.24	-	93,93,93,93	0
55	MG	AB	207	1/1	0.94	0.20	-	103,103,103,103	0
55	MG	AA	3417	1/1	0.93	0.28	-	67,67,67,67	0
55	MG	CA	1621	1/1	0.27	0.38	-	107,107,107,107	0
55	MG	BA	3527	1/1	0.57	0.31	-	97,97,97,97	0
55	MG	BA	3020	1/1	0.84	0.26	-	76,76,76,76	0
55	MG	BA	3103	1/1	0.89	0.19	-	82,82,82,82	0
55	MG	BA	3146	1/1	0.93	0.24	-	86,86,86,86	0
55	MG	AA	3304	1/1	0.51	0.32	-	90,90,90,90	0
55	MG	AA	3258	1/1	0.76	0.42	-	92,92,92,92	0
55	MG	BA	3333	1/1	0.85	0.27	-	73,73,73,73	0
55	MG	DA	1682	1/1	0.65	0.47	-	96,96,96,96	0
55	MG	DA	1650	1/1	0.90	0.47	-	95,95,95,95	0
55	MG	BA	3196	1/1	0.91	0.32	-	84,84,84,84	0
55	MG	CA	1723	1/1	0.79	0.39	-	106,106,106,106	0
55	MG	AA	3070	1/1	0.97	0.31	-	68,68,68,68	0
55	MG	BA	3124	1/1	0.80	0.39	-	102,102,102,102	0
55	MG	BA	3247	1/1	0.84	0.33	-	74,74,74,74	0
55	MG	AA	3303	1/1	0.85	0.39	-	95,95,95,95	0
55	MG	AA	3480	1/1	0.68	0.55	-	86,86,86,86	0
55	MG	AB	212	1/1	0.60	0.45	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3420	1/1	-0.35	0.18	-	136,136,136,136	0
55	MG	BA	3183	1/1	0.93	0.19	-	80,80,80,80	0
55	MG	AA	3377	1/1	0.78	0.55	-	94,94,94,94	0
55	MG	DA	1657	1/1	0.93	0.46	-	95,95,95,95	0
55	MG	BA	3038	1/1	0.90	0.27	-	78,78,78,78	0
55	MG	DA	1699	1/1	0.89	0.40	-	68,68,68,68	0
55	MG	CA	1692	1/1	0.89	0.11	-	127,127,127,127	0
55	MG	DA	1791	1/1	0.71	0.45	-	80,80,80,80	0
55	MG	AA	3524	1/1	0.50	0.41	-	94,94,94,94	0
55	MG	BA	3262	1/1	0.76	0.22	-	94,94,94,94	0
55	MG	CA	1627	1/1	0.96	0.25	-	65,65,65,65	0
55	MG	BA	3121	1/1	0.68	0.45	-	99,99,99,99	0
55	MG	CA	1666	1/1	0.90	0.20	-	70,70,70,70	0
55	MG	DA	1700	1/1	0.85	0.41	-	94,94,94,94	0
55	MG	DC	106	1/1	0.86	0.15	-	111,111,111,111	0
55	MG	BA	3045	1/1	0.71	0.26	-	88,88,88,88	0
55	MG	BA	3328	1/1	0.95	0.14	-	61,61,61,61	0
55	MG	AA	3469	1/1	0.65	0.49	-	103,103,103,103	0
55	MG	AA	3360	1/1	0.86	0.36	-	63,63,63,63	0
55	MG	CA	1684	1/1	0.88	0.31	-	101,101,101,101	0
55	MG	AA	3545	1/1	0.91	0.36	-	75,75,75,75	0
55	MG	CA	1618	1/1	0.94	0.28	-	94,94,94,94	0
55	MG	BA	3198	1/1	0.88	0.26	-	44,44,44,44	0
55	MG	BA	3285	1/1	0.98	0.19	-	45,45,45,45	0
55	MG	DA	1643	1/1	0.96	0.39	-	81,81,81,81	0
55	MG	BA	3498	1/1	0.80	0.15	-	99,99,99,99	0
55	MG	BA	3417	1/1	0.94	0.14	-	88,88,88,88	0
55	MG	BA	3120	1/1	0.82	0.17	-	81,81,81,81	0
55	MG	CA	1631	1/1	0.94	0.21	-	74,74,74,74	0
55	MG	BA	3076	1/1	0.78	0.37	-	91,91,91,91	0
55	MG	CA	1653	1/1	0.25	0.41	-	91,91,91,91	0
55	MG	CA	1741	1/1	0.87	0.24	-	80,80,80,80	0
55	MG	BA	3444	1/1	0.69	0.50	-	96,96,96,96	0
55	MG	BA	3378	1/1	0.71	0.20	-	78,78,78,78	0
55	MG	DA	1786	1/1	0.92	0.38	-	86,86,86,86	0
55	MG	AA	3531	1/1	0.82	0.45	-	96,96,96,96	0
55	MG	AA	3475	1/1	0.71	0.27	-	102,102,102,102	0
55	MG	CA	1773	1/1	0.42	0.36	-	101,101,101,101	0
55	MG	BA	3265	1/1	0.95	0.46	-	86,86,86,86	0
55	MG	AA	3038	1/1	0.82	0.55	-	80,80,80,80	0
55	MG	BA	3018	1/1	0.93	0.29	-	83,83,83,83	0
