wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 04:11 pm GMT

PDB ID	:	4V8X
Title	:	Structure of Thermus thermophilus ribosome
Authors	:	Feng, S.; Chen, Y.; Kamada, K.; Wang, H.; Tang, K.; Wang, M.; Gao, Y.G.
Deposited on	:	2013-07-19
Resolution	:	3.35 Å(reported)

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

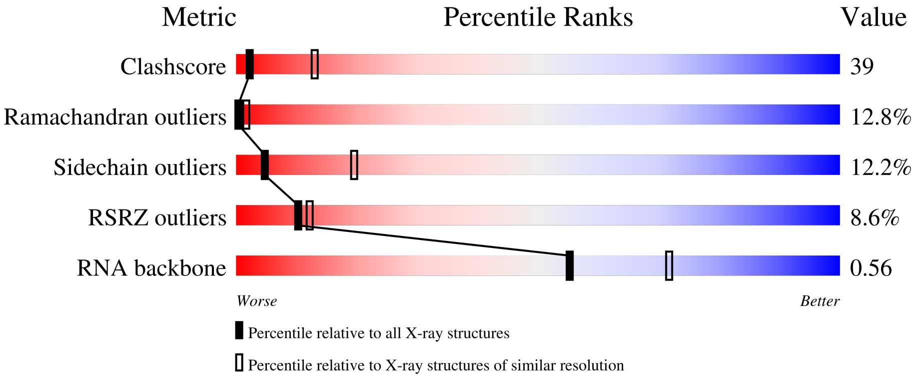
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

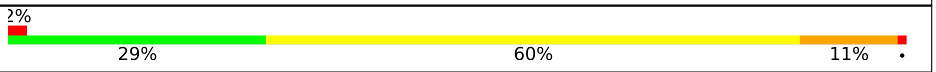
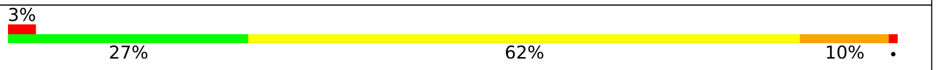
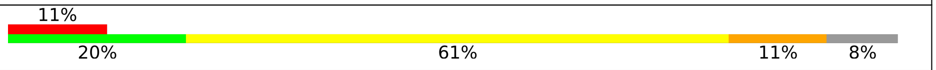
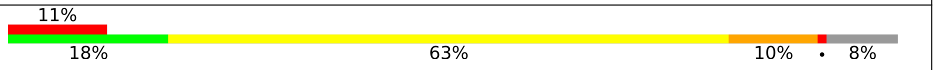
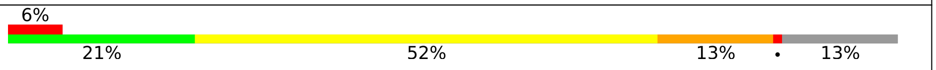
The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	1504	
1	CA	1504	
2	AB	256	
2	CB	256	
3	AC	239	

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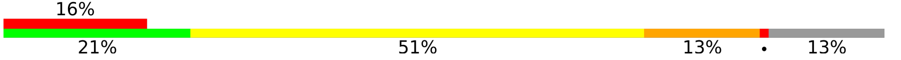
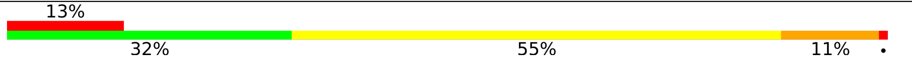
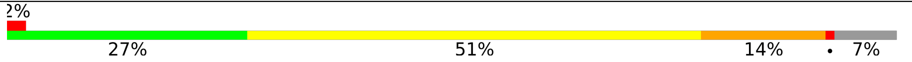
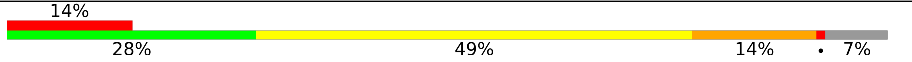
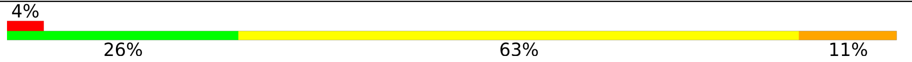
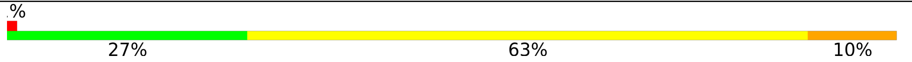
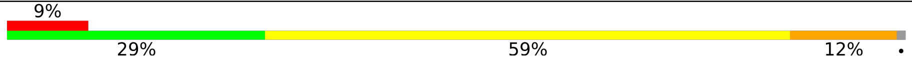
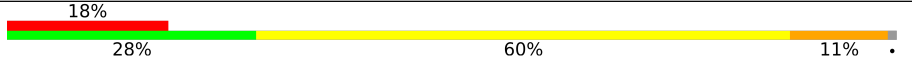
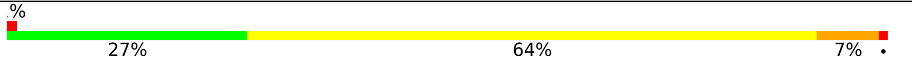
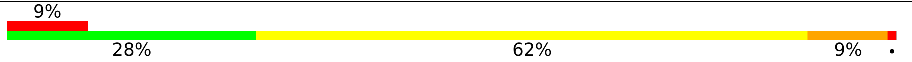
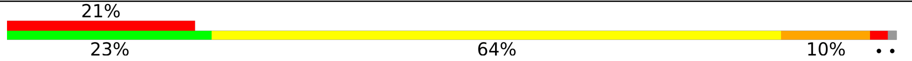
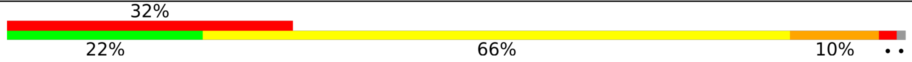
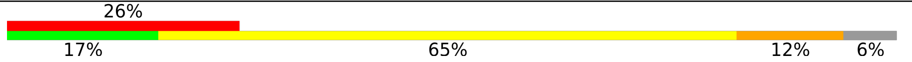
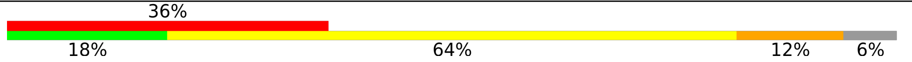
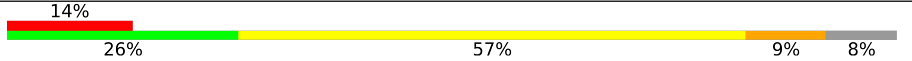
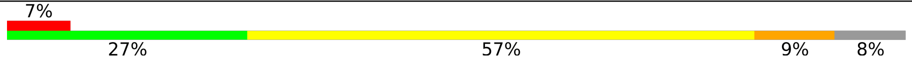
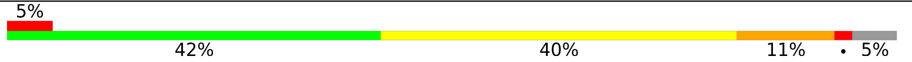
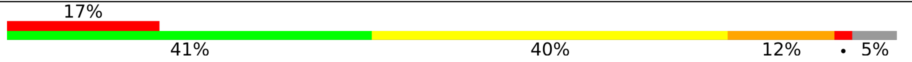
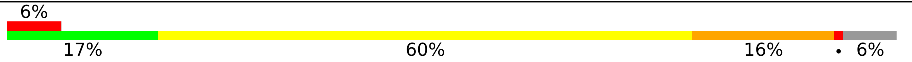
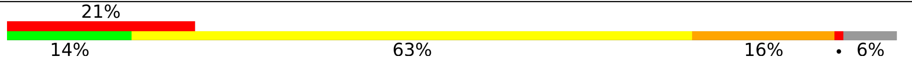
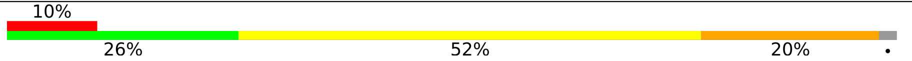
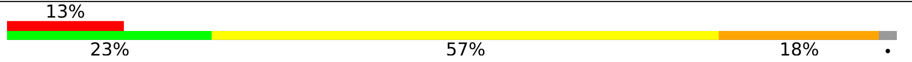
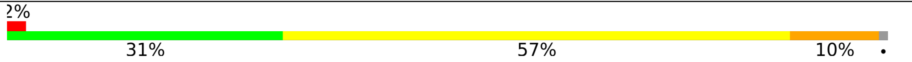
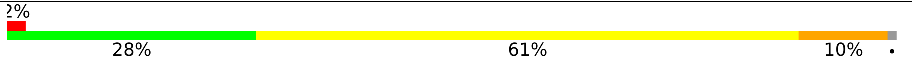
Mol	Chain	Length	Quality of chain
3	CC	239	 16% 21% 51% 13% • 13%
4	AD	209	 33% 55% 11% •
4	CD	209	 13% 32% 55% 11% •
5	AE	162	 2% 27% 51% 14% • 7%
5	CE	162	 14% 28% 49% 14% • 7%
6	AF	101	 4% 26% 63% 11%
6	CF	101	 % 27% 63% 10%
7	AG	156	 9% 29% 59% 12% •
7	CG	156	 18% 28% 60% 11% •
8	AH	138	 % 27% 64% 7% •
8	CH	138	 9% 28% 62% 9% •
9	AI	128	 21% 23% 64% 10% • •
9	CI	128	 32% 22% 66% 10% • •
10	AJ	105	 26% 17% 65% 12% 6%
10	CJ	105	 36% 18% 64% 12% 6%
11	AK	129	 14% 26% 57% 9% 8%
11	CK	129	 7% 27% 57% 9% 8%
12	AL	132	 5% 42% 40% 11% • 5%
12	CL	132	 17% 41% 40% 12% • 5%
13	AM	126	 6% 17% 60% 16% • 6%
13	CM	126	 21% 14% 63% 16% • 6%
14	AN	61	 10% 26% 52% 20% •
14	CN	61	 13% 23% 57% 18% •
15	AO	89	 2% 31% 57% 10% •
15	CO	89	 2% 28% 61% 10% •

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Mol	Chain	Length	Quality of chain
16	AP	88	2% 33% 52% 10% 5%
16	CP	88	34% 31% 51% 14% 5%
17	AQ	105	31% 58% 6% 5%
17	CQ	105	7% 33% 56% 6% 5%
18	AR	88	8% 24% 44% 11% 20%
18	CR	88	10% 25% 42% 13% 20%
19	AS	93	26% 14% 55% 12% • 15%
19	CS	93	33% 14% 56% 13% • 15%
20	AT	106	7% 25% 56% 13% 7%
20	CT	106	16% 21% 60% 11% • 7%
21	AU	27	44% 41% 41% 11% 7%
21	CU	27	63% 33% 41% 19% 7%
22	AV	77	% 38% 45% 16% •
23	AW	77	51% 26% 64% 10%
23	CV	77	% 43% 40% 16% •
23	CW	77	42% 23% 71% 5%
24	AX	25	12% 12% 16% 16% 56%
25	AY	84	19% 8% 61% 27% •
25	AZ	84	24% 17% 56% 27%
25	CY	84	44% 10% 58% 27% 5%
25	CZ	84	25% 18% 56% 26%
26	B0	85	12% 38% 51% 11% •
26	D0	85	12% 40% 48% 11% •
27	B1	98	2% 32% 47% 15% • •
27	D1	98	2% 21% 55% 17% • •

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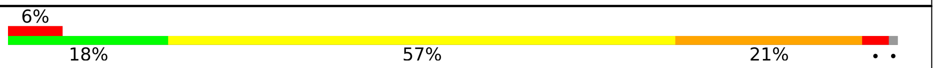
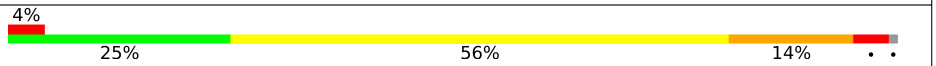
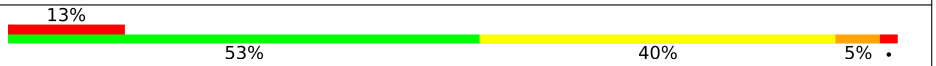
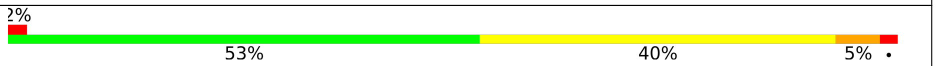
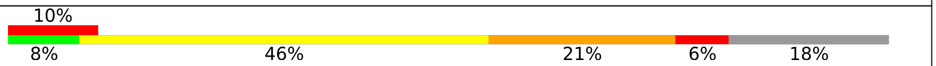
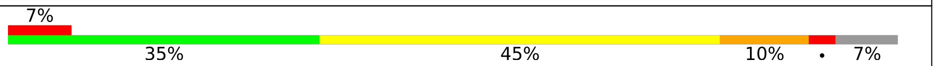
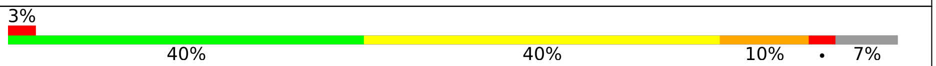
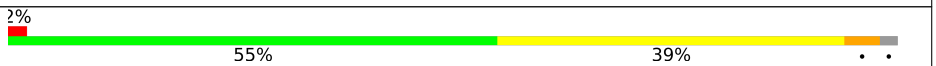
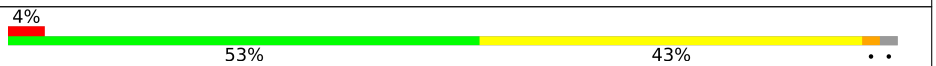
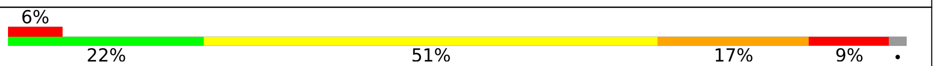
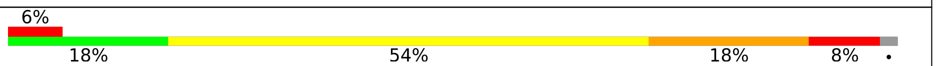
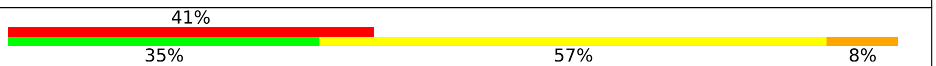
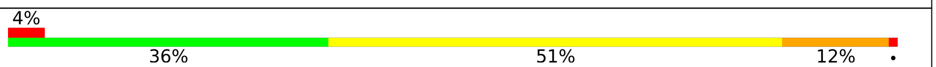
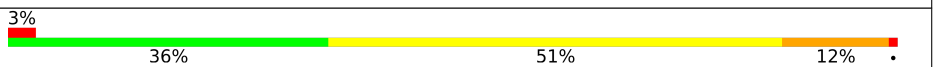
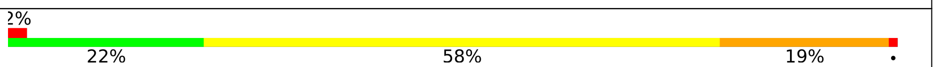
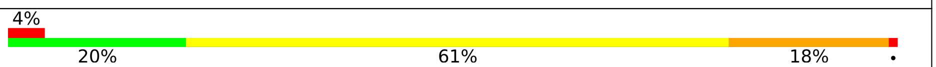
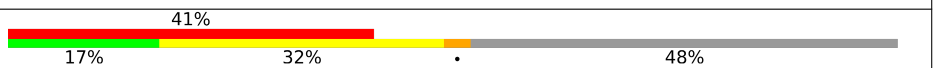
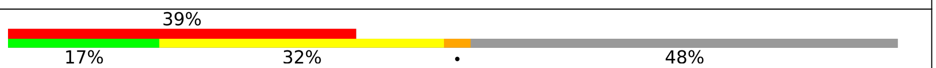
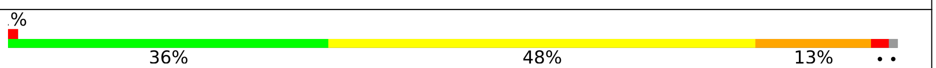
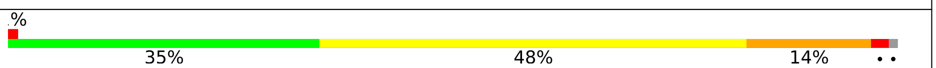
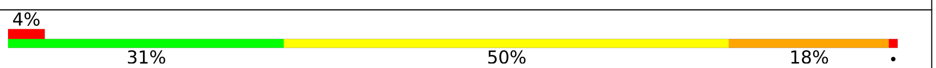
Mol	Chain	Length	Quality of chain
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2848	
36	DA	2848	
37	BB	119	
37	DB	119	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	

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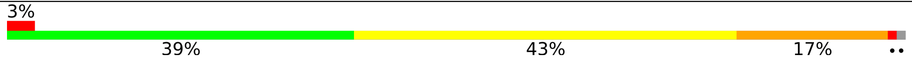
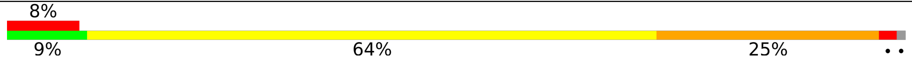
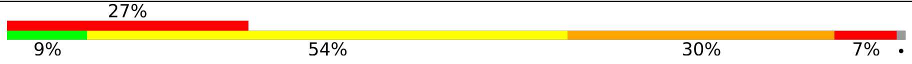
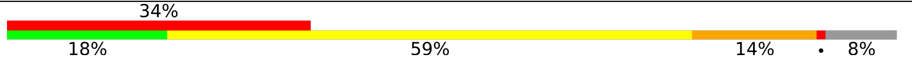
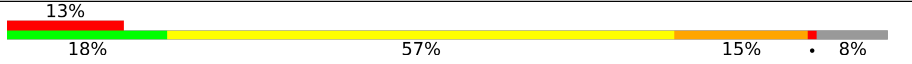
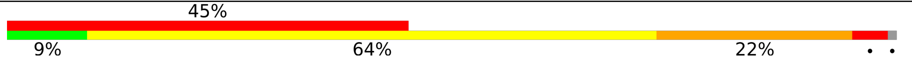
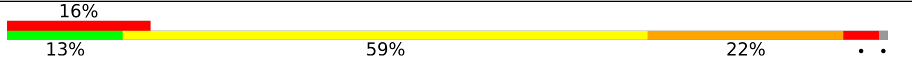
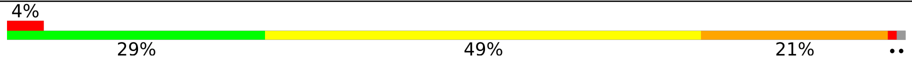
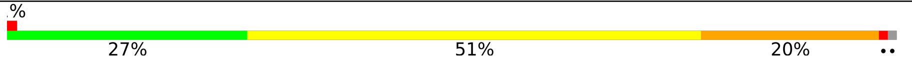
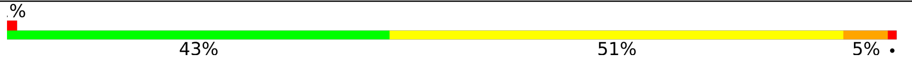
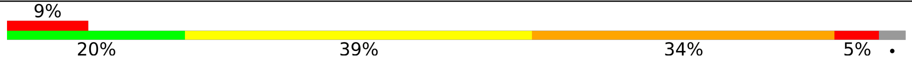
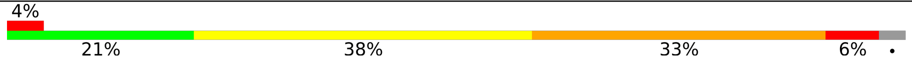
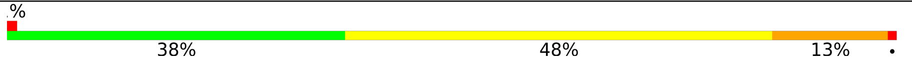
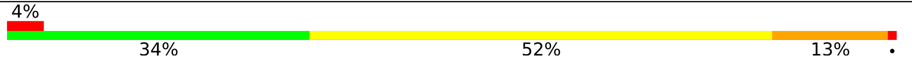
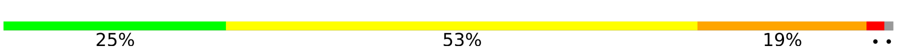
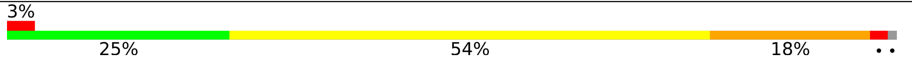
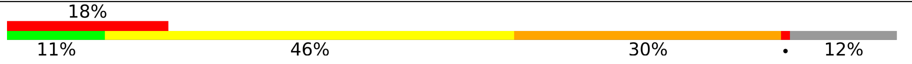
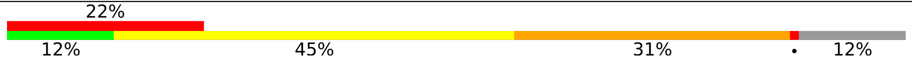
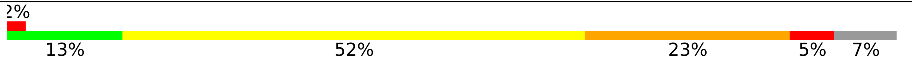
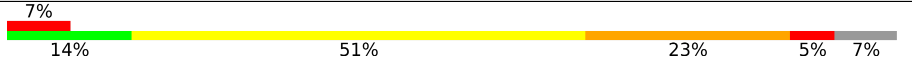
Mol	Chain	Length	Quality of chain
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BI	148	
44	DI	148	
45	BJ	130	
45	DJ	130	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52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

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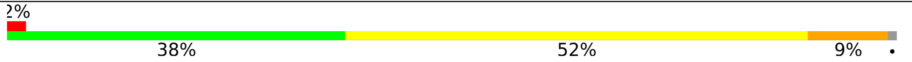
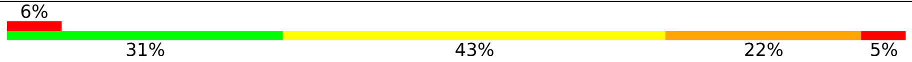
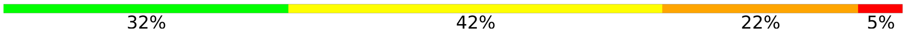
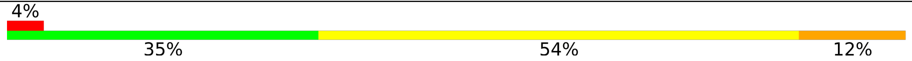
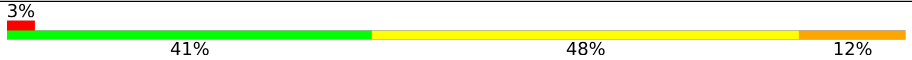
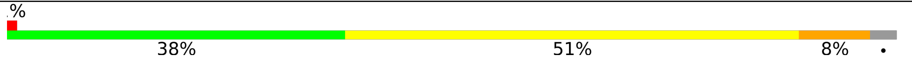
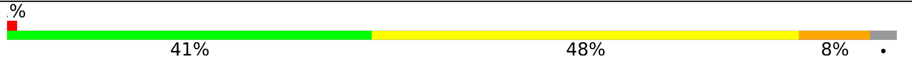
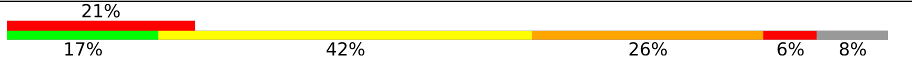
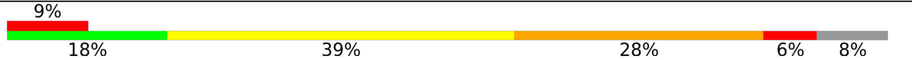
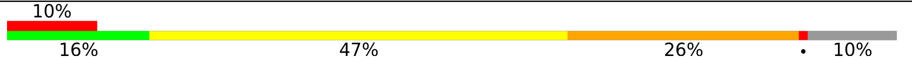
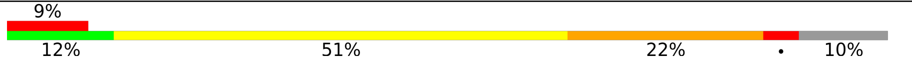
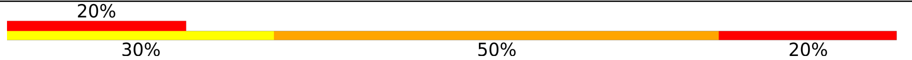
Mol	Chain	Length	Quality of chain
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	CX	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	OMU	AX	19	-	-	X	-
24	A2M	AX	20	-	-	X	X
24	A2M	AX	21	-	-	X	-
59	OMU	CX	19	-	-	X	-
59	A2M	CX	20	-	-	X	-
59	A2M	CX	21	-	-	X	-
60	MG	AA	1601	-	-	-	X
60	MG	AA	1603	-	-	-	X
60	MG	AA	1606	-	-	-	X
60	MG	AA	1608	-	-	-	X
60	MG	AA	1612	-	-	-	X
60	MG	AA	1614	-	-	-	X
60	MG	AA	1623	-	-	-	X
60	MG	AA	1624	-	-	-	X
60	MG	AA	1625	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	1627	-	-	-	X
60	MG	AA	1633	-	-	-	X
60	MG	AA	1634	-	-	-	X
60	MG	AA	1636	-	-	-	X
60	MG	AA	1641	-	-	-	X
60	MG	AA	1642	-	-	-	X
60	MG	AA	1643	-	-	-	X
60	MG	AA	1645	-	-	-	X
60	MG	AA	1646	-	-	-	X
60	MG	AA	1649	-	-	-	X
60	MG	AA	1650	-	-	-	X
60	MG	AA	1661	-	-	-	X
60	MG	AA	1662	-	-	-	X
60	MG	AA	1665	-	-	-	X
60	MG	AA	1667	-	-	-	X
60	MG	AA	1670	-	-	-	X
60	MG	AA	1672	-	-	-	X
60	MG	AA	1674	-	-	-	X
60	MG	AA	1675	-	-	-	X
60	MG	AA	1686	-	-	-	X
60	MG	AV	101	-	-	-	X
60	MG	B1	101	-	-	-	X
60	MG	BA	2908	-	-	-	X
60	MG	BA	2920	-	-	-	X
60	MG	BA	2949	-	-	-	X
60	MG	BA	2960	-	-	-	X
60	MG	BA	2965	-	-	-	X
60	MG	BA	2970	-	-	-	X
60	MG	BA	2973	-	-	-	X
60	MG	BA	2977	-	-	-	X
60	MG	BA	2988	-	-	-	X
60	MG	BA	2995	-	-	-	X
60	MG	BA	2996	-	-	-	X
60	MG	BA	3002	-	-	-	X
60	MG	BA	3008	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3012	-	-	-	X
60	MG	BA	3015	-	-	-	X
60	MG	BA	3017	-	-	-	X
60	MG	BA	3018	-	-	-	X
60	MG	BA	3020	-	-	-	X
60	MG	BA	3022	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3030	-	-	-	X
60	MG	BA	3032	-	-	-	X
60	MG	BA	3040	-	-	-	X
60	MG	BA	3046	-	-	-	X
60	MG	BA	3051	-	-	-	X
60	MG	BA	3053	-	-	-	X
60	MG	BA	3060	-	-	-	X
60	MG	BA	3063	-	-	-	X
60	MG	BA	3064	-	-	-	X
60	MG	BA	3066	-	-	-	X
60	MG	BA	3080	-	-	-	X
60	MG	BA	3081	-	-	-	X
60	MG	BA	3083	-	-	-	X
60	MG	BA	3084	-	-	-	X
60	MG	BA	3086	-	-	-	X
60	MG	BA	3089	-	-	-	X
60	MG	BA	3090	-	-	-	X
60	MG	BA	3093	-	-	-	X
60	MG	BA	3094	-	-	-	X
60	MG	BA	3098	-	-	-	X
60	MG	BA	3100	-	-	-	X
60	MG	BA	3101	-	-	-	X
60	MG	BA	3102	-	-	-	X
60	MG	BA	3106	-	-	-	X
60	MG	BA	3107	-	-	-	X
60	MG	BA	3108	-	-	-	X
60	MG	BA	3109	-	-	-	X
60	MG	BA	3114	-	-	-	X
60	MG	BA	3115	-	-	-	X
60	MG	BA	3120	-	-	-	X
60	MG	BA	3121	-	-	-	X
60	MG	BA	3123	-	-	-	X
60	MG	BA	3124	-	-	-	X
60	MG	BA	3126	-	-	-	X
60	MG	BA	3128	-	-	-	X
60	MG	BA	3129	-	-	-	X
60	MG	BB	201	-	-	-	X
60	MG	BF	301	-	-	-	X
60	MG	CA	1601	-	-	-	X
60	MG	CA	1603	-	-	-	X
60	MG	CA	1604	-	-	-	X
60	MG	CA	1606	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	1607	-	-	-	X
60	MG	CA	1612	-	-	-	X
60	MG	CA	1613	-	-	-	X
60	MG	CA	1618	-	-	-	X
60	MG	CA	1622	-	-	-	X
60	MG	CA	1624	-	-	-	X
60	MG	CA	1626	-	-	-	X
60	MG	CA	1627	-	-	-	X
60	MG	CA	1629	-	-	-	X
60	MG	CA	1631	-	-	-	X
60	MG	CA	1633	-	-	-	X
60	MG	CA	1636	-	-	-	X
60	MG	CA	1637	-	-	-	X
60	MG	CA	1640	-	-	-	X
60	MG	CA	1641	-	-	-	X
60	MG	CA	1644	-	-	-	X
60	MG	CA	1650	-	-	-	X
60	MG	CA	1653	-	-	-	X
60	MG	CA	1654	-	-	-	X
60	MG	CA	1662	-	-	-	X
60	MG	CA	1664	-	-	-	X
60	MG	CA	1665	-	-	-	X
60	MG	CA	1666	-	-	-	X
60	MG	CA	1667	-	-	-	X
60	MG	CA	1671	-	-	-	X
60	MG	CA	1672	-	-	-	X
60	MG	CA	1677	-	-	-	X
60	MG	CA	1678	-	-	-	X
60	MG	CA	1680	-	-	-	X
60	MG	CA	1686	-	-	-	X
60	MG	CA	1687	-	-	-	X
60	MG	CA	1688	-	-	-	X
60	MG	CA	1689	-	-	-	X
60	MG	CA	1690	-	-	-	X
60	MG	CA	1691	-	-	-	X
60	MG	CA	1692	-	-	-	X
60	MG	CA	1694	-	-	-	X
60	MG	CA	1696	-	-	-	X
60	MG	CA	1698	-	-	-	X
60	MG	CA	1700	-	-	-	X
60	MG	CA	1702	-	-	-	X
60	MG	CG	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CV	102	-	-	-	X
60	MG	DA	2901	-	-	-	X
60	MG	DA	2929	-	-	-	X
60	MG	DA	2942	-	-	-	X
60	MG	DA	2949	-	-	-	X
60	MG	DA	2962	-	-	-	X
60	MG	DA	2964	-	-	-	X
60	MG	DA	2965	-	-	-	X
60	MG	DA	2969	-	-	-	X
60	MG	DA	2972	-	-	-	X
60	MG	DA	2975	-	-	-	X
60	MG	DA	2986	-	-	-	X
60	MG	DA	2990	-	-	-	X
60	MG	DA	2991	-	-	-	X
60	MG	DA	2998	-	-	-	X
60	MG	DA	3003	-	-	-	X
60	MG	DA	3004	-	-	-	X
60	MG	DA	3009	-	-	-	X
60	MG	DA	3010	-	-	-	X
60	MG	DA	3014	-	-	-	X
60	MG	DA	3018	-	-	-	X
60	MG	DA	3019	-	-	-	X
60	MG	DA	3024	-	-	-	X
60	MG	DA	3027	-	-	-	X
60	MG	DA	3029	-	-	-	X
60	MG	DA	3031	-	-	-	X
60	MG	DA	3035	-	-	-	X
60	MG	DA	3037	-	-	-	X
60	MG	DA	3039	-	-	-	X
60	MG	DA	3041	-	-	-	X
60	MG	DA	3046	-	-	-	X
60	MG	DA	3048	-	-	-	X
60	MG	DA	3056	-	-	-	X
60	MG	DA	3057	-	-	-	X
60	MG	DA	3058	-	-	-	X
60	MG	DA	3061	-	-	-	X
60	MG	DA	3063	-	-	-	X
60	MG	DA	3068	-	-	-	X
60	MG	DA	3070	-	-	-	X
60	MG	DA	3071	-	-	-	X
60	MG	DA	3072	-	-	-	X
60	MG	DA	3077	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3080	-	-	-	X
60	MG	DA	3081	-	-	-	X
60	MG	DA	3082	-	-	-	X
60	MG	DA	3083	-	-	-	X
60	MG	DA	3085	-	-	-	X
60	MG	DA	3088	-	-	-	X
60	MG	DA	3089	-	-	-	X
60	MG	DA	3090	-	-	-	X
60	MG	DA	3094	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3097	-	-	-	X
60	MG	DA	3098	-	-	-	X
60	MG	DA	3099	-	-	-	X
60	MG	DA	3100	-	-	-	X
60	MG	DA	3104	-	-	-	X
60	MG	DA	3106	-	-	-	X
60	MG	DA	3114	-	-	-	X
60	MG	DA	3115	-	-	-	X
60	MG	DA	3117	-	-	-	X
60	MG	DA	3122	-	-	-	X
60	MG	DA	3124	-	-	-	X
60	MG	DA	3125	-	-	-	X
60	MG	DA	3132	-	-	-	X
60	MG	DA	3135	-	-	-	X
60	MG	DA	3137	-	-	-	X
60	MG	DA	3141	-	-	-	X
60	MG	DB	201	-	-	-	X
60	MG	DR	201	-	-	-	X
60	MG	DX	101	-	-	-	X
61	ZN	AD	301	-	-	X	-

2 Entry composition ⓘ

There are 61 unique types of molecules in this entry. The entry contains 298206 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
			Total	C	N	O	P			
1	AA	1504	32329	14390	5992	10444	1503	0	0	0
1	CA	1504	32329	14390	5992	10444	1503	0	0	0

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

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

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

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

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

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

- 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
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	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 795 499 157 138 1	0	0	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 885 549 168 165 3	0	0	0
11	CK	119	Total C N O S 885 549 168 165 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	AL	125	Total C N O S 971 611 196 163 1	0	0	1
12	CL	125	Total C N O S 971 611 196 163 1	0	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	AM	119	Total C N O S 938 579 194 163 2	0	0	1
13	CM	119	Total C N O S 938 579 194 163 2	0	0	1

- 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 492 312 104 72 4	0	0	0
14	CN	60	Total C N O S 492 312 104 72 4	0	0	0

- 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 734 459 147 126 2	0	0	0
15	CO	88	Total C N O S 734 459 147 126 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total 1641	C 733	N 297	O 535	P 76	0	0	0

- Molecule 23 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0
23	CV	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0
23	CW	77	Total 1640	C 732	N 297	O 535	P 76	0	0	0

- Molecule 24 is a RNA chain called 5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP* AP*AP*AP *AP*AP*UP*G U2M A2M A2MP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total 239	C 111	N 49	O 69	P 10	0	0	0

- Molecule 25 is a protein called TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	84	Total 722	C 464	N 126	O 130	S 2	0	0	0
25	AZ	84	Total 723	C 464	N 126	O 131	S 2	0	0	0
25	CY	84	Total 722	C 464	N 126	O 130	S 2	0	0	0
25	CZ	84	Total 723	C 464	N 126	O 131	S 2	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total 662	C 410	N 140	O 111	S 1	0	0	0
26	D0	84	Total 662	C 410	N 140	O 111	S 1	0	0	0

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total 451	C 285	N 78	O 83	S 5	0	0	1
30	D4	58	Total 451	C 285	N 78	O 83	S 5	0	0	1

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	56	Total 428	C 267	N 87	O 69	S 5	0	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	D5	56	Total C N O S 428 267 87 69 5	0	0	1

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	B6	50	Total C N O S 433 270 88 71 4	0	0	0
32	D6	50	Total C N O S 433 270 88 71 4	0	0	0

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	B7	48	Total C N O S 410 251 103 54 2	0	0	1
33	D7	48	Total C N O S 410 251 103 54 2	0	0	1

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	B9	37	Total C N O S 307 188 68 47 4	0	0	0
35	D9	37	Total C N O S 307 188 68 47 4	0	0	0

- Molecule 36 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BA	2848	Total C N O P 61341 27300 11478 19716 2847	0	0	0
36	DA	2848	Total C N O P 61341 27300 11478 19716 2847	0	0	0

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	120	Total 937	C 590	N 174	O 172	S 1	0	0	0
38	DC	120	Total 937	C 590	N 174	O 172	S 1	0	0	0

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	165	Total 1260	C 800	N 234	O 225	S 1	0	0	1
43	DH	165	Total 1260	C 800	N 234	O 225	S 1	0	0	1

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L10.

