wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:59 PM GMT

PDB ID	:	4V7Z
Title	:	Structure of the Thermus thermophilus 70S ribosome complexed with telithromycin.
Authors	:	Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on	:	2010-08-18
Resolution	:	3.10 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

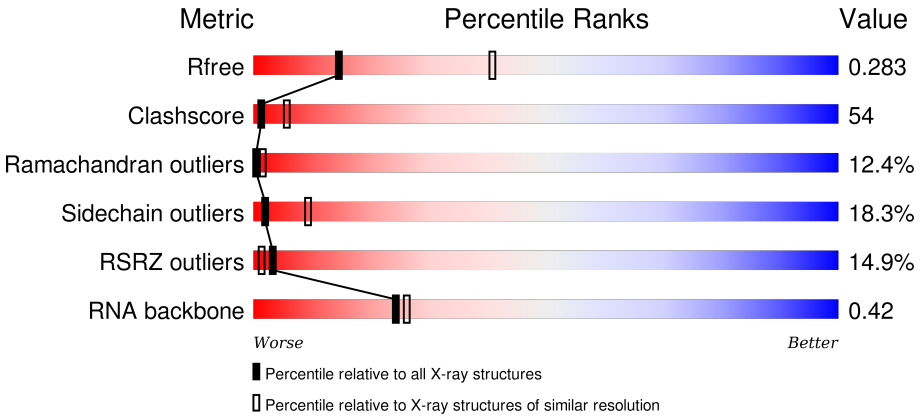
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	16% 15% 65% 19%
1	CA	1522	18% 16% 64% 19%
2	AB	256	20% 32% 50% 9% 8%
2	CB	256	23% 30% 52% 10% 8%

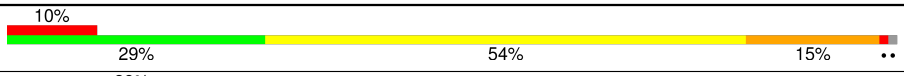
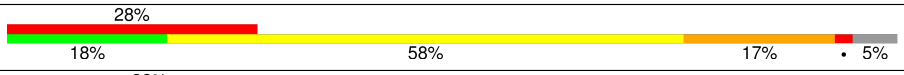
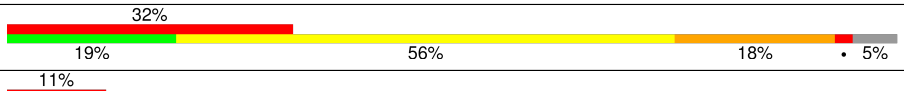
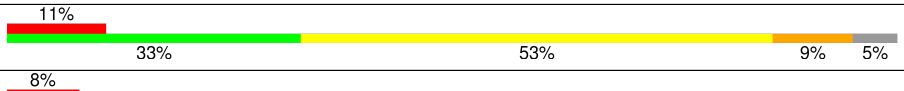
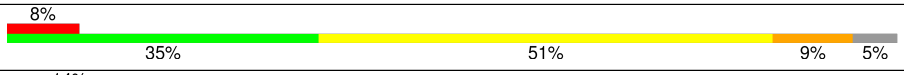
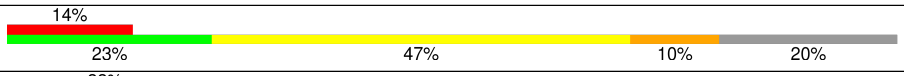
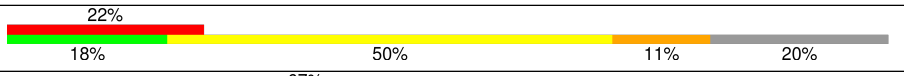
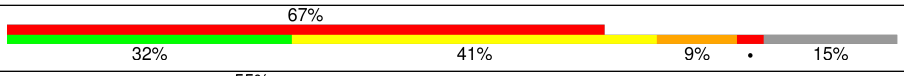
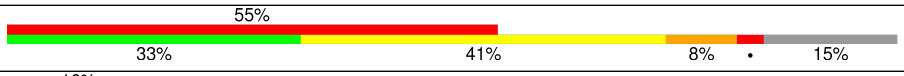
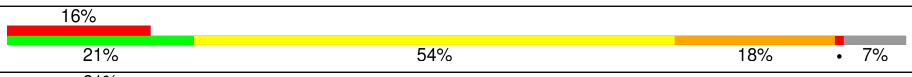
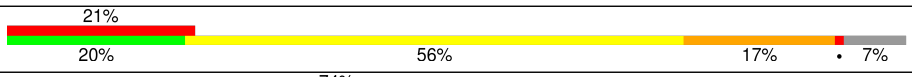
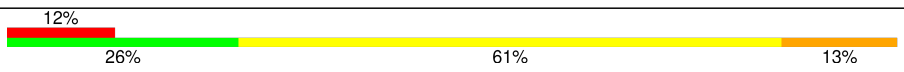
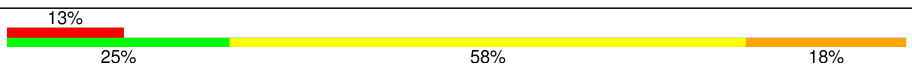
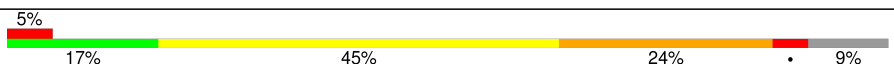
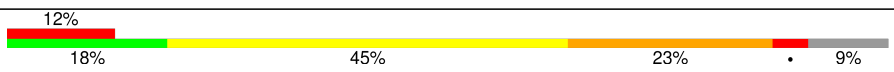
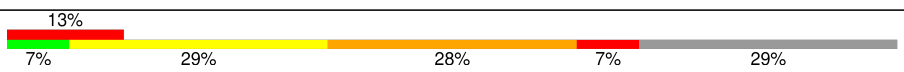
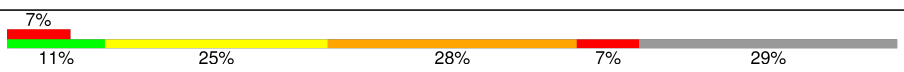
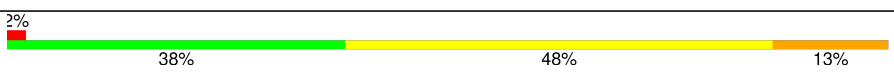
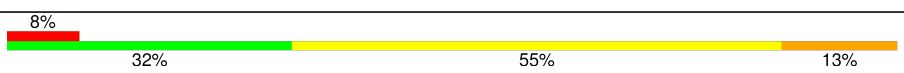
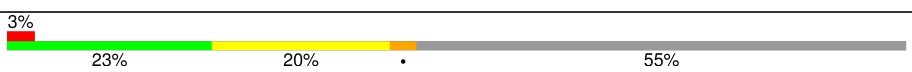
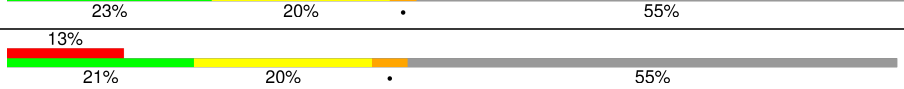
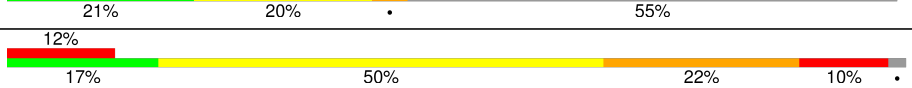
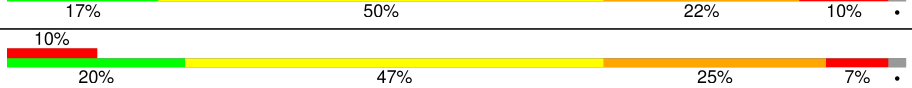
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	239	21% 31% 49% 6% • 13%
3	CC	239	23% 31% 49% 5% • 13%
4	AD	209	17% 23% 57% 18%
4	CD	209	8% 22% 59% 19%
5	AE	162	17% 30% 49% 12% • 7%
5	CE	162	25% 28% 50% 14% • 7%
6	AF	101	6% 12% 70% 18%
6	CF	101	20% 11% 70% 19%
7	AG	156	28% 46% 49% • •
7	CG	156	46% 46% 48% 5% •
8	AH	138	3% 23% 64% 11% •
8	CH	138	4% 25% 64% 9% •
9	AI	128	52% 36% 52% 9% • •
9	CI	128	62% 36% 54% 8% • •
10	AJ	105	56% 32% 52% 10% 6%
10	CJ	105	55% 31% 53% 10% 6%
11	AK	129	29% 23% 61% 6% • 8%
11	CK	129	32% 22% 63% 6% • 8%
12	AL	135	9% 22% 54% 16% • 7%
12	CL	135	23% 25% 52% 14% • 7%
13	AM	126	44% 32% 51% 8% • 9%
13	CM	126	46% 33% 50% 8% • 9%
14	AN	61	31% 41% 51% 5% • •
14	CN	61	23% 41% 51% 5% • •
15	AO	89	7% 27% 58% 12% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	B6	54	11% 39% 31% 9% 17%
28	D6	54	24% 9% 33% 33% 7% 17%
29	B7	49	4% 31% 55% 14%
29	D7	49	18% 29% 55% 16%
30	B8	65	12% 17% 49% 29%
30	D8	65	8% 18% 43% 32% 5%
31	BA	2787	3% 10% 47% 34% 7%
31	DA	2787	5% 9% 48% 34% 6%
32	BB	122	8% 8% 52% 34%
32	DB	122	15% 7% 53% 35%
33	BD	276	3% 26% 50% 22%
33	DD	276	3% 26% 52% 20%
34	BE	206	5% 22% 51% 24%
34	DE	206	8% 19% 54% 24%
35	BF	210	10% 25% 53% 18%
35	DF	210	11% 23% 56% 19%
36	BG	182	46% 20% 58% 20%
36	DG	182	52% 20% 58% 19%
37	BH	180	6% 27% 41% 17% 11%
37	DH	180	32% 26% 42% 16% 11%
38	BI	148	24% 22% 53% 21%
38	DI	148	50% 24% 49% 23%
39	BN	140	6% 15% 54% 27%
39	DN	140	6% 18% 52% 26%
40	BO	122	32% 52% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DO	122	29% 54% 16%
41	BP	150	7% 11% 39% 35% 12%
41	DP	150	16% 10% 42% 33% 12%
42	BQ	141	6% 24% 48% 22%
42	DQ	141	11% 23% 50% 21%
43	BR	118	3% 20% 53% 23%
43	DR	118	3% 23% 52% 21%
44	BS	112	17% 10% 47% 29% 12%
44	DS	112	29% 9% 48% 29% 12%
45	BT	146	8% 14% 42% 29% 5% 10%
45	DT	146	12% 14% 42% 29% 5% 10%
46	BU	118	5% 28% 54% 15%
46	DU	118	15% 29% 53% 16%
47	BV	101	10% 10% 49% 37% 5%
47	DV	101	20% 9% 50% 37% 5%
48	BW	113	24% 49% 26%
48	DW	113	2% 23% 52% 22%
49	BX	96	4% 14% 46% 32% 5%
49	DX	96	5% 11% 45% 34% 6%
50	BY	110	22% 14% 41% 34% 8%
50	DY	110	25% 12% 44% 32% 5% 8%
51	BZ	206	6% 22% 50% 12% 14%
51	DZ	206	13% 22% 48% 14% 14%

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
52	MG	AA	1606	-	-	-	X
52	MG	AA	1609	-	-	-	X
52	MG	AA	1610	-	-	-	X
52	MG	AA	1613	-	-	-	X
52	MG	AA	1614	-	-	-	X
52	MG	AA	1621	-	-	-	X
52	MG	AA	1623	-	-	-	X
52	MG	AA	1627	-	-	-	X
52	MG	AA	1629	-	-	-	X
52	MG	AA	1634	-	-	-	X
52	MG	AA	1647	-	-	-	X
52	MG	AA	1648	-	-	-	X
52	MG	AA	1649	-	-	-	X
52	MG	B5	101	-	-	-	X
52	MG	B7	101	-	-	-	X
52	MG	BA	3001	-	-	-	X
52	MG	BA	3002	-	-	-	X
52	MG	BA	3006	-	-	-	X
52	MG	BA	3008	-	-	-	X
52	MG	BA	3010	-	-	-	X
52	MG	BA	3012	-	-	-	X
52	MG	BA	3016	-	-	-	X
52	MG	BA	3018	-	-	-	X
52	MG	BA	3021	-	-	-	X
52	MG	BA	3023	-	-	-	X
52	MG	BA	3028	-	-	-	X
52	MG	BA	3032	-	-	-	X
52	MG	BA	3034	-	-	-	X
52	MG	BA	3037	-	-	-	X
52	MG	BA	3038	-	-	-	X
52	MG	BA	3039	-	-	-	X
52	MG	BA	3040	-	-	-	X
52	MG	BA	3041	-	-	-	X
52	MG	BA	3044	-	-	-	X
52	MG	BA	3046	-	-	-	X
52	MG	BA	3047	-	-	-	X
52	MG	BA	3049	-	-	-	X
52	MG	BA	3051	-	-	-	X
52	MG	BA	3052	-	-	-	X
52	MG	BA	3055	-	-	-	X
52	MG	BA	3060	-	-	-	X
52	MG	BA	3061	-	-	-	X
52	MG	BA	3063	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	BA	3066	-	-	-	X
52	MG	BA	3070	-	-	-	X
52	MG	BA	3071	-	-	-	X
52	MG	BA	3072	-	-	-	X
52	MG	BA	3074	-	-	-	X
52	MG	BA	3075	-	-	-	X
52	MG	BA	3080	-	-	-	X
52	MG	BA	3088	-	-	-	X
52	MG	BA	3089	-	-	-	X
52	MG	BA	3090	-	-	-	X
52	MG	BA	3091	-	-	-	X
52	MG	BA	3092	-	-	-	X
52	MG	BA	3093	-	-	-	X
52	MG	BA	3094	-	-	-	X
52	MG	BA	3096	-	-	-	X
52	MG	BA	3100	-	-	-	X
52	MG	BA	3101	-	-	-	X
52	MG	BA	3102	-	-	-	X
52	MG	BA	3109	-	-	-	X
52	MG	BA	3116	-	-	-	X
52	MG	BA	3117	-	-	-	X
52	MG	BA	3118	-	-	-	X
52	MG	BA	3122	-	-	-	X
52	MG	BA	3124	-	-	-	X
52	MG	BA	3126	-	-	-	X
52	MG	BA	3127	-	-	-	X
52	MG	BA	3138	-	-	-	X
52	MG	BA	3141	-	-	-	X
52	MG	BA	3144	-	-	-	X
52	MG	BA	3146	-	-	-	X
52	MG	BA	3148	-	-	-	X
52	MG	BA	3150	-	-	-	X
52	MG	BA	3156	-	-	-	X
52	MG	BA	3161	-	-	-	X
52	MG	BA	3164	-	-	-	X
52	MG	BA	3166	-	-	-	X
52	MG	BA	3173	-	-	-	X
52	MG	BA	3174	-	-	-	X
52	MG	BA	3176	-	-	-	X
52	MG	BA	3181	-	-	-	X
52	MG	BA	3190	-	-	-	X
52	MG	BA	3205	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	BA	3211	-	-	-	X
52	MG	BA	3214	-	-	-	X
52	MG	BA	3222	-	-	-	X
52	MG	BA	3225	-	-	-	X
52	MG	BA	3226	-	-	-	X
52	MG	BA	3228	-	-	-	X
52	MG	BA	3232	-	-	-	X
52	MG	BA	3234	-	-	-	X
52	MG	BA	3235	-	-	-	X
52	MG	BA	3237	-	-	-	X
52	MG	BA	3244	-	-	-	X
52	MG	BA	3247	-	-	-	X
52	MG	BA	3278	-	-	-	X
52	MG	BA	3280	-	-	-	X
52	MG	BA	3282	-	-	-	X
52	MG	BA	3284	-	-	-	X
52	MG	BA	3295	-	-	-	X
52	MG	BA	3309	-	-	-	X
52	MG	BA	3310	-	-	-	X
52	MG	BA	3315	-	-	-	X
52	MG	BA	3317	-	-	-	X
52	MG	BA	3319	-	-	-	X
52	MG	BA	3321	-	-	-	X
52	MG	BA	3332	-	-	-	X
52	MG	BA	3336	-	-	-	X
52	MG	BA	3337	-	-	-	X
52	MG	BA	3341	-	-	-	X
52	MG	BA	3352	-	-	-	X
52	MG	BD	301	-	-	-	X
52	MG	BX	101	-	-	-	X
52	MG	CA	1606	-	-	-	X
52	MG	CA	1607	-	-	-	X
52	MG	CA	1611	-	-	-	X
52	MG	CA	1621	-	-	-	X
52	MG	CA	1625	-	-	-	X
52	MG	CA	1627	-	-	-	X
52	MG	CA	1631	-	-	-	X
52	MG	CA	1632	-	-	-	X
52	MG	CA	1644	-	-	-	X
52	MG	CA	1645	-	-	-	X
52	MG	D5	101	-	-	-	X
52	MG	D7	101	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3001	-	-	-	X
52	MG	DA	3002	-	-	-	X
52	MG	DA	3004	-	-	-	X
52	MG	DA	3006	-	-	-	X
52	MG	DA	3007	-	-	-	X
52	MG	DA	3008	-	-	-	X
52	MG	DA	3009	-	-	-	X
52	MG	DA	3011	-	-	-	X
52	MG	DA	3015	-	-	-	X
52	MG	DA	3016	-	-	-	X
52	MG	DA	3017	-	-	-	X
52	MG	DA	3018	-	-	-	X
52	MG	DA	3019	-	-	-	X
52	MG	DA	3020	-	-	-	X
52	MG	DA	3022	-	-	-	X
52	MG	DA	3026	-	-	-	X
52	MG	DA	3027	-	-	-	X
52	MG	DA	3031	-	-	-	X
52	MG	DA	3033	-	-	-	X
52	MG	DA	3035	-	-	-	X
52	MG	DA	3036	-	-	-	X
52	MG	DA	3037	-	-	-	X
52	MG	DA	3038	-	-	-	X
52	MG	DA	3039	-	-	-	X
52	MG	DA	3040	-	-	-	X
52	MG	DA	3043	-	-	-	X
52	MG	DA	3045	-	-	-	X
52	MG	DA	3046	-	-	-	X
52	MG	DA	3048	-	-	-	X
52	MG	DA	3050	-	-	-	X
52	MG	DA	3051	-	-	-	X
52	MG	DA	3053	-	-	-	X
52	MG	DA	3054	-	-	-	X
52	MG	DA	3055	-	-	-	X
52	MG	DA	3056	-	-	-	X
52	MG	DA	3060	-	-	-	X
52	MG	DA	3062	-	-	-	X
52	MG	DA	3069	-	-	-	X
52	MG	DA	3070	-	-	-	X
52	MG	DA	3071	-	-	-	X
52	MG	DA	3073	-	-	-	X
52	MG	DA	3074	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3076	-	-	-	X
52	MG	DA	3079	-	-	-	X
52	MG	DA	3088	-	-	-	X
52	MG	DA	3090	-	-	-	X
52	MG	DA	3091	-	-	-	X
52	MG	DA	3093	-	-	-	X
52	MG	DA	3094	-	-	-	X
52	MG	DA	3096	-	-	-	X
52	MG	DA	3098	-	-	-	X
52	MG	DA	3103	-	-	-	X
52	MG	DA	3108	-	-	-	X
52	MG	DA	3109	-	-	-	X
52	MG	DA	3111	-	-	-	X
52	MG	DA	3115	-	-	-	X
52	MG	DA	3117	-	-	-	X
52	MG	DA	3120	-	-	-	X
52	MG	DA	3121	-	-	-	X
52	MG	DA	3134	-	-	-	X
52	MG	DA	3137	-	-	-	X
52	MG	DA	3139	-	-	-	X
52	MG	DA	3143	-	-	-	X
52	MG	DA	3147	-	-	-	X
52	MG	DA	3155	-	-	-	X
52	MG	DA	3156	-	-	-	X
52	MG	DA	3159	-	-	-	X
52	MG	DA	3161	-	-	-	X
52	MG	DA	3162	-	-	-	X
52	MG	DA	3165	-	-	-	X
52	MG	DA	3167	-	-	-	X
52	MG	DA	3173	-	-	-	X
52	MG	DA	3178	-	-	-	X
52	MG	DA	3191	-	-	-	X
52	MG	DA	3197	-	-	-	X
52	MG	DA	3205	-	-	-	X
52	MG	DA	3208	-	-	-	X
52	MG	DA	3211	-	-	-	X
52	MG	DA	3212	-	-	-	X
52	MG	DA	3216	-	-	-	X
52	MG	DA	3217	-	-	-	X
52	MG	DA	3218	-	-	-	X
52	MG	DA	3223	-	-	-	X
52	MG	DA	3227	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	MG	DA	3236	-	-	-	X
52	MG	DA	3239	-	-	-	X
52	MG	DA	3241	-	-	-	X
52	MG	DA	3252	-	-	-	X
52	MG	DA	3256	-	-	-	X
52	MG	DA	3259	-	-	-	X
52	MG	DA	3268	-	-	-	X
52	MG	DA	3270	-	-	-	X
52	MG	DA	3272	-	-	-	X
52	MG	DA	3274	-	-	-	X
52	MG	DA	3275	-	-	-	X
52	MG	DA	3278	-	-	-	X
52	MG	DA	3286	-	-	-	X
52	MG	DA	3288	-	-	-	X
52	MG	DA	3290	-	-	-	X
52	MG	DA	3292	-	-	-	X
52	MG	DA	3308	-	-	-	X
52	MG	DA	3313	-	-	-	X
52	MG	DA	3314	-	-	-	X
52	MG	DD	301	-	-	-	X
52	MG	DR	201	-	-	-	X
52	MG	DU	201	-	-	-	X
52	MG	DX	101	-	-	-	X
55	TEL	BA	3362	X	-	X	X
55	TEL	DA	3320	X	-	X	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278037 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 rRNA.

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

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- 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			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	INSERTION	UNP Q5SHN3
AL	3	ALA	-	INSERTION	UNP Q5SHN3
AL	4	LEU	-	INSERTION	UNP Q5SHN3
CL	2	VAL	-	INSERTION	UNP Q5SHN3
CL	3	ALA	-	INSERTION	UNP Q5SHN3
CL	4	LEU	-	INSERTION	UNP Q5SHN3

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

Continued on next page...

Continued from previous page...

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein Thx.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
22	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
23	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
24	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O	0	0	0
			157	93	32	32			
26	D4	32	Total	C	N	O	0	0	0
			157	93	32	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			

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

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

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

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

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

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

Continued on next page...

Continued from previous page...

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

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

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
42	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

Continued on next page...

Continued from previous page...

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

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BA	360	Total	Mg	0	0
			360	360		
52	CA	50	Total	Mg	0	0
			50	50		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	3	Total	Mg	0	0
			3	3		
52	DR	2	Total	Mg	0	0
			2	2		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	7	Total	Mg	0	0
			7	7		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	D8	1	Total	Mg	0	0
			1	1		
52	AA	52	Total	Mg	0	0
			52	52		
52	BQ	2	Total	Mg	0	0
			2	2		
52	D7	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
52	BR	1	Total Mg 1 1	0	0
52	DA	318	Total Mg 318 318	0	0
52	B7	1	Total Mg 1 1	0	0
52	DE	1	Total Mg 1 1	0	0
52	DX	1	Total Mg 1 1	0	0
52	DP	1	Total Mg 1 1	0	0
52	D5	1	Total Mg 1 1	0	0
52	BD	2	Total Mg 2 2	0	0
52	B0	1	Total Mg 1 1	0	0
52	DB	3	Total Mg 3 3	0	0

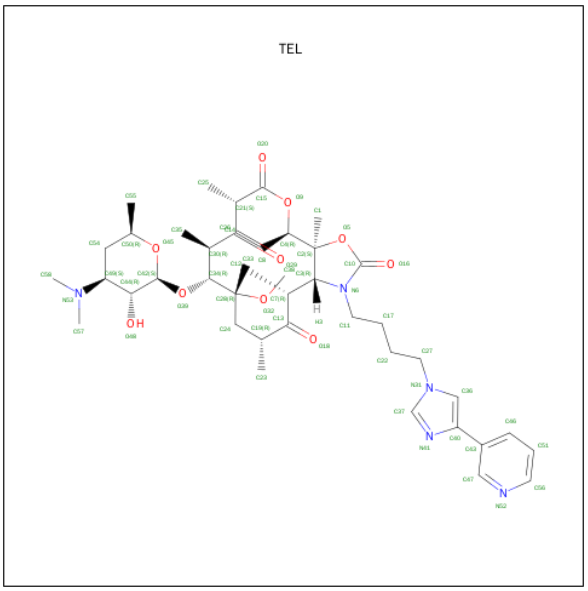
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BA	1	Total K 1 1	0	0
54	DA	1	Total K 1 1	0	0

- Molecule 55 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



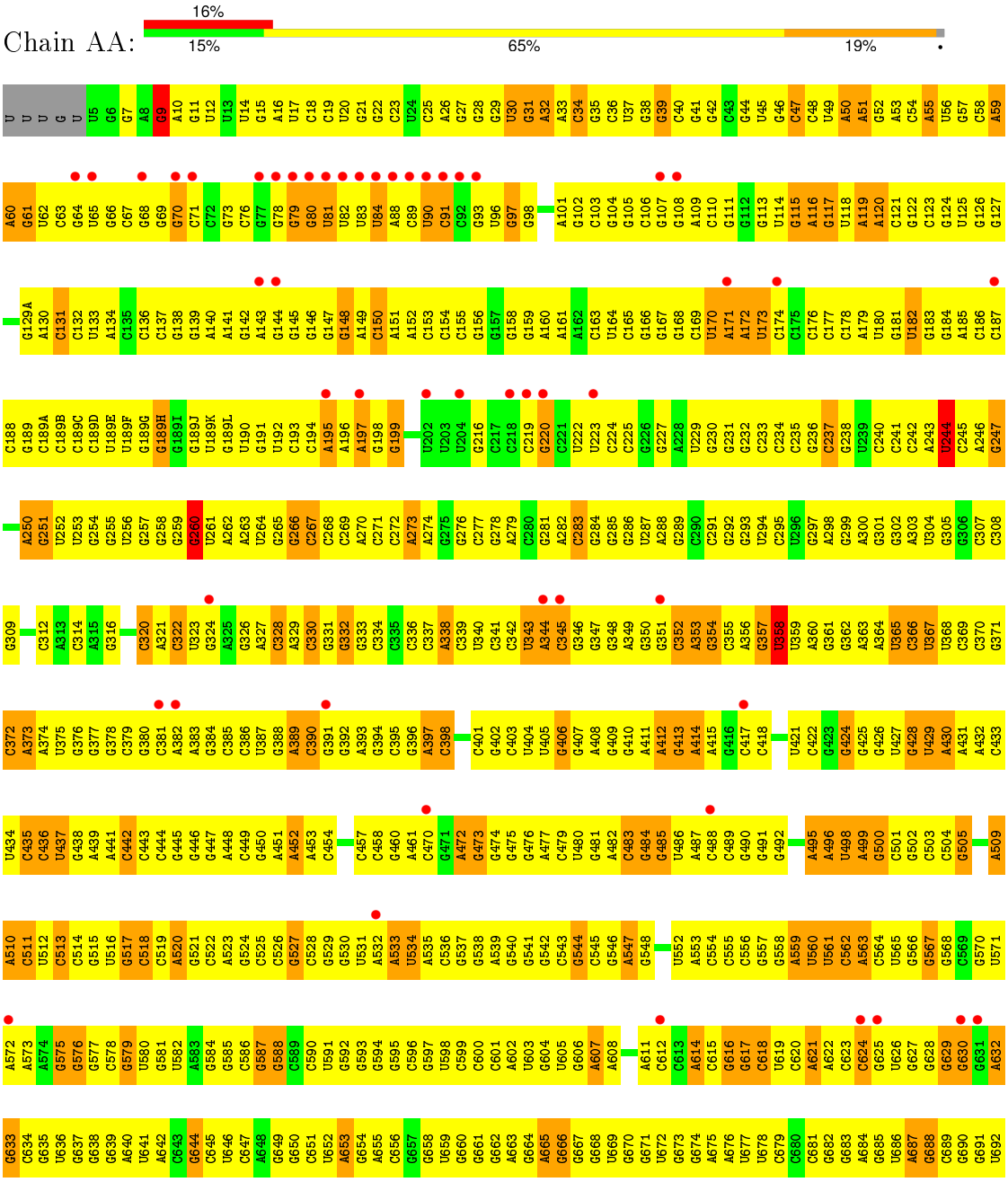
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			58	43	5	10		
55	DA	1	Total	C	N	O	0	0
			58	43	5	10		