55	MG	CA	1803	1/1	0.51	0.66	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3561	1/1	0.83	0.24	-	82,82,82,82	0
55	MG	BA	3400	1/1	0.95	0.28	-	74,74,74,74	0
55	MG	BA	3024	1/1	0.18	1.00	-	110,110,110,110	0
55	MG	AA	3293	1/1	0.90	0.20	-	77,77,77,77	0
55	MG	AA	3606	1/1	0.96	0.53	-	61,61,61,61	0
55	MG	AA	3218	1/1	0.90	0.40	-	73,73,73,73	0
55	MG	CA	1604	1/1	0.97	0.34	-	77,77,77,77	0
55	MG	AA	3333	1/1	0.90	0.47	-	95,95,95,95	0
55	MG	AA	3017	1/1	0.98	0.47	-	64,64,64,64	0
55	MG	CN	202	1/1	0.60	0.32	-	99,99,99,99	0
55	MG	CA	1656	1/1	0.81	0.52	-	88,88,88,88	0
55	MG	BA	3451	1/1	0.89	0.24	-	89,89,89,89	0
55	MG	AA	3554	1/1	0.82	0.46	-	74,74,74,74	0
55	MG	DA	1693	1/1	0.86	0.40	-	93,93,93,93	0
55	MG	BA	3368	1/1	0.75	0.30	-	106,106,106,106	0
55	MG	BA	3200	1/1	0.96	0.38	-	65,65,65,65	0
55	MG	AU	201	1/1	0.91	0.23	-	85,85,85,85	0
55	MG	CA	1809	1/1	0.61	0.39	-	79,79,79,79	0
55	MG	AA	3556	1/1	0.64	0.49	-	96,96,96,96	0
55	MG	AA	3039	1/1	0.77	0.67	-	82,82,82,82	0
55	MG	DA	1654	1/1	0.98	0.41	-	92,92,92,92	0
55	MG	AA	3331	1/1	0.83	0.46	-	76,76,76,76	0
55	MG	BA	3296	1/1	0.74	0.25	-	76,76,76,76	0
55	MG	DA	1702	1/1	0.70	0.36	-	99,99,99,99	0
55	MG	AA	3410	1/1	0.73	0.40	-	95,95,95,95	0
55	MG	AA	3481	1/1	0.90	0.15	-	112,112,112,112	0
55	MG	AA	3257	1/1	0.95	0.42	-	79,79,79,79	0
55	MG	BA	3110	1/1	0.85	0.38	-	92,92,92,92	0
55	MG	AA	3532	1/1	0.73	0.31	-	88,88,88,88	0
55	MG	BA	3115	1/1	0.87	0.28	-	79,79,79,79	0
55	MG	AA	3059	1/1	0.93	0.42	-	80,80,80,80	0
55	MG	AA	3196	1/1	0.89	0.21	-	61,61,61,61	0
55	MG	CA	1730	1/1	0.83	0.28	-	107,107,107,107	0
55	MG	AA	3519	1/1	0.87	0.16	-	53,53,53,53	0
55	MG	CA	1637	1/1	0.34	0.32	-	106,106,106,106	0
55	MG	AA	3255	1/1	0.89	0.44	-	88,88,88,88	0
55	MG	AA	3509	1/1	0.65	0.31	-	95,95,95,95	0
55	MG	AA	3316	1/1	0.72	0.18	-	83,83,83,83	0
55	MG	BA	3160	1/1	0.94	0.30	-	82,82,82,82	0
55	MG	CC	107	1/1	0.51	0.43	-	93,93,93,93	0
55	MG	CA	1607	1/1	0.96	0.40	-	93,93,93,93	0
55	MG	BA	3197	1/1	0.95	0.11	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3311	1/1	0.75	0.22	-	82,82,82,82	0
55	MG	BA	3506	1/1	0.85	0.20	-	74,74,74,74	0
55	MG	AA	3431	1/1	0.92	0.31	-	89,89,89,89	0
55	MG	AA	3378	1/1	0.87	0.53	-	84,84,84,84	0
55	MG	BA	3232	1/1	0.99	0.27	-	55,55,55,55	0
55	MG	AA	3575	1/1	0.93	0.39	-	42,42,42,42	0
55	MG	AA	3359	1/1	0.62	0.41	-	84,84,84,84	0
55	MG	CA	1690	1/1	0.80	0.40	-	102,102,102,102	0
55	MG	BA	3448	1/1	0.72	0.22	-	85,85,85,85	0
55	MG	AA	3219	1/1	0.92	0.41	-	81,81,81,81	0
55	MG	BA	3406	1/1	0.24	0.31	-	97,97,97,97	0
55	MG	BA	3082	1/1	0.93	0.37	-	76,76,76,76	0
55	MG	CA	1778	1/1	0.71	0.43	-	95,95,95,95	0
55	MG	AA	3314	1/1	0.93	0.52	-	80,80,80,80	0
55	MG	CA	1806	1/1	0.70	0.17	-	62,62,62,62	0
55	MG	CA	1641	1/1	0.99	0.23	-	65,65,65,65	0
55	MG	DA	1680	1/1	0.88	0.35	-	81,81,81,81	0
55	MG	AA	3347	1/1	0.40	0.33	-	92,92,92,92	0