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	1
			1113	710	211	185	7			
49	DQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	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	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
52	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

- Molecule 59 is a RNA chain called BACTERIAL TOXIN YOEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	10	Total 217	C 101	N 44	O 63	P 9	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	103	Total 103	Mg 103	0	0
60	AL	1	Total 1	Mg 1	0	0
60	AV	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	B0	1	Total 1	Mg 1	0	0
60	B1	2	Total 2	Mg 2	0	0
60	B5	2	Total 2	Mg 2	0	0
60	BA	236	Total 236	Mg 236	0	0
60	BB	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BP	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	CA	103	Total 103	Mg 103	0	0
60	CG	1	Total 1	Mg 1	0	0
60	CL	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	CV	2	Total Mg 2 2	0	0
60	D1	1	Total Mg 1 1	0	0
60	D5	1	Total Mg 1 1	0	0
60	DA	242	Total Mg 242 242	0	0
60	DB	1	Total Mg 1 1	0	0
60	DF	1	Total Mg 1 1	0	0
60	DR	1	Total Mg 1 1	0	0
60	DX	1	Total Mg 1 1	0	0

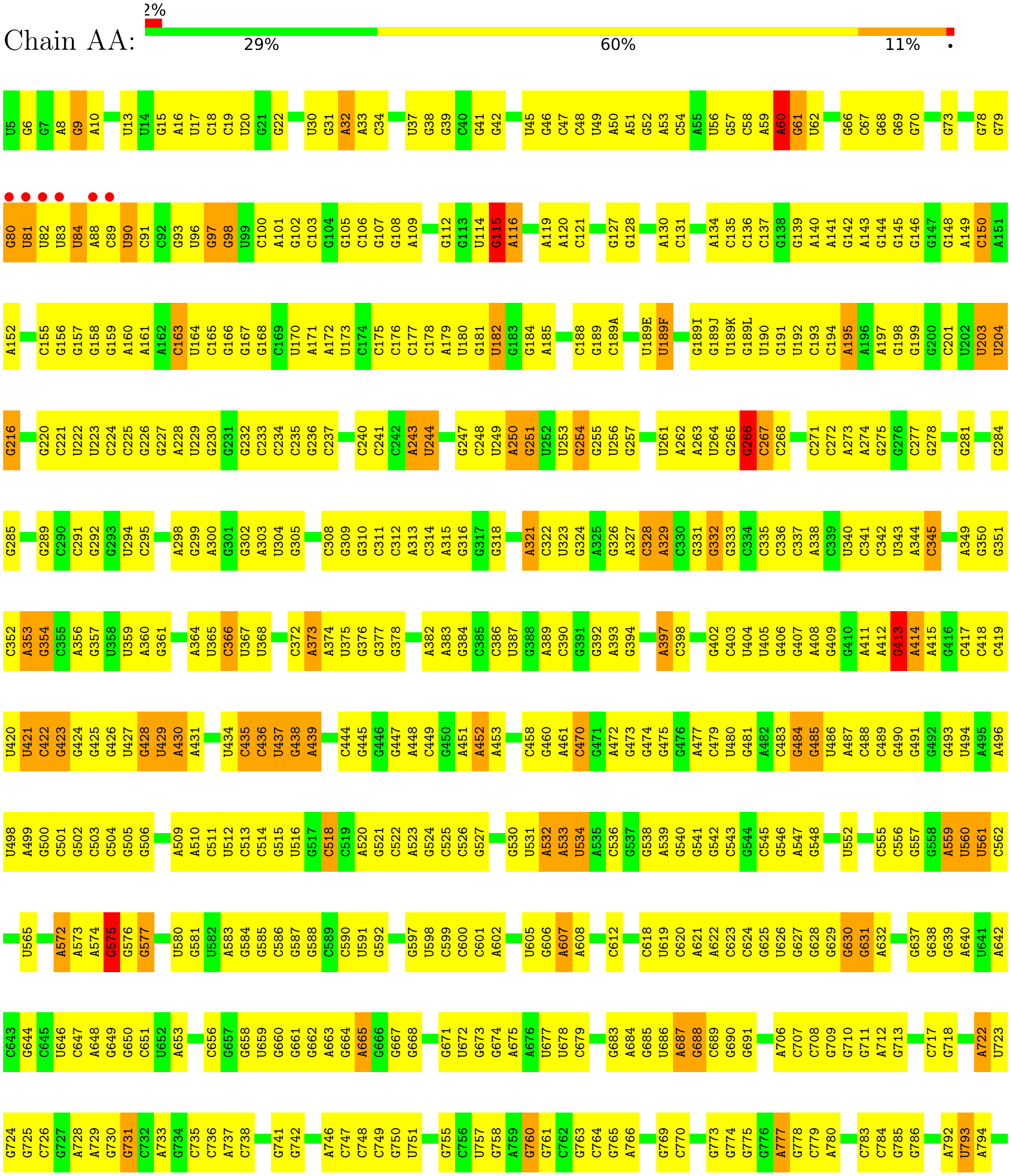
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

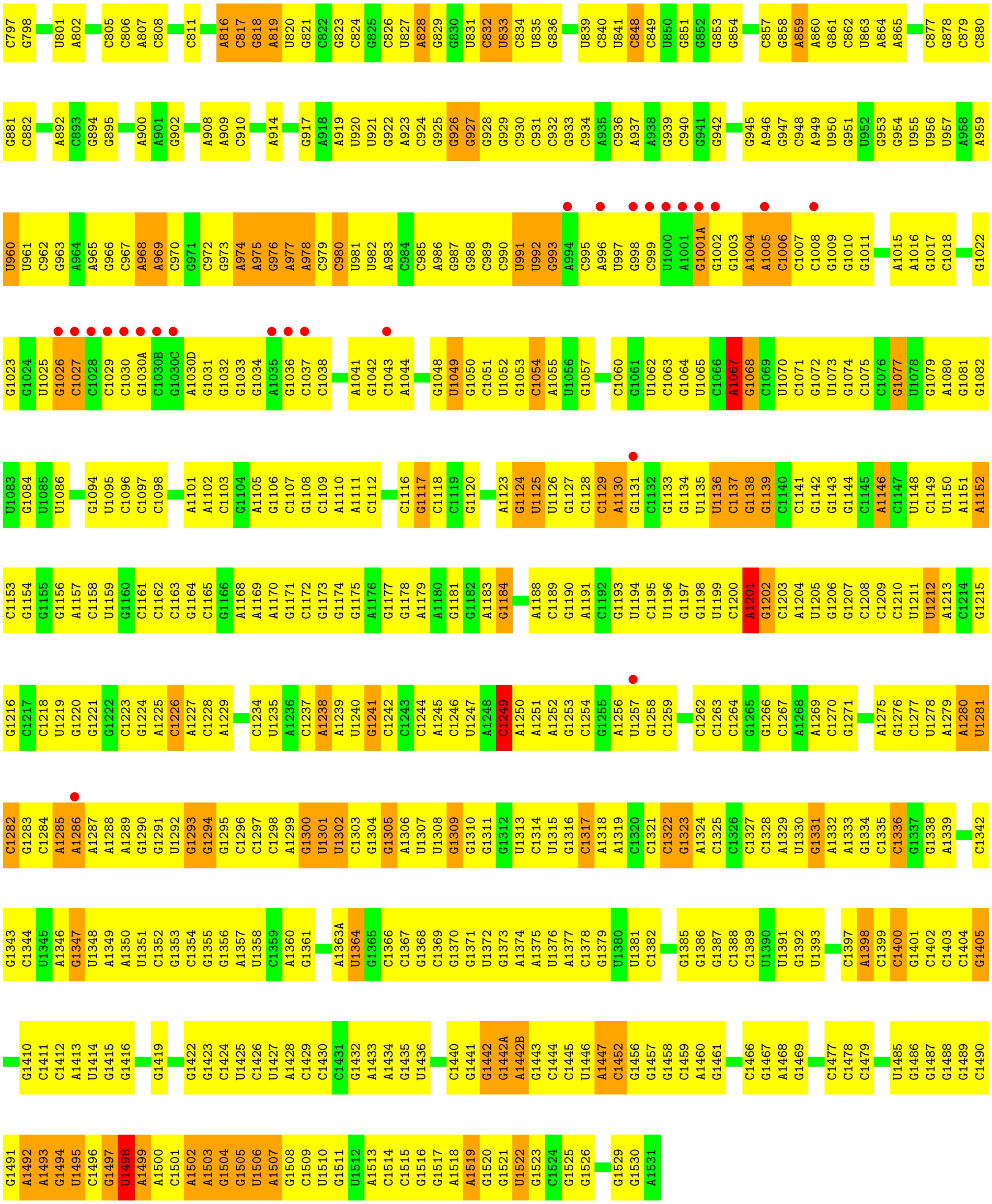
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AD	1	Total Zn 1 1	0	0
61	AN	1	Total Zn 1 1	0	0
61	CD	1	Total Zn 1 1	0	0
61	CN	1	Total Zn 1 1	0	0

3 Residue-property plots ⓘ

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

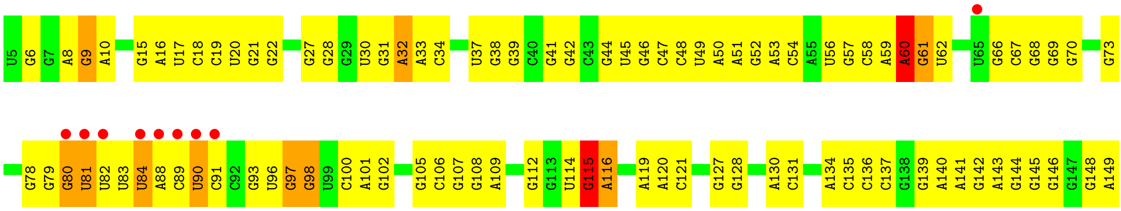
- Molecule 1: 16S ribosomal RNA

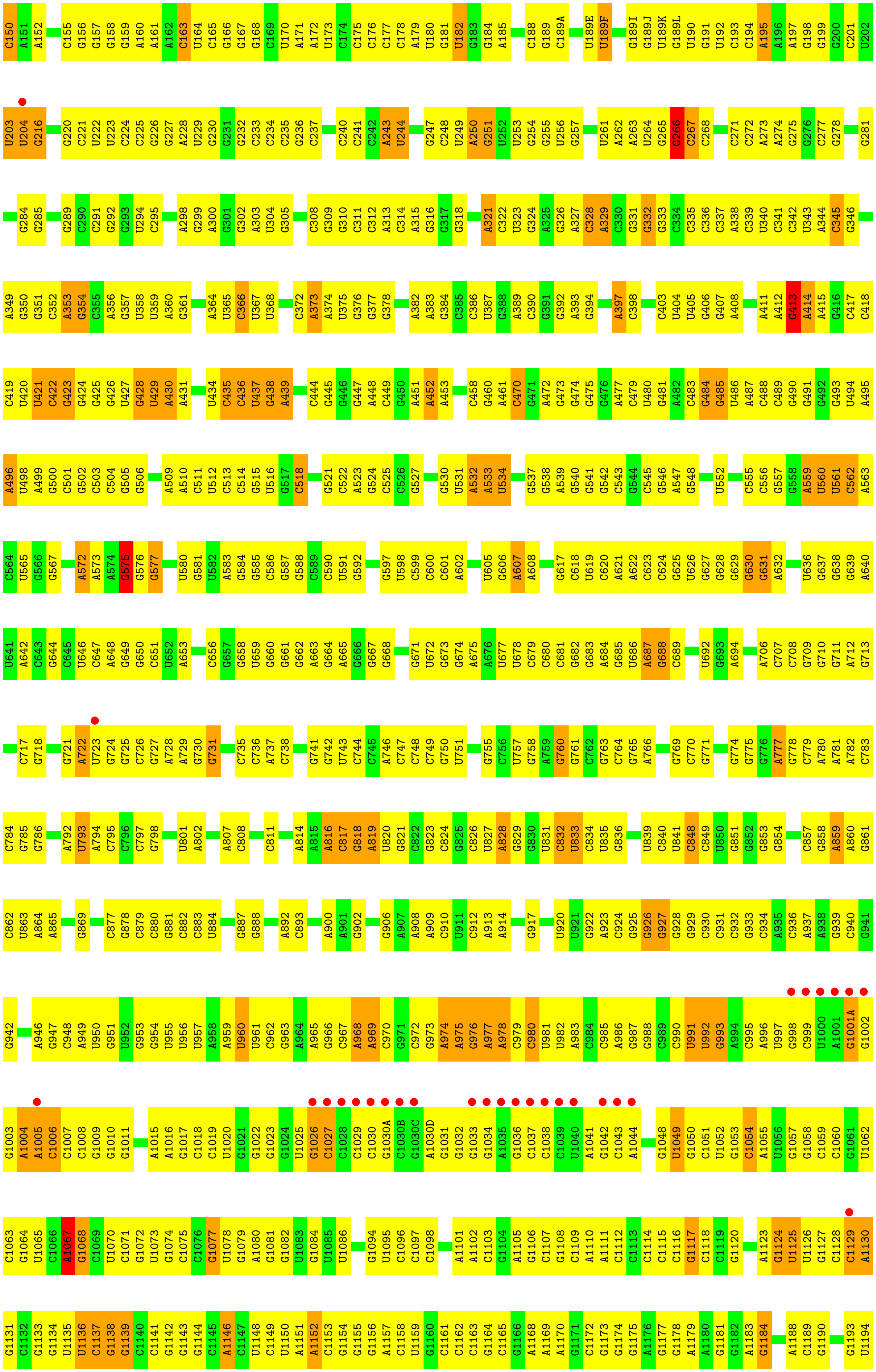




- Molecule 1: 16S ribosomal RNA

Chain CA:




C150 A151 A152 C155 G156 G157 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 G184 A185 C188 G189 C189A U189E U189F G189I G189J U189K G189L U190 G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U202
U203 U204 G216 G220 C221 U222 U223 G224 C225 G226 G227 A228 U229 G230 G231 G232 C233 G234 C235 G236 C237 C240 C241 C242 A243 U244 G247 C248 U249 A250 G251 U252 U253 G254 G255 U256 G257 U261 A262 A263 U264 G265 G266 C267 C268 C271 C272 A273 A274 G275 G276 C277 G278 G281
G284 G285 G289 C290 C291 G292 G293 U294 C295 A298 G299 A300 G301 G302 A303 U304 G305 C308 G309 G310 C311 G312 A313 C314 A315 G316 G317 G318 A321 C322 U323 G324 A325 C326 A327 C328 A329 C330 G331 G332 G333 C334 C335 C336 C337 A338 C339 U340 C341 C342 U343 A344 C345 G346
A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 A364 U365 C366 U367 U368 C372 A373 A374 U375 G376 G377 G378 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 A393 G394 A397 C398 C403 U404 U405 G406 G407 A408 A411 A412 G413 A414 A415 G416 C417 C418
C419 U420 U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 U434 C435 C436 U437 G438 A439 C444 G445 G446 G447 A448 C449 G450 A451 A452 A453 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 A477 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 G493 U494 A495
A496 U498 A499 G500 C501 G502 C503 C504 G505 G506 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 G521 C522 A523 G524 C525 C526 G527 G530 U531 A532 A533 U534 G537 G538 A539 G540 G541 G542 C543 G544 C545 G546 A547 G548 U552 C555 C556 G557 G558 A559 U560 U561 C562 A563
C564 U565 G566 G567 A572 A573 A574 G575 C576 G577 U580 G581 U582 A583 G584 G585 C586 G587 G588 C589 C590 U591 G592 G597 U598 C599 C600 C601 A602 U605 G606 A607 A608 C617 C618 U619 C620 A621 A622 C623 C624 G625 U626 C627 G628 G629 G630 G631 A632 U636 G637 G638 G639 A640
U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667 G668 G671 U672 G673 C674 A675 A676 U677 C678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 U692 G693 A694 A706 C707 C708 G709 G710 G711 A712 G713
C717 G718 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C735 C736 A737 C738 G741 G742 U743 C744 C745 A746 C747 C748 C749 G750 U751 G755 C756 U757 G758 A759 G760 G761 C762 G763 C764 G765 A766 G769 C770 G771 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783
C784 G785 G786 A792 U793 A794 C795 C796 C797 G798 U801 A802 A807 C808 C811 A814 A815 A816 C817 G818 A819 U820 G821 C822 G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 U839 C840 U841 C848 C849 U850 G851 G852 G853 G854 C857 G858 A859 A860 G861
C862 U863 A864 A865 G869 C877 G878 C879 C880 G881 C882 C883 U884 G887 G888 A892 C893 A900 A901 G902 G906 A907 A908 A909 C910 U911 C912 A913 A914 G917 U920 U921 G922 A923 C924 G925 G926 G927 G928 C929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941
G942 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002
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C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1094 U1095 C1096 C1097 C1098 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 C1115 C1116 G1117 C1118 C1119 G1120 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130
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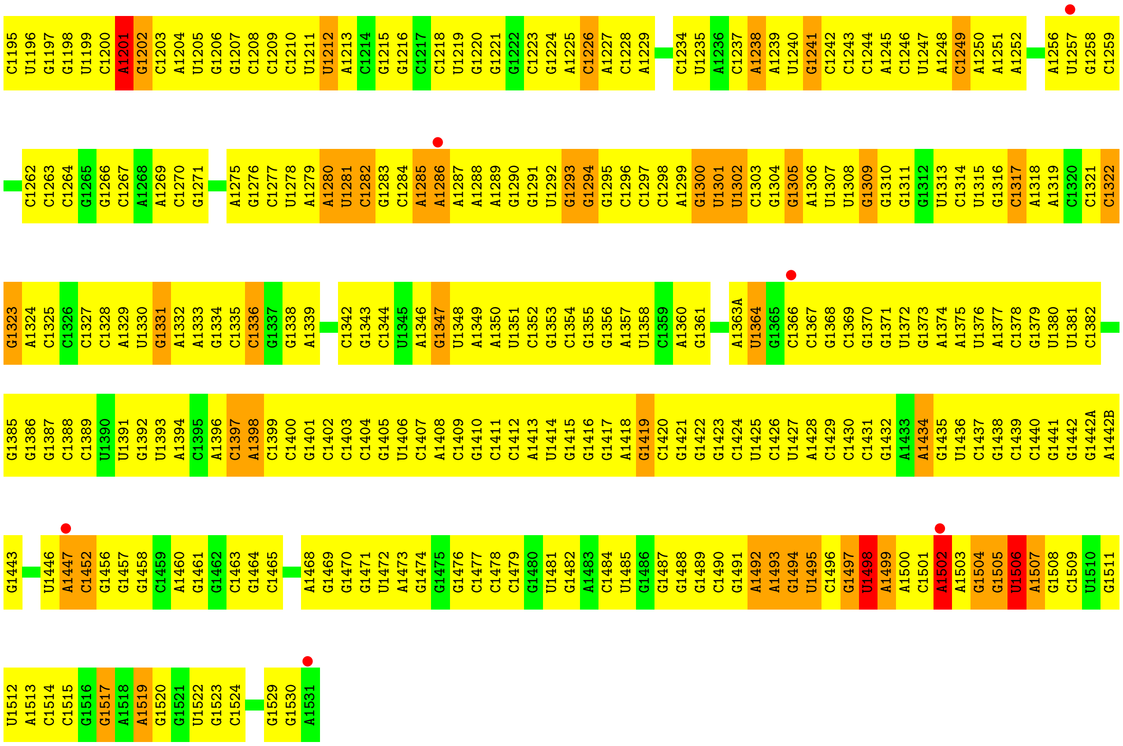
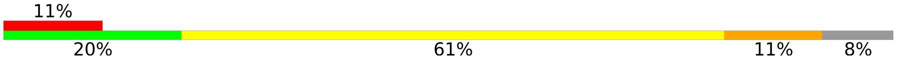
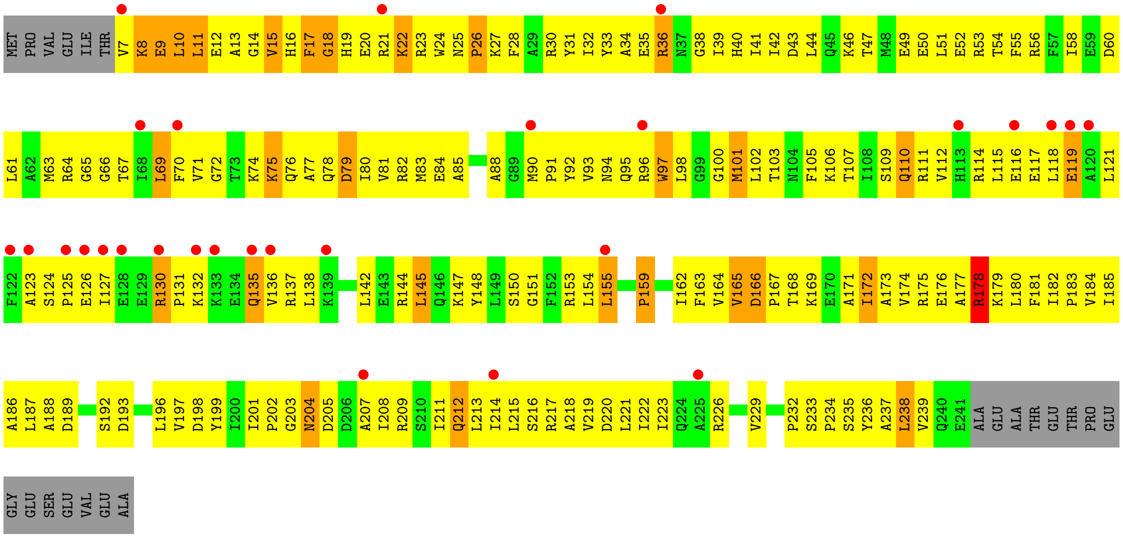


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

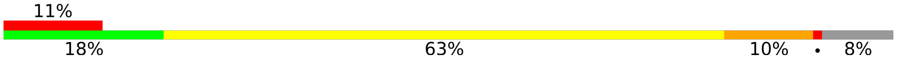
Chain AB:

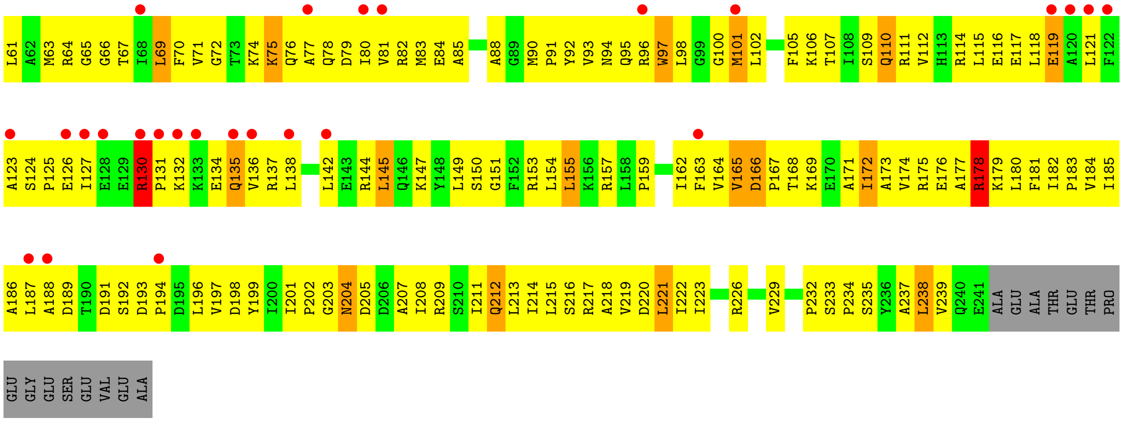




- Molecule 2: 30S RIBOSOMAL PROTEIN S2

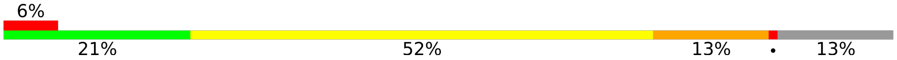
Chain CB:

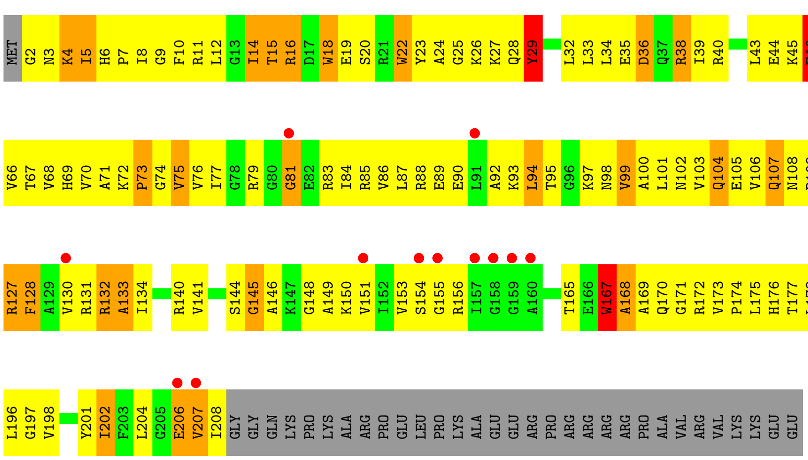




- Molecule 3: 30S RIBOSOMAL PROTEIN S3

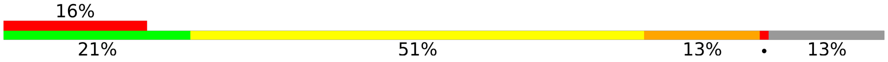
Chain AC:

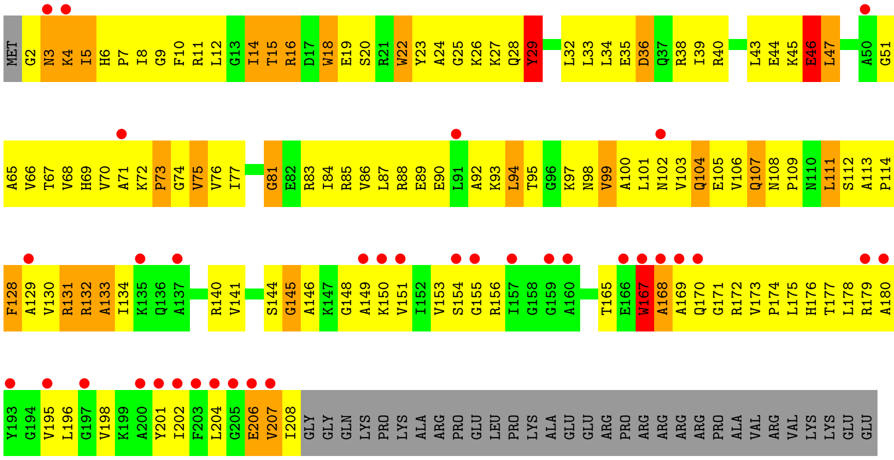




- Molecule 3: 30S RIBOSOMAL PROTEIN S3

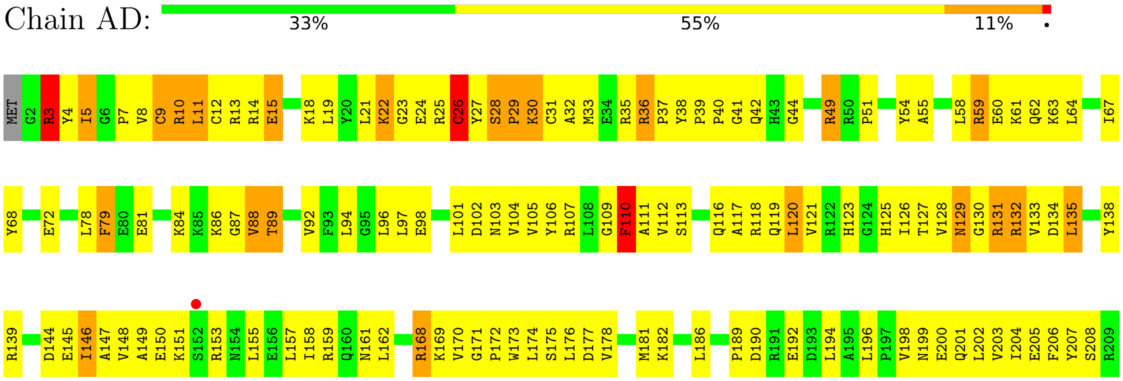
Chain CC:





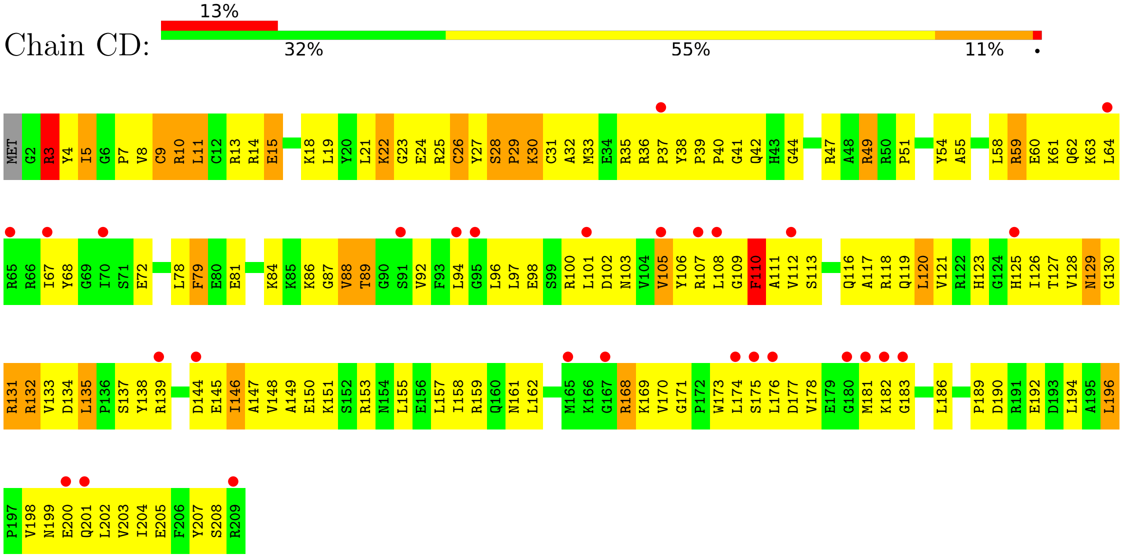
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



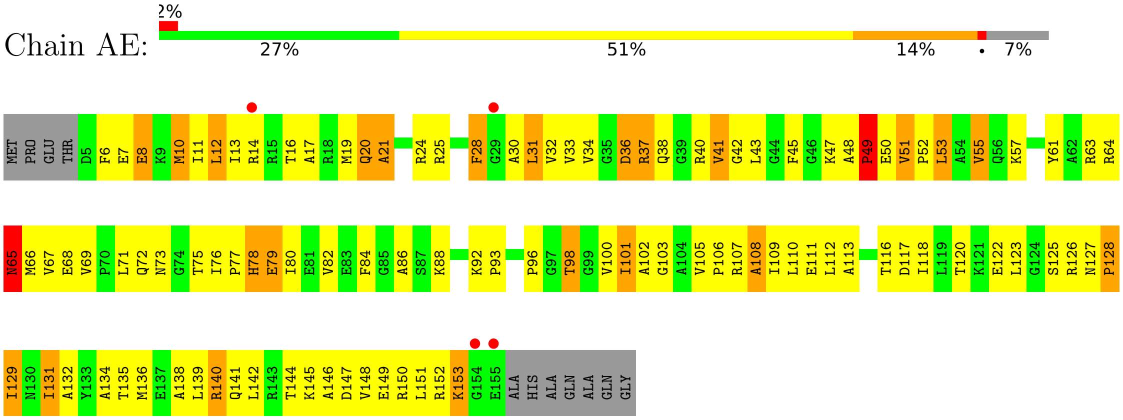
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



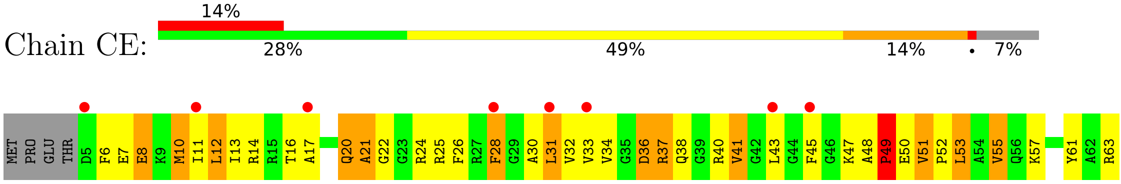
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

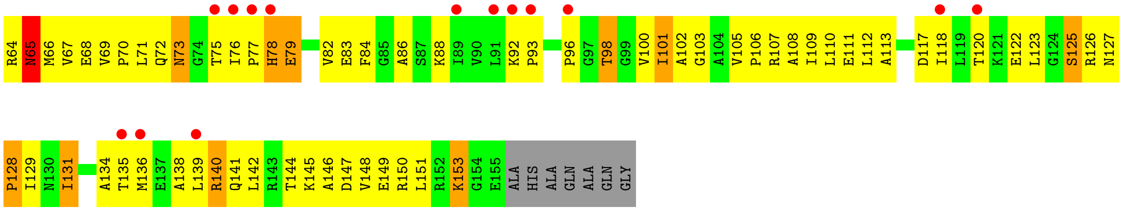
Chain AE:



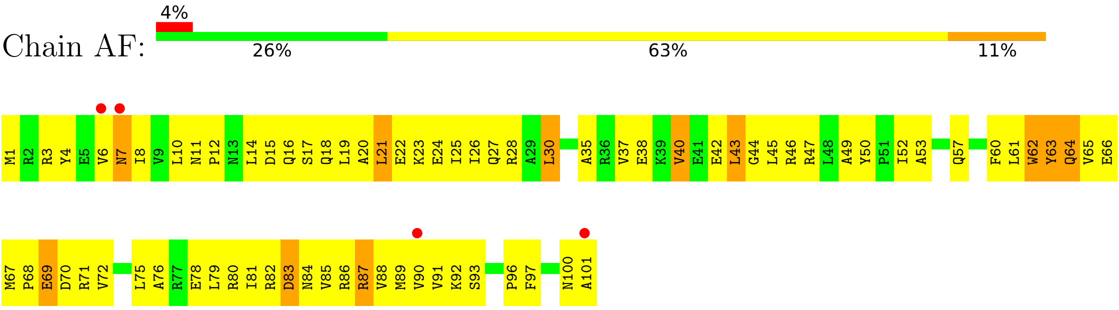
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:

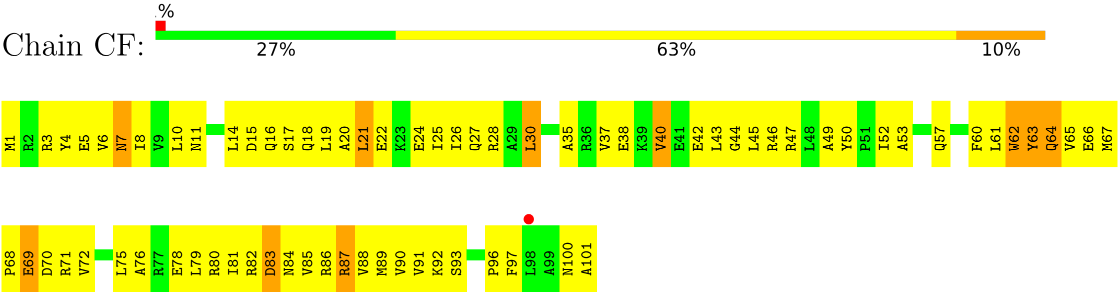




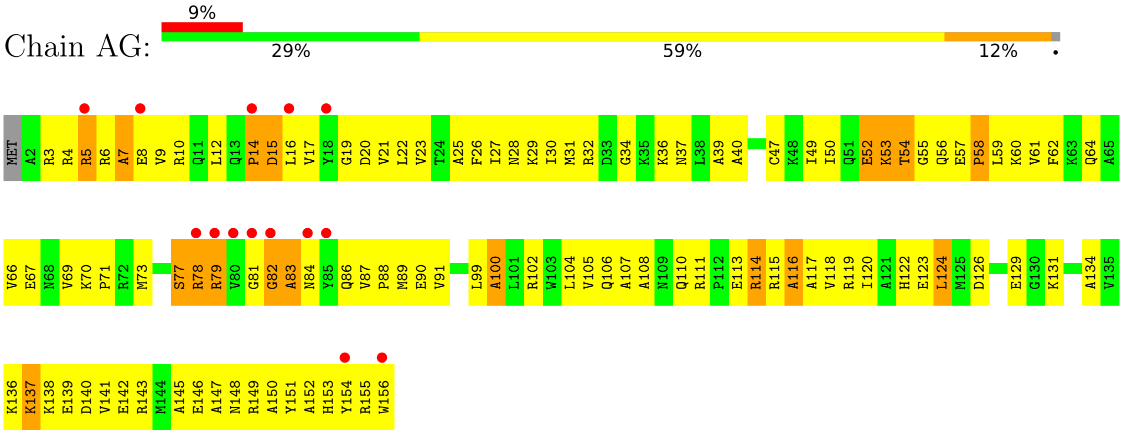
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



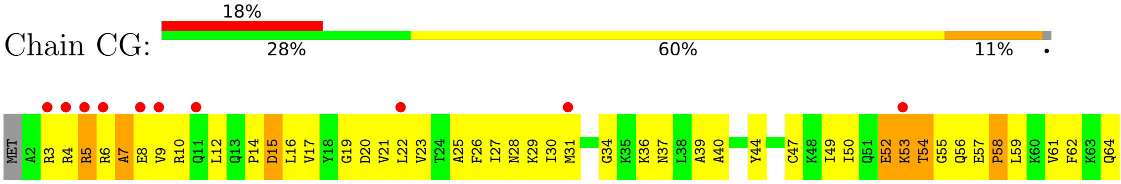
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

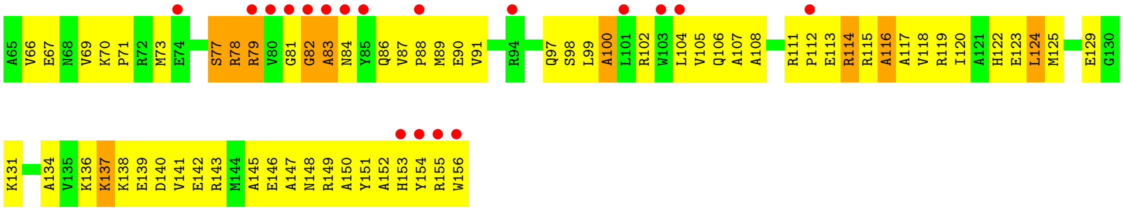


- Molecule 7: 30S RIBOSOMAL PROTEIN S7



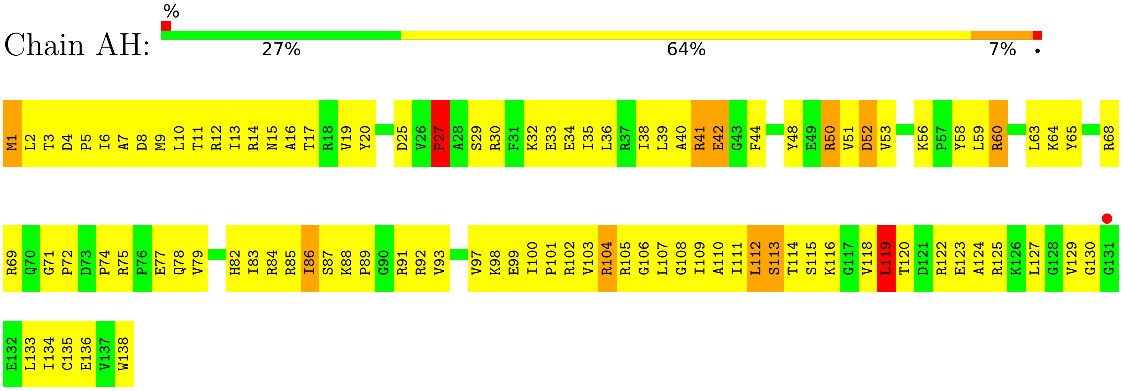
- Molecule 7: 30S RIBOSOMAL PROTEIN S7





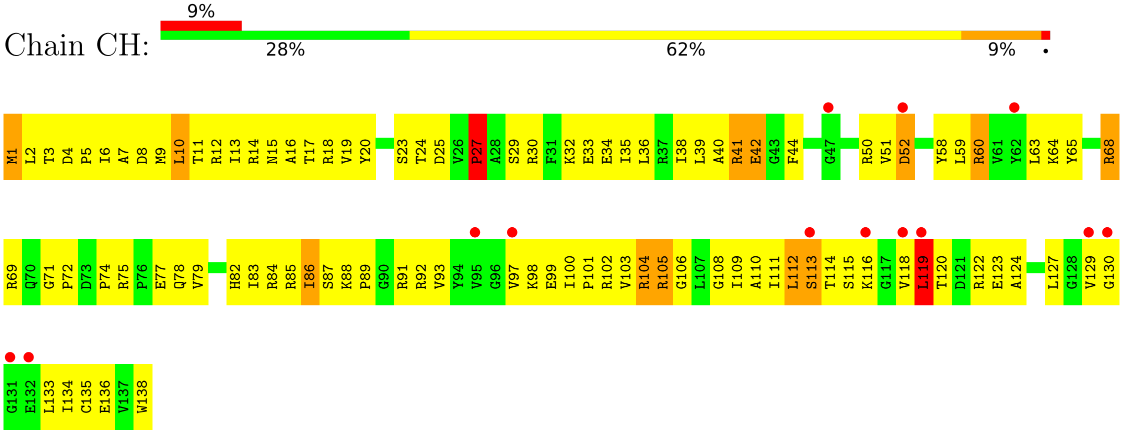
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



