



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2018 – 02:19 AM EST

PDB ID : 4V5E
Title : Insights into translational termination from the structure of RF2 bound to the ribosome
Authors : Weixlbaumer, A.; Jin, H.; Neubauer, C.; Voorhees, R.M.; Petry, S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-04-30
Resolution : 3.45 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

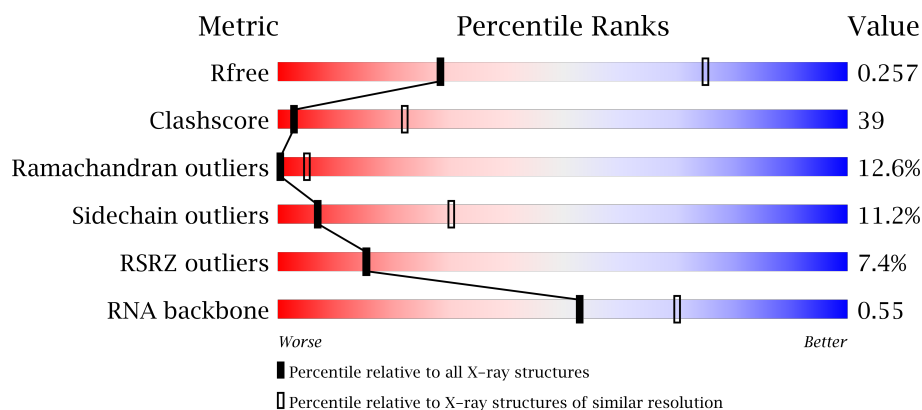
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)
RNA backbone	2435	1020 (4.02-2.86)

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	1522	<div> <div>2%</div> <div>26% 60% 12%</div> </div>
1	CA	1522	<div> <div>3%</div> <div>26% 60% 12%</div> </div>
2	AB	256	<div> <div>17%</div> <div>21% 58% 12% 8%</div> </div>
2	CB	256	<div> <div>6%</div> <div>21% 57% 12% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	8	
23	CX	8	
24	AY	351	
24	CY	351	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2901	
35	DA	2901	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

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Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
44	BJ	130	
44	DJ	130	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	

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Mol	Chain	Length	Quality of chain
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	DI	148	

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
60	MG	AA	1608	-	-	-	X
60	MG	AA	1611	-	-	-	X
60	MG	AA	1623	-	-	-	X
60	MG	AA	1625	-	-	-	X
60	MG	AA	1627	-	-	-	X
60	MG	AA	1632	-	-	-	X
60	MG	AA	1634	-	-	-	X
60	MG	AA	1650	-	-	-	X
60	MG	AA	1655	-	-	-	X
60	MG	AA	1656	-	-	-	X
60	MG	AA	1657	-	-	-	X
60	MG	AA	1669	-	-	-	X
60	MG	AA	1671	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	1672	-	-	-	X
60	MG	AA	1674	-	-	-	X
60	MG	AA	1683	-	-	-	X
60	MG	AA	1685	-	-	-	X
60	MG	AA	1714	-	-	-	X
60	MG	AA	1721	-	-	-	X
60	MG	AA	1735	-	-	-	X
60	MG	AA	1741	-	-	-	X
60	MG	AA	1745	-	-	-	X
60	MG	AA	1749	-	-	-	X
60	MG	AV	101	-	-	-	X
60	MG	AY	401	-	-	-	X
60	MG	B1	101	-	-	-	X
60	MG	B7	101	-	-	-	X
60	MG	BA	3004	-	-	-	X
60	MG	BA	3005	-	-	-	X
60	MG	BA	3009	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3012	-	-	-	X
60	MG	BA	3013	-	-	-	X
60	MG	BA	3015	-	-	-	X
60	MG	BA	3019	-	-	-	X
60	MG	BA	3020	-	-	-	X
60	MG	BA	3021	-	-	-	X
60	MG	BA	3023	-	-	-	X
60	MG	BA	3024	-	-	-	X
60	MG	BA	3026	-	-	-	X
60	MG	BA	3033	-	-	-	X
60	MG	BA	3035	-	-	-	X
60	MG	BA	3037	-	-	-	X
60	MG	BA	3042	-	-	-	X
60	MG	BA	3043	-	-	-	X
60	MG	BA	3044	-	-	-	X
60	MG	BA	3045	-	-	-	X
60	MG	BA	3049	-	-	-	X
60	MG	BA	3050	-	-	-	X
60	MG	BA	3051	-	-	-	X
60	MG	BA	3056	-	-	-	X
60	MG	BA	3058	-	-	-	X
60	MG	BA	3061	-	-	-	X
60	MG	BA	3062	-	-	-	X
60	MG	BA	3064	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3066	-	-	-	X
60	MG	BA	3067	-	-	-	X
60	MG	BA	3068	-	-	-	X
60	MG	BA	3069	-	-	-	X
60	MG	BA	3070	-	-	-	X
60	MG	BA	3071	-	-	-	X
60	MG	BA	3074	-	-	-	X
60	MG	BA	3076	-	-	-	X
60	MG	BA	3079	-	-	-	X
60	MG	BA	3082	-	-	-	X
60	MG	BA	3083	-	-	-	X
60	MG	BA	3088	-	-	-	X
60	MG	BA	3090	-	-	-	X
60	MG	BA	3098	-	-	-	X
60	MG	BA	3099	-	-	-	X
60	MG	BA	3101	-	-	-	X
60	MG	BA	3102	-	-	-	X
60	MG	BA	3103	-	-	-	X
60	MG	BA	3105	-	-	-	X
60	MG	BA	3106	-	-	-	X
60	MG	BA	3107	-	-	-	X
60	MG	BA	3108	-	-	-	X
60	MG	BA	3113	-	-	-	X
60	MG	BA	3114	-	-	-	X
60	MG	BA	3116	-	-	-	X
60	MG	BA	3123	-	-	-	X
60	MG	BA	3128	-	-	-	X
60	MG	BA	3138	-	-	-	X
60	MG	BA	3142	-	-	-	X
60	MG	BA	3145	-	-	-	X
60	MG	BA	3147	-	-	-	X
60	MG	BA	3155	-	-	-	X
60	MG	BA	3158	-	-	-	X
60	MG	BA	3159	-	-	-	X
60	MG	BA	3160	-	-	-	X
60	MG	BA	3163	-	-	-	X
60	MG	BA	3164	-	-	-	X
60	MG	BA	3165	-	-	-	X
60	MG	BA	3175	-	-	-	X
60	MG	BA	3182	-	-	-	X
60	MG	BA	3184	-	-	-	X
60	MG	BA	3185	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3188	-	-	-	X
60	MG	BA	3196	-	-	-	X
60	MG	BA	3201	-	-	-	X
60	MG	BA	3202	-	-	-	X
60	MG	BA	3206	-	-	-	X
60	MG	BA	3213	-	-	-	X
60	MG	BA	3214	-	-	-	X
60	MG	BA	3219	-	-	-	X
60	MG	BA	3224	-	-	-	X
60	MG	BA	3225	-	-	-	X
60	MG	BA	3228	-	-	-	X
60	MG	BA	3233	-	-	-	X
60	MG	BA	3243	-	-	-	X
60	MG	BA	3252	-	-	-	X
60	MG	BA	3257	-	-	-	X
60	MG	BA	3264	-	-	-	X
60	MG	BA	3267	-	-	-	X
60	MG	BA	3269	-	-	-	X
60	MG	BA	3271	-	-	-	X
60	MG	BA	3279	-	-	-	X
60	MG	BA	3280	-	-	-	X
60	MG	BA	3287	-	-	-	X
60	MG	BA	3296	-	-	-	X
60	MG	BA	3299	-	-	-	X
60	MG	BA	3300	-	-	-	X
60	MG	BA	3303	-	-	-	X
60	MG	BA	3305	-	-	-	X
60	MG	BA	3307	-	-	-	X
60	MG	BA	3318	-	-	-	X
60	MG	BA	3342	-	-	-	X
60	MG	BA	3346	-	-	-	X
60	MG	BA	3347	-	-	-	X
60	MG	BA	3348	-	-	-	X
60	MG	BA	3351	-	-	-	X
60	MG	BD	301	-	-	-	X
60	MG	CA	1603	-	-	-	X
60	MG	CA	1607	-	-	-	X
60	MG	CA	1610	-	-	-	X
60	MG	CA	1612	-	-	-	X
60	MG	CA	1616	-	-	-	X
60	MG	CA	1622	-	-	-	X
60	MG	CA	1624	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	1631	-	-	-	X
60	MG	CA	1633	-	-	-	X
60	MG	CA	1635	-	-	-	X
60	MG	CA	1645	-	-	-	X
60	MG	CA	1649	-	-	-	X
60	MG	CA	1669	-	-	-	X
60	MG	CA	1674	-	-	-	X
60	MG	CA	1686	-	-	-	X
60	MG	CA	1695	-	-	-	X
60	MG	CA	1719	-	-	-	X
60	MG	CA	1722	-	-	-	X
60	MG	CA	1736	-	-	-	X
60	MG	CA	1746	-	-	-	X
60	MG	CA	1750	-	-	-	X
60	MG	CV	101	-	-	-	X
60	MG	CY	401	-	-	-	X
60	MG	D1	101	-	-	-	X
60	MG	DA	3002	-	-	-	X
60	MG	DA	3005	-	-	-	X
60	MG	DA	3006	-	-	-	X
60	MG	DA	3010	-	-	-	X
60	MG	DA	3012	-	-	-	X
60	MG	DA	3013	-	-	-	X
60	MG	DA	3014	-	-	-	X
60	MG	DA	3016	-	-	-	X
60	MG	DA	3020	-	-	-	X
60	MG	DA	3021	-	-	-	X
60	MG	DA	3022	-	-	-	X
60	MG	DA	3024	-	-	-	X
60	MG	DA	3025	-	-	-	X
60	MG	DA	3027	-	-	-	X
60	MG	DA	3033	-	-	-	X
60	MG	DA	3034	-	-	-	X
60	MG	DA	3036	-	-	-	X
60	MG	DA	3038	-	-	-	X
60	MG	DA	3043	-	-	-	X
60	MG	DA	3044	-	-	-	X
60	MG	DA	3046	-	-	-	X
60	MG	DA	3048	-	-	-	X
60	MG	DA	3052	-	-	-	X
60	MG	DA	3053	-	-	-	X
60	MG	DA	3055	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3057	-	-	-	X
60	MG	DA	3059	-	-	-	X
60	MG	DA	3061	-	-	-	X
60	MG	DA	3062	-	-	-	X
60	MG	DA	3063	-	-	-	X
60	MG	DA	3065	-	-	-	X
60	MG	DA	3067	-	-	-	X
60	MG	DA	3068	-	-	-	X
60	MG	DA	3069	-	-	-	X
60	MG	DA	3070	-	-	-	X
60	MG	DA	3071	-	-	-	X
60	MG	DA	3072	-	-	-	X
60	MG	DA	3074	-	-	-	X
60	MG	DA	3075	-	-	-	X
60	MG	DA	3077	-	-	-	X
60	MG	DA	3079	-	-	-	X
60	MG	DA	3080	-	-	-	X
60	MG	DA	3081	-	-	-	X
60	MG	DA	3083	-	-	-	X
60	MG	DA	3084	-	-	-	X
60	MG	DA	3089	-	-	-	X
60	MG	DA	3091	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3097	-	-	-	X
60	MG	DA	3099	-	-	-	X
60	MG	DA	3100	-	-	-	X
60	MG	DA	3103	-	-	-	X
60	MG	DA	3104	-	-	-	X
60	MG	DA	3106	-	-	-	X
60	MG	DA	3107	-	-	-	X
60	MG	DA	3108	-	-	-	X
60	MG	DA	3109	-	-	-	X
60	MG	DA	3114	-	-	-	X
60	MG	DA	3116	-	-	-	X
60	MG	DA	3127	-	-	-	X
60	MG	DA	3129	-	-	-	X
60	MG	DA	3131	-	-	-	X
60	MG	DA	3139	-	-	-	X
60	MG	DA	3143	-	-	-	X
60	MG	DA	3146	-	-	-	X
60	MG	DA	3148	-	-	-	X
60	MG	DA	3151	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3152	-	-	-	X
60	MG	DA	3156	-	-	-	X
60	MG	DA	3157	-	-	-	X
60	MG	DA	3159	-	-	-	X
60	MG	DA	3160	-	-	-	X
60	MG	DA	3161	-	-	-	X
60	MG	DA	3162	-	-	-	X
60	MG	DA	3163	-	-	-	X
60	MG	DA	3165	-	-	-	X
60	MG	DA	3166	-	-	-	X
60	MG	DA	3167	-	-	-	X
60	MG	DA	3170	-	-	-	X
60	MG	DA	3184	-	-	-	X
60	MG	DA	3186	-	-	-	X
60	MG	DA	3196	-	-	-	X
60	MG	DA	3197	-	-	-	X
60	MG	DA	3203	-	-	-	X
60	MG	DA	3206	-	-	-	X
60	MG	DA	3207	-	-	-	X
60	MG	DA	3214	-	-	-	X
60	MG	DA	3215	-	-	-	X
60	MG	DA	3220	-	-	-	X
60	MG	DA	3225	-	-	-	X
60	MG	DA	3226	-	-	-	X
60	MG	DA	3229	-	-	-	X
60	MG	DA	3234	-	-	-	X
60	MG	DA	3238	-	-	-	X
60	MG	DA	3245	-	-	-	X
60	MG	DA	3253	-	-	-	X
60	MG	DA	3258	-	-	-	X
60	MG	DA	3259	-	-	-	X
60	MG	DA	3265	-	-	-	X
60	MG	DA	3267	-	-	-	X
60	MG	DA	3269	-	-	-	X
60	MG	DA	3271	-	-	-	X
60	MG	DA	3287	-	-	-	X
60	MG	DA	3295	-	-	-	X
60	MG	DA	3298	-	-	-	X
60	MG	DA	3299	-	-	-	X
60	MG	DA	3304	-	-	-	X
60	MG	DA	3305	-	-	-	X
60	MG	DA	3317	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3327	-	-	-	X
60	MG	DA	3344	-	-	-	X
60	MG	DA	3345	-	-	-	X
60	MG	DD	301	-	-	-	X
60	MG	DD	302	-	-	-	X
60	MG	DF	301	-	-	-	X
60	MG	DF	303	-	-	-	X
60	MG	DR	201	-	-	-	X
60	MG	DU	201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 304505 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			
12	CL	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			
13	CM	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	7			
23	CX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	7			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	351	Total	C	N	O	S	0	0	0
			2799	1751	503	537	8			
24	CY	351	Total	C	N	O	S	0	0	0
			2799	1751	503	537	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	303	GLU	ARG	conflict	UNP Q5SM01
CY	303	GLU	ARG	conflict	UNP Q5SM01

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
25	D0	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
29	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
34	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2886	Total	C	N	O	P	0	0	0
			62154	27663	11625	19981	2885			
35	DA	2886	Total	C	N	O	P	0	0	0
			62154	27663	11625	19981	2885			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
42	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			
44	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			
45	DK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
47	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
48	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
49	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
50	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
51	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
52	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
53	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
54	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
55	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
58	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 59 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DI	146	Total	C	N	O	S	0	0	1
			1133	724	201	207	1			

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	354	Total	Mg	0	0
			354	354		
60	CA	157	Total	Mg	0	0
			157	157		
60	DQ	1	Total	Mg	0	0
			1	1		
60	DF	3	Total	Mg	0	0
			3	3		
60	CV	7	Total	Mg	0	0
			7	7		
60	AW	5	Total	Mg	0	0
			5	5		
60	DU	1	Total	Mg	0	0
			1	1		
60	B1	1	Total	Mg	0	0
			1	1		
60	DY	1	Total	Mg	0	0
			1	1		
60	BP	1	Total	Mg	0	0
			1	1		
60	DC	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CY	1	Total 1	Mg 1	0	0
60	B5	2	Total 2	Mg 2	0	0
60	BB	4	Total 4	Mg 4	0	0
60	AE	1	Total 1	Mg 1	0	0
60	DB	4	Total 4	Mg 4	0	0
60	D3	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	7	Total 7	Mg 7	0	0
60	DR	1	Total 1	Mg 1	0	0
60	AA	157	Total 157	Mg 157	0	0
60	BQ	1	Total 1	Mg 1	0	0
60	D7	1	Total 1	Mg 1	0	0
60	BC	1	Total 1	Mg 1	0	0
60	AM	1	Total 1	Mg 1	0	0
60	BU	1	Total 1	Mg 1	0	0
60	CN	1	Total 1	Mg 1	0	0
60	DD	2	Total 2	Mg 2	0	0
60	DH	1	Total 1	Mg 1	0	0
60	B3	1	Total 1	Mg 1	0	0
60	DX	1	Total 1	Mg 1	0	0
60	DA	353	Total 353	Mg 353	0	0

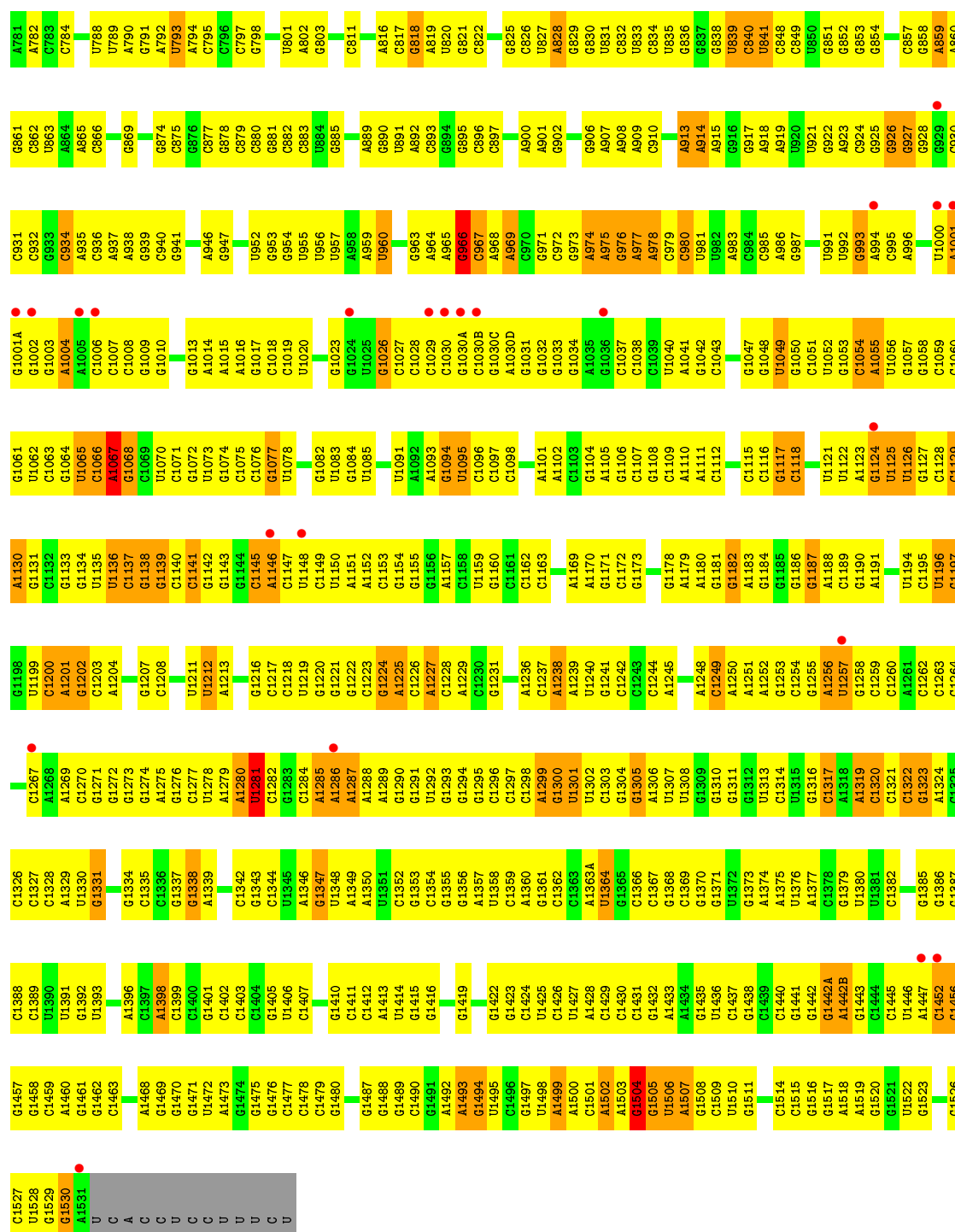
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B7	2	Total 2	Mg 2	0	0
60	AL	1	Total 1	Mg 1	0	0
60	D1	1	Total 1	Mg 1	0	0
60	BS	1	Total 1	Mg 1	0	0
60	CW	5	Total 5	Mg 5	0	0
60	D5	2	Total 2	Mg 2	0	0
60	BD	2	Total 2	Mg 2	0	0
60	AY	1	Total 1	Mg 1	0	0
60	CL	1	Total 1	Mg 1	0	0
60	BH	1	Total 1	Mg 1	0	0

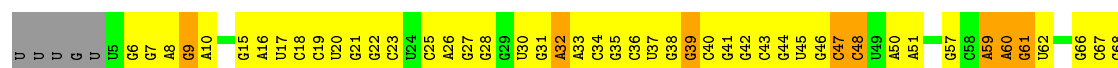
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CN	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0

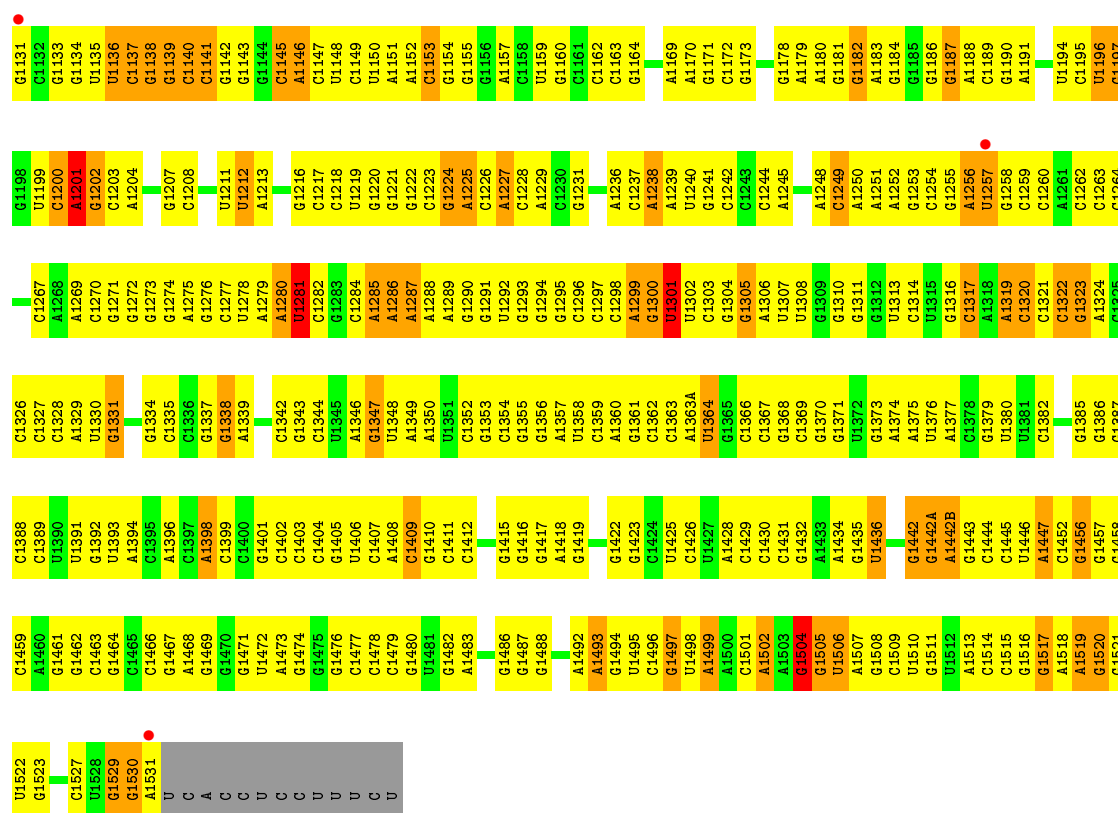


• Molecule 1: 16S ribosomal RNA

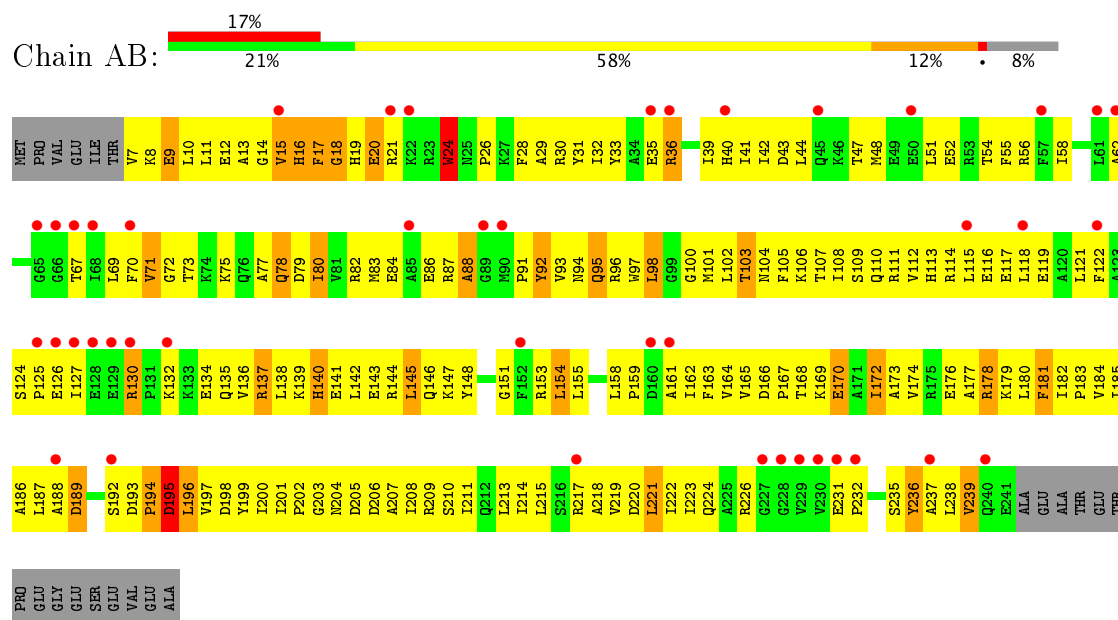
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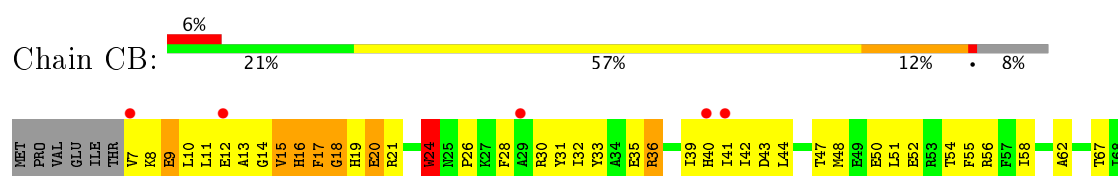
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A935	C936	A937	A938	A939	C940	C941	A946	C947	C948	U952	C953	C954	U955	U956	U957	A958	A959	U960	U961	C962	C963	A964	A965	C966	C967	A968	A969	C970	C971	C972	G973	A974	A975	C976	A977	A978	C979	C980	U981	U982	A983	C984	C985	A986	C987	U991	U992	C993	A994	C995	A996	U1000	A1001	U1001A	G1002						
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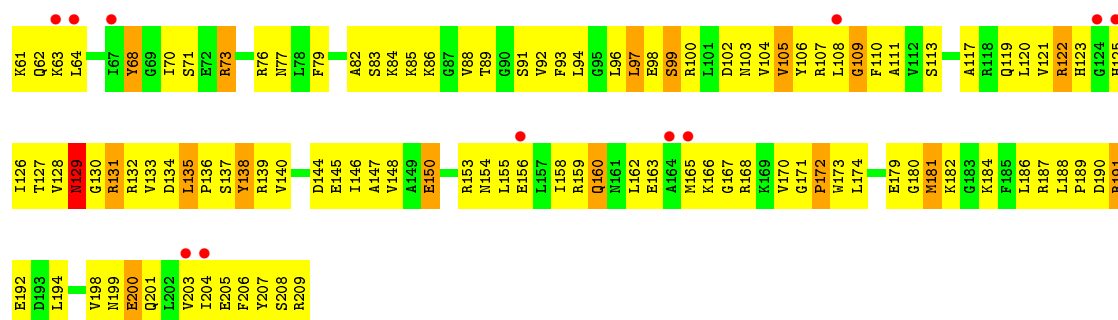
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



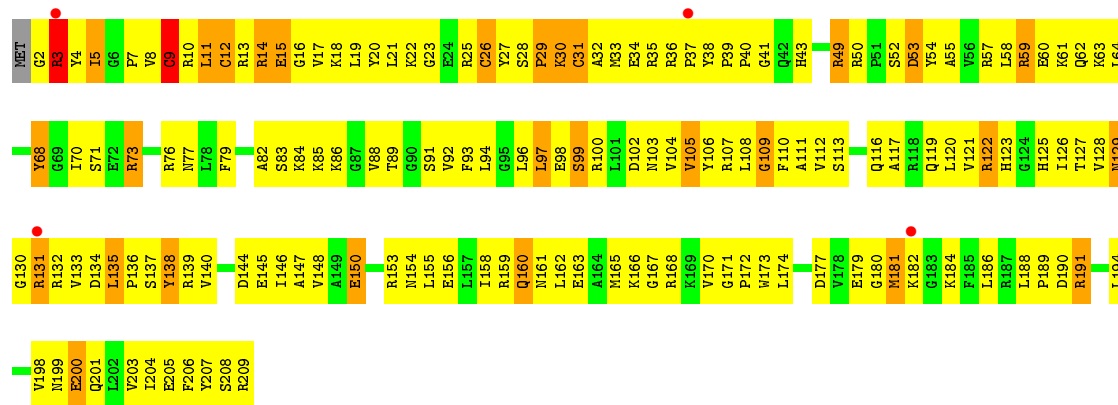
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



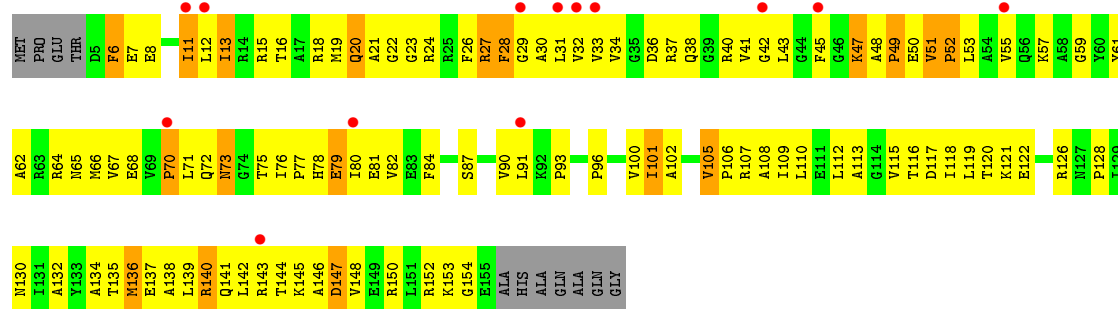




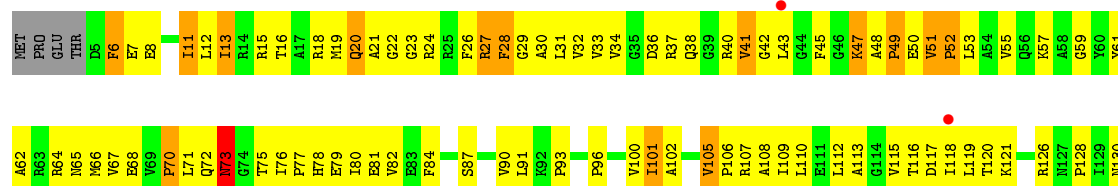
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

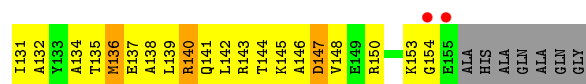


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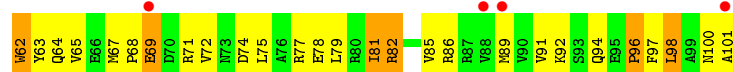


• Molecule 5: 30S RIBOSOMAL PROTEIN S5





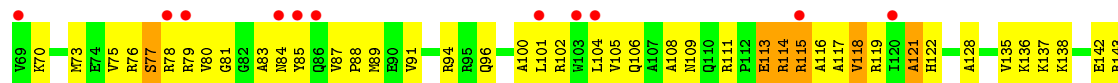
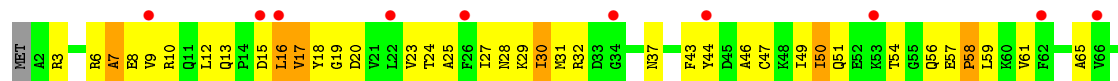
● Molecule 6: 30S RIBOSOMAL PROTEIN S6