55	MG	AA	3254	1/1	0.86	0.63	-	85,85,85,85	0
55	MG	BA	3387	1/1	0.71	0.48	-	107,107,107,107	0
55	MG	CA	1617	1/1	0.78	0.51	-	72,72,72,72	0
55	MG	CA	1622	1/1	0.94	0.15	-	86,86,86,86	0
55	MG	AA	3109	1/1	0.81	0.37	-	53,53,53,53	0
55	MG	BA	3303	1/1	0.45	0.37	-	89,89,89,89	0
55	MG	CA	1744	1/1	0.94	0.46	-	57,57,57,57	0
55	MG	DA	1608	1/1	0.80	0.24	-	92,92,92,92	0
55	MG	CA	1677	1/1	0.76	0.25	-	90,90,90,90	0
55	MG	BA	3410	1/1	0.73	0.43	-	94,94,94,94	0
55	MG	AA	3460	1/1	0.94	0.26	-	106,106,106,106	0
55	MG	CA	1772	1/1	0.93	0.21	-	83,83,83,83	0
55	MG	AA	3616	1/1	0.77	0.30	-	95,95,95,95	0
55	MG	CA	1675	1/1	0.88	0.24	-	97,97,97,97	0
55	MG	BA	3225	1/1	0.98	0.20	-	78,78,78,78	0
55	MG	AA	3467	1/1	0.79	0.39	-	87,87,87,87	0
55	MG	AA	3296	1/1	0.85	0.54	-	72,72,72,72	0
55	MG	BA	3223	1/1	0.88	0.27	-	64,64,64,64	0
55	MG	AA	3022	1/1	0.98	0.27	-	49,49,49,49	0
55	MG	AB	204	1/1	0.42	0.56	-	96,96,96,96	0
55	MG	AA	3062	1/1	0.90	0.37	-	86,86,86,86	0
55	MG	AA	3537	1/1	0.47	0.30	-	105,105,105,105	0
55	MG	DA	1777	1/1	0.63	0.40	-	87,87,87,87	0
55	MG	AA	3392	1/1	0.69	0.50	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1779	1/1	0.88	0.13	-	113,113,113,113	0
55	MG	BA	3095	1/1	0.40	0.38	-	112,112,112,112	0
55	MG	CA	1832	1/1	0.50	0.25	-	106,106,106,106	0
55	MG	AA	3329	1/1	0.85	0.16	-	94,94,94,94	0
55	MG	CA	1710	1/1	0.57	0.35	-	81,81,81,81	0
55	MG	AA	3586	1/1	0.90	0.14	-	53,53,53,53	0
55	MG	AA	3111	1/1	0.96	0.51	-	36,36,36,36	0
55	MG	BA	3362	1/1	0.82	0.14	-	71,71,71,71	0
55	MG	AB	210	1/1	0.97	0.38	-	65,65,65,65	0
55	MG	AA	3216	1/1	0.92	0.33	-	64,64,64,64	0
55	MG	CA	1672	1/1	0.50	0.26	-	106,106,106,106	0
55	MG	AA	3529	1/1	0.88	0.28	-	68,68,68,68	0
55	MG	AA	3330	1/1	0.93	0.34	-	60,60,60,60	0
55	MG	BA	3416	1/1	0.54	0.31	-	103,103,103,103	0
55	MG	AA	3193	1/1	0.37	0.69	-	96,96,96,96	0
55	MG	CA	1709	1/1	0.74	0.46	-	96,96,96,96	0
55	MG	AA	3187	1/1	0.92	0.46	-	87,87,87,87	0
55	MG	BA	3259	1/1	0.86	0.35	-	54,54,54,54	0
55	MG	CA	1616	1/1	0.76	0.24	-	103,103,103,103	0
55	MG	BA	3134	1/1	0.98	0.28	-	63,63,63,63	0
55	MG	CA	1729	1/1	0.76	0.34	-	94,94,94,94	0
55	MG	DA	1734	1/1	0.90	0.31	-	88,88,88,88	0
55	MG	BA	3150	1/1	0.88	0.40	-	96,96,96,96	0
55	MG	BA	3029	1/1	0.89	0.39	-	75,75,75,75	0
55	MG	CA	1657	1/1	0.96	0.32	-	63,63,63,63	0
55	MG	DA	1767	1/1	0.80	0.40	-	113,113,113,113	0
55	MG	BA	3388	1/1	0.91	0.32	-	87,87,87,87	0
55	MG	BA	3480	1/1	0.92	0.23	-	56,56,56,56	0
55	MG	DA	1765	1/1	0.79	0.20	-	93,93,93,93	0
55	MG	BA	3141	1/1	0.96	0.23	-	72,72,72,72	0
55	MG	BA	3503	1/1	0.90	0.13	-	69,69,69,69	0
55	MG	CA	1754	1/1	0.89	0.39	-	114,114,114,114	0
55	MG	DA	1607	1/1	0.71	0.32	-	92,92,92,92	0
55	MG	AA	3341	1/1	0.69	0.26	-	95,95,95,95	0
55	MG	AA	3614	1/1	0.97	0.55	-	78,78,78,78	0
55	MG	BA	3052	1/1	0.96	0.29	-	58,58,58,58	0
55	MG	BA	3014	1/1	0.96	0.27	-	72,72,72,72	0
55	MG	AA	3435	1/1	0.63	0.46	-	78,78,78,78	0