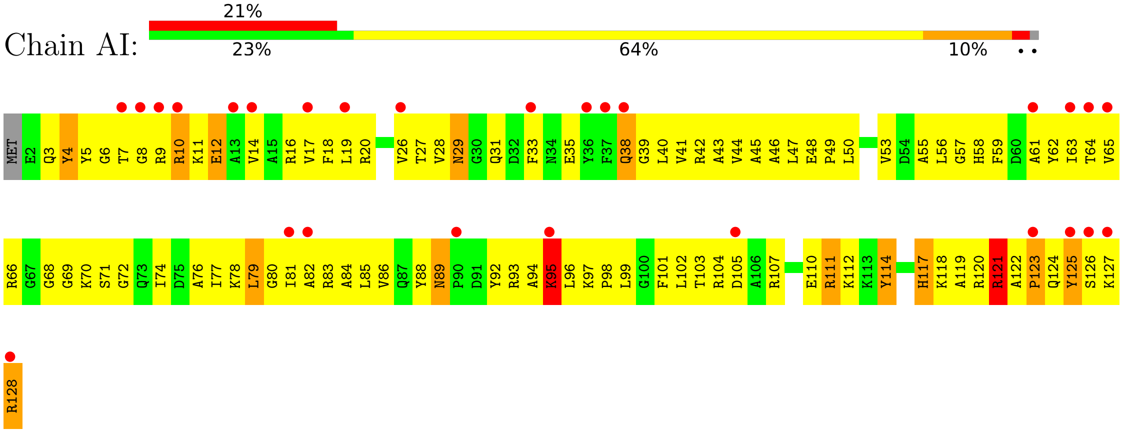
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



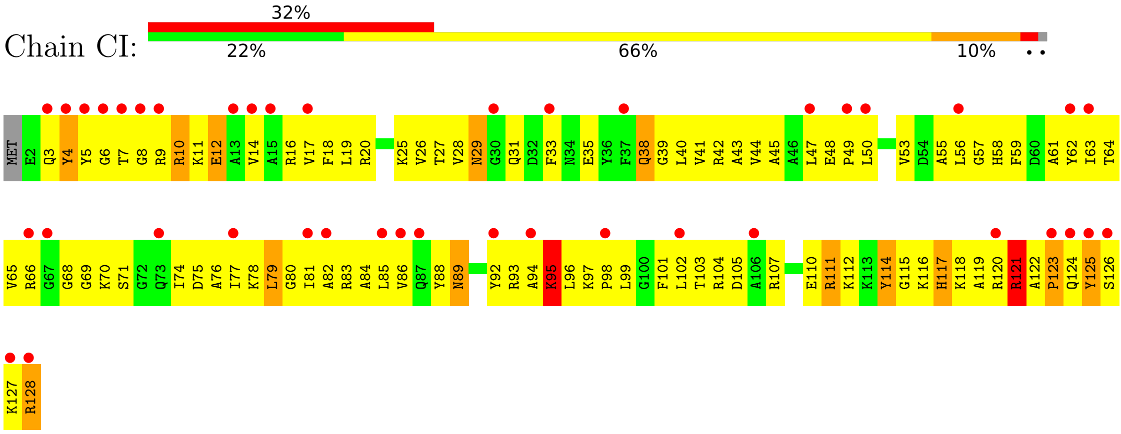
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



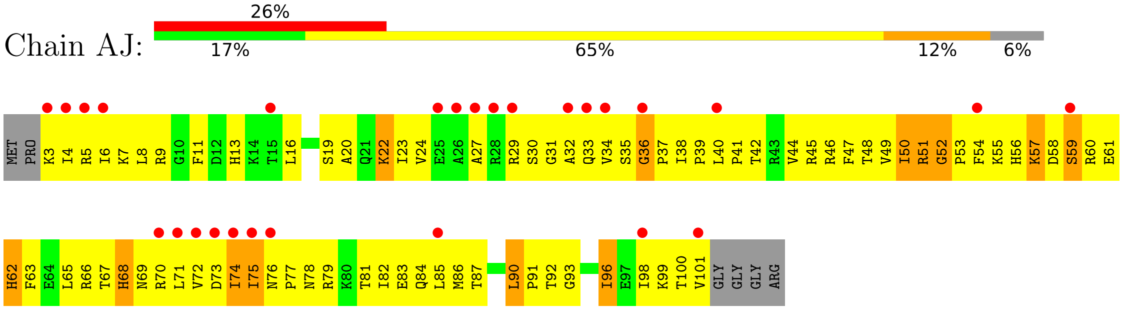
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



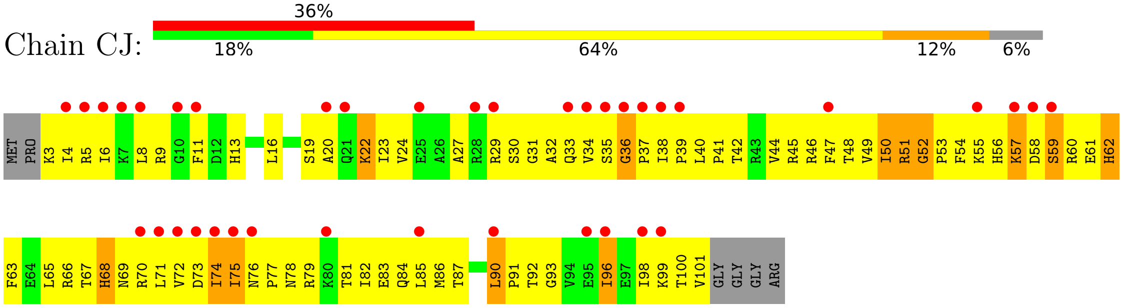
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



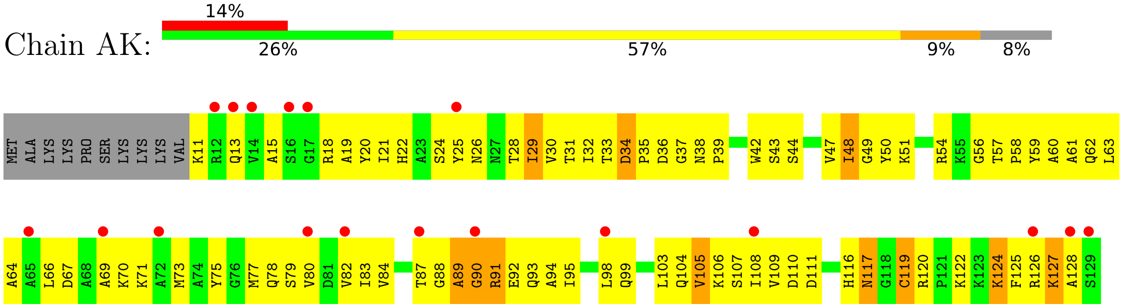
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



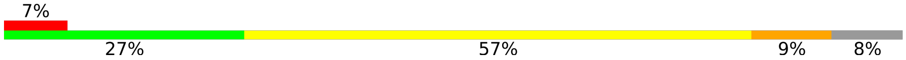
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

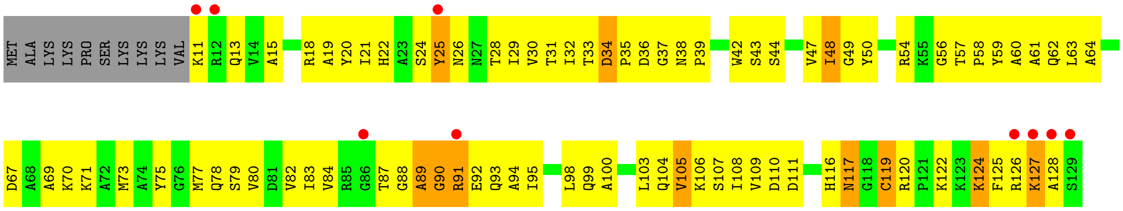
Chain AK:



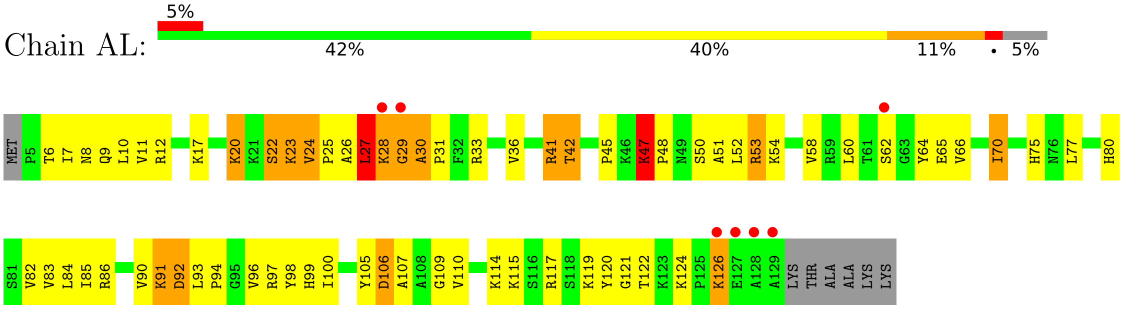
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:

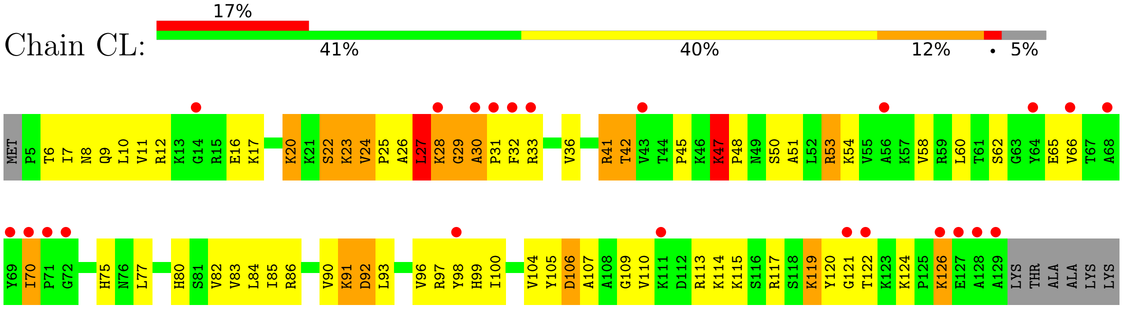




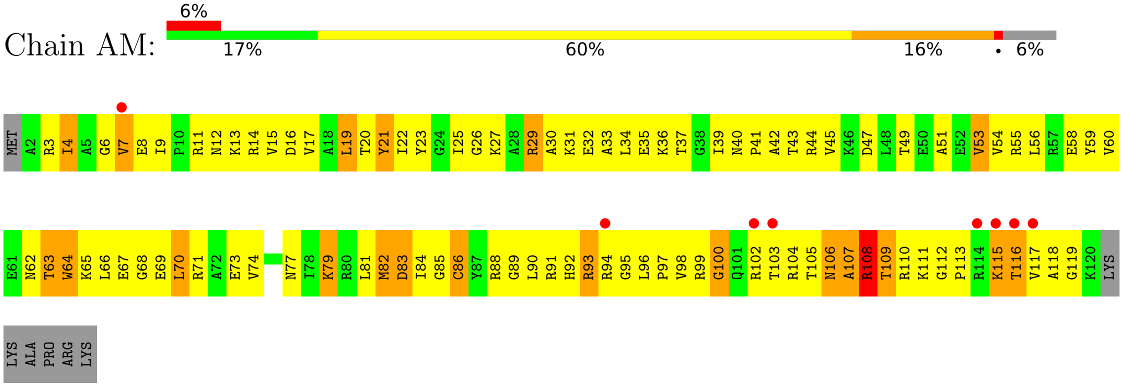
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



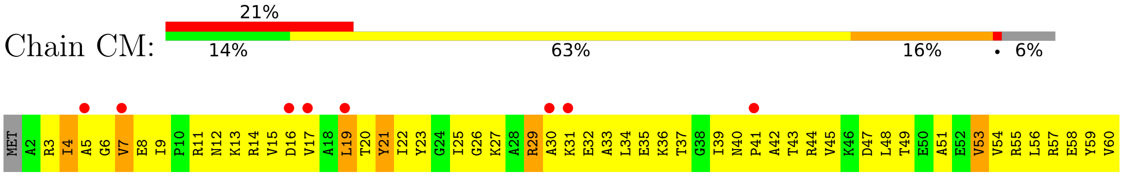
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

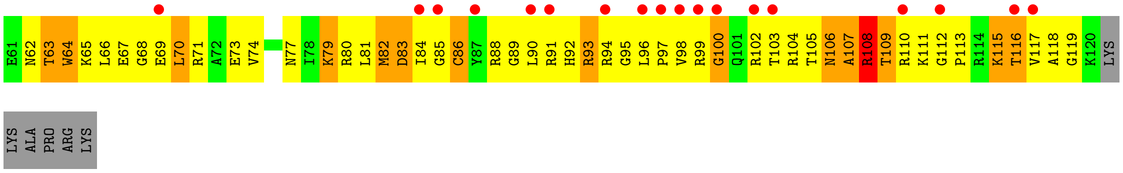


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

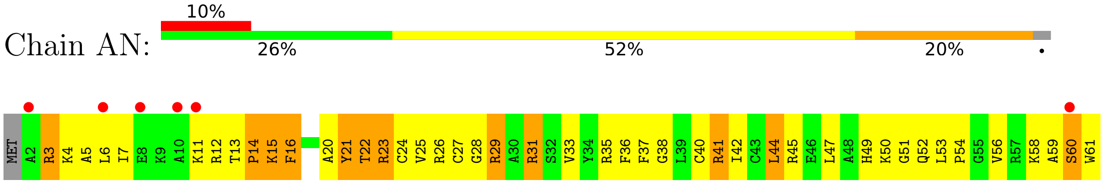


- Molecule 13: 30S RIBOSOMAL PROTEIN S13

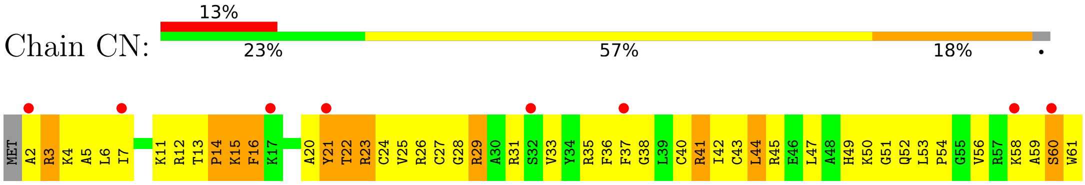




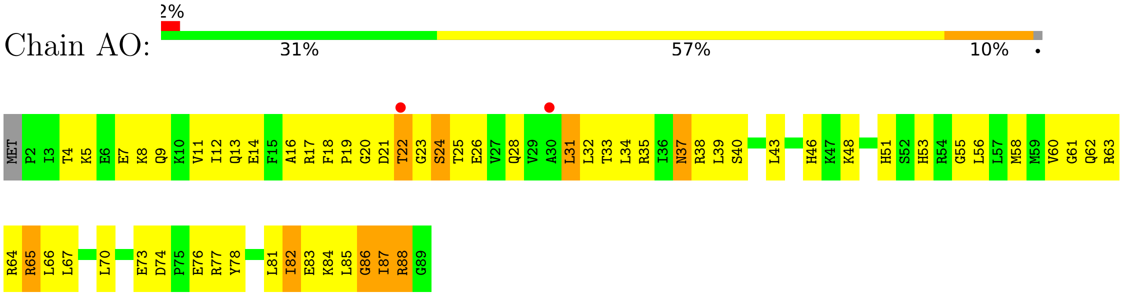
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



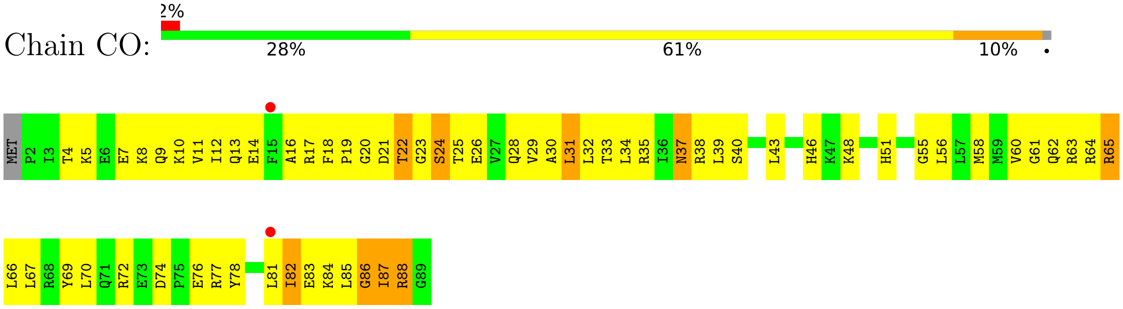
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



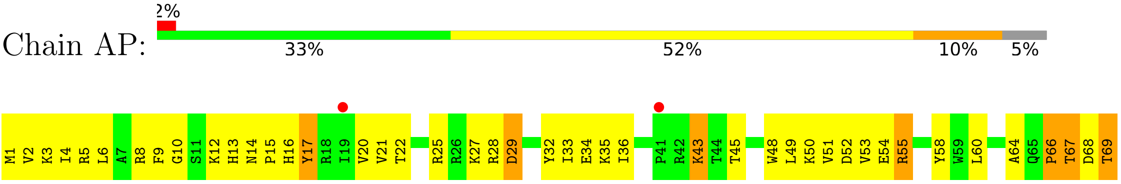
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

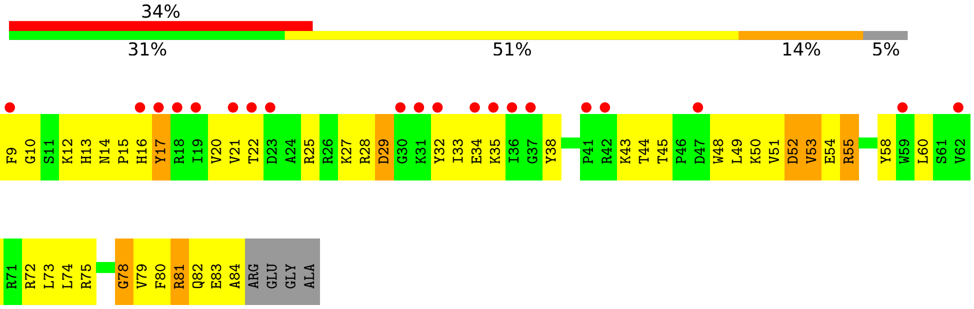


- Molecule 16: 30S RIBOSOMAL PROTEIN S16



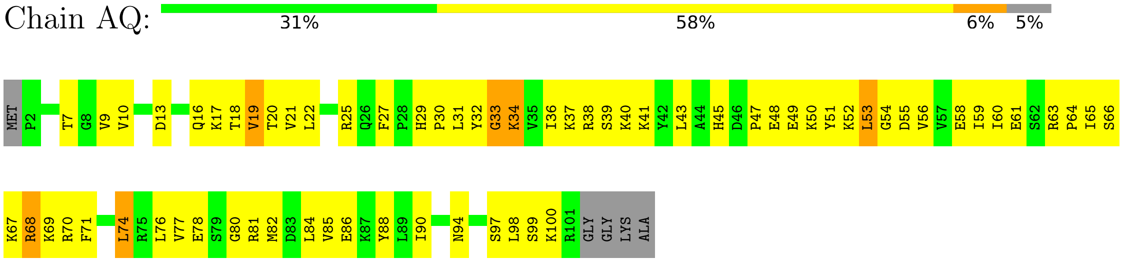
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



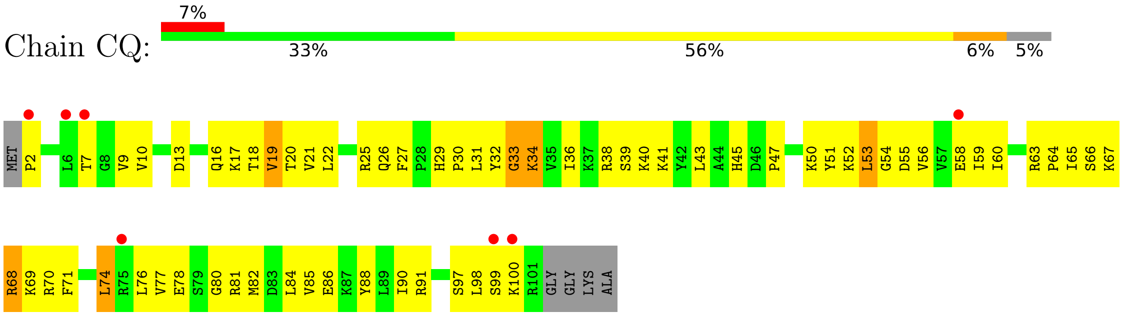
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



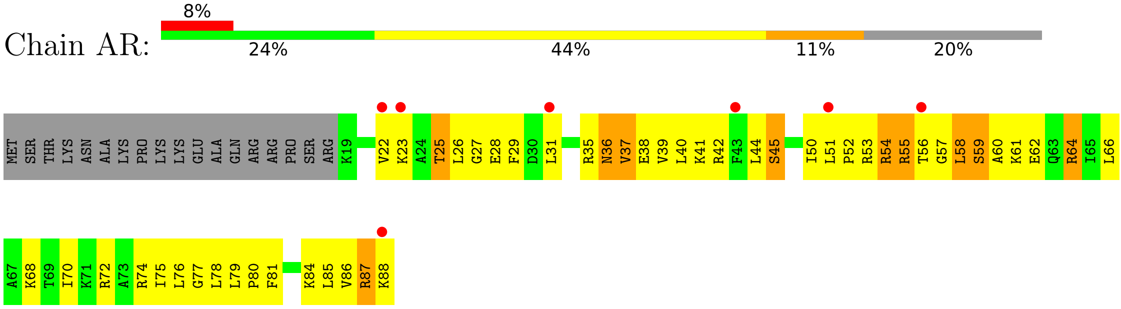
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



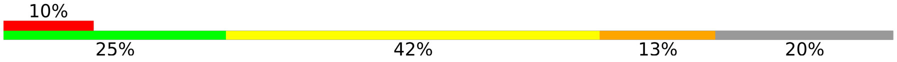
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

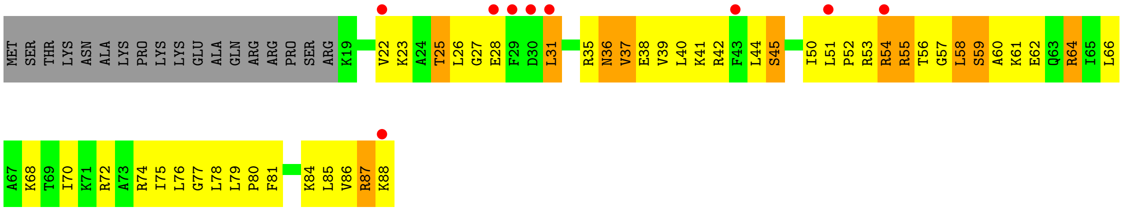
Chain AR:



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

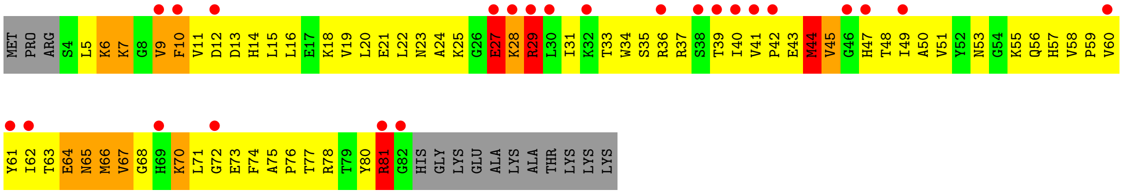
Chain CR:





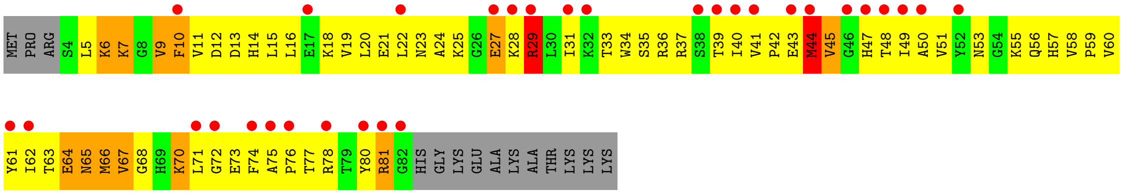
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



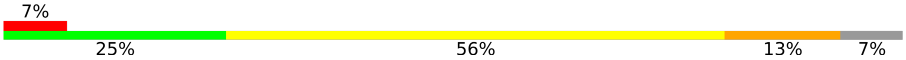
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

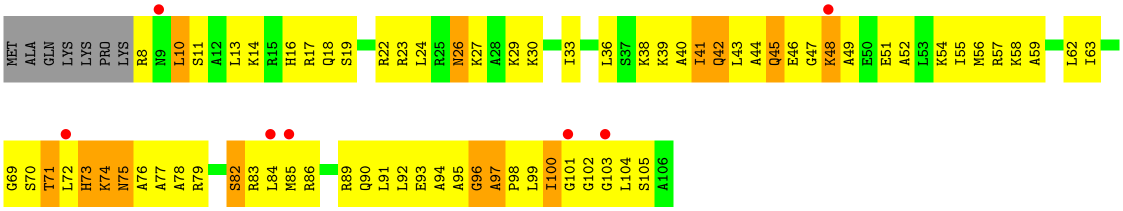
Chain CS:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

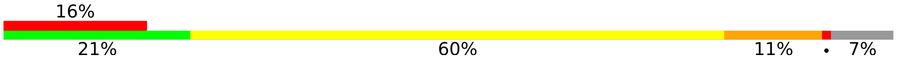
Chain AT:

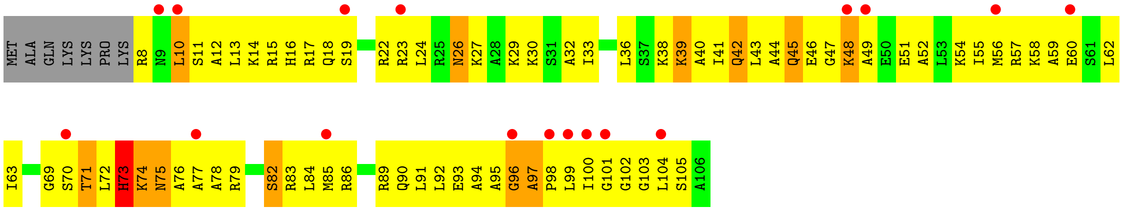




- Molecule 20: 30S RIBOSOMAL PROTEIN S20

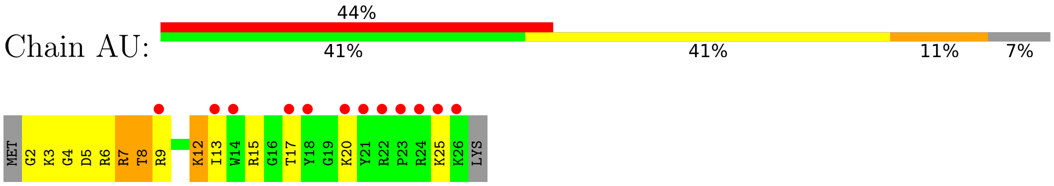
Chain CT:





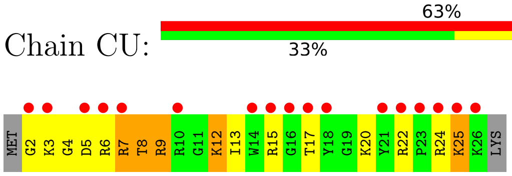
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



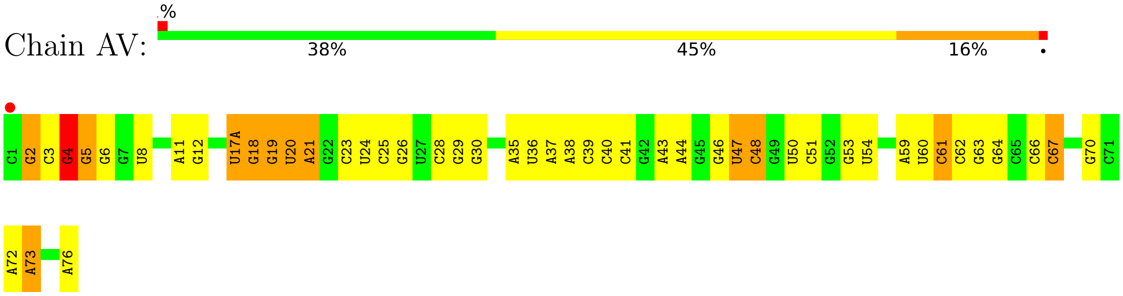
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



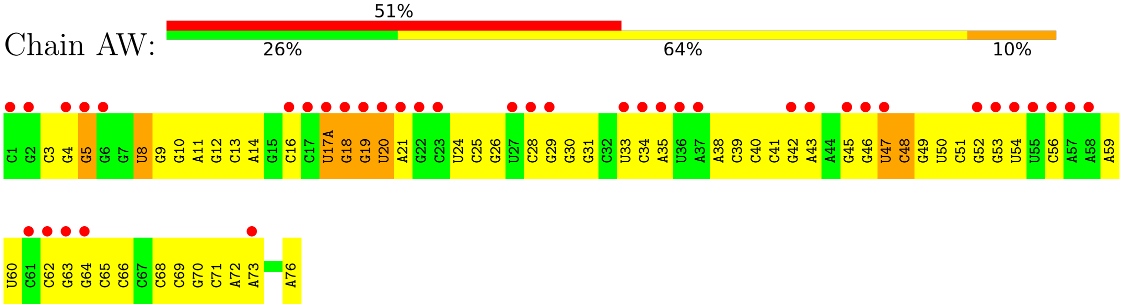
- Molecule 22: transfer RNA

Chain AV:



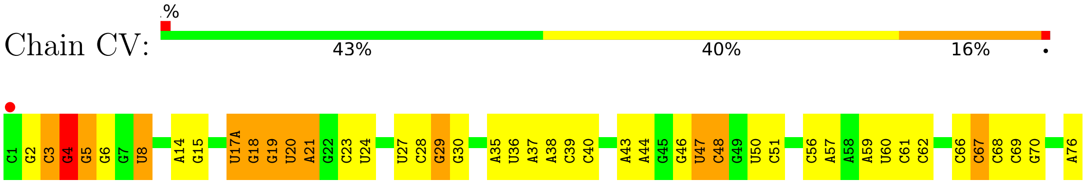
- Molecule 23: transfer RNA

Chain AW:



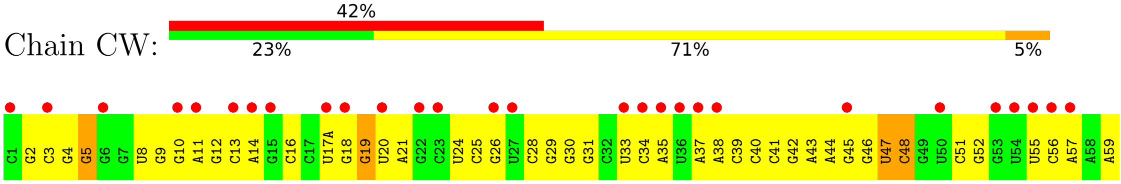
- Molecule 23: transfer RNA

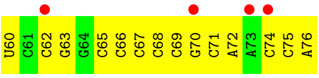
Chain CV:



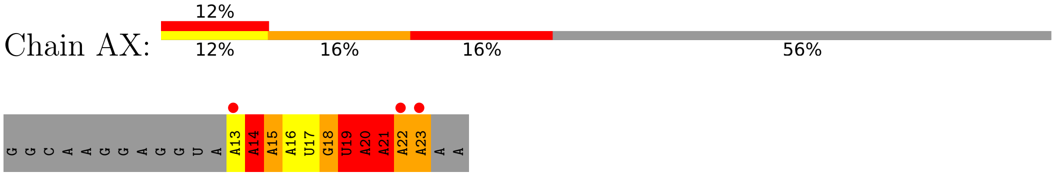
- Molecule 23: transfer RNA

Chain CW:

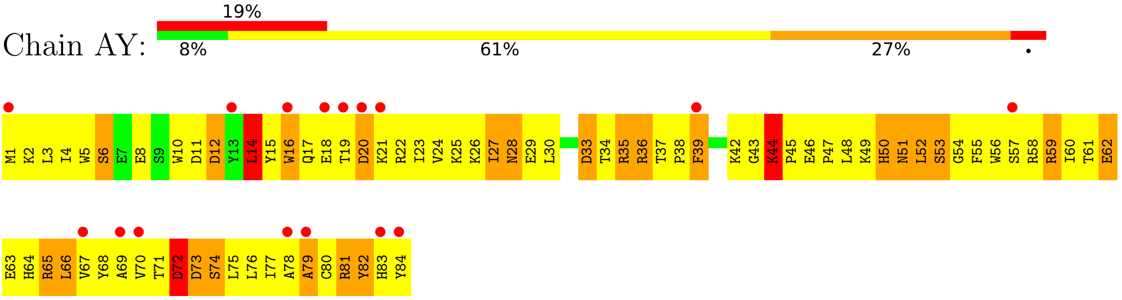




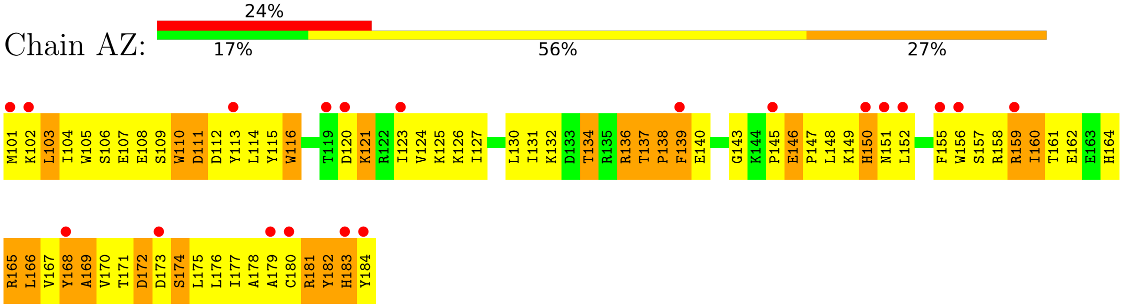
- Molecule 24: 5’-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*AP*AP*AP *AP*AP*UP*G U2M A2M A2MP*AP*AP*AP*A)-3’



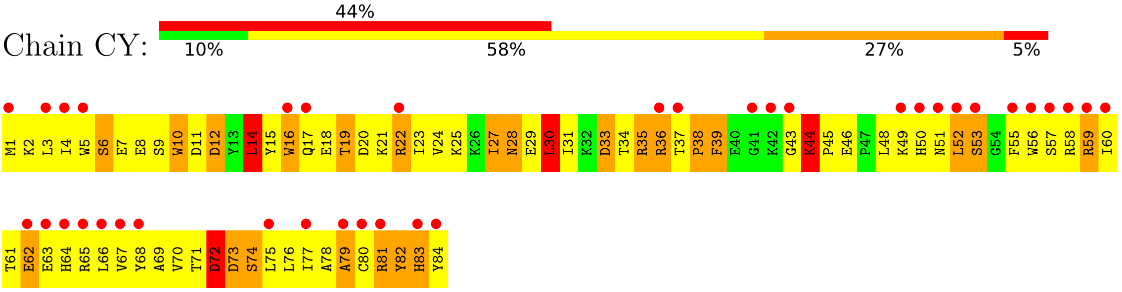
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM



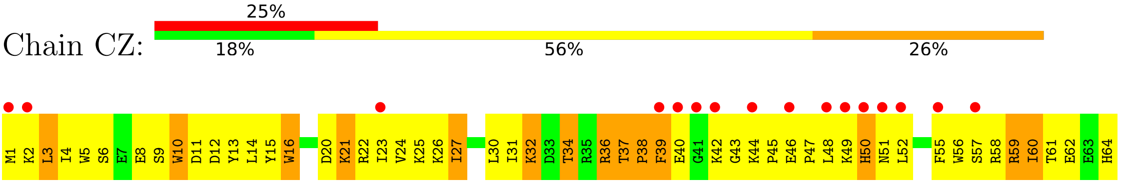
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

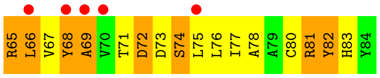


- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM



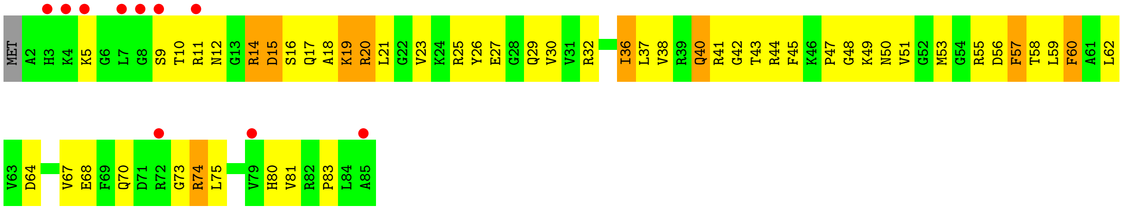
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM





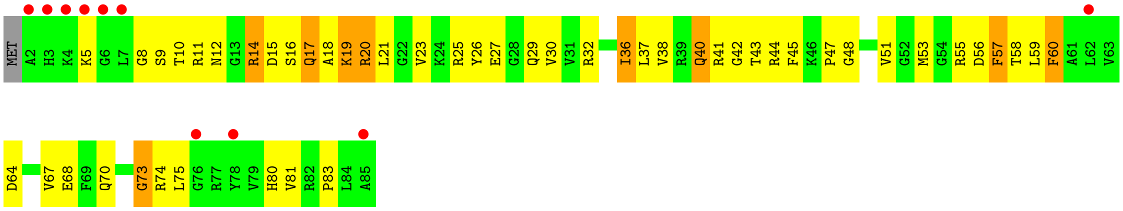
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



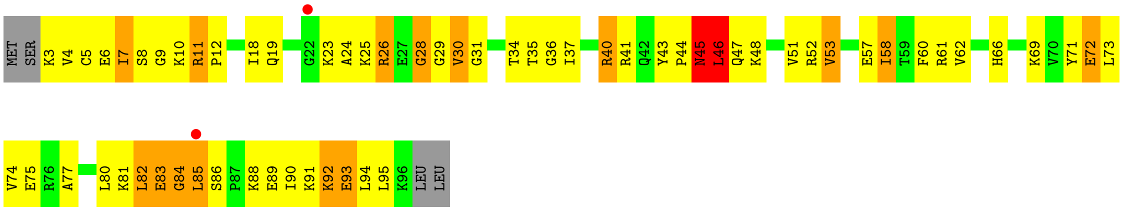
- Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:



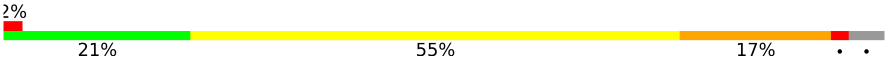
- Molecule 27: 50S RIBOSOMAL PROTEIN L28