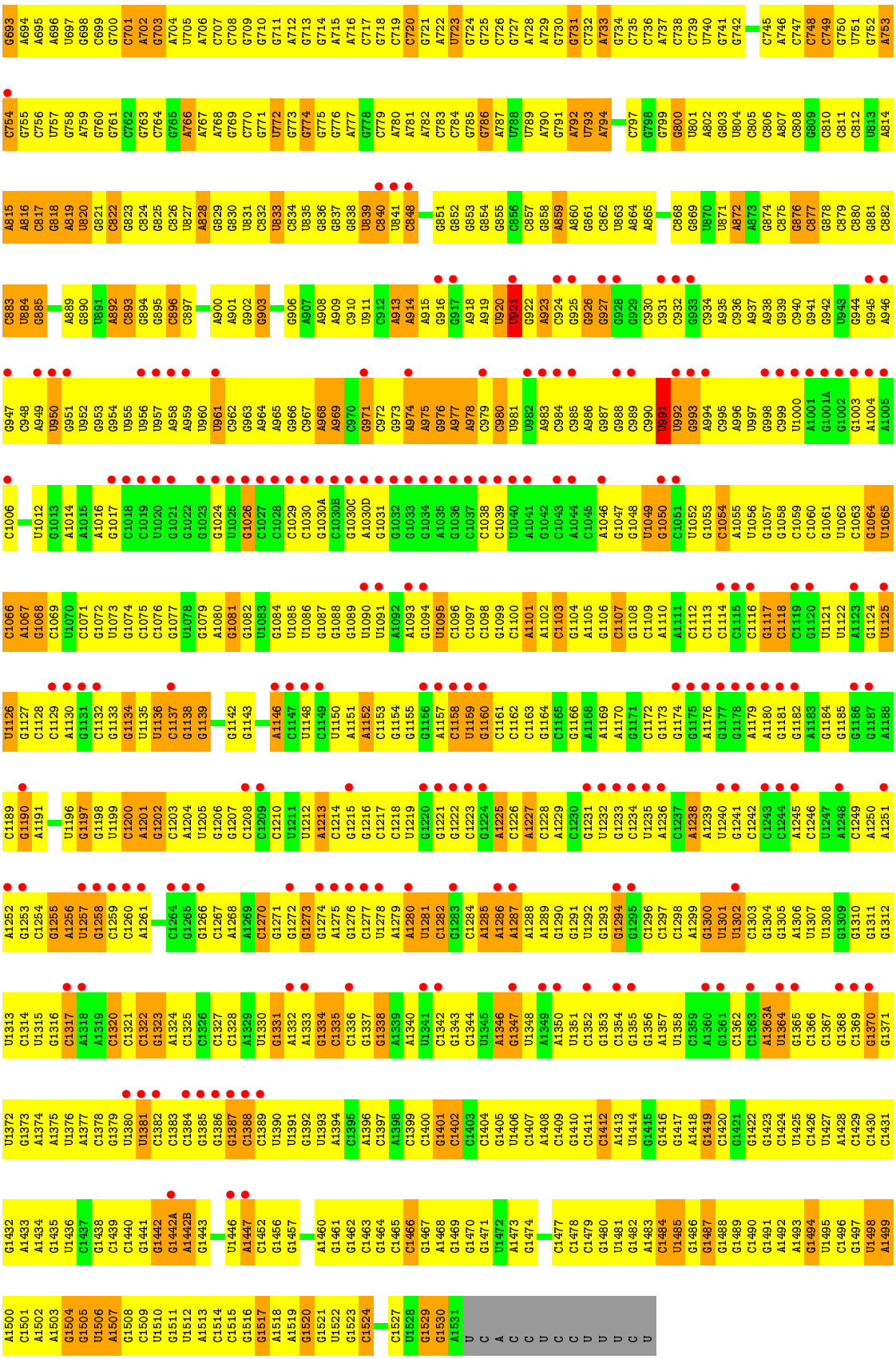
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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 rRNA

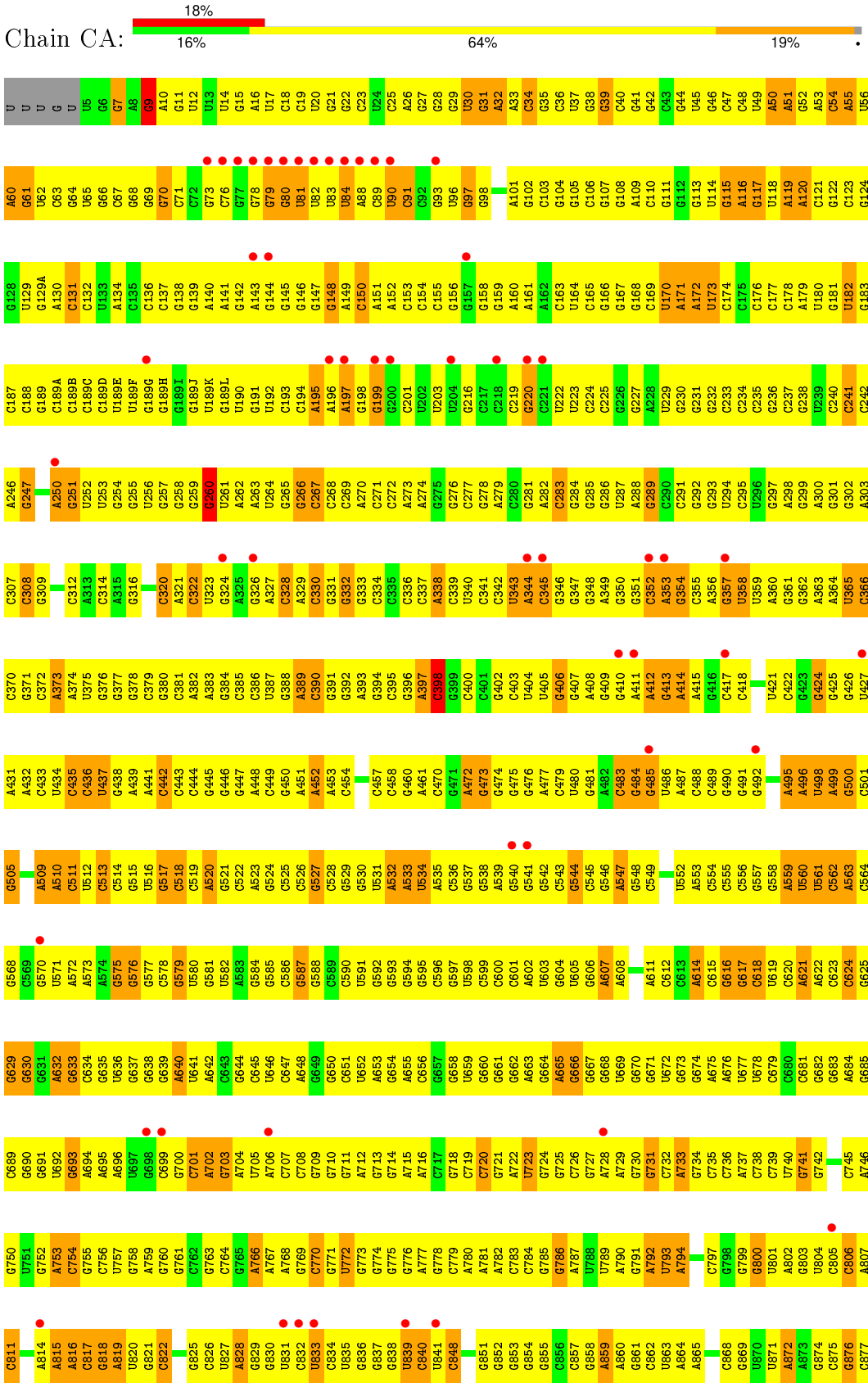
Chain AA:

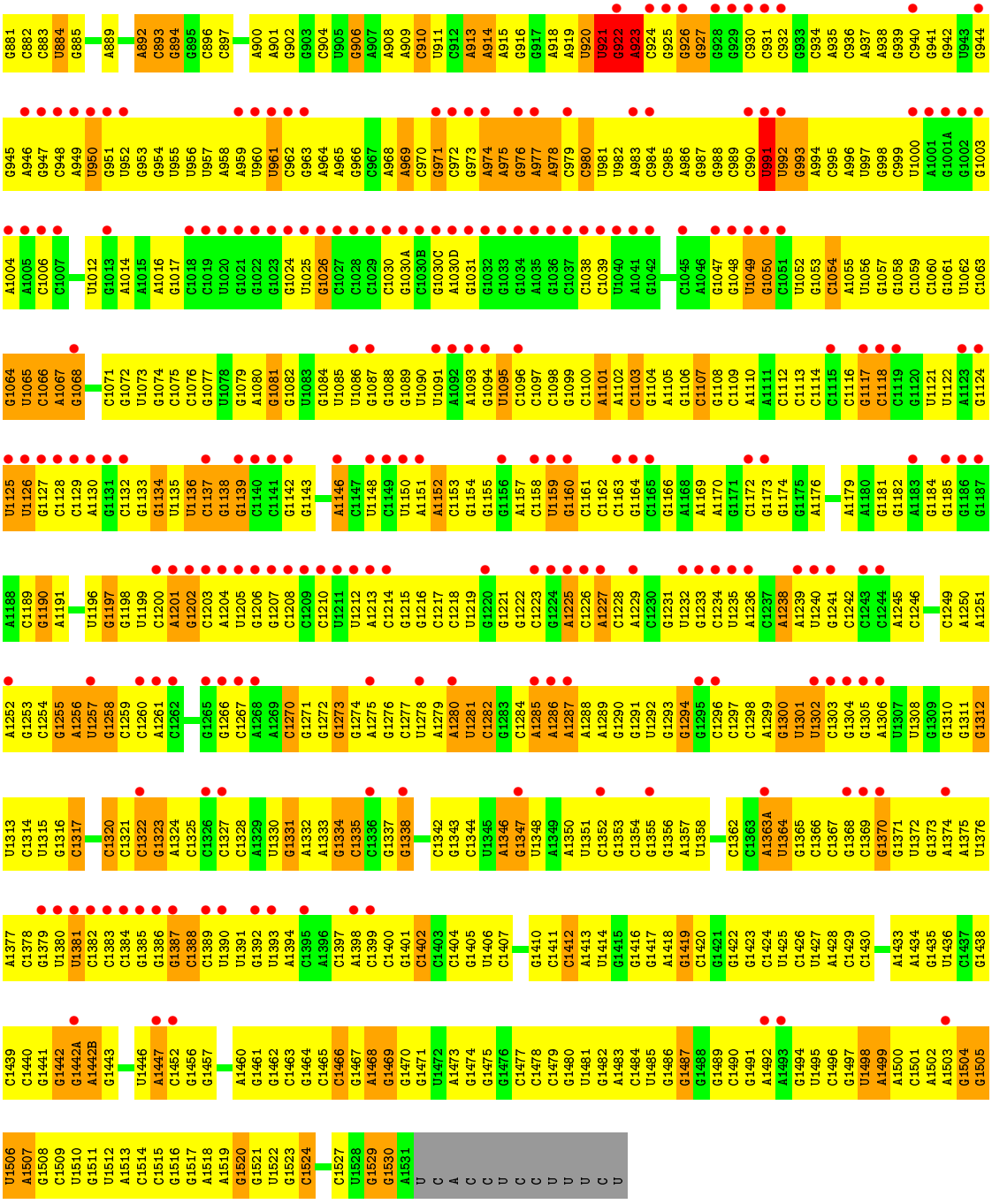




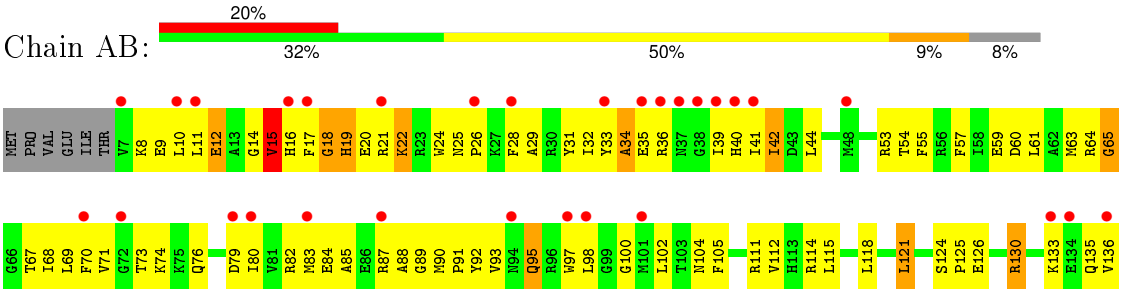
• Molecule 1: 16S rRNA

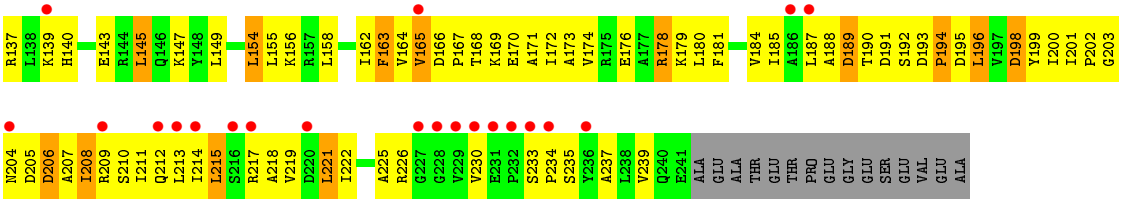
Chain CA:





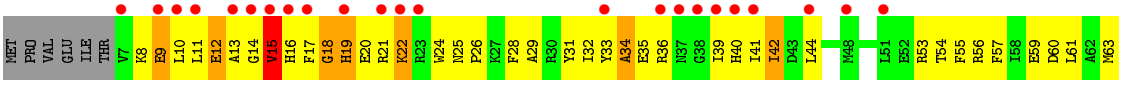
• Molecule 2: 30S ribosomal protein S2

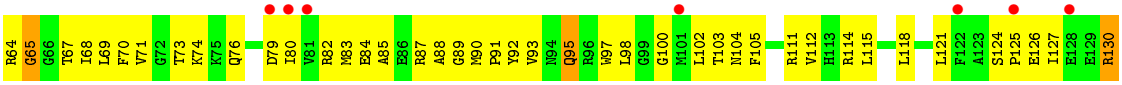


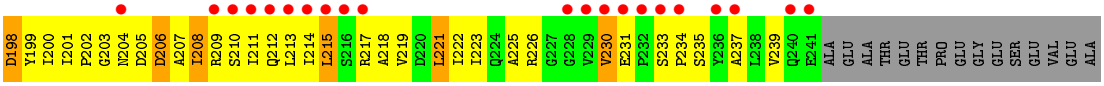


• Molecule 2: 30S ribosomal protein S2

Chain CB:

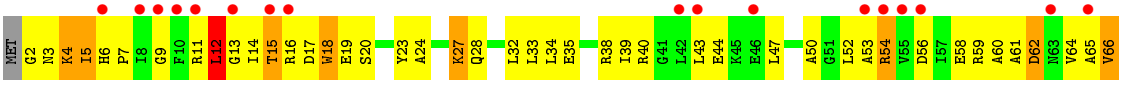


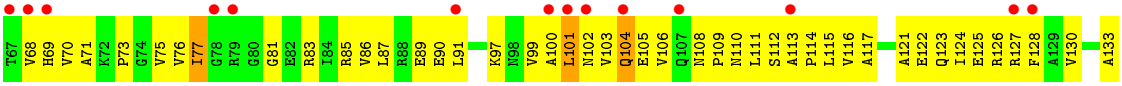


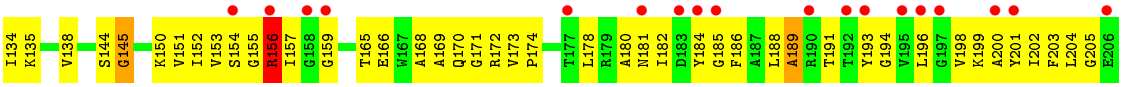


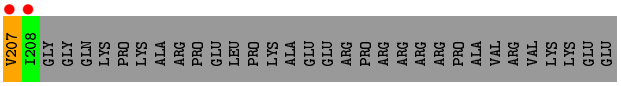
• Molecule 3: 30S ribosomal protein S3

Chain AC:



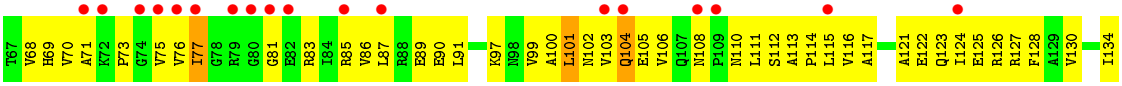


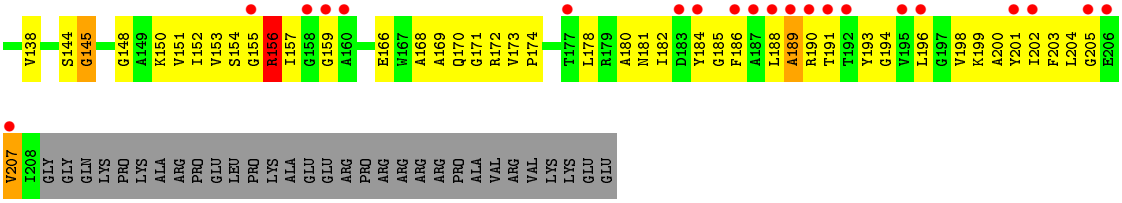




• Molecule 3: 30S ribosomal protein S3

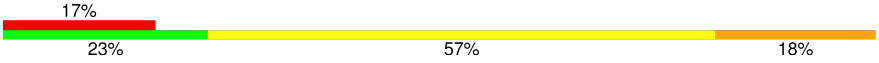
Chain CC:

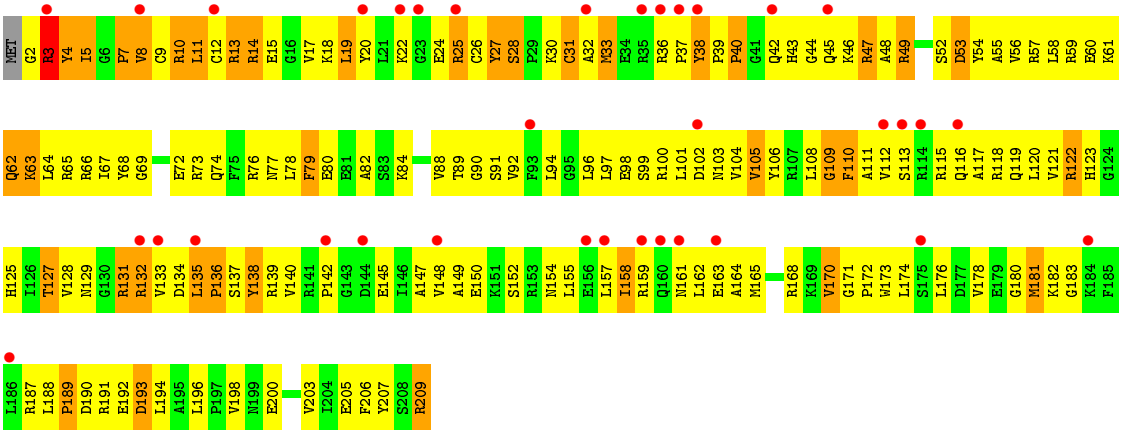




• Molecule 4: 30S ribosomal protein S4

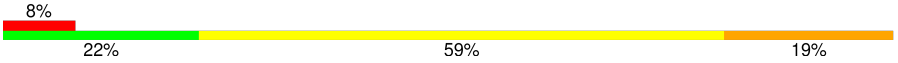
Chain AD:

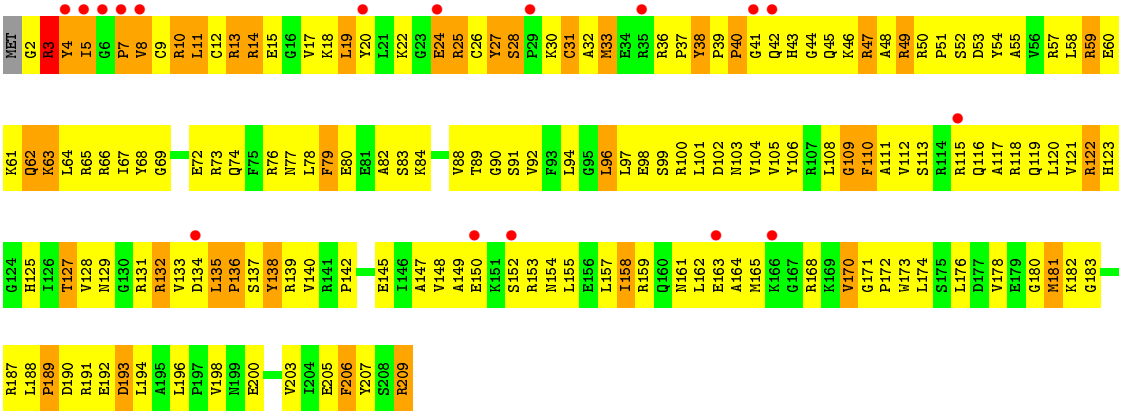




• Molecule 4: 30S ribosomal protein S4

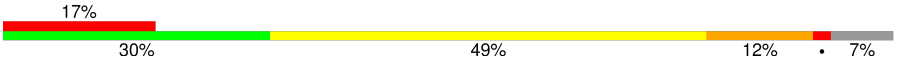
Chain CD:

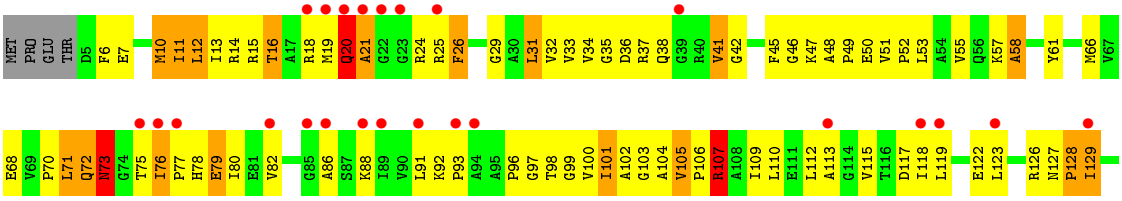


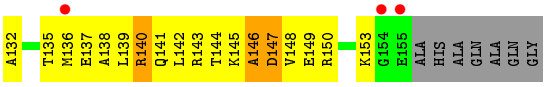


• Molecule 5: 30S ribosomal protein S5

Chain AE:

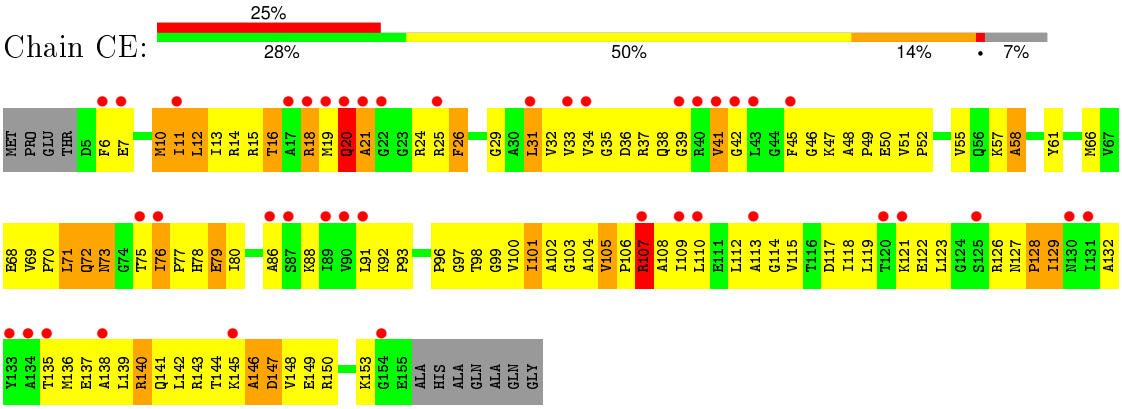






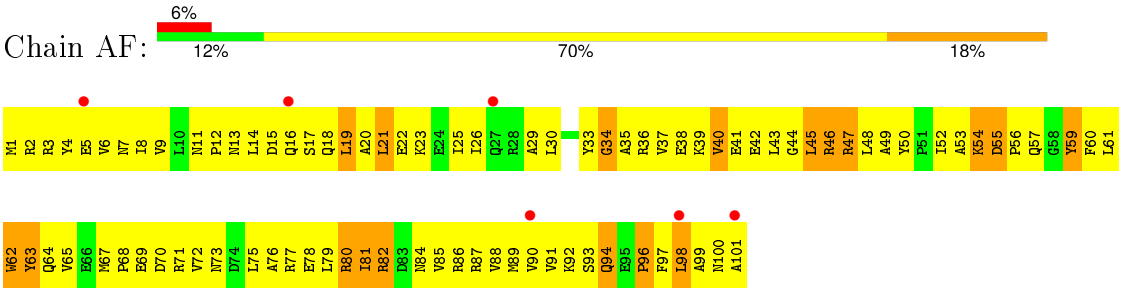
• Molecule 5: 30S ribosomal protein S5

Chain CE:



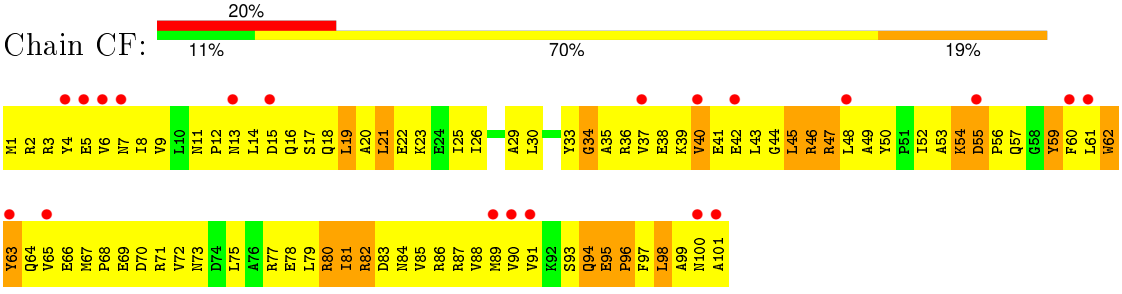
• Molecule 6: 30S ribosomal protein S6

Chain AF:



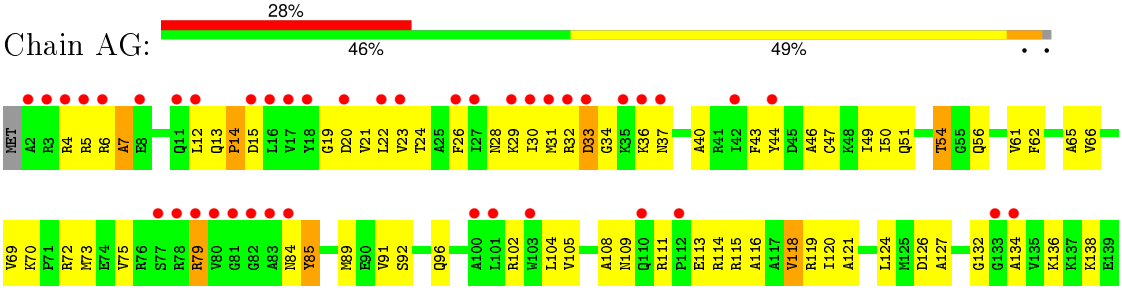
• Molecule 6: 30S ribosomal protein S6

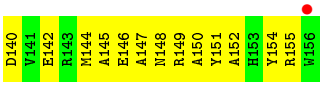
Chain CF:



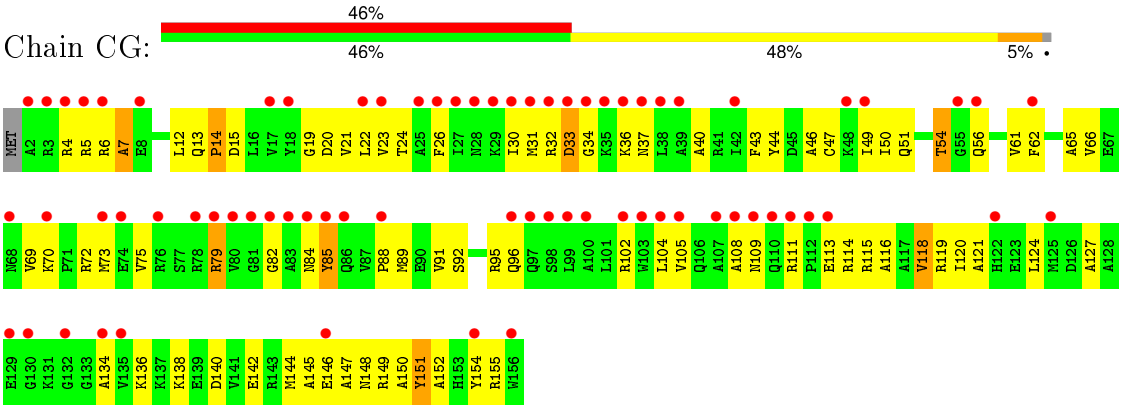
• Molecule 7: 30S ribosomal protein S7

Chain AG:

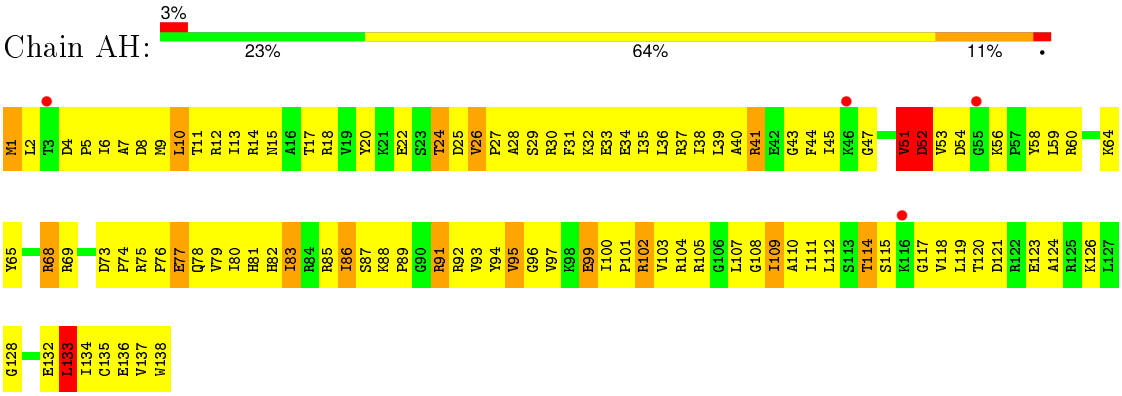




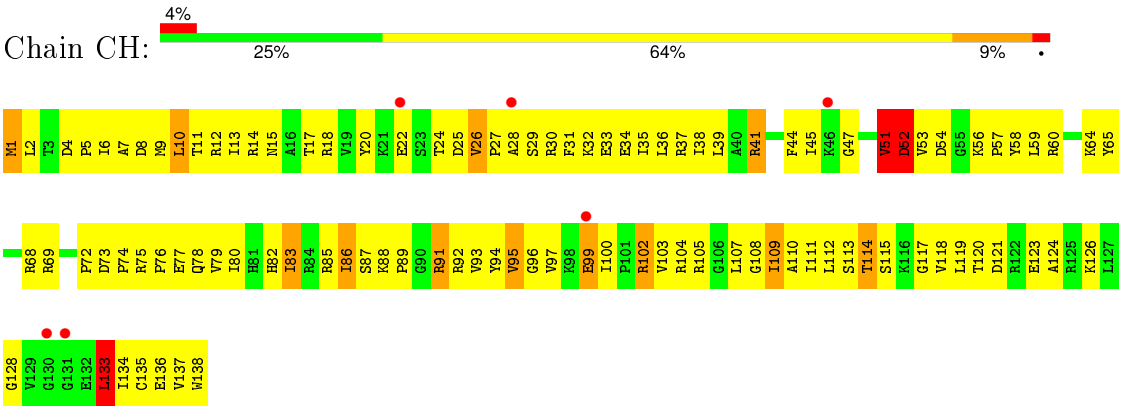
- Molecule 7: 30S ribosomal protein S7



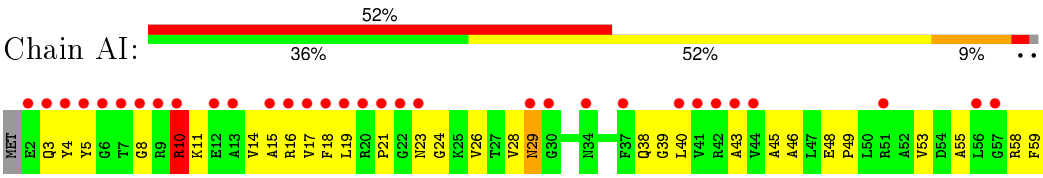
- Molecule 8: 30S ribosomal protein S8

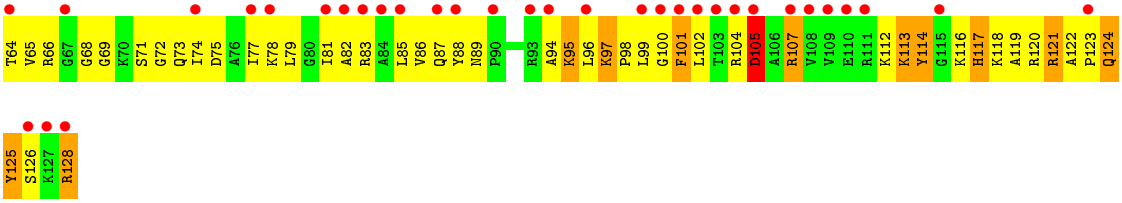


- Molecule 8: 30S ribosomal protein S8

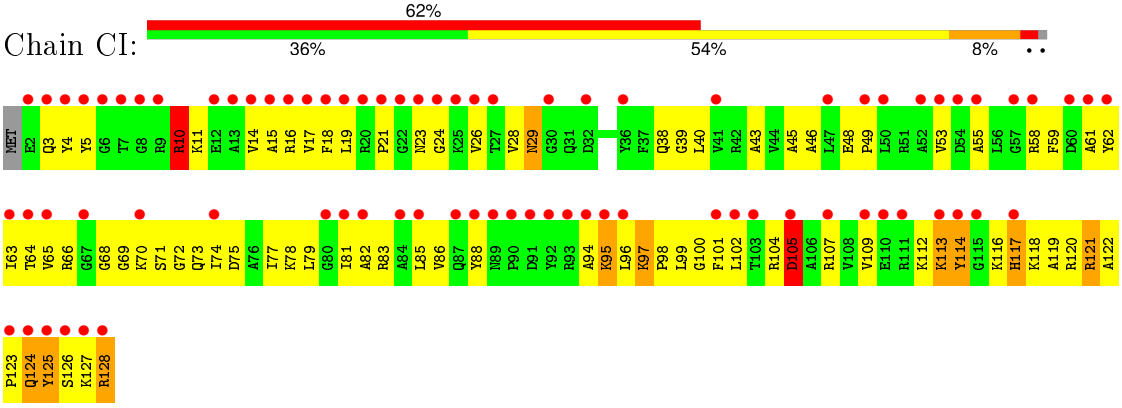


- Molecule 9: 30S ribosomal protein S9

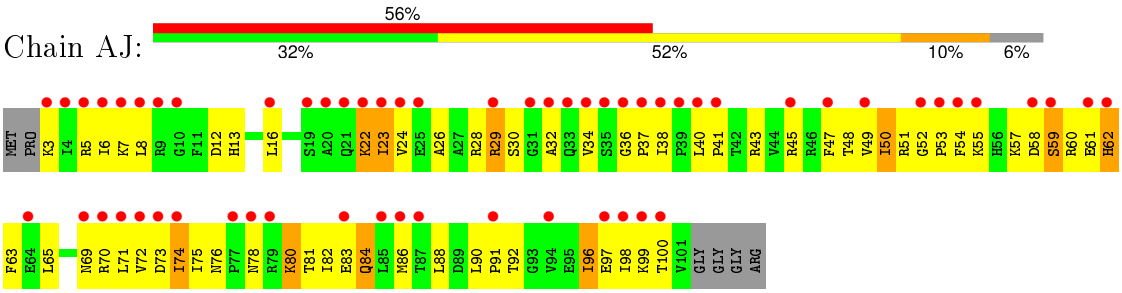




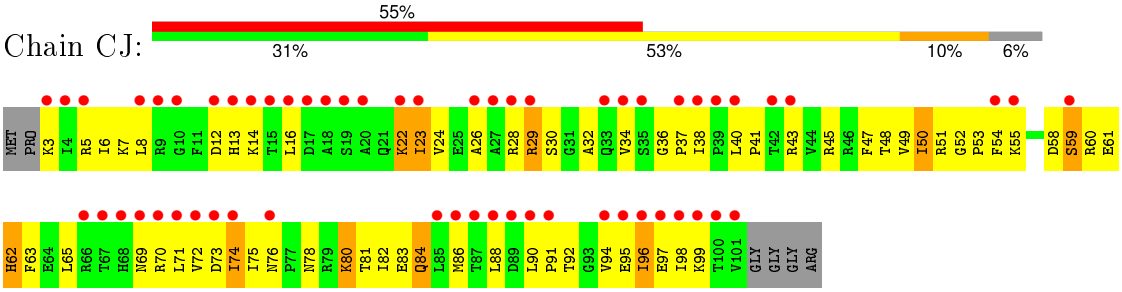
• Molecule 9: 30S ribosomal protein S9



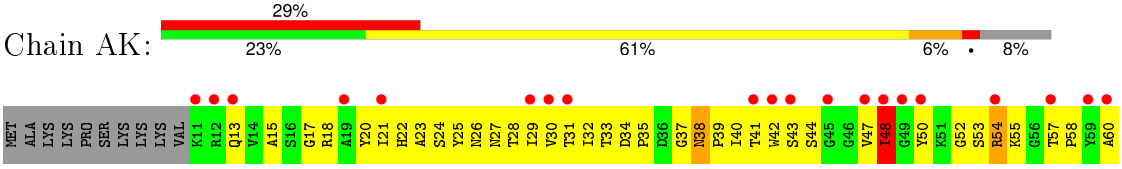
• Molecule 10: 30S ribosomal protein S10

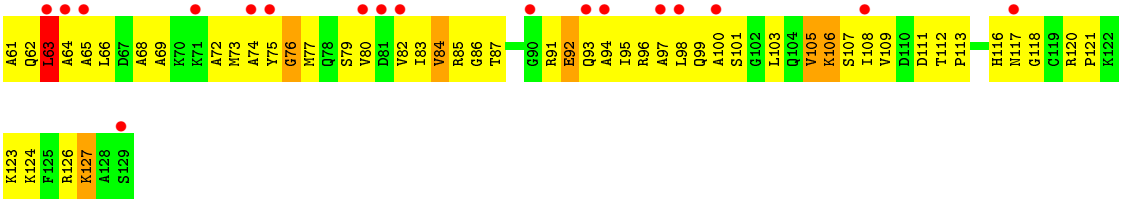


• Molecule 10: 30S ribosomal protein S10



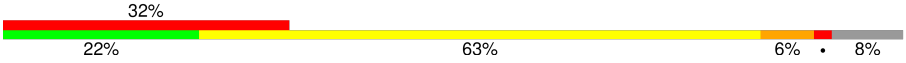
• Molecule 11: 30S ribosomal protein S11

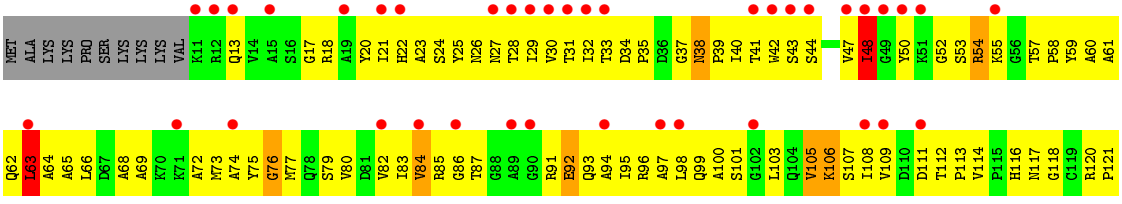


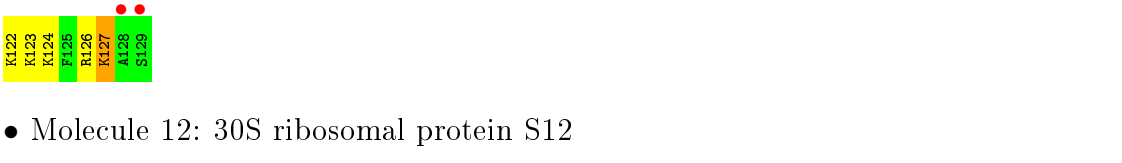


• Molecule 11: 30S ribosomal protein S11

Chain CK:

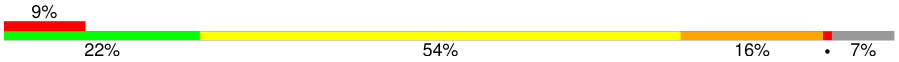


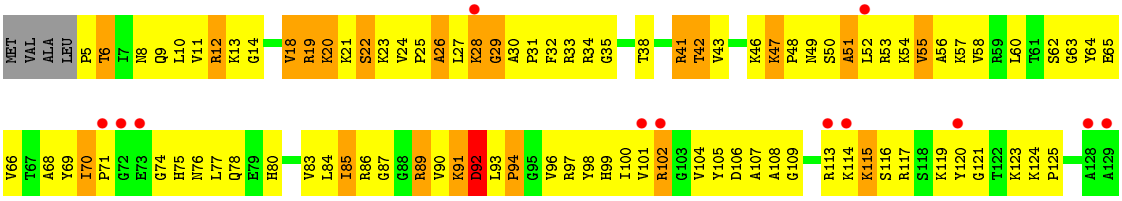


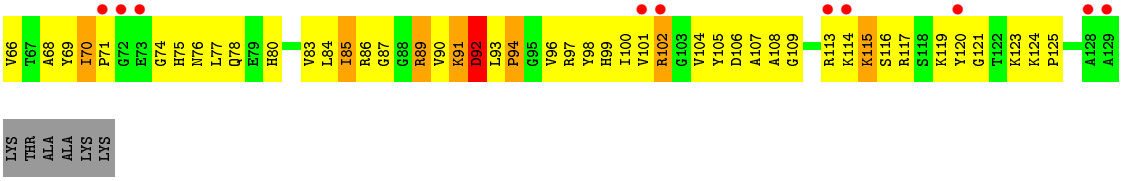


• Molecule 12: 30S ribosomal protein S12

Chain AL:

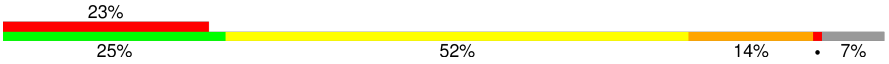


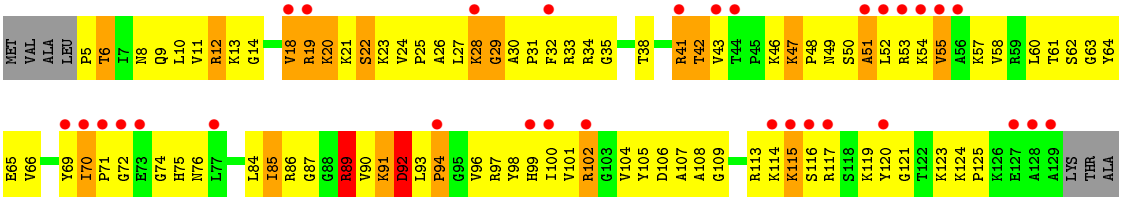


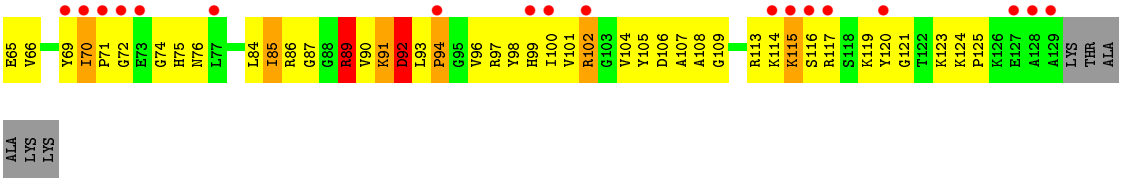


• Molecule 12: 30S ribosomal protein S12

Chain CL:

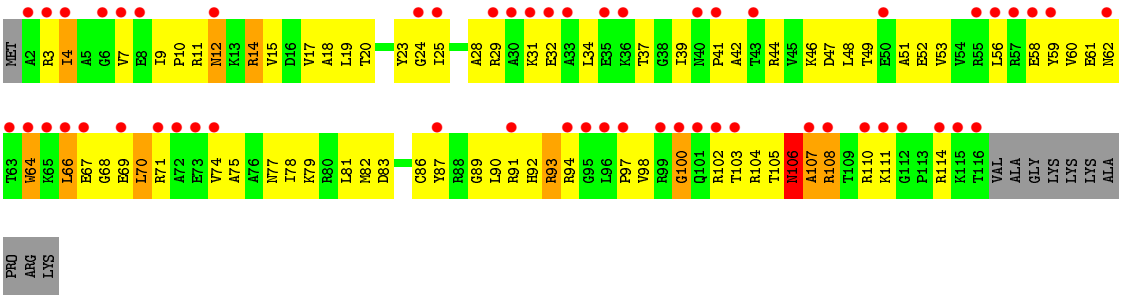




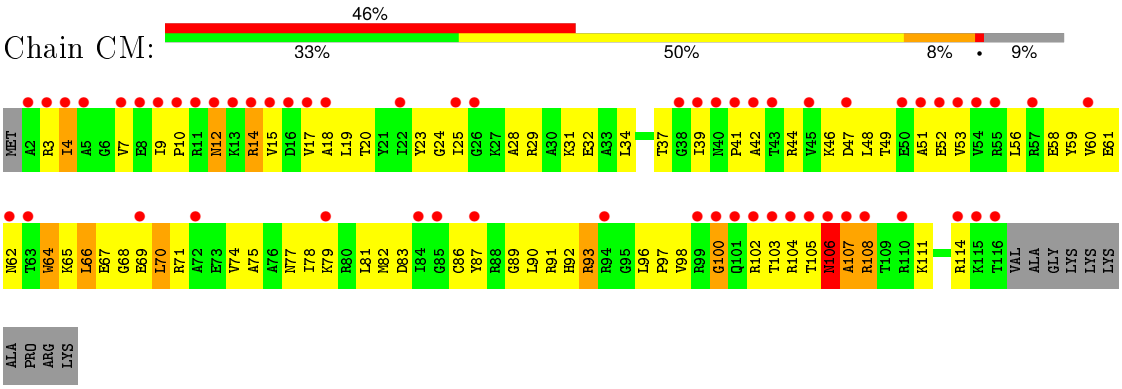


• Molecule 13: 30S ribosomal protein S13

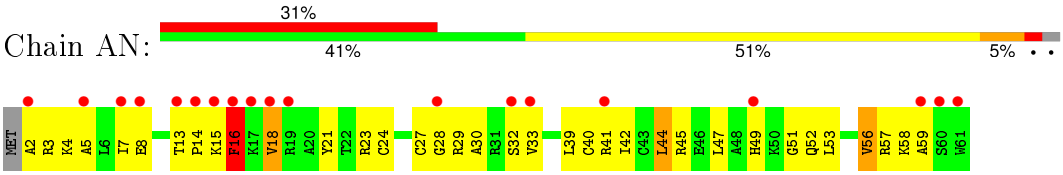
Chain AM:



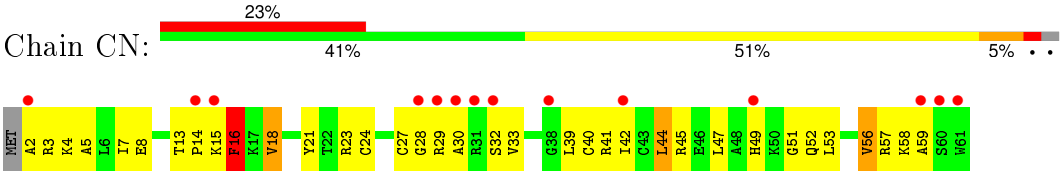
• Molecule 13: 30S ribosomal protein S13



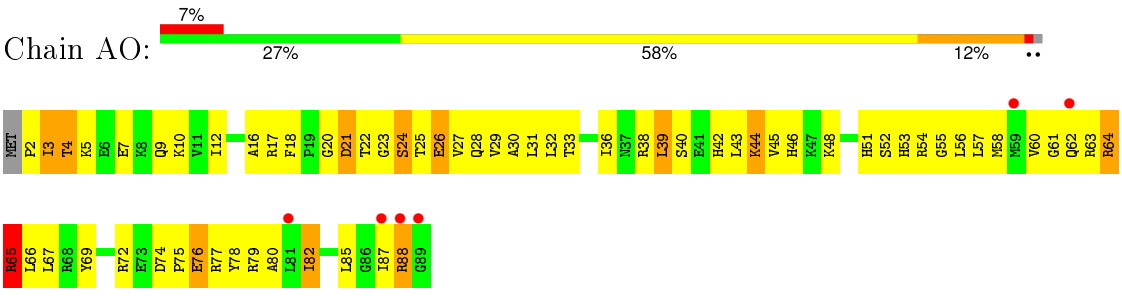
• Molecule 14: 30S ribosomal protein S14



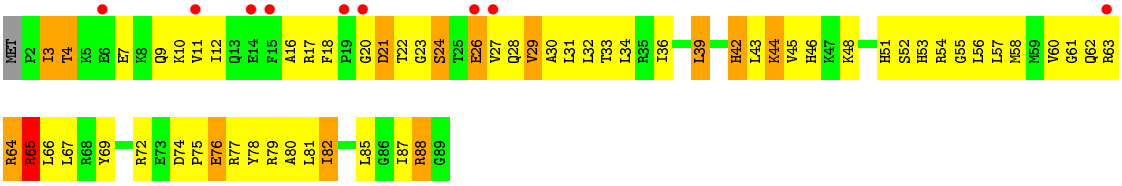
• Molecule 14: 30S ribosomal protein S14



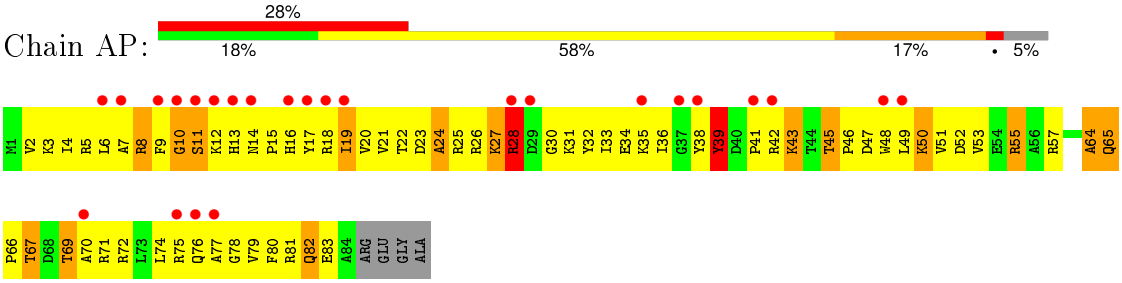
• Molecule 15: 30S ribosomal protein S15



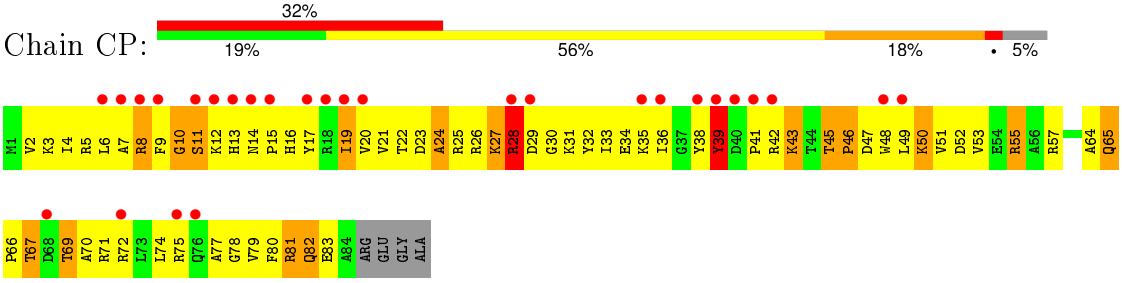
• Molecule 15: 30S ribosomal protein S15



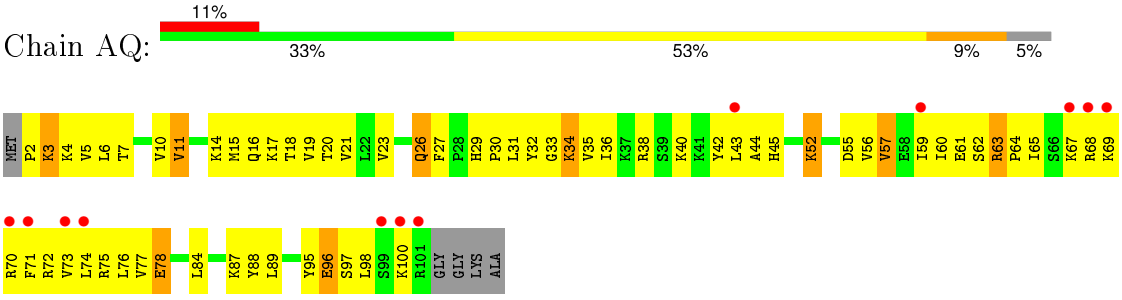
• Molecule 16: 30S ribosomal protein S16



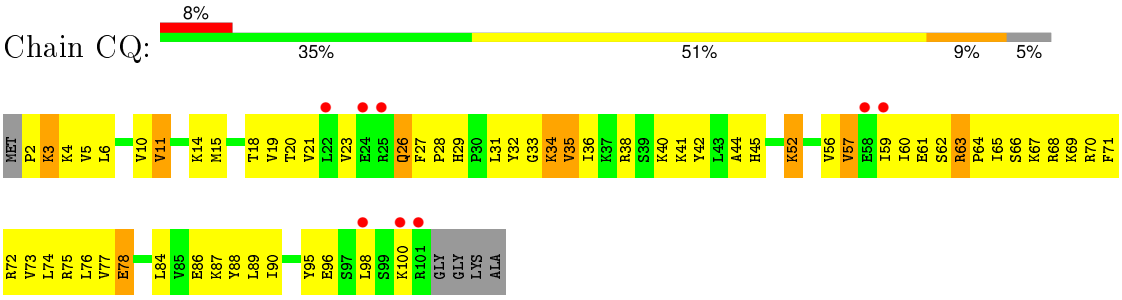
• Molecule 16: 30S ribosomal protein S16



• Molecule 17: 30S ribosomal protein S17

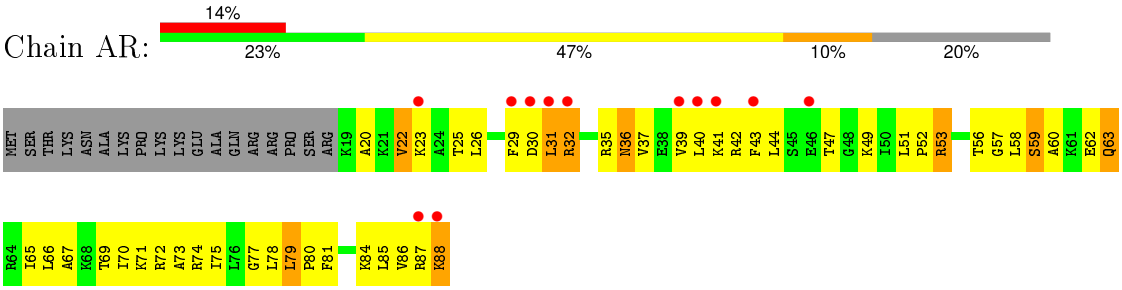


• Molecule 17: 30S ribosomal protein S17



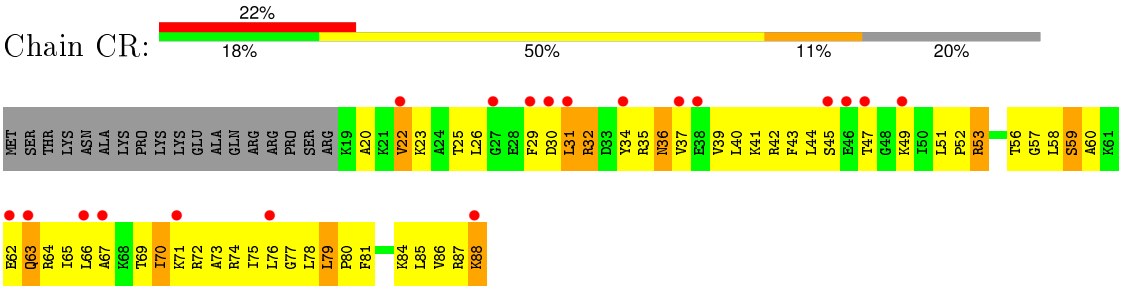
• Molecule 18: 30S ribosomal protein S18

Chain AR:



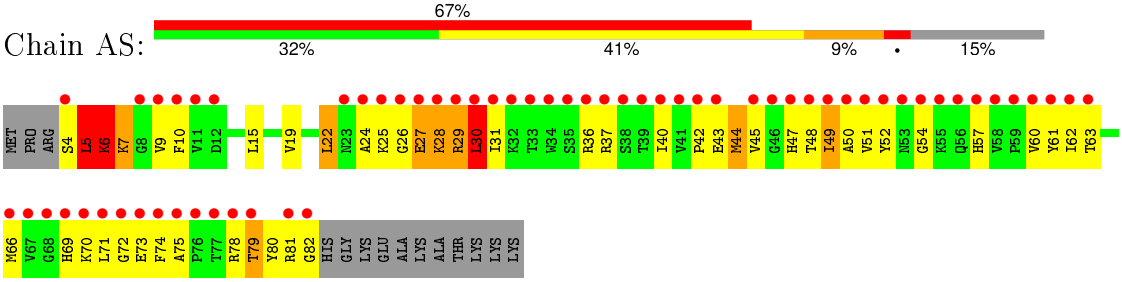
- Molecule 18: 30S ribosomal protein S18

Chain CR:



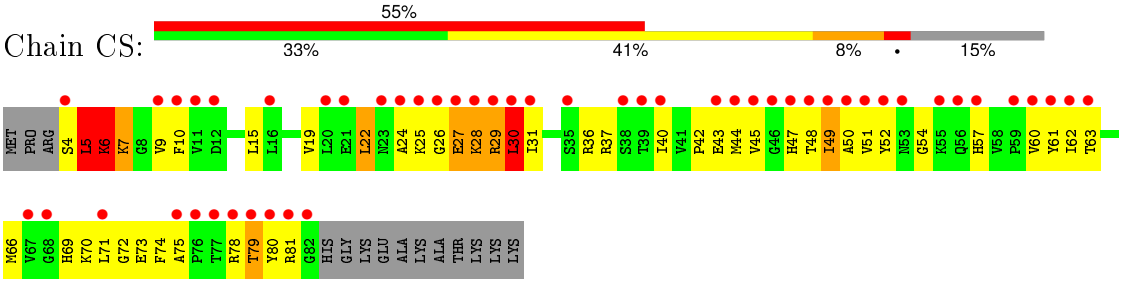
- Molecule 19: 30S ribosomal protein S19

Chain AS:



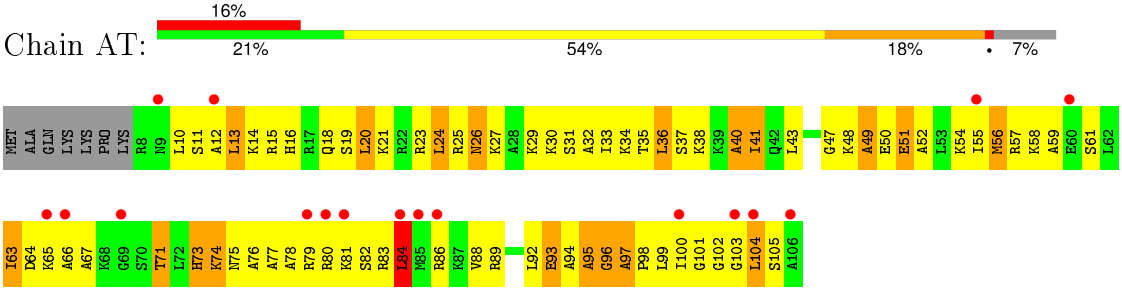
- Molecule 19: 30S ribosomal protein S19

Chain CS:



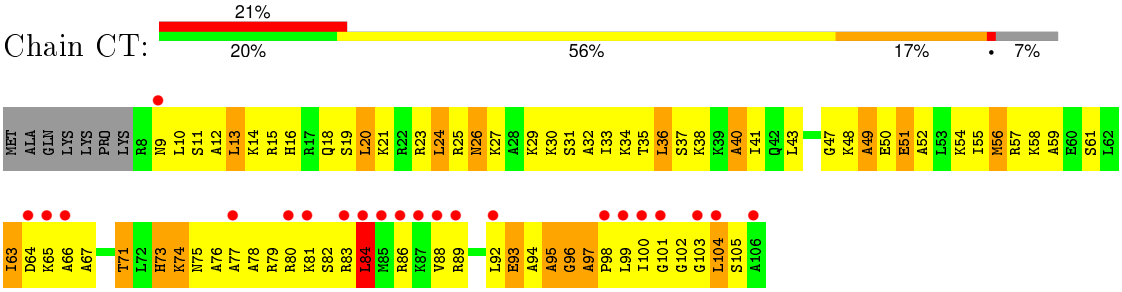
- Molecule 20: 30S ribosomal protein S20