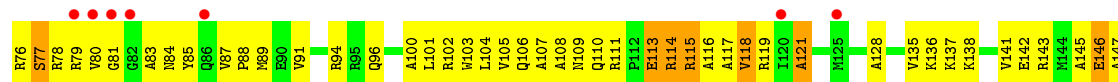
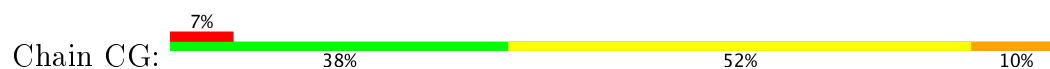
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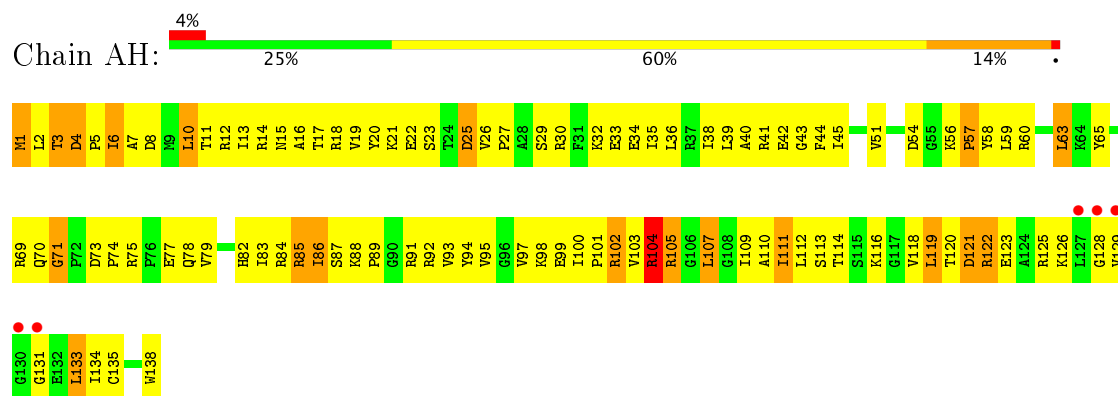
● Molecule 7: 30S RIBOSOMAL PROTEIN S7



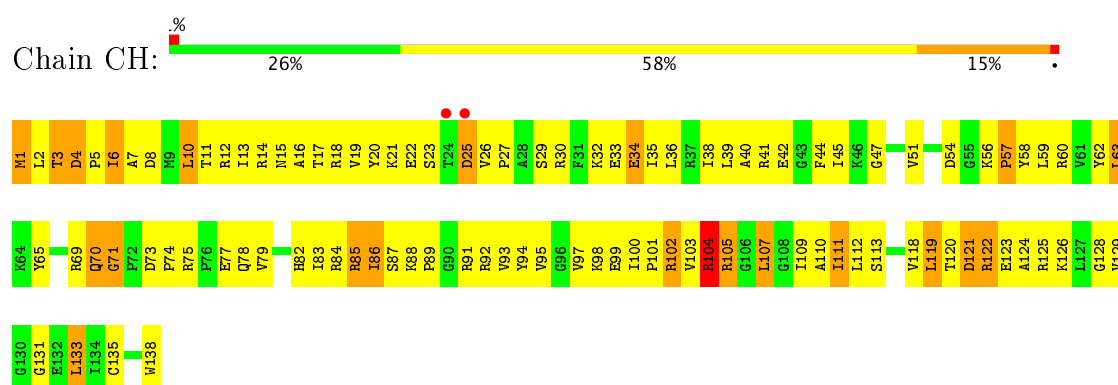
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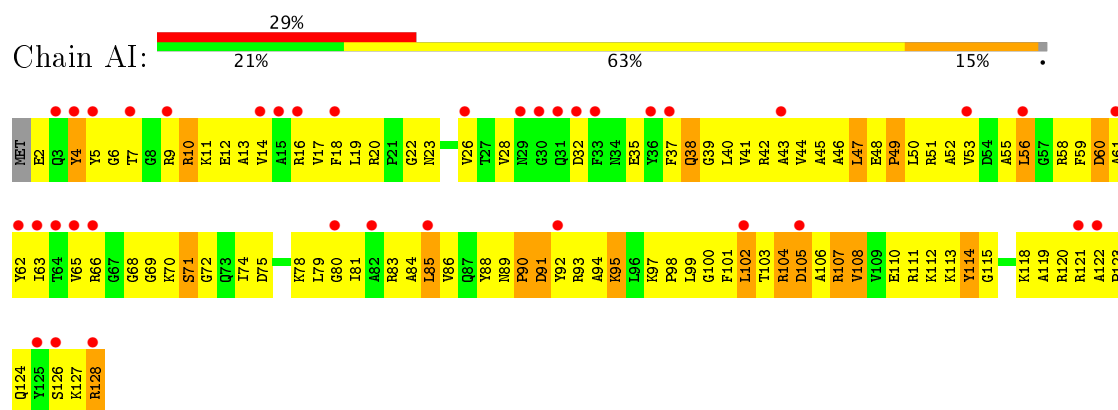
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



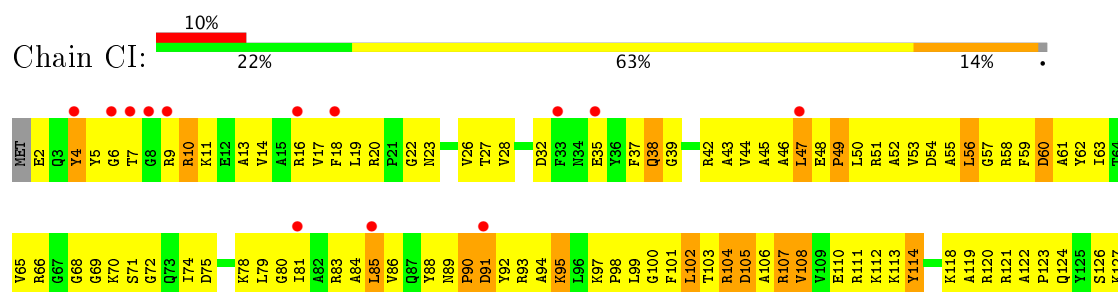
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



- Molecule 9: 30S RIBOSOMAL PROTEIN S9

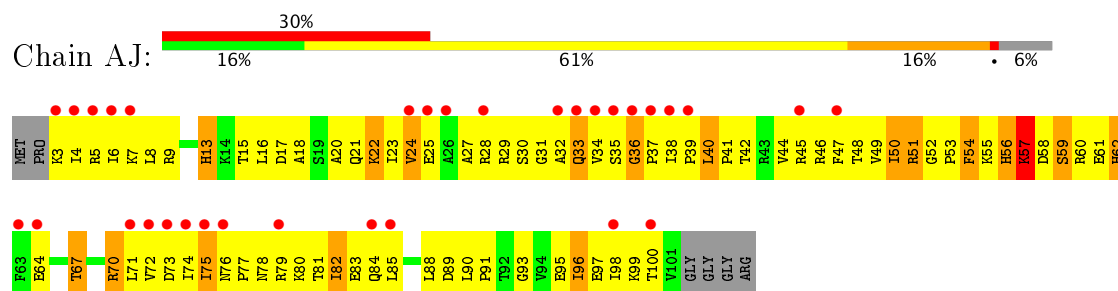


- Molecule 9: 30S RIBOSOMAL PROTEIN S9

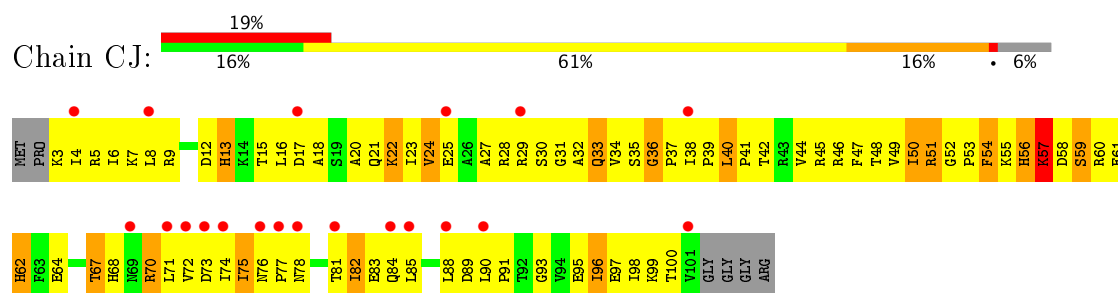


R128

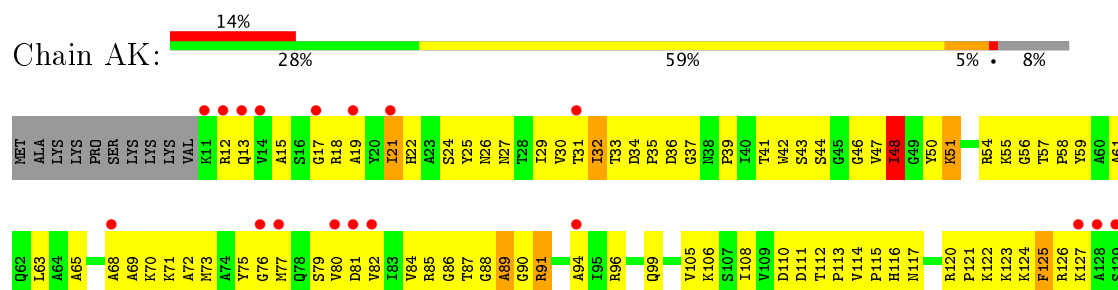
● Molecule 10: 30S RIBOSOMAL PROTEIN S10



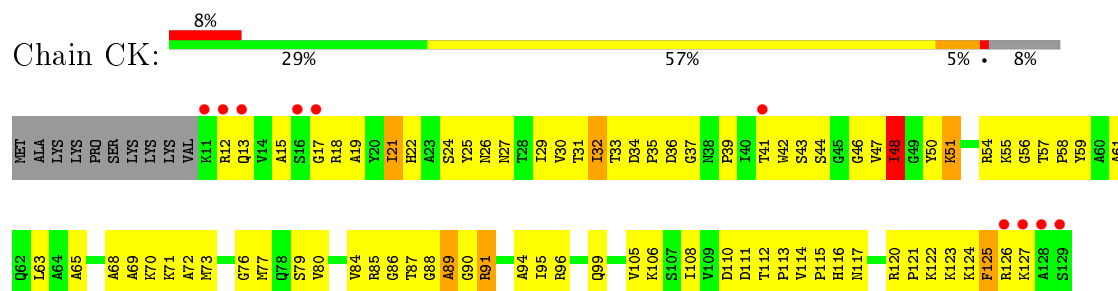
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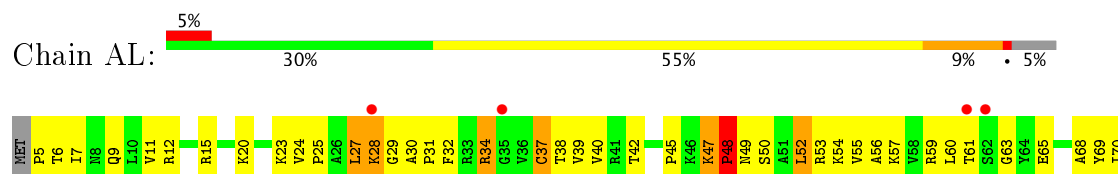
● Molecule 11: 30S RIBOSOMAL PROTEIN S11

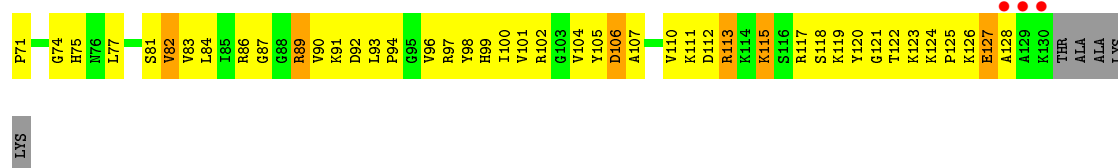


● Molecule 11: 30S RIBOSOMAL PROTEIN S11

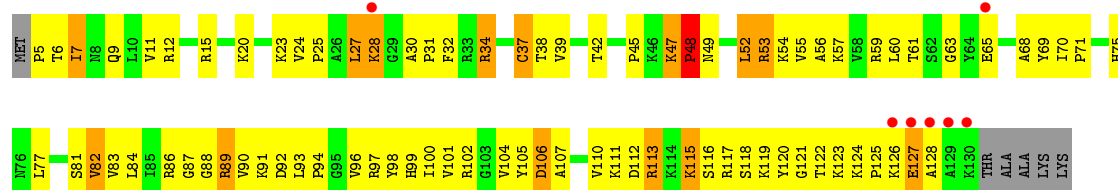


● Molecule 12: 30S RIBOSOMAL PROTEIN S12

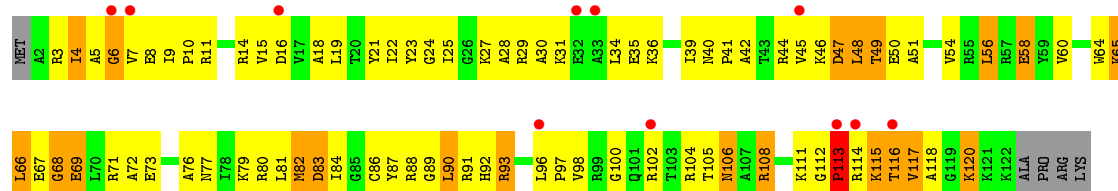




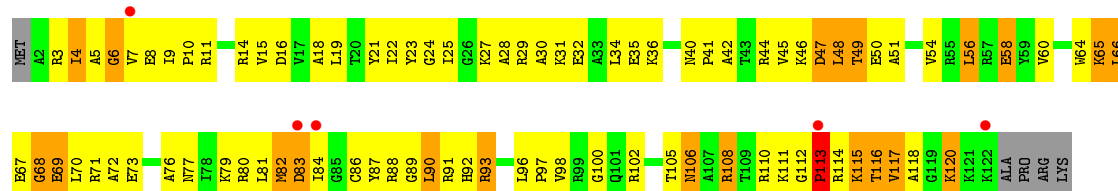
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



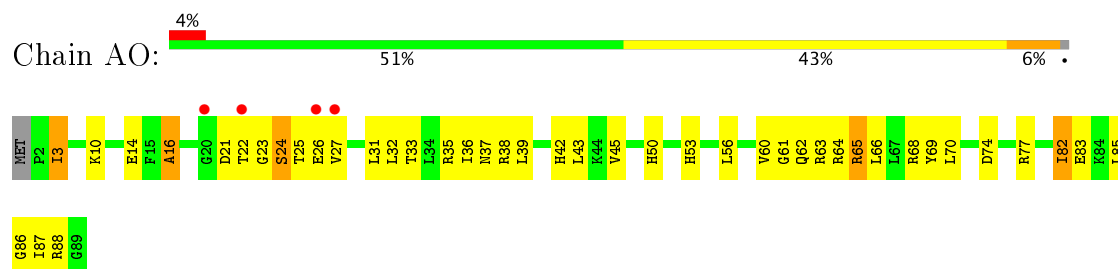
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



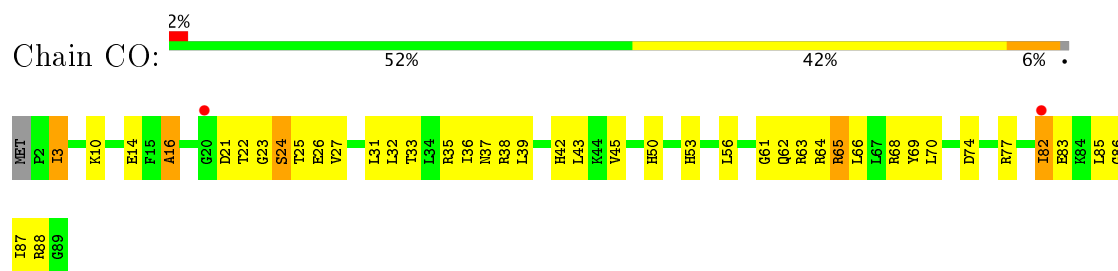
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



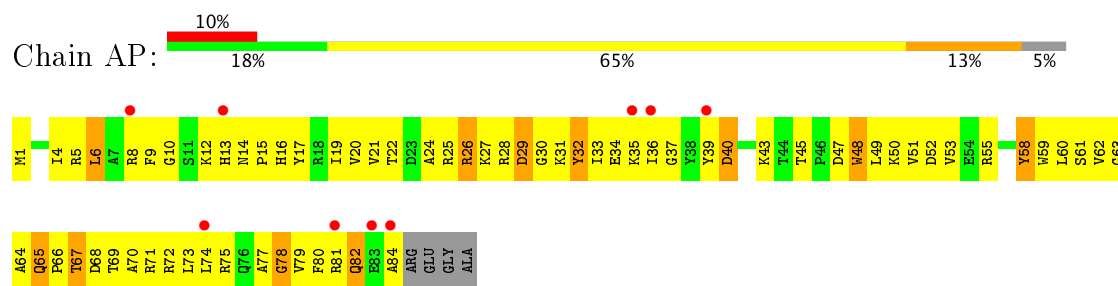
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



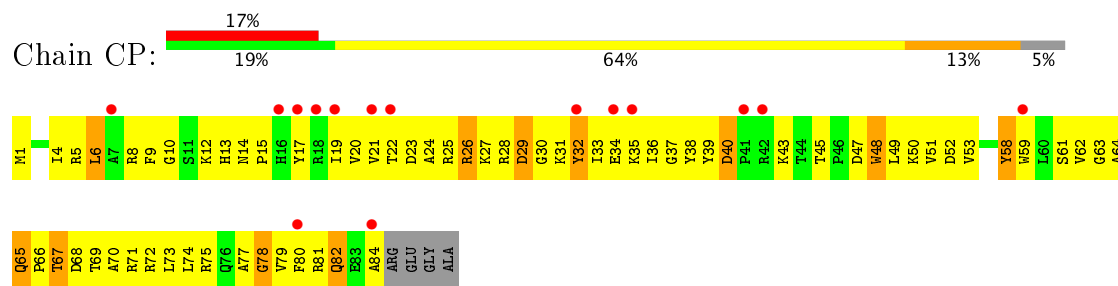
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



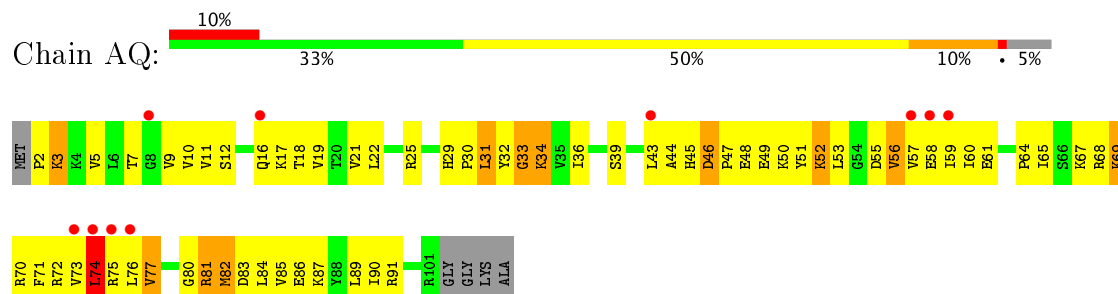
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

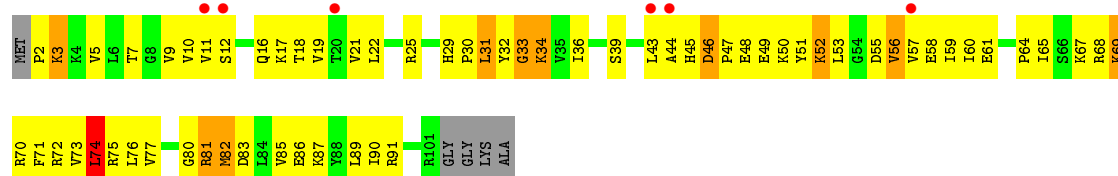


- Molecule 17: 30S RIBOSOMAL PROTEIN S17

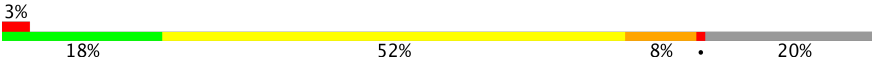


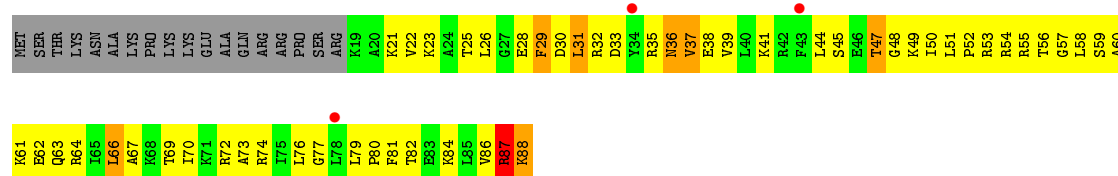
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ: 

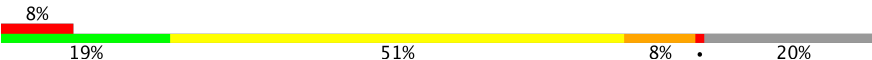


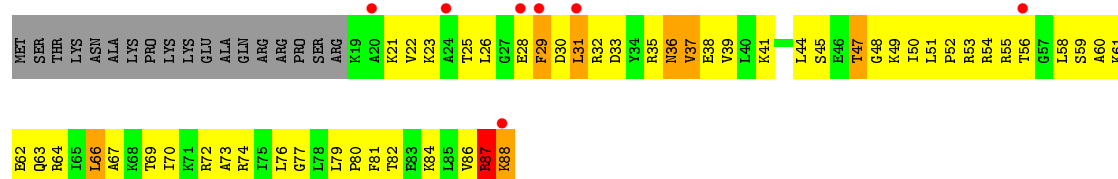
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 

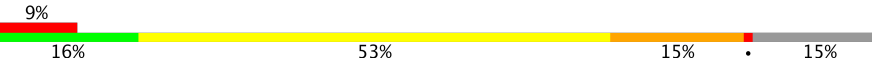


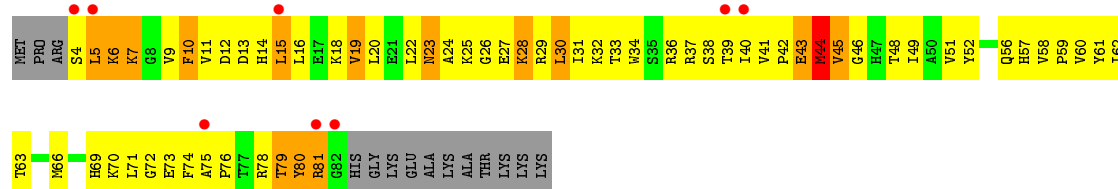
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR: 

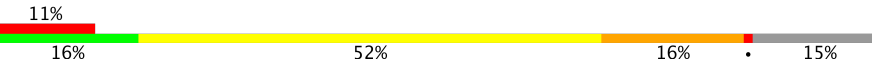


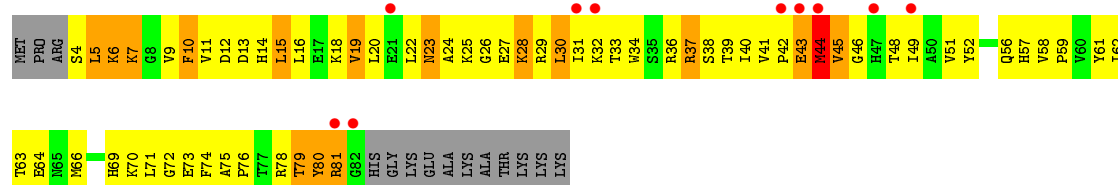
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 

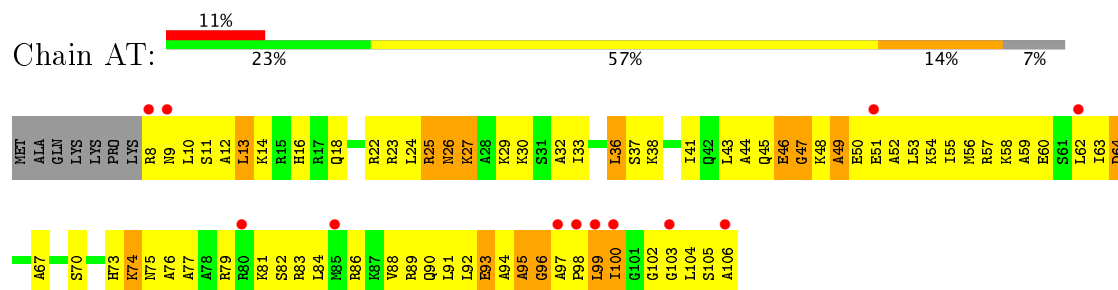


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

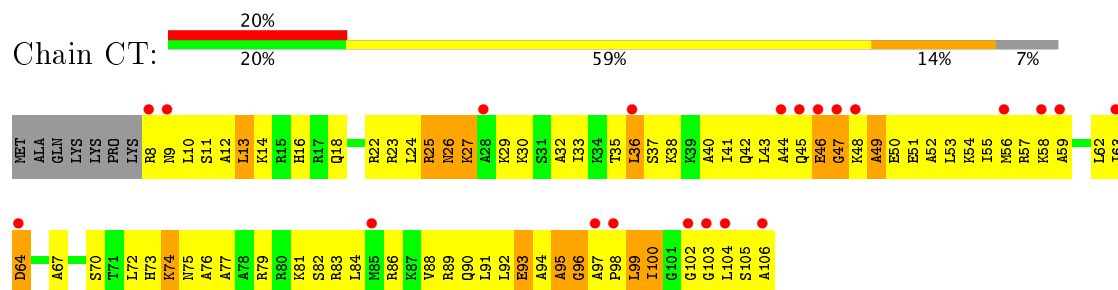
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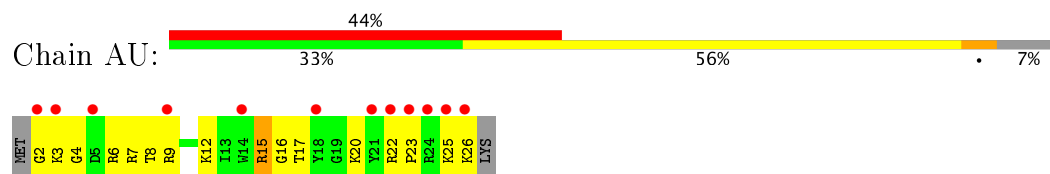
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



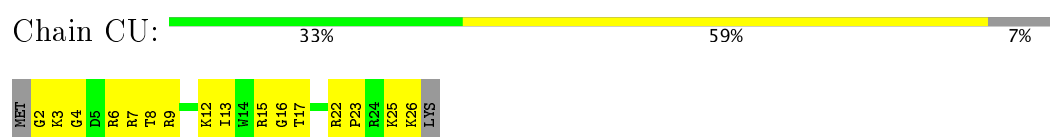
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



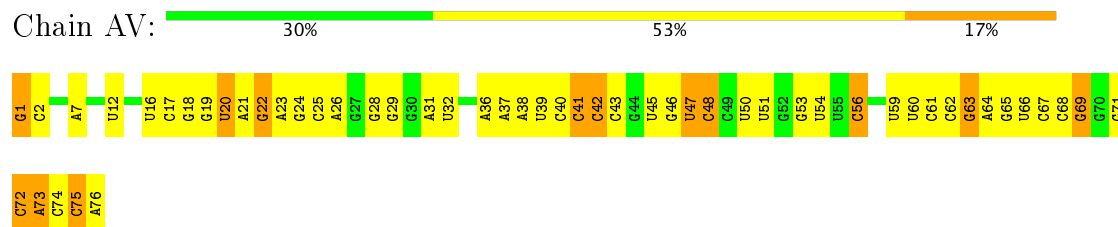
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



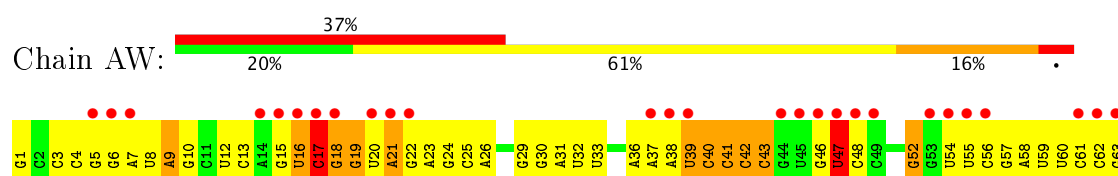
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

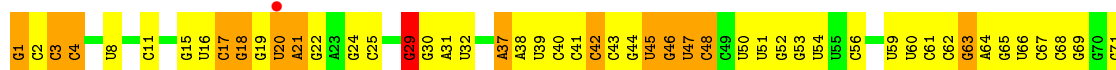


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

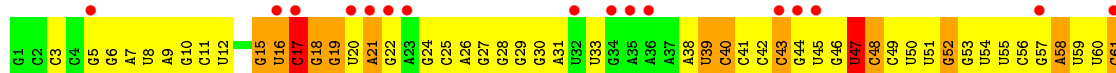




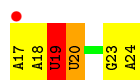
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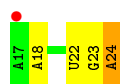
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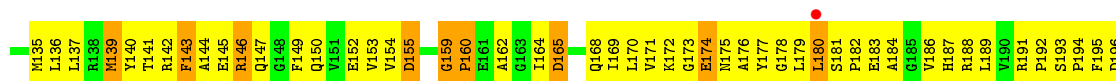
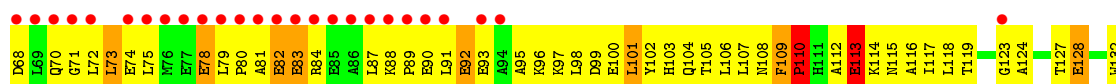
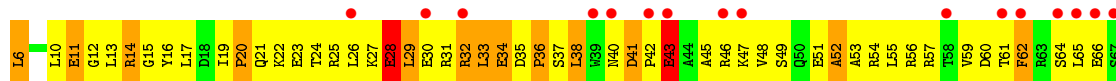
- Molecule 23: MRNA

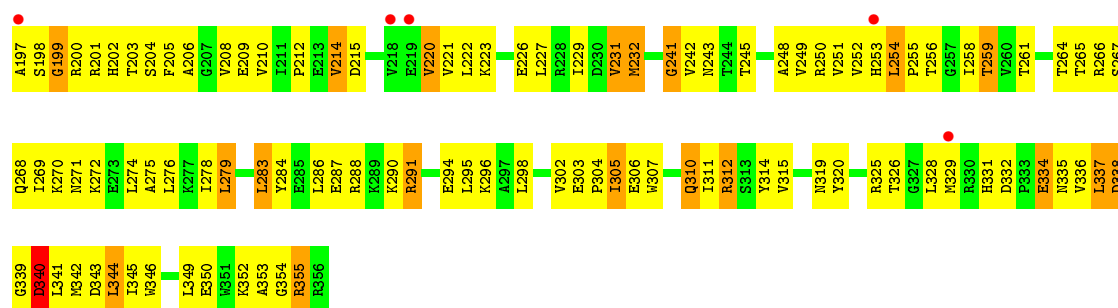


- Molecule 23: MRNA

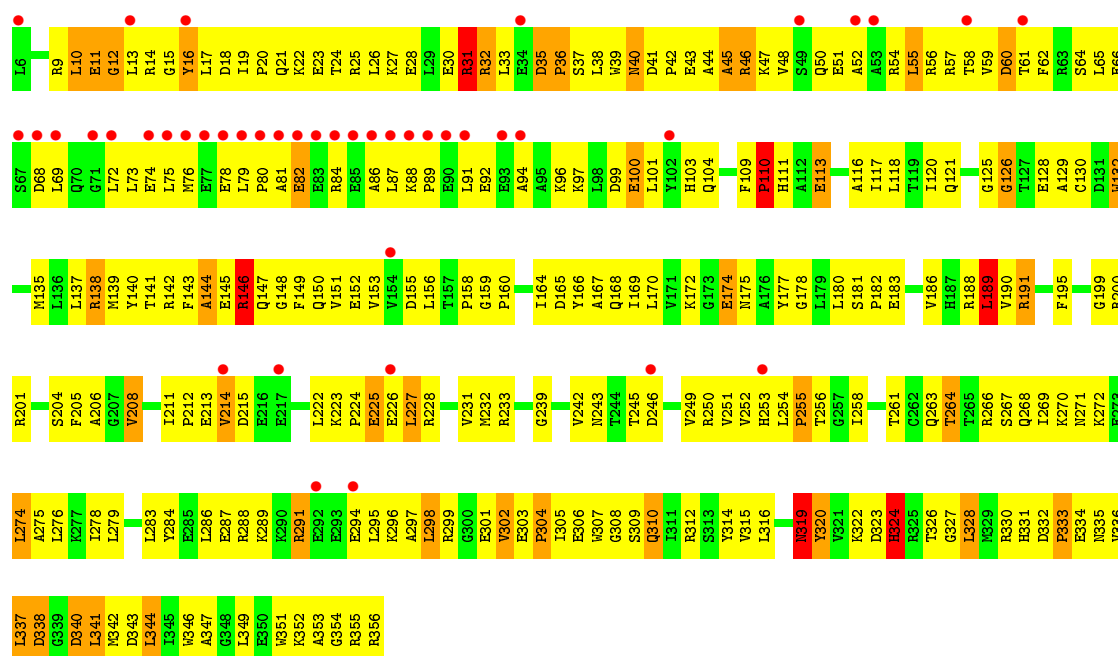


- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

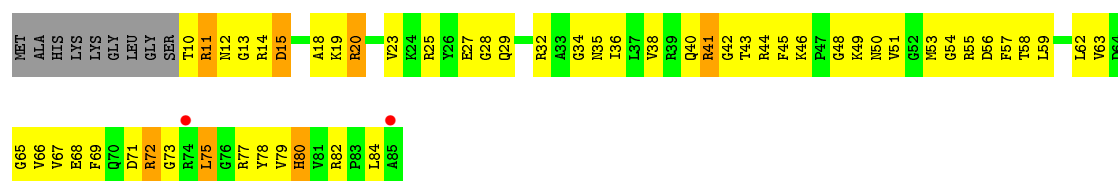




• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2



• Molecule 25: 50S RIBOSOMAL PROTEIN L27

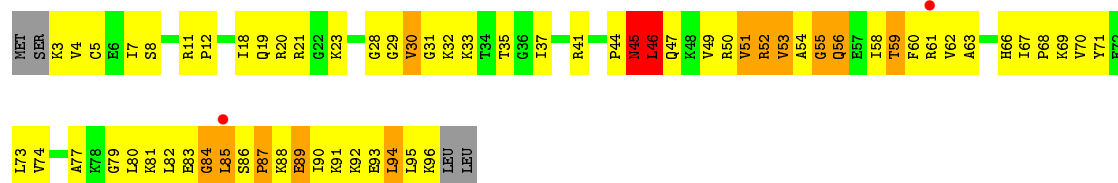


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

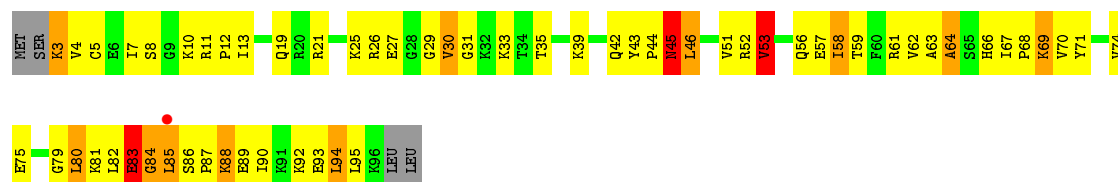




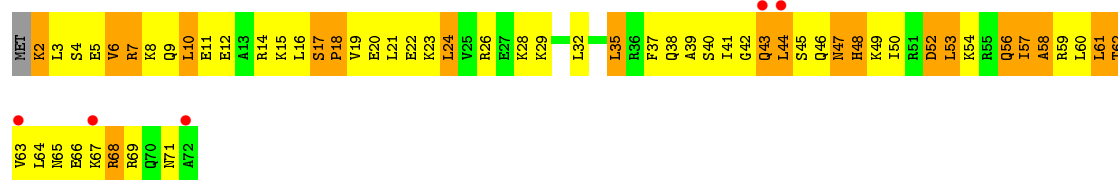
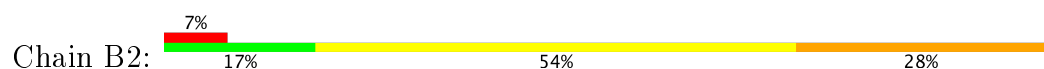
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