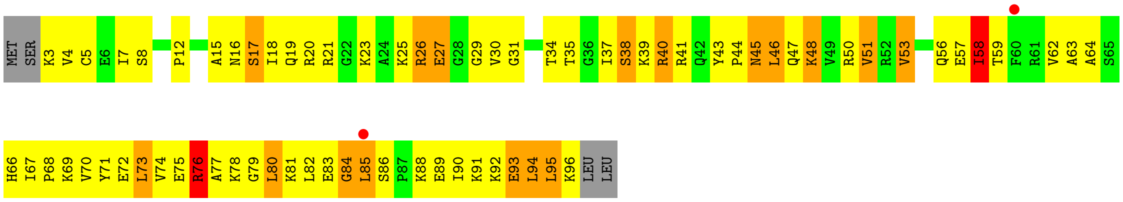
Chain B1:



- Molecule 27: 50S RIBOSOMAL PROTEIN L28

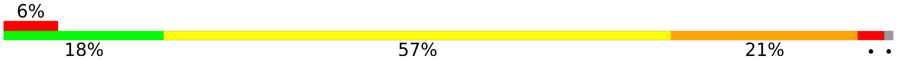
Chain D1:





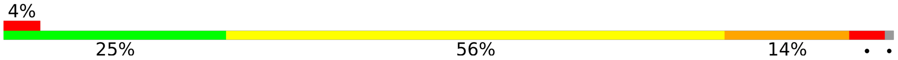
- Molecule 28: 50S RIBOSOMAL PROTEIN L29

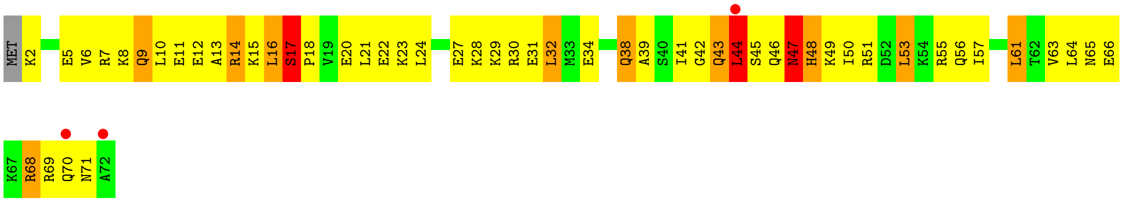
Chain B2:



- Molecule 28: 50S RIBOSOMAL PROTEIN L29

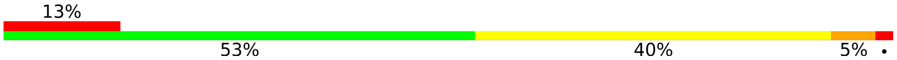
Chain D2:

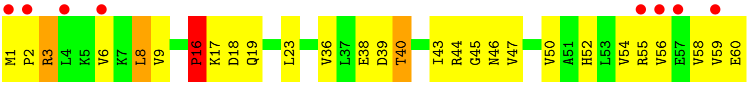




- Molecule 29: 50S RIBOSOMAL PROTEIN L30

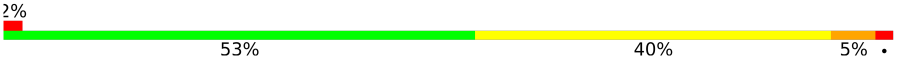
Chain B3:

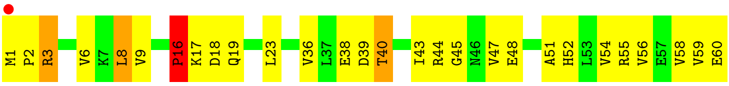




- Molecule 29: 50S RIBOSOMAL PROTEIN L30

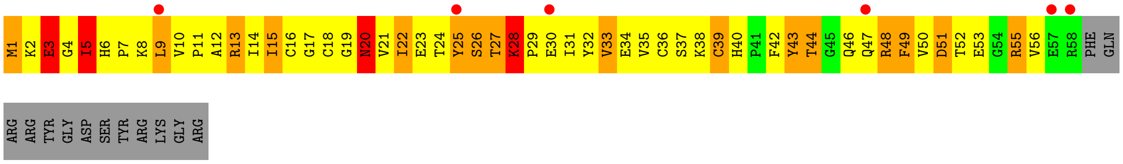
Chain D3:





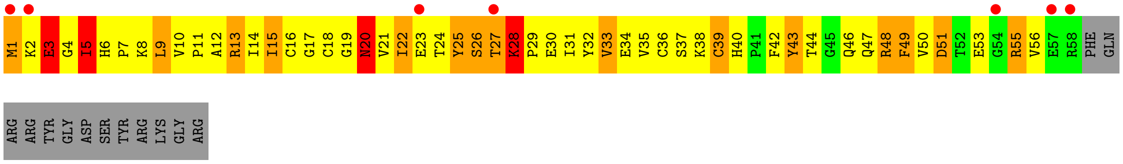
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:

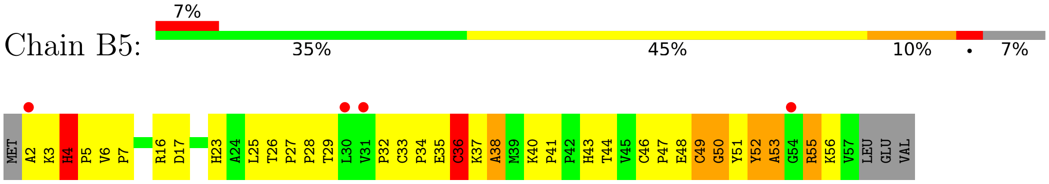


- Molecule 30: 50S RIBOSOMAL PROTEIN L31

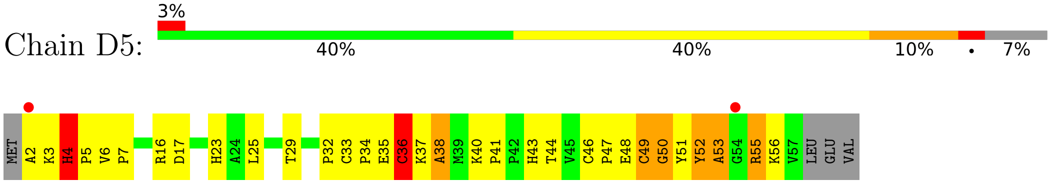
Chain D4:



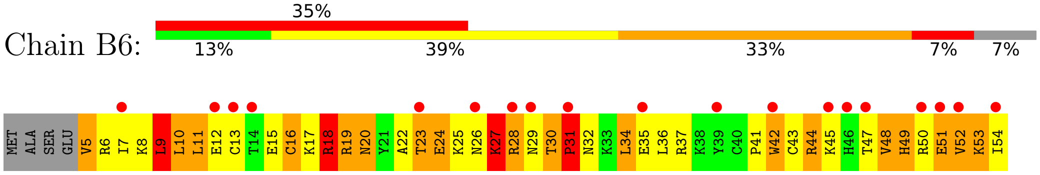
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



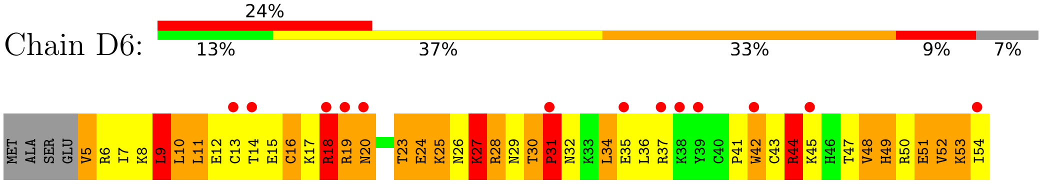
- Molecule 31: 50S RIBOSOMAL PROTEIN L32



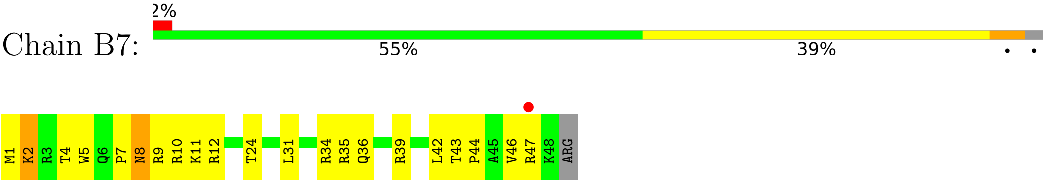
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



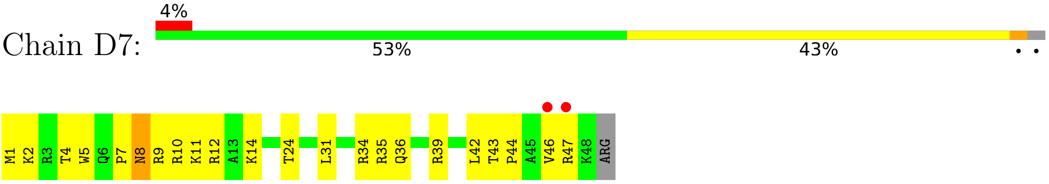
- Molecule 32: 50S RIBOSOMAL PROTEIN L33



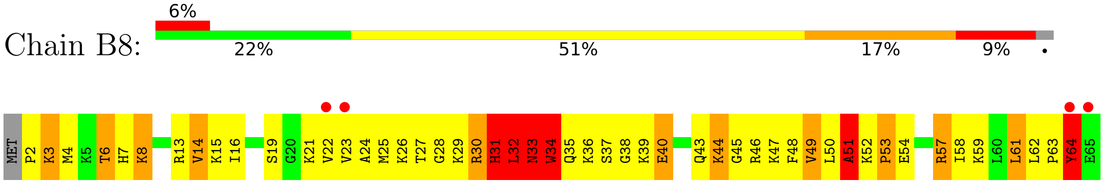
- Molecule 33: 50S RIBOSOMAL PROTEIN L34



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

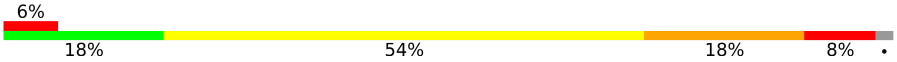


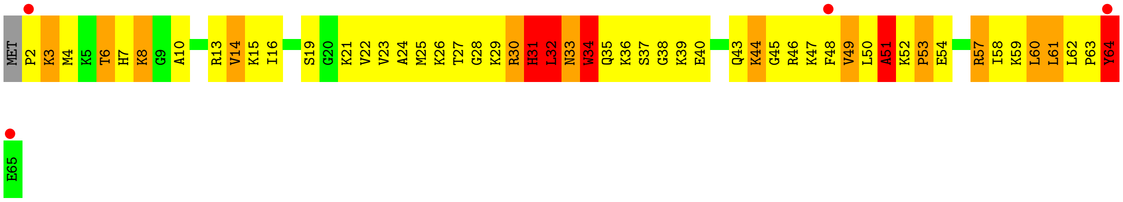
- Molecule 34: 50S RIBOSOMAL PROTEIN L35



- Molecule 34: 50S RIBOSOMAL PROTEIN L35

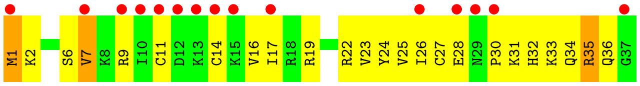
Chain D8:





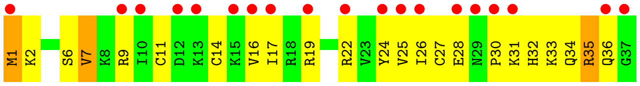
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



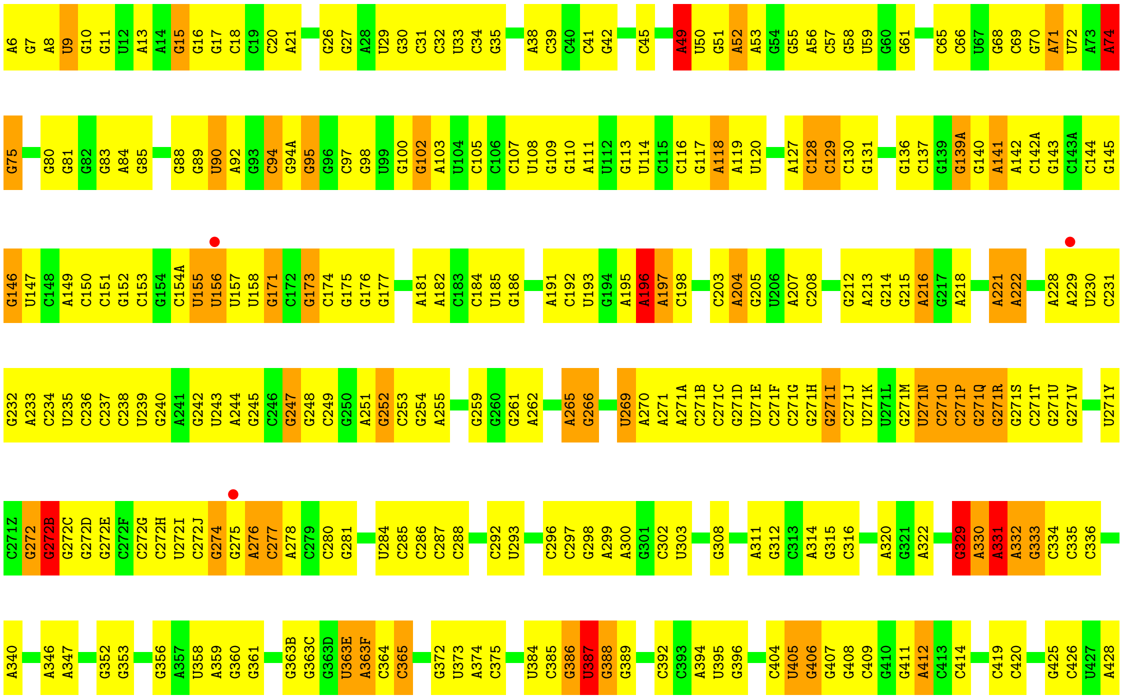
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

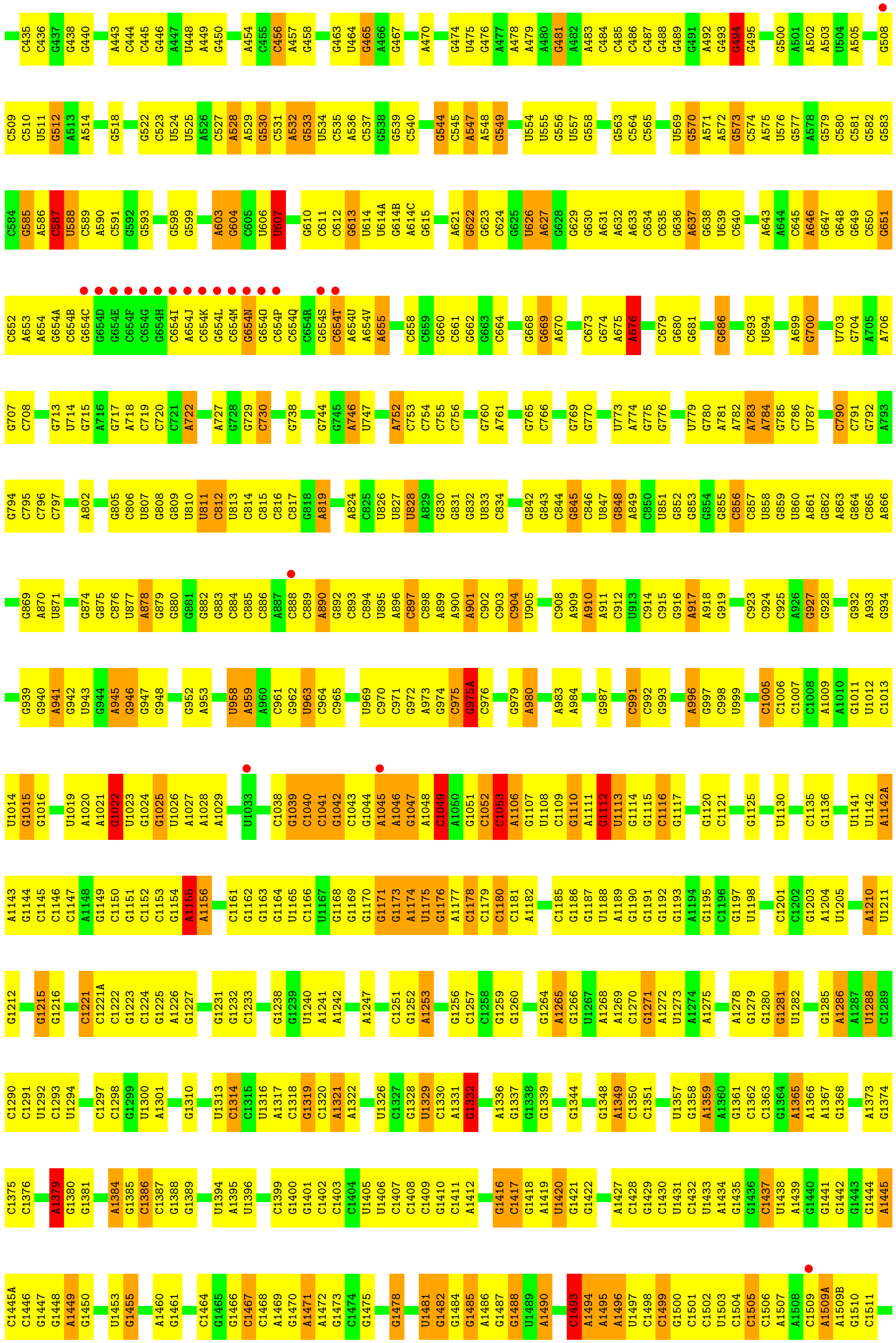
Chain D9:



- Molecule 36: 23S ribosomal RNA

Chain BA:

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C509 C510 U511 G512 A513 A514 G518 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 G544 C545 A547 A548 G549 U554 U555 G556 U557 G558 G563 C564 C565 U569 G570 A571 A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583
C584 G585 A586 C587 U588 C589 A590 C591 G592 G593 G598 G599 A603 G604 G605 U606 U607 G610 C611 C612 G613 U614 U614A G614B A614C G615 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 A643 A644 C645 A646 G647 G648 G649 C650 G651
C652 A653 A654 G654A C654B G654C G654D G654E C654F C654G G654H C654I A654J G654K G654L C654M G654N G654O C654P C654Q C654R G654S C654T A654U A654V A655 C658 C659 G660 C661 G662 G663 C664 G668 G669 A670 C673 G674 A675 A676 C679 G680 G681 G686 C693 U694 A699 G700 U703 G704 A705 A706
G707 C708 G713 U714 G715 A716 G717 A718 C719 C720 C721 A722 A727 G728 G729 C730 G738 G744 G745 A746 U747 A752 C753 C754 C755 C756 G760 A761 G765 C766 G769 G770 U773 A774 G775 G776 U779 G780 A781 A782 A783 A784 G785 C786 U787 C790 C791 G792 A793
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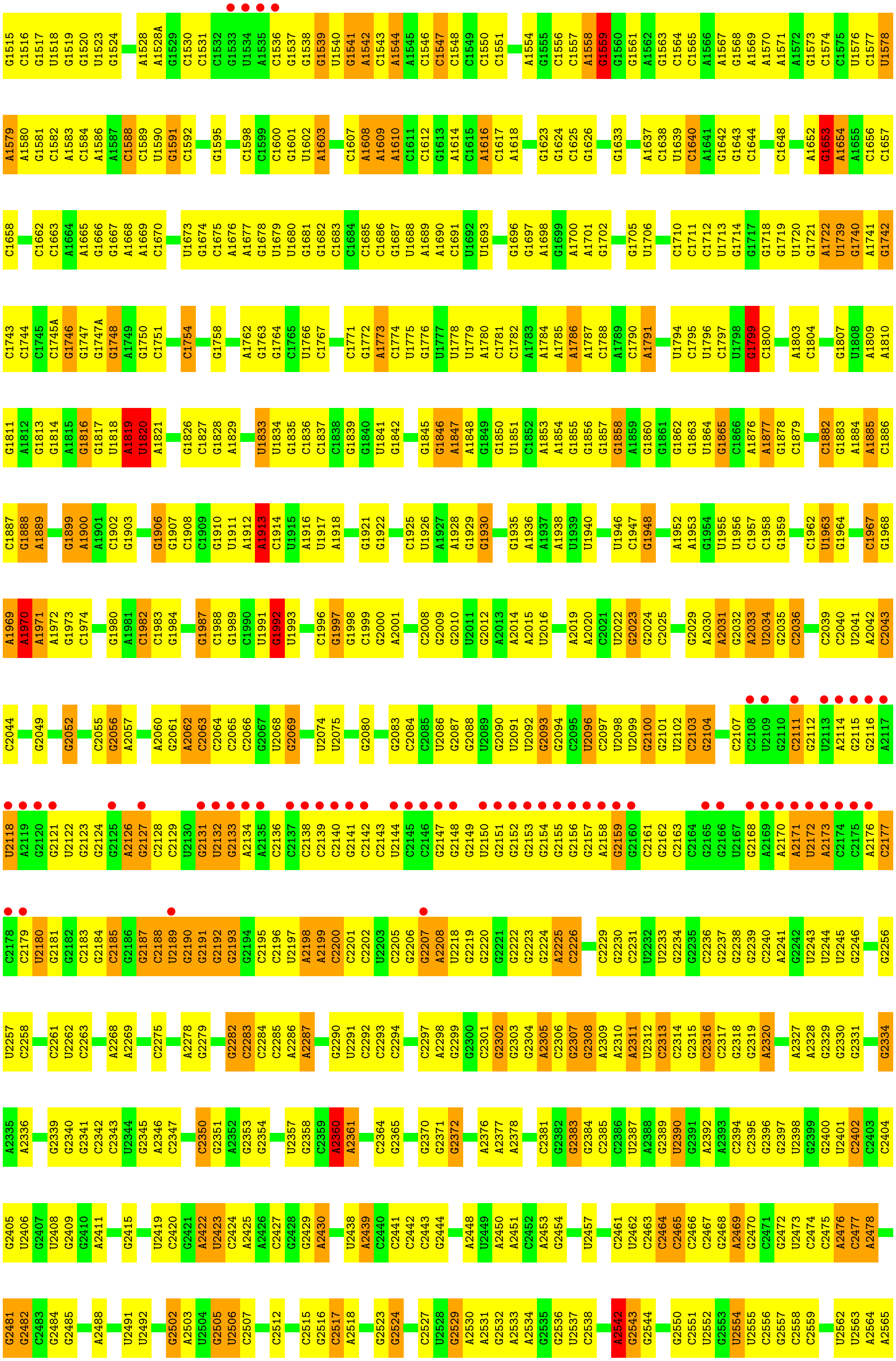
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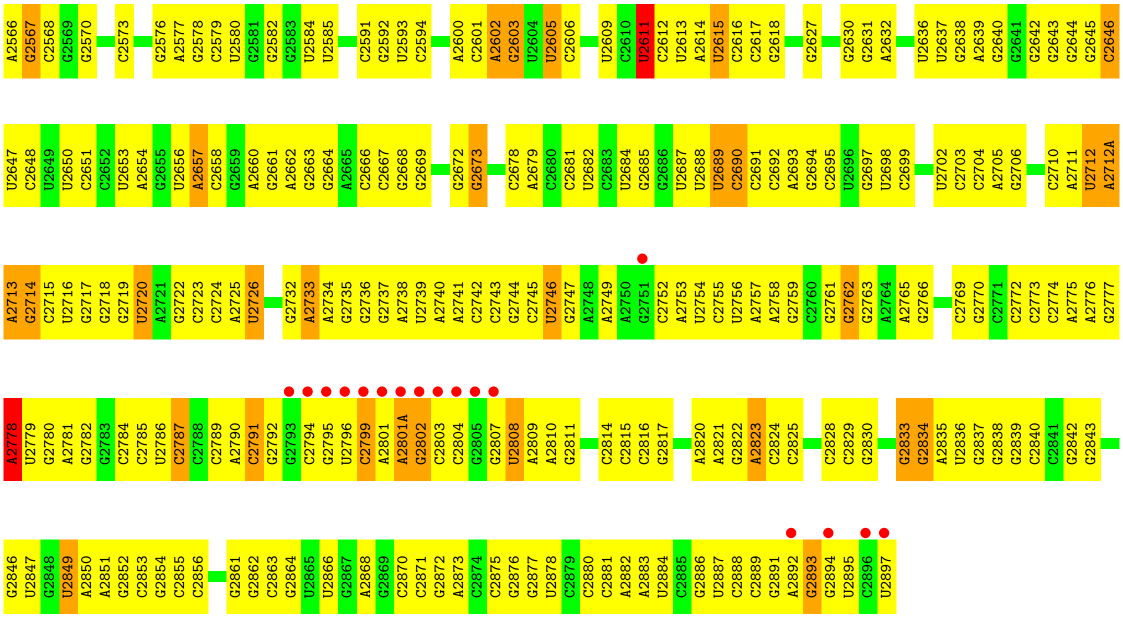
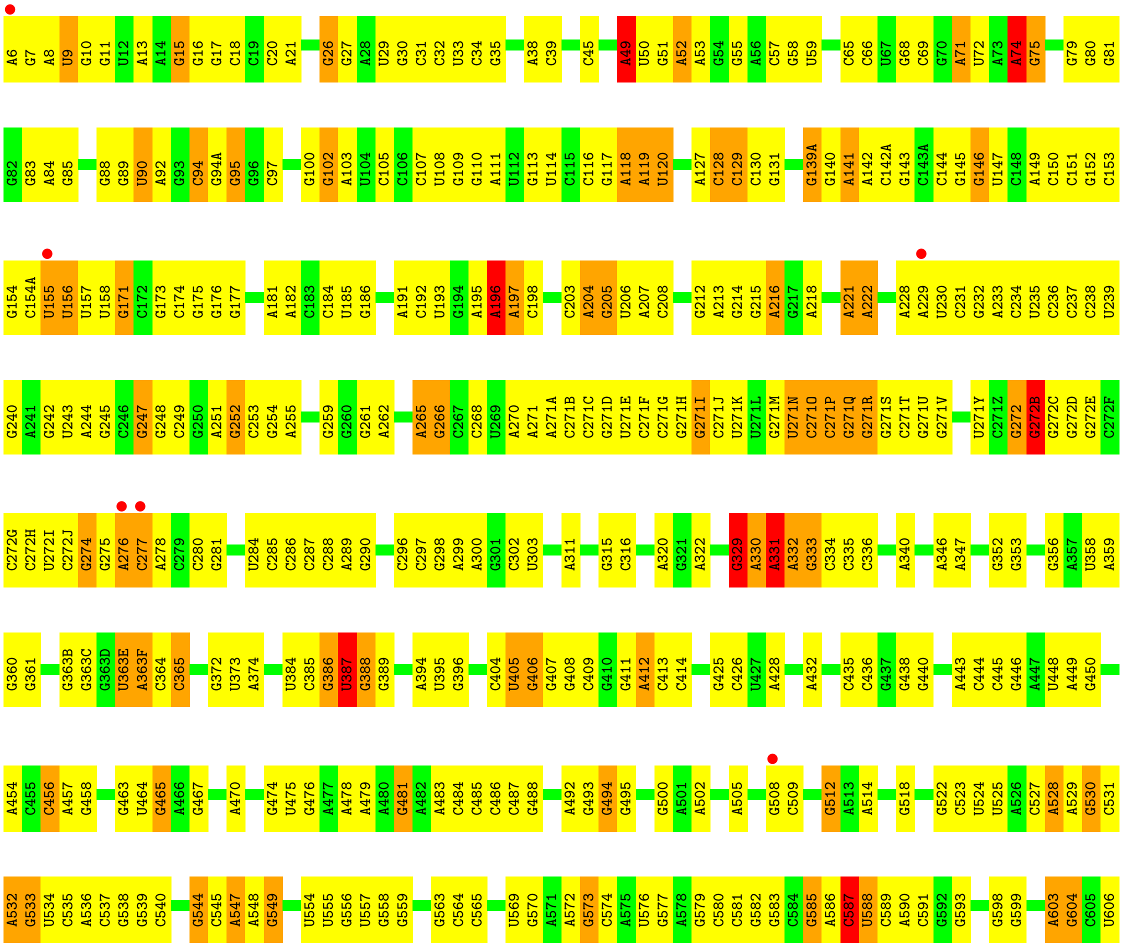
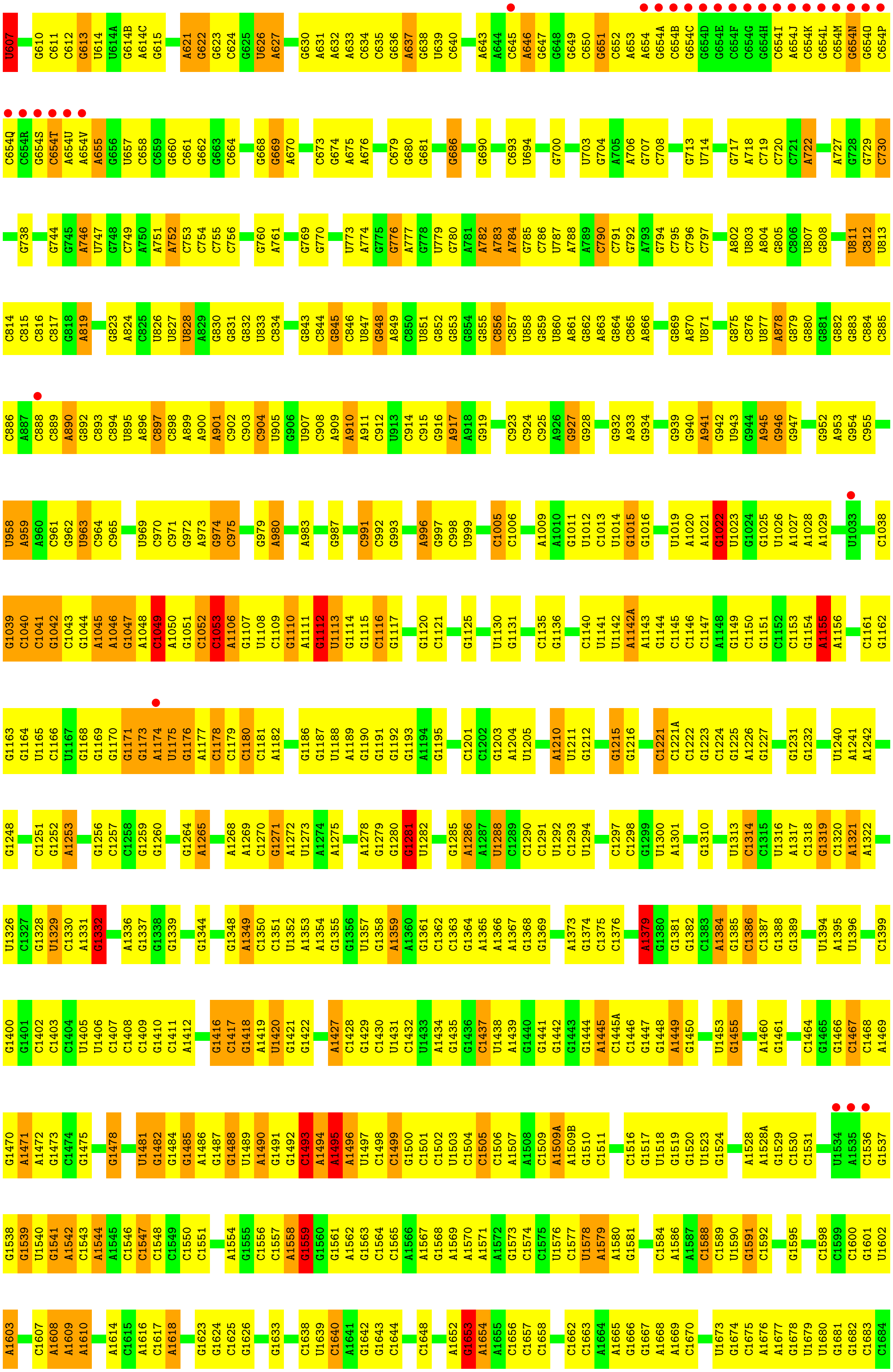


- Molecule 36: 23S ribosomal RNA

Chain DA:

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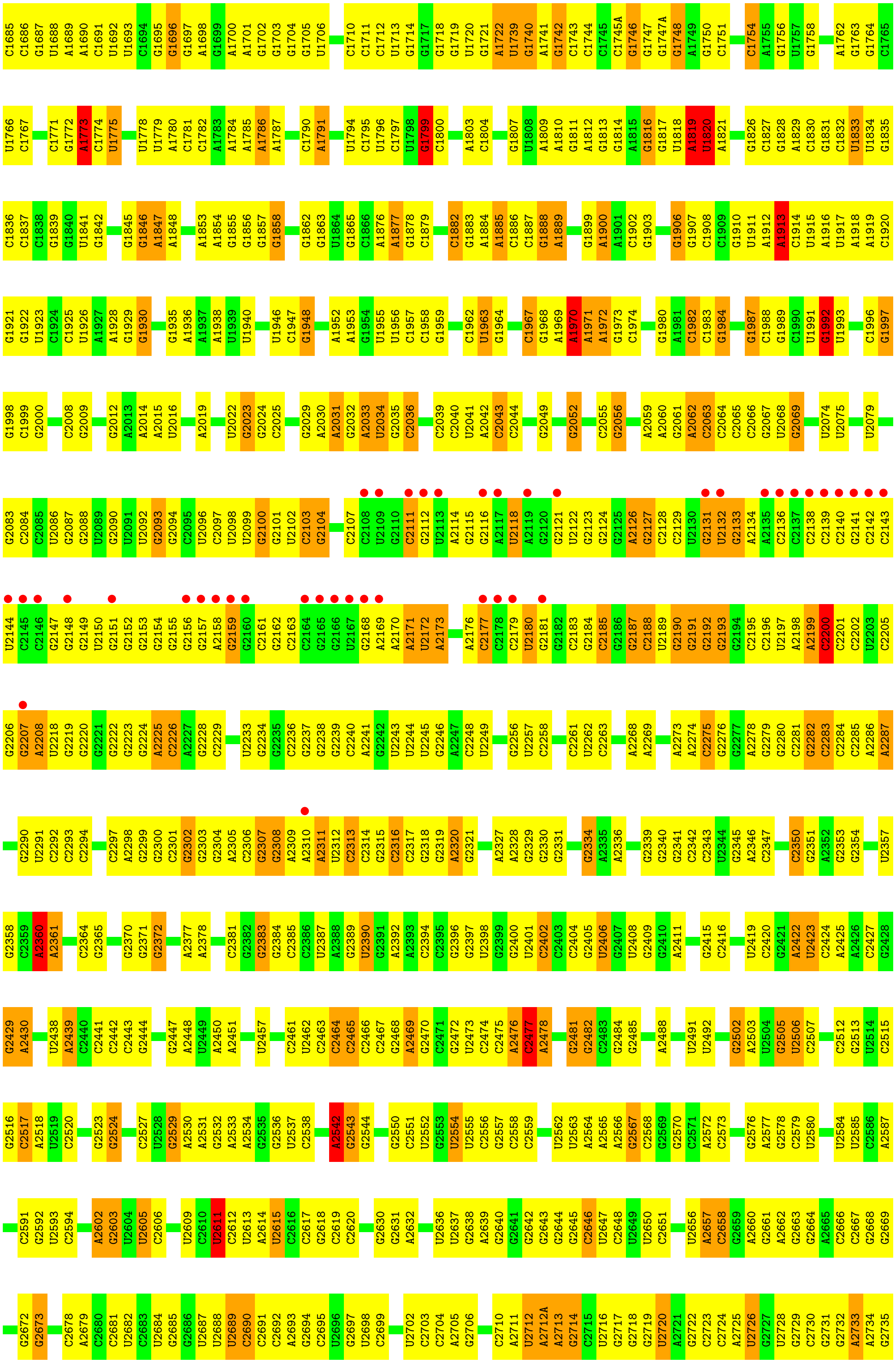
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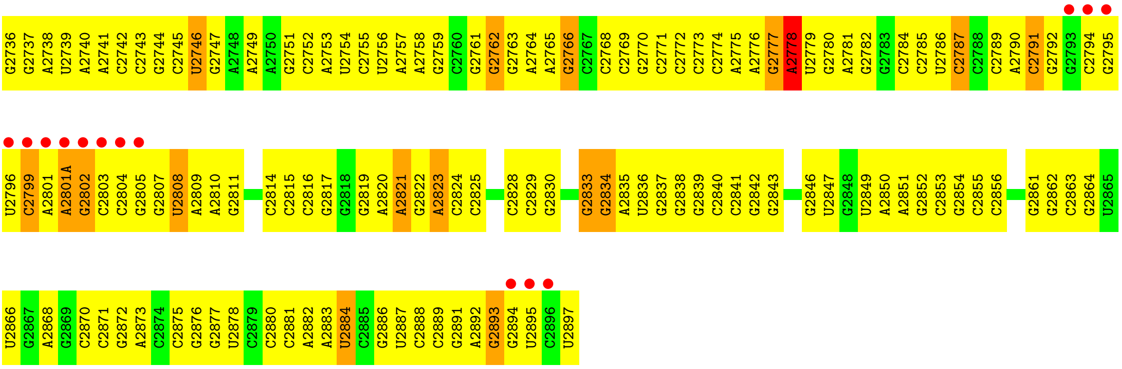

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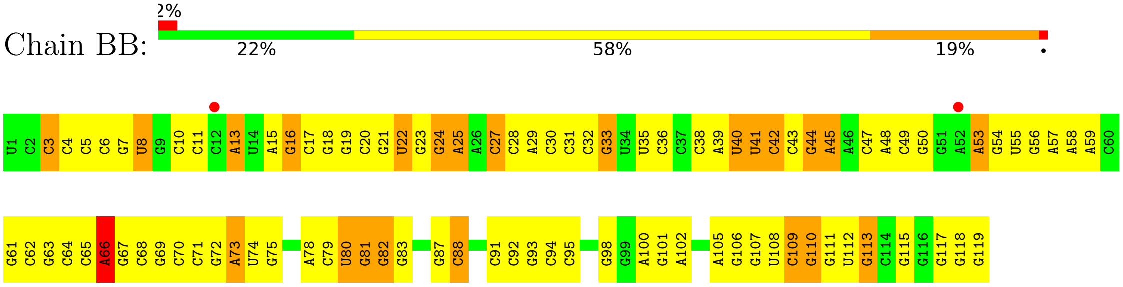
- Molecule 37: 5S ribosomal RNA



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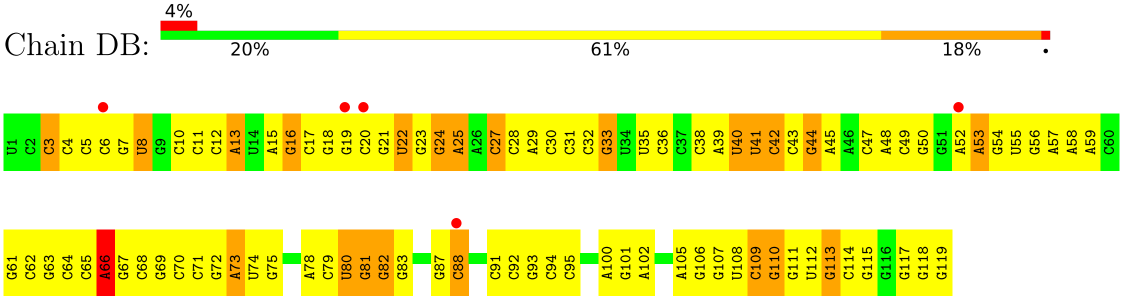
- Molecule 37: 5S ribosomal RNA