Chain AT:



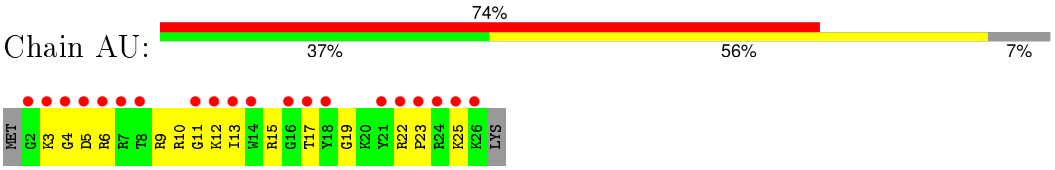
- Molecule 20: 30S ribosomal protein S20

Chain CT:



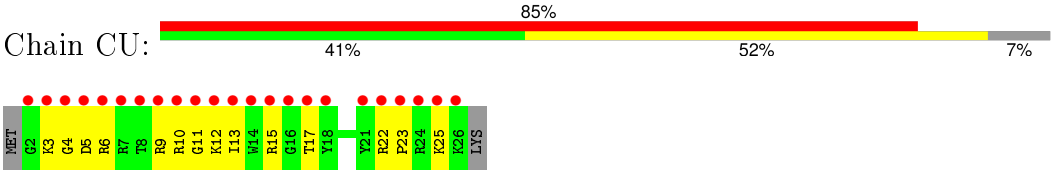
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



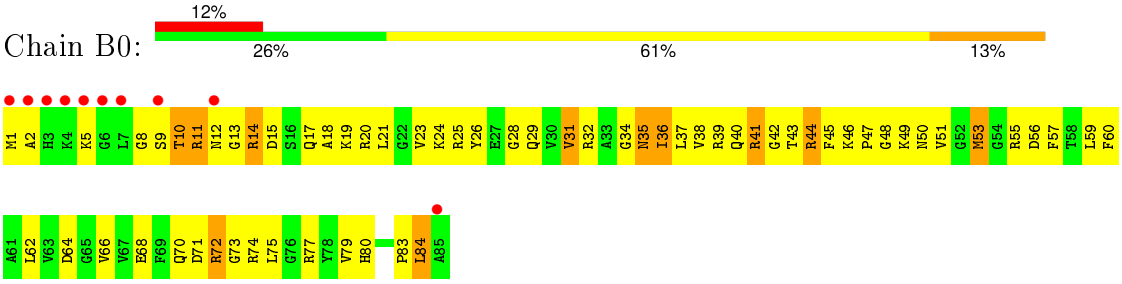
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



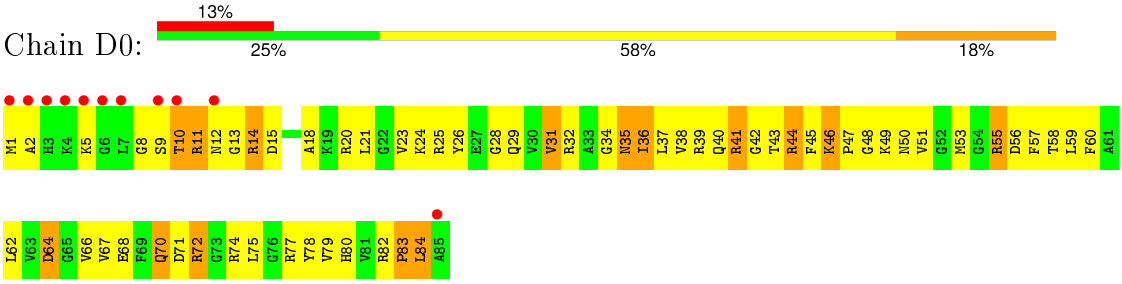
- Molecule 22: 50S ribosomal protein L27

Chain B0:



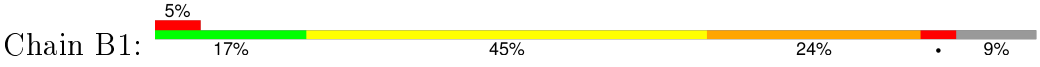
- Molecule 22: 50S ribosomal protein L27

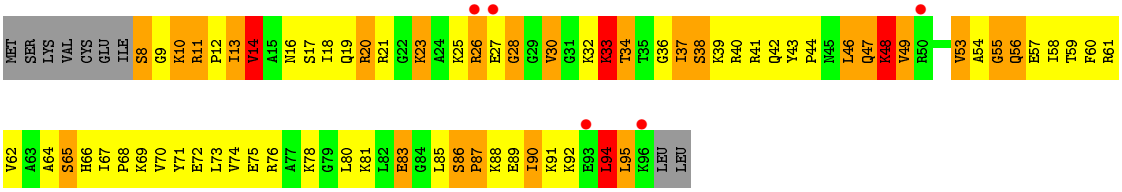
Chain D0:

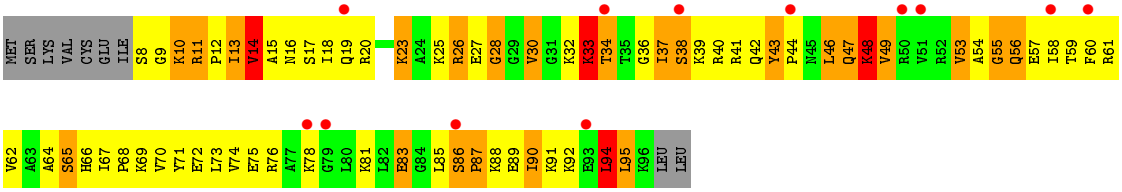


- Molecule 23: 50S ribosomal protein L28

Chain B1:





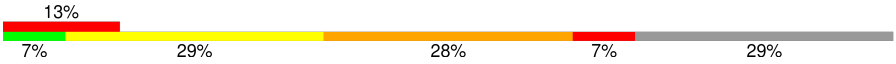


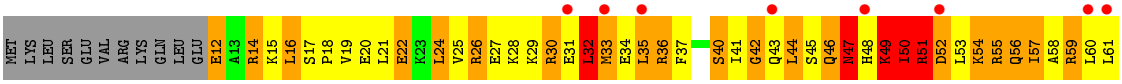
• Molecule 23: 50S ribosomal protein L28

Chain D1:

• Molecule 24: 50S ribosomal protein L29

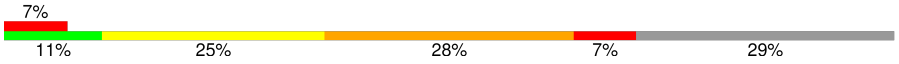
Chain B2:

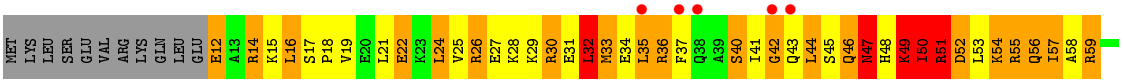




• Molecule 24: 50S ribosomal protein L29

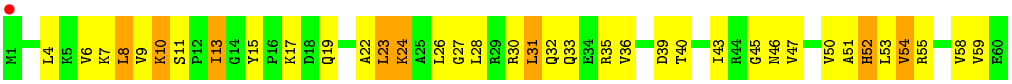
Chain D2:





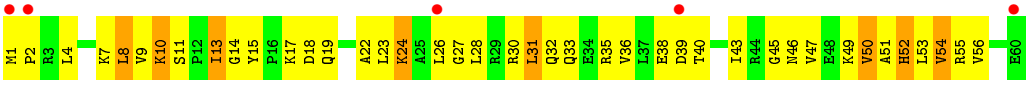
• Molecule 25: 50S ribosomal protein L30

Chain B3:



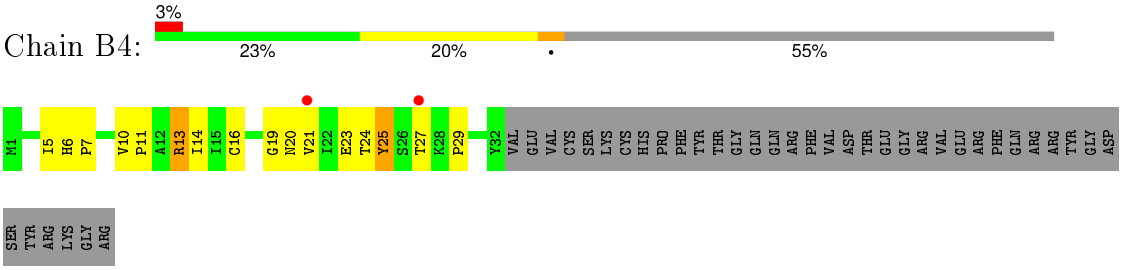
• Molecule 25: 50S ribosomal protein L30

Chain D3:



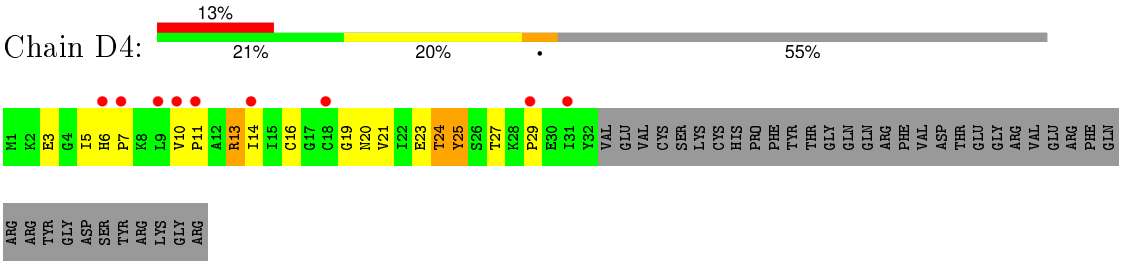
- Molecule 26: 50S ribosomal protein L31

Chain B4:



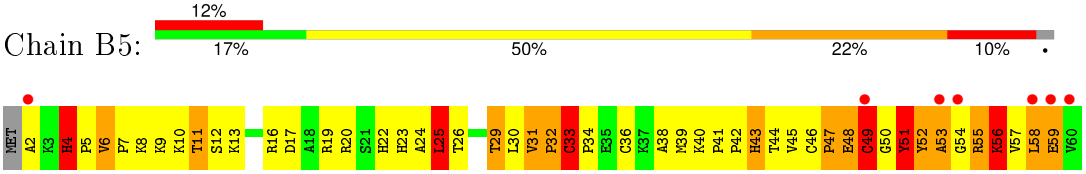
- Molecule 26: 50S ribosomal protein L31

Chain D4:



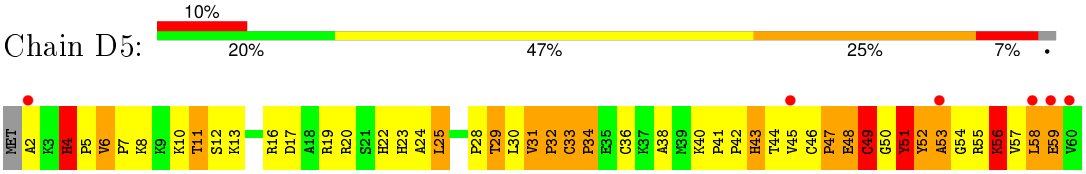
- Molecule 27: 50S ribosomal protein L32

Chain B5:



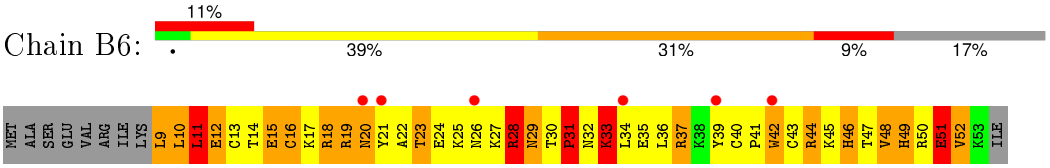
- Molecule 27: 50S ribosomal protein L32

Chain D5:



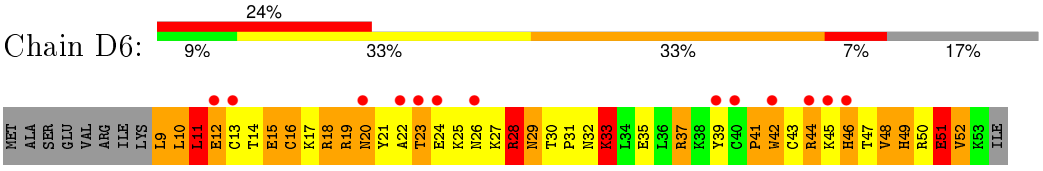
- Molecule 28: 50S ribosomal protein L33

Chain B6:



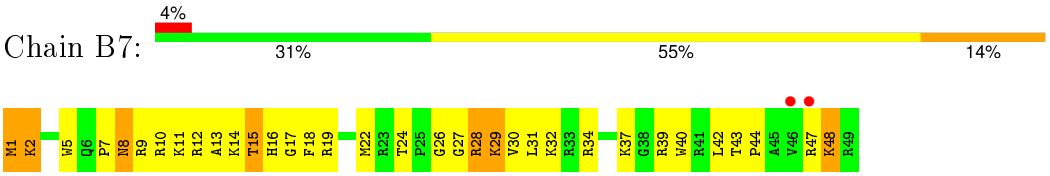
- Molecule 28: 50S ribosomal protein L33

Chain D6:



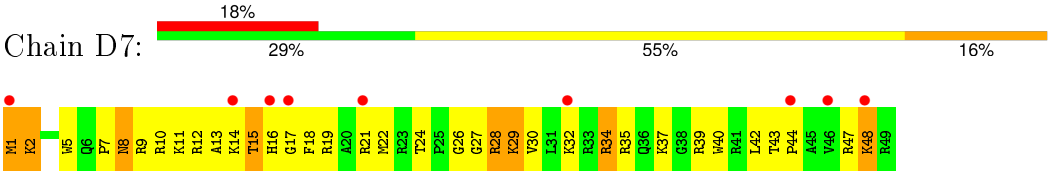
- Molecule 29: 50S ribosomal protein L34

Chain B7:



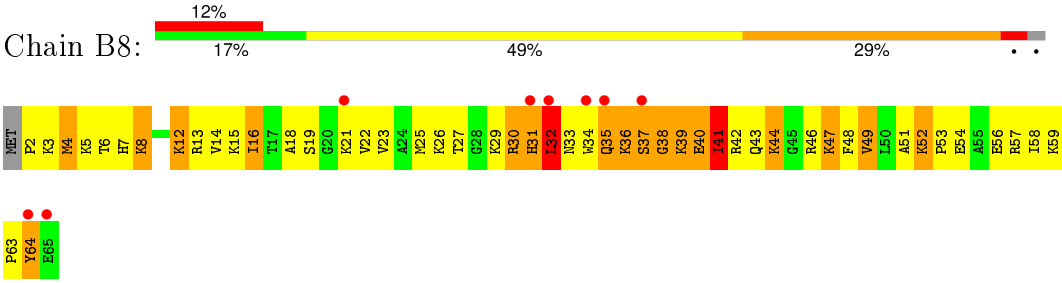
• Molecule 29: 50S ribosomal protein L34

Chain D7:



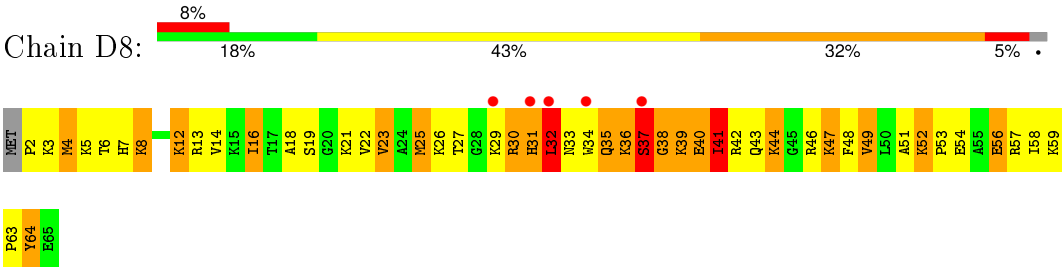
• Molecule 30: 50S ribosomal protein L35

Chain B8:



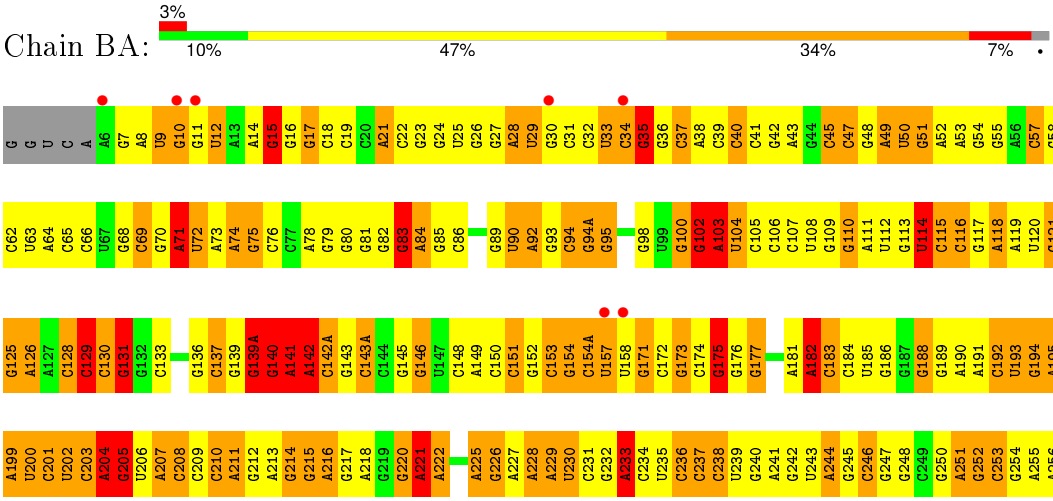
• Molecule 30: 50S ribosomal protein L35

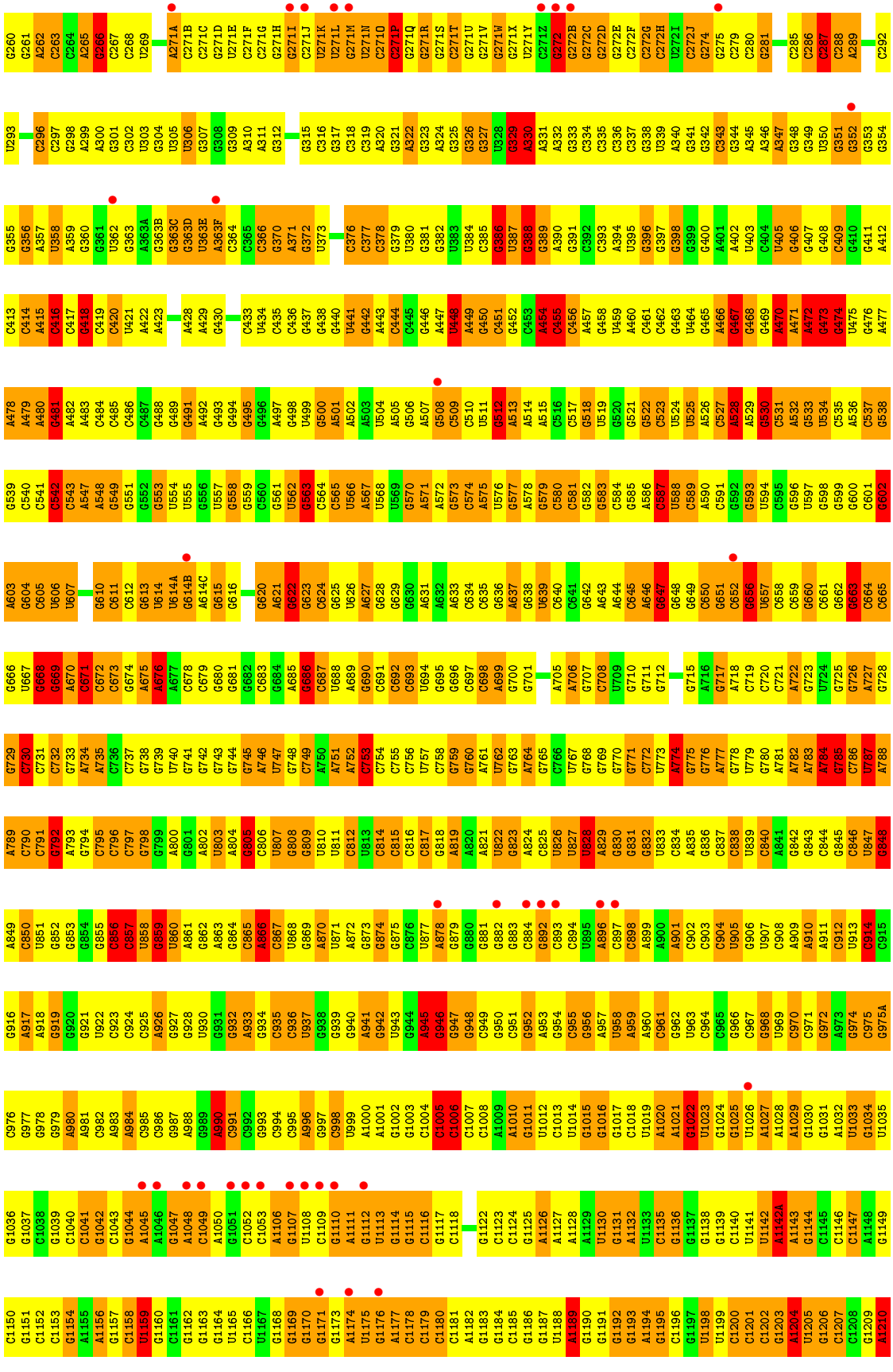
Chain D8:

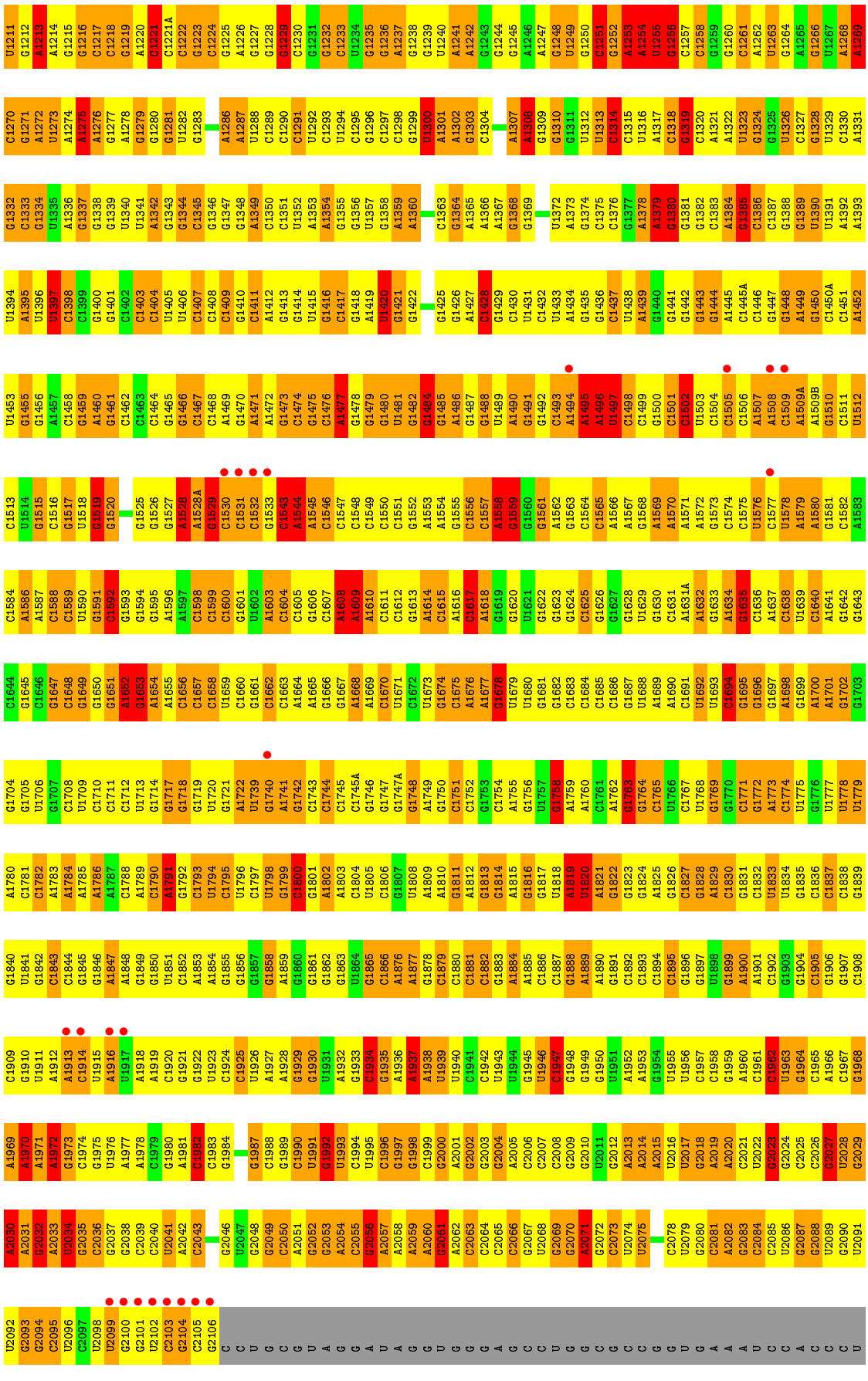


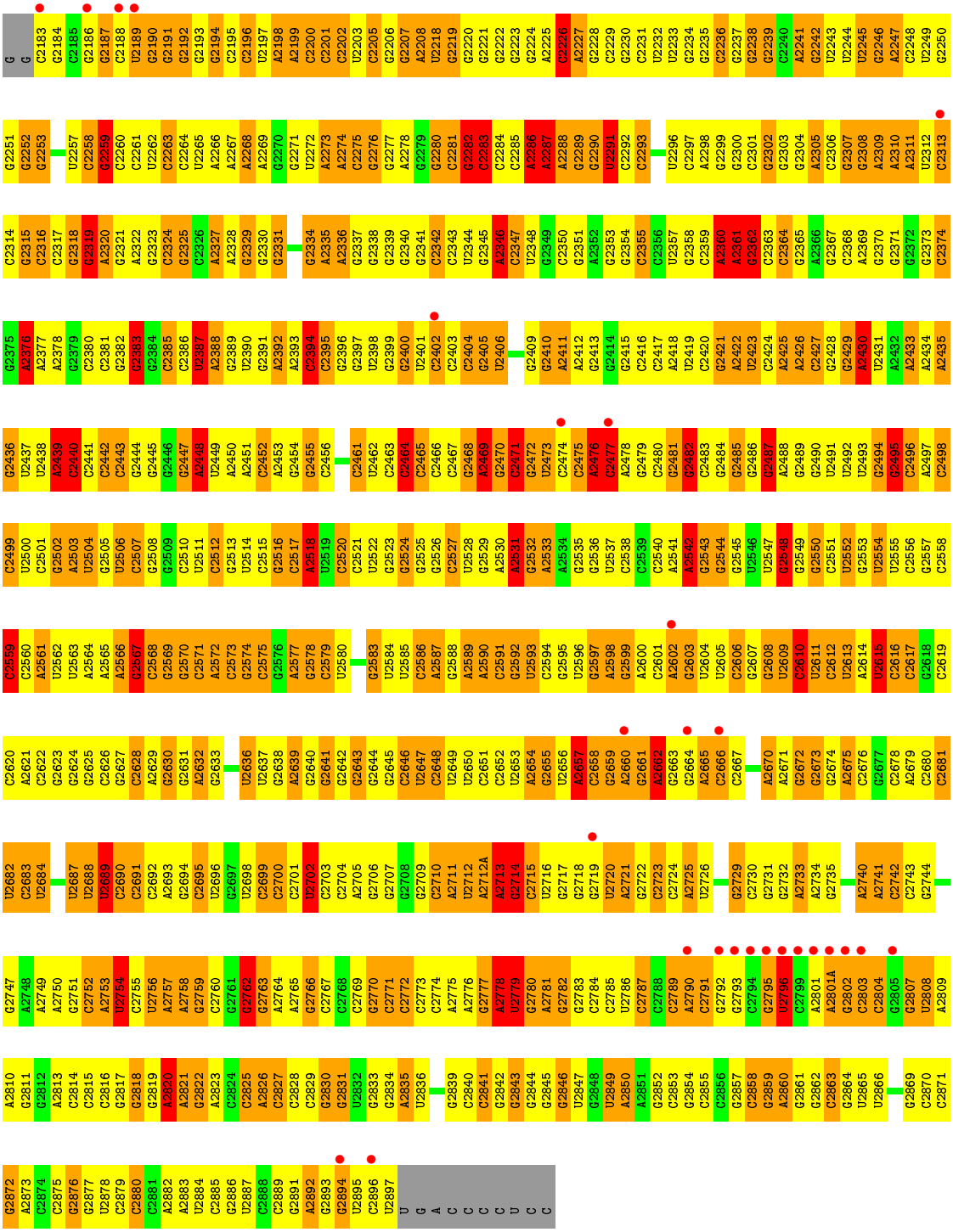
• Molecule 31: 23S ribosomal RNA

Chain BA:



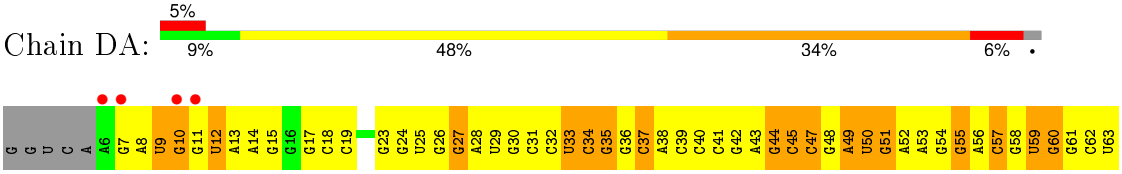


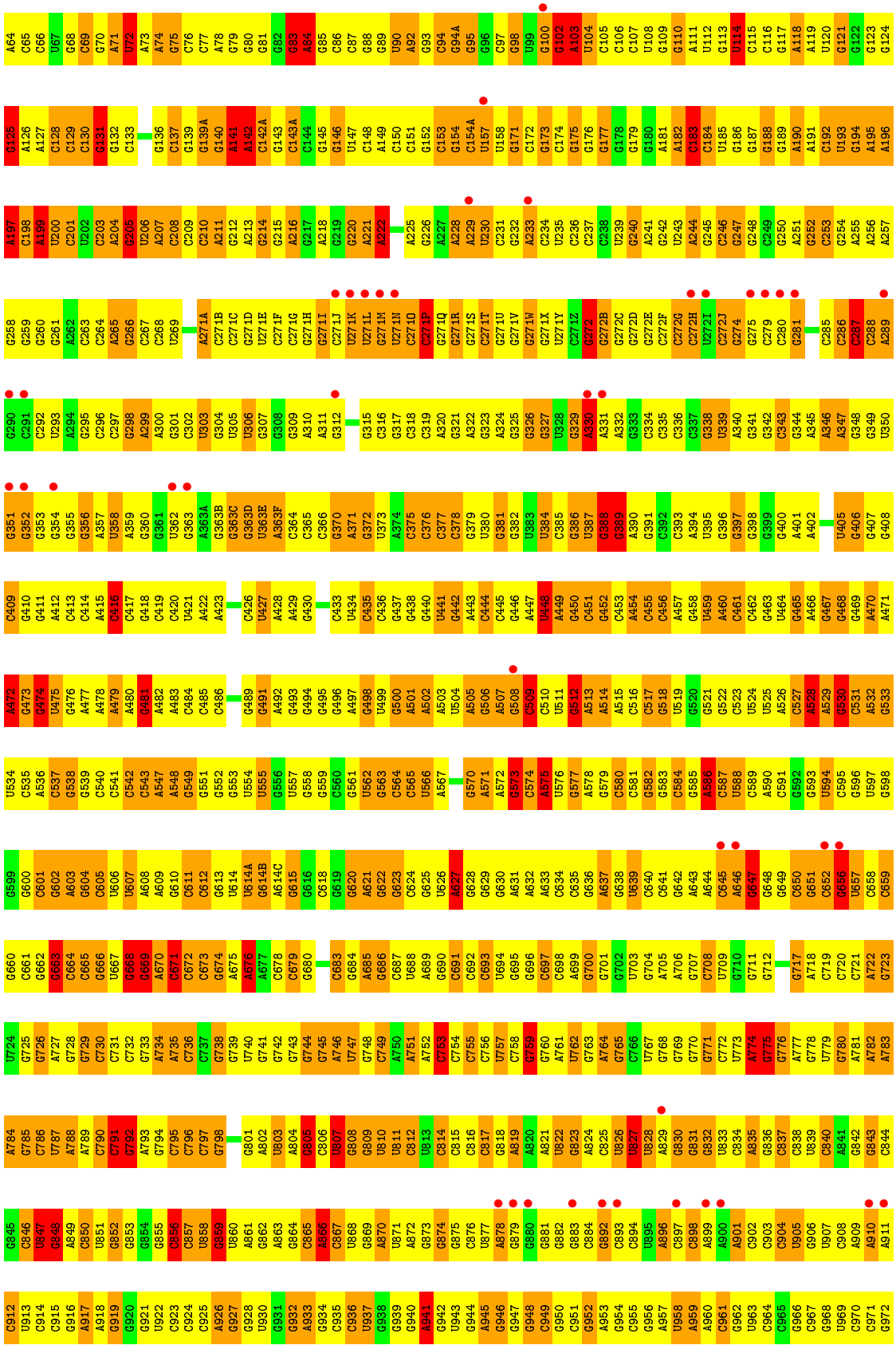


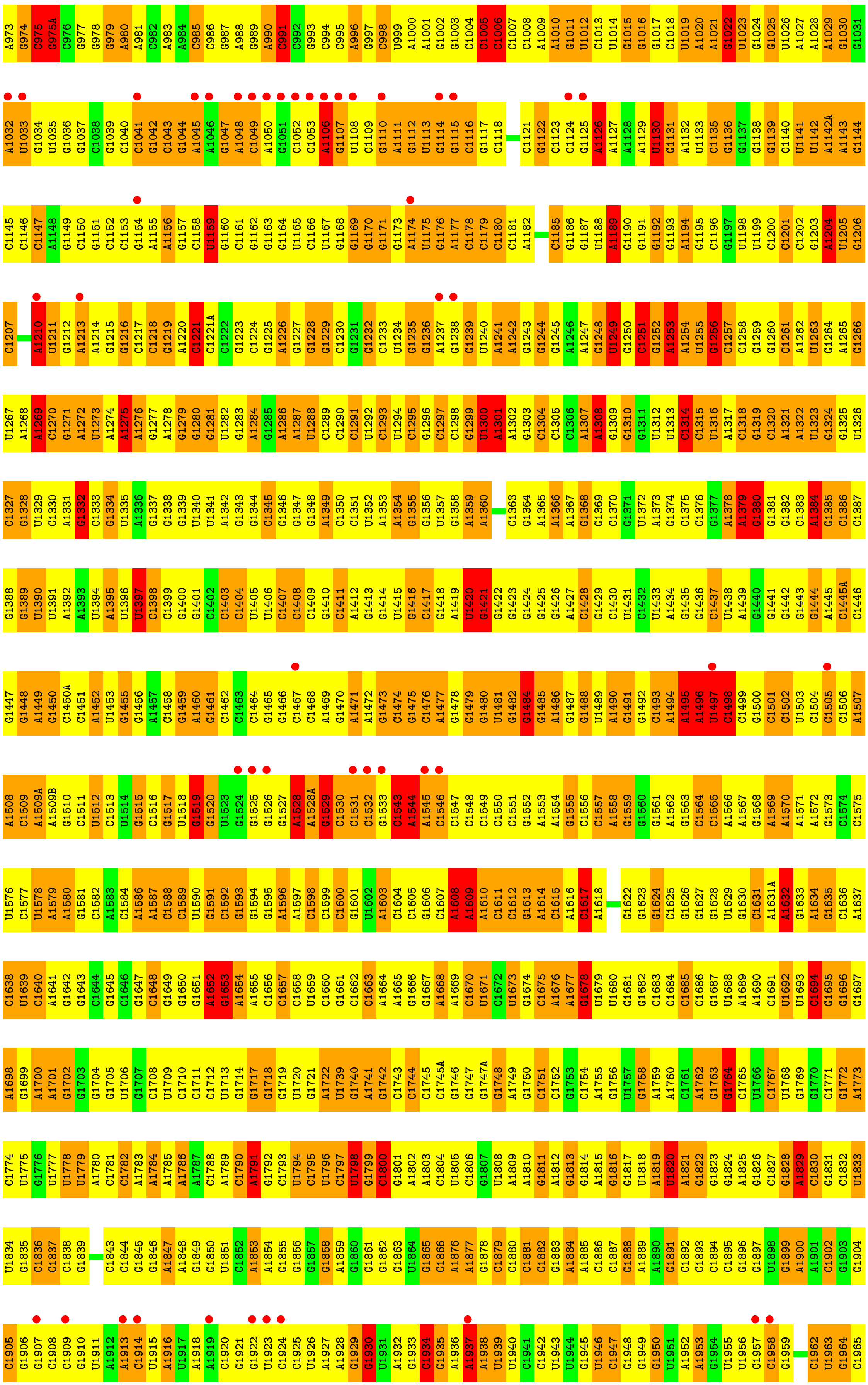


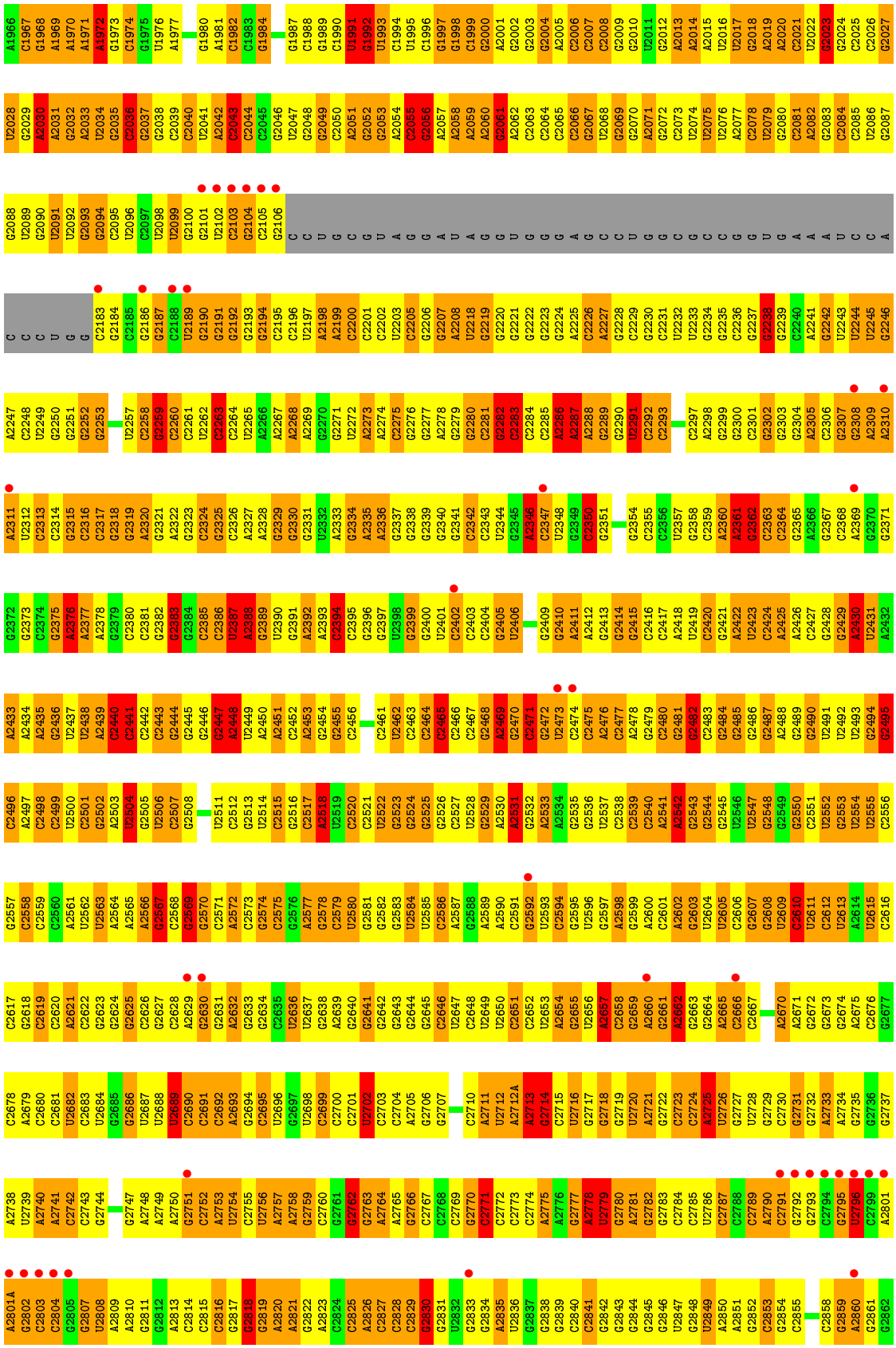
• Molecule 31: 23S ribosomal RNA

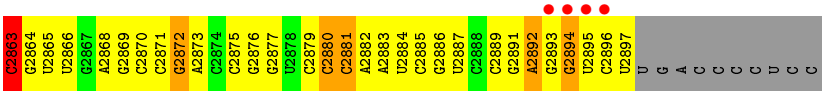
Chain DA:





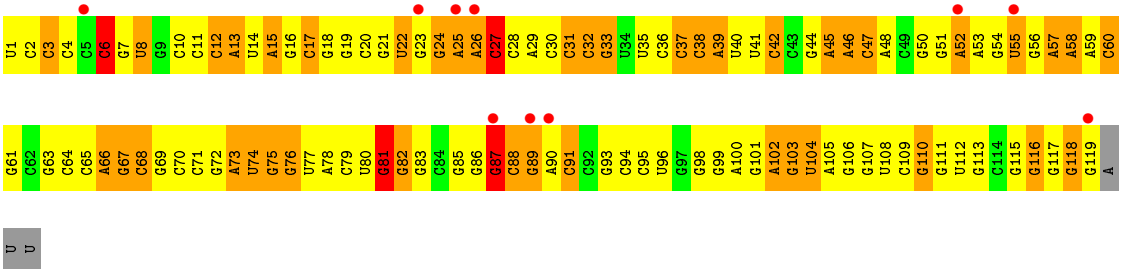

A973 G974 C975 G975A C976 G977 G978 G979 A980 A981 C982 A983 A984 G985 C986 G987 A988 G989 A990 C991 G992 G993 C994 C995 A996 G997 G998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031
A1032 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 — C1121 G1122 C1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144
C1145 C1146 C1147 A1148 G1149 C1150 G1151 C1152 C1153 G1154 A1155 A1156 G1157 C1158 U1159 G1160 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 — C1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 G1202 G1203 A1204 U1205 G1206
C1207 — A1210 U1211 G1212 A1213 A1214 G1215 G1216 C1217 C1218 G1219 A1220 C1221 C1221A C1222 G1223 C1224 G1225 A1226 G1227 G1228 G1229 C1230 G1231 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266
U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1279 G1280 G1281 U1282 G1283 A1284 G1285 A1286 A1287 U1288 C1289 C1290 C1291 U1292 C1293 U1294 C1295 G1296 C1297 C1298 G1299 U1300 A1301 A1302 G1303 C1304 C1305 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 A1322 U1323 G1324 G1325 U1326
C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 G1346 G1347 G1348 A1349 C1350 C1351 U1352 A1353 A1354 G1355 G1356 U1357 C1358 A1359 A1360 — C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 C1375 C1376 G1377 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 C1387
G1388 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 C1399 G1400 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 C1437 U1438 A1439 G1440 G1441 G1442 G1443 G1444 A1445 C1445A C1446
G1447 G1448 A1449 G1450 C1450A C1451 A1452 G1453 G1455 G1456 A1457 C1458 G1459 A1460 G1461 C1462 C1463 C1464 G1465 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474 G1475 C1476 A1477 G1478 G1479 C1480 U1481 G1482 G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 C1501 C1502 U1503 C1504 C1505 C1506 A1507
A1508 C1509 A1509A A1509B G1510 C1511 U1512 C1513 U1514 G1515 C1516 G1517 U1518 G1519 G1520 U1523 G1524 G1525 G1526 G1527 A1528 A1528A G1529 C1530 C1531 C1532 G1533 C1543 A1544 A1545 C1546 C1547 C1548 C1549 C1550 C1551 G1552 A1553 A1554 G1555 C1556 C1557 A1558 G1559 G1560 G1561 A1562 G1563 C1564 C1565 A1566 A1567 G1568 A1569 A1570 A1571 G1572 G1573 C1574 C1575
U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 G1595 A1596 A1597 C1598 C1599 C1600 G1601 U1602 A1603 C1604 C1605 G1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 — G1622 G1623 G1624 C1625 G1626 G1627 C1628 U1629 G1630 C1631 A1631A A1632 G1633 A1634 G1635 C1636 A1637
C1638 U1639 C1640 A1641 G1642 G1643 C1644 G1645 C1646 C1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1660 G1661 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 C1675 G1676 A1677 G1678 U1679 U1680 G1681 G1682 C1683 C1684 C1685 C1686 C1687 U1688 A1689 A1690 C1691 U1692 U1693 C1694 G1695 G1696 G1697
A1698 G1699 A1700 A1701 G1702 G1703 G1704 G1705 U1706 G1707 C1708 U1709 C1710 C1711 C1712 U1713 G1714 G1717 G1718 G1719 U1720 G1721 A1722 U1739 G1740 A1741 G1742 C1743 C1744 C1745 C1745A C1746 G1747 C1747A G1748 A1749 G1750 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1759 A1760 C1761 A1762 C1763 G1764 C1765 U1766 C1767 U1768 G1769 G1770 C1771 G1772 A1773
C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 C1806 G1807 U1808 A1809 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833
U1834 G1835 C1836 C1837 C1838 G1839 — C1843 C1844 G1845 G1846 A1847 A1848 G1849 G1850 U1851 C1852 A1853 A1854 G1855 G1856 G1857 G1858 A1859 G1860 G1861 G1862 G1863 U1864 G1865 C1866 A1876 A1877 G1878 C1879 C1880 C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 G1891 C1892 G1893 C1894 C1895 G1896 G1897 U1898 G1899 A1900 A1901 C1902 G1903 G1904
C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 U1946 C1947 G1948 G1949 G1950 U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1958 G1959 — C1962 U1963 G1964 C1965





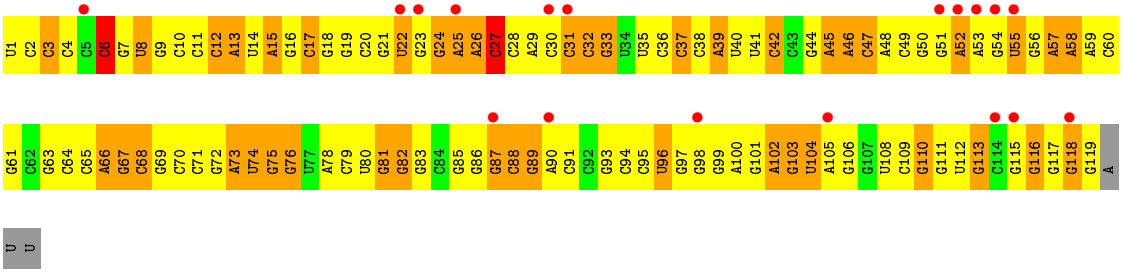
- Molecule 32: 5S ribosomal RNA

Chain BB:



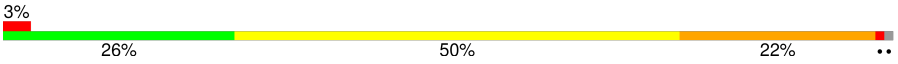
- Molecule 32: 5S ribosomal RNA

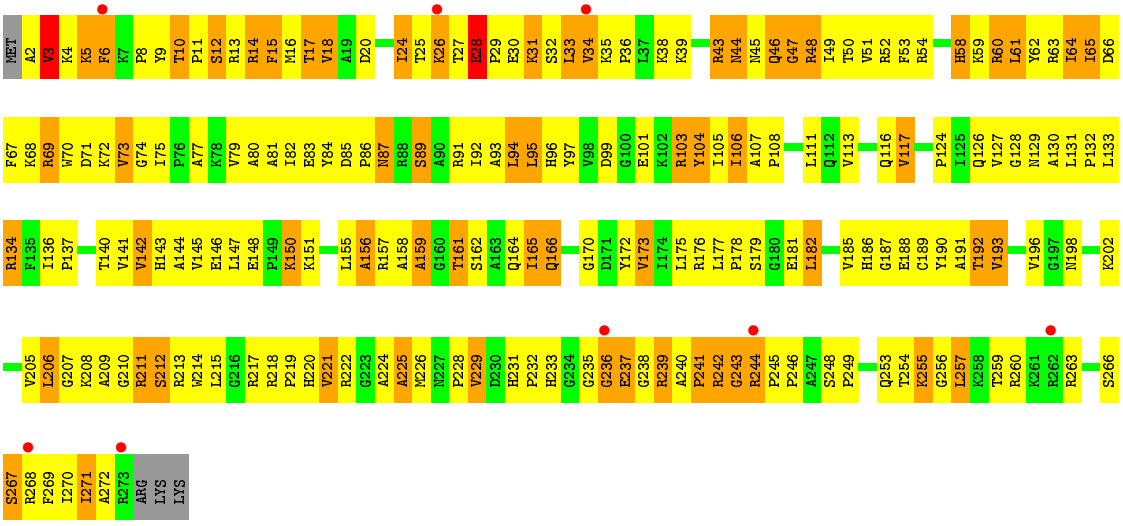
Chain DB:



- Molecule 33: 50S ribosomal protein L2

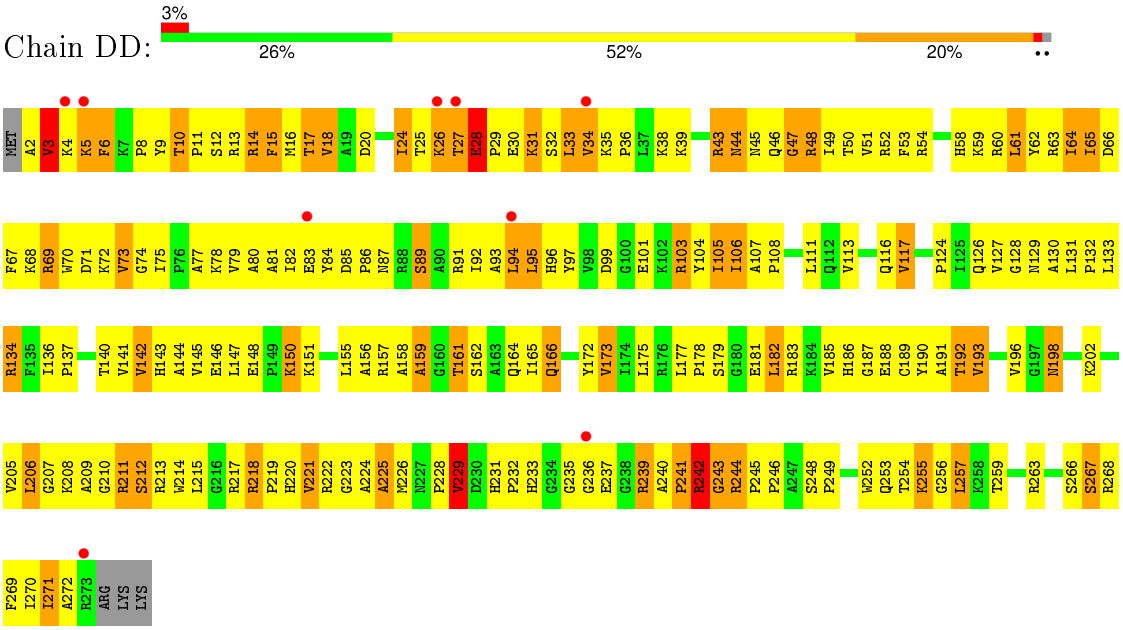
Chain BD:





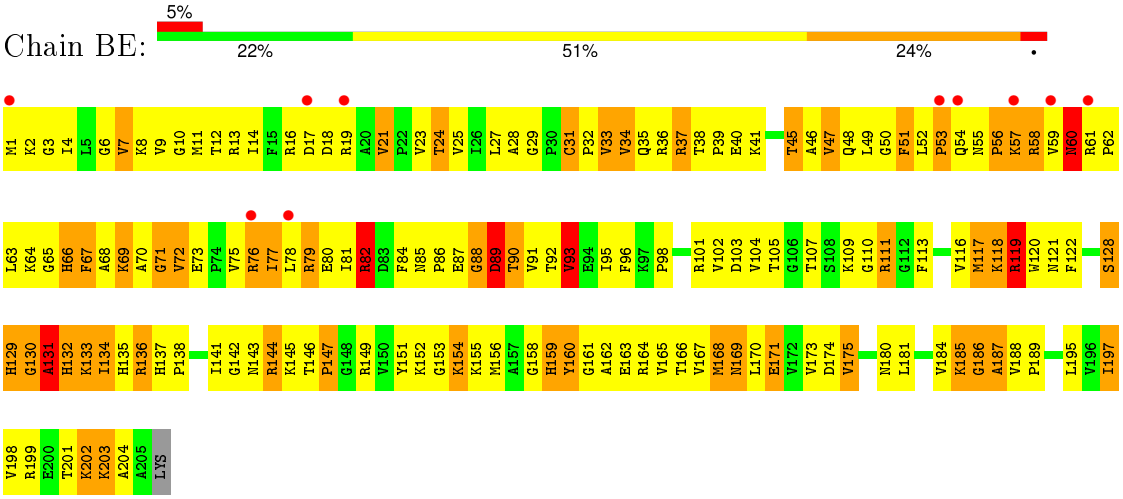
- Molecule 33: 50S ribosomal protein L2

Chain DD:



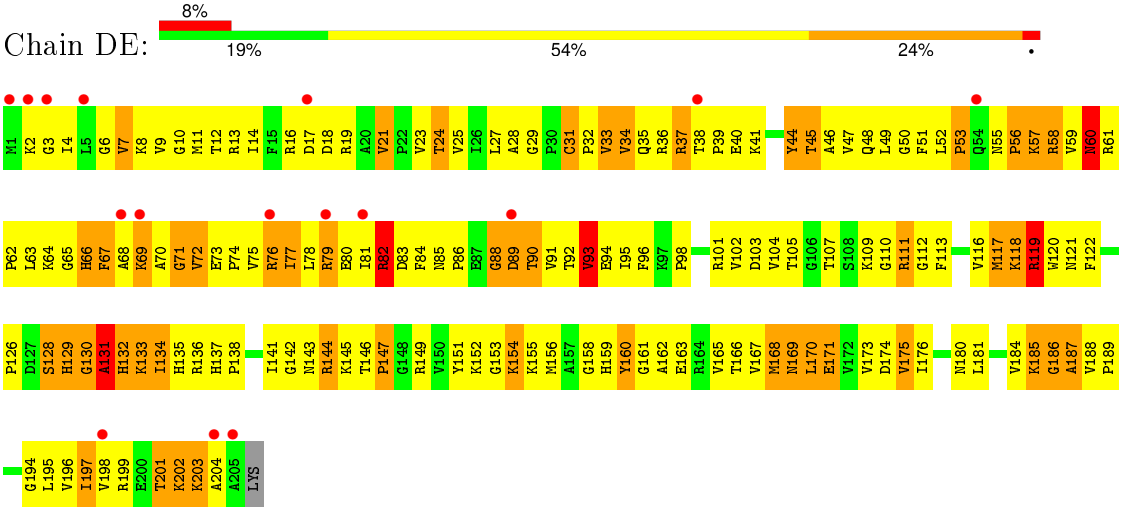
- Molecule 34: 50S ribosomal protein L3

Chain BE:



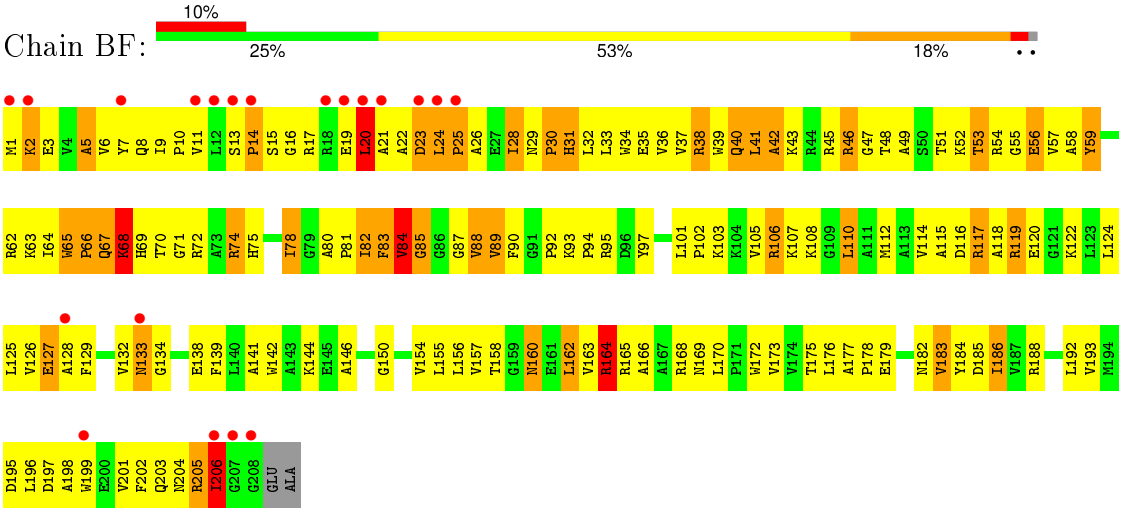
- Molecule 34: 50S ribosomal protein L3

Chain DE:



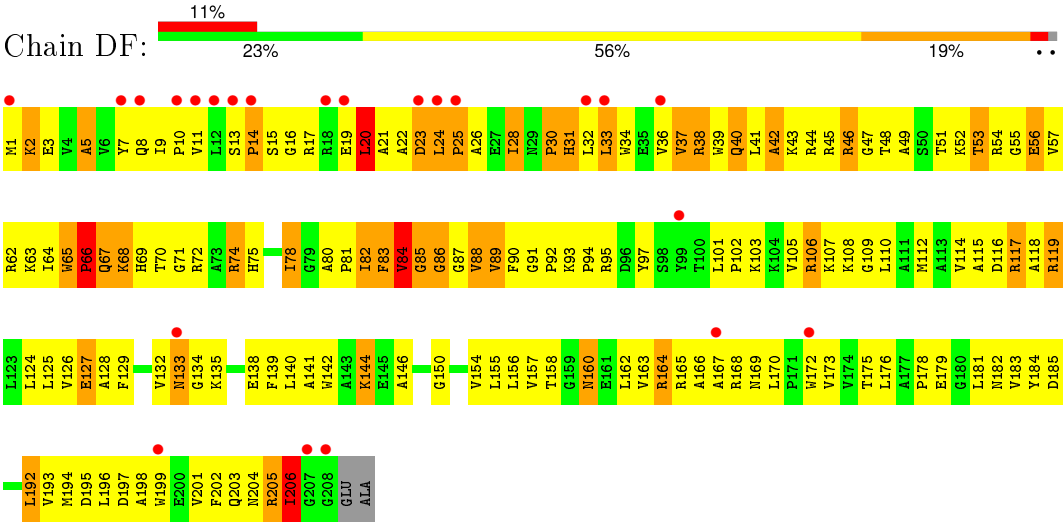
- Molecule 35: 50S ribosomal protein L4

Chain BF:



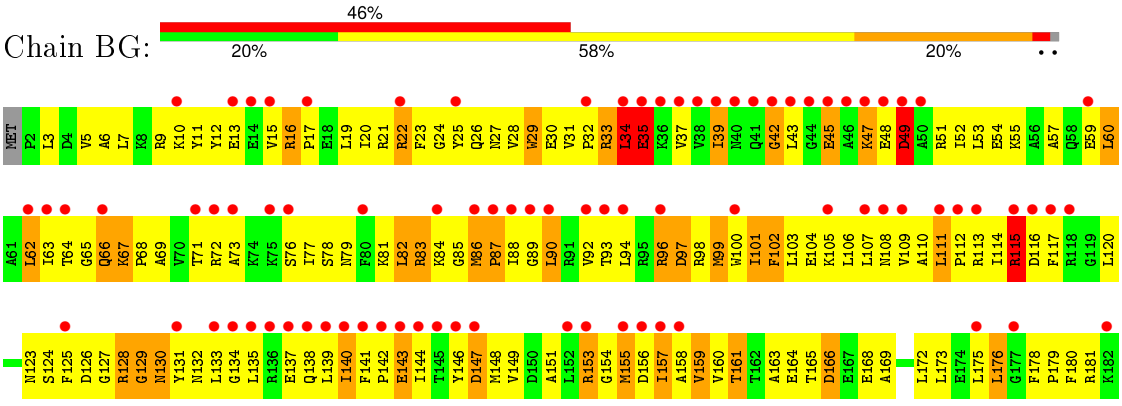
- Molecule 35: 50S ribosomal protein L4

Chain DF:



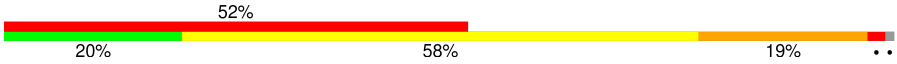
- Molecule 36: 50S ribosomal protein L5

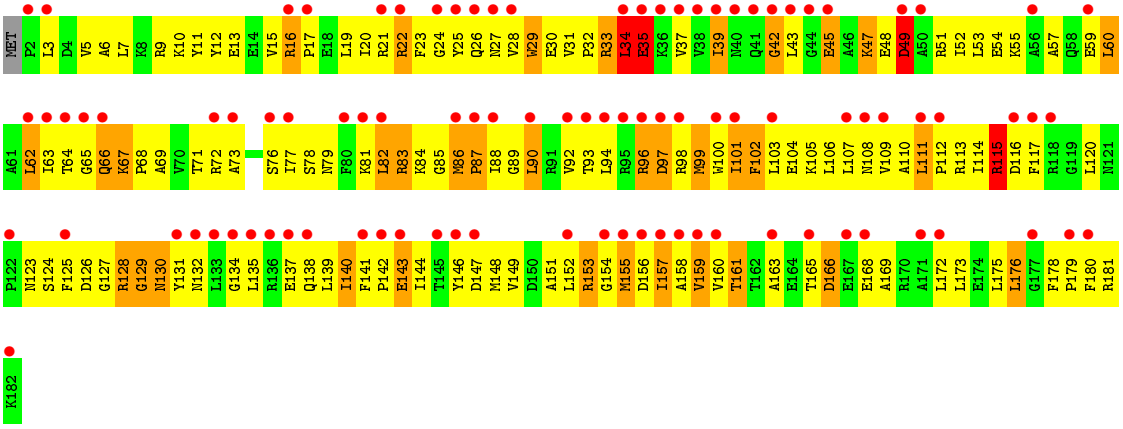
Chain BG:



- Molecule 36: 50S ribosomal protein L5

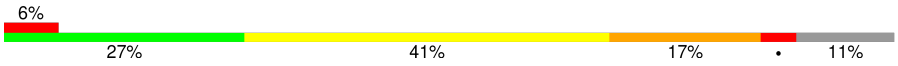
Chain DG:

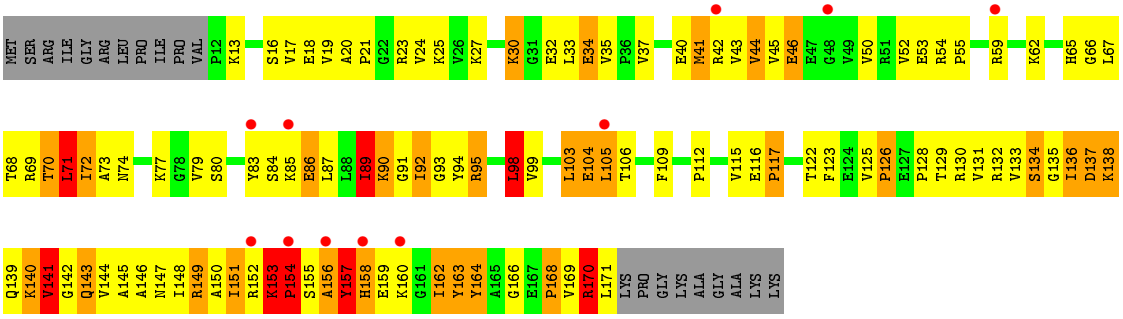




• Molecule 37: 50S ribosomal protein L6

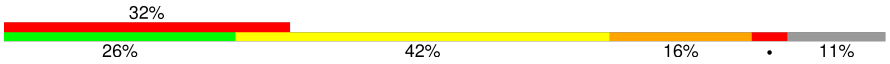
Chain BH:

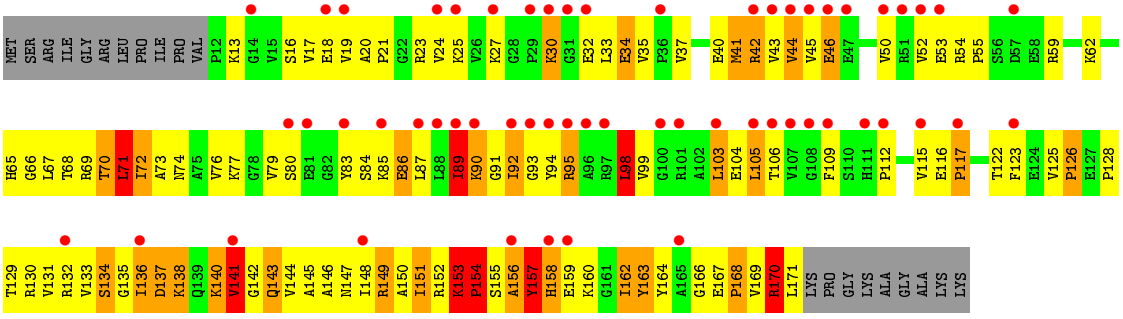




• Molecule 37: 50S ribosomal protein L6

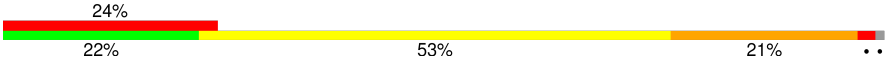
Chain DH:

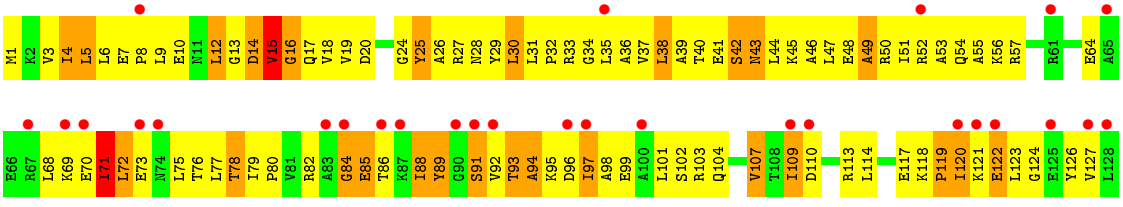


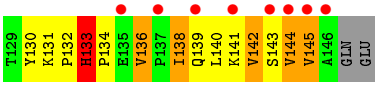


• Molecule 38: 50S ribosomal protein L9

Chain BI:

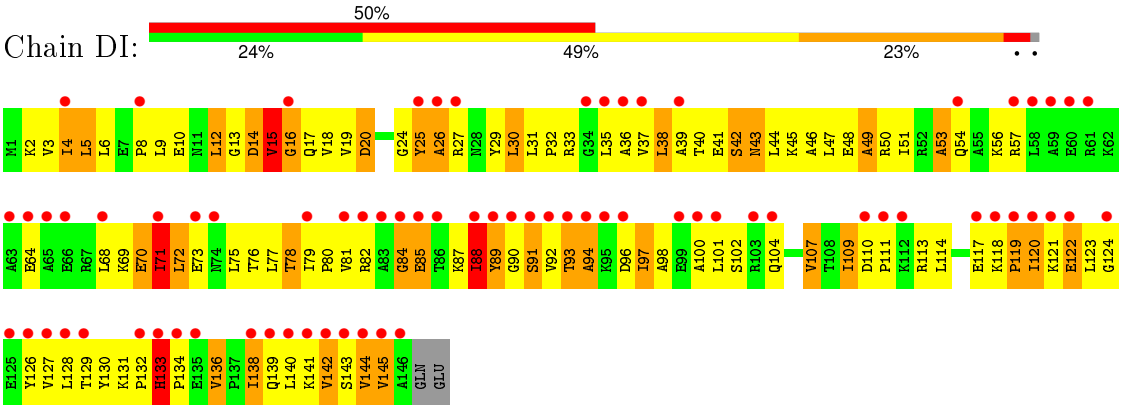






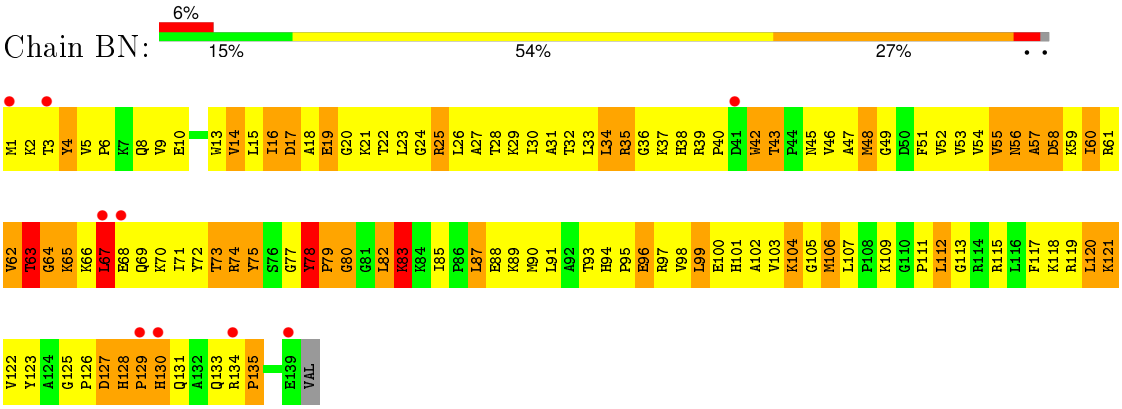
- Molecule 38: 50S ribosomal protein L9

Chain DI:



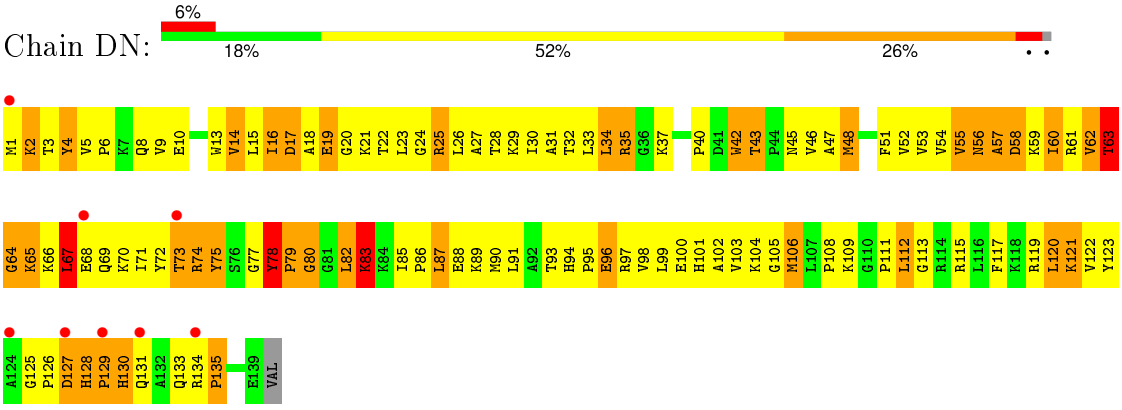
- Molecule 39: 50S ribosomal protein L13

Chain BN:



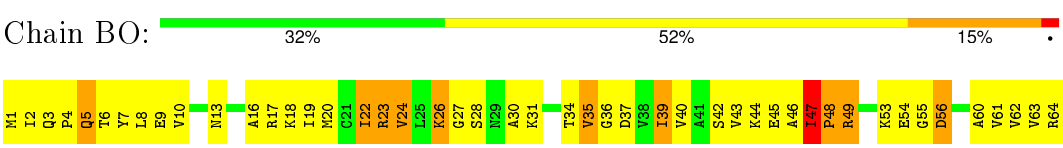
- Molecule 39: 50S ribosomal protein L13

Chain DN:



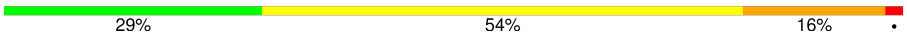
- Molecule 40: 50S ribosomal protein L14

Chain BO:



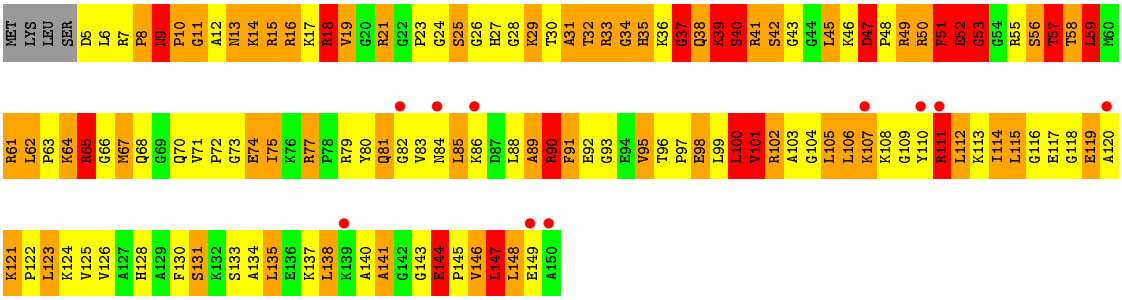
• Molecule 40: 50S ribosomal protein L14

Chain DO:



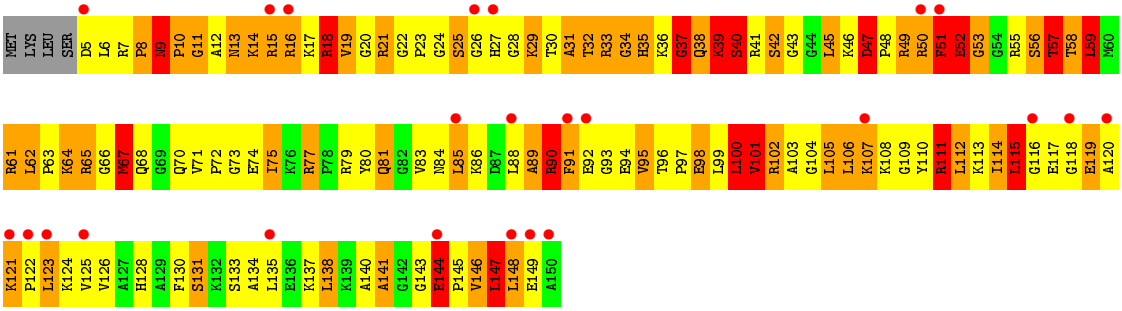
• Molecule 41: 50S ribosomal protein L15

Chain BP:



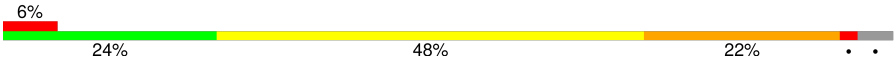
• Molecule 41: 50S ribosomal protein L15

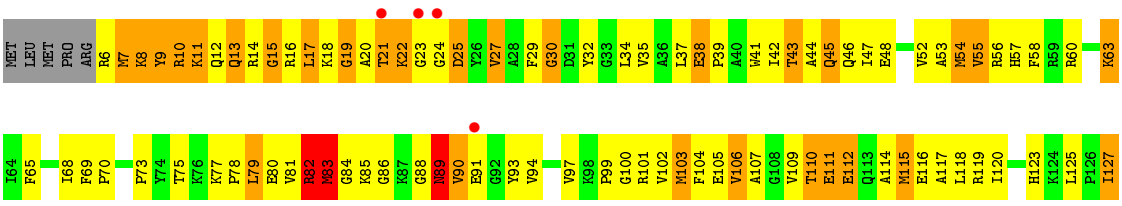
Chain DP:

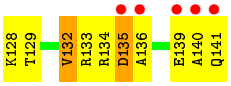


• Molecule 42: 50S ribosomal protein L16

Chain BQ:

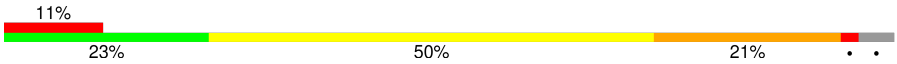


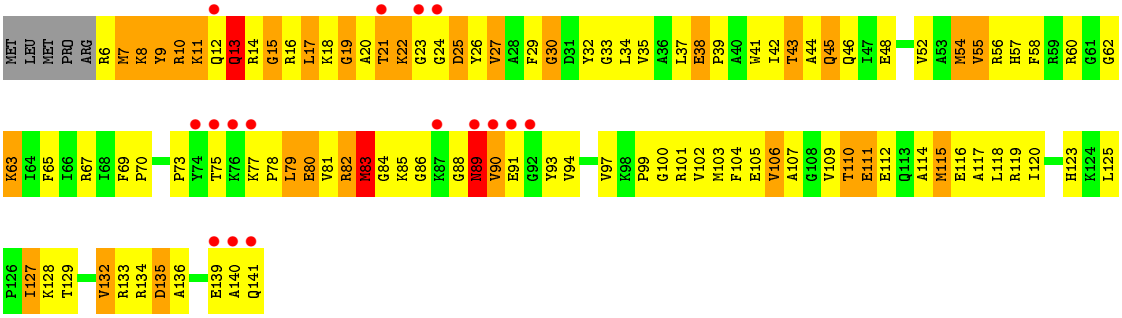




- Molecule 42: 50S ribosomal protein L16

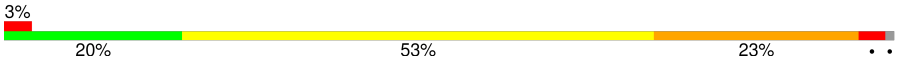
Chain DQ:

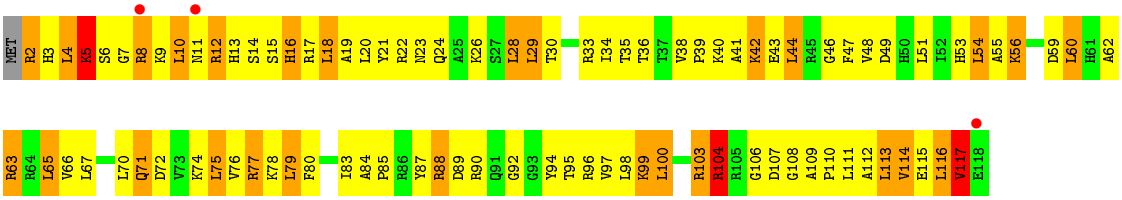




- Molecule 43: 50S ribosomal protein L17

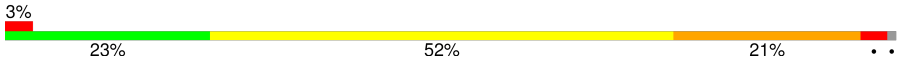
Chain BR:

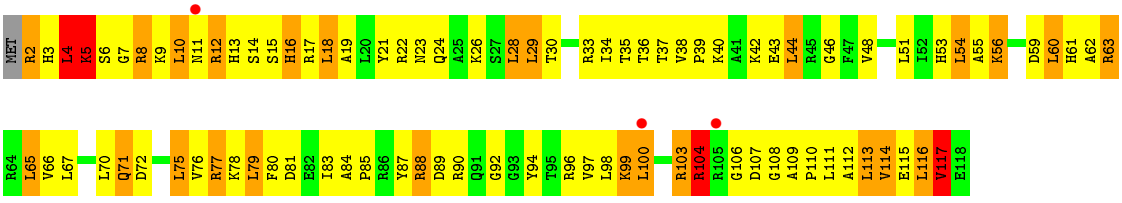




- Molecule 43: 50S ribosomal protein L17

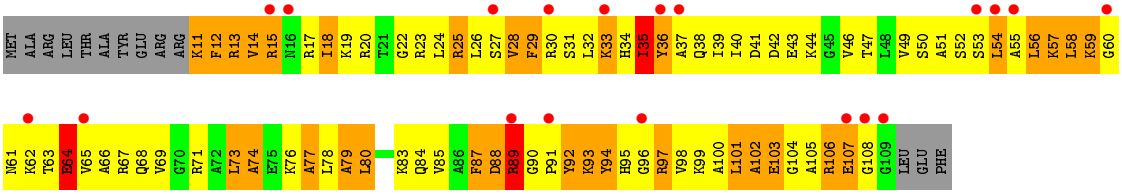
Chain DR:





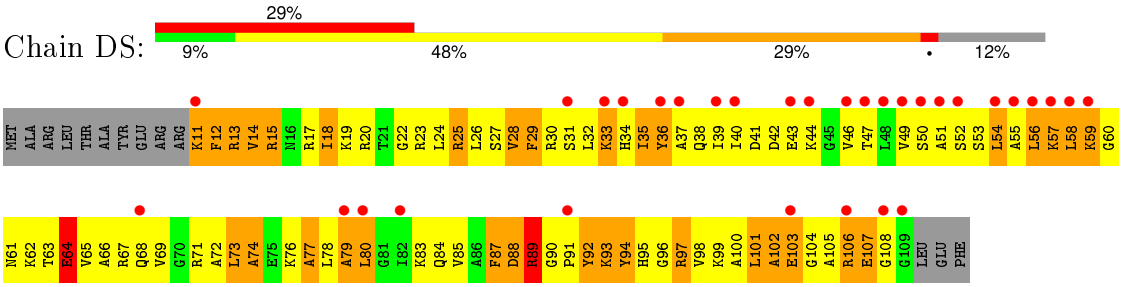
- Molecule 44: 50S ribosomal protein L18

Chain BS:



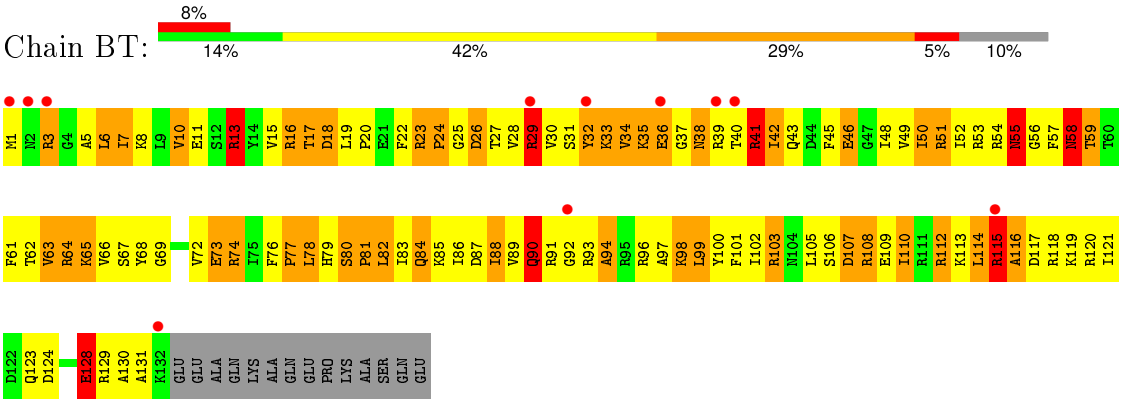
- Molecule 44: 50S ribosomal protein L18

Chain DS:



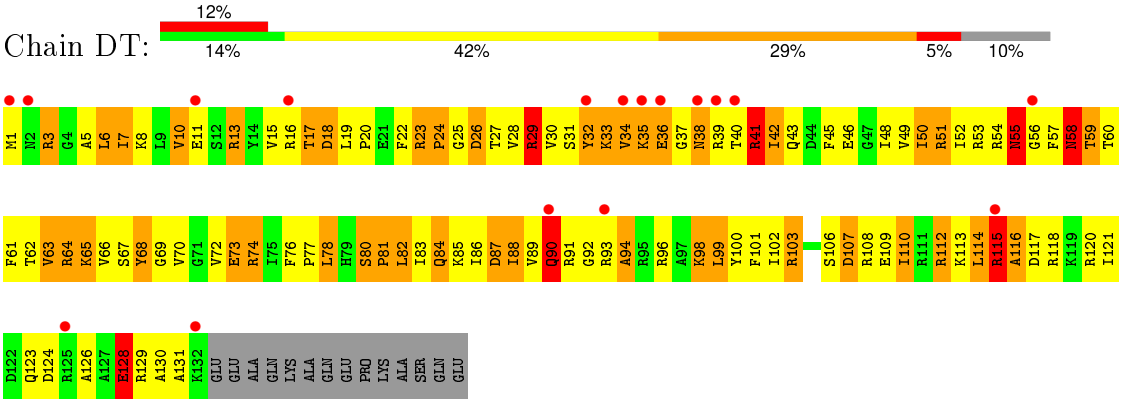
• Molecule 45: 50S ribosomal protein L19

Chain BT:



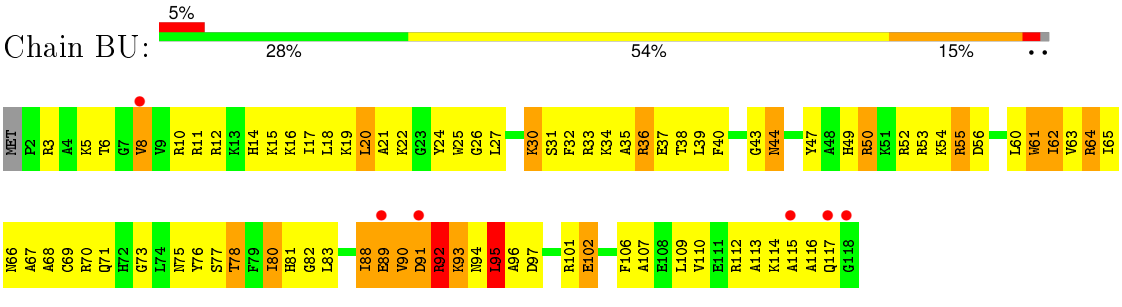
• Molecule 45: 50S ribosomal protein L19

Chain DT:



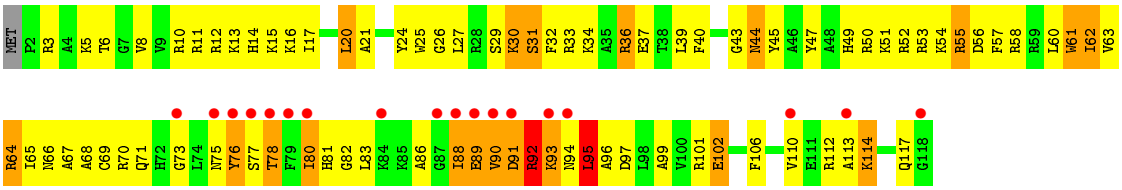
• Molecule 46: 50S ribosomal protein L20

Chain BU:



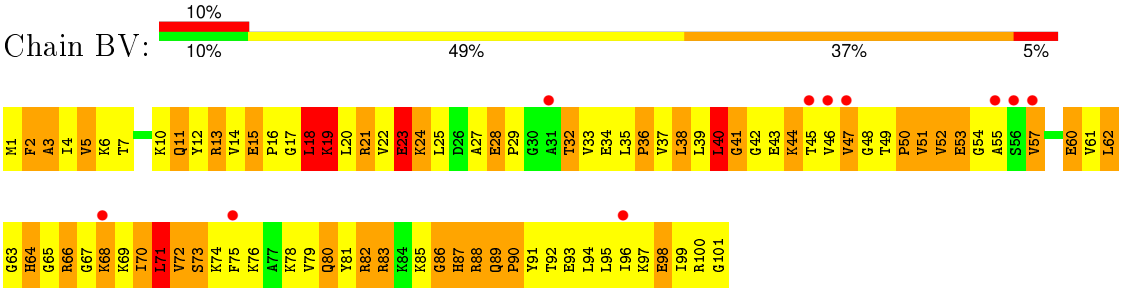
• Molecule 46: 50S ribosomal protein L20

Chain DU:



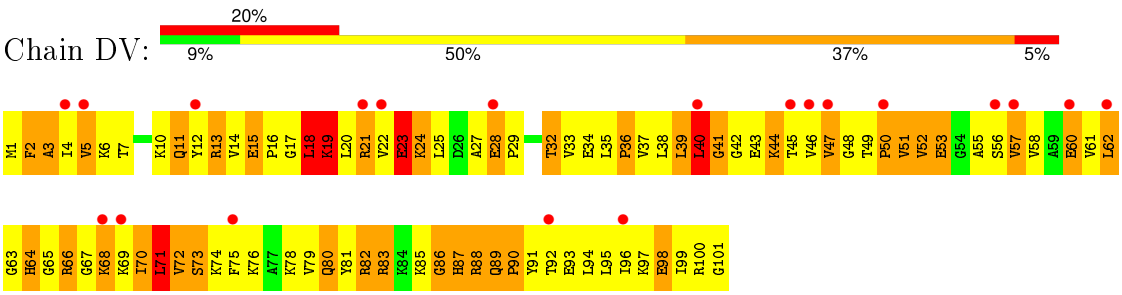
• Molecule 47: 50S ribosomal protein L21

Chain BV:



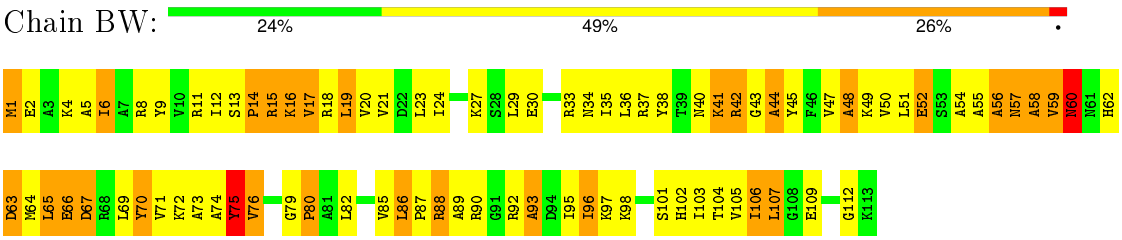
• Molecule 47: 50S ribosomal protein L21