55	MG	BA	3347	1/1	0.86	0.23	-	85,85,85,85	0
55	MG	AA	3421	1/1	0.74	0.56	-	94,94,94,94	0
55	MG	BA	3033	1/1	0.63	0.25	-	94,94,94,94	0
55	MG	CA	1764	1/1	0.74	0.20	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3053	1/1	0.95	0.36	-	65,65,65,65	0
55	MG	AA	3301	1/1	0.55	0.30	-	85,85,85,85	0
55	MG	AB	214	1/1	0.57	0.39	-	102,102,102,102	0
55	MG	AA	3569	1/1	0.94	0.31	-	60,60,60,60	0
55	MG	BA	3365	1/1	0.94	0.38	-	90,90,90,90	0
55	MG	CA	1756	1/1	0.87	0.13	-	113,113,113,113	0
55	MG	CA	1775	1/1	0.64	0.27	-	113,113,113,113	0
55	MG	BA	3166	1/1	0.96	0.32	-	40,40,40,40	0
55	MG	CA	1820	1/1	0.93	0.43	-	88,88,88,88	0
55	MG	AB	201	1/1	0.91	0.67	-	96,96,96,96	0
55	MG	AA	3182	1/1	0.68	0.47	-	88,88,88,88	0
55	MG	DA	1793	1/1	0.39	0.38	-	108,108,108,108	0
55	MG	AA	3283	1/1	0.97	0.38	-	91,91,91,91	0
55	MG	DA	1758	1/1	0.58	0.46	-	109,109,109,109	0
55	MG	CA	1665	1/1	0.90	0.53	-	74,74,74,74	0
55	MG	AA	3404	1/1	0.85	0.29	-	95,95,95,95	0
55	MG	BA	3349	1/1	0.90	0.28	-	93,93,93,93	0
55	MG	AA	3349	1/1	0.89	0.44	-	84,84,84,84	0
55	MG	DA	1803	1/1	0.79	0.49	-	100,100,100,100	0
55	MG	AA	3030	1/1	0.98	0.31	-	45,45,45,45	0
55	MG	BA	3301	1/1	0.46	0.32	-	106,106,106,106	0
55	MG	AA	3367	1/1	0.63	0.52	-	87,87,87,87	0
55	MG	AA	3388	1/1	0.88	0.51	-	85,85,85,85	0
55	MG	BA	3209	1/1	0.82	0.31	-	46,46,46,46	0
55	MG	AA	3535	1/1	0.93	0.16	-	103,103,103,103	0
55	MG	AA	3619	1/1	0.87	0.50	-	87,87,87,87	0
55	MG	BA	3403	1/1	0.96	0.19	-	77,77,77,77	0
55	MG	BA	3255	1/1	0.97	0.37	-	52,52,52,52	0
55	MG	DC	103	1/1	0.95	0.33	-	78,78,78,78	0
55	MG	AA	3580	1/1	0.87	0.30	-	78,78,78,78	0
55	MG	BA	3464	1/1	0.69	0.33	-	104,104,104,104	0
55	MG	AA	3132	1/1	0.46	0.57	-	106,106,106,106	0
55	MG	CA	1798	1/1	0.78	0.40	-	82,82,82,82	0
55	MG	BA	3215	1/1	0.99	0.32	-	66,66,66,66	0
55	MG	BA	3431	1/1	0.90	0.25	-	84,84,84,84	0
55	MG	BA	3436	1/1	0.77	0.28	-	94,94,94,94	0
55	MG	CA	1831	1/1	0.55	0.33	-	105,105,105,105	0
55	MG	AA	3499	1/1	0.76	0.67	-	93,93,93,93	0
55	MG	BA	3070	1/1	0.74	0.28	-	81,81,81,81	0
55	MG	CA	1753	1/1	0.57	0.23	-	107,107,107,107	0
55	MG	BA	3062	1/1	0.97	0.26	-	110,110,110,110	0
55	MG	BA	3468	1/1	0.46	0.28	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3026	1/1	0.82	0.31	-	72,72,72,72	0
55	MG	BA	3398	1/1	0.57	0.55	-	96,96,96,96	0
55	MG	AA	3204	1/1	0.97	0.31	-	44,44,44,44	0
55	MG	DA	1744	1/1	0.93	0.40	-	57,57,57,57	0
55	MG	BA	3389	1/1	0.78	0.17	-	96,96,96,96	0
55	MG	AA	3320	1/1	0.43	0.32	-	103,103,103,103	0
55	MG	BA	3151	1/1	0.56	0.27	-	96,96,96,96	0
55	MG	BA	3356	1/1	0.78	0.19	-	84,84,84,84	0
55	MG	BA	3465	1/1	0.36	0.34	-	97,97,97,97	0
55	MG	CA	1719	1/1	0.68	0.35	-	85,85,85,85	0
55	MG	AA	3557	1/1	0.78	0.49	-	100,100,100,100	0
55	MG	CA	1747	1/1	0.85	0.43	-	83,83,83,83	0
55	MG	BA	3116	1/1	0.30	0.22	-	107,107,107,107	0
55	MG	AA	3226	1/1	0.94	0.30	-	77,77,77,77	0