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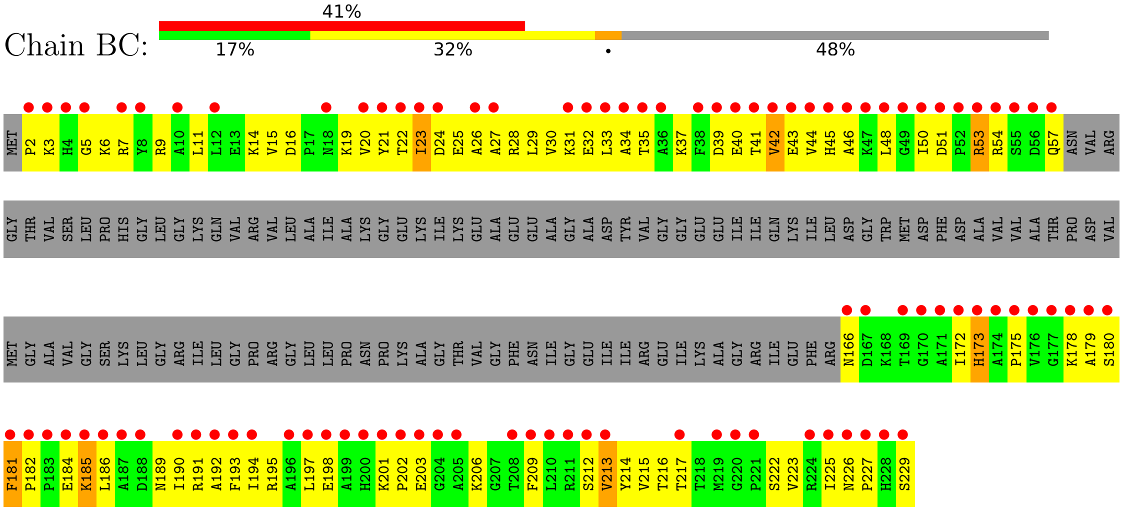
- Molecule 38: 50S RIBOSOMAL PROTEIN L1



Chain BC:

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- Molecule 38: 50S RIBOSOMAL PROTEIN L1

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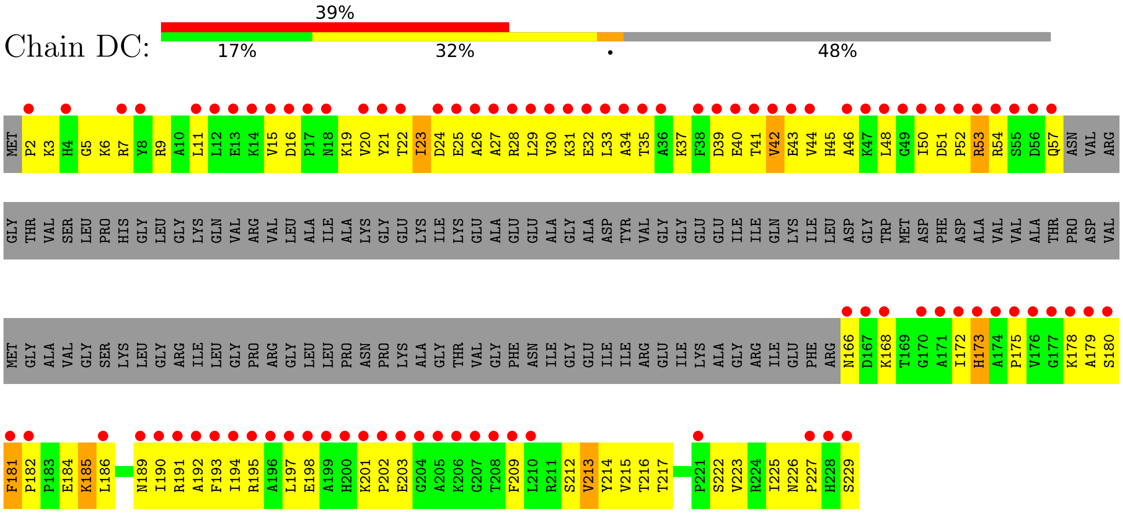
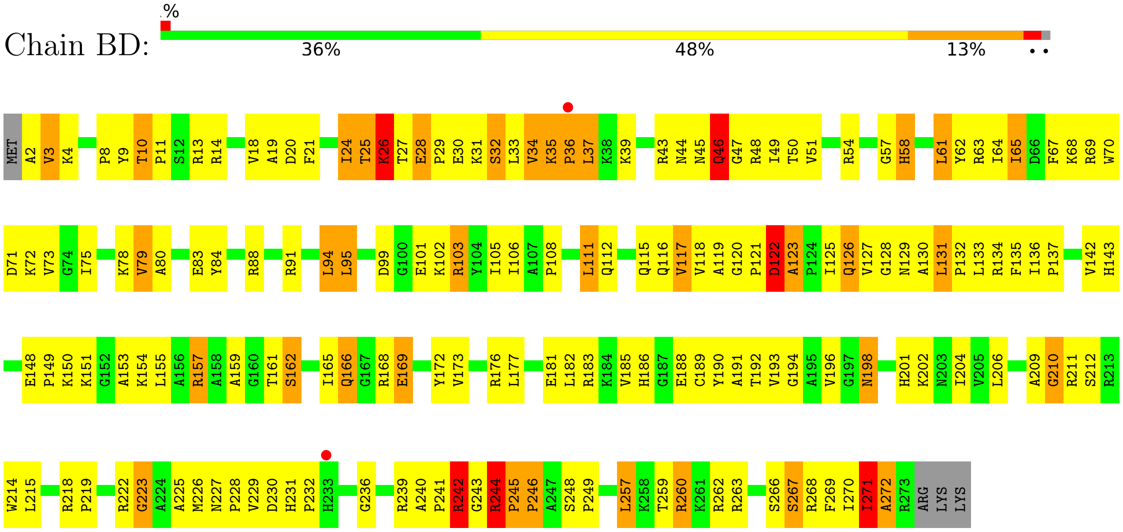


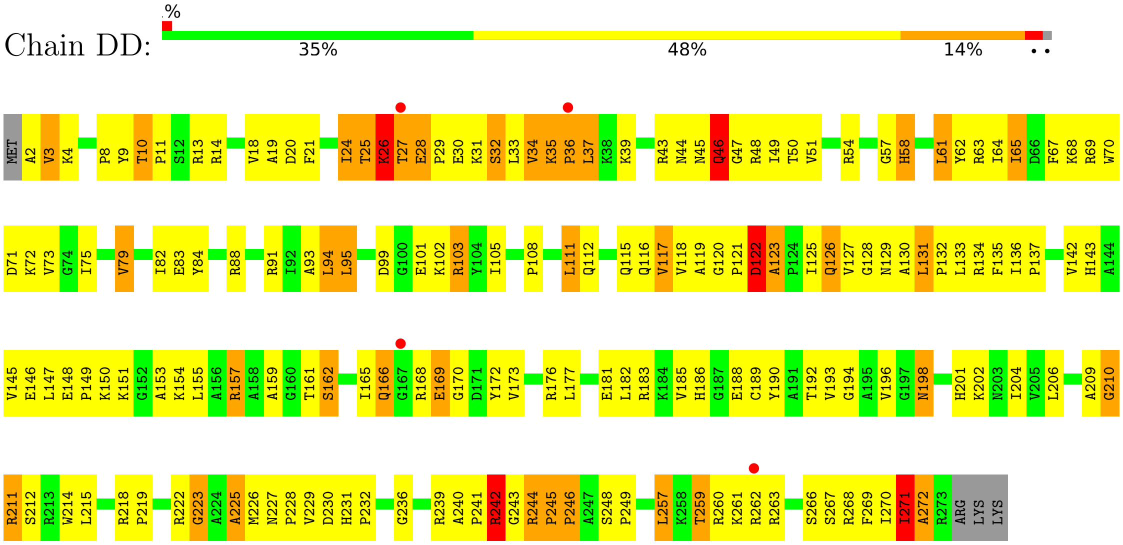
- Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain BD:



- Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD:



- Molecule 40: 50S RIBOSOMAL PROTEIN L3

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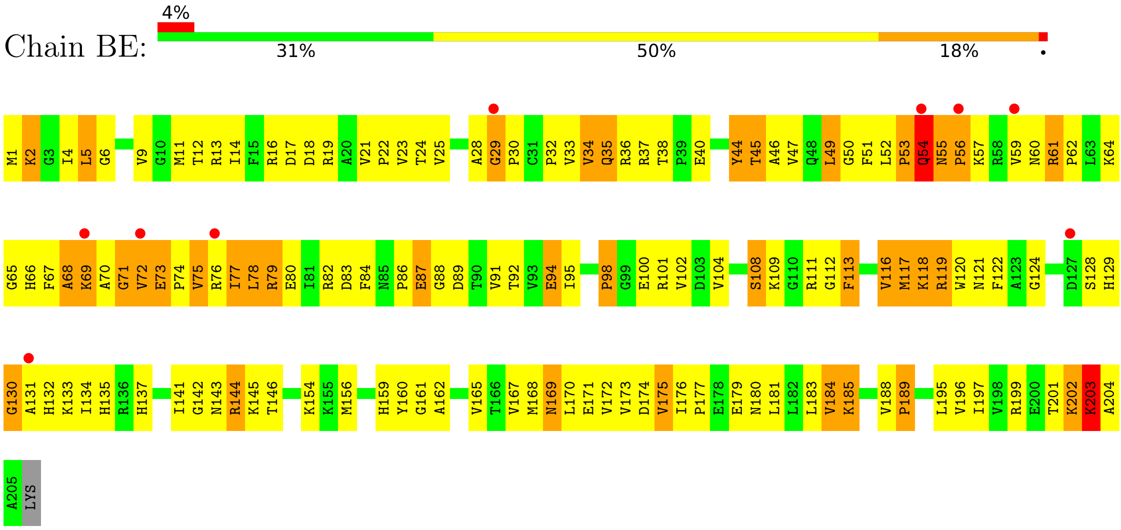
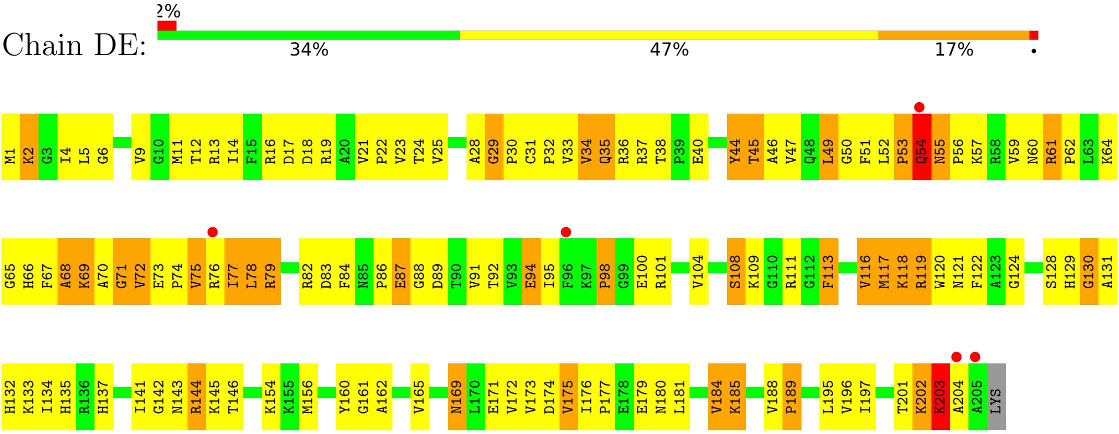


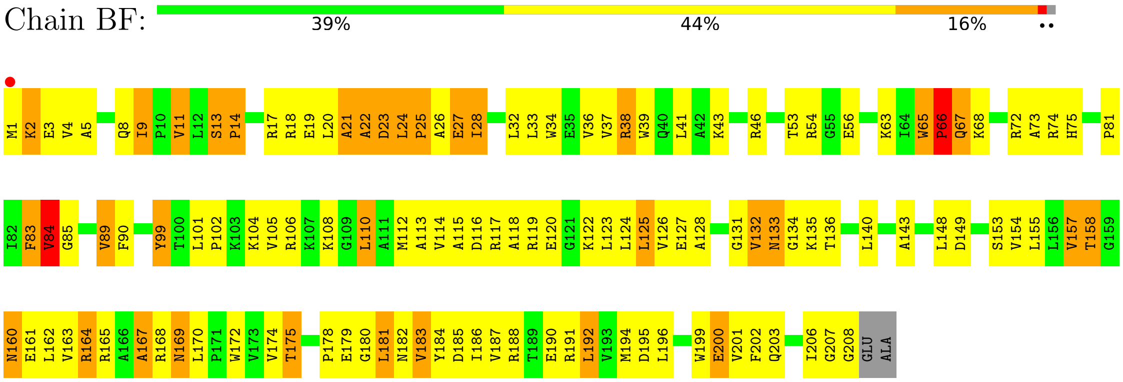
- Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE:



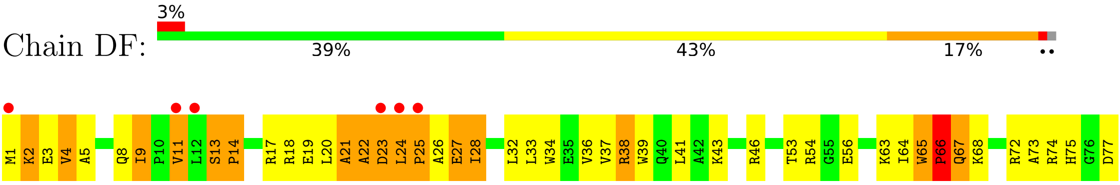
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

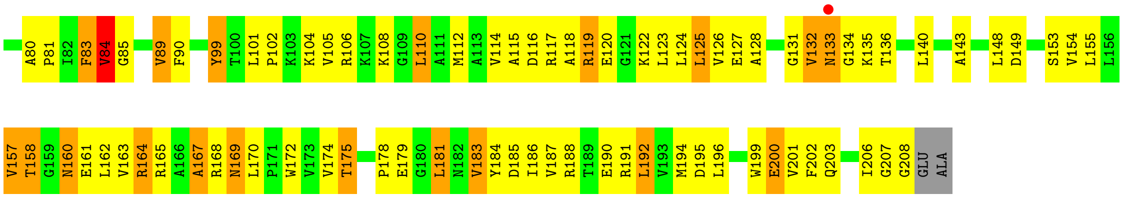
Chain BF:



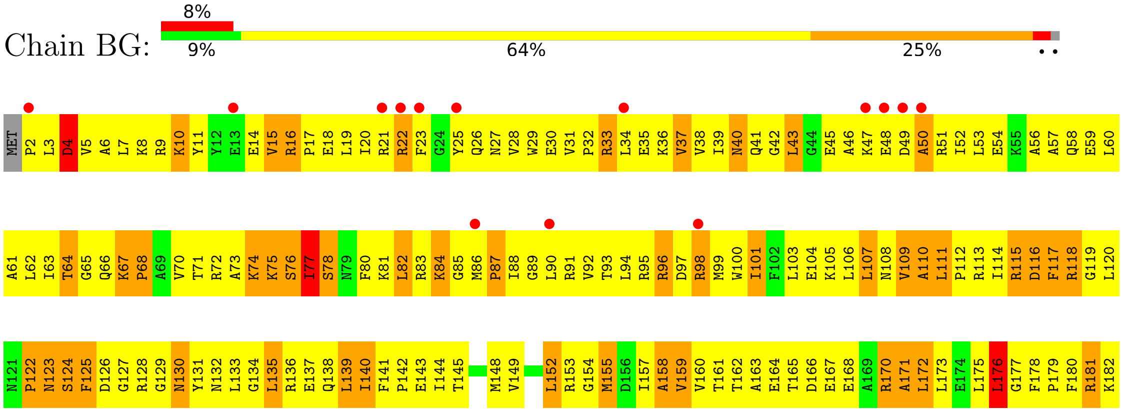
- Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:

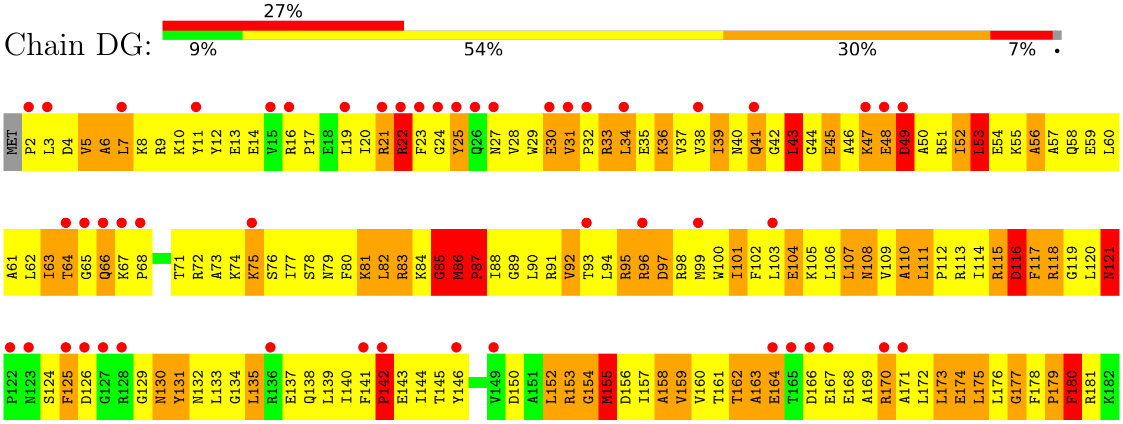




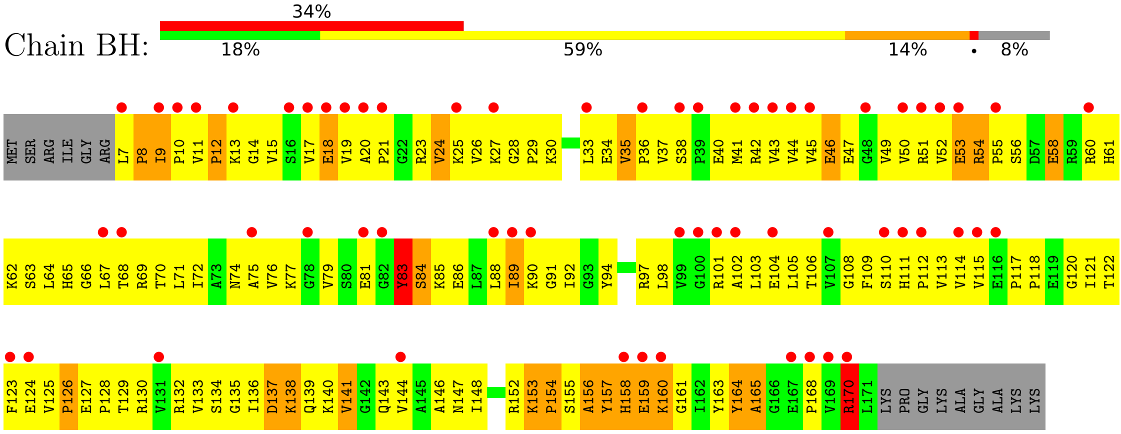
- Molecule 42: 50S RIBOSOMAL PROTEIN L5



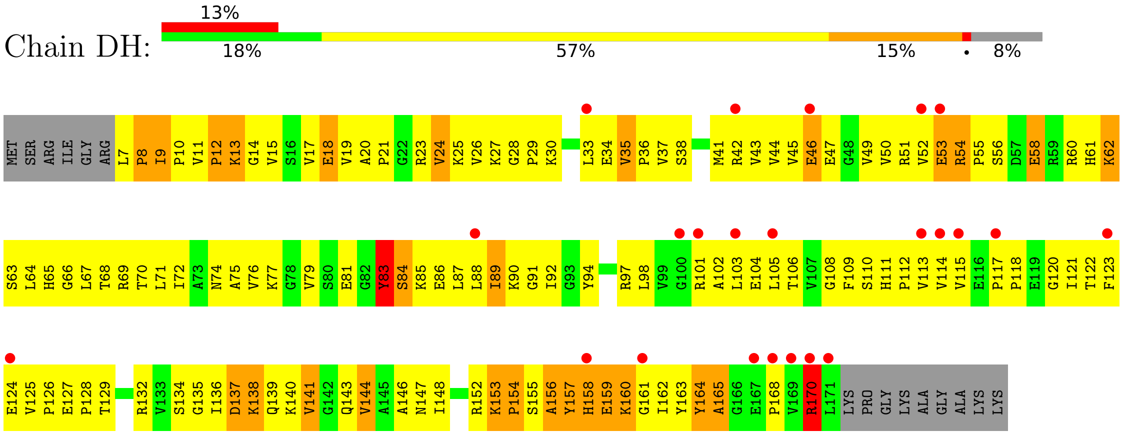
- Molecule 42: 50S RIBOSOMAL PROTEIN L5



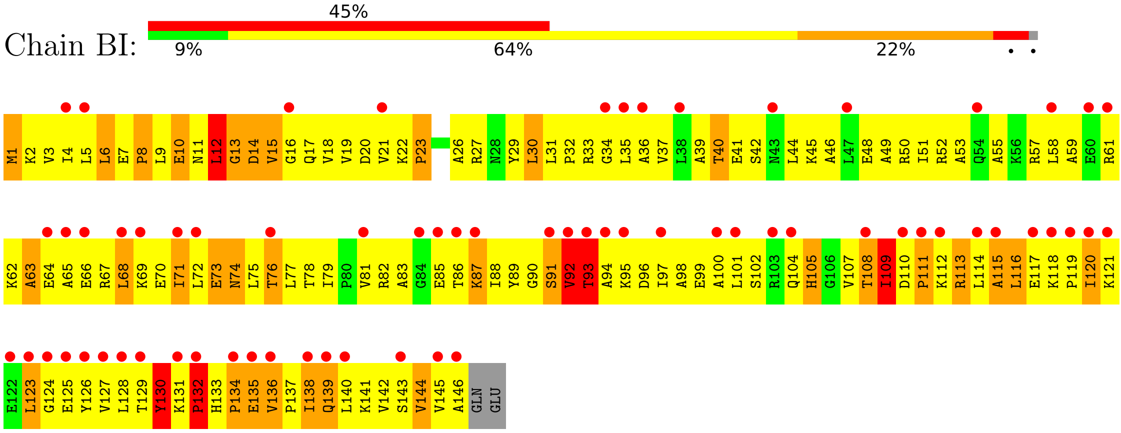
- Molecule 43: 50S RIBOSOMAL PROTEIN L6



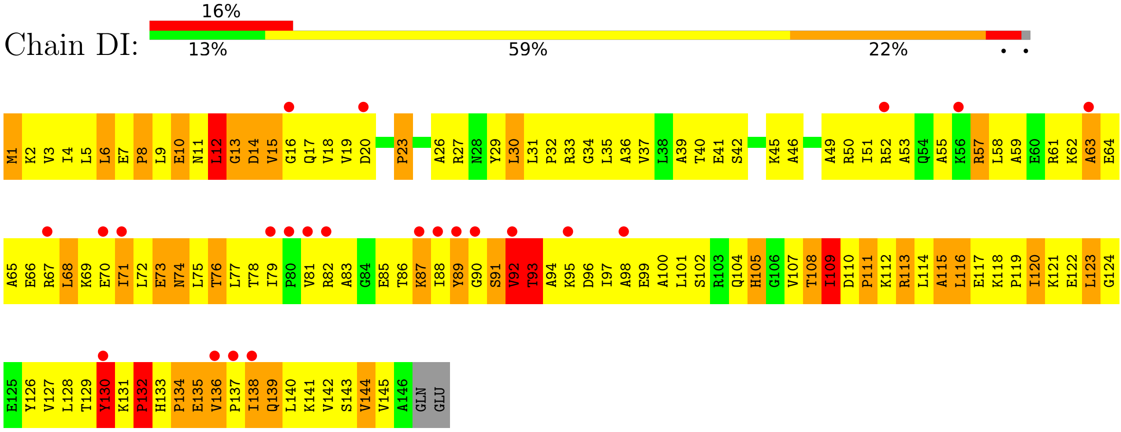
- Molecule 43: 50S RIBOSOMAL PROTEIN L6



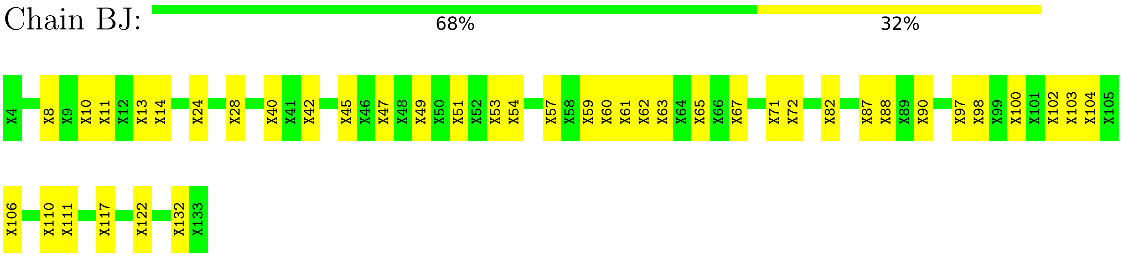
- Molecule 44: 50S RIBOSOMAL PROTEIN L9



- Molecule 44: 50S RIBOSOMAL PROTEIN L9

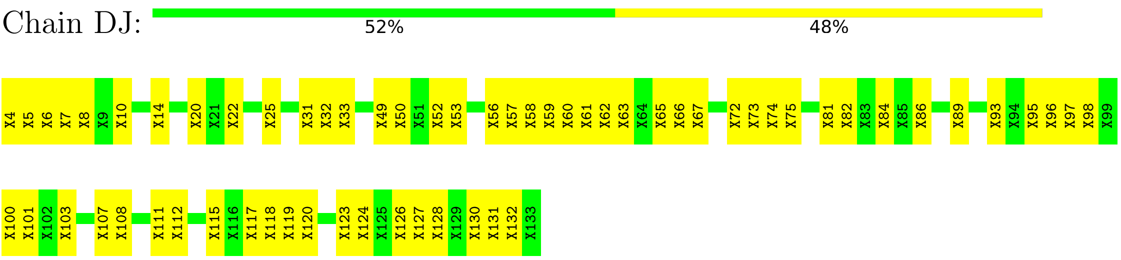


- Molecule 45: 50S RIBOSOMAL PROTEIN L10



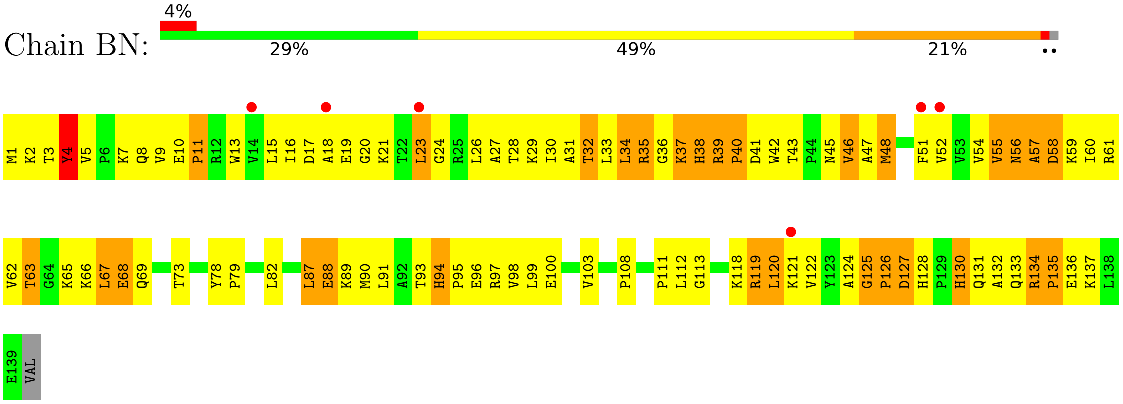
- Molecule 45: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



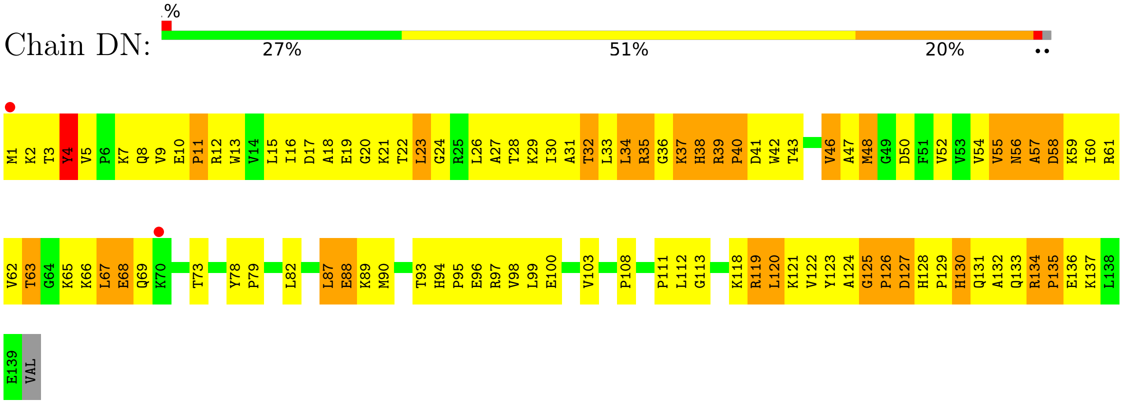
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



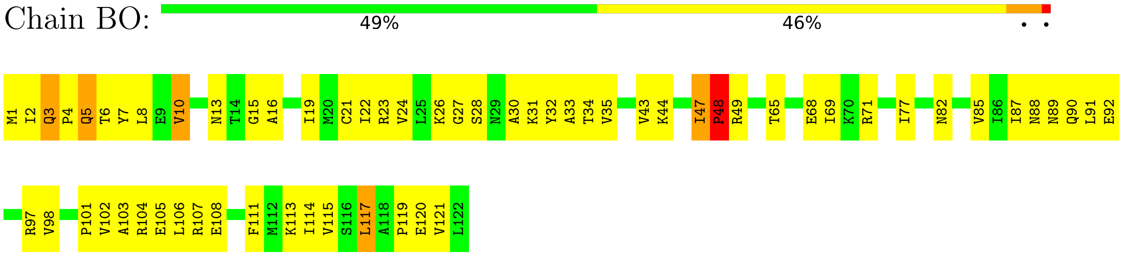
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



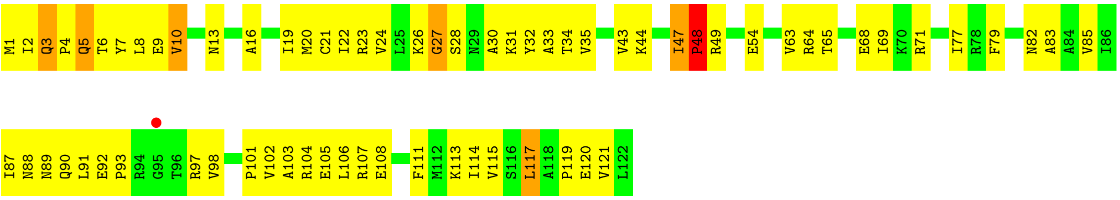
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



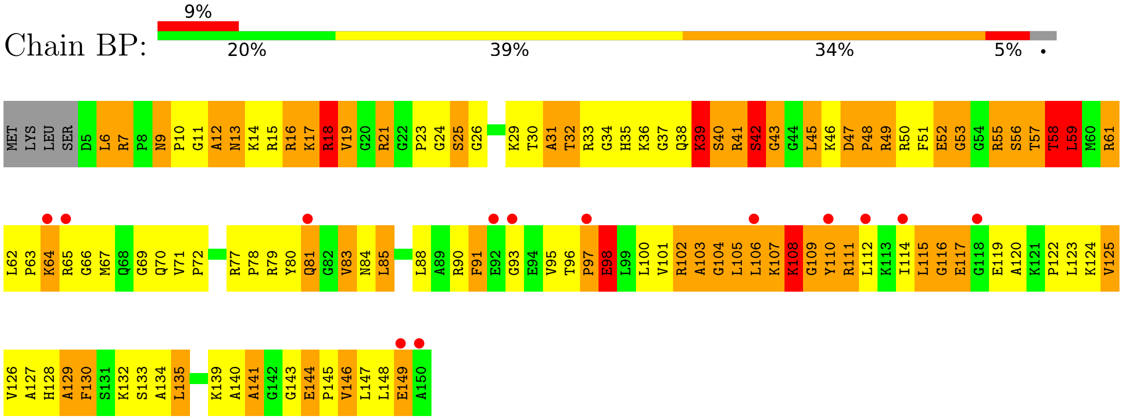
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO:



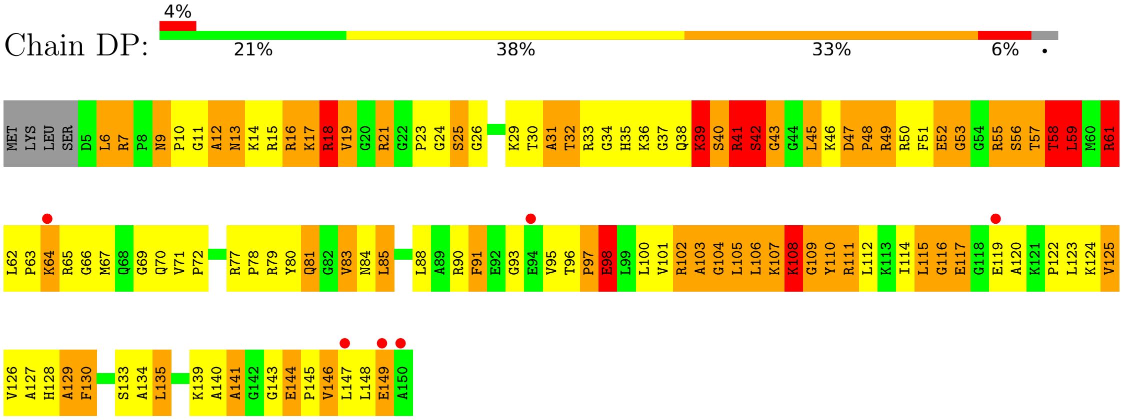
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:



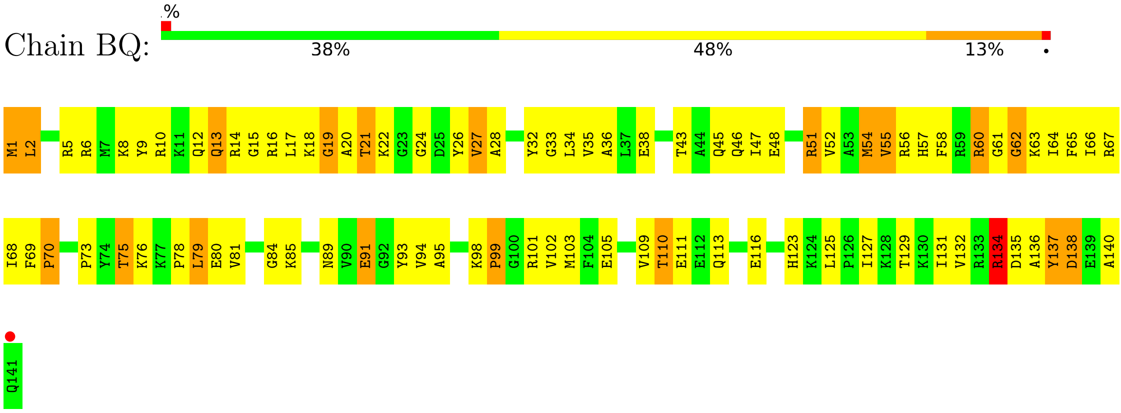
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



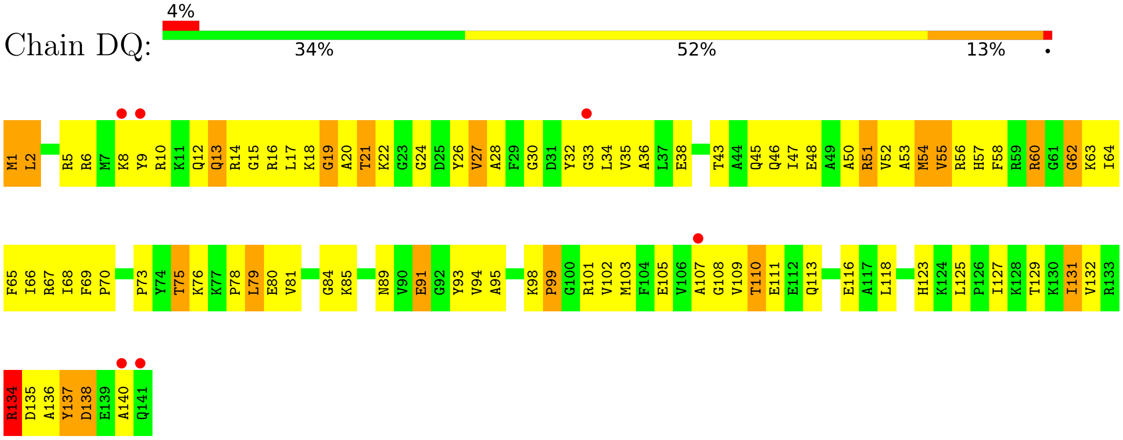
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



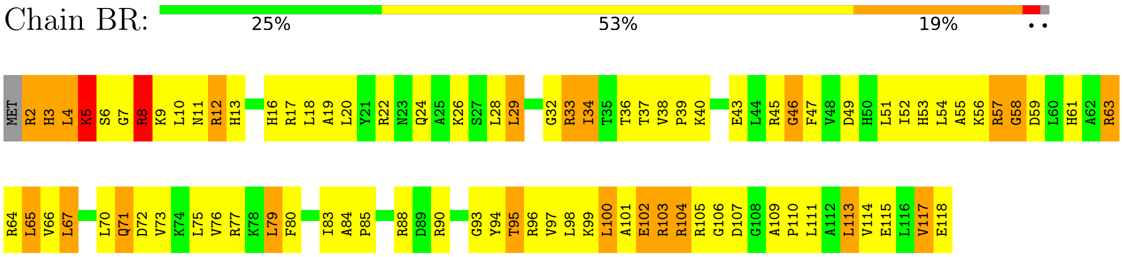
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



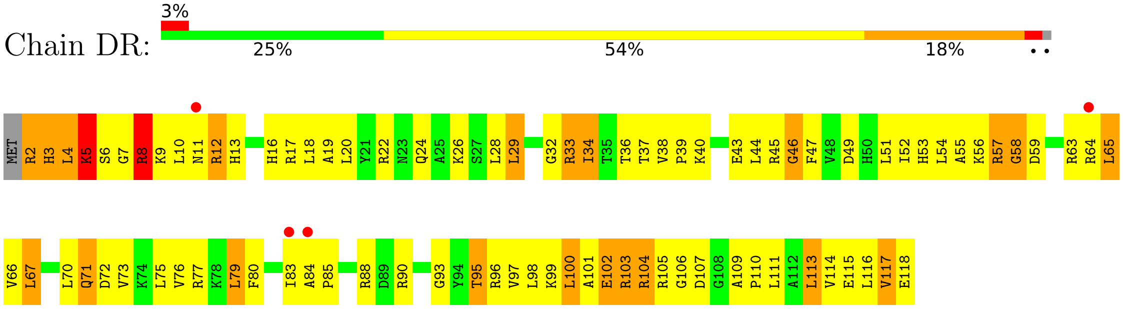
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