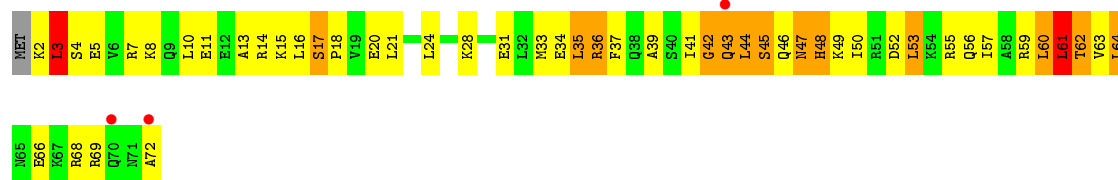
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



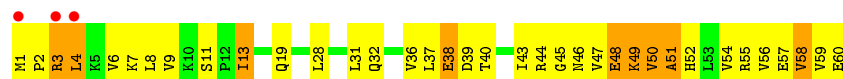
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



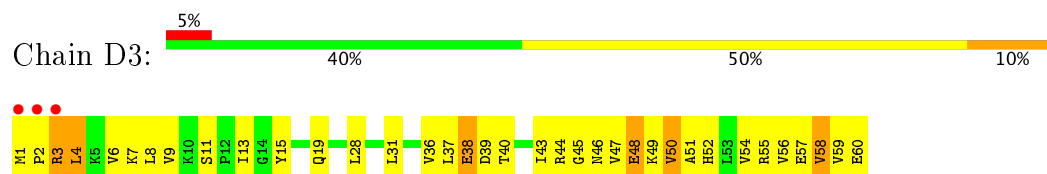
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



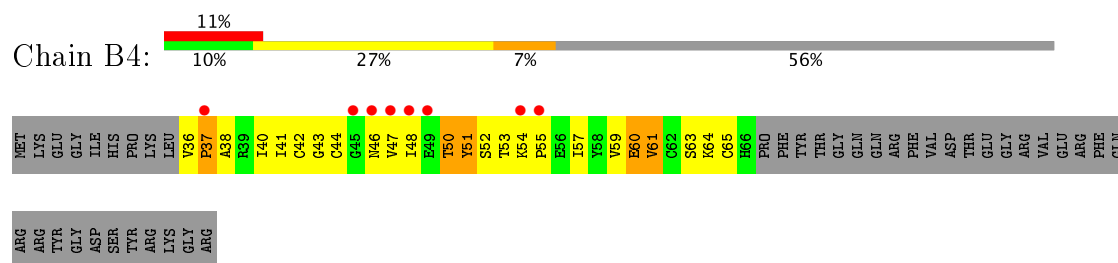
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



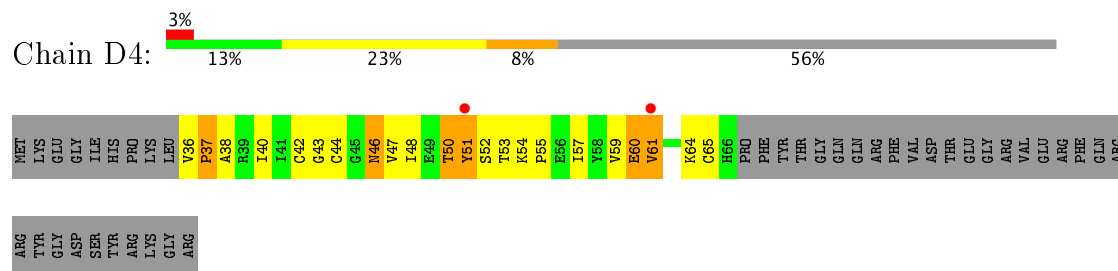
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



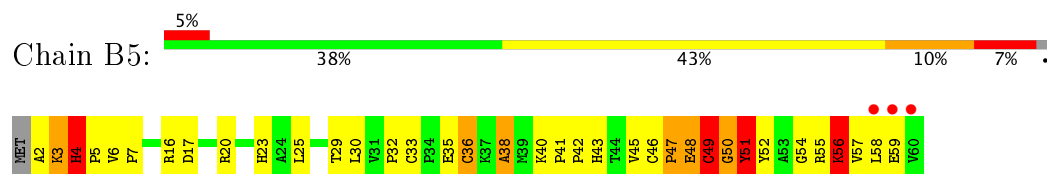
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



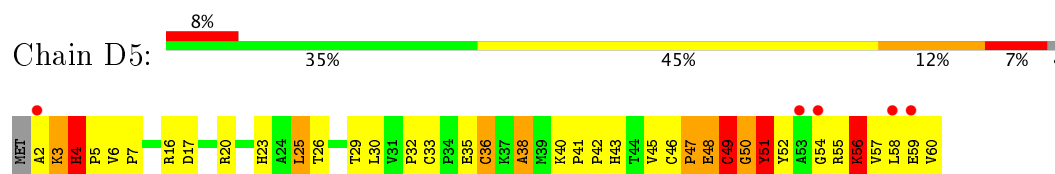
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



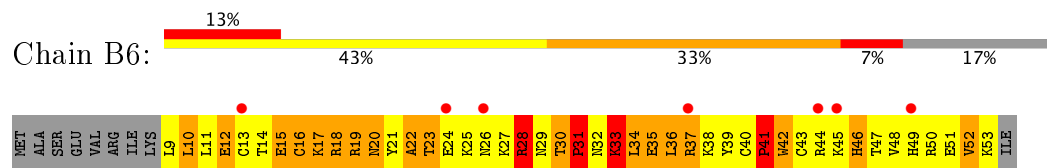
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 30: 50S RIBOSOMAL PROTEIN L32

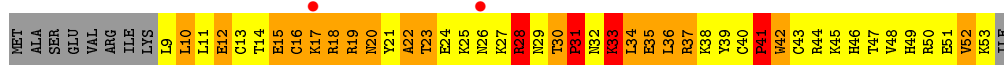


- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33





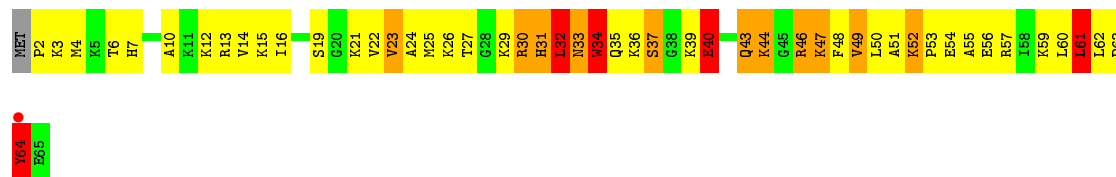
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



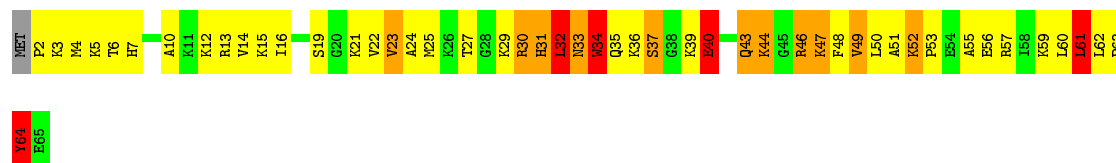
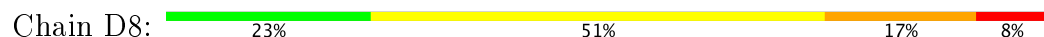
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



- Molecule 33: 50S RIBOSOMAL PROTEIN L35



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

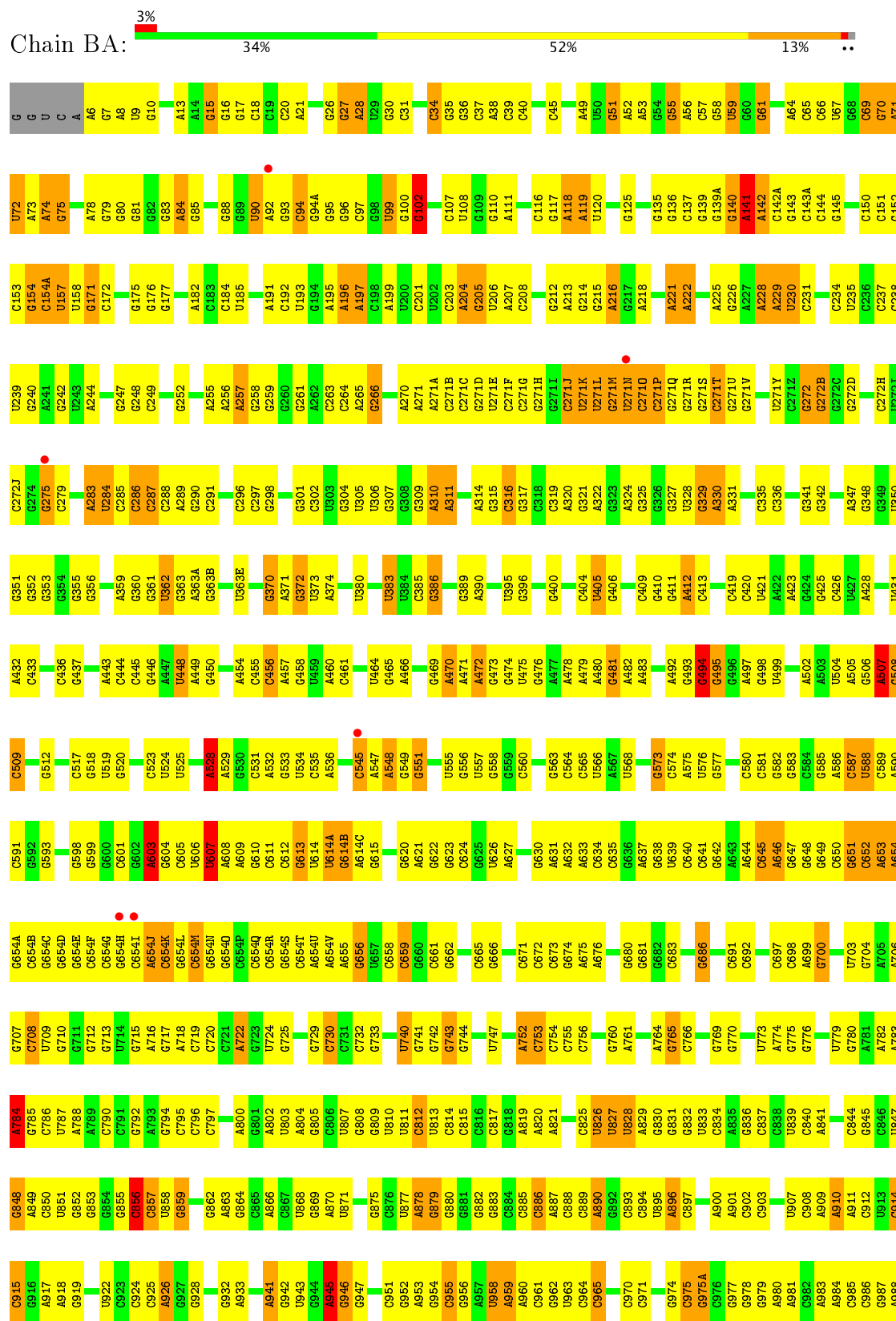


- Molecule 34: 50S RIBOSOMAL PROTEIN L36

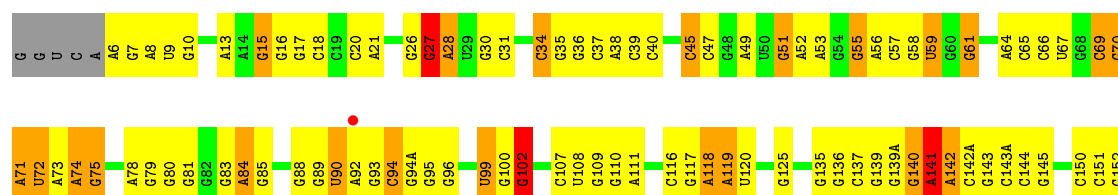


- Molecule 34: 50S RIBOSOMAL PROTEIN L36



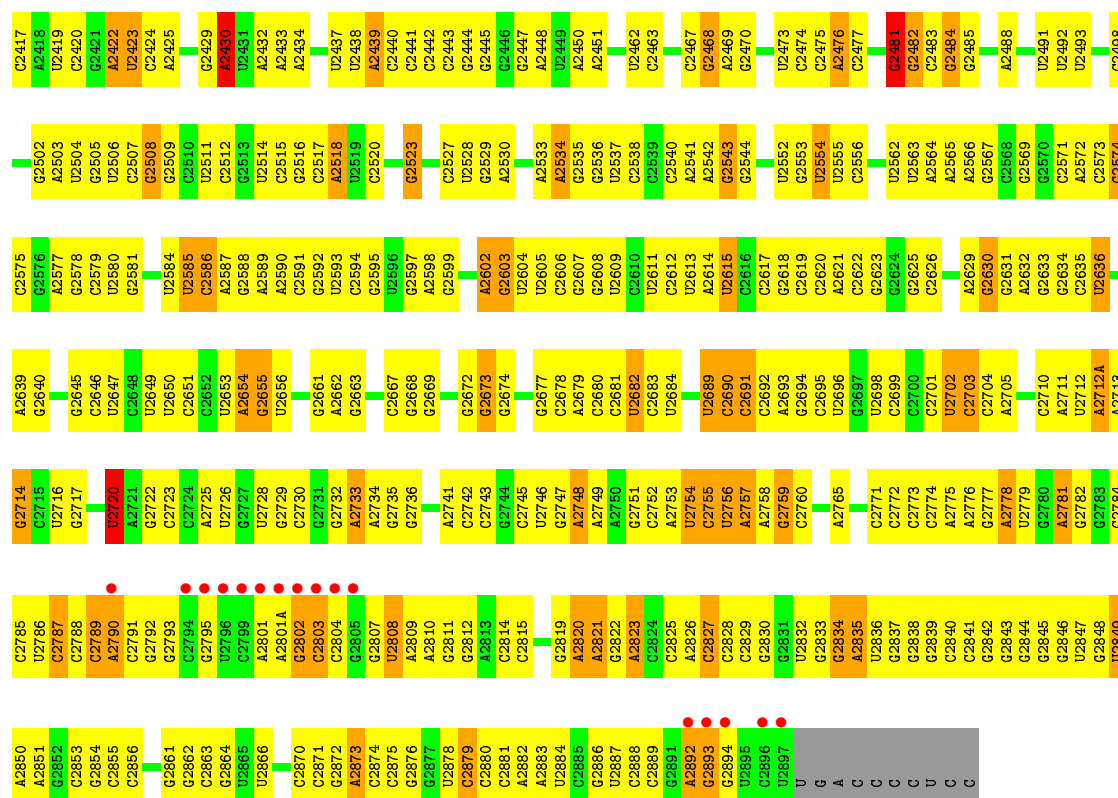






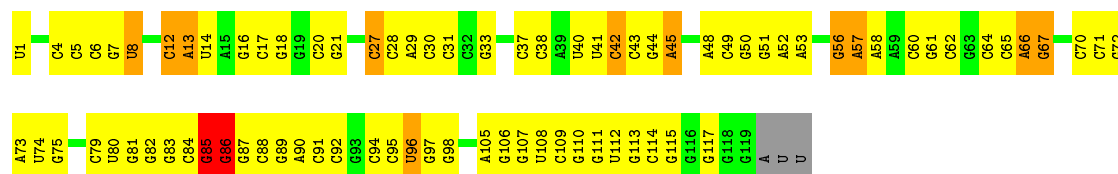






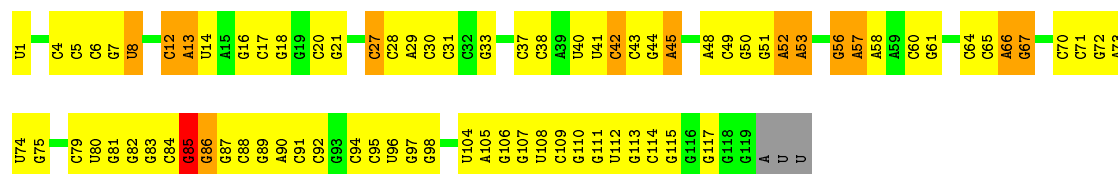
• Molecule 36: 5S RIBOSOMAL RNA

Chain BB: 31% 56% 9% ..



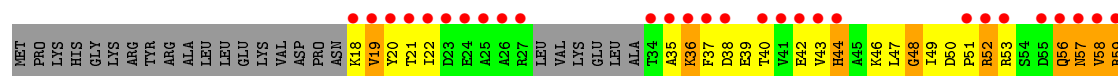
• Molecule 36: 5S RIBOSOMAL RNA

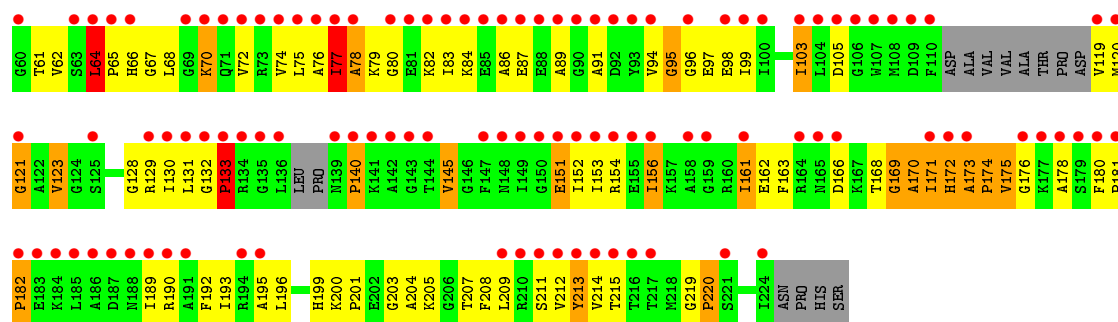
Chain DB: 31% 55% 11% ..



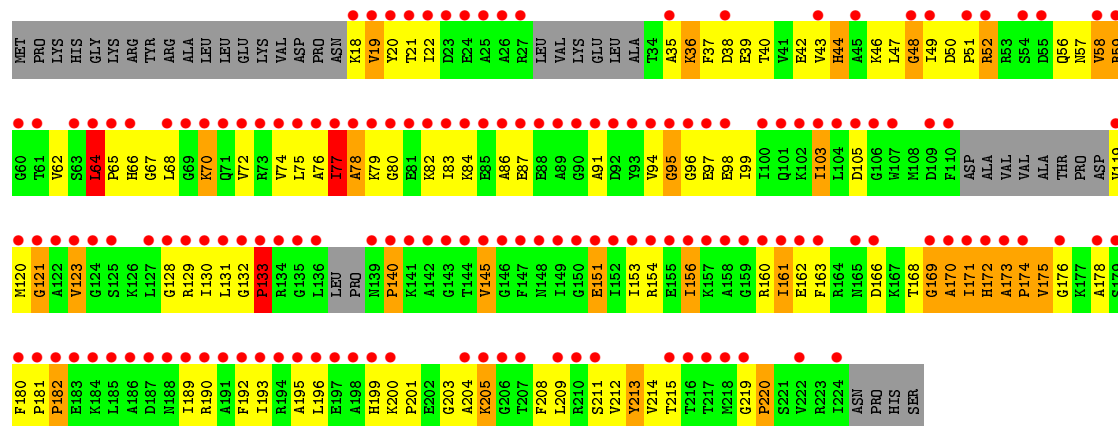
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC: 34% 59% 35% 13% 17%

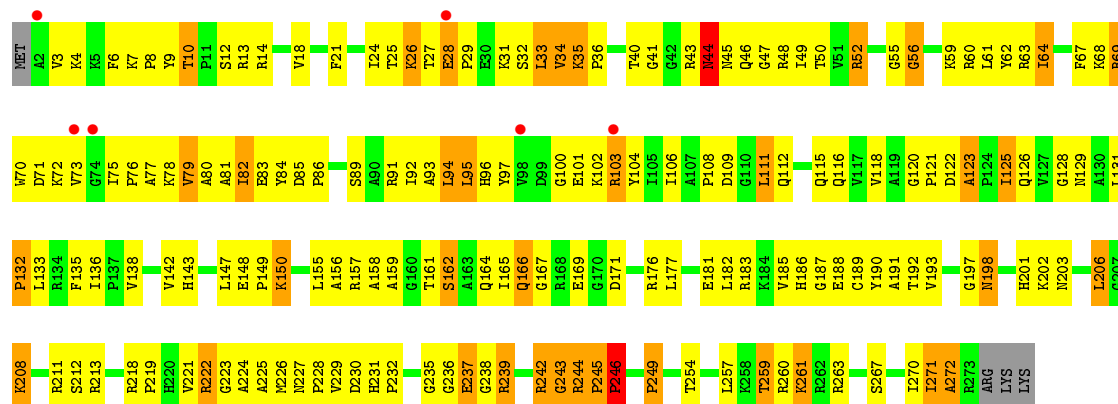




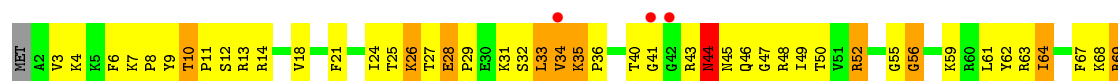
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

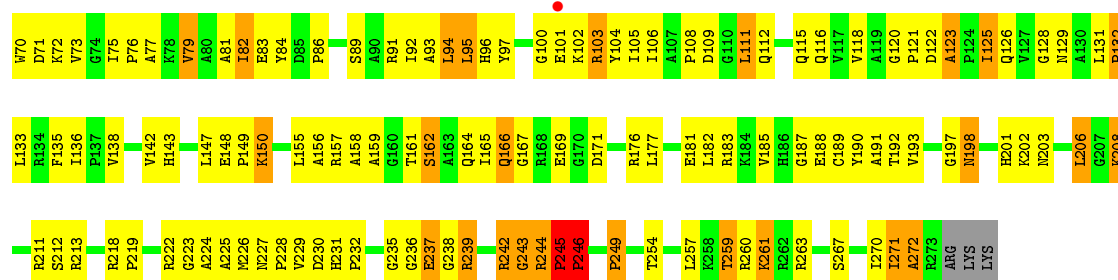


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

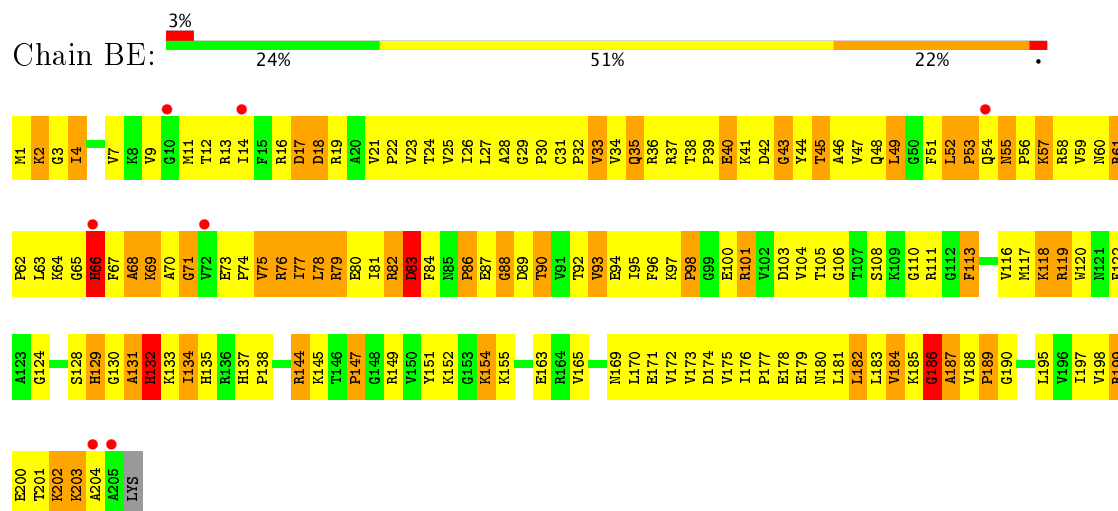


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

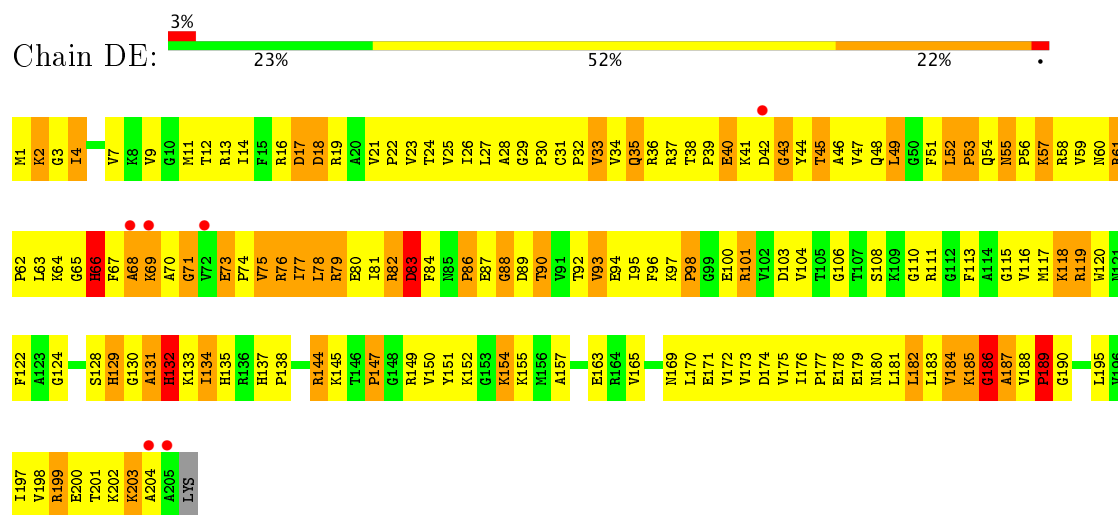




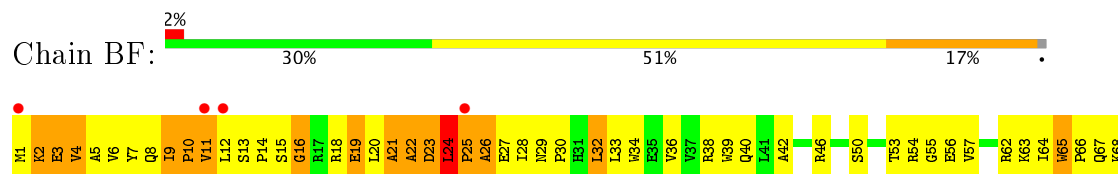
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

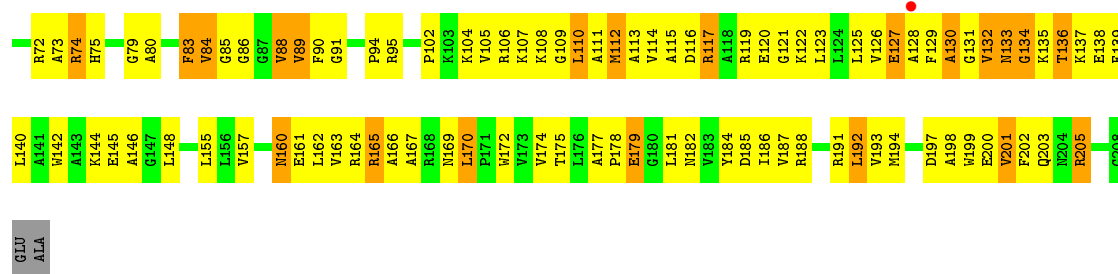


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

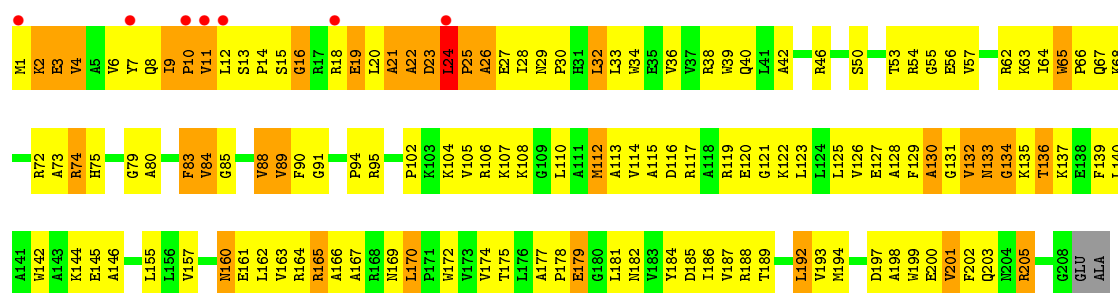


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

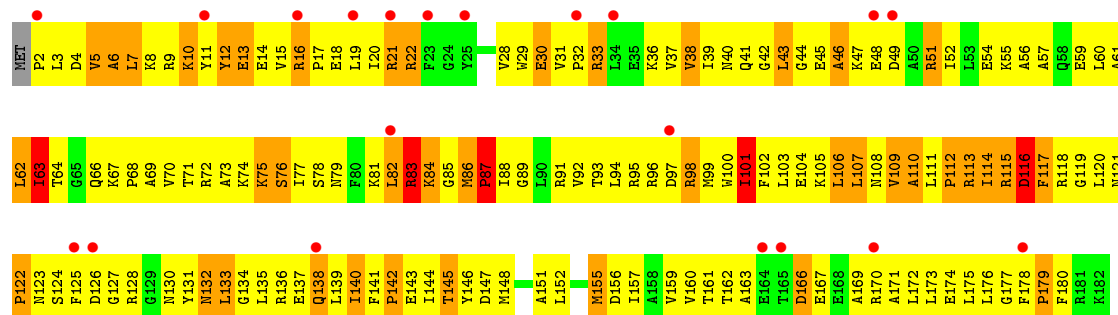
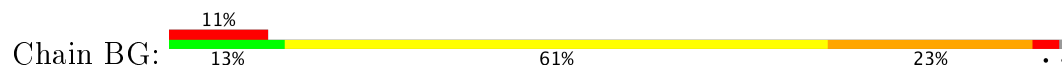