55	MG	BA	3176	1/1	0.87	0.20	-	79,79,79,79	0
55	MG	AA	3232	1/1	0.93	0.66	-	104,104,104,104	0
55	MG	DA	1769	1/1	0.77	0.34	-	79,79,79,79	0
55	MG	DA	1674	1/1	0.94	0.27	-	76,76,76,76	0
55	MG	AA	3041	1/1	0.95	0.33	-	66,66,66,66	0
55	MG	AA	3261	1/1	0.66	0.52	-	85,85,85,85	0
55	MG	DA	1796	1/1	0.94	0.25	-	97,97,97,97	0
55	MG	DA	1784	1/1	0.40	0.34	-	103,103,103,103	0
55	MG	DA	1766	1/1	0.79	0.53	-	116,116,116,116	0
55	MG	AA	3134	1/1	0.89	0.36	-	79,79,79,79	0
55	MG	CA	1648	1/1	0.93	0.40	-	79,79,79,79	0
55	MG	AA	3179	1/1	0.94	0.29	-	53,53,53,53	0
55	MG	BA	3360	1/1	0.86	0.32	-	83,83,83,83	0
55	MG	BA	3275	1/1	0.96	0.38	-	52,52,52,52	0
55	MG	AA	3344	1/1	0.86	0.46	-	68,68,68,68	0
55	MG	BA	3245	1/1	0.90	0.19	-	72,72,72,72	0
55	MG	CA	1784	1/1	0.85	0.46	-	101,101,101,101	0
55	MG	BA	3274	1/1	0.94	0.19	-	90,90,90,90	0
55	MG	BA	3281	1/1	0.86	0.32	-	92,92,92,92	0
55	MG	AA	3151	1/1	0.96	0.45	-	58,58,58,58	0
55	MG	AA	3061	1/1	0.96	0.26	-	79,79,79,79	0
55	MG	AA	3146	1/1	0.92	0.41	-	65,65,65,65	0
55	MG	BA	3332	1/1	0.59	0.23	-	100,100,100,100	0
55	MG	BA	3508	1/1	0.88	0.35	-	73,73,73,73	0
55	MG	AA	3617	1/1	0.94	0.47	-	92,92,92,92	0
55	MG	AA	3234	1/1	0.89	0.38	-	82,82,82,82	0
55	MG	AA	3284	1/1	0.96	0.44	-	81,81,81,81	0
55	MG	BA	3061	1/1	0.86	0.13	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3001	1/1	0.96	0.30	-	64,64,64,64	0
55	MG	CA	1629	1/1	0.69	0.15	-	95,95,95,95	0
55	MG	CA	1774	1/1	0.28	0.43	-	97,97,97,97	0
55	MG	AA	3368	1/1	0.96	0.48	-	90,90,90,90	0
55	MG	DC	101	1/1	0.87	0.12	-	95,95,95,95	0
55	MG	AA	3544	1/1	0.93	0.37	-	63,63,63,63	0
55	MG	AA	3239	1/1	0.94	0.45	-	60,60,60,60	0
55	MG	CA	1609	1/1	0.93	0.43	-	78,78,78,78	0
55	MG	BA	3059	1/1	0.96	0.26	-	50,50,50,50	0
55	MG	BA	3357	1/1	0.77	0.39	-	71,71,71,71	0
55	MG	DA	1727	1/1	0.88	0.36	-	86,86,86,86	0
55	MG	AA	3403	1/1	0.94	0.28	-	91,91,91,91	0
55	MG	BA	3164	1/1	0.52	0.22	-	99,99,99,99	0
55	MG	CA	1827	1/1	0.61	0.29	-	89,89,89,89	0
55	MG	AA	3282	1/1	0.94	0.39	-	78,78,78,78	0
55	MG	DA	1773	1/1	0.83	0.47	-	69,69,69,69	0
55	MG	BA	3454	1/1	0.64	0.42	-	105,105,105,105	0
55	MG	BA	3260	1/1	0.81	0.14	-	82,82,82,82	0
55	MG	AA	3298	1/1	0.89	0.59	-	73,73,73,73	0
55	MG	BA	3504	1/1	0.88	0.15	-	117,117,117,117	0
55	MG	BA	3122	1/1	0.82	0.33	-	95,95,95,95	0
55	MG	BA	3525	1/1	0.86	0.36	-	98,98,98,98	0
55	MG	AA	3295	1/1	0.79	0.66	-	102,102,102,102	0
55	MG	AF	302	1/1	0.69	0.33	-	93,93,93,93	0
55	MG	BA	3036	1/1	0.91	0.44	-	85,85,85,85	0
55	MG	AA	3246	1/1	0.93	0.52	-	73,73,73,73	0
55	MG	AA	3350	1/1	0.79	0.24	-	90,90,90,90	0
55	MG	CA	1783	1/1	0.41	0.86	-	106,106,106,106	0
55	MG	BA	3138	1/1	0.98	0.30	-	52,52,52,52	0
55	MG	DA	1804	1/1	0.51	0.34	-	123,123,123,123	0
55	MG	BA	3390	1/1	0.77	0.46	-	77,77,77,77	0
55	MG	AA	3382	1/1	0.34	0.50	-	102,102,102,102	0
55	MG	AA	3527	1/1	0.71	0.43	-	86,86,86,86	0
55	MG	AA	3622	1/1	0.85	0.53	-	65,65,65,65	0