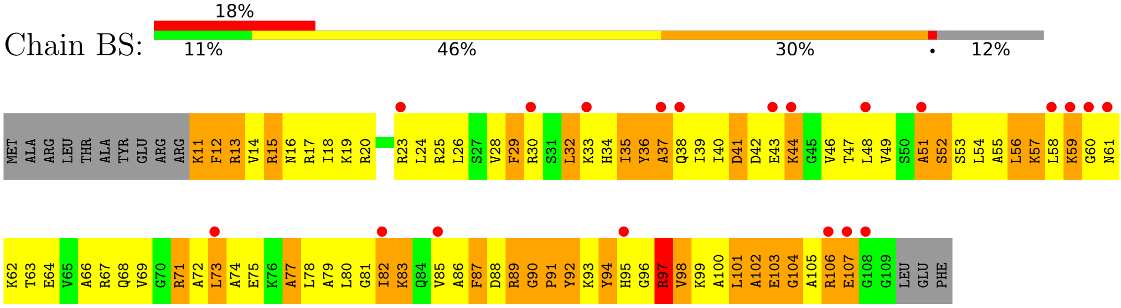
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



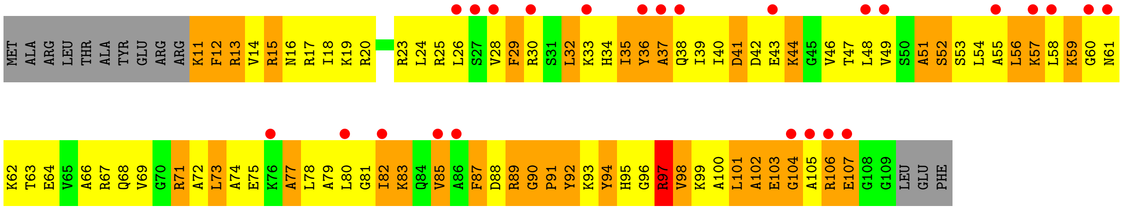
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



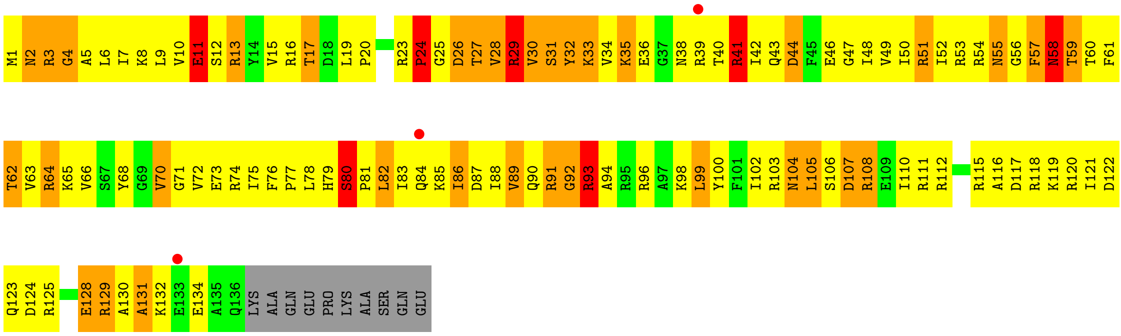
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



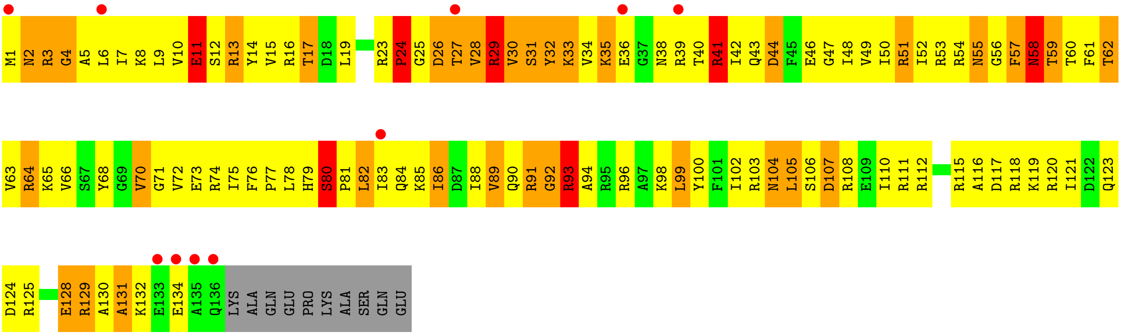
- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:



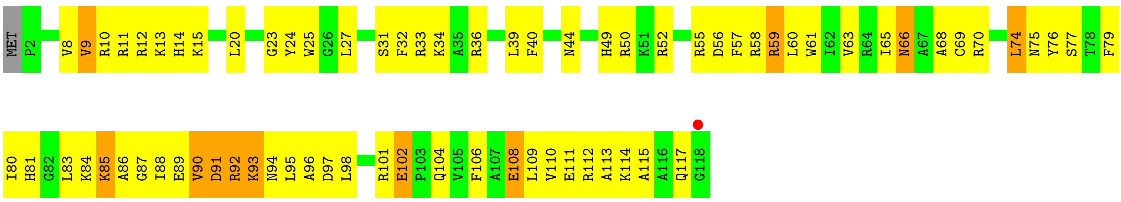
- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:



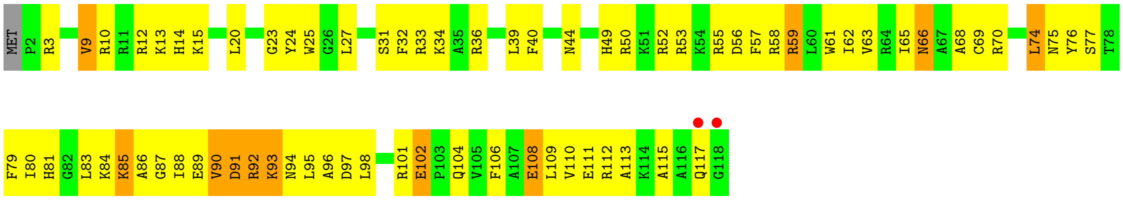
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



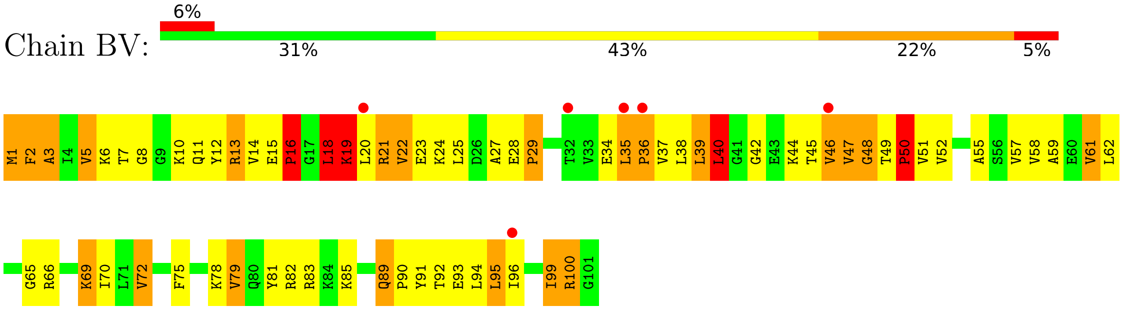
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



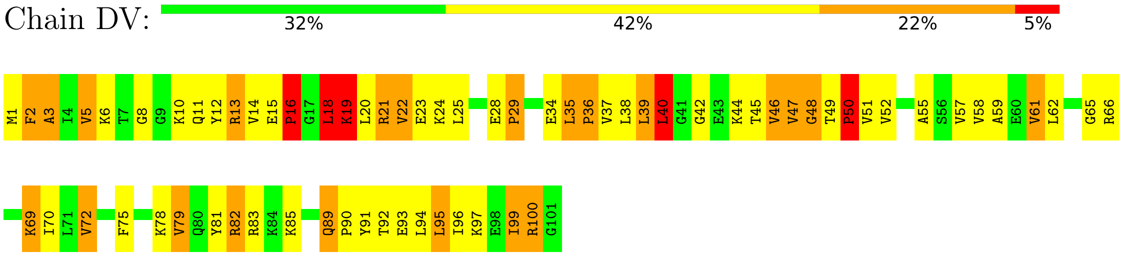
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



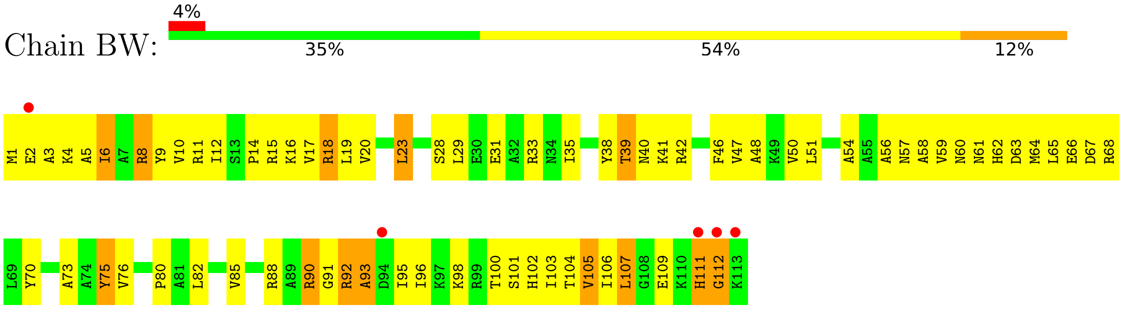
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



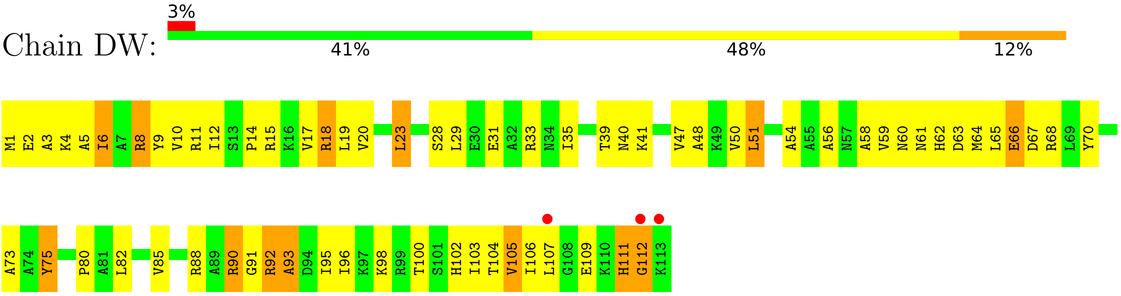
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



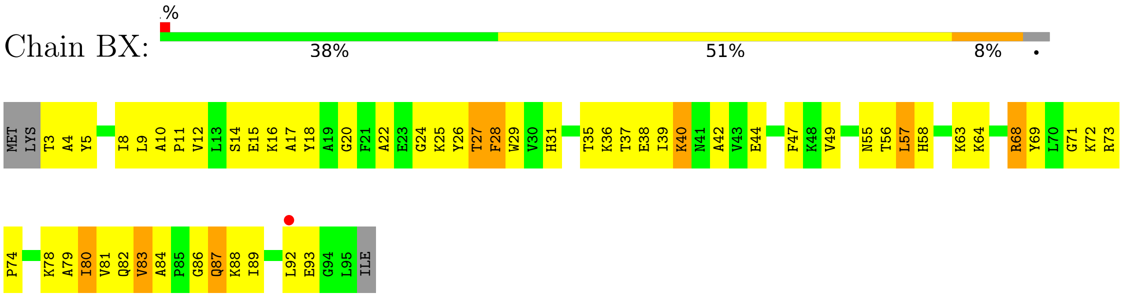
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



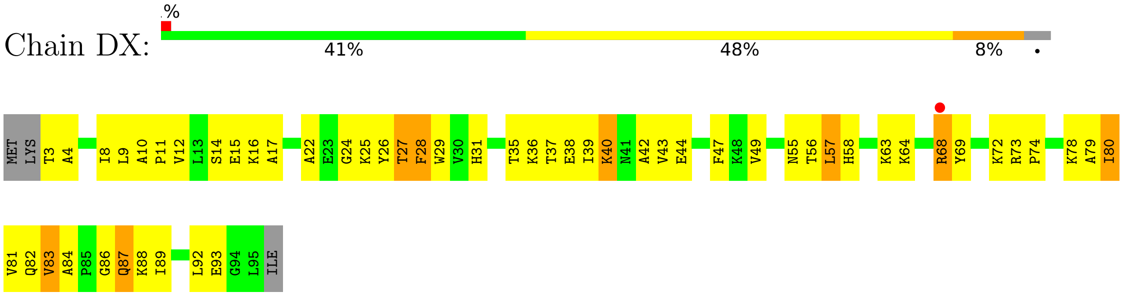
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



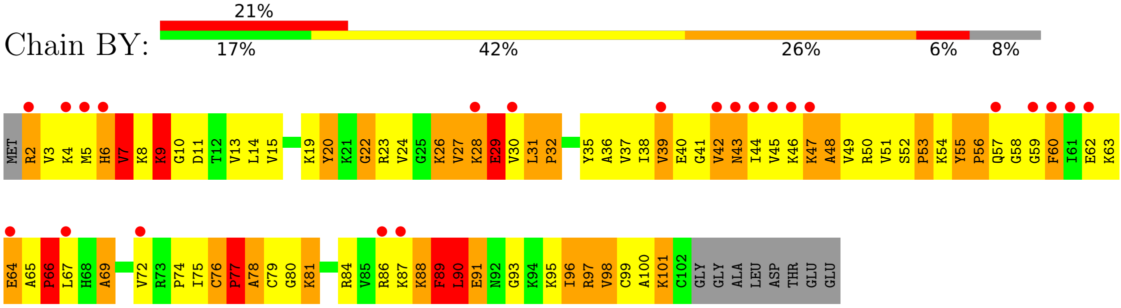
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



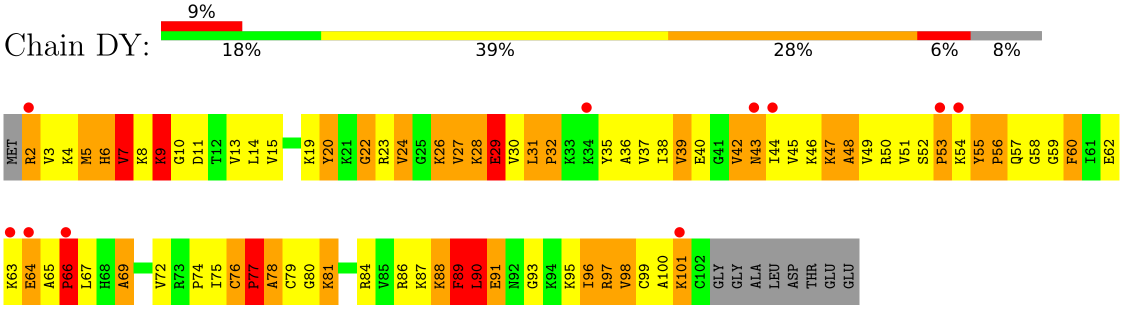
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



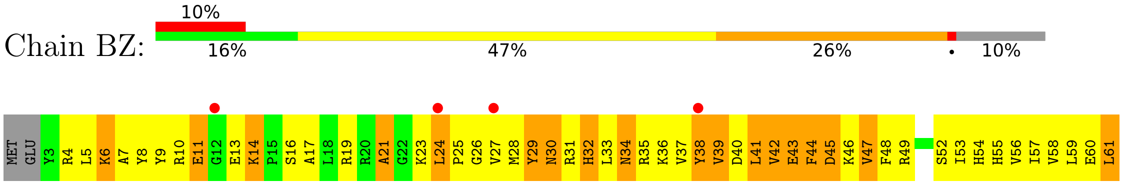
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

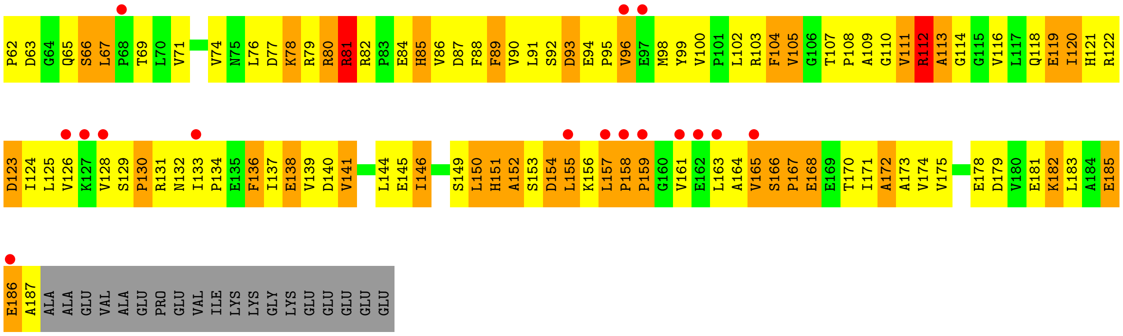
Chain DY:



- Molecule 58: 50S RIBOSOMAL PROTEIN L25

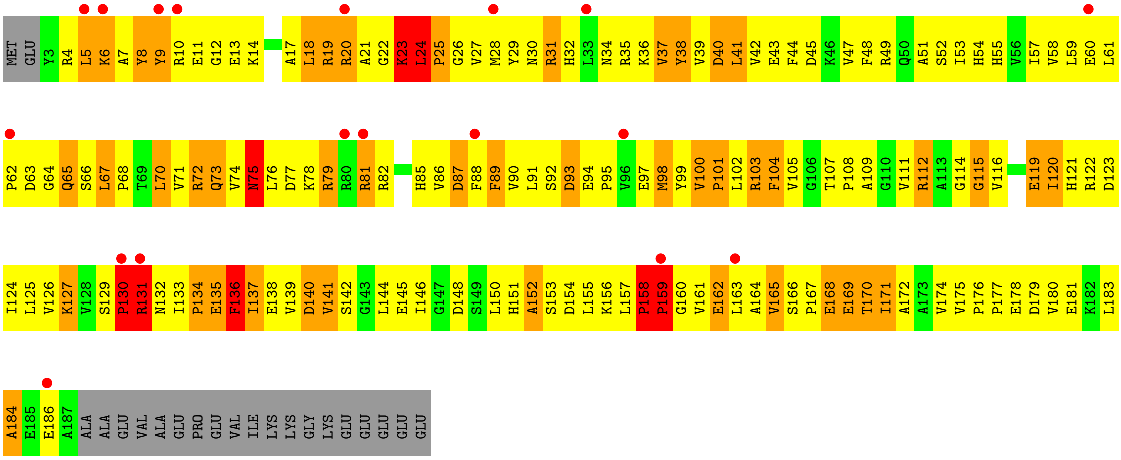
Chain BZ:





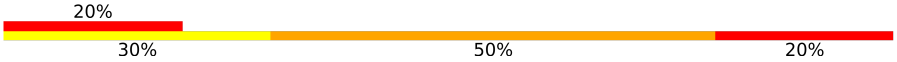
- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



- Molecule 59: BACTERIAL TOXIN YOEB

Chain CX:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.59Å 455.43Å 616.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.35 49.79 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.79-3.35) 99.7 (49.79-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.261 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	96.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 95.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	298206	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

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

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, OMU, A2M, 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	0.43	1/36190 (0.0%)	0.69	13/56486 (0.0%)
1	CA	0.41	1/36190 (0.0%)	0.70	15/56486 (0.0%)
2	AB	0.33	0/1936	0.62	0/2611
2	CB	0.33	0/1936	0.61	0/2611
3	AC	0.33	0/1637	0.59	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.38	0/1733	0.67	1/2318 (0.0%)
4	CD	0.35	0/1733	0.64	0/2318
5	AE	0.38	0/1163	0.67	0/1566
5	CE	0.37	0/1163	0.65	0/1566
6	AF	0.34	0/856	0.64	0/1154
6	CF	0.35	0/856	0.64	0/1154
7	AG	0.32	0/1276	0.55	0/1709
7	CG	0.30	0/1276	0.55	0/1709
8	AH	0.35	0/1136	0.69	0/1527
8	CH	0.33	0/1136	0.68	0/1527
9	AI	0.33	0/1027	0.60	0/1373
9	CI	0.32	0/1027	0.61	0/1373
10	AJ	0.35	0/808	0.62	0/1087
10	CJ	0.33	0/808	0.61	0/1087
11	AK	0.33	0/900	0.61	0/1213
11	CK	0.35	0/900	0.61	0/1213
12	AL	0.42	0/987	0.75	0/1322
12	CL	0.43	0/987	0.74	1/1322 (0.1%)
13	AM	0.33	0/943	0.84	3/1256 (0.2%)
13	CM	0.33	0/943	0.85	3/1256 (0.2%)
14	AN	0.36	0/501	0.94	3/664 (0.5%)
14	CN	0.37	0/501	0.92	3/664 (0.5%)
15	AO	0.36	0/745	0.61	0/992
15	CO	0.38	0/745	0.61	0/992
16	AP	0.39	0/717	0.63	0/965
16	CP	0.36	0/717	0.61	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.39	0/837	0.66	0/1119
17	CQ	0.37	0/837	0.65	0/1119
18	AR	0.37	0/579	1.06	3/768 (0.4%)
18	CR	0.36	0/579	0.97	3/768 (0.4%)
19	AS	0.43	0/643	0.92	3/867 (0.3%)
19	CS	0.51	0/643	0.98	3/867 (0.3%)
20	AT	0.35	0/765	0.61	0/1007
20	CT	0.32	0/765	0.60	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.49	0/1810	0.70	0/2821
23	AW	0.39	0/1832	0.69	0/2855
23	CV	0.44	0/1832	0.72	1/2855 (0.0%)
23	CW	0.37	0/1832	0.69	0/2855
24	AX	0.41	0/194	0.65	0/301
25	AY	0.41	0/742	0.63	1/1002 (0.1%)
25	AZ	0.40	0/743	0.63	0/1002
25	CY	0.48	0/742	0.69	2/1002 (0.2%)
25	CZ	0.47	0/743	0.64	0/1002
26	B0	0.39	0/671	0.68	0/892
26	D0	0.39	0/671	0.69	0/892
27	B1	0.43	0/739	0.81	1/983 (0.1%)
27	D1	0.47	0/739	0.78	0/983
28	B2	0.38	0/600	0.68	0/793
28	D2	0.47	0/600	0.76	1/793 (0.1%)
29	B3	0.38	0/473	0.65	0/636
29	D3	0.40	0/473	0.66	0/636
30	B4	0.39	0/461	0.70	0/623
30	D4	0.40	0/461	0.69	0/623
31	B5	0.51	0/442	0.86	0/598
31	D5	0.54	0/442	0.85	0/598
32	B6	0.46	0/440	0.83	0/586
32	D6	0.51	0/440	0.85	0/586
33	B7	0.48	0/418	0.68	0/552
33	D7	0.54	0/418	0.69	0/552
34	B8	0.57	0/516	0.97	4/681 (0.6%)
34	D8	0.56	0/516	0.97	5/681 (0.7%)
35	B9	0.36	0/310	0.61	0/407
35	D9	0.36	0/310	0.62	0/407
36	BA	0.53	5/68704 (0.0%)	0.74	50/107260 (0.0%)
36	DA	0.56	3/68704 (0.0%)	0.75	57/107260 (0.1%)
37	BB	0.39	0/2853	0.69	0/4451
37	DB	0.41	0/2853	0.70	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	BC	0.31	0/956	0.55	0/1288
38	DC	0.31	0/956	0.55	0/1288
39	BD	0.47	0/2155	0.82	2/2907 (0.1%)
39	DD	0.51	0/2155	0.83	3/2907 (0.1%)
40	BE	0.46	0/1597	0.78	1/2155 (0.0%)
40	DE	0.47	0/1597	0.78	1/2155 (0.0%)
41	BF	0.46	0/1659	0.76	1/2246 (0.0%)
41	DF	0.48	0/1659	0.76	1/2246 (0.0%)
42	BG	0.36	0/1498	0.66	0/2013
42	DG	0.42	0/1498	0.79	1/2013 (0.0%)
43	BH	0.38	0/1285	0.71	0/1741
43	DH	0.40	0/1285	0.72	0/1741
44	BI	0.37	0/1147	0.87	3/1553 (0.2%)
44	DI	0.39	0/1147	0.88	3/1553 (0.2%)
46	BN	0.42	0/1132	0.74	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.45	0/943	0.69	0/1269
47	DO	0.41	0/943	0.67	0/1269
48	BP	0.53	0/1131	1.06	6/1504 (0.4%)
48	DP	0.55	0/1131	1.08	7/1504 (0.5%)
49	BQ	0.44	0/1134	0.68	0/1517
49	DQ	0.42	0/1134	0.68	0/1517
50	BR	0.42	0/974	0.77	2/1302 (0.2%)
50	DR	0.44	0/974	0.79	2/1302 (0.2%)
51	BS	0.40	0/779	0.69	0/1038
51	DS	0.41	0/779	0.69	0/1038
52	BT	0.48	0/1138	0.83	3/1521 (0.2%)
52	DT	0.45	0/1138	0.81	3/1521 (0.2%)
53	BU	0.44	0/975	0.75	0/1297
53	DU	0.47	0/975	0.75	0/1297
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.75	0/1057
55	BW	0.44	0/907	0.72	0/1216
55	DW	0.46	0/907	0.74	0/1216
56	BX	0.44	0/740	0.69	0/995
56	DX	0.47	0/740	0.71	0/995
57	BY	0.51	0/789	0.79	1/1053 (0.1%)
57	DY	0.55	0/789	0.80	1/1053 (0.1%)
58	BZ	0.38	0/1500	0.71	0/2037
58	DZ	0.40	0/1500	0.74	1/2037 (0.0%)
59	CX	0.44	0/169	0.70	0/262
All	All	0.48	10/321535 (0.0%)	0.73	220/480333 (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	1	15
1	CA	0	13
22	AV	0	1
23	CV	0	2
24	AX	0	1
36	BA	7	51
36	DA	7	58
37	BB	0	2
37	DB	0	2
59	CX	0	1
All	All	15	146

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	975(A)	G	O3'-P	-12.04	1.46	1.61
1	AA	413	G	O3'-P	-8.20	1.51	1.61
1	CA	413	G	O3'-P	-7.59	1.52	1.61
36	BA	783	A	C5-C6	-5.78	1.35	1.41
36	BA	2506	U	N1-C2	5.66	1.43	1.38

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	AR	64	ARG	NE-CZ-NH2	-15.72	112.44	120.30
19	CS	81	ARG	NE-CZ-NH1	15.12	127.86	120.30
18	AR	64	ARG	NE-CZ-NH1	14.85	127.73	120.30
13	CM	29	ARG	NE-CZ-NH2	-13.53	113.53	120.30
13	CM	29	ARG	NE-CZ-NH1	13.37	126.99	120.30

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	115	G	C3'
36	BA	49	A	C3'
36	BA	331	A	C3'
36	BA	752	A	C3'
36	BA	1799	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	U	Sidechain
1	AA	254	G	Sidechain
1	AA	318	G	Sidechain
1	AA	436	C	Sidechain
1	AA	575	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16317	1251	0
1	CA	32329	0	16317	1322	1
2	AB	1901	0	1951	294	0
2	CB	1901	0	1951	300	0
3	AC	1613	0	1677	234	0
3	CC	1613	0	1677	234	0
4	AD	1703	0	1766	193	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	133	0
6	AF	843	0	857	109	0
6	CF	843	0	857	111	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	136	0
8	AH	1116	0	1177	129	0
8	CH	1116	0	1177	125	0
9	AI	1010	0	1035	149	0
9	CI	1010	0	1035	152	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	162	0
11	AK	885	0	904	107	0
11	CK	885	0	904	106	0
12	AL	971	0	1057	109	0
12	CL	971	0	1057	112	0
13	AM	938	0	991	143	0
13	CM	938	0	991	152	0
14	AN	492	0	530	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	531	70	0
15	AO	734	0	771	75	0
15	CO	734	0	771	70	0
16	AP	701	0	720	69	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	75	0
17	CQ	824	0	891	73	0
18	AR	574	0	644	84	0
18	CR	574	0	644	82	0
19	AS	630	0	652	109	0
19	CS	630	0	652	106	0
20	AT	763	0	861	85	0
20	CT	763	0	861	95	0
21	AU	209	0	221	23	0
21	CU	209	0	221	25	0
22	AV	1641	0	839	55	0
23	AW	1640	0	837	57	0
23	CV	1640	0	837	55	0
23	CW	1640	0	837	64	0
24	AX	239	0	127	94	0
25	AY	722	0	713	147	0
25	AZ	723	0	710	110	0
25	CY	722	0	713	149	0
25	CZ	723	0	713	103	0
26	B0	662	0	688	79	0
26	D0	662	0	688	75	0
27	B1	732	0	808	87	0
27	D1	732	0	808	91	0
28	B2	598	0	653	88	0
28	D2	598	0	653	67	0
29	B3	468	0	523	27	0
29	D3	468	0	523	27	0
30	B4	451	0	449	126	0
30	D4	451	0	449	109	0
31	B5	428	0	445	65	0
31	D5	428	0	445	65	0
32	B6	433	0	461	109	0
32	D6	433	0	461	110	0
33	B7	410	0	454	29	0
33	D7	410	0	454	27	0
34	B8	508	0	576	119	0
34	D8	508	0	576	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B9	307	0	338	34	0
35	D9	307	0	338	31	0
36	BA	61341	0	30927	1969	0
36	DA	61341	0	30928	1948	0
37	BB	2551	0	1295	125	0
37	DB	2551	0	1295	119	0
38	BC	937	0	957	96	0
38	DC	937	0	957	101	0
39	BD	2105	0	2182	253	0
39	DD	2105	0	2182	266	0
40	BE	1564	0	1629	215	0
40	DE	1564	0	1629	213	0
41	BF	1624	0	1677	185	0
41	DF	1624	0	1677	168	0
42	BG	1474	0	1534	329	0
42	DG	1474	0	1534	389	0
43	BH	1260	0	1326	180	0
43	DH	1260	0	1326	175	0
44	BI	1132	0	1218	282	1
44	DI	1132	0	1218	279	0
45	BJ	651	0	177	28	0
45	DJ	651	0	174	64	0
46	BN	1105	0	1180	154	0
46	DN	1105	0	1180	160	0
47	BO	933	0	996	86	0
47	DO	933	0	996	97	0
48	BP	1114	0	1187	297	0
48	DP	1114	0	1187	294	0
49	BQ	1113	0	1171	105	0
49	DQ	1113	0	1171	112	0
50	BR	960	0	1021	139	0
50	DR	960	0	1021	130	0
51	BS	771	0	832	166	0
51	DS	771	0	832	173	0
52	BT	1124	0	1181	226	0
52	DT	1124	0	1181	211	0
53	BU	958	0	1014	125	0
53	DU	958	0	1015	123	0
54	BV	779	0	852	135	0
54	DV	779	0	852	139	0
55	BW	896	0	953	90	0
55	DW	896	0	953	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BX	726	0	778	74	0
56	DX	726	0	778	71	0
57	BY	776	0	870	182	0
57	DY	776	0	870	176	0
58	BZ	1468	0	1492	253	0
58	DZ	1468	0	1492	348	0
59	CX	217	0	116	77	0
60	AA	103	0	0	0	0
60	AL	1	0	0	0	0
60	AV	1	0	0	0	0
60	AX	1	0	0	0	0
60	B0	1	0	0	0	0
60	B1	2	0	0	0	0
60	B5	2	0	0	0	0
60	BA	236	0	0	0	0
60	BB	2	0	0	0	0
60	BF	1	0	0	0	0
60	BP	1	0	0	0	0
60	BX	1	0	0	0	0
60	CA	103	0	0	0	0
60	CG	1	0	0	0	0
60	CL	1	0	0	0	0
60	CV	2	0	0	0	0
60	D1	1	0	0	0	0
60	D5	1	0	0	0	0
60	DA	242	0	0	0	0
60	DB	1	0	0	0	0
60	DF	1	0	0	0	0
60	DR	1	0	0	0	0
60	DX	1	0	0	0	0
61	AD	1	0	0	2	0
61	AN	1	0	0	0	0
61	CD	1	0	0	1	0
61	CN	1	0	0	1	0
All	All	298206	0	202858	19516	1

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 19516 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:19:OMU:CM2	25:AY:51:ASN:HD21	1.10	1.58
4:CD:26:CYS:SG	61:CD:301:ZN:ZN	1.01	1.49
1:AA:1493:A:C8	24:AX:20:A2M:HM'3	1.49	1.48
1:AA:1493:A:C8	24:AX:20:A2M:CM'	1.98	1.46
1:AA:1493:A:N7	24:AX:20:A2M:CM'	1.89	1.34

All (1) 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)
44:BI:121:LYS:NZ	1:CA:358:U:OP1[4_555]	2.13	0.07

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%)	128 (55%)	77 (33%)	28 (12%)	0	2
2	CB	233/256 (91%)	129 (55%)	75 (32%)	29 (12%)	0	2
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	1
3	CC	205/239 (86%)	125 (61%)	53 (26%)	27 (13%)	0	1
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	6
4	CD	206/209 (99%)	139 (68%)	51 (25%)	16 (8%)	1	6
5	AE	149/162 (92%)	106 (71%)	31 (21%)	12 (8%)	1	6
5	CE	149/162 (92%)	107 (72%)	29 (20%)	13 (9%)	1	5
6	AF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	8
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	8
7	AG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	0	2
7	CG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	0	2
8	AH	136/138 (99%)	99 (73%)	25 (18%)	12 (9%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	0	4
9	AI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	4
9	CI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	4
10	AJ	97/105 (92%)	69 (71%)	21 (22%)	7 (7%)	1	8
10	CJ	97/105 (92%)	72 (74%)	18 (19%)	7 (7%)	1	8
11	AK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	0	4
11	CK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	0	4
12	AL	123/132 (93%)	87 (71%)	26 (21%)	10 (8%)	1	6
12	CL	123/132 (93%)	88 (72%)	25 (20%)	10 (8%)	1	6
13	AM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	1
13	CM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	1
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	1
14	CN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	1
15	AO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	8
15	CO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	1	8
16	AP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	7
16	CP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	7
17	AQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	2	15
17	CQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	2	15
18	AR	68/88 (77%)	41 (60%)	17 (25%)	10 (15%)	0	1
18	CR	68/88 (77%)	42 (62%)	16 (24%)	10 (15%)	0	1
19	AS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	1
19	CS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	1
20	AT	97/106 (92%)	59 (61%)	26 (27%)	12 (12%)	0	2
20	CT	97/106 (92%)	58 (60%)	26 (27%)	13 (13%)	0	1
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	1
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
25	AY	82/84 (98%)	53 (65%)	13 (16%)	16 (20%)	0	0
25	AZ	82/84 (98%)	54 (66%)	20 (24%)	8 (10%)	0	4
25	CY	82/84 (98%)	50 (61%)	16 (20%)	16 (20%)	0	0
25	CZ	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	2	15
26	D0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	1	11
27	B1	92/98 (94%)	67 (73%)	12 (13%)	13 (14%)	0	1
27	D1	92/98 (94%)	66 (72%)	14 (15%)	12 (13%)	0	1
28	B2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	1
28	D2	69/72 (96%)	45 (65%)	16 (23%)	8 (12%)	0	2
29	B3	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	3	23
29	D3	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	3	23
30	B4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
30	D4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
31	B5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	1
31	D5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	1
32	B6	48/54 (89%)	25 (52%)	7 (15%)	16 (33%)	0	0
32	D6	48/54 (89%)	26 (54%)	7 (15%)	15 (31%)	0	0
33	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	32
33	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
34	B8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	1
34	D8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	1
35	B9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	5
35	D9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	5
38	BC	116/229 (51%)	84 (72%)	26 (22%)	6 (5%)	2	14
38	DC	116/229 (51%)	85 (73%)	25 (22%)	6 (5%)	2	14
39	BD	270/276 (98%)	205 (76%)	37 (14%)	28 (10%)	0	3
39	DD	270/276 (98%)	202 (75%)	41 (15%)	27 (10%)	0	3
40	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
40	DE	203/206 (98%)	145 (71%)	35 (17%)	23 (11%)	0	2
41	BF	206/210 (98%)	155 (75%)	29 (14%)	22 (11%)	0	3
41	DF	206/210 (98%)	157 (76%)	26 (13%)	23 (11%)	0	2
42	BG	177/182 (97%)	105 (59%)	33 (19%)	39 (22%)	0	0
42	DG	177/182 (97%)	80 (45%)	47 (27%)	50 (28%)	0	0
43	BH	163/180 (91%)	98 (60%)	39 (24%)	26 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DH	163/180 (91%)	98 (60%)	38 (23%)	27 (17%)	0	1
44	BI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	0
44	DI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	0
46	BN	137/140 (98%)	96 (70%)	23 (17%)	18 (13%)	0	1
46	DN	137/140 (98%)	95 (69%)	25 (18%)	17 (12%)	0	2
47	BO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	29
47	DO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	5	29
48	BP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
49	BQ	139/141 (99%)	109 (78%)	17 (12%)	13 (9%)	0	4
49	DQ	139/141 (99%)	107 (77%)	20 (14%)	12 (9%)	1	5
50	BR	115/118 (98%)	89 (77%)	14 (12%)	12 (10%)	0	3
50	DR	115/118 (98%)	89 (77%)	13 (11%)	13 (11%)	0	2
51	BS	97/112 (87%)	51 (53%)	23 (24%)	23 (24%)	0	0
51	DS	97/112 (87%)	50 (52%)	23 (24%)	24 (25%)	0	0
52	BT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	0
52	DT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	0
53	BU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	2	14
53	DU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	2	14
54	BV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	1
54	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	1
55	BW	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	2	13
55	DW	111/113 (98%)	96 (86%)	9 (8%)	6 (5%)	2	13
56	BX	91/96 (95%)	71 (78%)	17 (19%)	3 (3%)	4	24
56	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	4	24
57	BY	99/110 (90%)	42 (42%)	25 (25%)	32 (32%)	0	0
57	DY	99/110 (90%)	41 (41%)	26 (26%)	32 (32%)	0	0
58	BZ	183/206 (89%)	102 (56%)	40 (22%)	41 (22%)	0	0
58	DZ	183/206 (89%)	85 (46%)	58 (32%)	40 (22%)	0	0
All	All	11928/12922 (92%)	7972 (67%)	2431 (20%)	1525 (13%)	0	2

5 of 1525 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	10	LEU
2	AB	75	LYS
2	AB	123	ALA
2	AB	155	LEU