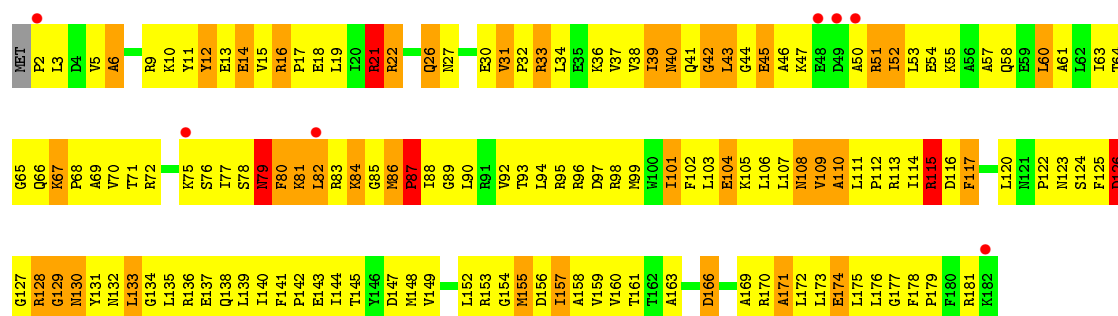
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



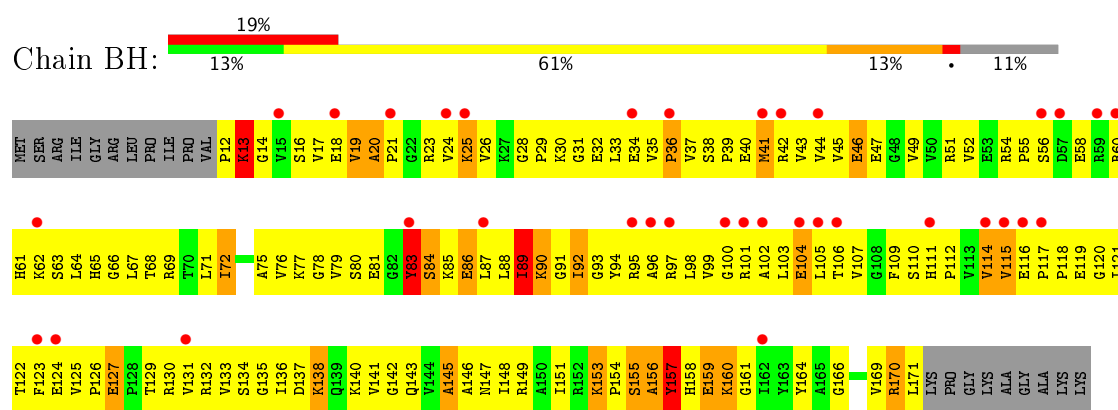
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



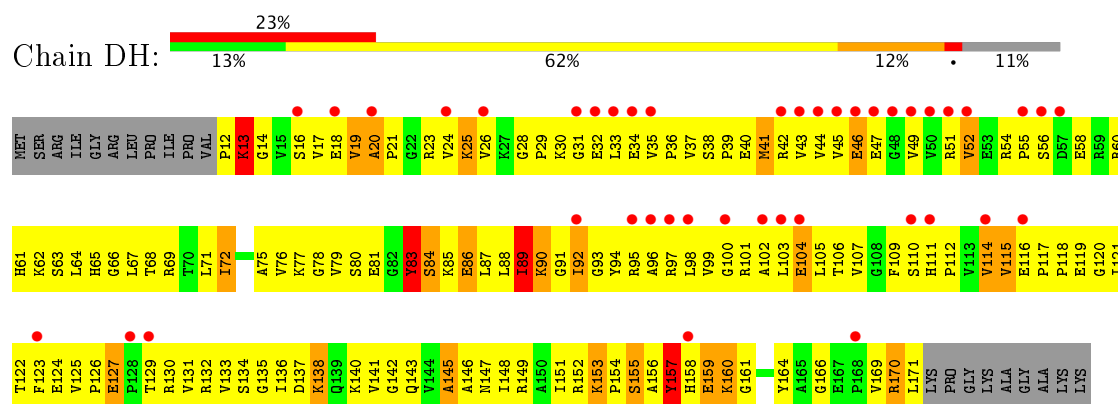
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



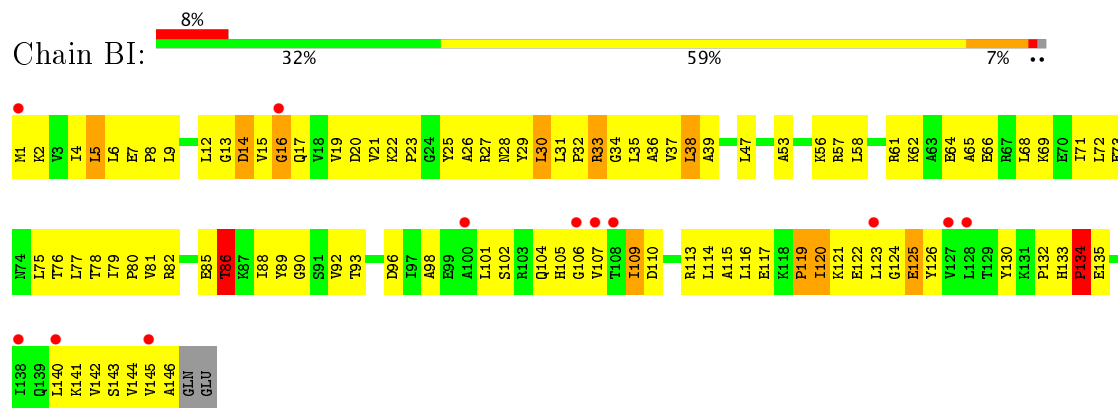
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



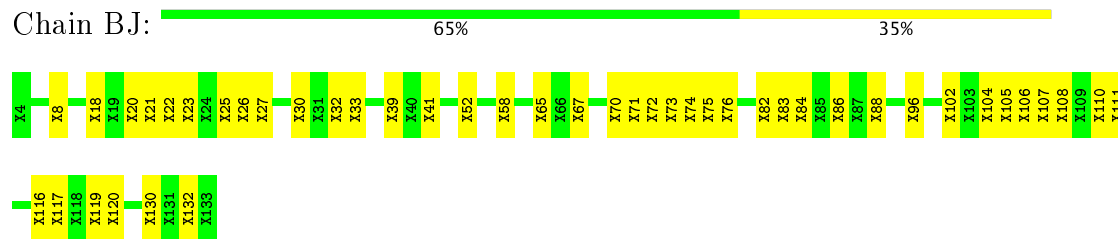
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: 50S RIBOSOMAL PROTEIN L9



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



• Molecule 44: 50S RIBOSOMAL PROTEIN L10

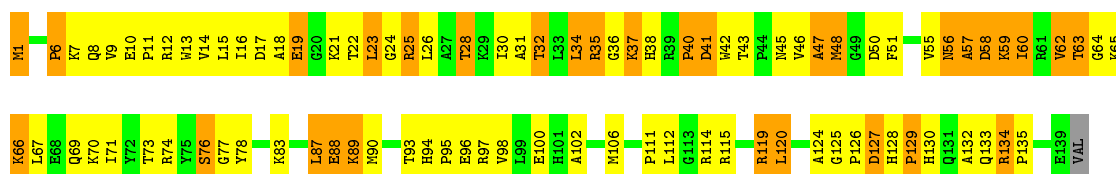
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

- Molecule 45: 50S RIBOSOMAL PROTEIN L11

• Molecule 46: 50S RIBOSOMAL PROTEIN L13

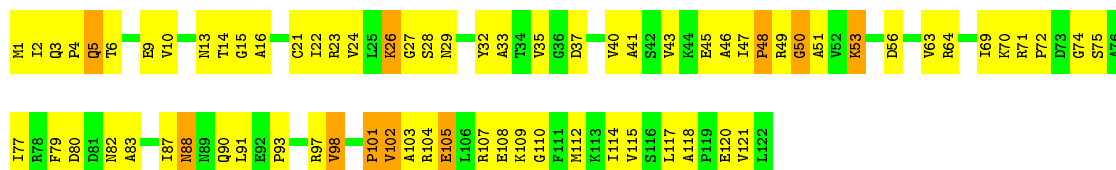
- Molecule 46: 50S RIBOSOMAL PROTEIN L13





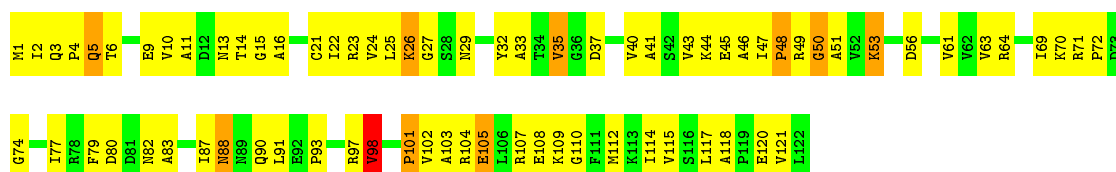
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO: 41% 51% 8%



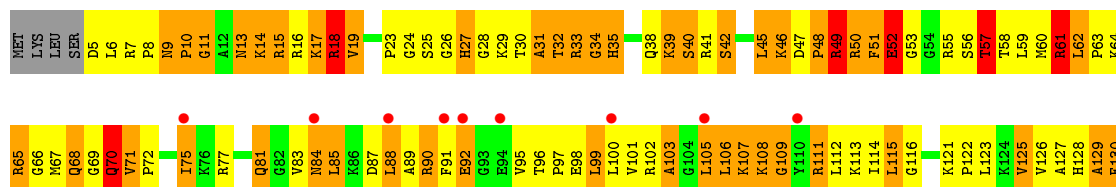
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO: 39% 52% 7%



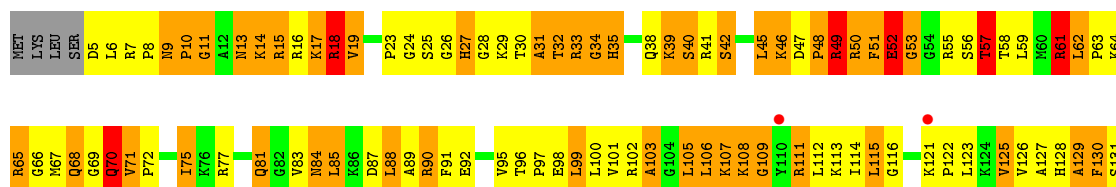
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP: 7% 20% 39% 33% 5%

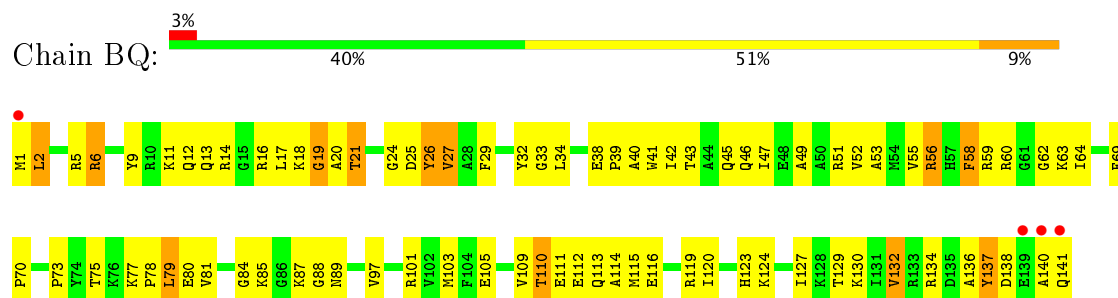


• Molecule 48: 50S RIBOSOMAL PROTEIN L15

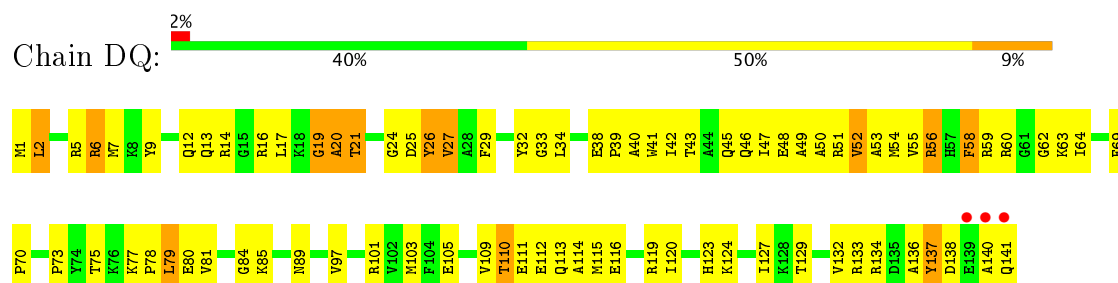
Chain DP: 3% 21% 39% 33% 5%



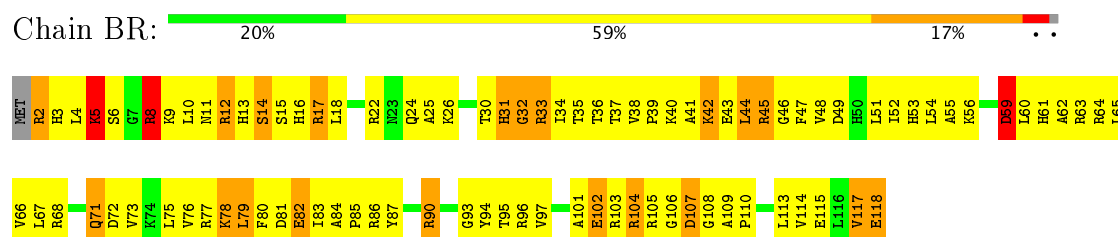
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



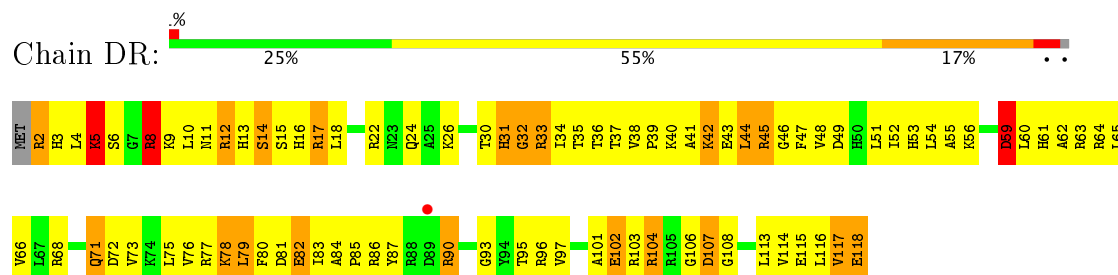
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



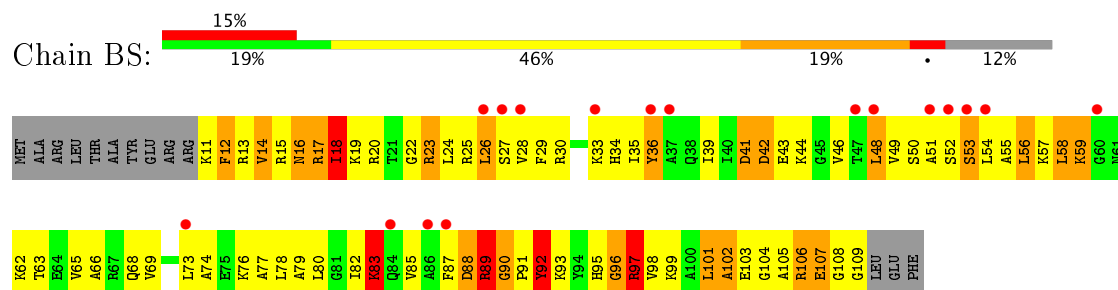
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



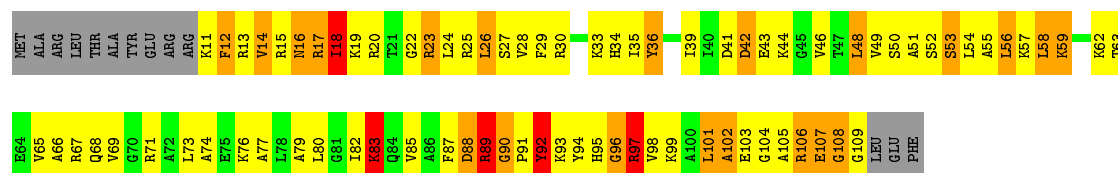

- Molecule 50: 50S RIBOSOMAL PROTEIN L17



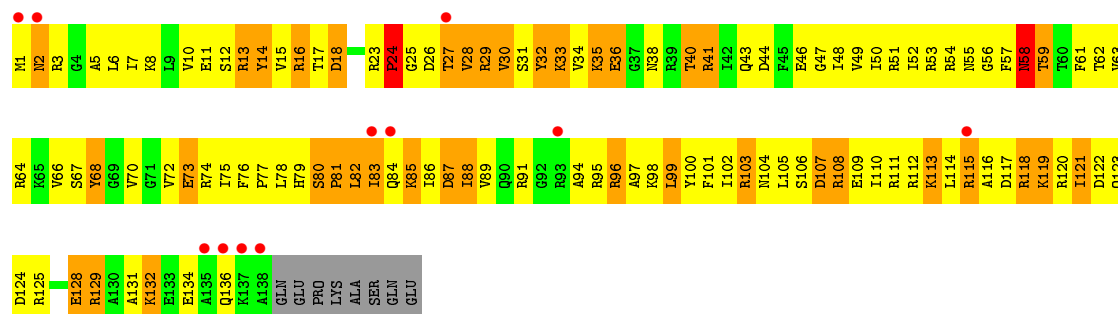

- Molecule 51: 50S RIBOSOMAL PROTEIN L18



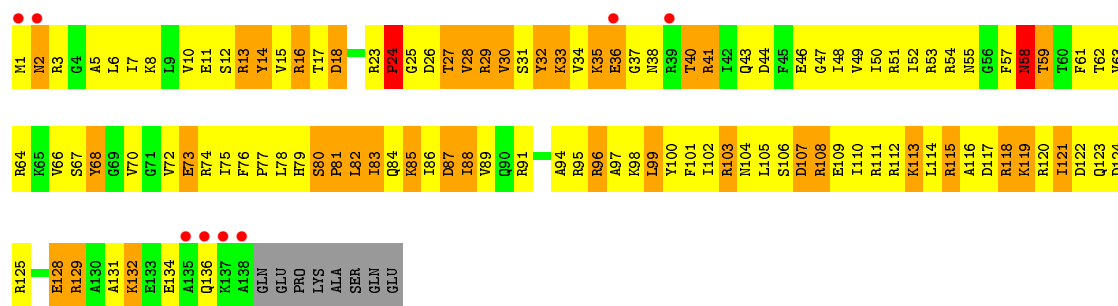
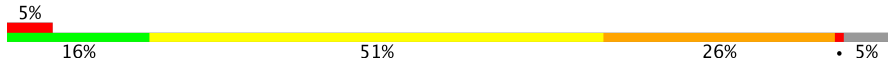
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS: 

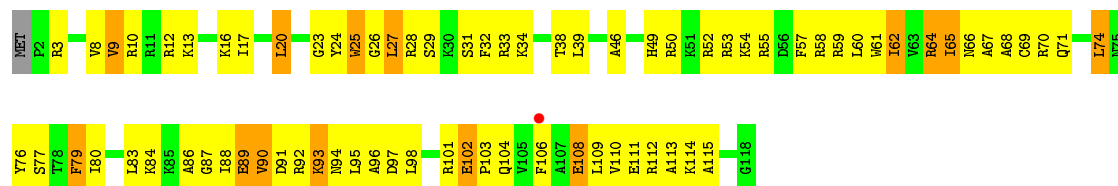
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT: 

• Molecule 52: 50S RIBOSOMAL PROTEIN L19

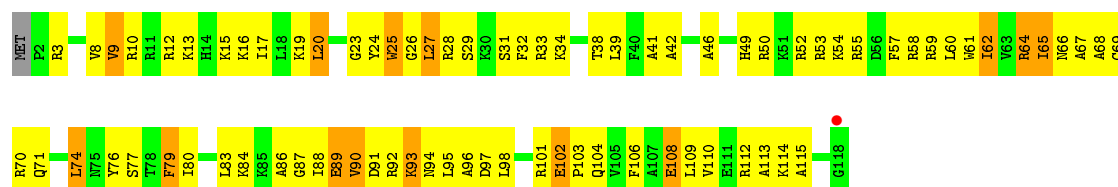
Chain DT: 

• Molecule 53: 50S RIBOSOMAL PROTEIN L20

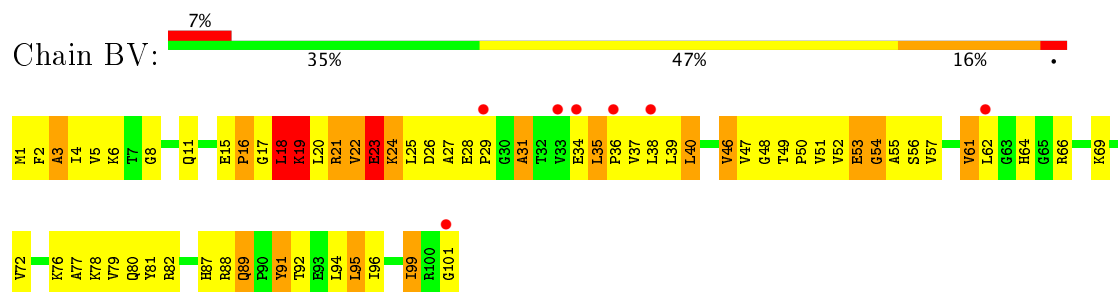
Chain BU: 

• Molecule 53: 50S RIBOSOMAL PROTEIN L20

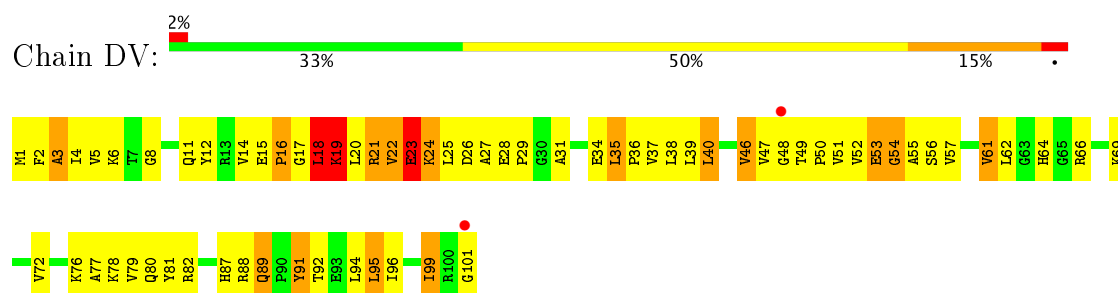
Chain DU: 



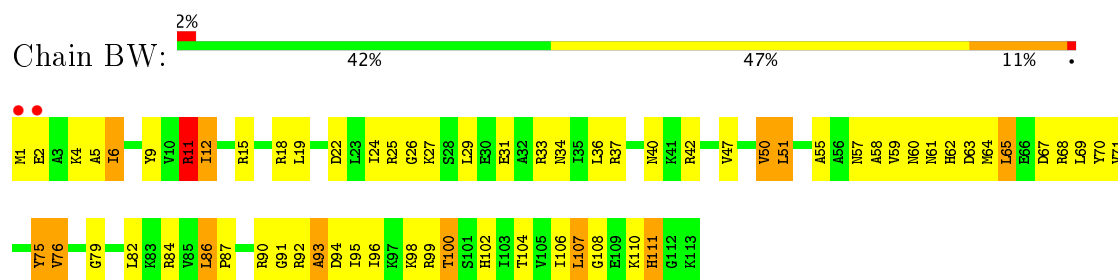
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



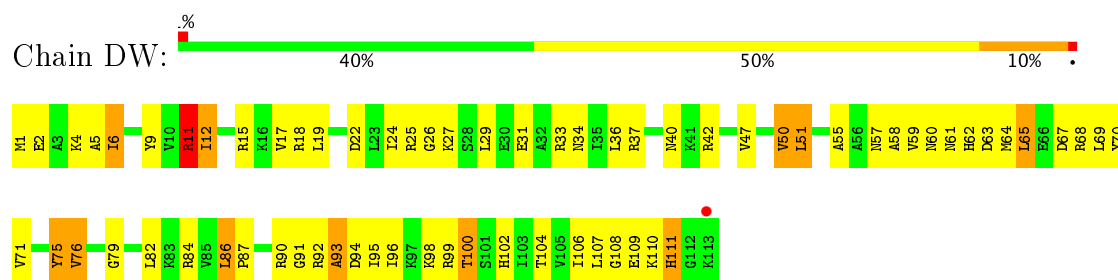
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



• Molecule 55: 50S RIBOSOMAL PROTEIN L22

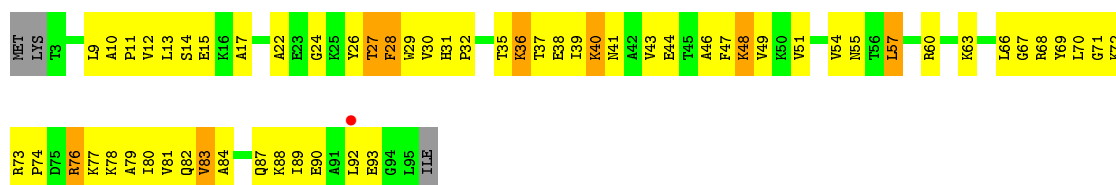


• Molecule 55: 50S RIBOSOMAL PROTEIN L22



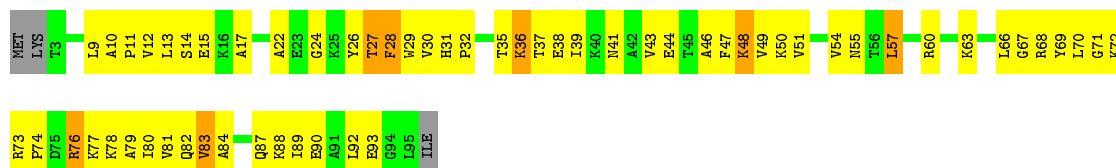
• Molecule 56: 50S RIBOSOMAL PROTEIN L23





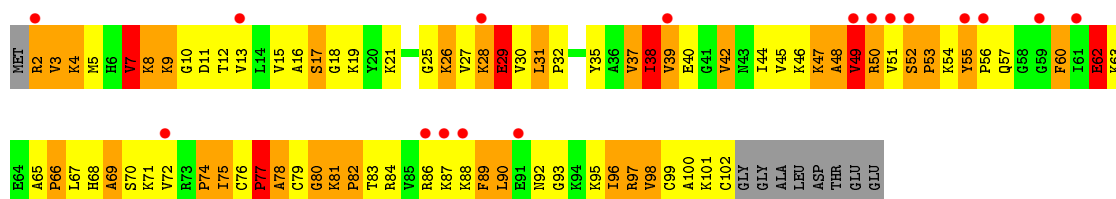
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX: 34% 55% 7%



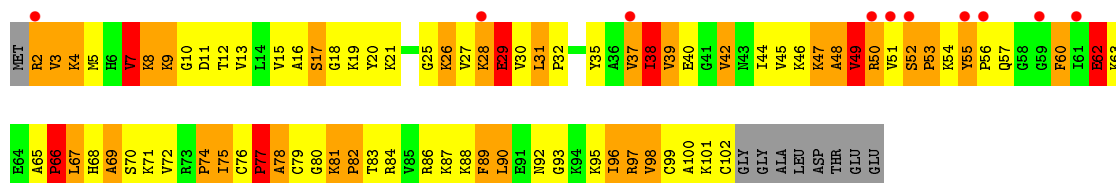
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY: 15% 17% 40% 29% 5% 8%



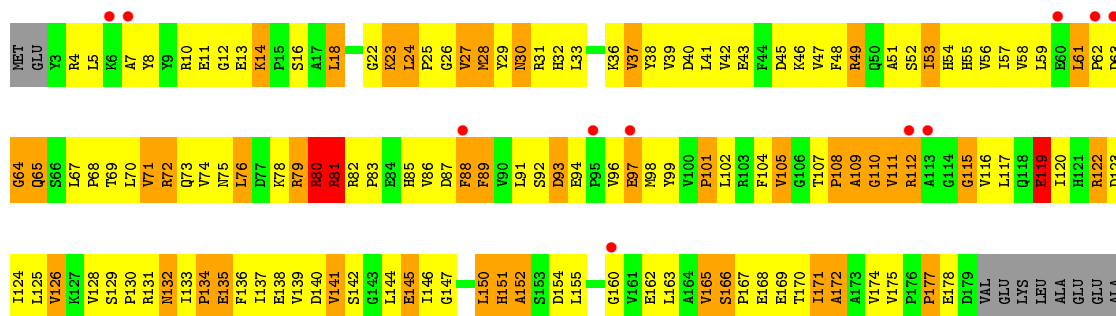
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY: 9% 16% 41% 28% 6% 8%



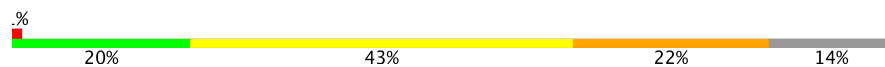
• Molecule 58: 50S RIBOSOMAL PROTEIN L25

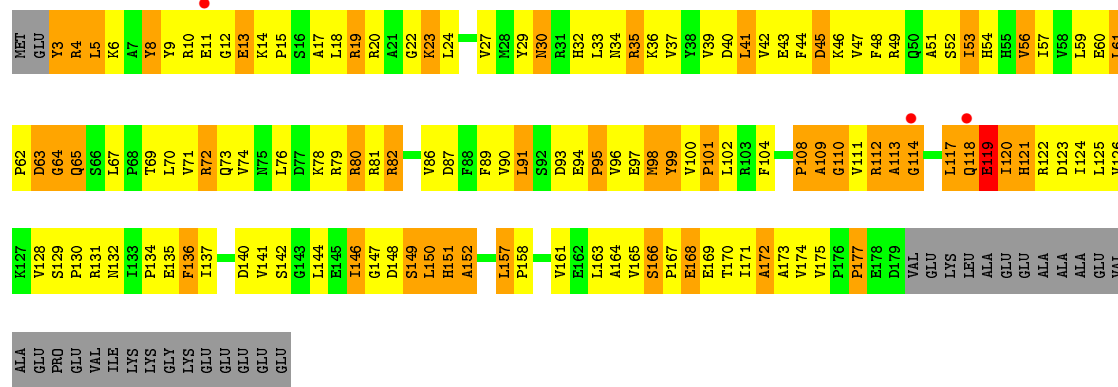
Chain BZ: 5% 19% 44% 21% 14%



ALA
ALA
GLU
VAL
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU
GLU

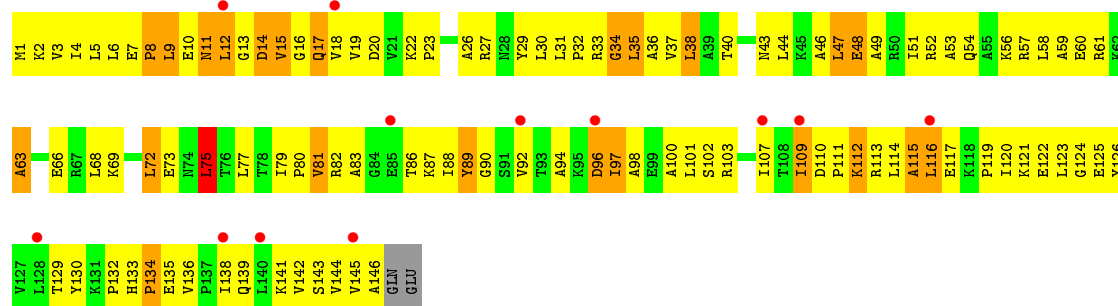
• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ: 