55	MG	CA	1655	1/1	0.84	0.52	-	95,95,95,95	0
55	MG	BA	3377	1/1	0.90	0.31	-	81,81,81,81	0
55	MG	AB	203	1/1	0.95	0.42	-	69,69,69,69	0
55	MG	BA	3148	1/1	0.93	0.23	-	91,91,91,91	0
55	MG	AA	3594	1/1	0.80	0.57	-	105,105,105,105	0
55	MG	AA	3181	1/1	0.94	0.39	-	66,66,66,66	0
55	MG	BA	3185	1/1	0.79	0.41	-	68,68,68,68	0
55	MG	DA	1751	1/1	0.90	0.34	-	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3286	1/1	0.98	0.24	-	85,85,85,85	0
55	MG	BA	3334	1/1	0.59	0.14	-	103,103,103,103	0
55	MG	BA	3137	1/1	0.96	0.30	-	48,48,48,48	0
55	MG	DA	1738	1/1	0.89	0.37	-	85,85,85,85	0
55	MG	BA	3433	1/1	0.81	0.24	-	88,88,88,88	0
55	MG	DA	1642	1/1	0.72	0.25	-	110,110,110,110	0
55	MG	CC	106	1/1	0.95	0.21	-	92,92,92,92	0
55	MG	BB	206	1/1	0.75	0.12	-	102,102,102,102	0
55	MG	CA	1605	1/1	0.97	0.27	-	86,86,86,86	0
55	MG	BA	3473	1/1	0.85	0.26	-	78,78,78,78	0
55	MG	BA	3102	1/1	0.92	0.11	-	86,86,86,86	0
55	MG	AA	3338	1/1	0.86	0.47	-	51,51,51,51	0
55	MG	AA	3488	1/1	0.85	0.25	-	93,93,93,93	0
55	MG	DA	1787	1/1	0.55	0.37	-	114,114,114,114	0
55	MG	AA	3076	1/1	0.94	0.38	-	82,82,82,82	0
55	MG	CA	1785	1/1	0.90	0.57	-	89,89,89,89	0
55	MG	BA	3271	1/1	0.92	0.32	-	84,84,84,84	0
55	MG	DA	1792	1/1	0.91	0.22	-	81,81,81,81	0
55	MG	DA	1720	1/1	0.75	0.32	-	96,96,96,96	0
55	MG	BB	212	1/1	0.27	0.31	-	104,104,104,104	0
55	MG	DA	1713	1/1	0.26	0.36	-	111,111,111,111	0
55	MG	CA	1782	1/1	0.78	0.56	-	94,94,94,94	0
55	MG	BA	3460	1/1	0.82	0.17	-	101,101,101,101	0
55	MG	AA	3559	1/1	0.83	0.33	-	83,83,83,83	0
55	MG	AA	3613	1/1	0.85	0.31	-	76,76,76,76	0
55	MG	BA	3458	1/1	0.90	0.24	-	71,71,71,71	0
55	MG	AA	3201	1/1	0.81	0.34	-	85,85,85,85	0
55	MG	BA	3154	1/1	0.96	0.14	-	46,46,46,46	0
55	MG	CA	1766	1/1	0.74	0.53	-	108,108,108,108	0
55	MG	AA	3273	1/1	0.54	0.29	-	101,101,101,101	0
55	MG	BA	3354	1/1	0.86	0.30	-	90,90,90,90	0
55	MG	AA	3398	1/1	0.83	0.36	-	73,73,73,73	0
55	MG	AA	3235	1/1	0.59	0.46	-	84,84,84,84	0
55	MG	DA	1676	1/1	0.96	0.43	-	82,82,82,82	0
55	MG	AA	3117	1/1	0.92	0.31	-	54,54,54,54	0
55	MG	BA	3263	1/1	0.90	0.24	-	84,84,84,84	0
55	MG	DA	1736	1/1	0.90	0.48	-	65,65,65,65	0
55	MG	BA	3375	1/1	0.58	0.30	-	75,75,75,75	0
55	MG	DA	1750	1/1	0.89	0.19	-	84,84,84,84	0
55	MG	AA	3095	1/1	0.96	0.29	-	89,89,89,89	0
55	MG	AA	3369	1/1	0.70	0.53	-	93,93,93,93	0
55	MG	AA	3183	1/1	0.86	0.32	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1719	1/1	0.29	0.56	-	112,112,112,112	0
55	MG	CA	1670	1/1	0.88	0.29	-	70,70,70,70	0
55	MG	DA	1703	1/1	0.23	0.37	-	115,115,115,115	0
55	MG	CA	1732	1/1	0.93	0.33	-	69,69,69,69	0
55	MG	AA	3402	1/1	0.58	0.46	-	92,92,92,92	0
55	MG	BA	3320	1/1	0.83	0.28	-	77,77,77,77	0
55	MG	AA	3409	1/1	0.43	0.54	-	104,104,104,104	0
55	MG	AA	3471	1/1	0.95	0.45	-	85,85,85,85	0
55	MG	AA	3429	1/1	0.81	0.44	-	90,90,90,90	0
55	MG	AA	3620	1/1	0.66	0.35	-	115,115,115,115	0