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%)	189 (94%)	13 (6%)	17	48
2	CB	202/220 (92%)	191 (95%)	11 (5%)	22	54
3	AC	160/188 (85%)	146 (91%)	14 (9%)	10	34
3	CC	160/188 (85%)	147 (92%)	13 (8%)	11	38
4	AD	180/181 (99%)	162 (90%)	18 (10%)	7	29
4	CD	180/181 (99%)	162 (90%)	18 (10%)	7	29
5	AE	115/123 (94%)	98 (85%)	17 (15%)	3	13
5	CE	115/123 (94%)	98 (85%)	17 (15%)	3	13
6	AF	90/90 (100%)	84 (93%)	6 (7%)	16	47
6	CF	90/90 (100%)	84 (93%)	6 (7%)	16	47
7	AG	126/127 (99%)	120 (95%)	6 (5%)	25	57
7	CG	126/127 (99%)	121 (96%)	5 (4%)	31	62
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	37
8	CH	119/119 (100%)	108 (91%)	11 (9%)	9	32
9	AI	98/99 (99%)	89 (91%)	9 (9%)	9	32
9	CI	98/99 (99%)	89 (91%)	9 (9%)	9	32
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	12	39
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	12	39
11	AK	90/99 (91%)	87 (97%)	3 (3%)	38	67
11	CK	90/99 (91%)	87 (97%)	3 (3%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/109 (95%)	95 (91%)	9 (9%)	10	35
12	CL	104/109 (95%)	95 (91%)	9 (9%)	10	35
13	AM	94/101 (93%)	83 (88%)	11 (12%)	5	21
13	CM	94/101 (93%)	83 (88%)	11 (12%)	5	21
14	AN	49/50 (98%)	46 (94%)	3 (6%)	18	50
14	CN	49/50 (98%)	46 (94%)	3 (6%)	18	50
15	AO	79/80 (99%)	73 (92%)	6 (8%)	13	41
15	CO	79/80 (99%)	73 (92%)	6 (8%)	13	41
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	30
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	22	54
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	22	54
18	AR	61/77 (79%)	61 (100%)	0	100	100
18	CR	61/77 (79%)	60 (98%)	1 (2%)	62	81
19	AS	69/80 (86%)	60 (87%)	9 (13%)	4	17
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	21
20	AT	76/82 (93%)	68 (90%)	8 (10%)	7	26
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9	32
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	26
25	AY	78/78 (100%)	65 (83%)	13 (17%)	2	9
25	AZ	78/78 (100%)	57 (73%)	21 (27%)	0	1
25	CY	78/78 (100%)	64 (82%)	14 (18%)	2	7
25	CZ	78/78 (100%)	56 (72%)	22 (28%)	0	1
26	B0	66/67 (98%)	56 (85%)	10 (15%)	3	12
26	D0	66/67 (98%)	56 (85%)	10 (15%)	3	12
27	B1	78/83 (94%)	69 (88%)	9 (12%)	5	22
27	D1	78/83 (94%)	66 (85%)	12 (15%)	2	12
28	B2	66/67 (98%)	56 (85%)	10 (15%)	3	12
28	D2	66/67 (98%)	56 (85%)	10 (15%)	3	12
29	B3	51/52 (98%)	46 (90%)	5 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D3	51/52 (98%)	46 (90%)	5 (10%)	8	30
30	B4	51/63 (81%)	39 (76%)	12 (24%)	1	2
30	D4	51/63 (81%)	39 (76%)	12 (24%)	1	2
31	B5	47/52 (90%)	42 (89%)	5 (11%)	6	26
31	D5	47/52 (90%)	42 (89%)	5 (11%)	6	26
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	3
32	D6	49/52 (94%)	36 (74%)	13 (26%)	0	1
33	B7	40/42 (95%)	36 (90%)	4 (10%)	7	29
33	D7	40/42 (95%)	36 (90%)	4 (10%)	7	29
34	B8	53/55 (96%)	42 (79%)	11 (21%)	1	4
34	D8	53/55 (96%)	43 (81%)	10 (19%)	1	6
35	B9	34/34 (100%)	32 (94%)	2 (6%)	19	51
35	D9	34/34 (100%)	32 (94%)	2 (6%)	19	51
38	BC	99/181 (55%)	96 (97%)	3 (3%)	41	69
38	DC	99/181 (55%)	96 (97%)	3 (3%)	41	69
39	BD	213/218 (98%)	188 (88%)	25 (12%)	5	21
39	DD	213/218 (98%)	187 (88%)	26 (12%)	5	19
40	BE	165/166 (99%)	143 (87%)	22 (13%)	4	16
40	DE	165/166 (99%)	144 (87%)	21 (13%)	4	18
41	BF	165/166 (99%)	145 (88%)	20 (12%)	5	20
41	DF	165/166 (99%)	145 (88%)	20 (12%)	5	20
42	BG	155/156 (99%)	137 (88%)	18 (12%)	5	21
42	DG	155/156 (99%)	121 (78%)	34 (22%)	1	3
43	BH	137/148 (93%)	127 (93%)	10 (7%)	14	43
43	DH	137/148 (93%)	127 (93%)	10 (7%)	14	43
44	BI	122/124 (98%)	105 (86%)	17 (14%)	3	15
44	DI	122/124 (98%)	105 (86%)	17 (14%)	3	15
46	BN	117/119 (98%)	98 (84%)	19 (16%)	2	10
46	DN	117/119 (98%)	98 (84%)	19 (16%)	2	10
47	BO	100/100 (100%)	94 (94%)	6 (6%)	19	50
47	DO	100/100 (100%)	94 (94%)	6 (6%)	19	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BP	112/116 (97%)	84 (75%)	28 (25%)	0	2
48	DP	112/116 (97%)	84 (75%)	28 (25%)	0	2
49	BQ	110/111 (99%)	95 (86%)	15 (14%)	3	16
49	DQ	110/111 (99%)	95 (86%)	15 (14%)	3	16
50	BR	100/101 (99%)	83 (83%)	17 (17%)	2	9
50	DR	100/101 (99%)	83 (83%)	17 (17%)	2	9
51	BS	77/88 (88%)	60 (78%)	17 (22%)	1	3
51	DS	77/88 (88%)	60 (78%)	17 (22%)	1	3
52	BT	118/127 (93%)	98 (83%)	20 (17%)	2	9
52	DT	118/127 (93%)	99 (84%)	19 (16%)	2	10
53	BU	92/94 (98%)	83 (90%)	9 (10%)	8	30
53	DU	92/94 (98%)	83 (90%)	9 (10%)	8	30
54	BV	82/82 (100%)	61 (74%)	21 (26%)	0	2
54	DV	82/82 (100%)	62 (76%)	20 (24%)	0	2
55	BW	91/92 (99%)	78 (86%)	13 (14%)	3	14
55	DW	91/92 (99%)	77 (85%)	14 (15%)	2	12
56	BX	74/78 (95%)	68 (92%)	6 (8%)	11	38
56	DX	74/78 (95%)	68 (92%)	6 (8%)	11	38
57	BY	84/91 (92%)	67 (80%)	17 (20%)	1	4
57	DY	84/91 (92%)	67 (80%)	17 (20%)	1	4
58	BZ	162/179 (90%)	137 (85%)	25 (15%)	2	12
58	DZ	162/179 (90%)	131 (81%)	31 (19%)	1	5
All	All	10102/10740 (94%)	8871 (88%)	1231 (12%)	5	19

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	DE	169	ASN
54	DV	13	ARG
42	DG	22	ARG
40	DE	154	LYS
48	DP	13	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
33	D7	8	ASN
50	DR	71	GLN
39	DD	58	HIS
42	DG	27	ASN
56	DX	55	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	214 (14%)	30 (1%)
1	CA	1503/1504 (99%)	209 (13%)	31 (2%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	10 (13%)	1 (1%)
23	CV	76/77 (98%)	12 (15%)	0
23	CW	76/77 (98%)	10 (13%)	1 (1%)
24	AX	10/25 (40%)	8 (80%)	1 (10%)
36	BA	2847/2848 (99%)	500 (17%)	49 (1%)
36	DA	2847/2848 (99%)	498 (17%)	47 (1%)
37	BB	118/119 (99%)	25 (21%)	2 (1%)
37	DB	118/119 (99%)	25 (21%)	2 (1%)
59	CX	9/10 (90%)	6 (66%)	2 (22%)
All	All	9259/9285 (99%)	1532 (16%)	166 (1%)

5 of 1532 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	30	U
1	AA	31	G
1	AA	32	A

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	CX	19	OMU
36	DA	1819	A
36	DA	74	A
36	DA	614(C)	A
36	DA	2062	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	A2M	AX	20	24,60	18,25,26	0.61	0	18,36,39	1.35	1 (5%)
22	5MU	AV	54	22	19,22,23	0.33	0	28,32,35	0.36	0
24	OMU	AX	19	24	19,22,23	0.61	1 (5%)	26,31,34	0.94	1 (3%)
59	OMU	CX	19	59	19,22,23	0.56	0	26,31,34	0.76	1 (3%)
59	A2M	CX	21	59	18,25,26	0.62	0	18,36,39	0.79	0
59	A2M	CX	20	59	18,25,26	0.62	0	18,36,39	1.25	2 (11%)
24	A2M	AX	21	24	18,25,26	0.62	0	18,36,39	1.74	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	A2M	AX	20	24,60	-	2/5/27/28	0/3/3/3
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2
24	OMU	AX	19	24	-	3/9/27/28	0/2/2/2
59	OMU	CX	19	59	-	2/9/27/28	0/2/2/2
59	A2M	CX	21	59	-	3/5/27/28	0/3/3/3
59	A2M	CX	20	59	-	2/5/27/28	0/3/3/3
24	A2M	AX	21	24	-	2/5/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	19	OMU	O2'-CM2	-2.18	1.34	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AX	21	A2M	CM'-O2'-C2'	-6.75	96.81	114.52
24	AX	20	A2M	CM'-O2'-C2'	-4.87	101.75	114.52
59	CX	20	A2M	CM'-O2'-C2'	-4.43	102.89	114.52
24	AX	19	OMU	CM2-O2'-C2'	-4.34	103.14	114.52
59	CX	19	OMU	CM2-O2'-C2'	3.32	123.24	114.52

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AX	19	OMU	C1'-C2'-O2'-CM2
24	AX	20	A2M	O4'-C4'-C5'-O5'
24	AX	21	A2M	C4'-C5'-O5'-P
59	CX	21	A2M	C4'-C5'-O5'-P
59	CX	21	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	20	A2M	31	0
22	AV	54	5MU	1	0
24	AX	19	OMU	14	0
59	CX	19	OMU	10	0
59	CX	21	A2M	20	0
59	CX	20	A2M	30	0
24	AX	21	A2M	21	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 711 ligands modelled in this entry, 711 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
42	DG	1
42	BG	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	5.57
1	CM	69:GLU	C	70:LEU	N	4.17
1	AM	69:GLU	C	70:LEU	N	4.16
1	CM	112:GLY	C	113:PRO	N	3.94
1	AM	112:GLY	C	113:PRO	N	3.93

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	1504/1504 (100%)	0.05	31 (2%)	63	67	63, 109, 201, 216	0
1	CA	1504/1504 (100%)	0.23	44 (2%)	51	54	65, 139, 211, 216	0
2	AB	235/256 (91%)	0.53	28 (11%)	4	5	87, 146, 195, 216	0
2	CB	235/256 (91%)	0.61	27 (11%)	4	5	86, 165, 206, 216	0
3	AC	207/239 (86%)	0.42	14 (6%)	17	20	83, 143, 188, 216	0
3	CC	207/239 (86%)	0.99	38 (18%)	1	1	100, 164, 200, 216	0
4	AD	208/209 (99%)	0.09	1 (0%)	91	93	70, 104, 147, 167	0
4	CD	208/209 (99%)	0.82	28 (13%)	3	3	95, 151, 199, 216	0
5	AE	151/162 (93%)	0.35	4 (2%)	56	58	62, 102, 142, 216	0
5	CE	151/162 (93%)	0.91	22 (14%)	2	2	60, 125, 168, 210	0
6	AF	101/101 (100%)	0.16	4 (3%)	38	40	73, 128, 164, 183	0
6	CF	101/101 (100%)	-0.09	1 (0%)	82	86	63, 112, 156, 181	0
7	AG	155/156 (99%)	0.35	14 (9%)	9	11	91, 136, 181, 210	0
7	CG	155/156 (99%)	0.73	28 (18%)	1	1	91, 153, 194, 216	0
8	AH	138/138 (100%)	0.28	1 (0%)	87	91	73, 108, 147, 193	0
8	CH	138/138 (100%)	0.68	13 (9%)	8	10	89, 132, 183, 213	0
9	AI	127/128 (99%)	1.05	27 (21%)	0	1	95, 155, 190, 216	0
9	CI	127/128 (99%)	1.76	41 (32%)	0	0	113, 170, 211, 216	0
10	AJ	99/105 (94%)	1.43	27 (27%)	0	0	88, 159, 208, 216	0
10	CJ	99/105 (94%)	2.07	38 (38%)	0	0	122, 174, 215, 216	0
11	AK	119/129 (92%)	0.93	18 (15%)	2	2	70, 120, 170, 212	0
11	CK	119/129 (92%)	0.39	9 (7%)	13	16	70, 120, 167, 195	0
12	AL	125/132 (94%)	0.48	7 (5%)	24	26	60, 89, 139, 216	0
12	CL	125/132 (94%)	0.88	23 (18%)	1	1	77, 113, 157, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	119/126 (94%)	0.47	8 (6%) 17 20	80, 143, 183, 216	0
13	CM	119/126 (94%)	1.12	26 (21%) 0 1	97, 167, 210, 216	0
14	AN	60/61 (98%)	0.70	6 (10%) 7 8	84, 136, 187, 204	0
14	CN	60/61 (98%)	0.74	8 (13%) 3 4	92, 154, 192, 206	0
15	AO	88/89 (98%)	0.32	2 (2%) 60 63	66, 108, 148, 177	0
15	CO	88/89 (98%)	0.13	2 (2%) 60 63	70, 114, 149, 174	0
16	AP	84/88 (95%)	0.50	2 (2%) 59 61	70, 94, 143, 199	0
16	CP	84/88 (95%)	1.76	30 (35%) 0 0	99, 138, 175, 208	0
17	AQ	100/105 (95%)	0.15	0 100 100	70, 99, 129, 161	0
17	CQ	100/105 (95%)	0.55	7 (7%) 16 18	90, 125, 158, 179	0
18	AR	70/88 (79%)	0.85	7 (10%) 7 8	87, 128, 170, 181	0
18	CR	70/88 (79%)	0.87	9 (12%) 3 4	77, 118, 168, 186	0
19	AS	79/93 (84%)	1.43	24 (30%) 0 0	111, 163, 209, 216	0
19	CS	79/93 (84%)	2.10	31 (39%) 0 0	122, 169, 213, 216	0
20	AT	99/106 (93%)	0.46	7 (7%) 16 18	71, 107, 163, 187	0
20	CT	99/106 (93%)	1.06	17 (17%) 1 1	93, 143, 181, 216	0
21	AU	25/27 (92%)	2.34	12 (48%) 0 0	99, 143, 176, 193	0
21	CU	25/27 (92%)	3.20	17 (68%) 0 0	102, 155, 182, 191	0
22	AV	76/77 (98%)	-0.22	1 (1%) 77 80	71, 108, 162, 206	0
23	AW	77/77 (100%)	2.31	39 (50%) 0 0	151, 218, 220, 221	0
23	CV	77/77 (100%)	-0.12	1 (1%) 77 80	76, 126, 184, 211	0
23	CW	77/77 (100%)	1.85	32 (41%) 0 0	151, 218, 220, 221	0
24	AX	8/25 (32%)	1.89	3 (37%) 0 0	52, 100, 165, 180	0
25	AY	84/84 (100%)	1.08	16 (19%) 1 1	105, 142, 171, 199	0
25	AZ	84/84 (100%)	0.99	20 (23%) 0 0	121, 166, 197, 200	0
25	CY	84/84 (100%)	1.97	37 (44%) 0 0	103, 160, 194, 200	0
25	CZ	84/84 (100%)	1.30	21 (25%) 0 0	132, 182, 200, 200	0
26	B0	84/85 (98%)	0.62	10 (11%) 4 5	69, 103, 160, 207	0
26	D0	84/85 (98%)	1.02	10 (11%) 4 5	76, 107, 163, 198	0
27	B1	94/98 (95%)	0.30	2 (2%) 63 67	55, 87, 144, 208	0
27	D1	94/98 (95%)	0.30	2 (2%) 63 67	53, 83, 132, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	B2	71/72 (98%)	0.26	4 (5%) 24 26	81, 122, 156, 205	0
28	D2	71/72 (98%)	-0.12	3 (4%) 36 38	51, 84, 123, 188	0
29	B3	60/60 (100%)	0.97	8 (13%) 3 4	66, 97, 144, 212	0
29	D3	60/60 (100%)	0.29	1 (1%) 70 73	61, 92, 159, 199	0
30	B4	58/71 (81%)	0.29	6 (10%) 6 7	104, 171, 212, 216	0
30	D4	58/71 (81%)	0.83	7 (12%) 4 4	145, 180, 214, 216	0
31	B5	56/60 (93%)	0.19	4 (7%) 16 18	49, 92, 147, 216	0
31	D5	56/60 (93%)	0.01	2 (3%) 42 45	49, 83, 151, 216	0
32	B6	50/54 (92%)	1.81	19 (38%) 0 0	89, 132, 180, 182	0
32	D6	50/54 (92%)	1.37	13 (26%) 0 0	97, 140, 188, 210	0
33	B7	48/49 (97%)	0.09	1 (2%) 63 67	50, 73, 123, 163	0
33	D7	48/49 (97%)	0.11	2 (4%) 36 38	42, 57, 101, 161	0
34	B8	64/65 (98%)	0.47	4 (6%) 20 22	57, 85, 144, 170	0
34	D8	64/65 (98%)	0.45	4 (6%) 20 22	48, 85, 142, 210	0
35	B9	37/37 (100%)	2.06	15 (40%) 0 0	94, 118, 162, 186	0
35	D9	37/37 (100%)	2.15	19 (51%) 0 0	93, 119, 162, 173	0
36	BA	2848/2848 (100%)	0.10	101 (3%) 44 46	46, 88, 203, 216	0
36	DA	2848/2848 (100%)	0.10	92 (3%) 47 50	43, 82, 203, 216	0
37	BB	119/119 (100%)	-0.12	2 (1%) 70 73	88, 144, 195, 212	0
37	DB	119/119 (100%)	0.30	5 (4%) 36 38	90, 173, 210, 216	0
38	BC	120/229 (52%)	4.07	95 (79%) 0 0	139, 202, 216, 216	0
38	DC	120/229 (52%)	3.81	90 (75%) 0 0	145, 202, 216, 216	0
39	BD	272/276 (98%)	0.08	2 (0%) 87 91	45, 83, 120, 188	0
39	DD	272/276 (98%)	0.09	4 (1%) 73 76	45, 77, 113, 185	0
40	BE	205/206 (99%)	0.20	9 (4%) 34 37	50, 89, 166, 201	0
40	DE	205/206 (99%)	0.42	5 (2%) 59 61	37, 89, 146, 194	0
41	BF	208/210 (99%)	-0.05	1 (0%) 91 93	49, 88, 164, 216	0
41	DF	208/210 (99%)	0.08	7 (3%) 45 47	36, 82, 164, 211	0
42	BG	181/182 (99%)	0.49	14 (7%) 13 15	100, 143, 188, 212	0
42	DG	181/182 (99%)	1.30	50 (27%) 0 0	109, 171, 215, 216	0
43	BH	165/180 (91%)	1.68	61 (36%) 0 0	98, 166, 214, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	DH	165/180 (91%)	0.71	23 (13%) 2 3	67, 127, 186, 216	0
44	BI	146/148 (98%)	2.76	67 (45%) 0 0	84, 172, 216, 216	0
44	DI	146/148 (98%)	1.08	23 (15%) 2 2	69, 144, 211, 216	0
45	BJ	0/130	-	-	-	-
45	DJ	0/130	-	-	-	-
46	BN	139/140 (99%)	0.40	6 (4%) 35 38	63, 97, 149, 192	0
46	DN	139/140 (99%)	0.05	2 (1%) 75 78	54, 90, 144, 175	0
47	BO	122/122 (100%)	-0.01	0 100 100	48, 78, 111, 141	0
47	DO	122/122 (100%)	0.24	1 (0%) 86 89	60, 89, 121, 138	0
48	BP	146/150 (97%)	0.57	13 (8%) 9 11	51, 103, 161, 216	0
48	DP	146/150 (97%)	0.36	6 (4%) 37 39	51, 105, 162, 210	0
49	BQ	141/141 (100%)	0.05	1 (0%) 87 91	65, 96, 134, 209	0
49	DQ	141/141 (100%)	0.43	6 (4%) 35 38	67, 103, 149, 208	0
50	BR	117/118 (99%)	0.09	0 100 100	55, 89, 123, 137	0
50	DR	117/118 (99%)	0.31	4 (3%) 45 47	51, 84, 121, 145	0
51	BS	99/112 (88%)	1.04	20 (20%) 1 1	93, 141, 189, 208	0
51	DS	99/112 (88%)	1.27	25 (25%) 0 0	91, 154, 199, 216	0
52	BT	136/146 (93%)	0.19	3 (2%) 62 65	64, 97, 176, 216	0
52	DT	136/146 (93%)	0.41	10 (7%) 14 17	68, 110, 189, 215	0
53	BU	117/118 (99%)	-0.02	1 (0%) 84 87	53, 86, 139, 210	0
53	DU	117/118 (99%)	-0.07	2 (1%) 70 73	45, 75, 122, 215	0
54	BV	101/101 (100%)	0.28	6 (5%) 22 25	53, 109, 158, 206	0
54	DV	101/101 (100%)	0.08	0 100 100	38, 93, 133, 216	0
55	BW	113/113 (100%)	0.28	5 (4%) 34 37	55, 80, 132, 199	0
55	DW	113/113 (100%)	0.20	3 (2%) 54 57	40, 72, 121, 209	0
56	BX	93/96 (96%)	0.21	1 (1%) 80 84	63, 106, 136, 155	0
56	DX	93/96 (96%)	0.13	1 (1%) 80 84	55, 79, 117, 164	0
57	BY	101/110 (91%)	1.37	23 (22%) 0 0	62, 114, 180, 206	0
57	DY	101/110 (91%)	0.71	10 (9%) 7 8	56, 102, 168, 211	0
58	BZ	185/206 (89%)	0.53	20 (10%) 5 6	85, 131, 186, 216	0
58	DZ	185/206 (89%)	0.38	18 (9%) 7 9	88, 144, 202, 215	0
59	CX	7/10 (70%)	1.59	2 (28%) 0 0	110, 144, 193, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	21436/22467 (95%)	0.45	1849 (8%)	10	12	36, 111, 202, 221	0

The worst 5 of 1849 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	AL	129	ALA	19.7
44	BI	119	PRO	16.5
44	BI	100	ALA	15.9
44	DI	88	ILE	15.1
5	AE	155	GLU	14.1