• Molecule 59: 50S RIBOSOMAL PROTEIN L9

Chain DI: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.34Å 450.91Å 614.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.45 49.57 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.57-3.45) 99.6 (49.57-3.45)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.257 0.210 , 0.257	Depositor DCC
R_{free} test set	33079 reflections (4.55%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 88.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	304505	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.39	0/36190	0.69	9/56486 (0.0%)
1	CA	0.41	0/36190	0.69	11/56486 (0.0%)
2	AB	0.32	0/1936	0.61	0/2611
2	CB	0.32	0/1936	0.61	0/2611
3	AC	0.32	0/1637	0.57	0/2207
3	CC	0.35	0/1637	0.57	0/2207
4	AD	0.34	0/1733	0.58	0/2318
4	CD	0.36	0/1733	0.59	0/2318
5	AE	0.36	0/1163	0.61	0/1566
5	CE	0.37	0/1163	0.62	0/1566
6	AF	0.29	0/856	0.58	0/1154
6	CF	0.29	0/856	0.58	0/1154
7	AG	0.30	0/1276	0.54	0/1709
7	CG	0.33	0/1276	0.56	0/1709
8	AH	0.32	0/1136	0.62	0/1527
8	CH	0.33	0/1136	0.63	0/1527
9	AI	0.31	0/1029	0.60	0/1378
9	CI	0.33	0/1029	0.61	0/1378
10	AJ	0.33	0/808	0.60	0/1087
10	CJ	0.34	0/808	0.61	0/1087
11	AK	0.32	0/900	0.60	0/1213
11	CK	0.33	0/900	0.60	0/1213
12	AL	0.40	0/992	0.74	0/1329
12	CL	0.40	0/992	0.75	0/1329
13	AM	0.32	0/966	0.65	0/1294
13	CM	0.34	0/966	0.66	0/1294
14	AN	0.35	0/501	0.58	0/664
14	CN	0.38	0/501	0.60	0/664
15	AO	0.31	0/745	0.54	0/992
15	CO	0.32	0/745	0.55	0/992
16	AP	0.37	0/717	0.63	0/965
16	CP	0.37	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/837	0.60	0/1119
17	CQ	0.37	0/837	0.60	0/1119
18	AR	0.32	0/579	0.61	0/768
18	CR	0.32	0/579	0.62	0/768
19	AS	0.37	0/643	0.60	0/867
19	CS	0.39	0/643	0.60	0/867
20	AT	0.29	0/765	0.55	0/1007
20	CT	0.29	0/765	0.56	0/1007
21	AU	0.44	0/213	0.53	0/279
21	CU	0.43	0/213	0.54	0/279
22	AV	0.52	0/1809	0.77	1/2819 (0.0%)
22	AW	0.42	0/1809	0.78	5/2819 (0.2%)
22	CV	0.53	0/1809	0.78	2/2819 (0.1%)
22	CW	0.39	0/1809	0.76	4/2819 (0.1%)
23	AX	0.53	0/185	0.79	1/286 (0.3%)
23	CX	0.56	0/185	0.71	0/286
24	AY	0.34	0/2847	0.66	0/3846
24	CY	0.36	0/2847	0.70	1/3846 (0.0%)
25	B0	0.42	0/615	0.72	0/819
25	D0	0.44	0/615	0.73	0/819
26	B1	0.44	0/739	0.79	1/983 (0.1%)
26	D1	0.49	0/739	0.77	0/983
27	B2	0.39	0/600	0.73	0/793
27	D2	0.44	0/600	0.75	1/793 (0.1%)
28	B3	0.44	0/473	0.74	0/636
28	D3	0.45	0/473	0.73	0/636
29	B4	0.38	0/229	0.53	0/311
29	D4	0.41	0/229	0.53	0/311
30	B5	0.46	0/473	0.83	0/639
30	D5	0.45	0/473	0.85	0/639
31	B6	0.62	1/388 (0.3%)	0.97	0/520
31	D6	0.71	1/388 (0.3%)	1.00	0/520
32	B7	0.48	0/427	0.70	0/563
32	D7	0.48	0/427	0.69	0/563
33	B8	0.63	0/516	0.88	0/681
33	D8	0.67	0/516	0.91	0/681
34	B9	0.42	0/302	0.77	1/397 (0.3%)
34	D9	0.45	0/302	0.77	1/397 (0.3%)
35	BA	0.53	1/69614 (0.0%)	0.74	40/108679 (0.0%)
35	DA	0.56	3/69614 (0.0%)	0.75	40/108679 (0.0%)
36	BB	0.50	2/2853 (0.1%)	0.87	4/4451 (0.1%)
36	DB	0.52	1/2853 (0.0%)	0.84	3/4451 (0.1%)
37	BC	0.36	0/1145	0.65	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.35	0/1145	0.66	7/1556 (0.4%)
38	BD	0.45	0/2155	0.68	1/2907 (0.0%)
38	DD	0.47	0/2155	0.68	1/2907 (0.0%)
39	BE	0.43	0/1597	0.76	1/2155 (0.0%)
39	DE	0.44	0/1597	0.76	1/2155 (0.0%)
40	BF	0.48	0/1659	0.77	0/2246
40	DF	0.49	0/1659	0.77	0/2246
41	BG	0.37	0/1499	0.69	0/2016
41	DG	0.41	0/1499	0.76	1/2016 (0.0%)
42	BH	0.36	0/1246	0.69	1/1684 (0.1%)
42	DH	0.37	0/1246	0.69	1/1684 (0.1%)
43	BI	0.31	0/1147	0.60	0/1553
45	BK	0.31	0/1057	0.57	0/1432
45	DK	0.31	0/1057	0.57	0/1432
46	BN	0.38	0/1132	0.69	0/1527
46	DN	0.41	0/1132	0.70	0/1527
47	BO	0.42	0/943	0.71	0/1269
47	DO	0.40	0/943	0.71	0/1269
48	BP	0.41	0/1131	0.78	1/1504 (0.1%)
48	DP	0.44	0/1131	0.78	1/1504 (0.1%)
49	BQ	0.44	0/1143	0.71	0/1527
49	DQ	0.46	0/1143	0.72	0/1527
50	BR	0.36	0/974	0.71	1/1302 (0.1%)
50	DR	0.37	0/974	0.72	1/1302 (0.1%)
51	BS	0.45	0/779	0.85	1/1038 (0.1%)
51	DS	0.56	0/779	0.89	1/1038 (0.1%)
52	BT	0.40	0/1156	0.74	0/1544
52	DT	0.41	0/1156	0.75	0/1544
53	BU	0.47	0/975	0.77	1/1297 (0.1%)
53	DU	0.47	0/975	0.80	1/1297 (0.1%)
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.76	0/1057
55	BW	0.39	0/907	0.67	0/1216
55	DW	0.41	0/907	0.69	0/1216
56	BX	0.43	0/740	0.71	0/995
56	DX	0.44	0/740	0.72	0/995
57	BY	0.50	0/789	0.80	0/1053
57	DY	0.49	0/789	0.81	0/1053
58	BZ	0.41	0/1436	0.72	0/1951
58	DZ	0.41	0/1436	0.77	0/1951
59	DI	0.36	0/1148	0.73	0/1554
All	All	0.47	9/327803 (0.0%)	0.72	154/489223 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	9
1	CA	0	10
22	AW	3	0
22	CV	0	2
22	CW	3	0
23	AX	0	1
30	B5	0	1
30	D5	0	2
35	BA	2	40
35	DA	3	46
All	All	11	111

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DB	86	G	P-OP2	-7.68	1.35	1.49
35	BA	568	U	C4-O4	7.25	1.29	1.23
36	BB	86	G	P-OP1	-7.23	1.36	1.49
36	BB	96	U	C2-O2	-6.42	1.16	1.22
31	D6	42	TRP	CB-CG	6.09	1.61	1.50

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	85	G	OP1-P-O3'	-22.67	55.33	105.20
36	DB	85	G	OP2-P-O3'	-19.05	63.30	105.20
36	BB	85	G	OP2-P-O3'	13.54	134.99	105.20
36	DB	85	G	OP1-P-O3'	12.71	133.15	105.20
36	DB	86	G	O5'-P-OP2	11.85	124.92	110.70

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AW	17	C	C1'
22	AW	47	U	C1'
22	AW	70	G	C3'
35	BA	1784	A	C3'
35	BA	1799	G	C3'

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	110	C	Sidechain
1	AA	324	G	Sidechain
1	AA	38	G	Sidechain
1	AA	388	G	Sidechain
1	AA	498	U	Sidechain

5.2 Too-close contacts [i](#)

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	32329	0	16318	1300	0
1	CA	32329	0	16318	1291	0
2	AB	1901	0	1951	253	0
2	CB	1901	0	1951	256	0
3	AC	1613	0	1677	193	0
3	CC	1613	0	1677	190	0
4	AD	1703	0	1763	215	0
4	CD	1703	0	1763	213	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	93	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	112	0
7	CG	1257	0	1296	112	0
8	AH	1116	0	1177	160	0
8	CH	1116	0	1177	152	0
9	AI	1011	0	1043	164	0
9	CI	1011	0	1043	172	0
10	AJ	795	0	840	170	0
10	CJ	795	0	840	165	0
11	AK	885	0	904	101	0
11	CK	885	0	904	104	0
12	AL	976	0	1062	99	0
12	CL	976	0	1062	93	0
13	AM	956	0	1021	104	0
13	CM	956	0	1021	106	0
14	AN	492	0	529	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	57	0
15	AO	734	0	771	52	0
15	CO	734	0	771	48	0
16	AP	701	0	720	100	0
16	CP	701	0	720	106	0
17	AQ	824	0	891	69	0
17	CQ	824	0	891	70	0
18	AR	574	0	644	78	0
18	CR	574	0	644	78	0
19	AS	630	0	652	97	0
19	CS	630	0	652	97	0
20	AT	763	0	861	112	0
20	CT	763	0	861	110	0
21	AU	209	0	221	18	0
21	CU	209	0	221	18	0
22	AV	1619	0	822	76	0
22	AW	1619	0	822	98	0
22	CV	1619	0	822	83	0
22	CW	1619	0	822	92	0
23	AX	166	0	87	17	0
23	CX	166	0	87	7	0
24	AY	2799	0	2809	362	0
24	CY	2799	0	2809	344	0
25	B0	607	0	628	82	0
25	D0	607	0	628	82	0
26	B1	732	0	808	113	0
26	D1	732	0	808	108	0
27	B2	598	0	653	85	0
27	D2	598	0	653	78	0
28	B3	468	0	523	59	3
28	D3	468	0	523	60	0
29	B4	226	0	229	33	0
29	D4	226	0	229	36	0
30	B5	459	0	480	64	0
30	D5	459	0	480	72	0
31	B6	381	0	391	117	0
31	D6	381	0	391	123	0
32	B7	419	0	467	25	0
32	D7	419	0	467	29	0
33	B8	508	0	576	122	0
33	D8	508	0	576	130	0
34	B9	299	0	324	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D9	299	0	324	31	0
35	BA	62154	0	31337	2153	0
35	DA	62154	0	31337	2168	9
36	BB	2551	0	1295	103	6
36	DB	2551	0	1295	103	0
37	BC	1142	0	865	110	0
37	DC	1142	0	865	103	0
38	BD	2105	0	2182	255	0
38	DD	2105	0	2182	246	0
39	BE	1564	0	1629	245	0
39	DE	1564	0	1629	252	0
40	BF	1624	0	1677	227	0
40	DF	1624	0	1677	226	0
41	BG	1474	0	1535	288	0
41	DG	1474	0	1535	249	0
42	BH	1223	0	1282	214	0
42	DH	1223	0	1282	212	0
43	BI	1132	0	1218	120	0
44	BJ	651	0	146	35	0
44	DJ	651	0	146	36	0
45	BK	1038	0	1089	157	0
45	DK	1038	0	1089	184	0
46	BN	1105	0	1180	129	0
46	DN	1105	0	1180	122	0
47	BO	933	0	996	92	0
47	DO	933	0	996	94	0
48	BP	1114	0	1187	261	0
48	DP	1114	0	1187	259	0
49	BQ	1122	0	1179	121	0
49	DQ	1122	0	1179	123	0
50	BR	960	0	1021	134	0
50	DR	960	0	1020	134	0
51	BS	771	0	832	147	0
51	DS	771	0	832	149	0
52	BT	1142	0	1202	231	0
52	DT	1142	0	1202	231	0
53	BU	958	0	1015	134	0
53	DU	958	0	1015	139	0
54	BV	779	0	852	144	0
54	DV	779	0	852	149	0
55	BW	896	0	953	76	0
55	DW	896	0	953	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BX	726	0	778	67	0
56	DX	726	0	778	65	0
57	BY	776	0	870	181	0
57	DY	776	0	870	182	0
58	BZ	1404	0	1432	232	0
58	DZ	1404	0	1432	245	0
59	DI	1133	0	1220	185	0
60	AA	157	0	0	0	0
60	AE	1	0	0	0	0
60	AL	1	0	0	0	0
60	AM	1	0	0	0	0
60	AV	7	0	0	0	0
60	AW	5	0	0	0	0
60	AY	1	0	0	0	0
60	B1	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	0	0
60	BA	354	0	0	0	0
60	BB	4	0	0	0	0
60	BC	1	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BH	1	0	0	0	0
60	BP	1	0	0	0	0
60	BQ	1	0	0	0	0
60	BS	1	0	0	0	0
60	BU	1	0	0	0	0
60	CA	157	0	0	0	0
60	CL	1	0	0	0	0
60	CN	1	0	0	0	0
60	CV	7	0	0	0	0
60	CW	5	0	0	0	0
60	CY	1	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	0	0
60	D5	2	0	0	0	0
60	D7	1	0	0	0	0
60	DA	353	0	0	0	0
60	DB	4	0	0	0	0
60	DC	1	0	0	0	0
60	DD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DF	3	0	0	0	0
60	DH	1	0	0	0	0
60	DQ	1	0	0	0	0
60	DR	1	0	0	0	0
60	DU	1	0	0	0	0
60	DX	1	0	0	0	0
60	DY	1	0	0	0	0
61	AD	1	0	0	0	0
61	AN	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	CN	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	304505	0	207553	19769	9

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 39.

The worst 5 of 19769 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)
26:D1:81:LYS:CE	35:DA:271(H):G:H5'	1.21	1.60
26:B1:81:LYS:HE2	35:BA:271(H):G:C5'	1.23	1.59
26:D1:81:LYS:HE2	35:DA:271(H):G:C5'	1.31	1.54
26:B1:81:LYS:CE	35:BA:271(H):G:H5'	1.10	1.53
35:BA:1887:C:H2'	35:BA:1888:G:H5''	1.22	1.18

The worst 5 of 9 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)
28:B3:48:GLU:O	35:DA:654(L):G:OP2[3_455]	1.99	0.21
36:BB:97:G:N7	35:DA:654(J):A:OP1[3_455]	2.05	0.15
36:BB:97:G:OP2	35:DA:654(I):C:O2'[3_455]	2.06	0.14
36:BB:96:U:C3'	35:DA:654(I):C:O2'[3_455]	2.09	0.11
36:BB:96:U:O2	35:DA:654(K):C:OP1[3_455]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	155 (66%)	58 (25%)	20 (9%)	1	11
2	CB	233/256 (91%)	156 (67%)	56 (24%)	21 (9%)	1	9
3	AC	205/239 (86%)	125 (61%)	57 (28%)	23 (11%)	0	6
3	CC	205/239 (86%)	128 (62%)	55 (27%)	22 (11%)	0	7
4	AD	206/209 (99%)	134 (65%)	49 (24%)	23 (11%)	0	6
4	CD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	7
5	AE	149/162 (92%)	98 (66%)	36 (24%)	15 (10%)	1	8
5	CE	149/162 (92%)	100 (67%)	34 (23%)	15 (10%)	1	8
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	14
6	CF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	14
7	AG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	1	14
7	CG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	1	14
8	AH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	1	10
8	CH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	1	10
9	AI	125/128 (98%)	83 (66%)	30 (24%)	12 (10%)	1	9
9	CI	125/128 (98%)	82 (66%)	31 (25%)	12 (10%)	1	9
10	AJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	0	5
10	CJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	0	5
11	AK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	4	34
11	CK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	4	34
12	AL	124/132 (94%)	89 (72%)	26 (21%)	9 (7%)	1	13
12	CL	124/132 (94%)	90 (73%)	25 (20%)	9 (7%)	1	13
13	AM	119/126 (94%)	82 (69%)	23 (19%)	14 (12%)	0	6
13	CM	119/126 (94%)	84 (71%)	21 (18%)	14 (12%)	0	6
14	AN	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0	4
15	AO	86/89 (97%)	59 (69%)	23 (27%)	4 (5%)	3	25
15	CO	86/89 (97%)	57 (66%)	25 (29%)	4 (5%)	3	25
16	AP	82/88 (93%)	51 (62%)	22 (27%)	9 (11%)	0	7
16	CP	82/88 (93%)	53 (65%)	20 (24%)	9 (11%)	0	7
17	AQ	98/105 (93%)	68 (69%)	17 (17%)	13 (13%)	0	4
17	CQ	98/105 (93%)	69 (70%)	17 (17%)	12 (12%)	0	5
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	8
18	CR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	8
19	AS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	3
19	CS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	3
20	AT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	0	6
20	CT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	0	6
21	AU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	10
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	10
24	AY	349/351 (99%)	246 (70%)	70 (20%)	33 (10%)	1	9
24	CY	349/351 (99%)	256 (73%)	61 (18%)	32 (9%)	1	9
25	B0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	11
25	D0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	11
26	B1	92/98 (94%)	65 (71%)	15 (16%)	12 (13%)	0	4
26	D1	92/98 (94%)	72 (78%)	12 (13%)	8 (9%)	1	10
27	B2	69/72 (96%)	40 (58%)	17 (25%)	12 (17%)	0	2
27	D2	69/72 (96%)	39 (56%)	20 (29%)	10 (14%)	0	3
28	B3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	8
28	D3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	8
29	B4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	4
29	D4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	4
30	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	2
30	D5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	2
31	B6	43/54 (80%)	17 (40%)	12 (28%)	14 (33%)	0	0
31	D6	43/54 (80%)	17 (40%)	13 (30%)	13 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	3
33	D8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	3
34	B9	34/37 (92%)	23 (68%)	11 (32%)	0	100	100
34	D9	34/37 (92%)	24 (71%)	10 (29%)	0	100	100
37	BC	183/229 (80%)	64 (35%)	71 (39%)	48 (26%)	0	1
37	DC	183/229 (80%)	65 (36%)	72 (39%)	46 (25%)	0	1
38	BD	270/276 (98%)	199 (74%)	39 (14%)	32 (12%)	0	6
38	DD	270/276 (98%)	198 (73%)	40 (15%)	32 (12%)	0	6
39	BE	203/206 (98%)	124 (61%)	45 (22%)	34 (17%)	0	2
39	DE	203/206 (98%)	123 (61%)	44 (22%)	36 (18%)	0	2
40	BF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	6
40	DF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	6
41	BG	179/182 (98%)	92 (51%)	54 (30%)	33 (18%)	0	2
41	DG	179/182 (98%)	107 (60%)	46 (26%)	26 (14%)	0	3
42	BH	158/180 (88%)	90 (57%)	38 (24%)	30 (19%)	0	2
42	DH	158/180 (88%)	91 (58%)	36 (23%)	31 (20%)	0	2
43	BI	144/148 (97%)	100 (69%)	28 (19%)	16 (11%)	0	7
45	BK	139/147 (95%)	88 (63%)	33 (24%)	18 (13%)	0	5
45	DK	139/147 (95%)	87 (63%)	34 (24%)	18 (13%)	0	5
46	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	3
46	DN	137/140 (98%)	99 (72%)	18 (13%)	20 (15%)	0	3
47	BO	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	2	23
47	DO	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	1	16
48	BP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
48	DP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
49	BQ	139/141 (99%)	111 (80%)	19 (14%)	9 (6%)	1	16
49	DQ	139/141 (99%)	114 (82%)	16 (12%)	9 (6%)	1	16
50	BR	115/118 (98%)	72 (63%)	29 (25%)	14 (12%)	0	5
50	DR	115/118 (98%)	70 (61%)	31 (27%)	14 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	97/112 (87%)	55 (57%)	22 (23%)	20 (21%)	0	1
51	DS	97/112 (87%)	54 (56%)	22 (23%)	21 (22%)	0	1
52	BT	136/146 (93%)	84 (62%)	23 (17%)	29 (21%)	0	1
52	DT	136/146 (93%)	85 (62%)	22 (16%)	29 (21%)	0	1
53	BU	115/118 (98%)	78 (68%)	27 (24%)	10 (9%)	1	10
53	DU	115/118 (98%)	77 (67%)	28 (24%)	10 (9%)	1	10
54	BV	99/101 (98%)	72 (73%)	13 (13%)	14 (14%)	0	3
54	DV	99/101 (98%)	72 (73%)	14 (14%)	13 (13%)	0	4
55	BW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	2	21
55	DW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	2	21
56	BX	91/96 (95%)	75 (82%)	14 (15%)	2 (2%)	8	43
56	DX	91/96 (95%)	74 (81%)	16 (18%)	1 (1%)	17	58
57	BY	99/110 (90%)	46 (46%)	20 (20%)	33 (33%)	0	0
57	DY	99/110 (90%)	47 (48%)	20 (20%)	32 (32%)	0	0
58	BZ	175/206 (85%)	102 (58%)	41 (23%)	32 (18%)	0	2
58	DZ	175/206 (85%)	110 (63%)	36 (21%)	29 (17%)	0	2
59	DI	144/148 (97%)	81 (56%)	42 (29%)	21 (15%)	0	3
All	All	12652/13582 (93%)	8336 (66%)	2725 (22%)	1591 (13%)	0	5

5 of 1591 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	95	GLN
2	AB	195	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	184 (91%)	18 (9%)	11	42
2	CB	202/220 (92%)	184 (91%)	18 (9%)	11	42
3	AC	160/188 (85%)	149 (93%)	11 (7%)	18	55
3	CC	160/188 (85%)	150 (94%)	10 (6%)	21	59
4	AD	180/181 (99%)	159 (88%)	21 (12%)	6	28
4	CD	180/181 (99%)	159 (88%)	21 (12%)	6	28
5	AE	115/123 (94%)	103 (90%)	12 (10%)	8	35
5	CE	115/123 (94%)	101 (88%)	14 (12%)	6	27
6	AF	90/90 (100%)	86 (96%)	4 (4%)	33	69
6	CF	90/90 (100%)	86 (96%)	4 (4%)	33	69
7	AG	126/127 (99%)	117 (93%)	9 (7%)	17	54
7	CG	126/127 (99%)	118 (94%)	8 (6%)	21	59
8	AH	119/119 (100%)	105 (88%)	14 (12%)	6	28
8	CH	119/119 (100%)	105 (88%)	14 (12%)	6	28
9	AI	98/99 (99%)	88 (90%)	10 (10%)	8	35
9	CI	98/99 (99%)	88 (90%)	10 (10%)	8	35
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	7	29
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	7	29
11	AK	90/99 (91%)	84 (93%)	6 (7%)	19	57
11	CK	90/99 (91%)	84 (93%)	6 (7%)	19	57
12	AL	104/109 (95%)	98 (94%)	6 (6%)	23	60
12	CL	104/109 (95%)	96 (92%)	8 (8%)	15	49
13	AM	96/101 (95%)	83 (86%)	13 (14%)	4	23
13	CM	96/101 (95%)	83 (86%)	13 (14%)	4	23
14	AN	49/50 (98%)	46 (94%)	3 (6%)	22	59
14	CN	49/50 (98%)	46 (94%)	3 (6%)	22	59
15	AO	79/80 (99%)	76 (96%)	3 (4%)	38	72
15	CO	79/80 (99%)	76 (96%)	3 (4%)	38	72
16	AP	72/74 (97%)	64 (89%)	8 (11%)	7	31
16	CP	72/74 (97%)	64 (89%)	8 (11%)	7	31
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	59	84
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	59	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	57 (93%)	4 (7%)	19	57
18	CR	61/77 (79%)	57 (93%)	4 (7%)	19	57
19	AS	69/80 (86%)	61 (88%)	8 (12%)	6	29
19	CS	69/80 (86%)	61 (88%)	8 (12%)	6	29
20	AT	76/82 (93%)	70 (92%)	6 (8%)	14	48
20	CT	76/82 (93%)	70 (92%)	6 (8%)	14	48
21	AU	19/22 (86%)	18 (95%)	1 (5%)	26	62
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	298/298 (100%)	264 (89%)	34 (11%)	7	29
24	CY	298/298 (100%)	264 (89%)	34 (11%)	7	29
25	B0	61/67 (91%)	58 (95%)	3 (5%)	29	65
25	D0	61/67 (91%)	58 (95%)	3 (5%)	29	65
26	B1	78/83 (94%)	70 (90%)	8 (10%)	8	35
26	D1	78/83 (94%)	66 (85%)	12 (15%)	3	17
27	B2	66/67 (98%)	55 (83%)	11 (17%)	2	14
27	D2	66/67 (98%)	59 (89%)	7 (11%)	8	34
28	B3	51/52 (98%)	47 (92%)	4 (8%)	15	48
28	D3	51/52 (98%)	48 (94%)	3 (6%)	23	60
29	B4	27/63 (43%)	25 (93%)	2 (7%)	16	51
29	D4	27/63 (43%)	24 (89%)	3 (11%)	7	31
30	B5	51/52 (98%)	45 (88%)	6 (12%)	6	28
30	D5	51/52 (98%)	44 (86%)	7 (14%)	4	22
31	B6	43/52 (83%)	32 (74%)	11 (26%)	0	3
31	D6	43/52 (83%)	32 (74%)	11 (26%)	0	3
32	B7	41/42 (98%)	39 (95%)	2 (5%)	29	65
32	D7	41/42 (98%)	39 (95%)	2 (5%)	29	65
33	B8	53/55 (96%)	41 (77%)	12 (23%)	1	5
33	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
34	B9	33/34 (97%)	28 (85%)	5 (15%)	3	18
34	D9	33/34 (97%)	28 (85%)	5 (15%)	3	18
37	BC	61/181 (34%)	55 (90%)	6 (10%)	9	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	61/181 (34%)	55 (90%)	6 (10%)	9	37
38	BD	213/218 (98%)	192 (90%)	21 (10%)	9	36
38	DD	213/218 (98%)	191 (90%)	22 (10%)	8	35
39	BE	165/166 (99%)	137 (83%)	28 (17%)	2	13
39	DE	165/166 (99%)	136 (82%)	29 (18%)	2	11
40	BF	165/166 (99%)	144 (87%)	21 (13%)	5	25
40	DF	165/166 (99%)	146 (88%)	19 (12%)	6	29
41	BG	155/156 (99%)	131 (84%)	24 (16%)	3	17
41	DG	155/156 (99%)	129 (83%)	26 (17%)	2	14
42	BH	132/148 (89%)	122 (92%)	10 (8%)	15	50
42	DH	132/148 (89%)	122 (92%)	10 (8%)	15	50
43	BI	122/124 (98%)	116 (95%)	6 (5%)	29	65
45	BK	106/111 (96%)	97 (92%)	9 (8%)	12	44
45	DK	106/111 (96%)	97 (92%)	9 (8%)	12	44
46	BN	117/119 (98%)	101 (86%)	16 (14%)	4	22
46	DN	117/119 (98%)	101 (86%)	16 (14%)	4	22
47	BO	100/100 (100%)	94 (94%)	6 (6%)	22	60
47	DO	100/100 (100%)	95 (95%)	5 (5%)	28	64
48	BP	112/116 (97%)	84 (75%)	28 (25%)	1	4
48	DP	112/116 (97%)	84 (75%)	28 (25%)	1	4
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	5	26
49	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	23
50	BR	100/101 (99%)	88 (88%)	12 (12%)	6	27
50	DR	100/101 (99%)	88 (88%)	12 (12%)	6	27
51	BS	77/88 (88%)	61 (79%)	16 (21%)	1	6
51	DS	77/88 (88%)	61 (79%)	16 (21%)	1	6
52	BT	120/127 (94%)	102 (85%)	18 (15%)	3	19
52	DT	120/127 (94%)	102 (85%)	18 (15%)	3	19
53	BU	92/94 (98%)	85 (92%)	7 (8%)	15	50
53	DU	92/94 (98%)	85 (92%)	7 (8%)	15	50
54	BV	82/82 (100%)	73 (89%)	9 (11%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	DV	82/82 (100%)	72 (88%)	10 (12%)	6	27
55	BW	91/92 (99%)	79 (87%)	12 (13%)	5	24
55	DW	91/92 (99%)	80 (88%)	11 (12%)	6	27
56	BX	74/78 (95%)	65 (88%)	9 (12%)	6	27
56	DX	74/78 (95%)	65 (88%)	9 (12%)	6	27
57	BY	84/91 (92%)	67 (80%)	17 (20%)	1	7
57	DY	84/91 (92%)	67 (80%)	17 (20%)	1	7
58	BZ	155/179 (87%)	128 (83%)	27 (17%)	2	12
58	DZ	155/179 (87%)	129 (83%)	26 (17%)	2	14
59	DI	122/124 (98%)	118 (97%)	4 (3%)	43	76
All	All	10446/11246 (93%)	9279 (89%)	1167 (11%)	7	30

5 of 1167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
55	BW	86	LEU
7	CG	114	ARG
52	DT	87	ASP
57	BY	15	VAL
2	CB	137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
51	BS	68	GLN
4	CD	74	GLN
49	DQ	123	HIS
53	BU	71	GLN
58	BZ	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	222 (14%)	34 (2%)
1	CA	1503/1522 (98%)	217 (14%)	34 (2%)
22	AV	75/76 (98%)	17 (22%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AW	75/76 (98%)	15 (20%)	3 (4%)
22	CV	75/76 (98%)	18 (24%)	0
22	CW	75/76 (98%)	16 (21%)	4 (5%)
23	AX	7/8 (87%)	1 (14%)	1 (14%)
23	CX	7/8 (87%)	1 (14%)	0
35	BA	2885/2901 (99%)	515 (17%)	58 (2%)
35	DA	2885/2901 (99%)	516 (17%)	57 (1%)
36	BB	118/122 (96%)	15 (12%)	3 (2%)
36	DB	118/122 (96%)	14 (11%)	3 (2%)
All	All	9326/9410 (99%)	1567 (16%)	198 (2%)