55	MG	DA	1779	1/1	0.82	0.34	-	91,91,91,91	0
55	MG	BA	3524	1/1	0.83	0.46	-	105,105,105,105	0
55	MG	A5	102	1/1	0.79	0.41	-	83,83,83,83	0
55	MG	CA	1736	1/1	0.80	0.26	-	88,88,88,88	0
55	MG	AA	3413	1/1	0.33	0.39	-	109,109,109,109	0
55	MG	BR	201	1/1	0.79	0.24	-	77,77,77,77	0
55	MG	AA	3415	1/1	0.82	0.47	-	87,87,87,87	0
55	MG	BA	3526	1/1	0.75	0.26	-	92,92,92,92	0
55	MG	BA	3068	1/1	0.69	0.28	-	93,93,93,93	0
55	MG	AA	3275	1/1	0.70	0.40	-	87,87,87,87	0
55	MG	DA	1611	1/1	0.66	0.38	-	100,100,100,100	0
55	MG	AA	3032	1/1	0.94	0.33	-	65,65,65,65	0
55	MG	DA	1696	1/1	0.94	0.32	-	66,66,66,66	0
55	MG	CA	1650	1/1	0.96	0.40	-	73,73,73,73	0
55	MG	CA	1697	1/1	0.89	0.76	-	92,92,92,92	0
55	MG	BA	3440	1/1	0.92	0.23	-	80,80,80,80	0
55	MG	CA	1633	1/1	0.76	0.30	-	83,83,83,83	0
55	MG	DA	1625	1/1	0.45	0.22	-	105,105,105,105	0
55	MG	AA	3264	1/1	0.73	0.55	-	80,80,80,80	0
55	MG	CA	1634	1/1	0.99	0.32	-	60,60,60,60	0
55	MG	AA	3079	1/1	0.87	0.23	-	92,92,92,92	0
55	MG	BA	3419	1/1	0.89	0.13	-	99,99,99,99	0
55	MG	AA	3169	1/1	0.65	0.35	-	89,89,89,89	0
55	MG	BA	3280	1/1	0.95	0.35	-	74,74,74,74	0
55	MG	DC	104	1/1	0.73	0.21	-	102,102,102,102	0
55	MG	AA	3205	1/1	0.97	0.35	-	55,55,55,55	0
55	MG	BB	203	1/1	0.88	0.29	-	76,76,76,76	0
55	MG	AA	3624	1/1	0.82	0.32	-	111,111,111,111	0
55	MG	BA	3041	1/1	0.61	0.48	-	104,104,104,104	0
55	MG	AA	3506	1/1	0.91	0.20	-	80,80,80,80	0
55	MG	AA	3381	1/1	0.73	0.72	-	90,90,90,90	0
55	MG	CA	1840	1/1	0.95	0.32	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	1662	1/1	0.86	0.45	-	78,78,78,78	0
55	MG	AA	3306	1/1	0.97	0.40	-	65,65,65,65	0
55	MG	CA	1777	1/1	0.97	0.35	-	92,92,92,92	0
55	MG	CA	1728	1/1	0.01	0.37	-	117,117,117,117	0
55	MG	AA	3593	1/1	0.75	0.50	-	95,95,95,95	0
55	MG	AA	3302	1/1	0.74	0.41	-	104,104,104,104	0
55	MG	AA	3096	1/1	0.73	0.32	-	89,89,89,89	0
55	MG	DA	1760	1/1	0.67	0.45	-	100,100,100,100	0
55	MG	DA	1620	1/1	0.93	0.30	-	85,85,85,85	0
55	MG	BA	3327	1/1	0.76	0.28	-	91,91,91,91	0
55	MG	AA	3211	1/1	0.89	0.32	-	58,58,58,58	0
55	MG	CA	1724	1/1	0.58	0.23	-	97,97,97,97	0
55	MG	AA	3510	1/1	0.82	0.53	-	84,84,84,84	0
55	MG	BA	3035	1/1	0.77	0.25	-	103,103,103,103	0
55	MG	BA	3476	1/1	0.79	0.18	-	68,68,68,68	0
55	MG	BA	3287	1/1	0.69	0.35	-	87,87,87,87	0
55	MG	AA	3361	1/1	0.68	0.54	-	93,93,93,93	0
55	MG	AA	3236	1/1	0.67	0.57	-	96,96,96,96	0
55	MG	BA	3202	1/1	0.83	0.23	-	69,69,69,69	0
55	MG	DA	1780	1/1	0.92	0.46	-	107,107,107,107	0
55	MG	AA	3203	1/1	0.98	0.47	-	65,65,65,65	0
55	MG	AA	3345	1/1	0.90	0.58	-	93,93,93,93	0
55	MG	BA	3019	1/1	0.79	0.24	-	100,100,100,100	0
55	MG	BA	3123	1/1	0.96	0.13	-	77,77,77,77	0
55	MG	DA	1770	1/1	0.71	0.35	-	95,95,95,95	0
55	MG	BA	3291	1/1	0.89	0.26	-	67,67,67,67	0
55	MG	BA	3090	1/1	0.62	0.33	-	109,109,109,109	0
55	MG	CA	1763	1/1	0.95	0.44	-	81,81,81,81	0
55	MG	AA	3288	1/1	0.95	0.61	-	90,90,90,90	0