Chain DV:



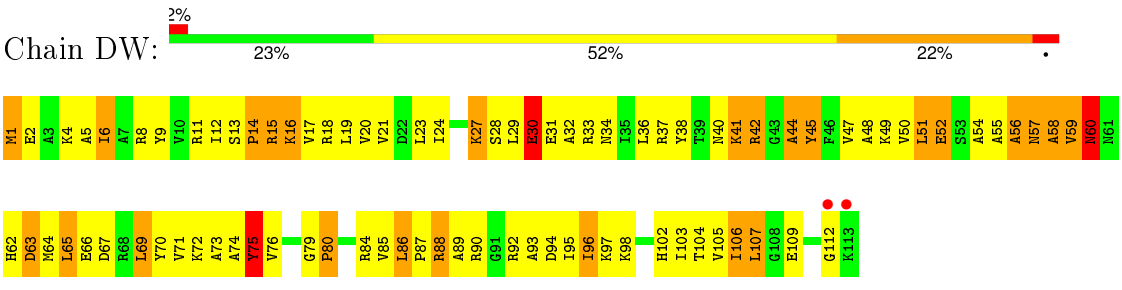
• Molecule 48: 50S ribosomal protein L22

Chain BW:



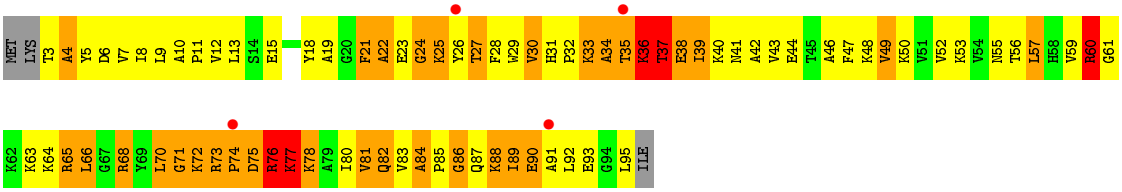
• Molecule 48: 50S ribosomal protein L22

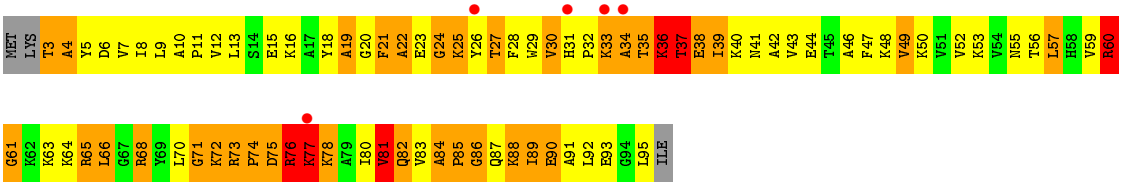
Chain DW:



• Molecule 49: 50S ribosomal protein L23

Chain BX:



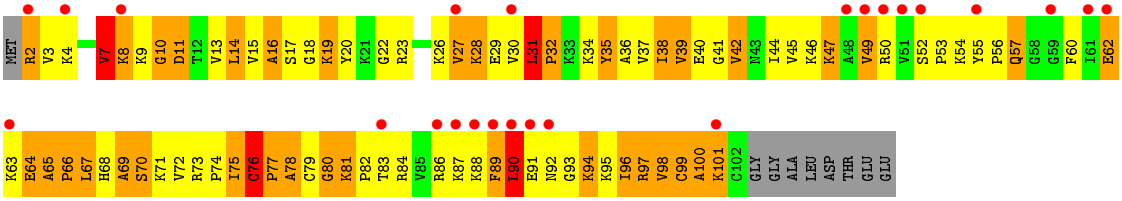


- Molecule 49: 50S ribosomal protein L23

Chain DX:

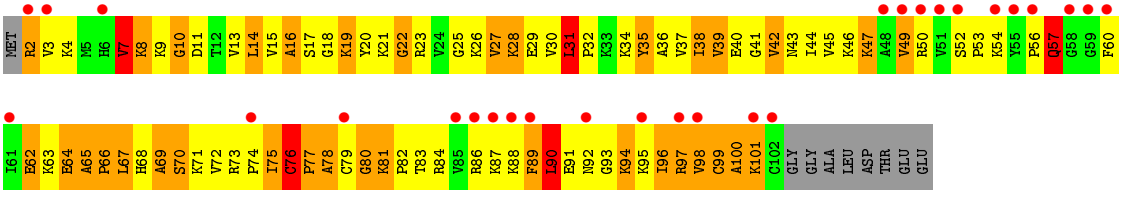
- Molecule 50: 50S ribosomal protein L24

Chain BY:



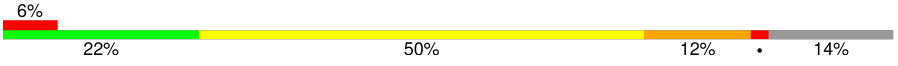
- Molecule 50: 50S ribosomal protein L24

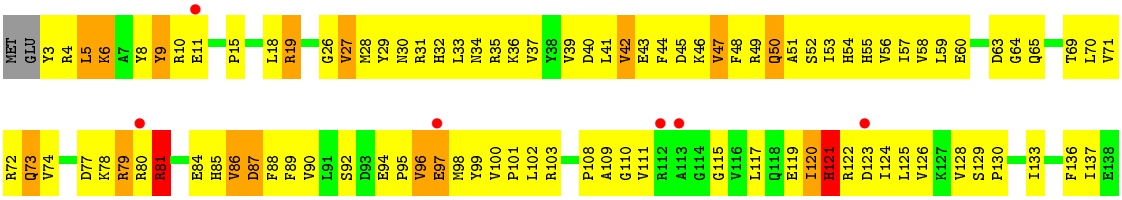
Chain DY:

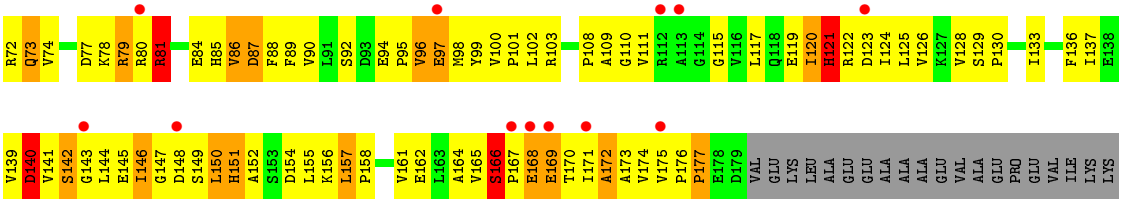


- Molecule 51: 50S ribosomal protein L25

Chain BZ:



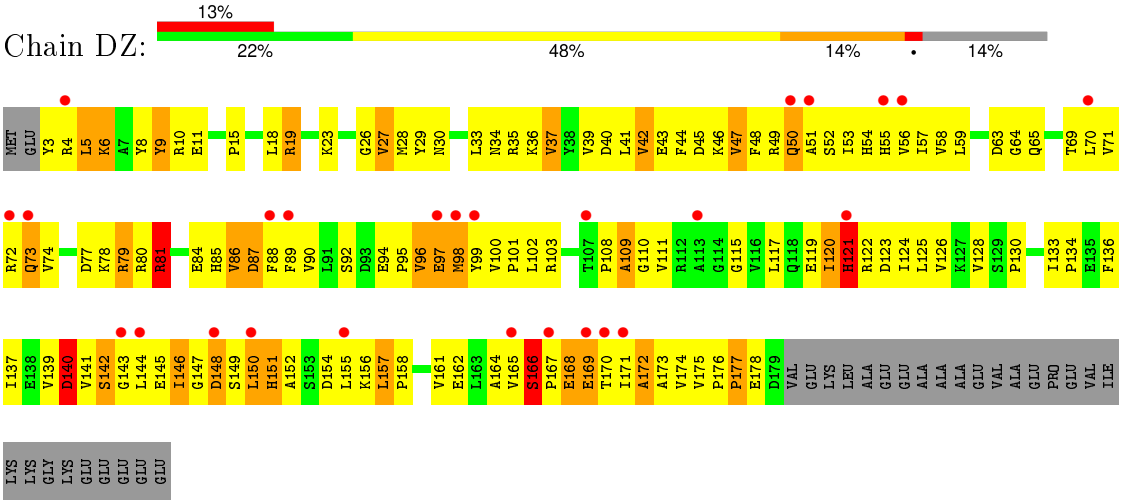




GLY LYS GLU GLU GLU GLU GLU

- Molecule 51: 50S ribosomal protein L25

Chain DZ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	207.32Å 437.99Å 614.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.10 48.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.97-3.10) 91.4 (48.97-3.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.12Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.246 , 0.284 0.247 , 0.283	Depositor DCC
R_{free} test set	45926 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	88.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 97.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 914156 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	278037	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.54	2/36190 (0.0%)	0.91	51/56486 (0.1%)
1	CA	0.52	2/36190 (0.0%)	0.92	61/56486 (0.1%)
2	AB	0.28	0/1936	0.49	0/2611
2	CB	0.28	0/1936	0.48	0/2611
3	AC	0.27	0/1637	0.45	0/2207
3	CC	0.27	0/1637	0.44	0/2207
4	AD	0.32	0/1733	0.54	0/2318
4	CD	0.34	0/1733	0.55	0/2318
5	AE	0.36	0/1163	0.55	0/1566
5	CE	0.34	0/1163	0.55	0/1566
6	AF	0.35	0/856	0.57	0/1154
6	CF	0.35	0/856	0.56	0/1154
7	AG	0.26	0/1276	0.43	0/1709
7	CG	0.26	0/1276	0.43	0/1709
8	AH	0.36	0/1136	0.56	0/1527
8	CH	0.35	0/1136	0.56	0/1527
9	AI	0.28	0/1028	0.44	0/1375
9	CI	0.28	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.27	0/808	0.48	0/1087
11	AK	0.34	0/900	0.55	0/1213
11	CK	0.33	0/900	0.55	0/1213
12	AL	0.40	0/987	0.65	0/1322
12	CL	0.40	0/987	0.66	0/1322
13	AM	0.28	0/928	0.48	0/1238
13	CM	0.28	0/928	0.48	0/1238
14	AN	0.28	0/501	0.46	0/664
14	CN	0.29	0/501	0.46	0/664
15	AO	0.35	0/745	0.55	0/992
15	CO	0.34	0/745	0.54	0/992
16	AP	0.34	0/717	0.55	0/965
16	CP	0.34	0/717	0.56	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.35	0/837	0.56	0/1119
17	CQ	0.35	0/837	0.55	0/1119
18	AR	0.35	0/579	0.57	0/768
18	CR	0.34	0/579	0.57	0/768
19	AS	0.28	0/643	0.45	0/867
19	CS	0.29	0/643	0.45	0/867
20	AT	0.34	0/765	0.53	0/1007
20	CT	0.34	0/765	0.54	0/1007
21	AU	0.26	0/213	0.42	0/279
21	CU	0.28	0/213	0.43	0/279
22	B0	0.60	0/658	0.75	0/878
22	D0	0.54	0/658	0.73	0/878
23	B1	0.69	0/700	0.97	0/931
23	D1	0.61	0/700	0.92	1/931 (0.1%)
24	B2	0.61	0/423	0.92	1/560 (0.2%)
24	D2	0.55	0/423	0.88	1/560 (0.2%)
25	B3	0.62	0/473	0.71	0/636
25	D3	0.45	0/473	0.66	0/636
26	B4	0.26	0/156	0.53	0/215
26	D4	0.28	0/156	0.52	0/215
27	B5	0.83	2/473 (0.4%)	1.04	3/639 (0.5%)
27	D5	0.67	0/473	1.01	3/639 (0.5%)
28	B6	0.73	0/387	0.91	2/517 (0.4%)
28	D6	0.60	0/387	0.85	1/517 (0.2%)
29	B7	0.67	0/427	0.83	0/563
29	D7	0.61	0/427	0.81	0/563
30	B8	0.72	0/516	0.98	1/681 (0.1%)
30	D8	0.61	0/516	0.94	1/681 (0.1%)
31	BA	1.17	111/65745 (0.2%)	1.49	1343/102639 (1.3%)
31	DA	0.89	28/65745 (0.0%)	1.45	1209/102639 (1.2%)
32	BB	0.87	0/2853	1.26	35/4451 (0.8%)
32	DB	0.63	0/2853	1.18	25/4451 (0.6%)
33	BD	0.63	0/2155	0.85	3/2907 (0.1%)
33	DD	0.58	0/2155	0.82	2/2907 (0.1%)
34	BE	0.69	0/1597	0.87	2/2155 (0.1%)
34	DE	0.58	0/1597	0.83	0/2155
35	BF	0.65	2/1659 (0.1%)	0.77	0/2246
35	DF	0.53	1/1659 (0.1%)	0.74	0/2246
36	BG	0.37	0/1498	0.61	1/2013 (0.0%)
36	DG	0.35	0/1498	0.59	1/2013 (0.0%)
37	BH	0.57	0/1246	0.71	0/1684
37	DH	0.41	0/1246	0.66	0/1684
38	BI	0.40	0/1147	0.65	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DI	0.43	0/1147	0.66	1/1553 (0.1%)
39	BN	0.71	0/1132	0.83	0/1527
39	DN	0.56	0/1132	0.76	0/1527
40	BO	0.62	0/943	0.74	0/1269
40	DO	0.53	0/943	0.73	0/1269
41	BP	0.65	0/1131	0.98	5/1504 (0.3%)
41	DP	0.56	0/1131	0.94	4/1504 (0.3%)
42	BQ	0.66	0/1100	0.80	1/1470 (0.1%)
42	DQ	0.55	0/1100	0.74	0/1470
43	BR	0.69	0/974	0.82	1/1302 (0.1%)
43	DR	0.57	0/974	0.80	2/1302 (0.2%)
44	BS	0.52	0/779	0.75	0/1038
44	DS	0.43	0/779	0.72	0/1038
45	BT	0.58	0/1114	0.82	0/1488
45	DT	0.52	0/1114	0.79	0/1488
46	BU	0.70	0/975	0.80	2/1297 (0.2%)
46	DU	0.56	0/975	0.74	1/1297 (0.1%)
47	BV	0.69	0/789	0.89	0/1054
47	DV	0.54	0/789	0.84	1/1054 (0.1%)
48	BW	0.76	0/907	0.91	1/1216 (0.1%)
48	DW	0.61	0/907	0.88	0/1216
49	BX	0.72	0/740	0.92	0/995
49	DX	0.63	0/740	0.90	0/995
50	BY	0.65	0/789	0.86	0/1053
50	DY	0.53	0/789	0.81	0/1053
51	BZ	0.46	0/1436	0.62	1/1951 (0.1%)
51	DZ	0.40	0/1436	0.61	1/1951 (0.1%)
All	All	0.79	148/301000 (0.0%)	1.17	2768/449812 (0.6%)

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	CA	1	0
22	B0	0	1
22	D0	0	1
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
27	B5	0	1
27	D5	0	1
31	BA	18	0
31	DA	18	0
33	BD	0	4
33	DD	0	2
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	3
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	2
49	DX	0	3
All	All	37	42

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	1142(A)	A	N9-C4	-11.15	1.31	1.37
31	BA	783	A	N9-C4	-10.64	1.31	1.37
31	BA	669	G	C4'-C3'	-10.15	1.42	1.53
31	BA	774	A	N9-C4	-9.61	1.32	1.37
31	DA	1142(A)	A	N9-C4	-9.23	1.32	1.37

The worst 5 of 2768 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	55	A	C8-N9-C4	-18.55	98.38	105.80
1	AA	55	A	N7-C8-N9	17.45	122.53	113.80
31	BA	1332	G	N3-C4-C5	16.73	136.96	128.60
31	BA	1332	G	N3-C4-N9	-16.73	115.96	126.00
31	BA	814	C	C6-N1-C2	15.82	126.63	120.30

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	472	A	C3'
31	BA	669	G	C4',C3',C1'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3'
31	BA	1379	A	C1'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	B0	11	ARG	Peptide
23	B1	30	VAL	Peptide
24	B2	54	LYS	Peptide
27	B5	51	TYR	Peptide
33	BD	47	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	2214	12
1	CA	32329	0	16318	2202	2
2	AB	1901	0	1951	203	0
2	CB	1901	0	1951	204	0
3	AC	1613	0	1677	143	0
3	CC	1613	0	1677	145	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1764	232	0
5	AE	1147	0	1207	126	0
5	CE	1147	0	1207	145	0
6	AF	843	0	857	116	0
6	CF	843	0	857	125	0
7	AG	1257	0	1296	77	0
7	CG	1257	0	1296	81	0
8	AH	1116	0	1177	144	0
8	CH	1116	0	1177	137	0
9	AI	1011	0	1042	112	0
9	CI	1011	0	1042	107	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	102	0
10	CJ	795	0	840	105	0
11	AK	885	0	904	109	0
11	CK	885	0	904	116	0
12	AL	971	0	1057	136	0
12	CL	971	0	1057	131	0
13	AM	921	0	976	97	0
13	CM	921	0	976	91	0
14	AN	492	0	532	46	0
14	CN	492	0	529	49	0
15	AO	734	0	771	81	0
15	CO	734	0	771	79	0
16	AP	701	0	720	103	0
16	CP	701	0	720	110	0
17	AQ	824	0	891	81	0
17	CQ	824	0	891	78	0
18	AR	574	0	644	86	0
18	CR	574	0	644	86	0
19	AS	630	0	652	53	0
19	CS	630	0	652	50	0
20	AT	763	0	861	93	0
20	CT	763	0	861	94	0
21	AU	209	0	221	14	0
21	CU	209	0	221	12	0
22	B0	650	0	654	90	0
22	D0	650	0	654	95	0
23	B1	693	0	764	149	0
23	D1	693	0	764	156	0
24	B2	421	0	461	141	0
24	D2	421	0	461	136	0
25	B3	468	0	523	47	0
25	D3	468	0	523	70	0
26	B4	157	0	69	7	0
26	D4	157	0	69	8	0
27	B5	459	0	480	100	0
27	D5	459	0	480	100	0
28	B6	381	0	390	102	0
28	D6	381	0	390	95	0
29	B7	419	0	467	54	0
29	D7	419	0	467	57	0
30	B8	508	0	576	156	0
30	D8	508	0	576	151	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29589	4119	0
31	DA	58698	0	29591	4387	0
32	BB	2551	0	1295	239	0
32	DB	2551	0	1295	231	0
33	BD	2105	0	2182	402	0
33	DD	2105	0	2182	406	0
34	BE	1564	0	1629	278	0
34	DE	1564	0	1629	278	0
35	BF	1624	0	1677	214	0
35	DF	1624	0	1677	209	0
36	BG	1474	0	1534	220	0
36	DG	1474	0	1534	223	0
37	BH	1223	0	1282	170	0
37	DH	1223	0	1282	162	0
38	BI	1132	0	1218	167	2
38	DI	1132	0	1218	158	12
39	BN	1105	0	1180	231	0
39	DN	1105	0	1180	231	0
40	BO	933	0	996	138	0
40	DO	933	0	996	133	0
41	BP	1114	0	1187	372	0
41	DP	1114	0	1187	345	0
42	BQ	1080	0	1127	195	0
42	DQ	1080	0	1127	195	0
43	BR	960	0	1021	136	0
43	DR	960	0	1021	146	0
44	BS	771	0	832	166	0
44	DS	771	0	832	172	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	213	0
46	BU	958	0	1015	171	0
46	DU	958	0	1015	177	0
47	BV	779	0	851	265	0
47	DV	779	0	851	258	0
48	BW	896	0	953	110	0
48	DW	896	0	953	128	0
49	BX	726	0	778	203	0
49	DX	726	0	777	199	0
50	BY	776	0	870	193	0
50	DY	776	0	870	191	0
51	BZ	1404	0	1432	190	0
51	DZ	1404	0	1432	196	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	52	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	B7	1	0	0	0	0
52	BA	360	0	0	0	0
52	BB	7	0	0	0	0
52	BD	2	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	50	0	0	0	0
52	D5	1	0	0	0	0
52	D7	1	0	0	0	0
52	D8	1	0	0	0	0
52	DA	318	0	0	0	0
52	DB	3	0	0	0	0
52	DD	2	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	2	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	58	0	65	32	0
55	DA	58	0	65	34	0
All	All	278037	0	189235	24925	14

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 54.

The worst 5 of 24925 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)
1:CA:921:U:H1'	1:CA:922:G:C4	1.55	1.40
55:DA:3320:TEL:C14	55:DA:3320:TEL:H11	1.64	1.28
55:BA:3362:TEL:C14	55:BA:3362:TEL:H11	1.64	1.24
33:BD:35:LYS:HD2	33:BD:104:TYR:CD1	1.73	1.22
26:B4:13:ARG:HA	36:BG:101:ILE:HG13	1.22	1.19

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:358:U:OP2	38:DI:90:GLY:N[2_655]	1.80	0.40
1:AA:55:A:C8	38:DI:82:ARG:NE[2_655]	1.98	0.22
1:AA:55:A:O4'	38:DI:82:ARG:NE[2_655]	1.98	0.22
1:AA:358:U:O4'	38:DI:89:TYR:CD1[2_655]	1.99	0.21
1:AA:359:U:O5'	38:DI:87:LYS:O[2_655]	1.99	0.21

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	233/256 (91%)	168 (72%)	49 (21%)	16 (7%)	1 8
2	CB	233/256 (91%)	169 (72%)	48 (21%)	16 (7%)	1 8
3	AC	205/239 (86%)	152 (74%)	40 (20%)	13 (6%)	2 10
3	CC	205/239 (86%)	153 (75%)	40 (20%)	12 (6%)	2 12
4	AD	206/209 (99%)	131 (64%)	49 (24%)	26 (13%)	0 1
4	CD	206/209 (99%)	130 (63%)	48 (23%)	28 (14%)	0 1
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1 4
5	CE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1 4
6	AF	99/101 (98%)	69 (70%)	18 (18%)	12 (12%)	0 2
6	CF	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	AG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	5 26
7	CG	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	5 26
8	AH	136/138 (99%)	100 (74%)	26 (19%)	10 (7%)	1 7
8	CH	136/138 (99%)	99 (73%)	28 (21%)	9 (7%)	1 9
9	AI	123/128 (96%)	85 (69%)	27 (22%)	11 (9%)	1 5
9	CI	123/128 (96%)	86 (70%)	26 (21%)	11 (9%)	1 5
10	AJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	5 27
10	CJ	97/105 (92%)	76 (78%)	18 (19%)	3 (3%)	5 27
11	AK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1 8
11	CK	117/129 (91%)	86 (74%)	23 (20%)	8 (7%)	1 8
12	AL	123/135 (91%)	76 (62%)	26 (21%)	21 (17%)	0 0
12	CL	123/135 (91%)	77 (63%)	24 (20%)	22 (18%)	0 0
13	AM	107/126 (85%)	75 (70%)	26 (24%)	6 (6%)	2 13
13	CM	107/126 (85%)	74 (69%)	27 (25%)	6 (6%)	2 13
14	AN	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	1 5
14	CN	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	1 5
15	AO	86/89 (97%)	56 (65%)	21 (24%)	9 (10%)	1 3
15	CO	86/89 (97%)	56 (65%)	21 (24%)	9 (10%)	1 3
16	AP	82/88 (93%)	48 (58%)	21 (26%)	13 (16%)	0 0
16	CP	82/88 (93%)	48 (58%)	21 (26%)	13 (16%)	0 0
17	AQ	98/105 (93%)	76 (78%)	17 (17%)	5 (5%)	2 15
17	CQ	98/105 (93%)	76 (78%)	17 (17%)	5 (5%)	2 15
18	AR	68/88 (77%)	43 (63%)	20 (29%)	5 (7%)	1 7
18	CR	68/88 (77%)	42 (62%)	19 (28%)	7 (10%)	1 4
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1 6
19	CS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1 6
20	AT	97/106 (92%)	58 (60%)	24 (25%)	15 (16%)	0 0
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0 0
21	AU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3 19
21	CU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3 19
22	B0	83/85 (98%)	67 (81%)	9 (11%)	7 (8%)	1 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	D0	83/85 (98%)	62 (75%)	14 (17%)	7 (8%)	1 6
23	B1	87/98 (89%)	43 (49%)	27 (31%)	17 (20%)	0 0
23	D1	87/98 (89%)	44 (51%)	26 (30%)	17 (20%)	0 0
24	B2	49/72 (68%)	25 (51%)	14 (29%)	10 (20%)	0 0
24	D2	49/72 (68%)	26 (53%)	13 (26%)	10 (20%)	0 0
25	B3	58/60 (97%)	48 (83%)	9 (16%)	1 (2%)	11 43
25	D3	58/60 (97%)	44 (76%)	13 (22%)	1 (2%)	11 43
26	B4	30/71 (42%)	7 (23%)	11 (37%)	12 (40%)	0 0
26	D4	30/71 (42%)	6 (20%)	11 (37%)	13 (43%)	0 0
27	B5	57/60 (95%)	37 (65%)	8 (14%)	12 (21%)	0 0
27	D5	57/60 (95%)	36 (63%)	8 (14%)	13 (23%)	0 0
28	B6	41/54 (76%)	19 (46%)	10 (24%)	12 (29%)	0 0
28	D6	41/54 (76%)	18 (44%)	11 (27%)	12 (29%)	0 0
29	B7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	9 37
29	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	9 37
30	B8	62/65 (95%)	37 (60%)	15 (24%)	10 (16%)	0 0
30	D8	62/65 (95%)	38 (61%)	13 (21%)	11 (18%)	0 0
33	BD	270/276 (98%)	203 (75%)	50 (18%)	17 (6%)	2 10
33	DD	270/276 (98%)	202 (75%)	52 (19%)	16 (6%)	2 12
34	BE	203/206 (98%)	133 (66%)	43 (21%)	27 (13%)	0 1
34	DE	203/206 (98%)	136 (67%)	39 (19%)	28 (14%)	0 1
35	BF	206/210 (98%)	138 (67%)	44 (21%)	24 (12%)	0 2
35	DF	206/210 (98%)	137 (66%)	45 (22%)	24 (12%)	0 2
36	BG	177/182 (97%)	110 (62%)	46 (26%)	21 (12%)	0 2
36	DG	177/182 (97%)	109 (62%)	47 (27%)	21 (12%)	0 2
37	BH	158/180 (88%)	98 (62%)	38 (24%)	22 (14%)	0 1
37	DH	158/180 (88%)	97 (61%)	37 (23%)	24 (15%)	0 0
38	BI	144/148 (97%)	86 (60%)	36 (25%)	22 (15%)	0 0
38	DI	144/148 (97%)	83 (58%)	38 (26%)	23 (16%)	0 0
39	BN	137/140 (98%)	93 (68%)	29 (21%)	15 (11%)	0 3
39	DN	137/140 (98%)	97 (71%)	25 (18%)	15 (11%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	BO	120/122 (98%)	96 (80%)	19 (16%)	5 (4%)	3 19
40	DO	120/122 (98%)	98 (82%)	17 (14%)	5 (4%)	3 19
41	BP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0 0
41	DP	144/150 (96%)	72 (50%)	29 (20%)	43 (30%)	0 0
42	BQ	134/141 (95%)	92 (69%)	29 (22%)	13 (10%)	1 4
42	DQ	134/141 (95%)	91 (68%)	29 (22%)	14 (10%)	1 3
43	BR	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	1 4
43	DR	115/118 (98%)	71 (62%)	34 (30%)	10 (9%)	1 5
44	BS	97/112 (87%)	43 (44%)	26 (27%)	28 (29%)	0 0
44	DS	97/112 (87%)	41 (42%)	29 (30%)	27 (28%)	0 0
45	BT	130/146 (89%)	80 (62%)	25 (19%)	25 (19%)	0 0
45	DT	130/146 (89%)	80 (62%)	26 (20%)	24 (18%)	0 0
46	BU	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	1 8
46	DU	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1 6
47	BV	97/101 (96%)	49 (50%)	24 (25%)	24 (25%)	0 0
47	DV	97/101 (96%)	47 (48%)	25 (26%)	25 (26%)	0 0
48	BW	111/113 (98%)	81 (73%)	11 (10%)	19 (17%)	0 0
48	DW	111/113 (98%)	78 (70%)	15 (14%)	18 (16%)	0 0
49	BX	91/96 (95%)	45 (50%)	22 (24%)	24 (26%)	0 0
49	DX	91/96 (95%)	45 (50%)	21 (23%)	25 (28%)	0 0
50	BY	99/110 (90%)	41 (41%)	25 (25%)	33 (33%)	0 0
50	DY	99/110 (90%)	41 (41%)	27 (27%)	31 (31%)	0 0
51	BZ	175/206 (85%)	117 (67%)	41 (23%)	17 (10%)	1 4
51	DZ	175/206 (85%)	116 (66%)	41 (23%)	18 (10%)	1 4
All	All	11148/12060 (92%)	7385 (66%)	2386 (21%)	1377 (12%)	0 1

5 of 1377 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	34	ALA
2	AB	165	VAL
2	AB	194	PRO
3	AC	54	ARG