5 of 1567 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2439	A
1	CA	372	C
35	DA	2225	A
35	BA	2542	A
1	CA	30	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1098 ligands modelled in this entry, 1098 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.12	38 (2%) 58 51	43, 106, 183, 201	0
1	CA	1504/1522 (98%)	0.04	46 (3%) 49 43	35, 87, 183, 201	0
2	AB	235/256 (91%)	0.77	43 (18%) 1 2	76, 137, 191, 201	0
2	CB	235/256 (91%)	0.32	15 (6%) 20 19	51, 117, 180, 201	0
3	AC	207/239 (86%)	0.84	27 (13%) 4 6	71, 130, 177, 201	0
3	CC	207/239 (86%)	0.07	2 (0%) 82 76	48, 96, 159, 200	0
4	AD	208/209 (99%)	0.55	22 (10%) 7 8	53, 116, 168, 199	0
4	CD	208/209 (99%)	0.15	4 (1%) 67 61	41, 95, 158, 183	0
5	AE	151/162 (93%)	0.41	13 (8%) 11 12	48, 102, 156, 179	0
5	CE	151/162 (93%)	-0.05	4 (2%) 56 49	29, 86, 145, 193	0
6	AF	101/101 (100%)	0.87	15 (14%) 3 4	75, 120, 170, 189	0
6	CF	101/101 (100%)	0.35	6 (5%) 23 21	60, 116, 162, 184	0
7	AG	155/156 (99%)	0.82	25 (16%) 2 3	64, 137, 182, 201	0
7	CG	155/156 (99%)	0.22	11 (7%) 17 16	42, 89, 143, 193	0
8	AH	138/138 (100%)	0.38	5 (3%) 43 39	50, 101, 152, 201	0
8	CH	138/138 (100%)	0.11	2 (1%) 75 70	50, 97, 148, 188	0
9	AI	127/128 (99%)	1.40	37 (29%) 1 1	66, 148, 192, 201	0
9	CI	127/128 (99%)	0.61	13 (10%) 7 9	43, 97, 148, 183	0
10	AJ	99/105 (94%)	1.82	32 (32%) 0 0	64, 154, 198, 201	0
10	CJ	99/105 (94%)	0.98	20 (20%) 1 1	44, 122, 197, 201	0
11	AK	119/129 (92%)	0.87	18 (15%) 3 4	52, 100, 155, 172	0
11	CK	119/129 (92%)	0.32	10 (8%) 12 13	49, 89, 165, 183	0
12	AL	126/132 (95%)	0.46	7 (5%) 25 23	42, 81, 146, 193	0
12	CL	126/132 (95%)	0.40	7 (5%) 25 23	37, 75, 148, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AM	121/126 (96%)	0.83	11 (9%)	10 11	69, 133, 191, 201	0
13	CM	121/126 (96%)	0.27	5 (4%)	38 33	26, 96, 156, 189	0
14	AN	60/61 (98%)	0.79	6 (10%)	8 9	76, 124, 173, 187	0
14	CN	60/61 (98%)	-0.03	0	100 100	40, 82, 118, 155	0
15	AO	88/89 (98%)	0.54	4 (4%)	34 29	43, 100, 153, 177	0
15	CO	88/89 (98%)	0.43	2 (2%)	61 54	55, 92, 138, 155	0
16	AP	84/88 (95%)	0.71	9 (10%)	7 8	59, 104, 142, 201	0
16	CP	84/88 (95%)	1.16	15 (17%)	2 2	56, 106, 157, 201	0
17	AQ	100/105 (95%)	0.49	10 (10%)	8 9	54, 96, 137, 165	0
17	CQ	100/105 (95%)	0.43	6 (6%)	23 21	53, 99, 152, 162	0
18	AR	70/88 (79%)	0.47	3 (4%)	36 31	62, 116, 160, 183	0
18	CR	70/88 (79%)	0.66	7 (10%)	8 9	51, 101, 157, 183	0
19	AS	79/93 (84%)	0.96	8 (10%)	8 9	91, 140, 191, 201	0
19	CS	79/93 (84%)	0.84	10 (12%)	4 6	51, 103, 193, 201	0
20	AT	99/106 (93%)	0.83	12 (12%)	5 7	55, 112, 165, 201	0
20	CT	99/106 (93%)	1.04	21 (21%)	1 1	68, 115, 177, 201	0
21	AU	25/27 (92%)	1.78	12 (48%)	0 0	78, 131, 167, 178	0
21	CU	25/27 (92%)	0.45	0	100 100	58, 85, 117, 123	0
22	AV	76/76 (100%)	-0.09	0	100 100	42, 85, 152, 176	0
22	AW	76/76 (100%)	1.60	28 (36%)	0 0	48, 184, 201, 201	0
22	CV	76/76 (100%)	-0.27	1 (1%)	77 71	35, 65, 135, 185	0
22	CW	76/76 (100%)	1.15	16 (21%)	1 1	30, 166, 198, 201	0
23	AX	8/8 (100%)	0.42	1 (12%)	4 6	67, 76, 160, 166	0
23	CX	8/8 (100%)	0.17	1 (12%)	4 6	46, 62, 153, 170	0
24	AY	351/351 (100%)	0.78	48 (13%)	3 5	31, 109, 190, 201	0
24	CY	351/351 (100%)	0.66	43 (12%)	5 6	25, 95, 188, 201	0
25	B0	76/85 (89%)	0.09	2 (2%)	56 49	25, 64, 105, 177	0
25	D0	76/85 (89%)	0.20	2 (2%)	56 49	10, 43, 103, 179	0
26	B1	94/98 (95%)	0.09	2 (2%)	64 58	23, 61, 123, 173	0
26	D1	94/98 (95%)	-0.08	1 (1%)	80 74	18, 52, 109, 155	0
27	B2	71/72 (98%)	0.35	5 (7%)	17 17	36, 85, 156, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.03	3 (4%) 37 32	27, 76, 144, 186	0
28	B3	60/60 (100%)	0.33	3 (5%) 30 26	19, 56, 131, 197	0
28	D3	60/60 (100%)	0.31	3 (5%) 30 26	20, 51, 112, 201	0
29	B4	31/71 (43%)	1.24	8 (25%) 1 1	99, 184, 201, 201	0
29	D4	31/71 (43%)	0.38	2 (6%) 20 18	51, 140, 184, 200	0
30	B5	59/60 (98%)	0.01	3 (5%) 29 25	22, 74, 170, 190	0
30	D5	59/60 (98%)	0.26	5 (8%) 11 13	7, 55, 183, 201	0
31	B6	45/54 (83%)	1.00	7 (15%) 2 3	39, 85, 140, 198	0
31	D6	45/54 (83%)	0.45	2 (4%) 35 30	24, 65, 117, 183	0
32	B7	49/49 (100%)	0.13	3 (6%) 22 21	7, 48, 129, 165	0
32	D7	49/49 (100%)	-0.01	1 (2%) 65 60	7, 37, 113, 189	0
33	B8	64/65 (98%)	-0.05	1 (1%) 72 66	17, 51, 125, 160	0
33	D8	64/65 (98%)	-0.20	0 100 100	8, 40, 120, 162	0
34	B9	36/37 (97%)	0.50	2 (5%) 25 23	45, 69, 127, 147	0
34	D9	36/37 (97%)	0.75	5 (13%) 3 5	40, 74, 133, 162	0
35	BA	2886/2901 (99%)	-0.06	91 (3%) 48 42	16, 58, 179, 201	0
35	DA	2886/2901 (99%)	-0.02	103 (3%) 43 39	14, 51, 181, 201	0
36	BB	119/122 (97%)	-0.07	0 100 100	46, 105, 160, 186	0
36	DB	119/122 (97%)	-0.21	0 100 100	34, 65, 99, 129	0
37	BC	191/229 (83%)	4.65	136 (71%) 0 0	91, 174, 201, 201	0
37	DC	191/229 (83%)	4.55	157 (82%) 0 0	104, 177, 201, 201	0
38	BD	272/276 (98%)	0.12	6 (2%) 62 55	27, 71, 122, 165	0
38	DD	272/276 (98%)	0.00	4 (1%) 74 68	25, 66, 108, 168	0
39	BE	205/206 (99%)	0.13	7 (3%) 46 40	22, 69, 152, 201	0
39	DE	205/206 (99%)	0.25	6 (2%) 52 45	16, 67, 144, 197	0
40	BF	208/210 (99%)	-0.19	5 (2%) 59 52	9, 52, 134, 194	0
40	DF	208/210 (99%)	-0.12	7 (3%) 46 40	9, 48, 140, 179	0
41	BG	181/182 (99%)	0.66	20 (11%) 6 8	64, 118, 173, 200	0
41	DG	181/182 (99%)	0.05	7 (3%) 40 35	30, 76, 137, 201	0
42	BH	160/180 (88%)	1.00	35 (21%) 1 1	50, 123, 181, 201	0
42	DH	160/180 (88%)	1.21	42 (26%) 1 1	63, 137, 186, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.69	12 (8%) 12 13	41, 138, 187, 200	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	1.97	56 (39%) 0 0	85, 158, 195, 201	0
45	DK	141/147 (95%)	1.98	57 (40%) 0 0	99, 158, 197, 201	0
46	BN	139/140 (99%)	-0.01	2 (1%) 75 70	30, 70, 129, 164	0
46	DN	139/140 (99%)	-0.07	0 100 100	24, 62, 122, 186	0
47	BO	122/122 (100%)	-0.23	0 100 100	28, 64, 101, 158	0
47	DO	122/122 (100%)	-0.12	0 100 100	25, 68, 101, 120	0
48	BP	146/150 (97%)	0.76	11 (7%) 15 15	27, 89, 163, 200	0
48	DP	146/150 (97%)	0.27	4 (2%) 55 49	25, 72, 147, 201	0
49	BQ	141/141 (100%)	0.01	4 (2%) 53 47	23, 65, 127, 198	0
49	DQ	141/141 (100%)	-0.18	3 (2%) 64 58	14, 53, 105, 196	0
50	BR	117/118 (99%)	-0.08	0 100 100	33, 72, 126, 156	0
50	DR	117/118 (99%)	0.05	1 (0%) 84 78	26, 68, 122, 150	0
51	BS	99/112 (88%)	0.88	17 (17%) 2 2	60, 104, 165, 188	0
51	DS	99/112 (88%)	-0.14	0 100 100	25, 61, 120, 171	0
52	BT	138/146 (94%)	0.27	11 (7%) 13 14	44, 87, 164, 201	0
52	DT	138/146 (94%)	0.26	8 (5%) 24 22	39, 87, 172, 199	0
53	BU	117/118 (99%)	-0.22	1 (0%) 84 78	18, 55, 112, 140	0
53	DU	117/118 (99%)	-0.32	1 (0%) 84 78	12, 45, 111, 190	0
54	BV	101/101 (100%)	0.28	7 (6%) 18 17	34, 79, 137, 185	0
54	DV	101/101 (100%)	0.07	2 (1%) 65 60	25, 66, 141, 201	0
55	BW	113/113 (100%)	-0.03	2 (1%) 69 62	25, 57, 114, 201	0
55	DW	113/113 (100%)	-0.16	1 (0%) 84 78	16, 47, 115, 170	0
56	BX	93/96 (96%)	0.16	1 (1%) 80 74	31, 74, 129, 155	0
56	DX	93/96 (96%)	-0.10	0 100 100	33, 67, 114, 160	0
57	BY	101/110 (91%)	0.88	17 (16%) 2 2	27, 84, 157, 201	0
57	DY	101/110 (91%)	0.61	10 (9%) 8 9	25, 81, 162, 201	0
58	BZ	177/206 (85%)	0.38	11 (6%) 21 20	36, 98, 156, 201	0
58	DZ	177/206 (85%)	-0.02	3 (1%) 70 64	30, 83, 130, 192	0
59	DI	146/148 (98%)	0.56	12 (8%) 12 13	28, 109, 155, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22210/23252 (95%)	0.32	1641 (7%) 15 15	7, 84, 181, 201	0

The worst 5 of 1641 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	215	THR	21.8
37	BC	214	VAL	21.6
37	BC	165	ASN	20.9
37	BC	108	MET	15.9
48	BP	150	ALA	15.7