55	MG	BA	3344	1/1	0.39	0.36	-	101,101,101,101	0
55	MG	AA	3384	1/1	0.67	0.56	-	87,87,87,87	0
55	MG	AA	3220	1/1	0.96	0.41	-	70,70,70,70	0
55	MG	BA	3487	1/1	0.87	0.19	-	66,66,66,66	0
55	MG	BA	3483	1/1	0.95	0.33	-	34,34,34,34	0
55	MG	AA	3120	1/1	0.69	0.32	-	86,86,86,86	0
55	MG	AA	3370	1/1	0.45	0.22	-	106,106,106,106	0
55	MG	BA	3015	1/1	0.92	0.20	-	71,71,71,71	0
55	MG	AA	3494	1/1	0.80	0.37	-	88,88,88,88	0
55	MG	BA	3519	1/1	0.75	0.24	-	107,107,107,107	0
55	MG	BA	3370	1/1	0.71	0.23	-	98,98,98,98	0
55	MG	CA	1821	1/1	0.57	0.38	-	94,94,94,94	0
55	MG	DA	1761	1/1	0.90	0.40	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3395	1/1	0.67	0.52	-	80,80,80,80	0
55	MG	BA	3372	1/1	0.90	0.38	-	105,105,105,105	0
55	MG	BA	3221	1/1	0.98	0.25	-	37,37,37,37	0
55	MG	CA	1676	1/1	0.87	0.29	-	76,76,76,76	0
55	MG	BA	3017	1/1	0.97	0.34	-	50,50,50,50	0
55	MG	BA	3091	1/1	0.74	0.37	-	86,86,86,86	0
55	MG	AA	3313	1/1	0.84	0.44	-	70,70,70,70	0
55	MG	CA	1815	1/1	0.72	0.27	-	91,91,91,91	0
55	MG	AA	3015	1/1	0.96	0.40	-	44,44,44,44	0
55	MG	CA	1750	1/1	0.83	0.51	-	104,104,104,104	0
55	MG	DA	1790	1/1	0.89	0.49	-	100,100,100,100	0
55	MG	AA	3104	1/1	0.73	0.34	-	80,80,80,80	0
55	MG	BA	3034	1/1	0.75	0.28	-	81,81,81,81	0
55	MG	BA	3143	1/1	0.94	0.21	-	63,63,63,63	0
55	MG	AA	3136	1/1	0.92	0.14	-	61,61,61,61	0
55	MG	BA	3032	1/1	0.82	0.37	-	110,110,110,110	0
55	MG	B5	101	1/1	0.96	0.20	-	61,61,61,61	0
55	MG	BA	3432	1/1	0.73	0.35	-	88,88,88,88	0
55	MG	BA	3077	1/1	0.72	0.24	-	101,101,101,101	0
55	MG	BA	3177	1/1	0.91	0.27	-	75,75,75,75	0
55	MG	AA	3335	1/1	0.63	0.65	-	91,91,91,91	0
55	MG	DA	1762	1/1	0.85	0.21	-	109,109,109,109	0
55	MG	BA	3222	1/1	0.96	0.18	-	54,54,54,54	0
55	MG	AA	3626	1/1	0.49	0.62	-	96,96,96,96	0
55	MG	BA	3044	1/1	0.75	0.48	-	104,104,104,104	0
55	MG	CA	1742	1/1	0.90	0.13	-	115,115,115,115	0
55	MG	CA	1826	1/1	0.83	0.28	-	81,81,81,81	0
55	MG	BB	209	1/1	0.78	0.31	-	95,95,95,95	0
55	MG	AA	3461	1/1	0.70	0.39	-	105,105,105,105	0
55	MG	CA	1640	1/1	0.66	0.35	-	85,85,85,85	0
55	MG	CA	1768	1/1	0.46	0.33	-	105,105,105,105	0
55	MG	BA	3353	1/1	0.79	0.22	-	84,84,84,84	0
55	MG	CA	1790	1/1	0.75	0.27	-	89,89,89,89	0
55	MG	AA	3133	1/1	0.97	0.51	-	46,46,46,46	0
55	MG	DA	1663	1/1	0.45	0.26	-	103,103,103,103	0
55	MG	BA	3066	1/1	0.91	0.21	-	86,86,86,86	0
55	MG	AA	3394	1/1	0.62	0.36	-	99,99,99,99	0
55	MG	BA	3276	1/1	0.94	0.14	-	88,88,88,88	0
55	MG	BA	3252	1/1	0.87	0.31	-	86,86,86,86	0
55	MG	DA	1705	1/1	0.97	0.35	-	97,97,97,97	0
55	MG	AA	3602	1/1	0.86	0.19	-	59,59,59,59	0
55	MG	AA	3087	1/1	0.94	0.45	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1761	1/1	0.82	0.42	-	66,66,66,66	0
55	MG	BA	3522	1/1	0.87	0.43	-	84,84,84,84	0
55	MG	AA	3241	1/1	0.82	0.68	-	80,80,80,80	0
55	MG	BA	3428	1/1	0.95	0.11	-	89,89,89,89	0
55	MG	AA	3248	1/1	0.93	0.51	-	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.