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

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. 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	B-factors(Å^2)	Q<0.9
59	A2M	CX	20	23/24	0.59	0.36	168,174,200,200	0
24	A2M	AX	20	23/24	0.60	0.43	158,164,194,194	0
24	A2M	AX	21	23/24	0.83	0.35	140,147,161,184	0
59	OMU	CX	19	21/22	0.85	0.29	117,161,200,200	0
24	OMU	AX	19	21/22	0.85	0.29	99,130,198,198	0
59	A2M	CX	21	23/24	0.87	0.29	177,179,187,190	0
22	5MU	AV	54	21/22	0.93	0.23	114,133,152,153	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
60	MG	AA	1618	1/1	-0.30	0.38	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1633	1/1	-0.20	0.59	78,78,78,78	0
60	MG	CA	1640	1/1	-0.10	1.19	102,102,102,102	0
60	MG	DA	3009	1/1	-0.07	0.88	168,168,168,168	0
60	MG	CA	1607	1/1	-0.06	0.42	101,101,101,101	0
60	MG	CA	1666	1/1	-0.02	0.60	137,137,137,137	1
60	MG	CA	1647	1/1	0.02	0.32	97,97,97,97	0
60	MG	BA	3094	1/1	0.05	0.97	100,100,100,100	0
60	MG	CA	1692	1/1	0.06	0.67	117,117,117,117	0
60	MG	BA	3017	1/1	0.11	0.66	117,117,117,117	0
60	MG	CA	1627	1/1	0.13	0.68	162,162,162,162	0
60	MG	AA	1623	1/1	0.13	0.66	100,100,100,100	0
60	MG	DA	2964	1/1	0.15	1.25	109,109,109,109	0
60	MG	AA	1612	1/1	0.18	1.12	102,102,102,102	0
60	MG	AA	1642	1/1	0.18	0.67	102,102,102,102	0
60	MG	BA	3101	1/1	0.21	0.83	123,123,123,123	0
60	MG	CA	1672	1/1	0.25	0.89	109,109,109,109	0
60	MG	AA	1645	1/1	0.25	1.24	99,99,99,99	0
60	MG	CA	1637	1/1	0.26	0.57	141,141,141,141	0
60	MG	BA	3045	1/1	0.28	0.21	88,88,88,88	0
60	MG	AA	1662	1/1	0.31	1.06	127,127,127,127	0
60	MG	BA	2901	1/1	0.31	0.30	145,145,145,145	0
60	MG	DA	3041	1/1	0.31	2.16	154,154,154,154	0
60	MG	BA	3001	1/1	0.32	0.20	157,157,157,157	0
60	MG	BA	3097	1/1	0.34	0.37	88,88,88,88	0
60	MG	BA	3051	1/1	0.35	0.75	72,72,72,72	0
60	MG	BA	3063	1/1	0.35	0.64	136,136,136,136	0
60	MG	DA	3082	1/1	0.35	0.77	77,77,77,77	0
60	MG	BA	3086	1/1	0.36	0.61	114,114,114,114	0
60	MG	CA	1650	1/1	0.36	1.29	127,127,127,127	0
60	MG	AA	1646	1/1	0.36	0.97	125,125,125,125	0
60	MG	AA	1638	1/1	0.37	0.13	139,139,139,139	1
60	MG	BA	3089	1/1	0.37	0.52	155,155,155,155	0
60	MG	AA	1627	1/1	0.38	1.24	101,101,101,101	0
60	MG	BA	2995	1/1	0.39	0.43	105,105,105,105	0
60	MG	AA	1665	1/1	0.39	2.52	121,121,121,121	0
60	MG	CA	1626	1/1	0.39	1.39	102,102,102,102	0
60	MG	DA	2901	1/1	0.40	0.79	136,136,136,136	0
60	MG	AA	1603	1/1	0.40	1.36	94,94,94,94	0
60	MG	AA	1652	1/1	0.40	0.35	103,103,103,103	1
60	MG	CA	1678	1/1	0.40	0.56	86,86,86,86	1
60	MG	BA	3030	1/1	0.40	0.75	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
60	MG	DA	3096	1/1	0.42	1.00	124,124,124,124	0
60	MG	CA	1612	1/1	0.43	0.56	102,102,102,102	0
60	MG	CA	1698	1/1	0.43	1.21	145,145,145,145	0
60	MG	BA	3084	1/1	0.44	0.85	126,126,126,126	0
60	MG	DA	3057	1/1	0.44	0.47	92,92,92,92	0
60	MG	DA	3081	1/1	0.45	0.57	104,104,104,104	0
60	MG	CA	1667	1/1	0.45	1.45	83,83,83,83	1
60	MG	BB	201	1/1	0.45	1.05	84,84,84,84	0
60	MG	BA	3046	1/1	0.46	0.49	112,112,112,112	0
60	MG	BA	3053	1/1	0.46	0.81	122,122,122,122	0
60	MG	DA	2990	1/1	0.46	0.65	88,88,88,88	0
60	MG	DA	3103	1/1	0.46	0.32	82,82,82,82	0
60	MG	DA	3099	1/1	0.47	0.62	108,108,108,108	0
60	MG	CA	1668	1/1	0.47	0.32	93,93,93,93	0
60	MG	DA	3122	1/1	0.47	1.24	79,79,79,79	0
60	MG	DA	2986	1/1	0.48	0.75	87,87,87,87	0
60	MG	BA	2977	1/1	0.48	1.11	107,107,107,107	0
60	MG	DA	2991	1/1	0.48	0.42	126,126,126,126	0
60	MG	DA	3048	1/1	0.49	0.62	129,129,129,129	0
60	MG	CA	1624	1/1	0.50	1.65	119,119,119,119	0
60	MG	CA	1665	1/1	0.50	0.60	111,111,111,111	1
60	MG	DA	3058	1/1	0.50	0.49	104,104,104,104	0
60	MG	AA	1675	1/1	0.51	0.43	93,93,93,93	0
60	MG	AA	1643	1/1	0.51	0.65	106,106,106,106	0
60	MG	BA	2988	1/1	0.52	0.69	117,117,117,117	0
60	MG	DA	3114	1/1	0.52	0.76	96,96,96,96	0
60	MG	DA	3018	1/1	0.52	0.42	114,114,114,114	0
60	MG	BA	3102	1/1	0.53	0.52	108,108,108,108	0
60	MG	CA	1634	1/1	0.54	0.34	122,122,122,122	0
60	MG	AA	1634	1/1	0.54	1.60	120,120,120,120	0
60	MG	DA	3004	1/1	0.54	0.52	113,113,113,113	0
60	MG	BA	3093	1/1	0.54	0.78	99,99,99,99	0
60	MG	DA	3071	1/1	0.54	0.87	123,123,123,123	0
60	MG	AA	1601	1/1	0.54	0.87	100,100,100,100	0
60	MG	DA	3008	1/1	0.55	0.24	92,92,92,92	0
60	MG	CA	1606	1/1	0.55	0.48	118,118,118,118	0
60	MG	DA	3117	1/1	0.55	0.92	123,123,123,123	0
60	MG	CA	1690	1/1	0.55	0.80	100,100,100,100	0
60	MG	BA	3088	1/1	0.56	0.39	105,105,105,105	0
60	MG	BA	3126	1/1	0.56	1.74	131,131,131,131	0
60	MG	BA	3100	1/1	0.56	0.48	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	1677	1/1	0.56	0.86	88,88,88,88	0
60	MG	AA	1691	1/1	0.56	0.38	96,96,96,96	0
60	MG	BA	3107	1/1	0.57	0.51	87,87,87,87	0
60	MG	DA	3019	1/1	0.57	0.88	112,112,112,112	0
60	MG	CA	1691	1/1	0.57	1.46	105,105,105,105	0
60	MG	BA	3098	1/1	0.57	0.68	89,89,89,89	0
60	MG	AA	1606	1/1	0.57	1.07	98,98,98,98	0
60	MG	AA	1641	1/1	0.58	0.59	93,93,93,93	0
60	MG	CA	1658	1/1	0.58	0.39	93,93,93,93	0
60	MG	DA	3106	1/1	0.59	0.77	143,143,143,143	0
60	MG	CA	1639	1/1	0.59	0.37	99,99,99,99	0
60	MG	CA	1686	1/1	0.59	0.54	94,94,94,94	0
60	MG	DA	3010	1/1	0.59	0.59	92,92,92,92	0
60	MG	DA	3124	1/1	0.59	1.96	98,98,98,98	0
60	MG	DA	3141	1/1	0.59	0.67	92,92,92,92	0
60	MG	AA	1649	1/1	0.60	0.72	124,124,124,124	0
60	MG	DA	3115	1/1	0.60	0.50	162,162,162,162	0
60	MG	DA	3098	1/1	0.61	0.61	107,107,107,107	0
60	MG	DA	3135	1/1	0.61	1.42	103,103,103,103	0
60	MG	CA	1662	1/1	0.61	0.69	113,113,113,113	0
60	MG	DA	3035	1/1	0.62	0.51	105,105,105,105	0
60	MG	CA	1644	1/1	0.62	0.68	94,94,94,94	0
60	MG	BA	2985	1/1	0.62	0.36	87,87,87,87	0
60	MG	DA	3055	1/1	0.62	0.26	106,106,106,106	0
60	MG	CA	1700	1/1	0.62	0.52	113,113,113,113	0
60	MG	CA	1702	1/1	0.62	1.22	96,96,96,96	0
60	MG	CA	1604	1/1	0.62	0.71	115,115,115,115	0
60	MG	DF	301	1/1	0.62	0.30	100,100,100,100	0
60	MG	CA	1601	1/1	0.63	0.87	86,86,86,86	0
60	MG	BA	3121	1/1	0.63	0.47	112,112,112,112	0
60	MG	DA	3088	1/1	0.64	0.80	110,110,110,110	0
60	MG	AA	1636	1/1	0.64	0.76	142,142,142,142	0
60	MG	AA	1608	1/1	0.65	0.44	81,81,81,81	0
60	MG	CG	201	1/1	0.65	0.53	83,83,83,83	1
60	MG	DA	3137	1/1	0.65	0.57	121,121,121,121	0
60	MG	DA	3090	1/1	0.65	0.69	106,106,106,106	0
60	MG	AA	1660	1/1	0.65	0.31	105,105,105,105	0
60	MG	AA	1604	1/1	0.66	0.39	132,132,132,132	0
60	MG	CA	1659	1/1	0.66	0.35	104,104,104,104	1
60	MG	BA	3064	1/1	0.66	0.48	86,86,86,86	0
60	MG	DA	3063	1/1	0.67	0.92	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3068	1/1	0.67	1.07	102,102,102,102	0
60	MG	DA	3031	1/1	0.67	0.83	92,92,92,92	0
60	MG	DA	3077	1/1	0.67	0.61	96,96,96,96	0
60	MG	BA	3114	1/1	0.67	1.60	130,130,130,130	0
60	MG	DA	3037	1/1	0.67	0.44	74,74,74,74	0
60	MG	BA	3020	1/1	0.67	0.63	103,103,103,103	0
60	MG	CA	1671	1/1	0.67	0.59	95,95,95,95	0
60	MG	CA	1653	1/1	0.67	0.61	127,127,127,127	0
60	MG	BA	3124	1/1	0.67	0.84	120,120,120,120	0
60	MG	DA	3029	1/1	0.67	0.65	99,99,99,99	0
60	MG	AA	1672	1/1	0.68	1.41	136,136,136,136	0
60	MG	BA	3007	1/1	0.68	0.33	125,125,125,125	0
60	MG	BA	3012	1/1	0.68	1.21	91,91,91,91	0
60	MG	AA	1677	1/1	0.68	0.24	114,114,114,114	0
60	MG	BA	3090	1/1	0.68	1.40	123,123,123,123	0
60	MG	BA	3083	1/1	0.69	0.52	87,87,87,87	0
60	MG	AA	1667	1/1	0.69	0.97	118,118,118,118	0
60	MG	DA	3022	1/1	0.69	0.31	81,81,81,81	0
60	MG	DA	3097	1/1	0.69	0.54	112,112,112,112	0
60	MG	DA	2972	1/1	0.69	0.60	100,100,100,100	0
60	MG	DA	3080	1/1	0.69	0.74	130,130,130,130	0
60	MG	DA	3102	1/1	0.69	0.38	80,80,80,80	0
60	MG	BA	3018	1/1	0.69	1.54	109,109,109,109	0
60	MG	CV	102	1/1	0.69	1.68	132,132,132,132	1
60	MG	DR	201	1/1	0.69	1.03	117,117,117,117	0
60	MG	BA	2966	1/1	0.70	0.40	92,92,92,92	0
60	MG	CA	1664	1/1	0.70	0.96	112,112,112,112	0
60	MG	BA	3115	1/1	0.70	0.84	85,85,85,85	0
60	MG	BA	2970	1/1	0.70	1.24	86,86,86,86	0
60	MG	BA	3106	1/1	0.70	0.74	97,97,97,97	0
60	MG	DA	2965	1/1	0.70	0.57	96,96,96,96	0
60	MG	DA	2969	1/1	0.70	0.83	84,84,84,84	0
60	MG	CA	1654	1/1	0.70	0.47	107,107,107,107	0
60	MG	AA	1686	1/1	0.70	1.39	99,99,99,99	0
60	MG	DA	3070	1/1	0.70	0.84	79,79,79,79	0
60	MG	DA	3100	1/1	0.70	0.81	113,113,113,113	0
60	MG	BA	3108	1/1	0.70	0.47	102,102,102,102	0
60	MG	CA	1696	1/1	0.71	1.18	162,162,162,162	0
60	MG	BA	2908	1/1	0.71	1.25	103,103,103,103	0
60	MG	DA	2929	1/1	0.71	0.70	94,94,94,94	0
60	MG	BA	2960	1/1	0.71	0.58	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3003	1/1	0.71	0.90	69,69,69,69	1
60	MG	AA	1624	1/1	0.71	0.66	111,111,111,111	0
60	MG	AA	1670	1/1	0.71	1.39	130,130,130,130	0
60	MG	CA	1633	1/1	0.72	0.66	93,93,93,93	0
60	MG	DA	3046	1/1	0.72	0.84	76,76,76,76	0
60	MG	BA	3022	1/1	0.72	0.46	125,125,125,125	0
60	MG	DA	3014	1/1	0.72	0.78	77,77,77,77	0
60	MG	CA	1688	1/1	0.72	0.95	103,103,103,103	0
60	MG	DA	3094	1/1	0.72	0.45	87,87,87,87	0
60	MG	CA	1618	1/1	0.72	0.55	83,83,83,83	0
60	MG	CA	1623	1/1	0.72	0.20	82,82,82,82	0
60	MG	DA	2999	1/1	0.72	0.22	94,94,94,94	0
60	MG	BA	3109	1/1	0.72	0.59	101,101,101,101	0
60	MG	AA	1689	1/1	0.72	0.27	98,98,98,98	0
60	MG	BA	3043	1/1	0.72	0.24	83,83,83,83	0
60	MG	DA	3056	1/1	0.73	0.47	126,126,126,126	0
60	MG	BA	3113	1/1	0.73	0.34	126,126,126,126	0
60	MG	BA	3080	1/1	0.73	0.58	115,115,115,115	0
60	MG	CA	1616	1/1	0.73	0.17	105,105,105,105	0
60	MG	CA	1641	1/1	0.73	1.46	94,94,94,94	0
60	MG	CA	1643	1/1	0.73	0.24	105,105,105,105	0
60	MG	BA	3006	1/1	0.73	0.39	91,91,91,91	0
60	MG	DA	3072	1/1	0.73	0.41	102,102,102,102	0
60	MG	DA	3017	1/1	0.73	0.12	97,97,97,97	0
60	MG	DB	201	1/1	0.73	0.43	69,69,69,69	0
60	MG	BA	3129	1/1	0.73	0.63	84,84,84,84	0
60	MG	DA	2962	1/1	0.73	0.48	89,89,89,89	0
60	MG	DX	101	1/1	0.73	0.73	72,72,72,72	1
60	MG	DA	2942	1/1	0.74	0.93	90,90,90,90	0
60	MG	CA	1685	1/1	0.74	0.33	115,115,115,115	0
60	MG	DA	3024	1/1	0.74	0.72	106,106,106,106	0
60	MG	CA	1699	1/1	0.74	0.38	134,134,134,134	0
60	MG	DA	3061	1/1	0.74	0.45	94,94,94,94	0
60	MG	BA	3011	1/1	0.74	0.77	106,106,106,106	0
60	MG	BA	2965	1/1	0.74	0.40	111,111,111,111	0
60	MG	BA	3096	1/1	0.74	0.32	84,84,84,84	0
60	MG	DA	3039	1/1	0.74	0.69	85,85,85,85	0
60	MG	BA	3008	1/1	0.74	0.67	96,96,96,96	0
60	MG	BF	301	1/1	0.74	0.55	100,100,100,100	0
60	MG	CA	1680	1/1	0.74	0.64	148,148,148,148	0
60	MG	DA	3105	1/1	0.74	0.33	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3002	1/1	0.75	1.08	97,97,97,97	0
60	MG	BA	2975	1/1	0.75	0.32	92,92,92,92	0
60	MG	DA	2998	1/1	0.75	0.52	91,91,91,91	0
60	MG	AA	1661	1/1	0.75	0.96	94,94,94,94	0
60	MG	CA	1670	1/1	0.75	0.09	153,153,153,153	0
60	MG	BA	3015	1/1	0.75	0.56	94,94,94,94	0
60	MG	DA	2949	1/1	0.75	0.91	102,102,102,102	0
60	MG	DA	3044	1/1	0.75	0.23	79,79,79,79	0
60	MG	CA	1629	1/1	0.76	0.98	95,95,95,95	0
60	MG	CA	1632	1/1	0.76	0.15	79,79,79,79	0
60	MG	BA	2920	1/1	0.76	1.17	98,98,98,98	0
60	MG	CA	1609	1/1	0.76	0.14	84,84,84,84	0
60	MG	CA	1636	1/1	0.76	0.51	90,90,90,90	0
60	MG	B1	101	1/1	0.76	0.56	113,113,113,113	0
60	MG	DA	3083	1/1	0.76	1.08	112,112,112,112	0
60	MG	CA	1613	1/1	0.76	0.41	89,89,89,89	0
60	MG	BA	3026	1/1	0.76	0.32	85,85,85,85	0
60	MG	DA	3091	1/1	0.76	0.34	107,107,107,107	0
60	MG	AA	1674	1/1	0.76	0.97	87,87,87,87	1
60	MG	CA	1622	1/1	0.76	0.51	93,93,93,93	0
60	MG	BA	3120	1/1	0.76	0.52	111,111,111,111	0
60	MG	CA	1603	1/1	0.76	0.86	113,113,113,113	0
60	MG	BA	3032	1/1	0.76	0.70	98,98,98,98	0
60	MG	AA	1650	1/1	0.76	0.71	111,111,111,111	0
60	MG	DA	2953	1/1	0.77	0.33	65,65,65,65	0
60	MG	BA	3066	1/1	0.77	0.99	113,113,113,113	0
60	MG	DA	3002	1/1	0.77	0.36	95,95,95,95	0
60	MG	BA	3078	1/1	0.77	0.33	104,104,104,104	0
60	MG	AA	1622	1/1	0.77	0.28	128,128,128,128	0
60	MG	AV	101	1/1	0.77	0.57	83,83,83,83	1
60	MG	BA	3035	1/1	0.77	0.18	86,86,86,86	0
60	MG	BA	3123	1/1	0.77	0.60	80,80,80,80	0
60	MG	DA	3085	1/1	0.77	0.51	86,86,86,86	0
60	MG	DA	3104	1/1	0.77	0.64	118,118,118,118	0
60	MG	AA	1635	1/1	0.77	0.30	111,111,111,111	0
60	MG	BA	2982	1/1	0.77	0.26	100,100,100,100	0
60	MG	DA	2975	1/1	0.78	1.21	138,138,138,138	0
60	MG	DA	3125	1/1	0.78	0.40	72,72,72,72	0
60	MG	DA	3132	1/1	0.78	0.57	120,120,120,120	0
60	MG	BA	2973	1/1	0.78	0.66	92,92,92,92	0
60	MG	BA	3081	1/1	0.78	0.64	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1614	1/1	0.78	0.58	98,98,98,98	0
60	MG	CA	1689	1/1	0.78	0.69	75,75,75,75	0
60	MG	BA	2949	1/1	0.78	0.48	77,77,77,77	0
60	MG	DA	3034	1/1	0.78	0.29	72,72,72,72	0
60	MG	AA	1695	1/1	0.78	0.36	105,105,105,105	0
60	MG	BA	2996	1/1	0.79	1.04	106,106,106,106	0
60	MG	BA	2983	1/1	0.79	0.34	108,108,108,108	0
60	MG	BA	3040	1/1	0.79	1.06	99,99,99,99	0
60	MG	CA	1694	1/1	0.79	0.94	112,112,112,112	0
60	MG	BA	3073	1/1	0.79	0.29	100,100,100,100	0
60	MG	CA	1687	1/1	0.79	0.41	119,119,119,119	0
60	MG	DA	3043	1/1	0.79	0.30	96,96,96,96	0
60	MG	AA	1625	1/1	0.79	0.46	85,85,85,85	0
60	MG	BA	3060	1/1	0.79	0.86	83,83,83,83	0
60	MG	CA	1675	1/1	0.80	0.31	122,122,122,122	0
60	MG	DA	3027	1/1	0.80	0.90	92,92,92,92	0
60	MG	BA	3128	1/1	0.80	0.45	117,117,117,117	0
60	MG	BA	3058	1/1	0.80	0.48	88,88,88,88	0
60	MG	DA	3128	1/1	0.80	1.26	92,92,92,92	0
60	MG	CA	1631	1/1	0.80	0.98	111,111,111,111	0
60	MG	AA	1651	1/1	0.80	0.32	113,113,113,113	0
60	MG	CA	1669	1/1	0.80	0.28	113,113,113,113	0
60	MG	DA	2951	1/1	0.80	1.03	91,91,91,91	0
60	MG	DA	3089	1/1	0.80	1.21	92,92,92,92	0
60	MG	BA	3038	1/1	0.80	0.34	90,90,90,90	0
60	MG	AA	1699	1/1	0.80	0.64	109,109,109,109	0
60	MG	AA	1693	1/1	0.80	0.96	119,119,119,119	0
60	MG	BA	2942	1/1	0.81	0.86	107,107,107,107	0
60	MG	AA	1609	1/1	0.81	0.86	106,106,106,106	0
60	MG	DA	3121	1/1	0.81	0.61	104,104,104,104	0
60	MG	DA	2956	1/1	0.81	0.48	63,63,63,63	0
60	MG	CA	1608	1/1	0.81	0.17	113,113,113,113	0
60	MG	CA	1652	1/1	0.81	0.77	148,148,148,148	0
60	MG	BA	3042	1/1	0.81	0.46	78,78,78,78	0
60	MG	CA	1703	1/1	0.81	0.31	107,107,107,107	0
60	MG	BA	3085	1/1	0.81	0.59	118,118,118,118	0
60	MG	BA	2976	1/1	0.81	0.50	66,66,66,66	0
60	MG	BA	2984	1/1	0.81	0.84	95,95,95,95	0
60	MG	CA	1660	1/1	0.81	0.84	95,95,95,95	0
60	MG	DA	2935	1/1	0.81	0.81	68,68,68,68	0
60	MG	BA	3062	1/1	0.81	0.61	89,89,89,89	0
60	MG	CA	1663	1/1	0.81	0.37	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1656	1/1	0.82	0.25	140,140,140,140	0
60	MG	B0	101	1/1	0.82	0.50	98,98,98,98	0
60	MG	BA	2969	1/1	0.82	0.45	61,61,61,61	0
60	MG	BA	3025	1/1	0.82	0.74	95,95,95,95	0
60	MG	DA	3086	1/1	0.82	0.56	78,78,78,78	0
60	MG	DA	2961	1/1	0.82	0.61	90,90,90,90	0
60	MG	DA	2996	1/1	0.82	0.36	63,63,63,63	0
60	MG	BA	2955	1/1	0.82	1.12	109,109,109,109	0
60	MG	DA	3142	1/1	0.82	0.21	81,81,81,81	0
60	MG	DA	2963	1/1	0.82	0.53	70,70,70,70	0
60	MG	AA	1671	1/1	0.82	1.00	96,96,96,96	0
60	MG	BA	3118	1/1	0.82	1.47	110,110,110,110	0
60	MG	BA	2963	1/1	0.82	0.68	103,103,103,103	0
60	MG	BA	3016	1/1	0.83	0.23	102,102,102,102	0
60	MG	DA	3118	1/1	0.83	0.63	73,73,73,73	0
60	MG	DA	3013	1/1	0.83	0.98	89,89,89,89	0
60	MG	AA	1640	1/1	0.83	0.51	64,64,64,64	1
60	MG	CA	1611	1/1	0.83	0.42	97,97,97,97	0
60	MG	DA	3042	1/1	0.83	0.35	81,81,81,81	0
60	MG	BX	101	1/1	0.83	1.30	110,110,110,110	1
60	MG	BA	2905	1/1	0.83	0.44	58,58,58,58	0
60	MG	DA	3000	1/1	0.83	0.52	77,77,77,77	0
60	MG	DA	3047	1/1	0.83	0.23	112,112,112,112	0
60	MG	AA	1688	1/1	0.83	1.14	113,113,113,113	0
60	MG	DA	3053	1/1	0.83	0.40	71,71,71,71	0
60	MG	BA	3082	1/1	0.83	0.44	101,101,101,101	0
60	MG	BA	2952	1/1	0.83	0.83	87,87,87,87	0
60	MG	DA	2980	1/1	0.83	1.16	111,111,111,111	0
60	MG	BA	2992	1/1	0.83	0.54	61,61,61,61	0
60	MG	BA	3125	1/1	0.84	0.46	91,91,91,91	0
60	MG	DA	3101	1/1	0.84	0.12	88,88,88,88	0
60	MG	BA	3076	1/1	0.84	0.57	108,108,108,108	0
60	MG	BA	2971	1/1	0.84	0.13	52,52,52,52	0
60	MG	BA	2993	1/1	0.84	0.75	92,92,92,92	0
60	MG	DA	3023	1/1	0.84	0.38	103,103,103,103	0
60	MG	BA	2950	1/1	0.84	0.93	81,81,81,81	0
60	MG	AA	1637	1/1	0.84	0.55	99,99,99,99	0
60	MG	BA	3019	1/1	0.84	0.39	74,74,74,74	0
60	MG	CA	1655	1/1	0.84	0.68	111,111,111,111	0
60	MG	DA	2903	1/1	0.84	1.02	85,85,85,85	0
60	MG	BA	3049	1/1	0.84	0.44	65,65,65,65	0
60	MG	BA	2997	1/1	0.84	0.13	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1617	1/1	0.84	0.46	104,104,104,104	0
60	MG	DA	3001	1/1	0.84	0.28	69,69,69,69	0
60	MG	AA	1613	1/1	0.84	1.48	114,114,114,114	0
60	MG	AA	1620	1/1	0.84	0.24	134,134,134,134	0
60	MG	BA	2921	1/1	0.84	0.34	98,98,98,98	0
60	MG	DA	3136	1/1	0.84	0.21	94,94,94,94	0
60	MG	DA	3045	1/1	0.84	0.96	104,104,104,104	0
60	MG	DA	3007	1/1	0.84	0.26	82,82,82,82	0
60	MG	BA	2930	1/1	0.84	1.33	117,117,117,117	0
60	MG	AA	1681	1/1	0.84	0.91	99,99,99,99	0
60	MG	BA	3037	1/1	0.84	0.82	79,79,79,79	0
60	MG	B5	102	1/1	0.84	0.56	79,79,79,79	0
60	MG	CA	1697	1/1	0.84	0.86	126,126,126,126	0
60	MG	AA	1639	1/1	0.85	0.41	98,98,98,98	1
60	MG	DA	2981	1/1	0.85	0.83	105,105,105,105	0
60	MG	D5	101	1/1	0.85	0.35	56,56,56,56	0
60	MG	DA	2960	1/1	0.85	0.67	59,59,59,59	0
60	MG	BA	3105	1/1	0.85	0.16	68,68,68,68	0
60	MG	DA	2992	1/1	0.85	0.38	75,75,75,75	0
60	MG	BA	3029	1/1	0.85	0.33	139,139,139,139	0
60	MG	CA	1615	1/1	0.85	0.69	127,127,127,127	0
60	MG	BA	3024	1/1	0.85	0.45	96,96,96,96	0
60	MG	DA	2940	1/1	0.85	0.73	72,72,72,72	0
60	MG	BA	3055	1/1	0.85	0.62	87,87,87,87	0
60	MG	BA	2902	1/1	0.85	0.33	155,155,155,155	0
60	MG	BA	3047	1/1	0.85	0.21	105,105,105,105	0
60	MG	DA	3075	1/1	0.85	0.36	75,75,75,75	0
60	MG	AA	1663	1/1	0.86	0.77	83,83,83,83	0
60	MG	CA	1682	1/1	0.86	0.16	151,151,151,151	0
60	MG	CA	1610	1/1	0.86	0.20	116,116,116,116	0
60	MG	BA	3072	1/1	0.86	0.85	89,89,89,89	0
60	MG	AA	1678	1/1	0.86	0.54	121,121,121,121	0
60	MG	CA	1628	1/1	0.86	0.42	66,66,66,66	0
60	MG	BA	3075	1/1	0.86	0.19	100,100,100,100	0
60	MG	DA	2979	1/1	0.86	0.32	57,57,57,57	0
60	MG	AA	1621	1/1	0.86	0.38	95,95,95,95	0
60	MG	BA	2937	1/1	0.86	0.75	70,70,70,70	0
60	MG	DA	2984	1/1	0.86	0.60	120,120,120,120	0
60	MG	BA	3132	1/1	0.86	0.48	116,116,116,116	0
60	MG	BA	2953	1/1	0.86	1.12	113,113,113,113	0
60	MG	DA	3069	1/1	0.87	0.58	73,73,73,73	0
60	MG	AA	1664	1/1	0.87	0.26	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3021	1/1	0.87	0.28	81,81,81,81	0
60	MG	BA	2994	1/1	0.87	0.27	77,77,77,77	0
60	MG	BA	2938	1/1	0.87	0.30	67,67,67,67	0
60	MG	DA	3127	1/1	0.87	1.24	112,112,112,112	0
60	MG	AA	1648	1/1	0.87	0.72	92,92,92,92	0
60	MG	DA	3078	1/1	0.87	0.71	122,122,122,122	0
60	MG	BA	3130	1/1	0.87	0.30	111,111,111,111	0
60	MG	BA	3104	1/1	0.87	0.24	115,115,115,115	0
60	MG	BA	3068	1/1	0.87	1.41	103,103,103,103	0
60	MG	DA	3011	1/1	0.87	0.38	88,88,88,88	0
60	MG	BA	2919	1/1	0.87	0.50	75,75,75,75	0
60	MG	BA	2932	1/1	0.87	0.36	61,61,61,61	0
60	MG	DA	3015	1/1	0.87	0.47	76,76,76,76	0
60	MG	CA	1642	1/1	0.87	1.27	97,97,97,97	0
60	MG	BA	3014	1/1	0.87	0.39	74,74,74,74	0
60	MG	BA	3087	1/1	0.88	0.97	112,112,112,112	0
60	MG	CA	1684	1/1	0.88	0.38	101,101,101,101	0
60	MG	CA	1646	1/1	0.88	0.55	119,119,119,119	0
60	MG	DA	3033	1/1	0.88	0.19	100,100,100,100	0
60	MG	BA	3023	1/1	0.88	1.15	79,79,79,79	0
60	MG	DA	3093	1/1	0.88	0.48	86,86,86,86	0
60	MG	BA	3103	1/1	0.88	1.04	107,107,107,107	0
60	MG	BA	3079	1/1	0.88	0.88	72,72,72,72	0
60	MG	BA	3122	1/1	0.88	0.74	84,84,84,84	0
60	MG	DA	2997	1/1	0.88	0.18	79,79,79,79	0
60	MG	DA	3134	1/1	0.88	0.73	89,89,89,89	0
60	MG	DA	3016	1/1	0.88	0.16	83,83,83,83	0
60	MG	AA	1657	1/1	0.88	0.34	121,121,121,121	0
60	MG	AA	1631	1/1	0.88	0.69	87,87,87,87	0
60	MG	AA	1632	1/1	0.88	0.77	75,75,75,75	0
60	MG	BA	3013	1/1	0.88	0.30	72,72,72,72	0
60	MG	BA	2987	1/1	0.88	0.72	100,100,100,100	0
60	MG	BA	3031	1/1	0.88	0.85	108,108,108,108	0
60	MG	AA	1615	1/1	0.88	0.95	84,84,84,84	0
60	MG	DA	3025	1/1	0.88	0.56	51,51,51,51	0
60	MG	AA	1647	1/1	0.89	0.39	104,104,104,104	0
60	MG	CA	1681	1/1	0.89	0.25	113,113,113,113	1
60	MG	AA	1629	1/1	0.89	0.52	65,65,65,65	1
60	MG	DA	3131	1/1	0.89	0.80	102,102,102,102	0
60	MG	BA	3009	1/1	0.89	0.98	117,117,117,117	0
60	MG	DA	2985	1/1	0.89	0.26	85,85,85,85	0
60	MG	BB	202	1/1	0.89	0.90	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3112	1/1	0.89	0.81	83,83,83,83	0
60	MG	CV	101	1/1	0.89	0.40	67,67,67,67	0
60	MG	BA	3021	1/1	0.89	0.14	79,79,79,79	0
60	MG	DA	3020	1/1	0.89	0.23	50,50,50,50	0
60	MG	AA	1628	1/1	0.89	0.48	87,87,87,87	0
60	MG	BA	2939	1/1	0.89	0.47	50,50,50,50	0
60	MG	DA	3059	1/1	0.89	1.06	110,110,110,110	0
60	MG	DA	2978	1/1	0.89	0.53	85,85,85,85	0
60	MG	BA	2998	1/1	0.90	0.62	88,88,88,88	0
60	MG	BA	2990	1/1	0.90	0.36	81,81,81,81	0
60	MG	BA	2931	1/1	0.90	0.41	72,72,72,72	0
60	MG	BA	2945	1/1	0.90	0.93	73,73,73,73	0
60	MG	AA	1703	1/1	0.90	1.31	102,102,102,102	0
60	MG	DA	3074	1/1	0.90	0.71	96,96,96,96	0
60	MG	AA	1611	1/1	0.90	0.22	82,82,82,82	0
60	MG	AA	1701	1/1	0.90	0.65	71,71,71,71	0
60	MG	BA	2909	1/1	0.90	0.50	64,64,64,64	0
60	MG	DA	3049	1/1	0.90	0.50	85,85,85,85	0
60	MG	BA	3116	1/1	0.90	0.27	91,91,91,91	0
60	MG	BA	3131	1/1	0.90	0.59	79,79,79,79	0
60	MG	BA	3091	1/1	0.90	0.46	79,79,79,79	0
60	MG	DA	2993	1/1	0.90	0.31	79,79,79,79	0
60	MG	DA	2994	1/1	0.90	0.60	52,52,52,52	0
60	MG	DA	2908	1/1	0.90	0.93	83,83,83,83	0
60	MG	BA	3092	1/1	0.90	0.57	82,82,82,82	0
60	MG	DA	3116	1/1	0.90	0.86	104,104,104,104	0
60	MG	CA	1645	1/1	0.90	0.21	68,68,68,68	0
60	MG	BA	2948	1/1	0.91	0.35	67,67,67,67	0
60	MG	BA	2904	1/1	0.91	0.76	56,56,56,56	0
60	MG	BA	2927	1/1	0.91	0.67	59,59,59,59	0
60	MG	DA	2970	1/1	0.91	0.13	47,47,47,47	0
60	MG	BA	2968	1/1	0.91	1.08	72,72,72,72	0
60	MG	CA	1625	1/1	0.91	0.59	96,96,96,96	0
60	MG	DA	2915	1/1	0.91	0.41	64,64,64,64	0
60	MG	DA	2916	1/1	0.91	0.81	53,53,53,53	0
60	MG	DA	3095	1/1	0.91	0.33	98,98,98,98	0
60	MG	BA	3052	1/1	0.91	0.23	99,99,99,99	0
60	MG	DA	3130	1/1	0.91	1.38	115,115,115,115	0
60	MG	BA	2916	1/1	0.91	0.30	71,71,71,71	0
60	MG	BA	2940	1/1	0.91	0.53	64,64,64,64	0
60	MG	AA	1685	1/1	0.91	0.30	66,66,66,66	0
60	MG	BA	3059	1/1	0.91	0.47	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	2999	1/1	0.91	0.77	121,121,121,121	0
60	MG	BA	3110	1/1	0.91	1.16	101,101,101,101	0
60	MG	DA	3138	1/1	0.91	0.42	113,113,113,113	0
60	MG	BA	3111	1/1	0.91	0.93	103,103,103,103	0
60	MG	AA	1673	1/1	0.91	0.09	79,79,79,79	0
60	MG	BA	2961	1/1	0.91	0.73	78,78,78,78	0
60	MG	DA	2995	1/1	0.91	0.74	75,75,75,75	0
60	MG	BA	3136	1/1	0.91	0.64	106,106,106,106	0
60	MG	BA	3028	1/1	0.91	0.46	89,89,89,89	0
60	MG	DA	2922	1/1	0.92	0.41	59,59,59,59	0
60	MG	DA	2924	1/1	0.92	0.23	87,87,87,87	0
60	MG	BA	2991	1/1	0.92	0.47	122,122,122,122	0
60	MG	DA	2983	1/1	0.92	0.32	93,93,93,93	0
60	MG	BA	2967	1/1	0.92	0.67	57,57,57,57	0
60	MG	AA	1690	1/1	0.92	0.82	96,96,96,96	0
60	MG	CA	1617	1/1	0.92	0.14	93,93,93,93	0
60	MG	DA	2948	1/1	0.92	0.63	60,60,60,60	0
60	MG	CA	1676	1/1	0.92	0.32	119,119,119,119	0
60	MG	CA	1602	1/1	0.92	0.14	92,92,92,92	0
60	MG	DA	3054	1/1	0.92	0.79	80,80,80,80	0
60	MG	CA	1638	1/1	0.92	0.37	81,81,81,81	0
60	MG	AA	1659	1/1	0.92	1.13	113,113,113,113	0
60	MG	DA	2958	1/1	0.92	0.23	96,96,96,96	0
60	MG	BA	3054	1/1	0.92	0.41	94,94,94,94	0
60	MG	DA	3133	1/1	0.92	0.73	87,87,87,87	0
60	MG	CA	1661	1/1	0.92	0.41	81,81,81,81	0
60	MG	BA	2946	1/1	0.92	0.29	66,66,66,66	0
60	MG	AA	1607	1/1	0.92	0.16	107,107,107,107	0
60	MG	BA	3077	1/1	0.92	0.36	84,84,84,84	0
60	MG	BA	3044	1/1	0.92	0.77	108,108,108,108	0
60	MG	AA	1668	1/1	0.92	0.61	109,109,109,109	0
60	MG	AA	1696	1/1	0.92	0.82	90,90,90,90	0
60	MG	DA	2913	1/1	0.92	0.49	70,70,70,70	0
60	MG	AA	1619	1/1	0.92	0.17	72,72,72,72	0
60	MG	CA	1648	1/1	0.92	0.14	71,71,71,71	0
60	MG	DA	3076	1/1	0.92	0.29	119,119,119,119	0
61	ZN	CN	101	1/1	0.92	0.04	153,153,153,153	0
60	MG	AA	1692	1/1	0.93	1.16	101,101,101,101	0
60	MG	CA	1695	1/1	0.93	0.74	80,80,80,80	0
60	MG	BA	3095	1/1	0.93	0.21	97,97,97,97	0
60	MG	BA	3074	1/1	0.93	0.20	104,104,104,104	0
60	MG	AA	1700	1/1	0.93	1.33	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	2989	1/1	0.93	0.68	87,87,87,87	0
60	MG	BA	2933	1/1	0.93	0.66	77,77,77,77	0
60	MG	BA	2951	1/1	0.93	0.22	63,63,63,63	0
60	MG	AA	1683	1/1	0.93	0.43	89,89,89,89	0
60	MG	BA	2918	1/1	0.93	0.87	64,64,64,64	0
60	MG	CL	201	1/1	0.93	0.51	87,87,87,87	1
60	MG	BA	2954	1/1	0.93	0.34	66,66,66,66	0
60	MG	BA	3056	1/1	0.93	0.28	55,55,55,55	0
60	MG	AA	1687	1/1	0.93	0.20	74,74,74,74	0
60	MG	BA	2957	1/1	0.93	0.38	63,63,63,63	0
60	MG	DA	3065	1/1	0.93	0.90	75,75,75,75	0
60	MG	BA	2903	1/1	0.93	0.79	97,97,97,97	0
60	MG	DA	2904	1/1	0.93	0.82	49,49,49,49	0
60	MG	DA	3119	1/1	0.93	0.90	75,75,75,75	0
60	MG	DA	2905	1/1	0.93	0.45	59,59,59,59	0
60	MG	BA	3061	1/1	0.93	0.62	71,71,71,71	0
60	MG	BA	3039	1/1	0.93	0.50	67,67,67,67	0
60	MG	DA	3073	1/1	0.93	0.56	87,87,87,87	0
60	MG	DA	2914	1/1	0.93	0.42	49,49,49,49	0
60	MG	BP	201	1/1	0.93	0.21	71,71,71,71	0
60	MG	BA	2978	1/1	0.93	0.81	134,134,134,134	0
60	MG	AA	1655	1/1	0.93	0.36	94,94,94,94	1
60	MG	DA	2987	1/1	0.93	0.18	86,86,86,86	0
60	MG	DA	2989	1/1	0.93	0.59	79,79,79,79	0
60	MG	DA	3030	1/1	0.93	0.31	101,101,101,101	0
60	MG	BA	3065	1/1	0.93	1.01	122,122,122,122	0
60	MG	DA	3032	1/1	0.93	0.55	67,67,67,67	0
60	MG	AA	1698	1/1	0.93	1.43	80,80,80,80	0
60	MG	DA	2932	1/1	0.93	0.60	64,64,64,64	0
60	MG	BA	2964	1/1	0.93	0.42	80,80,80,80	0
60	MG	DA	2936	1/1	0.93	0.24	59,59,59,59	0
60	MG	CA	1605	1/1	0.93	0.20	104,104,104,104	0
60	MG	BA	2906	1/1	0.93	0.40	100,100,100,100	0
60	MG	DA	3092	1/1	0.93	0.47	86,86,86,86	0
60	MG	DA	2945	1/1	0.93	0.22	57,57,57,57	0
60	MG	DA	2947	1/1	0.93	0.18	51,51,51,51	0
60	MG	BA	2944	1/1	0.94	0.40	58,58,58,58	0
60	MG	BA	3069	1/1	0.94	0.18	87,87,87,87	0
60	MG	DA	2919	1/1	0.94	0.85	73,73,73,73	0
60	MG	BA	3070	1/1	0.94	0.86	118,118,118,118	0
60	MG	AX	101	1/1	0.94	0.74	96,96,96,96	0
60	MG	DA	3060	1/1	0.94	0.48	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
60	MG	CA	1635	1/1	0.94	0.12	98,98,98,98	0
60	MG	DA	3062	1/1	0.94	0.38	49,49,49,49	0
60	MG	DA	2931	1/1	0.94	0.44	52,52,52,52	0
60	MG	DA	3107	1/1	0.94	0.68	59,59,59,59	0
60	MG	DA	3110	1/1	0.94	0.74	63,63,63,63	0
60	MG	BA	2956	1/1	0.94	0.61	64,64,64,64	0
60	MG	DA	3113	1/1	0.94	0.49	96,96,96,96	0
60	MG	AA	1610	1/1	0.94	0.31	84,84,84,84	0
60	MG	AA	1626	1/1	0.94	0.16	99,99,99,99	0
60	MG	BA	3005	1/1	0.94	0.70	85,85,85,85	0
60	MG	BA	3135	1/1	0.94	0.47	83,83,83,83	0
60	MG	DA	3028	1/1	0.94	0.57	123,123,123,123	0
60	MG	DA	2943	1/1	0.94	0.24	59,59,59,59	0
60	MG	AA	1666	1/1	0.94	0.27	84,84,84,84	0
60	MG	BA	2974	1/1	0.94	0.95	68,68,68,68	0
60	MG	BA	2962	1/1	0.94	0.76	64,64,64,64	0
60	MG	CA	1620	1/1	0.94	1.10	115,115,115,115	0
60	MG	DA	3126	1/1	0.94	0.79	76,76,76,76	0
60	MG	DA	2950	1/1	0.94	0.36	55,55,55,55	0
60	MG	AA	1697	1/1	0.94	1.11	127,127,127,127	0
60	MG	CA	1673	1/1	0.94	0.48	116,116,116,116	0
60	MG	DA	3038	1/1	0.94	0.62	77,77,77,77	0
60	MG	BA	3117	1/1	0.94	0.49	72,72,72,72	0
60	MG	AA	1684	1/1	0.94	0.85	103,103,103,103	0
60	MG	BA	3119	1/1	0.94	0.98	99,99,99,99	0
60	MG	DA	3087	1/1	0.94	0.69	68,68,68,68	0
60	MG	D1	101	1/1	0.94	0.92	92,92,92,92	0
60	MG	BA	2929	1/1	0.94	0.71	65,65,65,65	0
60	MG	CA	1651	1/1	0.94	0.10	144,144,144,144	0
60	MG	BA	3027	1/1	0.94	0.56	51,51,51,51	0
60	MG	BA	2980	1/1	0.94	0.61	82,82,82,82	0
60	MG	CA	1683	1/1	0.94	0.13	93,93,93,93	0
60	MG	BA	2913	1/1	0.94	0.53	59,59,59,59	0
60	MG	DA	3050	1/1	0.94	1.43	105,105,105,105	0
60	MG	CA	1630	1/1	0.94	0.18	105,105,105,105	0
61	ZN	AN	101	1/1	0.94	0.04	153,153,153,153	0
61	ZN	CD	301	1/1	0.94	0.10	106,106,106,106	0
60	MG	CA	1657	1/1	0.94	0.28	56,56,56,56	1
60	MG	CA	1679	1/1	0.95	0.55	79,79,79,79	0
60	MG	BA	3067	1/1	0.95	0.21	93,93,93,93	0
60	MG	BA	2936	1/1	0.95	0.76	58,58,58,58	0
60	MG	BA	2959	1/1	0.95	0.48	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
60	MG	DA	3120	1/1	0.95	0.49	71,71,71,71	0
60	MG	DA	3026	1/1	0.95	0.35	78,78,78,78	0
60	MG	CA	1614	1/1	0.95	0.29	87,87,87,87	0
60	MG	BA	3057	1/1	0.95	0.52	73,73,73,73	0
60	MG	BA	2941	1/1	0.95	0.58	49,49,49,49	0
60	MG	BA	3036	1/1	0.95	0.30	97,97,97,97	0
60	MG	DA	2971	1/1	0.95	0.64	66,66,66,66	0
60	MG	B5	101	1/1	0.95	0.42	76,76,76,76	0
60	MG	DA	2938	1/1	0.95	0.34	45,45,45,45	0
60	MG	BA	3000	1/1	0.95	0.46	52,52,52,52	1
60	MG	DA	2941	1/1	0.95	0.24	45,45,45,45	0
60	MG	DA	3036	1/1	0.95	0.50	59,59,59,59	0
60	MG	CA	1621	1/1	0.95	0.13	96,96,96,96	0
60	MG	BA	3050	1/1	0.95	0.83	116,116,116,116	0
60	MG	DA	2902	1/1	0.95	0.15	152,152,152,152	0
60	MG	DA	3040	1/1	0.95	0.41	64,64,64,64	0
60	MG	BA	2986	1/1	0.95	0.63	81,81,81,81	0
60	MG	CA	1674	1/1	0.95	0.28	137,137,137,137	0
60	MG	CA	1693	1/1	0.95	0.55	65,65,65,65	0
60	MG	DA	2907	1/1	0.95	0.66	51,51,51,51	0
60	MG	DA	3108	1/1	0.95	0.53	61,61,61,61	0
60	MG	BA	3134	1/1	0.95	0.73	75,75,75,75	0
60	MG	BA	2972	1/1	0.95	0.75	76,76,76,76	0
60	MG	DA	2955	1/1	0.95	0.26	54,54,54,54	0
60	MG	BA	3041	1/1	0.95	0.52	71,71,71,71	0
60	MG	BA	2943	1/1	0.95	0.80	56,56,56,56	0
60	MG	AA	1658	1/1	0.96	0.65	92,92,92,92	0
60	MG	DA	2946	1/1	0.96	0.32	57,57,57,57	0
60	MG	BA	2923	1/1	0.96	0.50	78,78,78,78	0
60	MG	BA	2925	1/1	0.96	0.32	97,97,97,97	0
60	MG	AA	1676	1/1	0.96	0.25	104,104,104,104	0
60	MG	BA	3133	1/1	0.96	1.11	73,73,73,73	0
60	MG	AA	1605	1/1	0.96	0.33	66,66,66,66	0
60	MG	BA	3010	1/1	0.96	0.42	88,88,88,88	0
60	MG	DA	2954	1/1	0.96	0.25	57,57,57,57	0
60	MG	BA	2907	1/1	0.96	0.56	55,55,55,55	0
60	MG	DA	2909	1/1	0.96	0.68	55,55,55,55	0
60	MG	AA	1653	1/1	0.96	0.40	94,94,94,94	0
60	MG	B1	102	1/1	0.96	0.71	83,83,83,83	0
60	MG	DA	3123	1/1	0.96	0.62	82,82,82,82	0
60	MG	BA	2979	1/1	0.96	0.22	103,103,103,103	0
60	MG	DA	3006	1/1	0.96	0.52	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
60	MG	BA	3033	1/1	0.96	0.41	92,92,92,92	0
60	MG	DA	2918	1/1	0.96	0.66	59,59,59,59	0
60	MG	BA	3034	1/1	0.96	0.15	82,82,82,82	0
60	MG	DA	3129	1/1	0.96	0.28	113,113,113,113	0
60	MG	DA	2921	1/1	0.96	0.46	49,49,49,49	0
60	MG	AA	1654	1/1	0.96	0.50	139,139,139,139	0
60	MG	DA	2923	1/1	0.96	0.29	52,52,52,52	0
60	MG	CA	1649	1/1	0.96	0.12	82,82,82,82	0
60	MG	DA	2926	1/1	0.96	0.74	47,47,47,47	0
60	MG	DA	2974	1/1	0.96	0.70	92,92,92,92	0
60	MG	DA	2928	1/1	0.96	0.41	42,42,42,42	0
60	MG	BA	2981	1/1	0.96	0.15	88,88,88,88	0
60	MG	DA	2930	1/1	0.96	0.47	55,55,55,55	0
60	MG	DA	3140	1/1	0.96	0.69	77,77,77,77	0
60	MG	BA	3099	1/1	0.96	0.25	117,117,117,117	0
60	MG	CA	1701	1/1	0.96	0.53	58,58,58,58	0
60	MG	BA	2914	1/1	0.96	0.39	83,83,83,83	0
60	MG	AA	1694	1/1	0.96	0.54	102,102,102,102	0
60	MG	AA	1702	1/1	0.96	0.76	74,74,74,74	0
60	MG	AA	1682	1/1	0.96	0.39	98,98,98,98	0
60	MG	AL	201	1/1	0.96	0.40	125,125,125,125	1
60	MG	BA	3127	1/1	0.96	0.42	84,84,84,84	0
60	MG	BA	3004	1/1	0.96	0.31	63,63,63,63	0
60	MG	AA	1616	1/1	0.97	0.40	84,84,84,84	0
60	MG	DA	3052	1/1	0.97	0.27	57,57,57,57	0
60	MG	AA	1669	1/1	0.97	0.28	96,96,96,96	0
60	MG	DA	2988	1/1	0.97	0.22	111,111,111,111	0
60	MG	DA	2967	1/1	0.97	0.66	51,51,51,51	0
60	MG	BA	2926	1/1	0.97	0.40	58,58,58,58	0
60	MG	BA	2917	1/1	0.97	0.85	58,58,58,58	0
60	MG	AA	1679	1/1	0.97	0.61	100,100,100,100	0
60	MG	BA	3071	1/1	0.97	0.44	61,61,61,61	0
60	MG	DA	2973	1/1	0.97	0.63	51,51,51,51	0
60	MG	DA	2937	1/1	0.97	0.34	45,45,45,45	0
60	MG	AA	1680	1/1	0.97	0.30	75,75,75,75	0
60	MG	DA	2977	1/1	0.97	0.15	104,104,104,104	0
60	MG	DA	3139	1/1	0.97	0.87	69,69,69,69	0
60	MG	DA	3064	1/1	0.97	0.24	66,66,66,66	0
60	MG	DA	2906	1/1	0.97	0.33	67,67,67,67	0
60	MG	BA	2912	1/1	0.97	0.78	71,71,71,71	0
60	MG	DA	2959	1/1	0.97	0.62	61,61,61,61	0
60	MG	AA	1602	1/1	0.97	0.59	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	2982	1/1	0.97	0.80	75,75,75,75	0
60	MG	DA	2925	1/1	0.97	0.42	58,58,58,58	0
60	MG	BA	2922	1/1	0.97	0.49	53,53,53,53	0
60	MG	DA	3005	1/1	0.97	0.58	53,53,53,53	0
60	MG	DA	2911	1/1	0.97	0.57	62,62,62,62	0
60	MG	BA	3048	1/1	0.98	0.27	87,87,87,87	0
60	MG	BA	2947	1/1	0.98	0.65	88,88,88,88	0
60	MG	DA	2912	1/1	0.98	0.52	45,45,45,45	0
60	MG	BA	2958	1/1	0.98	0.18	76,76,76,76	0
60	MG	DA	2927	1/1	0.98	0.79	52,52,52,52	0
60	MG	BA	2924	1/1	0.98	0.27	52,52,52,52	0
60	MG	DA	2966	1/1	0.98	0.69	48,48,48,48	0
60	MG	DA	3051	1/1	0.98	0.29	56,56,56,56	0
60	MG	BA	2915	1/1	0.98	0.35	51,51,51,51	0
60	MG	BA	3003	1/1	0.98	0.66	68,68,68,68	0
60	MG	DA	2917	1/1	0.98	0.86	58,58,58,58	0
60	MG	DA	3079	1/1	0.98	0.15	131,131,131,131	0
60	MG	DA	3012	1/1	0.98	0.30	53,53,53,53	0
60	MG	BA	2911	1/1	0.98	0.75	74,74,74,74	0
60	MG	DA	2933	1/1	0.98	0.50	53,53,53,53	0
60	MG	DA	3109	1/1	0.98	0.66	45,45,45,45	0
60	MG	DA	2952	1/1	0.98	0.47	56,56,56,56	0
60	MG	DA	3111	1/1	0.98	1.00	62,62,62,62	0
60	MG	DA	3084	1/1	0.98	0.21	103,103,103,103	0
60	MG	DA	2934	1/1	0.98	0.40	86,86,86,86	0
60	MG	CA	1619	1/1	0.98	0.10	67,67,67,67	0
60	MG	DA	2920	1/1	0.98	0.17	75,75,75,75	0
60	MG	CA	1656	1/1	0.98	0.60	90,90,90,90	0
60	MG	DA	2957	1/1	0.98	0.55	66,66,66,66	0
60	MG	AA	1644	1/1	0.98	0.09	141,141,141,141	0
61	ZN	AD	301	1/1	0.98	0.17	106,106,106,106	0
60	MG	DA	2939	1/1	0.98	0.51	41,41,41,41	0
60	MG	DA	3066	1/1	0.98	0.52	102,102,102,102	0
60	MG	DA	3067	1/1	0.98	0.50	52,52,52,52	0
60	MG	DA	2910	1/1	0.99	0.34	57,57,57,57	0
60	MG	BA	2935	1/1	0.99	0.50	110,110,110,110	0
60	MG	BA	2928	1/1	0.99	0.99	63,63,63,63	0
60	MG	BA	3112	1/1	0.99	0.64	47,47,47,47	0
60	MG	BA	2910	1/1	0.99	0.25	75,75,75,75	0
60	MG	DA	2976	1/1	0.99	0.68	53,53,53,53	0
60	MG	AA	1630	1/1	0.99	0.10	109,109,109,109	1
60	MG	DA	2968	1/1	0.99	0.48	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
60	MG	DA	2944	1/1	0.99	0.41	74,74,74,74	0
60	MG	BA	2934	1/1	0.99	0.47	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.