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(Å ²)	Q<0.9
60	MG	DA	3024	1/1	0.94	0.98	85.85	49,49,49,49	0
60	MG	DA	3025	1/1	0.92	0.76	83.71	56,56,56,56	0
60	MG	BA	3066	1/1	0.96	0.94	75.90	50,50,50,50	0
60	MG	BA	3102	1/1	0.92	0.76	68.68	47,47,47,47	0
60	MG	DA	3038	1/1	0.97	0.58	57.92	47,47,47,47	0
60	MG	DA	3065	1/1	0.95	0.56	53.57	53,53,53,53	0
60	MG	BA	3045	1/1	0.87	0.80	52.63	47,47,47,47	0
60	MG	DA	3163	1/1	0.96	0.65	51.89	50,50,50,50	0
60	MG	BA	3043	1/1	0.96	0.79	51.76	47,47,47,47	0
60	MG	DA	3100	1/1	0.79	0.69	50.94	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3165	1/1	0.95	0.70	49.77	47,47,47,47	0
60	MG	DA	3006	1/1	0.93	0.75	49.21	47,47,47,47	0
60	MG	BA	3103	1/1	0.93	0.58	46.56	50,50,50,50	0
60	MG	CA	1631	1/1	0.78	0.83	46.51	53,53,53,53	0
60	MG	DA	3220	1/1	0.91	0.84	46.34	49,49,49,49	0
60	MG	DA	3143	1/1	0.64	0.45	45.98	47,47,47,47	1
60	MG	BA	3123	1/1	0.87	0.62	45.00	53,53,53,53	0
60	MG	DA	3203	1/1	0.96	0.46	44.46	47,47,47,47	0
60	MG	BA	3099	1/1	0.88	0.80	43.81	55,55,55,55	0
60	MG	BA	3049	1/1	0.97	0.66	43.71	47,47,47,47	0
60	MG	DA	3265	1/1	0.96	0.61	43.49	53,53,53,53	0
60	MG	BA	3042	1/1	0.93	1.00	43.29	47,47,47,47	0
60	MG	BA	3106	1/1	0.95	0.73	42.57	51,51,51,51	0
60	MG	DA	3053	1/1	0.97	0.61	41.95	47,47,47,47	0
60	MG	BA	3158	1/1	0.96	0.86	39.93	49,49,49,49	0
60	MG	BA	3348	1/1	0.95	0.59	39.10	55,55,55,55	0
60	MG	AA	1655	1/1	0.81	0.41	38.00	52,52,52,52	0
60	MG	BA	3108	1/1	0.96	0.71	37.92	52,52,52,52	0
60	MG	BA	3303	1/1	0.82	0.74	37.58	55,55,55,55	0
60	MG	DA	3258	1/1	0.89	0.83	37.28	51,51,51,51	1
60	MG	DA	3079	1/1	0.93	0.47	36.34	56,56,56,56	0
60	MG	DA	3245	1/1	0.95	0.58	35.82	53,53,53,53	0
60	MG	DA	3046	1/1	0.87	0.74	35.77	47,47,47,47	0
60	MG	BA	3101	1/1	0.95	0.68	35.66	47,47,47,47	0
60	MG	BA	3264	1/1	0.97	0.58	35.30	53,53,53,53	0
60	MG	DA	3269	1/1	0.88	0.59	34.90	52,52,52,52	0
60	MG	BA	3033	1/1	0.95	0.56	33.65	47,47,47,47	0
60	MG	DA	3057	1/1	0.94	0.67	33.43	47,47,47,47	0
60	MG	BA	3287	1/1	0.65	0.41	32.84	51,51,51,51	0
60	MG	BA	3269	1/1	0.80	0.53	32.62	52,52,52,52	0
60	MG	CA	1622	1/1	0.94	0.84	32.42	57,57,57,57	0
60	MG	BA	3024	1/1	0.91	0.65	32.32	56,56,56,56	0
60	MG	BA	3116	1/1	0.96	0.39	32.16	47,47,47,47	0
60	MG	BA	3228	1/1	0.92	0.80	31.97	52,52,52,52	0
60	MG	DA	3166	1/1	0.86	0.65	31.91	47,47,47,47	0
60	MG	BA	3044	1/1	0.92	0.84	31.61	56,56,56,56	0
60	MG	BA	3147	1/1	0.95	0.42	31.40	51,51,51,51	0
60	MG	DA	3061	1/1	0.95	0.49	31.34	47,47,47,47	0
60	MG	BA	3305	1/1	0.96	0.71	31.05	55,55,55,55	0
60	MG	CA	1645	1/1	0.88	0.70	30.60	50,50,50,50	0
60	MG	DA	3055	1/1	0.90	0.58	30.59	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3113	1/1	0.93	0.52	29.24	47,47,47,47	0
60	MG	CA	1736	1/1	0.86	0.61	28.99	55,55,55,55	0
60	MG	DA	3225	1/1	0.73	0.76	28.61	51,51,51,51	0
60	MG	DA	3062	1/1	0.96	0.43	28.41	48,48,48,48	0
60	MG	DA	3081	1/1	0.93	0.55	28.35	52,52,52,52	0
60	MG	BA	3082	1/1	0.81	0.67	28.25	51,51,51,51	0
60	MG	DA	3327	1/1	0.67	0.46	28.05	55,55,55,55	0
60	MG	DA	3034	1/1	0.95	0.58	27.71	47,47,47,47	0
60	MG	DA	3151	1/1	0.95	0.52	27.17	51,51,51,51	0
60	MG	DA	3010	1/1	0.95	0.64	26.71	47,47,47,47	0
60	MG	BA	3071	1/1	0.94	0.40	26.68	47,47,47,47	0
60	MG	BA	3023	1/1	0.96	0.78	26.64	49,49,49,49	0
60	MG	DA	3295	1/1	0.95	0.76	26.45	55,55,55,55	0
60	MG	DA	3161	1/1	0.95	0.31	25.91	47,47,47,47	0
60	MG	DA	3067	1/1	0.95	0.61	25.85	50,50,50,50	0
60	MG	BA	3280	1/1	0.90	0.49	25.70	57,57,57,57	0
60	MG	BA	3064	1/1	0.93	0.52	25.65	53,53,53,53	0
60	MG	DA	3159	1/1	0.95	0.84	25.65	49,49,49,49	0
60	MG	DA	3103	1/1	0.81	0.49	25.54	47,47,47,47	0
60	MG	DA	3215	1/1	0.88	0.50	25.31	48,48,48,48	0
60	MG	DA	3152	1/1	0.95	0.46	25.20	47,47,47,47	0
60	MG	BA	3056	1/1	0.98	0.62	25.08	47,47,47,47	0
60	MG	BA	3020	1/1	0.97	0.57	24.17	47,47,47,47	0
60	MG	BA	3219	1/1	0.92	0.86	24.14	49,49,49,49	0
60	MG	BA	3224	1/1	0.86	0.43	23.84	51,51,51,51	0
60	MG	BA	3058	1/1	0.93	0.70	23.81	55,55,55,55	0
60	MG	DA	3080	1/1	0.96	0.55	23.25	49,49,49,49	0
60	MG	DA	3059	1/1	0.86	0.77	23.01	55,55,55,55	0
60	MG	BA	3243	1/1	0.94	0.57	22.87	53,53,53,53	0
60	MG	DA	3104	1/1	0.96	0.42	22.74	50,50,50,50	0
60	MG	BA	3160	1/1	0.97	0.31	22.63	47,47,47,47	0
60	MG	DA	3002	1/1	0.88	0.95	22.28	54,54,54,54	1
60	MG	BA	3351	1/1	0.85	0.49	22.19	55,55,55,55	0
60	MG	DA	3089	1/1	0.97	0.65	21.74	48,48,48,48	0
60	MG	BA	3088	1/1	0.99	0.57	21.58	48,48,48,48	0
60	MG	DA	3021	1/1	0.97	0.53	21.48	47,47,47,47	0
60	MG	DA	3107	1/1	0.97	0.61	21.46	51,51,51,51	0
60	MG	DA	3036	1/1	0.96	0.40	21.38	55,55,55,55	0
60	MG	BA	3068	1/1	0.98	0.49	21.36	47,47,47,47	0
60	MG	DA	3139	1/1	0.94	0.65	21.21	50,50,50,50	0
60	MG	BA	3005	1/1	0.95	0.70	21.19	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3185	1/1	0.92	0.61	21.06	50,50,50,50	0
60	MG	AA	1714	1/1	0.91	0.55	20.82	59,59,59,59	0
60	MG	BA	3035	1/1	0.98	0.38	20.72	55,55,55,55	0
60	MG	DA	3146	1/1	0.93	0.46	20.39	47,47,47,47	0
60	MG	DA	3304	1/1	0.96	0.70	20.38	55,55,55,55	0
60	MG	CA	1624	1/1	0.90	0.38	20.23	51,51,51,51	0
60	MG	BA	3061	1/1	0.97	0.45	19.76	48,48,48,48	0
60	MG	BA	3105	1/1	0.74	0.49	19.76	47,47,47,47	0
60	MG	AA	1656	1/1	0.86	0.67	19.72	47,47,47,47	0
60	MG	DA	3005	1/1	0.95	0.44	19.60	53,53,53,53	0
60	MG	DA	3043	1/1	0.93	1.02	19.57	47,47,47,47	0
60	MG	BA	3062	1/1	0.95	0.51	19.56	47,47,47,47	0
60	MG	BA	3300	1/1	0.96	0.32	19.53	55,55,55,55	0
60	MG	BA	3021	1/1	0.98	0.40	19.27	47,47,47,47	0
60	MG	BA	3296	1/1	0.83	0.67	19.23	55,55,55,55	0
60	MG	BA	3201	1/1	0.56	0.44	19.23	52,52,52,52	0
60	MG	BA	3107	1/1	0.95	0.37	19.15	51,51,51,51	0
60	MG	BA	3013	1/1	0.98	0.40	18.71	47,47,47,47	0
60	MG	DA	3013	1/1	0.95	0.55	18.62	49,49,49,49	0
60	MG	BA	3090	1/1	0.98	0.46	18.17	48,48,48,48	0
60	MG	BA	3214	1/1	0.80	0.33	18.07	48,48,48,48	0
60	MG	AV	101	1/1	0.96	0.41	17.96	49,49,49,49	0
60	MG	BA	3069	1/1	0.97	0.36	17.93	48,48,48,48	0
60	MG	BA	3050	1/1	0.98	0.33	17.86	47,47,47,47	0
60	MG	DA	3012	1/1	0.86	0.34	17.44	47,47,47,47	0
60	MG	DA	3063	1/1	0.94	0.55	16.93	47,47,47,47	0
60	MG	DA	3020	1/1	0.98	0.54	16.86	47,47,47,47	0
60	MG	DA	3287	1/1	0.74	0.45	16.60	51,51,51,51	0
60	MG	BA	3257	1/1	0.94	0.36	16.57	51,51,51,51	0
60	MG	CA	1695	1/1	0.86	0.38	16.46	56,56,56,56	0
60	MG	AA	1632	1/1	0.91	0.47	16.45	53,53,53,53	0
60	MG	BA	3213	1/1	0.93	0.43	16.35	58,58,58,58	0
60	MG	BA	3083	1/1	0.98	0.51	16.34	47,47,47,47	0
60	MG	DA	3052	1/1	0.96	0.56	16.29	51,51,51,51	0
60	MG	BA	3138	1/1	0.92	0.34	15.92	50,50,50,50	0
60	MG	AA	1650	1/1	0.83	0.45	15.77	47,47,47,47	0
60	MG	DA	3160	1/1	0.92	0.33	15.69	55,55,55,55	0
60	MG	BA	3009	1/1	0.96	0.65	15.58	47,47,47,47	0
60	MG	DA	3044	1/1	0.98	0.54	15.52	47,47,47,47	0
60	MG	CA	1719	1/1	0.72	0.38	15.47	55,55,55,55	1
60	MG	DA	3186	1/1	0.96	0.54	15.29	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1741	1/1	0.92	0.49	15.24	55,55,55,55	0
60	MG	DF	303	1/1	0.86	0.69	15.19	59,59,59,59	0
60	MG	AY	401	1/1	0.89	0.54	15.14	55,55,55,55	0
60	MG	BA	3037	1/1	0.98	0.40	14.91	47,47,47,47	0
60	MG	DA	3099	1/1	0.96	0.36	14.90	54,54,54,54	0
60	MG	BA	3012	1/1	0.94	0.59	14.79	49,49,49,49	0
60	MG	DA	3197	1/1	0.94	0.58	14.58	47,47,47,47	0
60	MG	DA	3165	1/1	0.91	0.28	14.30	47,47,47,47	0
60	MG	DA	3226	1/1	0.93	0.42	14.23	51,51,51,51	0
60	MG	BA	3019	1/1	0.95	0.54	14.13	47,47,47,47	0
60	MG	AA	1735	1/1	0.83	0.55	14.10	55,55,55,55	0
60	MG	DA	3074	1/1	0.97	0.43	14.06	52,52,52,52	0
60	MG	DA	3106	1/1	0.79	0.40	13.88	47,47,47,47	0
60	MG	DA	3109	1/1	0.95	0.41	13.80	52,52,52,52	0
60	MG	AA	1745	1/1	0.94	0.66	13.74	55,55,55,55	0
60	MG	DD	301	1/1	0.92	0.58	13.62	47,47,47,47	0
60	MG	DA	3184	1/1	0.97	0.50	13.30	49,49,49,49	0
60	MG	DA	3096	1/1	0.97	0.45	13.08	60,60,60,60	0
60	MG	DA	3077	1/1	0.94	0.35	12.87	48,48,48,48	0
60	MG	BA	3307	1/1	0.84	0.33	12.82	55,55,55,55	0
60	MG	DA	3345	1/1	0.97	0.37	12.80	55,55,55,55	0
60	MG	DA	3196	1/1	0.95	0.35	12.72	52,52,52,52	0
60	MG	CV	101	1/1	0.97	0.58	12.63	49,49,49,49	0
60	MG	DA	3271	1/1	0.96	0.48	12.61	51,51,51,51	0
60	MG	DA	3114	1/1	0.96	0.38	12.59	47,47,47,47	0
60	MG	DA	3148	1/1	0.98	0.38	12.26	51,51,51,51	0
60	MG	DA	3022	1/1	0.98	0.22	12.20	47,47,47,47	0
60	MG	DA	3075	1/1	0.96	0.52	12.14	47,47,47,47	0
60	MG	CA	1669	1/1	0.96	0.30	12.11	47,47,47,47	0
60	MG	BA	3271	1/1	0.95	0.61	12.06	51,51,51,51	0
60	MG	BA	3202	1/1	0.97	0.35	12.04	47,47,47,47	0
60	MG	DA	3207	1/1	0.99	0.48	12.00	47,47,47,47	0
60	MG	BA	3070	1/1	0.98	0.39	11.96	50,50,50,50	0
60	MG	DA	3157	1/1	0.93	0.35	11.81	48,48,48,48	0
60	MG	DA	3068	1/1	0.90	0.40	11.61	50,50,50,50	0
60	MG	B7	101	1/1	0.90	0.54	11.52	49,49,49,49	0
60	MG	DA	3162	1/1	0.77	0.35	11.38	47,47,47,47	0
60	MG	DA	3127	1/1	0.79	0.32	11.36	52,52,52,52	0
60	MG	DA	3070	1/1	0.96	0.35	11.35	48,48,48,48	0
60	MG	DA	3084	1/1	0.98	0.36	11.28	47,47,47,47	0
60	MG	CA	1633	1/1	0.90	0.93	11.28	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3299	1/1	0.97	0.42	11.11	55,55,55,55	0
60	MG	DA	3206	1/1	0.88	0.33	10.93	50,50,50,50	0
60	MG	CA	1610	1/1	0.90	0.51	10.68	48,48,48,48	0
60	MG	BA	3026	1/1	0.94	0.39	10.53	47,47,47,47	0
60	MG	BA	3142	1/1	0.72	0.40	10.51	47,47,47,47	0
60	MG	DA	3097	1/1	0.85	0.51	10.43	56,56,56,56	0
60	MG	DA	3214	1/1	0.96	0.37	10.32	58,58,58,58	0
60	MG	DA	3253	1/1	0.88	0.35	10.29	49,49,49,49	0
60	MG	DA	3069	1/1	0.98	0.33	10.27	47,47,47,47	0
60	MG	BA	3051	1/1	0.97	0.35	10.26	51,51,51,51	0
60	MG	CA	1635	1/1	0.90	0.42	10.25	49,49,49,49	0
60	MG	AA	1634	1/1	0.90	0.68	10.08	52,52,52,52	0
60	MG	BD	301	1/1	0.94	0.49	10.05	47,47,47,47	0
60	MG	CA	1603	1/1	0.97	0.35	9.93	61,61,61,61	0
60	MG	BA	3079	1/1	0.94	0.44	9.66	49,49,49,49	0
60	MG	DA	3033	1/1	0.81	0.27	9.65	53,53,53,53	0
60	MG	BA	3159	1/1	0.91	0.32	9.40	55,55,55,55	0
60	MG	BA	3004	1/1	0.90	0.29	9.28	53,53,53,53	0
60	MG	BA	3098	1/1	0.99	0.28	9.21	54,54,54,54	0
60	MG	DA	3344	1/1	0.90	0.54	9.09	55,55,55,55	0
60	MG	DA	3108	1/1	0.98	0.21	8.93	51,51,51,51	0
60	MG	BA	3233	1/1	0.94	0.62	8.79	47,47,47,47	0
60	MG	BA	3011	1/1	0.97	0.30	8.77	47,47,47,47	0
60	MG	BA	3164	1/1	0.98	0.25	8.69	47,47,47,47	0
60	MG	DA	3016	1/1	0.97	0.51	8.66	47,47,47,47	0
60	MG	CA	1686	1/1	0.94	0.33	8.31	57,57,57,57	0
60	MG	DA	3267	1/1	0.93	0.32	8.10	54,54,54,54	0
60	MG	BA	3188	1/1	0.91	0.36	8.01	57,57,57,57	0
60	MG	DA	3027	1/1	0.93	0.46	7.97	47,47,47,47	0
60	MG	BA	3015	1/1	0.99	0.48	7.95	47,47,47,47	0
60	MG	DA	3317	1/1	0.82	0.31	7.87	55,55,55,55	0
60	MG	BA	3347	1/1	0.97	0.31	7.63	55,55,55,55	0
60	MG	AA	1625	1/1	0.95	0.28	7.31	51,51,51,51	0
60	MG	DA	3072	1/1	0.98	0.24	6.97	47,47,47,47	0
60	MG	BA	3076	1/1	0.95	0.24	6.91	48,48,48,48	0
60	MG	BA	3342	1/1	0.95	0.28	6.90	55,55,55,55	0
60	MG	CY	401	1/1	0.95	0.56	6.84	55,55,55,55	0
60	MG	AA	1749	1/1	0.98	0.36	6.77	55,55,55,55	0
60	MG	AA	1685	1/1	0.94	0.26	6.72	57,57,57,57	0
60	MG	CA	1649	1/1	0.94	0.42	6.67	47,47,47,47	0
60	MG	BA	3067	1/1	0.89	0.32	6.60	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3234	1/1	0.97	0.54	6.52	47,47,47,47	0
60	MG	DA	3014	1/1	0.99	0.31	6.33	47,47,47,47	0
60	MG	BA	3128	1/1	0.94	0.21	6.30	50,50,50,50	0
60	MG	BA	3074	1/1	0.95	0.40	6.20	47,47,47,47	0
60	MG	BA	3318	1/1	0.83	0.29	6.19	55,55,55,55	0
60	MG	BA	3206	1/1	0.95	0.30	6.17	47,47,47,47	0
60	MG	BA	3182	1/1	0.96	0.38	6.17	49,49,49,49	0
60	MG	BA	3252	1/1	0.97	0.33	6.04	49,49,49,49	0
60	MG	B1	101	1/1	0.92	0.56	6.03	55,55,55,55	0
60	MG	DA	3156	1/1	0.97	0.34	6.02	51,51,51,51	0
60	MG	DA	3170	1/1	0.91	0.48	5.99	49,49,49,49	1
60	MG	CA	1722	1/1	0.75	0.39	5.84	55,55,55,55	0
60	MG	DA	3298	1/1	0.94	0.30	5.82	55,55,55,55	0
60	MG	BA	3196	1/1	0.95	0.47	5.82	47,47,47,47	0
60	MG	AA	1623	1/1	0.94	0.53	5.70	57,57,57,57	0
60	MG	BA	3114	1/1	0.97	0.25	5.65	48,48,48,48	0
60	MG	BA	3163	1/1	0.96	0.41	5.53	53,53,53,53	0
60	MG	DA	3048	1/1	0.98	0.25	5.27	47,47,47,47	0
60	MG	BA	3145	1/1	0.97	0.29	5.25	47,47,47,47	0
60	MG	BA	3225	1/1	0.85	0.33	5.25	51,51,51,51	0
60	MG	CA	1616	1/1	0.95	0.37	5.23	54,54,54,54	0
60	MG	DA	3116	1/1	0.94	0.34	5.23	50,50,50,50	0
60	MG	AA	1627	1/1	0.89	0.31	5.18	53,53,53,53	0
60	MG	DA	3305	1/1	0.93	0.24	5.07	55,55,55,55	0
60	MG	DA	3071	1/1	0.98	0.30	5.07	50,50,50,50	0
60	MG	DA	3091	1/1	0.94	0.40	4.86	48,48,48,48	0
60	MG	DA	3238	1/1	0.77	0.24	4.75	47,47,47,47	0
60	MG	CA	1750	1/1	0.95	0.24	4.72	55,55,55,55	0
60	MG	BA	3346	1/1	0.87	0.46	4.68	55,55,55,55	0
60	MG	DA	3299	1/1	0.88	0.37	4.60	55,55,55,55	0
60	MG	AA	1674	1/1	0.94	0.22	4.57	50,50,50,50	0
60	MG	BA	3155	1/1	0.97	0.31	4.53	51,51,51,51	0
60	MG	DA	3259	1/1	0.85	0.35	4.49	58,58,58,58	0
60	MG	BA	3279	1/1	0.96	0.19	4.31	55,55,55,55	0
60	MG	AA	1721	1/1	0.95	0.41	4.03	55,55,55,55	1
60	MG	CA	1607	1/1	0.91	0.32	3.97	47,47,47,47	0
60	MG	D1	101	1/1	0.98	0.41	3.81	55,55,55,55	0
60	MG	BA	3184	1/1	0.97	0.43	3.77	47,47,47,47	0
60	MG	AA	1669	1/1	0.96	0.29	3.77	47,47,47,47	0
60	MG	DA	3083	1/1	0.74	0.29	3.74	51,51,51,51	0
60	MG	DA	3167	1/1	0.79	0.23	3.72	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1683	1/1	0.68	0.45	3.67	47,47,47,47	0
60	MG	AA	1671	1/1	0.95	0.32	3.54	47,47,47,47	0
60	MG	DA	3229	1/1	0.80	0.38	3.52	52,52,52,52	0
60	MG	BA	3175	1/1	0.81	0.30	3.06	49,49,49,49	1
60	MG	DU	201	1/1	0.97	0.50	3.04	48,48,48,48	0
60	MG	BA	3267	1/1	0.96	0.24	2.98	54,54,54,54	0
60	MG	AA	1608	1/1	0.95	0.26	2.82	47,47,47,47	0
60	MG	CA	1612	1/1	0.84	0.28	2.76	56,56,56,56	0
60	MG	DA	3131	1/1	0.97	0.20	2.71	48,48,48,48	0
60	MG	CA	1746	1/1	0.98	0.23	2.52	55,55,55,55	0
60	MG	DA	3129	1/1	0.94	0.21	2.49	50,50,50,50	0
60	MG	AA	1657	1/1	0.54	0.27	2.29	54,54,54,54	0
60	MG	DF	301	1/1	0.85	0.27	2.27	47,47,47,47	0
60	MG	CA	1674	1/1	0.82	0.21	2.25	50,50,50,50	0
60	MG	DD	302	1/1	0.94	0.46	2.22	47,47,47,47	0
60	MG	AA	1672	1/1	0.94	0.25	2.21	53,53,53,53	0
60	MG	DR	201	1/1	0.99	0.33	2.06	47,47,47,47	0
60	MG	BA	3047	1/1	0.92	0.31	1.94	47,47,47,47	0
60	MG	AA	1754	1/1	0.84	0.26	1.69	55,55,55,55	0
60	MG	AA	1694	1/1	0.64	0.21	1.68	56,56,56,56	0
60	MG	BA	3032	1/1	0.80	0.17	1.51	53,53,53,53	0
60	MG	AA	1611	1/1	0.89	0.49	1.40	48,48,48,48	0
60	MG	BF	301	1/1	0.93	0.29	1.40	47,47,47,47	0
60	MG	CA	1658	1/1	0.93	0.25	1.40	49,49,49,49	0
60	MG	BA	3237	1/1	0.71	0.27	1.37	67,67,67,67	0
60	MG	BA	3130	1/1	0.97	0.19	1.36	48,48,48,48	0
60	MG	CA	1671	1/1	0.95	0.19	1.20	47,47,47,47	0
60	MG	BA	3321	1/1	0.95	0.20	0.89	55,55,55,55	0
60	MG	BA	3205	1/1	0.92	0.17	0.83	50,50,50,50	0
60	MG	AA	1679	1/1	0.83	0.19	0.82	53,53,53,53	0
60	MG	AA	1654	1/1	0.97	0.15	0.78	53,53,53,53	0
60	MG	AA	1658	1/1	0.90	0.27	0.77	49,49,49,49	0
60	MG	AA	1610	1/1	0.88	0.28	0.68	55,55,55,55	0
60	MG	DA	3320	1/1	0.97	0.20	0.67	55,55,55,55	0
60	MG	AL	201	1/1	0.77	0.25	0.57	51,51,51,51	1
60	MG	BA	3248	1/1	0.88	0.26	0.53	56,56,56,56	1
60	MG	AA	1722	1/1	0.97	0.27	0.24	55,55,55,55	0
60	MG	CA	1754	1/1	0.87	0.24	0.23	55,55,55,55	0
61	ZN	CD	301	1/1	0.99	0.27	0.23	52,52,52,52	0
60	MG	CA	1675	1/1	0.79	0.18	-0.02	48,48,48,48	1
60	MG	AA	1621	1/1	0.88	0.22	-0.05	56,56,56,56	0
60	MG	CA	1626	1/1	0.95	0.17	-0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3313	1/1	0.95	0.18	-0.19	55,55,55,55	0
60	MG	AA	1635	1/1	0.80	0.19	-0.31	47,47,47,47	0
60	MG	AA	1675	1/1	0.64	0.18	-0.33	48,48,48,48	0
60	MG	DA	3312	1/1	0.93	0.16	-0.39	55,55,55,55	0
60	MG	BA	3263	1/1	0.95	0.15	-0.42	56,56,56,56	0
60	MG	AA	1636	1/1	0.95	0.20	-0.56	49,49,49,49	0
61	ZN	AD	301	1/1	0.98	0.20	-0.64	52,52,52,52	0
60	MG	AA	1617	1/1	0.84	0.17	-0.73	54,54,54,54	0
60	MG	BA	3166	1/1	0.94	0.10	-1.01	47,47,47,47	0
60	MG	BA	3152	1/1	0.84	0.12	-1.30	50,50,50,50	0
60	MG	BA	3306	1/1	0.92	0.18	-1.33	55,55,55,55	0
61	ZN	CN	102	1/1	1.00	0.12	-1.42	60,60,60,60	0
60	MG	AA	1734	1/1	0.91	0.16	-1.53	55,55,55,55	0
60	MG	CA	1678	1/1	0.93	0.13	-1.55	49,49,49,49	0
60	MG	CA	1620	1/1	0.94	0.19	-1.56	56,56,56,56	0
61	ZN	AN	101	1/1	0.98	0.10	-1.56	60,60,60,60	1
61	ZN	D9	101	1/1	1.00	0.11	-1.64	55,55,55,55	1
60	MG	AA	1678	1/1	0.98	0.05	-1.81	49,49,49,49	0
60	MG	AA	1751	1/1	0.99	0.07	-1.87	55,55,55,55	0
60	MG	AA	1682	1/1	0.91	0.13	-1.91	53,53,53,53	0
60	MG	CA	1682	1/1	0.98	0.11	-2.13	53,53,53,53	0
60	MG	AW	103	1/1	0.90	0.09	-2.26	54,54,54,54	0
61	ZN	B9	101	1/1	0.99	0.06	-2.38	55,55,55,55	0
60	MG	BA	3236	1/1	0.81	0.13	-2.53	47,47,47,47	0
60	MG	CA	1696	1/1	0.98	0.10	-2.86	62,62,62,62	0
60	MG	AA	1633	1/1	0.92	0.12	-2.93	55,55,55,55	0
60	MG	CA	1653	1/1	0.98	0.07	-3.33	53,53,53,53	0
60	MG	DA	3306	1/1	0.91	0.10	-3.75	55,55,55,55	0
60	MG	AA	1748	1/1	0.65	0.40	-	55,55,55,55	0
60	MG	DA	3073	1/1	0.93	0.60	-	53,53,53,53	0
60	MG	AA	1710	1/1	0.88	0.13	-	55,55,55,55	0
60	MG	DA	3273	1/1	0.96	0.29	-	58,58,58,58	0
60	MG	DA	3050	1/1	0.94	0.52	-	47,47,47,47	0
60	MG	CN	101	1/1	0.92	0.36	-	55,55,55,55	0
60	MG	BA	3007	1/1	0.95	0.49	-	52,52,52,52	0
60	MG	BA	3177	1/1	0.91	0.84	-	47,47,47,47	0
60	MG	BA	3086	1/1	0.96	0.54	-	48,48,48,48	0
60	MG	BC	301	1/1	0.56	0.53	-	52,52,52,52	1
60	MG	AA	1612	1/1	0.93	0.13	-	52,52,52,52	0
60	MG	BA	3339	1/1	0.84	0.24	-	55,55,55,55	0
60	MG	DA	3255	1/1	0.94	0.46	-	60,60,60,60	0
60	MG	CA	1707	1/1	0.84	0.63	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1680	1/1	0.97	0.30	-	49,49,49,49	0
60	MG	BA	3040	1/1	0.97	0.60	-	47,47,47,47	0
60	MG	BA	3014	1/1	0.97	0.59	-	53,53,53,53	0
60	MG	BA	3277	1/1	0.91	0.74	-	57,57,57,57	0
60	MG	BA	3081	1/1	0.98	0.36	-	47,47,47,47	0
60	MG	DA	3135	1/1	0.95	0.51	-	54,54,54,54	0
60	MG	DB	204	1/1	0.91	0.20	-	55,55,55,55	0
60	MG	BA	3246	1/1	0.90	0.38	-	55,55,55,55	0
60	MG	AA	1725	1/1	0.89	1.06	-	54,54,54,54	0
60	MG	DA	3286	1/1	0.96	0.24	-	60,60,60,60	0
60	MG	DA	3054	1/1	0.91	0.35	-	51,51,51,51	0
60	MG	BA	3120	1/1	0.92	0.62	-	50,50,50,50	0
60	MG	DA	3085	1/1	0.89	0.42	-	47,47,47,47	0
60	MG	DA	3201	1/1	0.95	0.42	-	60,60,60,60	0
60	MG	BA	3034	1/1	0.94	0.35	-	50,50,50,50	0
60	MG	DA	3308	1/1	0.93	0.14	-	55,55,55,55	0
60	MG	DA	3123	1/1	0.91	0.25	-	64,64,64,64	1
60	MG	AA	1605	1/1	0.97	0.11	-	50,50,50,50	0
60	MG	AA	1673	1/1	0.81	0.12	-	52,52,52,52	0
60	MG	AA	1747	1/1	0.69	0.35	-	55,55,55,55	1
60	MG	BA	3046	1/1	0.98	0.43	-	47,47,47,47	0
60	MG	CA	1625	1/1	0.77	0.62	-	53,53,53,53	0
60	MG	BA	3266	1/1	0.88	0.55	-	59,59,59,59	0
60	MG	BA	3085	1/1	0.97	0.17	-	47,47,47,47	0
60	MG	CW	102	1/1	0.96	0.29	-	60,60,60,60	0
60	MG	DA	3316	1/1	0.86	0.60	-	55,55,55,55	0
60	MG	DA	3256	1/1	0.93	0.62	-	55,55,55,55	0
60	MG	DA	3348	1/1	0.95	0.32	-	55,55,55,55	0
60	MG	DA	3136	1/1	0.92	0.93	-	58,58,58,58	0
60	MG	CA	1670	1/1	0.54	0.72	-	69,69,69,69	0
60	MG	BA	3149	1/1	0.97	0.53	-	54,54,54,54	0
60	MG	BA	3354	1/1	0.90	0.40	-	55,55,55,55	0
60	MG	BA	3322	1/1	0.93	0.38	-	55,55,55,55	0
60	MG	BA	3282	1/1	0.87	0.43	-	57,57,57,57	0
60	MG	CA	1712	1/1	0.93	0.50	-	47,47,47,47	0
60	MG	AA	1742	1/1	0.83	0.34	-	55,55,55,55	0
60	MG	DY	201	1/1	0.93	0.28	-	55,55,55,55	0
60	MG	BA	3250	1/1	0.90	0.45	-	52,52,52,52	0
60	MG	CA	1605	1/1	0.90	0.60	-	59,59,59,59	0
60	MG	BA	3249	1/1	0.81	0.43	-	56,56,56,56	0
60	MG	BA	3183	1/1	0.81	0.63	-	56,56,56,56	0
60	MG	BA	3294	1/1	0.77	0.12	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3212	1/1	0.59	0.49	-	55,55,55,55	0
60	MG	AA	1718	1/1	0.68	0.23	-	55,55,55,55	0
60	MG	BA	3262	1/1	0.98	0.18	-	63,63,63,63	1
60	MG	AA	1666	1/1	0.82	0.58	-	57,57,57,57	0
60	MG	CA	1637	1/1	0.85	0.26	-	52,52,52,52	0
60	MG	DA	3274	1/1	0.83	0.51	-	63,63,63,63	0
60	MG	DA	3039	1/1	0.96	0.38	-	51,51,51,51	0
60	MG	AA	1604	1/1	0.95	0.39	-	61,61,61,61	0
60	MG	DA	3205	1/1	0.82	0.55	-	57,57,57,57	0
60	MG	BA	3109	1/1	0.95	0.30	-	48,48,48,48	0
60	MG	DA	3035	1/1	0.94	0.40	-	50,50,50,50	0
60	MG	DA	3281	1/1	0.80	0.37	-	57,57,57,57	0
60	MG	BA	3316	1/1	0.94	0.46	-	55,55,55,55	0
60	MG	BA	3135	1/1	0.66	0.71	-	58,58,58,58	0
60	MG	DA	3015	1/1	0.99	0.54	-	53,53,53,53	0
60	MG	AA	1644	1/1	0.88	0.36	-	49,49,49,49	0
60	MG	CA	1752	1/1	0.97	0.19	-	55,55,55,55	1
60	MG	DA	3173	1/1	0.93	0.23	-	58,58,58,58	0
60	MG	CA	1756	1/1	0.92	0.34	-	55,55,55,55	1
60	MG	DB	202	1/1	0.96	0.74	-	55,55,55,55	0
60	MG	DA	3102	1/1	0.97	0.74	-	47,47,47,47	0
60	MG	BA	3192	1/1	0.90	0.26	-	65,65,65,65	0
60	MG	AA	1620	1/1	0.92	0.29	-	55,55,55,55	0
60	MG	AV	103	1/1	0.92	0.26	-	54,54,54,54	1
60	MG	BA	3226	1/1	0.90	0.46	-	56,56,56,56	0
60	MG	BA	3054	1/1	0.88	0.77	-	47,47,47,47	0
60	MG	BA	3096	1/1	0.90	0.43	-	56,56,56,56	0
60	MG	AW	104	1/1	0.94	0.13	-	56,56,56,56	0
60	MG	DA	3247	1/1	0.83	0.32	-	55,55,55,55	1
60	MG	AA	1652	1/1	0.91	0.39	-	47,47,47,47	0
60	MG	AA	1613	1/1	0.59	0.27	-	56,56,56,56	0
60	MG	AA	1691	1/1	0.92	0.47	-	59,59,59,59	0
60	MG	DA	3149	1/1	0.86	0.24	-	47,47,47,47	0
60	MG	BA	3010	1/1	0.91	0.60	-	52,52,52,52	0
60	MG	BA	3112	1/1	0.90	0.33	-	48,48,48,48	0
60	MG	AA	1628	1/1	0.95	0.37	-	70,70,70,70	0
60	MG	CA	1748	1/1	0.91	0.44	-	55,55,55,55	1
60	MG	CA	1703	1/1	0.97	0.29	-	47,47,47,47	0
60	MG	DA	3278	1/1	0.96	0.66	-	51,51,51,51	0
60	MG	CA	1727	1/1	0.91	0.21	-	56,56,56,56	0
60	MG	AA	1702	1/1	0.98	0.34	-	47,47,47,47	0
60	MG	DA	3341	1/1	0.96	0.49	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3075	1/1	0.94	0.38	-	47,47,47,47	0
60	MG	BA	3025	1/1	0.94	0.44	-	55,55,55,55	0
60	MG	DA	3124	1/1	0.94	0.46	-	53,53,53,53	0
60	MG	AA	1739	1/1	0.88	0.20	-	55,55,55,55	1
60	MG	BA	3119	1/1	0.92	0.77	-	49,49,49,49	0
60	MG	DA	3105	1/1	0.80	0.83	-	48,48,48,48	0
60	MG	DA	3130	1/1	0.95	0.24	-	56,56,56,56	0
60	MG	BA	3291	1/1	0.94	0.37	-	54,54,54,54	0
60	MG	B5	102	1/1	0.91	0.61	-	53,53,53,53	0
60	MG	CA	1630	1/1	0.95	0.27	-	47,47,47,47	0
60	MG	AA	1707	1/1	0.91	0.46	-	49,49,49,49	0
60	MG	DA	3347	1/1	0.90	0.25	-	55,55,55,55	0
60	MG	CA	1734	1/1	0.83	0.20	-	55,55,55,55	1
60	MG	DA	3008	1/1	0.90	0.36	-	52,52,52,52	0
60	MG	AA	1638	1/1	0.82	0.25	-	52,52,52,52	0
60	MG	CV	105	1/1	0.85	0.23	-	50,50,50,50	0
60	MG	CA	1606	1/1	0.84	0.32	-	58,58,58,58	0
60	MG	BA	3170	1/1	0.95	0.40	-	50,50,50,50	0
60	MG	CA	1666	1/1	0.88	0.56	-	57,57,57,57	0
60	MG	AA	1649	1/1	0.88	0.15	-	53,53,53,53	0
60	MG	DA	3319	1/1	0.63	0.47	-	55,55,55,55	0
60	MG	BA	3028	1/1	0.99	0.45	-	52,52,52,52	0
60	MG	CA	1676	1/1	0.65	0.49	-	58,58,58,58	0
60	MG	DA	3288	1/1	0.90	0.20	-	66,66,66,66	0
60	MG	CA	1717	1/1	0.80	0.41	-	52,52,52,52	0
60	MG	DA	3262	1/1	0.83	0.32	-	52,52,52,52	0
60	MG	DA	3250	1/1	0.91	0.45	-	56,56,56,56	0
60	MG	DA	3087	1/1	0.81	0.58	-	48,48,48,48	0
60	MG	DA	3007	1/1	0.95	0.71	-	53,53,53,53	0
60	MG	BA	3340	1/1	0.93	0.60	-	55,55,55,55	0
60	MG	BA	3146	1/1	0.94	0.65	-	47,47,47,47	0
60	MG	BA	3136	1/1	0.96	0.79	-	50,50,50,50	0
60	MG	DA	3260	1/1	0.70	0.52	-	59,59,59,59	0
60	MG	DA	3326	1/1	0.90	0.55	-	55,55,55,55	0
60	MG	DA	3264	1/1	0.93	0.14	-	56,56,56,56	0
60	MG	CA	1619	1/1	0.96	0.26	-	55,55,55,55	0
60	MG	BA	3230	1/1	0.88	0.78	-	54,54,54,54	0
60	MG	DA	3180	1/1	0.75	0.22	-	52,52,52,52	0
60	MG	CA	1656	1/1	0.92	0.82	-	47,47,47,47	0
60	MG	CA	1693	1/1	0.83	0.74	-	59,59,59,59	0
60	MG	CA	1623	1/1	0.97	0.42	-	48,48,48,48	0
60	MG	CA	1735	1/1	0.96	0.16	-	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3095	1/1	0.98	0.75	-	47,47,47,47	0
60	MG	BA	3029	1/1	0.91	0.34	-	55,55,55,55	0
60	MG	DA	3224	1/1	0.79	0.43	-	52,52,52,52	0
60	MG	AV	104	1/1	0.94	0.10	-	54,54,54,54	0
60	MG	DA	3240	1/1	0.24	0.91	-	55,55,55,55	1
60	MG	DX	101	1/1	0.89	0.22	-	55,55,55,55	0
60	MG	AA	1642	1/1	0.47	0.32	-	55,55,55,55	0
60	MG	BA	3002	1/1	0.88	0.30	-	67,67,67,67	0
60	MG	AA	1696	1/1	0.80	0.31	-	62,62,62,62	0
60	MG	BA	3187	1/1	0.84	0.40	-	48,48,48,48	0
60	MG	DA	3223	1/1	0.88	0.34	-	49,49,49,49	0
60	MG	DB	203	1/1	0.90	0.73	-	55,55,55,55	0
60	MG	DA	3078	1/1	0.98	0.86	-	51,51,51,51	0
60	MG	BA	3232	1/1	0.93	0.51	-	53,53,53,53	0
60	MG	CA	1714	1/1	0.96	0.47	-	64,64,64,64	0
60	MG	DA	3280	1/1	0.79	0.69	-	57,57,57,57	0
60	MG	BA	3060	1/1	0.97	0.57	-	47,47,47,47	0
60	MG	BA	3173	1/1	0.87	0.33	-	56,56,56,56	0
60	MG	CA	1723	1/1	0.93	0.10	-	55,55,55,55	0
60	MG	BA	3216	1/1	0.92	0.28	-	49,49,49,49	0
60	MG	AA	1728	1/1	0.94	0.30	-	55,55,55,55	0
60	MG	BA	3195	1/1	0.87	0.42	-	52,52,52,52	0
60	MG	BA	3179	1/1	0.76	0.34	-	59,59,59,59	0
60	MG	BA	3323	1/1	0.95	0.84	-	55,55,55,55	0
60	MG	DA	3145	1/1	0.91	0.40	-	49,49,49,49	0
60	MG	AA	1640	1/1	0.94	0.41	-	48,48,48,48	0
60	MG	AA	1602	1/1	0.92	0.37	-	52,52,52,52	0
60	MG	CA	1685	1/1	0.88	0.35	-	47,47,47,47	0
60	MG	AA	1756	1/1	0.96	0.16	-	55,55,55,55	1
60	MG	AA	1647	1/1	0.80	0.37	-	62,62,62,62	0
60	MG	CA	1628	1/1	0.96	0.31	-	56,56,56,56	0
60	MG	AV	106	1/1	0.86	0.05	-	57,57,57,57	0
60	MG	CA	1615	1/1	0.65	0.69	-	64,64,64,64	0
60	MG	DA	3064	1/1	0.95	0.41	-	56,56,56,56	0
60	MG	DA	3003	1/1	0.76	0.43	-	67,67,67,67	0
60	MG	AA	1726	1/1	0.92	0.29	-	56,56,56,56	0
60	MG	BA	3337	1/1	0.83	0.16	-	55,55,55,55	0
60	MG	CA	1690	1/1	0.90	0.20	-	59,59,59,59	0
60	MG	DA	3049	1/1	0.93	0.43	-	47,47,47,47	0
60	MG	BB	201	1/1	0.88	0.56	-	67,67,67,67	0
60	MG	CA	1663	1/1	0.76	0.24	-	51,51,51,51	0
60	MG	BA	3302	1/1	0.96	0.64	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1738	1/1	0.95	0.10	-	55,55,55,55	0
60	MG	DA	3303	1/1	0.92	0.73	-	55,55,55,55	0
60	MG	DA	3279	1/1	0.92	0.28	-	55,55,55,55	0
60	MG	DA	3199	1/1	0.93	0.54	-	53,53,53,53	0
60	MG	BA	3038	1/1	0.98	0.45	-	51,51,51,51	0
60	MG	DA	3040	1/1	0.89	0.30	-	68,68,68,68	0
60	MG	BA	3087	1/1	0.97	0.32	-	49,49,49,49	0
60	MG	AV	105	1/1	0.87	0.21	-	50,50,50,50	1
60	MG	BA	3207	1/1	0.88	0.55	-	60,60,60,60	0
60	MG	DA	3185	1/1	0.86	0.53	-	56,56,56,56	0
60	MG	DA	3134	1/1	0.37	0.64	-	64,64,64,64	0
60	MG	BA	3260	1/1	0.95	0.18	-	57,57,57,57	0
60	MG	DA	3094	1/1	0.96	0.44	-	51,51,51,51	0
60	MG	AA	1661	1/1	0.97	0.48	-	52,52,52,52	0
60	MG	AA	1717	1/1	0.88	0.26	-	66,66,66,66	0
60	MG	DA	3342	1/1	0.96	0.27	-	55,55,55,55	0
60	MG	CA	1711	1/1	0.91	0.15	-	55,55,55,55	0
60	MG	AA	1690	1/1	0.95	0.67	-	52,52,52,52	0
60	MG	DA	3182	1/1	0.88	0.27	-	56,56,56,56	0
60	MG	DA	3121	1/1	0.97	0.41	-	50,50,50,50	0
60	MG	BA	3157	1/1	0.99	0.11	-	53,53,53,53	0
60	MG	DA	3200	1/1	0.88	0.97	-	58,58,58,58	0
60	MG	AA	1615	1/1	0.93	0.81	-	53,53,53,53	0
60	MG	AA	1711	1/1	0.91	0.29	-	47,47,47,47	0
60	MG	BA	3273	1/1	0.88	0.46	-	58,58,58,58	0
60	MG	BA	3349	1/1	0.90	0.50	-	55,55,55,55	0
60	MG	DA	3141	1/1	0.94	0.36	-	56,56,56,56	0
60	MG	AA	1697	1/1	0.81	0.35	-	52,52,52,52	0
60	MG	DA	3335	1/1	0.90	0.50	-	55,55,55,55	0
60	MG	CA	1749	1/1	0.87	0.38	-	55,55,55,55	0
60	MG	CA	1609	1/1	0.94	0.36	-	55,55,55,55	0
60	MG	DA	3249	1/1	0.87	0.19	-	56,56,56,56	0
60	MG	BA	3080	1/1	0.84	0.66	-	52,52,52,52	0
60	MG	DA	3332	1/1	0.93	0.49	-	55,55,55,55	0
60	MG	DA	3218	1/1	0.97	0.53	-	51,51,51,51	0
60	MG	BA	3222	1/1	0.79	0.29	-	49,49,49,49	0
60	MG	CA	1617	1/1	0.90	0.29	-	51,51,51,51	0
60	MG	CA	1643	1/1	0.58	0.56	-	49,49,49,49	0
60	MG	DA	3125	1/1	0.93	0.22	-	49,49,49,49	0
60	MG	D3	101	1/1	0.94	0.48	-	58,58,58,58	0
60	MG	DA	3041	1/1	0.97	0.35	-	47,47,47,47	0
60	MG	DA	3241	1/1	0.97	0.10	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1660	1/1	0.82	0.20	-	58,58,58,58	0
60	MG	BU	201	1/1	0.83	0.41	-	48,48,48,48	0
60	MG	BA	3141	1/1	0.82	0.57	-	49,49,49,49	0
60	MG	BA	3144	1/1	0.93	0.42	-	49,49,49,49	0
60	MG	BA	3008	1/1	0.97	0.41	-	55,55,55,55	0
60	MG	AA	1743	1/1	0.84	0.61	-	55,55,55,55	0
60	MG	B5	101	1/1	0.98	0.35	-	49,49,49,49	0
60	MG	BA	3330	1/1	0.92	0.25	-	55,55,55,55	0
60	MG	CA	1614	1/1	0.90	0.81	-	53,53,53,53	0
60	MG	CA	1668	1/1	0.91	0.82	-	58,58,58,58	0
60	MG	BA	3240	1/1	0.96	0.59	-	58,58,58,58	1
60	MG	CA	1738	1/1	0.90	0.94	-	55,55,55,55	0
60	MG	BA	3227	1/1	0.66	0.66	-	55,55,55,55	0
60	MG	AA	1626	1/1	0.97	0.30	-	53,53,53,53	0
60	MG	DA	3235	1/1	0.88	0.28	-	49,49,49,49	0
60	MG	BA	3072	1/1	0.87	0.72	-	53,53,53,53	0
60	MG	DA	3231	1/1	0.71	0.51	-	54,54,54,54	1
60	MG	DA	3282	1/1	0.79	0.35	-	57,57,57,57	0
60	MG	BA	3115	1/1	0.96	0.53	-	50,50,50,50	0
60	MG	CA	1721	1/1	0.89	0.27	-	58,58,58,58	0
60	MG	BA	3301	1/1	0.68	0.54	-	55,55,55,55	0
60	MG	BA	3312	1/1	0.93	0.74	-	55,55,55,55	0
60	MG	AA	1737	1/1	0.82	0.67	-	55,55,55,55	0
60	MG	DA	3026	1/1	0.96	0.45	-	55,55,55,55	0
60	MG	BA	3084	1/1	0.94	0.37	-	47,47,47,47	0
60	MG	DA	3088	1/1	0.95	0.42	-	49,49,49,49	0
60	MG	CA	1641	1/1	0.77	0.38	-	55,55,55,55	0
60	MG	AA	1659	1/1	0.56	0.30	-	57,57,57,57	0
60	MG	BA	3239	1/1	0.79	0.38	-	55,55,55,55	0
60	MG	DA	3115	1/1	0.93	0.23	-	48,48,48,48	0
60	MG	CA	1644	1/1	0.81	0.13	-	57,57,57,57	0
60	MG	DA	3296	1/1	0.93	0.60	-	55,55,55,55	0
60	MG	DA	3090	1/1	0.92	0.66	-	48,48,48,48	0
60	MG	BP	201	1/1	0.97	0.22	-	49,49,49,49	0
60	MG	AA	1606	1/1	0.93	0.30	-	59,59,59,59	0
60	MG	BA	3238	1/1	0.94	0.09	-	55,55,55,55	1
60	MG	CA	1745	1/1	0.88	0.24	-	55,55,55,55	0
60	MG	DA	3004	1/1	0.95	0.38	-	61,61,61,61	0
60	MG	AA	1637	1/1	0.69	0.52	-	53,53,53,53	0
60	MG	BA	3235	1/1	0.94	0.21	-	60,60,60,60	0
60	MG	BD	302	1/1	0.92	0.62	-	47,47,47,47	0
60	MG	AA	1700	1/1	0.91	0.27	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1667	1/1	0.83	0.27	-	47,47,47,47	0
60	MG	CA	1647	1/1	0.80	0.24	-	62,62,62,62	0
60	MG	AA	1732	1/1	0.65	0.52	-	55,55,55,55	0
60	MG	DA	3315	1/1	0.90	0.29	-	55,55,55,55	0
60	MG	AA	1720	1/1	0.74	0.50	-	58,58,58,58	1
60	MG	BA	3186	1/1	0.97	0.90	-	51,51,51,51	0
60	MG	CA	1667	1/1	0.89	0.41	-	47,47,47,47	0
60	MG	DA	3176	1/1	0.76	0.41	-	58,58,58,58	0
60	MG	AA	1607	1/1	0.97	0.42	-	58,58,58,58	0
60	MG	BA	3343	1/1	0.92	0.53	-	55,55,55,55	0
60	MG	CA	1700	1/1	0.86	0.26	-	54,54,54,54	0
60	MG	BA	3027	1/1	0.95	0.31	-	50,50,50,50	0
60	MG	DA	3323	1/1	0.87	0.50	-	55,55,55,55	0
60	MG	BA	3234	1/1	0.80	0.81	-	52,52,52,52	0
60	MG	CL	201	1/1	0.93	0.58	-	51,51,51,51	1
60	MG	BA	3272	1/1	0.89	0.26	-	59,59,59,59	1
60	MG	CA	1683	1/1	0.87	0.25	-	47,47,47,47	0
60	MG	BA	3319	1/1	0.74	0.33	-	55,55,55,55	0
60	MG	BB	204	1/1	0.92	0.22	-	55,55,55,55	0
60	MG	BA	3331	1/1	0.95	0.22	-	55,55,55,55	0
60	MG	AA	1701	1/1	0.89	0.31	-	51,51,51,51	0
60	MG	CA	1636	1/1	0.95	0.65	-	53,53,53,53	0
60	MG	DA	3174	1/1	0.94	0.37	-	52,52,52,52	0
60	MG	AA	1676	1/1	0.86	0.38	-	58,58,58,58	0
60	MG	CA	1684	1/1	0.89	0.14	-	49,49,49,49	0
60	MG	DA	3227	1/1	0.76	0.34	-	56,56,56,56	0
60	MG	DA	3082	1/1	0.97	0.74	-	47,47,47,47	0
60	MG	CA	1673	1/1	0.87	0.48	-	52,52,52,52	1
60	MG	AA	1646	1/1	0.88	0.74	-	50,50,50,50	0
60	MG	DA	3284	1/1	0.96	0.89	-	57,57,57,57	0
60	MG	DA	3221	1/1	0.92	0.55	-	54,54,54,54	0
60	MG	AA	1630	1/1	0.92	0.70	-	51,51,51,51	0
60	MG	AA	1660	1/1	0.90	0.11	-	58,58,58,58	0
60	MG	BA	3286	1/1	0.88	0.24	-	60,60,60,60	0
60	MG	AA	1687	1/1	0.81	0.21	-	48,48,48,48	0
60	MG	DA	3228	1/1	0.87	0.37	-	55,55,55,55	0
60	MG	DA	3011	1/1	0.82	0.56	-	52,52,52,52	0
60	MG	AA	1619	1/1	0.97	0.60	-	49,49,49,49	0
60	MG	DA	3244	1/1	0.96	0.49	-	47,47,47,47	0
60	MG	DA	3213	1/1	0.84	0.32	-	55,55,55,55	0
60	MG	CA	1639	1/1	0.92	0.29	-	48,48,48,48	0
60	MG	DA	3246	1/1	0.98	0.24	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3351	1/1	0.77	0.67	-	55,55,55,55	0
60	MG	BA	3297	1/1	0.96	0.49	-	55,55,55,55	0
60	MG	CA	1718	1/1	0.77	0.43	-	66,66,66,66	0
60	MG	CA	1755	1/1	0.92	0.54	-	55,55,55,55	0
60	MG	DA	3337	1/1	0.74	0.25	-	55,55,55,55	0
60	MG	AA	1622	1/1	0.86	0.20	-	48,48,48,48	0
60	MG	BA	3204	1/1	0.93	0.40	-	57,57,57,57	0
60	MG	DA	3066	1/1	0.92	0.54	-	52,52,52,52	0
60	MG	AA	1740	1/1	0.93	0.38	-	55,55,55,55	0
60	MG	BA	3244	1/1	0.90	0.25	-	60,60,60,60	0
60	MG	BA	3140	1/1	0.89	0.49	-	56,56,56,56	0
60	MG	AA	1719	1/1	0.95	0.14	-	56,56,56,56	0
60	MG	CA	1709	1/1	0.69	0.37	-	65,65,65,65	0
60	MG	CA	1692	1/1	0.94	0.49	-	59,59,59,59	0
60	MG	AA	1629	1/1	0.95	0.27	-	56,56,56,56	0
60	MG	BA	3336	1/1	0.69	0.62	-	55,55,55,55	0
60	MG	DA	3188	1/1	0.83	0.39	-	48,48,48,48	0
60	MG	BA	3169	1/1	0.95	0.57	-	51,51,51,51	0
60	MG	CW	105	1/1	0.79	0.65	-	53,53,53,53	0
60	MG	BA	3329	1/1	0.89	0.35	-	55,55,55,55	1
60	MG	CA	1688	1/1	0.81	0.15	-	48,48,48,48	0
60	MG	BA	3100	1/1	0.90	0.83	-	51,51,51,51	0
60	MG	DA	3172	1/1	0.97	0.50	-	50,50,50,50	0
60	MG	DA	3031	1/1	0.92	0.73	-	47,47,47,47	0
60	MG	CA	1724	1/1	0.96	0.14	-	57,57,57,57	1
60	MG	AA	1645	1/1	0.88	0.16	-	57,57,57,57	0
60	MG	CA	1731	1/1	0.83	0.37	-	55,55,55,55	0
60	MG	AE	201	1/1	0.89	0.79	-	57,57,57,57	0
60	MG	CA	1638	1/1	0.93	0.59	-	53,53,53,53	0
60	MG	BA	3092	1/1	0.91	0.61	-	50,50,50,50	0
60	MG	BA	3171	1/1	0.93	0.15	-	58,58,58,58	0
60	MG	AA	1716	1/1	0.57	1.13	-	52,52,52,52	0
60	MG	BA	3003	1/1	0.94	0.30	-	61,61,61,61	0
60	MG	BA	3311	1/1	0.90	0.38	-	55,55,55,55	0
60	MG	BA	3251	1/1	0.85	0.51	-	61,61,61,61	0
60	MG	DA	3338	1/1	0.91	0.71	-	55,55,55,55	0
60	MG	AA	1662	1/1	0.90	0.14	-	52,52,52,52	0
60	MG	AA	1729	1/1	0.84	0.23	-	55,55,55,55	0
60	MG	DA	3154	1/1	0.96	0.25	-	53,53,53,53	0
60	MG	DA	3171	1/1	0.97	0.70	-	51,51,51,51	0
60	MG	AA	1755	1/1	0.86	0.62	-	55,55,55,55	0
60	MG	BA	3122	1/1	0.83	0.39	-	64,64,64,64	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3217	1/1	0.89	0.70	-	51,51,51,51	0
60	MG	DA	3328	1/1	0.66	0.34	-	55,55,55,55	1
60	MG	DA	3346	1/1	0.93	0.82	-	55,55,55,55	0
60	MG	CA	1648	1/1	0.81	0.29	-	53,53,53,53	1
60	MG	CA	1657	1/1	0.96	0.28	-	54,54,54,54	0
60	MG	CA	1753	1/1	0.80	0.89	-	55,55,55,55	1
60	MG	AA	1648	1/1	0.71	0.14	-	62,62,62,62	0
60	MG	CA	1618	1/1	0.93	0.31	-	49,49,49,49	0
60	MG	DA	3314	1/1	0.88	0.25	-	55,55,55,55	1
60	MG	DA	3300	1/1	0.92	0.48	-	55,55,55,55	0
60	MG	DA	3032	1/1	0.94	0.29	-	50,50,50,50	0
60	MG	BA	3332	1/1	0.92	0.11	-	55,55,55,55	0
60	MG	BA	3274	1/1	0.85	0.67	-	63,63,63,63	0
60	MG	BA	3258	1/1	0.83	0.32	-	58,58,58,58	0
60	MG	DA	3331	1/1	0.90	0.09	-	55,55,55,55	1
60	MG	BA	3247	1/1	0.87	0.20	-	59,59,59,59	0
60	MG	AA	1698	1/1	0.76	0.35	-	53,53,53,53	1
60	MG	AA	1750	1/1	0.91	0.23	-	55,55,55,55	0
60	MG	CV	102	1/1	0.94	0.35	-	54,54,54,54	0
60	MG	AA	1651	1/1	0.87	0.72	-	54,54,54,54	0
60	MG	DA	3047	1/1	0.89	0.35	-	47,47,47,47	0
60	MG	BA	3268	1/1	0.94	0.72	-	59,59,59,59	0
60	MG	BA	3036	1/1	0.92	0.24	-	53,53,53,53	0
60	MG	CA	1646	1/1	0.90	0.45	-	62,62,62,62	0
60	MG	DA	3037	1/1	0.87	0.36	-	53,53,53,53	0
60	MG	CW	101	1/1	0.68	0.58	-	56,56,56,56	1
60	MG	DA	3142	1/1	0.72	0.54	-	49,49,49,49	0
60	MG	DA	3028	1/1	0.97	0.37	-	50,50,50,50	0
60	MG	BA	3200	1/1	0.83	0.26	-	60,60,60,60	0
60	MG	DA	3009	1/1	0.95	0.54	-	55,55,55,55	0
60	MG	CA	1732	1/1	0.93	0.20	-	55,55,55,55	0
60	MG	DA	3086	1/1	0.95	0.14	-	47,47,47,47	0
60	MG	AA	1746	1/1	0.81	0.31	-	55,55,55,55	1
60	MG	BA	3117	1/1	0.89	0.39	-	52,52,52,52	0
60	MG	DA	3023	1/1	0.98	0.80	-	47,47,47,47	0
60	MG	DA	3343	1/1	0.84	0.53	-	55,55,55,55	0
60	MG	BA	3265	1/1	0.85	0.47	-	47,47,47,47	0
60	MG	DA	3324	1/1	0.93	0.51	-	55,55,55,55	0
60	MG	BA	3110	1/1	0.98	0.41	-	49,49,49,49	0
60	MG	DA	3133	1/1	0.83	0.33	-	57,57,57,57	0
60	MG	DA	3257	1/1	0.91	0.67	-	55,55,55,55	0
60	MG	D5	102	1/1	0.95	0.35	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3290	1/1	0.91	0.37	-	57,57,57,57	0
60	MG	AA	1668	1/1	0.75	0.61	-	58,58,58,58	0
60	MG	AA	1603	1/1	0.91	0.23	-	57,57,57,57	0
60	MG	BA	3304	1/1	0.92	0.65	-	55,55,55,55	0
60	MG	BA	3194	1/1	0.89	0.26	-	53,53,53,53	0
60	MG	BA	3006	1/1	0.96	0.82	-	53,53,53,53	0
60	MG	BA	3181	1/1	0.71	0.27	-	53,53,53,53	0
60	MG	BA	3057	1/1	0.89	0.47	-	47,47,47,47	0
60	MG	AA	1677	1/1	0.84	0.35	-	55,55,55,55	1
60	MG	BA	3156	1/1	0.95	0.50	-	48,48,48,48	0
60	MG	DA	3112	1/1	0.92	0.31	-	52,52,52,52	0
60	MG	DA	3193	1/1	0.58	0.41	-	65,65,65,65	0
60	MG	AA	1664	1/1	0.92	0.29	-	60,60,60,60	0
60	MG	AV	102	1/1	0.95	0.28	-	54,54,54,54	0
60	MG	CA	1742	1/1	0.94	0.69	-	55,55,55,55	0
60	MG	DA	3195	1/1	0.97	0.25	-	53,53,53,53	0
60	MG	BA	3309	1/1	0.78	0.22	-	55,55,55,55	0
60	MG	BA	3245	1/1	0.91	0.39	-	53,53,53,53	0
60	MG	DA	3128	1/1	0.93	0.30	-	56,56,56,56	0
60	MG	BA	3308	1/1	0.98	0.52	-	55,55,55,55	0
60	MG	BA	3022	1/1	0.98	1.00	-	47,47,47,47	0
60	MG	DA	3322	1/1	0.95	0.75	-	55,55,55,55	0
60	MG	BA	3353	1/1	0.94	0.54	-	55,55,55,55	0
60	MG	DA	3019	1/1	0.95	0.59	-	54,54,54,54	0
60	MG	BA	3256	1/1	0.96	0.68	-	55,55,55,55	0
60	MG	CA	1744	1/1	0.83	0.44	-	55,55,55,55	0
60	MG	CW	103	1/1	0.87	0.49	-	54,54,54,54	1
60	MG	BA	3338	1/1	0.69	0.33	-	55,55,55,55	0
60	MG	DA	3294	1/1	0.69	0.51	-	49,49,49,49	1
60	MG	BA	3104	1/1	0.91	0.72	-	48,48,48,48	0
60	MG	BA	3189	1/1	0.81	0.37	-	59,59,59,59	0
60	MG	DA	3113	1/1	0.93	0.31	-	48,48,48,48	0
60	MG	CA	1659	1/1	0.83	0.23	-	57,57,57,57	0
60	MG	BA	3211	1/1	0.93	0.26	-	59,59,59,59	1
60	MG	DA	3340	1/1	0.99	0.38	-	55,55,55,55	0
60	MG	CA	1705	1/1	0.77	0.45	-	49,49,49,49	1
60	MG	CA	1681	1/1	0.72	0.54	-	66,66,66,66	0
60	MG	BA	3324	1/1	0.81	0.37	-	55,55,55,55	0
60	MG	BA	3208	1/1	0.91	0.43	-	51,51,51,51	0
60	MG	AA	1753	1/1	0.90	0.45	-	55,55,55,55	1
60	MG	CA	1699	1/1	0.95	0.16	-	53,53,53,53	1
60	MG	DA	3029	1/1	0.98	0.32	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1687	1/1	0.65	0.44	-	58,58,58,58	0
60	MG	DA	3219	1/1	0.77	0.38	-	66,66,66,66	0
60	MG	DA	3045	1/1	0.91	0.44	-	56,56,56,56	0
60	MG	DA	3266	1/1	0.93	0.53	-	47,47,47,47	0
60	MG	BA	3126	1/1	0.82	0.30	-	52,52,52,52	0
60	MG	CA	1654	1/1	0.90	0.72	-	57,57,57,57	0
60	MG	BA	3335	1/1	0.88	0.54	-	55,55,55,55	0
60	MG	CA	1601	1/1	0.93	0.30	-	56,56,56,56	0
60	MG	CV	103	1/1	0.60	0.30	-	54,54,54,54	0
60	MG	CA	1702	1/1	0.92	0.38	-	51,51,51,51	0
60	MG	BA	3333	1/1	0.92	0.71	-	55,55,55,55	0
60	MG	BA	3253	1/1	0.81	0.55	-	54,54,54,54	0
60	MG	BA	3241	1/1	0.79	0.32	-	61,61,61,61	1
60	MG	BA	3190	1/1	0.93	0.43	-	54,54,54,54	0
60	MG	BA	3078	1/1	0.92	0.68	-	56,56,56,56	0
60	MG	BA	3133	1/1	0.81	0.40	-	64,64,64,64	0
60	MG	BA	3176	1/1	0.95	0.57	-	48,48,48,48	0
60	MG	DA	3058	1/1	0.98	0.62	-	47,47,47,47	0
60	MG	CW	104	1/1	0.84	0.36	-	56,56,56,56	0
60	MG	CA	1640	1/1	0.98	0.73	-	47,47,47,47	0
60	MG	DA	3169	1/1	0.93	0.39	-	47,47,47,47	0
60	MG	CA	1713	1/1	0.90	0.36	-	54,54,54,54	0
60	MG	DA	3254	1/1	0.91	0.24	-	54,54,54,54	0
60	MG	BA	3283	1/1	0.90	0.30	-	65,65,65,65	0
60	MG	BA	3131	1/1	0.84	0.38	-	59,59,59,59	0
60	MG	CA	1661	1/1	0.87	0.59	-	52,52,52,52	0
60	MG	DA	3313	1/1	0.94	0.77	-	55,55,55,55	0
60	MG	BA	3121	1/1	0.97	0.27	-	50,50,50,50	0
60	MG	CA	1664	1/1	0.88	0.49	-	60,60,60,60	0
60	MG	CA	1613	1/1	0.69	0.23	-	52,52,52,52	0
60	MG	BA	3059	1/1	0.99	0.31	-	48,48,48,48	0
60	MG	CA	1621	1/1	0.82	0.21	-	48,48,48,48	0
60	MG	DA	3119	1/1	0.98	0.50	-	49,49,49,49	0
60	MG	AA	1618	1/1	0.92	0.22	-	51,51,51,51	1
60	MG	DH	201	1/1	0.94	0.12	-	50,50,50,50	0
60	MG	CV	106	1/1	0.77	0.18	-	57,57,57,57	1
60	MG	AA	1609	1/1	0.98	0.25	-	52,52,52,52	0
60	MG	CA	1611	1/1	0.95	0.25	-	52,52,52,52	0
60	MG	BA	3167	1/1	0.89	0.31	-	53,53,53,53	0
60	MG	BA	3197	1/1	0.97	0.45	-	58,58,58,58	0
60	MG	BA	3111	1/1	0.92	0.26	-	52,52,52,52	0
60	MG	CA	1634	1/1	0.92	0.16	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3295	1/1	0.95	0.15	-	49,49,49,49	0
60	MG	DA	3179	1/1	0.94	0.90	-	47,47,47,47	0
60	MG	BA	3041	1/1	0.98	0.65	-	47,47,47,47	0
60	MG	BA	3127	1/1	0.92	0.24	-	56,56,56,56	0
60	MG	DA	3283	1/1	0.77	0.47	-	65,65,65,65	0
60	MG	BA	3223	1/1	0.96	0.40	-	52,52,52,52	0
60	MG	DA	3252	1/1	0.93	0.53	-	61,61,61,61	1
60	MG	BA	3161	1/1	0.71	0.28	-	47,47,47,47	0
60	MG	AA	1731	1/1	0.88	0.24	-	55,55,55,55	0
60	MG	DA	3291	1/1	0.97	0.69	-	54,54,54,54	0
60	MG	AA	1706	1/1	0.91	0.24	-	51,51,51,51	0
60	MG	DA	3056	1/1	0.96	0.43	-	47,47,47,47	0
60	MG	CV	104	1/1	0.93	0.08	-	54,54,54,54	0
60	MG	BA	3001	1/1	0.89	0.33	-	54,54,54,54	0
60	MG	DA	3334	1/1	0.75	0.29	-	55,55,55,55	0
60	MG	BA	3255	1/1	0.98	0.30	-	55,55,55,55	0
60	MG	DA	3222	1/1	0.83	0.71	-	53,53,53,53	0
60	MG	DA	3233	1/1	0.94	0.64	-	53,53,53,53	0
60	MG	BA	3139	1/1	0.81	0.48	-	50,50,50,50	0
60	MG	CA	1715	1/1	0.89	0.65	-	59,59,59,59	0
60	MG	AA	1733	1/1	0.80	0.28	-	55,55,55,55	0
60	MG	DA	3261	1/1	0.94	0.22	-	57,57,57,57	0
60	MG	DA	3175	1/1	0.96	0.46	-	56,56,56,56	0
60	MG	BA	3097	1/1	0.90	0.34	-	47,47,47,47	0
60	MG	AA	1703	1/1	0.93	0.25	-	62,62,62,62	0
60	MG	DA	3093	1/1	0.88	0.74	-	50,50,50,50	0
60	MG	AA	1624	1/1	0.95	0.34	-	48,48,48,48	0
60	MG	BA	3118	1/1	0.94	0.51	-	49,49,49,49	0
60	MG	AA	1693	1/1	0.80	0.47	-	61,61,61,61	0
60	MG	BA	3030	1/1	0.85	0.61	-	47,47,47,47	0
60	MG	CA	1627	1/1	0.87	0.20	-	70,70,70,70	0
60	MG	AA	1704	1/1	0.84	0.26	-	49,49,49,49	1
60	MG	DA	3117	1/1	0.94	0.28	-	47,47,47,47	0
60	MG	DA	3098	1/1	0.91	0.27	-	47,47,47,47	0
60	MG	AA	1757	1/1	0.94	0.34	-	55,55,55,55	0
60	MG	BA	3344	1/1	0.88	0.89	-	55,55,55,55	0
60	MG	BA	3259	1/1	0.85	0.28	-	59,59,59,59	0
60	MG	CA	1739	1/1	0.89	0.14	-	55,55,55,55	0
60	MG	BA	3017	1/1	0.97	0.43	-	52,52,52,52	0
60	MG	BA	3275	1/1	0.89	0.39	-	59,59,59,59	0
60	MG	BA	3095	1/1	0.91	0.61	-	60,60,60,60	0
60	MG	BA	3293	1/1	0.98	0.45	-	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1601	1/1	0.91	0.19	-	56,56,56,56	0
60	MG	DA	3001	1/1	0.84	0.30	-	57,57,57,57	0
60	MG	DA	3318	1/1	0.83	0.21	-	55,55,55,55	0
60	MG	DA	3292	1/1	0.95	0.53	-	55,55,55,55	0
60	MG	AA	1631	1/1	0.97	0.23	-	47,47,47,47	0
60	MG	AA	1709	1/1	0.87	0.55	-	50,50,50,50	0
60	MG	CA	1691	1/1	0.86	0.72	-	52,52,52,52	0
60	MG	DA	3339	1/1	0.96	0.38	-	55,55,55,55	0
60	MG	BA	3039	1/1	0.87	0.24	-	68,68,68,68	0
60	MG	BA	3341	1/1	0.76	0.60	-	55,55,55,55	0
60	MG	DA	3289	1/1	0.98	0.45	-	54,54,54,54	0
60	MG	CA	1729	1/1	0.69	0.34	-	55,55,55,55	1
60	MG	BA	3288	1/1	0.95	0.22	-	66,66,66,66	0
60	MG	BA	3325	1/1	0.88	0.34	-	55,55,55,55	0
60	MG	BA	3289	1/1	0.94	0.42	-	54,54,54,54	0
60	MG	BA	3298	1/1	0.95	0.44	-	55,55,55,55	0
60	MG	DC	301	1/1	0.45	0.64	-	52,52,52,52	1
60	MG	BA	3137	1/1	0.83	0.59	-	52,52,52,52	0
60	MG	CA	1672	1/1	0.95	0.45	-	53,53,53,53	0
60	MG	DA	3126	1/1	0.96	0.80	-	47,47,47,47	0
60	MG	BA	3254	1/1	0.86	0.61	-	60,60,60,60	0
60	MG	AM	201	1/1	0.70	0.57	-	47,47,47,47	0
60	MG	CA	1662	1/1	0.92	0.27	-	52,52,52,52	0
60	MG	BA	3053	1/1	0.95	0.19	-	51,51,51,51	0
60	MG	BA	3180	1/1	0.86	0.42	-	56,56,56,56	0
60	MG	BA	3125	1/1	0.97	0.71	-	47,47,47,47	0
60	MG	BS	201	1/1	0.75	0.49	-	55,55,55,55	0
60	MG	AA	1724	1/1	0.95	0.55	-	59,59,59,59	0
60	MG	DA	3110	1/1	0.95	0.30	-	48,48,48,48	0
60	MG	DA	3297	1/1	0.94	0.45	-	55,55,55,55	0
60	MG	CA	1651	1/1	0.67	0.42	-	47,47,47,47	0
60	MG	AA	1653	1/1	0.77	0.87	-	60,60,60,60	0
60	MG	BA	3065	1/1	0.94	0.24	-	52,52,52,52	0
60	MG	BA	3073	1/1	0.95	0.44	-	52,52,52,52	0
60	MG	CA	1710	1/1	0.84	0.27	-	50,50,50,50	0
60	MG	CA	1629	1/1	0.81	0.46	-	51,51,51,51	0
60	MG	DA	3309	1/1	0.82	0.49	-	55,55,55,55	1
60	MG	AA	1616	1/1	0.58	0.55	-	64,64,64,64	0
60	MG	BA	3199	1/1	0.68	0.70	-	58,58,58,58	0
60	MG	BA	3284	1/1	0.86	0.68	-	57,57,57,57	0
60	MG	CA	1679	1/1	0.76	0.40	-	53,53,53,53	1
60	MG	DA	3290	1/1	0.89	0.44	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3190	1/1	0.78	0.26	-	59,59,59,59	0
60	MG	BA	3231	1/1	0.90	0.40	-	51,51,51,51	0
60	MG	AA	1639	1/1	0.90	0.21	-	53,53,53,53	0
60	MG	BA	3328	1/1	0.72	0.59	-	55,55,55,55	0
60	MG	BA	3153	1/1	0.85	0.45	-	53,53,53,53	0
60	MG	BA	3052	1/1	0.97	0.53	-	47,47,47,47	0
60	MG	AA	1663	1/1	0.94	0.29	-	51,51,51,51	0
60	MG	DA	3232	1/1	0.91	0.17	-	51,51,51,51	0
60	MG	AA	1614	1/1	0.97	0.07	-	52,52,52,52	0
60	MG	BA	3094	1/1	0.90	0.60	-	47,47,47,47	0
60	MG	AA	1730	1/1	0.74	0.46	-	55,55,55,55	0
60	MG	AW	105	1/1	0.86	0.20	-	53,53,53,53	0
60	MG	AA	1692	1/1	0.73	0.70	-	59,59,59,59	0
60	MG	DA	3243	1/1	0.97	0.13	-	61,61,61,61	1
60	MG	BA	3281	1/1	0.93	0.39	-	57,57,57,57	0
60	MG	BA	3016	1/1	0.93	0.89	-	47,47,47,47	0
60	MG	BH	201	1/1	0.95	0.13	-	50,50,50,50	0
60	MG	DA	3329	1/1	0.91	0.29	-	55,55,55,55	0
60	MG	CA	1665	1/1	0.86	0.50	-	50,50,50,50	0
60	MG	DA	3321	1/1	0.90	0.22	-	55,55,55,55	0
60	MG	AA	1641	1/1	0.91	0.43	-	47,47,47,47	0
60	MG	BA	3317	1/1	0.96	0.74	-	55,55,55,55	0
60	MG	DF	302	1/1	0.87	0.24	-	53,53,53,53	0
60	MG	DA	3217	1/1	0.92	0.16	-	49,49,49,49	0
60	MG	CA	1743	1/1	0.93	0.28	-	55,55,55,55	0
60	MG	DA	3268	1/1	0.94	0.86	-	59,59,59,59	0
60	MG	D7	101	1/1	0.87	0.38	-	54,54,54,54	0
60	MG	DA	3333	1/1	0.77	0.38	-	55,55,55,55	0
60	MG	DA	3189	1/1	0.96	0.17	-	57,57,57,57	0
60	MG	CA	1655	1/1	0.69	0.67	-	52,52,52,52	0
60	MG	BA	3031	1/1	0.97	0.26	-	50,50,50,50	0
60	MG	CA	1730	1/1	0.72	0.40	-	55,55,55,55	0
60	MG	BA	3242	1/1	0.95	0.39	-	47,47,47,47	0
60	MG	CA	1652	1/1	0.82	0.91	-	60,60,60,60	0
60	MG	AA	1752	1/1	0.93	0.20	-	55,55,55,55	0
60	MG	AA	1708	1/1	0.84	0.30	-	65,65,65,65	0
60	MG	BA	3350	1/1	0.90	0.32	-	55,55,55,55	0
60	MG	AA	1715	1/1	0.90	0.23	-	55,55,55,55	0
60	MG	AA	1713	1/1	0.88	0.16	-	64,64,64,64	0
60	MG	DA	3270	1/1	0.95	0.61	-	67,67,67,67	0
60	MG	DA	3251	1/1	0.91	0.19	-	52,52,52,52	0
60	MG	AA	1727	1/1	0.85	0.65	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3193	1/1	0.95	0.28	-	53,53,53,53	0
60	MG	DA	3211	1/1	0.95	0.51	-	57,57,57,57	0
60	MG	CA	1747	1/1	0.86	0.40	-	55,55,55,55	1
60	MG	AA	1686	1/1	0.81	0.47	-	58,58,58,58	1
60	MG	BA	3154	1/1	0.94	0.34	-	48,48,48,48	0
60	MG	CA	1694	1/1	0.88	0.62	-	61,61,61,61	0
60	MG	CA	1733	1/1	0.75	0.53	-	55,55,55,55	0
60	MG	DA	3277	1/1	0.98	0.78	-	57,57,57,57	0
60	MG	BA	3327	1/1	0.89	0.47	-	55,55,55,55	0
60	MG	BB	203	1/1	0.92	0.67	-	55,55,55,55	0
60	MG	DA	3330	1/1	0.80	0.20	-	55,55,55,55	0
60	MG	DA	3060	1/1	0.97	0.47	-	48,48,48,48	0
60	MG	BA	3292	1/1	0.84	0.68	-	55,55,55,55	0
60	MG	CA	1708	1/1	0.84	0.25	-	49,49,49,49	0
60	MG	DB	201	1/1	0.75	0.90	-	67,67,67,67	0
60	MG	AA	1684	1/1	0.87	0.17	-	49,49,49,49	0
60	MG	BA	3174	1/1	0.90	0.32	-	58,58,58,58	0
60	MG	BA	3089	1/1	0.97	0.59	-	48,48,48,48	0
60	MG	B3	101	1/1	0.96	0.56	-	58,58,58,58	0
60	MG	AA	1680	1/1	0.96	0.40	-	49,49,49,49	0
60	MG	DA	3236	1/1	0.97	0.87	-	52,52,52,52	0
60	MG	DA	3137	1/1	0.97	0.65	-	50,50,50,50	0
60	MG	DA	3276	1/1	0.91	0.78	-	58,58,58,58	0
60	MG	BA	3093	1/1	0.97	0.42	-	51,51,51,51	0
60	MG	BA	3150	1/1	0.90	0.47	-	51,51,51,51	0
60	MG	DA	3204	1/1	0.96	0.33	-	52,52,52,52	0
60	MG	DA	3302	1/1	0.82	0.53	-	55,55,55,55	0
60	MG	CA	1720	1/1	0.79	0.15	-	56,56,56,56	0
60	MG	CA	1602	1/1	0.92	0.26	-	52,52,52,52	0
60	MG	DA	3030	1/1	0.86	0.41	-	55,55,55,55	0
60	MG	DA	3242	1/1	0.88	0.22	-	58,58,58,58	1
60	MG	DA	3177	1/1	0.46	0.56	-	49,49,49,49	0
60	MG	BA	3143	1/1	0.84	0.30	-	57,57,57,57	0
60	MG	CA	1716	1/1	0.80	0.28	-	55,55,55,55	0
60	MG	DA	3164	1/1	0.95	0.69	-	53,53,53,53	0
60	MG	DA	3293	1/1	0.88	0.24	-	52,52,52,52	0
60	MG	DA	3092	1/1	0.86	0.42	-	51,51,51,51	1
60	MG	DA	3285	1/1	0.82	0.27	-	55,55,55,55	0
60	MG	BA	3191	1/1	0.94	0.17	-	61,61,61,61	0
60	MG	BA	3210	1/1	0.95	0.41	-	57,57,57,57	0
60	MG	DA	3132	1/1	0.89	0.30	-	59,59,59,59	0
60	MG	AA	1736	1/1	0.88	0.25	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3198	1/1	0.96	0.69	-	53,53,53,53	0
60	MG	DA	3212	1/1	0.95	0.22	-	59,59,59,59	0
60	MG	DA	3158	1/1	0.87	0.46	-	53,53,53,53	0
60	MG	DA	3140	1/1	0.90	0.37	-	50,50,50,50	1
60	MG	DA	3101	1/1	0.95	0.52	-	51,51,51,51	0
60	MG	DA	3275	1/1	0.90	0.65	-	59,59,59,59	0
60	MG	DA	3349	1/1	0.79	0.55	-	55,55,55,55	0
60	MG	CA	1608	1/1	0.98	0.38	-	52,52,52,52	0
60	MG	CA	1704	1/1	0.97	0.64	-	62,62,62,62	0
60	MG	CA	1740	1/1	0.78	0.33	-	55,55,55,55	0
60	MG	BA	3326	1/1	0.91	0.81	-	55,55,55,55	0
60	MG	BA	3048	1/1	0.96	0.59	-	47,47,47,47	0
60	MG	DA	3216	1/1	0.88	0.54	-	60,60,60,60	0
60	MG	DA	3191	1/1	0.85	0.31	-	54,54,54,54	0
60	MG	BA	3215	1/1	0.92	0.71	-	60,60,60,60	0
60	MG	CA	1728	1/1	0.97	0.51	-	55,55,55,55	0
60	MG	AA	1705	1/1	0.78	0.22	-	51,51,51,51	0
60	MG	BA	3220	1/1	0.88	0.64	-	54,54,54,54	0
60	MG	DA	3310	1/1	0.94	0.23	-	55,55,55,55	0
60	MG	AA	1665	1/1	0.94	0.76	-	50,50,50,50	0
60	MG	DA	3311	1/1	0.96	0.64	-	55,55,55,55	0
60	MG	DA	3230	1/1	0.90	0.12	-	49,49,49,49	0
60	MG	DA	3352	1/1	0.79	0.55	-	55,55,55,55	0
60	MG	DA	3183	1/1	0.70	0.23	-	53,53,53,53	0
60	MG	BA	3162	1/1	0.91	0.82	-	50,50,50,50	0
60	MG	DA	3336	1/1	0.84	0.27	-	55,55,55,55	1
60	MG	AA	1695	1/1	0.85	0.31	-	62,62,62,62	0
60	MG	DA	3353	1/1	0.86	0.70	-	55,55,55,55	0
60	MG	AA	1712	1/1	0.85	0.41	-	54,54,54,54	0
60	MG	BA	3132	1/1	0.89	0.35	-	57,57,57,57	0
60	MG	DA	3051	1/1	0.97	0.19	-	47,47,47,47	0
60	MG	BA	3334	1/1	0.92	0.29	-	55,55,55,55	0
60	MG	DA	3350	1/1	0.94	0.43	-	55,55,55,55	0
60	MG	CA	1698	1/1	0.90	0.33	-	52,52,52,52	0
60	MG	BA	3278	1/1	0.97	0.29	-	51,51,51,51	0
60	MG	BA	3218	1/1	0.94	0.58	-	66,66,66,66	0
60	MG	CA	1741	1/1	0.92	0.54	-	55,55,55,55	0
60	MG	AA	1699	1/1	0.72	0.47	-	54,54,54,54	1
60	MG	CA	1725	1/1	0.93	0.38	-	59,59,59,59	0
60	MG	CA	1726	1/1	0.87	0.78	-	54,54,54,54	0
60	MG	DA	3150	1/1	0.99	0.60	-	54,54,54,54	0
60	MG	DA	3122	1/1	0.74	0.44	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1744	1/1	0.87	0.27	-	55,55,55,55	0
60	MG	DA	3210	1/1	0.86	0.59	-	66,66,66,66	0
60	MG	BA	3148	1/1	0.91	0.17	-	47,47,47,47	0
60	MG	DA	3118	1/1	0.87	0.41	-	52,52,52,52	0
60	MG	BA	3270	1/1	0.95	0.74	-	67,67,67,67	0
60	MG	DA	3237	1/1	0.90	0.69	-	60,60,60,60	0
60	MG	BA	3315	1/1	0.84	0.41	-	55,55,55,55	1
60	MG	DA	3018	1/1	0.92	0.47	-	52,52,52,52	0
60	MG	CA	1751	1/1	0.86	0.27	-	55,55,55,55	0
60	MG	DA	3076	1/1	0.94	0.37	-	47,47,47,47	0
60	MG	BA	3077	1/1	0.92	0.54	-	51,51,51,51	0
60	MG	DA	3325	1/1	0.90	0.91	-	55,55,55,55	0
60	MG	AA	1681	1/1	0.88	0.28	-	66,66,66,66	0
60	MG	BA	3352	1/1	0.95	0.34	-	55,55,55,55	0
60	MG	D5	101	1/1	0.95	0.16	-	49,49,49,49	0
60	MG	BA	3091	1/1	0.79	0.39	-	51,51,51,51	0
60	MG	DA	3194	1/1	0.91	0.49	-	53,53,53,53	0
60	MG	CA	1677	1/1	0.67	0.20	-	55,55,55,55	1
60	MG	DA	3138	1/1	0.85	0.47	-	52,52,52,52	0
60	MG	DA	3111	1/1	0.92	0.25	-	49,49,49,49	0
60	MG	AV	107	1/1	0.53	0.68	-	54,54,54,54	1
60	MG	AW	101	1/1	0.80	0.70	-	56,56,56,56	1
60	MG	BA	3310	1/1	0.91	0.21	-	55,55,55,55	0
60	MG	BA	3221	1/1	0.94	0.68	-	53,53,53,53	0
60	MG	BA	3285	1/1	0.89	0.25	-	55,55,55,55	0
60	MG	DA	3198	1/1	0.99	0.49	-	58,58,58,58	0
60	MG	CA	1701	1/1	0.96	0.46	-	51,51,51,51	0
60	MG	DQ	201	1/1	0.92	0.77	-	55,55,55,55	0
60	MG	CA	1697	1/1	0.93	0.15	-	62,62,62,62	0
60	MG	BA	3178	1/1	0.87	0.29	-	52,52,52,52	0
60	MG	BA	3124	1/1	0.89	0.32	-	49,49,49,49	0
60	MG	BA	3229	1/1	0.90	0.17	-	49,49,49,49	0
60	MG	DA	3272	1/1	0.82	0.33	-	59,59,59,59	1
60	MG	AA	1643	1/1	0.87	0.17	-	56,56,56,56	0
60	MG	DA	3153	1/1	0.93	0.12	-	50,50,50,50	0
60	MG	BA	3134	1/1	0.89	0.26	-	54,54,54,54	0
60	MG	DA	3042	1/1	0.96	0.78	-	47,47,47,47	0
60	MG	BA	3276	1/1	0.88	0.45	-	58,58,58,58	0
60	MG	DA	3017	1/1	0.92	0.66	-	47,47,47,47	0
60	MG	BB	202	1/1	0.96	0.44	-	55,55,55,55	0
60	MG	BA	3314	1/1	0.87	0.33	-	55,55,55,55	0
60	MG	DA	3147	1/1	0.96	0.43	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3155	1/1	0.99	0.40	-	48,48,48,48	0
60	MG	BA	3063	1/1	0.99	0.27	-	56,56,56,56	0
60	MG	CA	1642	1/1	0.93	0.61	-	56,56,56,56	0
60	MG	CA	1706	1/1	0.93	0.19	-	51,51,51,51	0
60	MG	DA	3178	1/1	0.89	0.50	-	48,48,48,48	0
60	MG	DA	3301	1/1	0.86	0.64	-	55,55,55,55	0
60	MG	CA	1632	1/1	0.84	0.12	-	55,55,55,55	0
60	MG	CA	1737	1/1	0.90	0.40	-	55,55,55,55	1
60	MG	BA	3151	1/1	0.86	0.31	-	47,47,47,47	0
60	MG	BA	3209	1/1	0.86	0.55	-	66,66,66,66	0
60	MG	DA	3239	1/1	0.76	0.24	-	67,67,67,67	1
60	MG	DA	3168	1/1	0.96	0.19	-	53,53,53,53	0
60	MG	DA	3263	1/1	0.84	0.44	-	63,63,63,63	0
60	MG	AA	1688	1/1	0.78	0.46	-	63,63,63,63	1
60	MG	CA	1650	1/1	0.95	0.66	-	54,54,54,54	0
60	MG	DA	3144	1/1	0.66	0.29	-	57,57,57,57	0
60	MG	AA	1670	1/1	0.87	0.29	-	69,69,69,69	0
60	MG	BA	3018	1/1	0.97	0.55	-	54,54,54,54	0
60	MG	AA	1689	1/1	0.59	0.96	-	59,59,59,59	1
60	MG	BQ	201	1/1	0.97	0.79	-	55,55,55,55	0
60	MG	CV	107	1/1	0.84	0.28	-	54,54,54,54	0
60	MG	DA	3209	1/1	0.89	0.49	-	51,51,51,51	0
60	MG	DA	3307	1/1	0.93	0.27	-	55,55,55,55	0
60	MG	DA	3248	1/1	0.98	0.15	-	59,59,59,59	1
60	MG	CA	1689	1/1	0.96	0.26	-	63,63,63,63	1
60	MG	BA	3168	1/1	0.92	0.39	-	47,47,47,47	0
60	MG	DA	3192	1/1	0.96	0.20	-	61,61,61,61	1
60	MG	B7	102	1/1	0.89	0.35	-	54,54,54,54	0
60	MG	BA	3055	1/1	0.96	0.66	-	47,47,47,47	0
60	MG	CA	1757	1/1	0.92	0.20	-	55,55,55,55	0
60	MG	BA	3172	1/1	0.93	0.34	-	52,52,52,52	0
60	MG	BA	3129	1/1	0.81	0.36	-	56,56,56,56	0
60	MG	BA	3320	1/1	0.77	0.45	-	55,55,55,55	0
60	MG	DA	3202	1/1	0.63	0.61	-	52,52,52,52	1
60	MG	AA	1723	1/1	0.90	0.34	-	57,57,57,57	0
60	MG	BA	3203	1/1	0.97	0.37	-	52,52,52,52	0
60	MG	CA	1604	1/1	0.96	0.21	-	50,50,50,50	0
60	MG	AW	102	1/1	0.88	0.13	-	60,60,60,60	1
60	MG	DA	3187	1/1	0.98	0.53	-	51,51,51,51	0
60	MG	BA	3345	1/1	0.91	0.24	-	55,55,55,55	0
60	MG	BA	3261	1/1	0.95	0.53	-	52,52,52,52	0
60	MG	DA	3181	1/1	0.74	0.64	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3208	1/1	0.96	0.25	-	60,60,60,60	0
60	MG	DA	3120	1/1	0.93	0.90	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.