5.3.2 Protein sidechains (i)

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%)	182 (90%)	20 (10%)	10	34
2	CB	202/220 (92%)	183 (91%)	19 (9%)	11	39
3	AC	160/188 (85%)	154 (96%)	6 (4%)	40	76
3	CC	160/188 (85%)	154 (96%)	6 (4%)	40	76
4	AD	180/181 (99%)	157 (87%)	23 (13%)	5	21
4	CD	180/181 (99%)	156 (87%)	24 (13%)	5	20
5	AE	115/123 (94%)	101 (88%)	14 (12%)	6	24
5	CE	115/123 (94%)	101 (88%)	14 (12%)	6	24
6	AF	90/90 (100%)	80 (89%)	10 (11%)	8	29
6	CF	90/90 (100%)	80 (89%)	10 (11%)	8	29
7	AG	126/127 (99%)	120 (95%)	6 (5%)	31	69
7	CG	126/127 (99%)	120 (95%)	6 (5%)	31	69
8	AH	119/119 (100%)	104 (87%)	15 (13%)	5	22
8	CH	119/119 (100%)	105 (88%)	14 (12%)	6	25
9	AI	98/99 (99%)	87 (89%)	11 (11%)	7	29
9	CI	98/99 (99%)	88 (90%)	10 (10%)	9	33
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	16
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	5	19
11	AK	90/99 (91%)	83 (92%)	7 (8%)	16	49
11	CK	90/99 (91%)	83 (92%)	7 (8%)	16	49
12	AL	104/111 (94%)	94 (90%)	10 (10%)	10	37
12	CL	104/111 (94%)	94 (90%)	10 (10%)	10	37
13	AM	93/101 (92%)	85 (91%)	8 (9%)	13	45
13	CM	93/101 (92%)	85 (91%)	8 (9%)	13	45
14	AN	49/50 (98%)	46 (94%)	3 (6%)	23	59
14	CN	49/50 (98%)	46 (94%)	3 (6%)	23	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9 33
15	CO	79/80 (99%)	71 (90%)	8 (10%)	9 33
16	AP	72/74 (97%)	61 (85%)	11 (15%)	3 14
16	CP	72/74 (97%)	61 (85%)	11 (15%)	3 14
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	13 45
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	13 45
18	AR	61/77 (79%)	55 (90%)	6 (10%)	10 36
18	CR	61/77 (79%)	55 (90%)	6 (10%)	10 36
19	AS	69/80 (86%)	60 (87%)	9 (13%)	5 21
19	CS	69/80 (86%)	60 (87%)	9 (13%)	5 21
20	AT	76/82 (93%)	65 (86%)	11 (14%)	4 16
20	CT	76/82 (93%)	64 (84%)	12 (16%)	3 13
21	AU	19/22 (86%)	19 (100%)	0	100 100
21	CU	19/22 (86%)	19 (100%)	0	100 100
22	B0	61/67 (91%)	48 (79%)	13 (21%)	1 6
22	D0	61/67 (91%)	48 (79%)	13 (21%)	1 6
23	B1	73/83 (88%)	51 (70%)	22 (30%)	0 1
23	D1	73/83 (88%)	53 (73%)	20 (27%)	0 1
24	B2	46/67 (69%)	28 (61%)	18 (39%)	0 0
24	D2	46/67 (69%)	28 (61%)	18 (39%)	0 0
25	B3	51/52 (98%)	41 (80%)	10 (20%)	1 7
25	D3	51/52 (98%)	42 (82%)	9 (18%)	2 10
27	B5	51/52 (98%)	39 (76%)	12 (24%)	1 4
27	D5	51/52 (98%)	41 (80%)	10 (20%)	1 7
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0 0
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0 0
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1 5
29	D7	41/42 (98%)	31 (76%)	10 (24%)	1 3
30	B8	53/55 (96%)	36 (68%)	17 (32%)	0 0
30	D8	53/55 (96%)	35 (66%)	18 (34%)	0 0
33	BD	213/218 (98%)	160 (75%)	53 (25%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	DD	213/218 (98%)	157 (74%)	56 (26%)	0 2
34	BE	165/166 (99%)	127 (77%)	38 (23%)	1 4
34	DE	165/166 (99%)	126 (76%)	39 (24%)	1 3
35	BF	165/166 (99%)	130 (79%)	35 (21%)	1 6
35	DF	165/166 (99%)	132 (80%)	33 (20%)	1 7
36	BG	155/156 (99%)	126 (81%)	29 (19%)	2 8
36	DG	155/156 (99%)	126 (81%)	29 (19%)	2 8
37	BH	132/148 (89%)	105 (80%)	27 (20%)	1 6
37	DH	132/148 (89%)	107 (81%)	25 (19%)	2 8
38	BI	122/124 (98%)	99 (81%)	23 (19%)	2 8
38	DI	122/124 (98%)	100 (82%)	22 (18%)	2 10
39	BN	117/119 (98%)	80 (68%)	37 (32%)	0 1
39	DN	117/119 (98%)	81 (69%)	36 (31%)	0 1
40	BO	100/100 (100%)	82 (82%)	18 (18%)	2 10
40	DO	100/100 (100%)	80 (80%)	20 (20%)	1 7
41	BP	112/116 (97%)	67 (60%)	45 (40%)	0 0
41	DP	112/116 (97%)	67 (60%)	45 (40%)	0 0
42	BQ	106/111 (96%)	81 (76%)	25 (24%)	1 3
42	DQ	106/111 (96%)	82 (77%)	24 (23%)	1 4
43	BR	100/101 (99%)	76 (76%)	24 (24%)	1 3
43	DR	100/101 (99%)	76 (76%)	24 (24%)	1 3
44	BS	77/88 (88%)	59 (77%)	18 (23%)	1 4
44	DS	77/88 (88%)	59 (77%)	18 (23%)	1 4
45	BT	116/127 (91%)	76 (66%)	40 (34%)	0 0
45	DT	116/127 (91%)	77 (66%)	39 (34%)	0 0
46	BU	92/94 (98%)	74 (80%)	18 (20%)	1 7
46	DU	92/94 (98%)	71 (77%)	21 (23%)	1 4
47	BV	82/82 (100%)	56 (68%)	26 (32%)	0 1
47	DV	82/82 (100%)	57 (70%)	25 (30%)	0 1
48	BW	91/92 (99%)	67 (74%)	24 (26%)	0 2
48	DW	91/92 (99%)	69 (76%)	22 (24%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	BX	74/78 (95%)	55 (74%)	19 (26%)	0 2
49	DX	74/78 (95%)	54 (73%)	20 (27%)	0 1
50	BY	84/91 (92%)	67 (80%)	17 (20%)	1 7
50	DY	84/91 (92%)	66 (79%)	18 (21%)	1 5
51	BZ	155/179 (87%)	132 (85%)	23 (15%)	4 16
51	DZ	155/179 (87%)	131 (84%)	24 (16%)	3 14
All	All	9322/9876 (94%)	7617 (82%)	1705 (18%)	2 9

5 of 1705 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BV	98	GLU
9	CI	114	TYR
46	DU	8	VAL
48	BW	101	SER
2	CB	145	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 256 such sidechains are listed below:

Mol	Chain	Res	Type
45	BT	90	GLN
5	CE	78	HIS
43	DR	31	HIS
48	BW	34	ASN
2	CB	146	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	307 (20%)	30 (1%)
1	CA	1503/1522 (98%)	307 (20%)	30 (1%)
31	BA	2723/2787 (97%)	822 (30%)	77 (2%)
31	DA	2723/2787 (97%)	827 (30%)	75 (2%)
32	BB	118/122 (96%)	42 (35%)	0
32	DB	118/122 (96%)	42 (35%)	0
All	All	8688/8862 (98%)	2347 (27%)	212 (2%)

5 of 2347 RNA backbone outliers are listed below:

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

5 of 212 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2422	A
1	CA	484	G
31	DA	2288	A
31	BA	2542	A
1	CA	30	U

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 827 ligands modelled in this entry, 825 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	TEL	BA	3362	-	59,62,62	1.68	6 (10%)	72,92,92	2.84	22 (30%)
55	TEL	DA	3320	-	59,62,62	1.68	6 (10%)	72,92,92	2.84	22 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	TEL	BA	3362	-	1/1/19/19	0/73/108/108	0/4/5/5
55	TEL	DA	3320	-	1/1/19/19	0/73/108/108	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3320	TEL	C43-C40	-7.33	1.37	1.48
55	BA	3362	TEL	C43-C40	-7.27	1.37	1.48
55	BA	3362	TEL	O5-C2	-4.63	1.40	1.47
55	DA	3320	TEL	O5-C2	-4.62	1.40	1.47
55	BA	3362	TEL	C36-N31	-4.21	1.31	1.38

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	BA	3362	TEL	C8-C4-C2	-15.41	92.52	115.25
55	DA	3320	TEL	C8-C4-C2	-15.41	92.52	115.25
55	BA	3362	TEL	C2-O5-C10	-7.63	102.94	109.28
55	DA	3320	TEL	C2-O5-C10	-7.62	102.95	109.28
55	BA	3362	TEL	C2-C3-C7	-5.48	107.03	117.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
55	DA	3320	TEL	C21
55	BA	3362	TEL	C21

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3362	TEL	32	0
55	DA	3320	TEL	34	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
47	DV	1
36	DG	1
36	BG	1
9	AI	1
9	CI	1
47	BV	1
28	D6	1
28	B6	1

The worst 5 of 14 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	5.74
1	BG	112:PRO	C	113:ARG	N	5.73
1	CM	69:GLU	C	70:LEU	N	4.94
1	AM	69:GLU	C	70:LEU	N	4.93
1	D6	46:HIS	C	47:THR	N	4.90

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	0.95	245 (16%) 2 1	64, 134, 200, 203	0
1	CA	1504/1522 (98%)	0.96	272 (18%) 2 1	67, 134, 200, 203	0
2	AB	235/256 (91%)	1.00	51 (21%) 1 0	122, 175, 196, 201	0
2	CB	235/256 (91%)	1.46	59 (25%) 1 0	123, 175, 196, 202	0
3	AC	207/239 (86%)	1.08	51 (24%) 1 0	122, 174, 194, 197	0
3	CC	207/239 (86%)	1.24	55 (26%) 1 0	122, 175, 195, 199	0
4	AD	208/209 (99%)	0.87	35 (16%) 2 1	89, 149, 187, 193	0
4	CD	208/209 (99%)	0.44	17 (8%) 14 5	86, 148, 186, 193	0
5	AE	151/162 (93%)	0.79	27 (17%) 2 1	88, 127, 174, 197	0
5	CE	151/162 (93%)	1.17	41 (27%) 1 0	90, 128, 174, 197	0
6	AF	101/101 (100%)	0.35	6 (5%) 26 11	95, 151, 183, 196	0
6	CF	101/101 (100%)	0.72	20 (19%) 1 0	96, 154, 184, 198	0
7	AG	155/156 (99%)	1.36	43 (27%) 1 0	146, 184, 197, 200	0
7	CG	155/156 (99%)	2.32	72 (46%) 0 0	146, 185, 197, 199	0
8	AH	138/138 (100%)	0.29	4 (2%) 55 31	92, 129, 167, 189	0
8	CH	138/138 (100%)	0.24	6 (4%) 39 18	92, 129, 166, 189	0
9	AI	127/128 (99%)	2.32	66 (51%) 0 0	143, 190, 200, 202	0
9	CI	127/128 (99%)	2.93	79 (62%) 0 0	144, 190, 199, 202	0
10	AJ	99/105 (94%)	2.52	59 (59%) 0 0	130, 184, 199, 200	0
10	CJ	99/105 (94%)	3.32	58 (58%) 0 0	134, 185, 199, 202	0
11	AK	119/129 (92%)	1.53	38 (31%) 1 0	87, 142, 187, 200	0
11	CK	119/129 (92%)	1.71	41 (34%) 0 0	86, 144, 189, 200	0
12	AL	125/135 (92%)	0.64	12 (9%) 10 3	76, 114, 168, 200	0
12	CL	125/135 (92%)	1.06	31 (24%) 1 0	80, 114, 169, 199	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	115/126 (91%)	2.29	55 (47%) 0 0	147, 192, 199, 201	0
13	CM	115/126 (91%)	2.56	58 (50%) 0 0	148, 192, 199, 202	0
14	AN	60/61 (98%)	1.89	19 (31%) 1 0	141, 183, 196, 199	0
14	CN	60/61 (98%)	1.43	14 (23%) 1 0	142, 182, 196, 198	0
15	AO	88/89 (98%)	0.40	6 (6%) 20 7	85, 123, 173, 189	0
15	CO	88/89 (98%)	0.63	9 (10%) 9 3	87, 124, 176, 186	0
16	AP	84/88 (95%)	1.33	25 (29%) 1 0	97, 128, 177, 192	0
16	CP	84/88 (95%)	1.35	28 (33%) 0 0	97, 126, 175, 191	0
17	AQ	100/105 (95%)	0.54	12 (12%) 6 2	82, 113, 158, 175	0
17	CQ	100/105 (95%)	0.30	8 (8%) 15 5	82, 114, 158, 176	0
18	AR	70/88 (79%)	0.89	12 (17%) 2 1	102, 140, 183, 193	0
18	CR	70/88 (79%)	1.65	19 (27%) 1 0	103, 140, 182, 196	0
19	AS	79/93 (84%)	3.85	62 (78%) 0 0	160, 194, 199, 199	0
19	CS	79/93 (84%)	3.09	51 (64%) 0 0	158, 193, 199, 200	0
20	AT	99/106 (93%)	0.65	17 (17%) 2 1	97, 133, 181, 196	0
20	CT	99/106 (93%)	0.91	22 (22%) 1 0	97, 132, 180, 197	0
21	AU	25/27 (92%)	4.36	20 (80%) 0 0	153, 185, 194, 195	0
21	CU	25/27 (92%)	5.55	23 (92%) 0 0	156, 186, 195, 196	0
22	B0	85/85 (100%)	0.80	10 (11%) 6 2	56, 78, 183, 200	0
22	D0	85/85 (100%)	0.47	11 (12%) 5 2	62, 82, 179, 199	0
23	B1	89/98 (90%)	0.40	5 (5%) 28 11	54, 86, 160, 184	0
23	D1	89/98 (90%)	0.56	12 (13%) 4 2	57, 88, 162, 191	0
24	B2	51/72 (70%)	0.78	9 (17%) 2 1	63, 105, 166, 192	0
24	D2	51/72 (70%)	0.56	5 (9%) 10 3	68, 110, 167, 192	0
25	B3	60/60 (100%)	-0.01	1 (1%) 73 52	49, 77, 143, 193	0
25	D3	60/60 (100%)	0.52	5 (8%) 14 5	54, 79, 145, 186	0
26	B4	32/71 (45%)	0.04	2 (6%) 23 9	140, 177, 199, 200	0
26	D4	32/71 (45%)	0.95	9 (28%) 1 0	139, 180, 199, 201	0
27	B5	58/60 (96%)	0.50	7 (12%) 6 2	40, 65, 182, 197	0
27	D5	58/60 (96%)	0.39	6 (10%) 9 3	42, 69, 186, 197	0
28	B6	45/54 (83%)	0.98	6 (13%) 4 2	52, 100, 167, 192	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	D6	45/54 (83%)	1.17	13 (28%) 1 0	57, 102, 169, 189	0
29	B7	49/49 (100%)	0.43	2 (4%) 41 19	42, 51, 132, 180	0
29	D7	49/49 (100%)	1.02	9 (18%) 2 1	45, 54, 132, 180	0
30	B8	64/65 (98%)	0.66	8 (12%) 5 2	53, 76, 137, 169	0
30	D8	64/65 (98%)	0.48	5 (7%) 16 5	55, 79, 140, 168	0
31	BA	2725/2787 (97%)	0.42	94 (3%) 49 24	38, 66, 177, 204	0
31	DA	2725/2787 (97%)	0.29	137 (5%) 32 13	44, 71, 181, 203	0
32	BB	119/122 (97%)	0.65	10 (8%) 14 4	56, 123, 191, 200	0
32	DB	119/122 (97%)	0.64	18 (15%) 3 1	64, 127, 194, 203	0
33	BD	272/276 (98%)	0.16	8 (2%) 55 31	42, 70, 130, 172	0
33	DD	272/276 (98%)	0.21	9 (3%) 50 26	47, 73, 128, 175	0
34	BE	205/206 (99%)	0.44	10 (4%) 33 14	40, 75, 166, 194	0
34	DE	205/206 (99%)	0.50	16 (7%) 16 5	46, 78, 169, 195	0
35	BF	208/210 (99%)	0.81	20 (9%) 10 3	39, 86, 178, 198	0
35	DF	208/210 (99%)	0.61	23 (11%) 7 2	44, 89, 182, 199	0
36	BG	181/182 (99%)	2.69	84 (46%) 0 0	116, 186, 200, 203	0
36	DG	181/182 (99%)	3.25	95 (52%) 0 0	119, 188, 200, 203	0
37	BH	160/180 (88%)	0.58	11 (6%) 20 7	81, 136, 181, 190	0
37	DH	160/180 (88%)	1.67	57 (35%) 0 0	87, 142, 186, 195	0
38	BI	146/148 (98%)	1.22	36 (24%) 1 0	74, 178, 197, 200	0
38	DI	146/148 (98%)	3.28	74 (50%) 0 0	76, 180, 198, 201	0
39	BN	139/140 (99%)	0.33	9 (6%) 22 8	51, 87, 154, 186	0
39	DN	139/140 (99%)	0.25	8 (5%) 26 11	56, 90, 155, 190	0
40	BO	122/122 (100%)	0.16	0 100 100	51, 79, 133, 168	0
40	DO	122/122 (100%)	0.07	0 100 100	54, 84, 136, 173	0
41	BP	146/150 (97%)	0.80	10 (6%) 20 7	43, 106, 165, 199	0
41	DP	146/150 (97%)	0.90	24 (16%) 2 1	42, 109, 168, 198	0
42	BQ	136/141 (96%)	0.59	9 (6%) 22 8	55, 88, 159, 190	0
42	DQ	136/141 (96%)	0.62	16 (11%) 6 2	59, 90, 160, 191	0
43	BR	117/118 (99%)	0.15	3 (2%) 59 35	43, 65, 134, 180	0
43	DR	117/118 (99%)	0.10	3 (2%) 59 35	47, 68, 136, 182	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BS	99/112 (88%)	1.22	19 (19%) 2 1	79, 134, 189, 198	0
44	DS	99/112 (88%)	1.86	32 (32%) 1 0	83, 136, 192, 198	0
45	BT	132/146 (90%)	0.50	11 (8%) 14 5	60, 105, 179, 192	0
45	DT	132/146 (90%)	0.60	17 (12%) 5 2	65, 107, 179, 195	0
46	BU	117/118 (99%)	0.41	6 (5%) 32 13	43, 71, 142, 190	0
46	DU	117/118 (99%)	0.70	18 (15%) 3 1	48, 76, 145, 194	0
47	BV	101/101 (100%)	0.80	10 (9%) 9 3	44, 117, 183, 198	0
47	DV	101/101 (100%)	1.14	20 (19%) 1 0	49, 120, 186, 197	0
48	BW	113/113 (100%)	-0.16	0 100 100	41, 58, 127, 188	0
48	DW	113/113 (100%)	-0.34	2 (1%) 71 50	43, 62, 130, 191	0
49	BX	93/96 (96%)	0.40	4 (4%) 39 18	50, 82, 151, 186	0
49	DX	93/96 (96%)	0.12	5 (5%) 29 12	57, 84, 153, 186	0
50	BY	101/110 (91%)	1.33	24 (23%) 1 0	61, 120, 197, 199	0
50	DY	101/110 (91%)	1.53	28 (27%) 1 0	68, 121, 195, 199	0
51	BZ	177/206 (85%)	0.40	13 (7%) 18 6	76, 129, 182, 196	0
51	DZ	177/206 (85%)	0.55	26 (14%) 3 1	80, 133, 185, 196	0
All	All	20062/20922 (95%)	0.82	2992 (14%) 3 1	38, 110, 197, 204	0

The worst 5 of 2992 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BF	208	GLY	36.2
2	CB	7	VAL	27.6
35	BF	207	GLY	25.8
31	DA	2802	G	22.1
44	DS	109	GLY	22.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3227	1/1	0.79	0.92	103.78	79,79,79,79	0
52	MG	DA	3018	1/1	0.99	0.68	101.13	34,34,34,34	0
52	MG	BA	3205	1/1	0.92	1.14	63.03	68,68,68,68	0
52	MG	DA	3036	1/1	0.96	1.02	58.34	54,54,54,54	0
52	MG	BA	3093	1/1	0.85	0.77	50.97	57,57,57,57	0
52	MG	DA	3275	1/1	0.85	0.75	50.35	72,72,72,72	0
52	MG	BA	3088	1/1	0.62	0.71	48.35	60,60,60,60	0
52	MG	BA	3295	1/1	0.90	0.89	47.18	79,79,79,79	0
52	MG	BA	3127	1/1	0.84	0.80	45.75	48,48,48,48	0
52	MG	BA	3173	1/1	0.95	0.59	42.99	46,46,46,46	0
52	MG	DA	3071	1/1	0.93	0.72	40.89	85,85,85,85	0
52	MG	DA	3038	1/1	0.89	0.83	39.84	68,68,68,68	0
52	MG	DA	3039	1/1	0.93	1.12	36.66	69,69,69,69	0
52	MG	DA	3054	1/1	0.92	0.65	36.25	47,47,47,47	0
52	MG	BA	3211	1/1	0.93	0.58	35.50	38,38,38,38	0
52	MG	DA	3143	1/1	0.94	0.52	34.66	43,43,43,43	0
52	MG	DA	3121	1/1	0.94	1.02	33.96	64,64,64,64	0
52	MG	BA	3039	1/1	0.86	1.03	33.85	57,57,57,57	0
52	MG	BA	3166	1/1	0.58	0.61	33.21	75,75,75,75	0
52	MG	BA	3228	1/1	0.89	0.90	32.44	56,56,56,56	0
52	MG	BA	3072	1/1	0.94	0.69	32.41	59,59,59,59	0
52	MG	DA	3147	1/1	0.98	0.58	32.19	35,35,35,35	0
52	MG	BA	3094	1/1	0.96	0.74	30.32	47,47,47,47	0
52	MG	BA	3337	1/1	0.93	0.98	29.48	61,61,61,61	0
52	MG	DA	3079	1/1	0.89	0.91	27.57	39,39,39,39	0
52	MG	DA	3162	1/1	0.90	0.64	26.24	80,80,80,80	0
52	MG	BA	3008	1/1	0.97	0.50	25.74	36,36,36,36	0
52	MG	BA	3100	1/1	0.96	0.47	25.06	40,40,40,40	0
52	MG	DA	3217	1/1	0.56	1.01	25.00	55,55,55,55	0
52	MG	BA	3138	1/1	0.92	0.81	24.54	42,42,42,42	0
52	MG	DA	3191	1/1	0.87	0.41	23.43	48,48,48,48	0
52	MG	DA	3031	1/1	0.96	0.67	23.05	61,61,61,61	0
52	MG	BA	3156	1/1	0.96	0.54	22.86	31,31,31,31	0
52	MG	BA	3146	1/1	0.85	0.43	22.73	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3016	1/1	0.76	0.54	22.66	54,54,54,54	0
52	MG	BA	3080	1/1	0.97	0.72	22.36	23,23,23,23	0
52	MG	DA	3211	1/1	0.91	0.93	22.26	62,62,62,62	0
52	MG	DA	3088	1/1	0.95	0.60	22.14	53,53,53,53	0
52	MG	BA	3150	1/1	0.80	0.49	22.09	50,50,50,50	0
52	MG	DA	3090	1/1	0.91	0.54	22.08	53,53,53,53	0
52	MG	DA	3292	1/1	0.86	0.74	21.82	60,60,60,60	0
52	MG	DA	3308	1/1	0.92	0.57	21.27	75,75,75,75	0
52	MG	BA	3214	1/1	0.95	0.54	21.03	55,55,55,55	0
52	MG	DA	3134	1/1	0.79	0.89	20.70	61,61,61,61	0
52	MG	DA	3173	1/1	0.96	0.53	20.39	48,48,48,48	0
52	MG	DA	3007	1/1	0.92	0.49	20.04	40,40,40,40	0
52	MG	BA	3038	1/1	0.99	0.58	19.60	25,25,25,25	0
52	MG	AA	1629	1/1	0.93	0.69	19.42	83,83,83,83	0
52	MG	BA	3047	1/1	0.95	0.63	19.07	41,41,41,41	0
52	MG	BA	3074	1/1	0.92	0.62	18.95	67,67,67,67	0
52	MG	DA	3091	1/1	0.97	0.61	18.83	44,44,44,44	0
52	MG	DA	3001	1/1	0.94	0.48	18.57	66,66,66,66	0
52	MG	DA	3093	1/1	0.91	0.71	18.11	49,49,49,49	0
52	MG	BA	3237	1/1	0.95	0.46	18.03	60,60,60,60	0
52	MG	BA	3090	1/1	0.91	0.47	17.84	22,22,22,22	0
52	MG	BA	3102	1/1	0.95	0.38	17.75	41,41,41,41	0
52	MG	DA	3216	1/1	0.95	0.88	17.47	78,78,78,78	0
52	MG	DA	3159	1/1	0.94	0.51	16.53	39,39,39,39	0
52	MG	DA	3073	1/1	0.85	0.53	16.41	55,55,55,55	0
52	MG	DA	3139	1/1	0.91	0.65	16.29	48,48,48,48	0
52	MG	BA	3040	1/1	0.94	0.67	16.03	49,49,49,49	0
52	MG	DA	3043	1/1	0.95	0.37	16.01	43,43,43,43	0
52	MG	DA	3046	1/1	0.91	0.41	15.84	49,49,49,49	0
52	MG	BA	3234	1/1	0.67	0.52	15.71	40,40,40,40	0
52	MG	BA	3006	1/1	0.99	0.52	15.66	27,27,27,27	0
52	MG	BA	3315	1/1	0.94	0.80	15.63	62,62,62,62	0
52	MG	BA	3096	1/1	0.99	0.60	15.58	33,33,33,33	0
52	MG	DA	3055	1/1	0.94	0.45	15.52	38,38,38,38	0
52	MG	BA	3037	1/1	0.96	0.44	15.48	14,14,14,14	0
52	MG	BA	3144	1/1	0.94	0.75	15.13	43,43,43,43	0
52	MG	DA	3205	1/1	0.90	0.44	15.00	64,64,64,64	0
52	MG	DA	3272	1/1	0.84	0.72	14.94	78,78,78,78	0
52	MG	CA	1627	1/1	0.88	0.70	14.88	76,76,76,76	0
52	MG	BA	3181	1/1	0.94	0.54	14.65	54,54,54,54	0
52	MG	DA	3098	1/1	0.94	0.45	14.53	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3049	1/1	0.92	0.47	14.52	26,26,26,26	0
52	MG	BA	3190	1/1	0.96	0.45	14.22	34,34,34,34	0
52	MG	CA	1645	1/1	0.90	0.86	14.16	64,64,64,64	0
52	MG	DA	3040	1/1	0.94	0.36	14.15	36,36,36,36	0
52	MG	DA	3035	1/1	0.98	0.62	13.99	41,41,41,41	0
52	MG	AA	1621	1/1	0.96	0.54	13.92	51,51,51,51	0
52	MG	BA	3336	1/1	0.97	0.50	13.83	61,61,61,61	0
52	MG	BA	3002	1/1	0.92	0.64	13.72	31,31,31,31	0
52	MG	CA	1632	1/1	0.97	0.33	13.63	76,76,76,76	0
52	MG	BA	3148	1/1	0.95	0.55	13.61	28,28,28,28	0
52	MG	BA	3225	1/1	0.96	0.46	13.48	23,23,23,23	0
52	MG	DA	3156	1/1	0.83	0.50	13.42	44,44,44,44	0
52	MG	BA	3226	1/1	0.92	0.45	13.22	42,42,42,42	0
52	MG	BA	3352	1/1	0.80	0.48	12.98	53,53,53,53	0
52	MG	BA	3161	1/1	0.85	0.41	12.65	65,65,65,65	0
52	MG	DA	3111	1/1	0.83	0.44	12.52	56,56,56,56	0
52	MG	AA	1610	1/1	0.88	0.26	12.19	115,115,115,115	0
52	MG	DA	3050	1/1	0.96	0.48	12.18	39,39,39,39	0
52	MG	DA	3022	1/1	0.98	0.40	12.03	38,38,38,38	0
52	MG	AA	1648	1/1	0.81	0.69	11.76	57,57,57,57	0
52	MG	BA	3044	1/1	0.99	0.45	11.58	19,19,19,19	0
52	MG	BA	3032	1/1	0.98	0.34	11.42	39,39,39,39	0
52	MG	DA	3313	1/1	0.81	0.57	11.33	64,64,64,64	0
52	MG	AA	1634	1/1	0.98	0.42	11.33	54,54,54,54	0
52	MG	DA	3033	1/1	0.98	0.44	11.06	63,63,63,63	0
52	MG	CA	1625	1/1	0.82	0.38	10.77	70,70,70,70	0
52	MG	DA	3094	1/1	0.78	0.40	10.76	75,75,75,75	0
52	MG	AA	1613	1/1	0.95	0.34	10.73	76,76,76,76	0
52	MG	DA	3178	1/1	0.95	0.41	10.72	52,52,52,52	0
52	MG	BA	3010	1/1	0.98	0.53	10.66	53,53,53,53	0
52	MG	BA	3023	1/1	0.96	0.34	10.53	31,31,31,31	0
52	MG	BA	3309	1/1	0.88	0.39	10.49	70,70,70,70	0
52	MG	DA	3137	1/1	0.97	0.57	10.43	49,49,49,49	0
52	MG	BA	3092	1/1	0.98	0.40	10.30	22,22,22,22	0
52	MG	BA	3001	1/1	0.96	0.30	10.24	55,55,55,55	0
52	MG	DA	3270	1/1	0.88	0.52	10.19	92,92,92,92	0
52	MG	BA	3232	1/1	0.92	0.43	10.01	43,43,43,43	0
52	MG	BA	3310	1/1	0.94	0.58	9.95	74,74,74,74	0
52	MG	BA	3101	1/1	0.98	0.34	9.92	17,17,17,17	0
52	MG	BA	3282	1/1	0.99	0.34	9.91	49,49,49,49	0
52	MG	B7	101	1/1	0.93	0.31	9.84	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3074	1/1	0.86	0.46	9.84	56,56,56,56	0
52	MG	DA	3053	1/1	0.97	0.72	9.81	90,90,90,90	0
52	MG	DA	3286	1/1	0.78	0.37	9.74	63,63,63,63	0
52	MG	DA	3045	1/1	0.78	0.49	9.67	51,51,51,51	0
52	MG	AA	1614	1/1	0.50	0.30	9.59	81,81,81,81	0
52	MG	AA	1649	1/1	0.99	0.42	9.43	68,68,68,68	0
52	MG	BA	3244	1/1	0.91	0.43	9.43	44,44,44,44	0
52	MG	DA	3019	1/1	0.98	0.54	9.34	42,42,42,42	0
52	MG	DA	3051	1/1	0.98	0.40	9.33	53,53,53,53	0
52	MG	DA	3002	1/1	0.88	0.57	9.28	41,41,41,41	0
52	MG	DA	3026	1/1	0.95	0.56	9.24	32,32,32,32	0
52	MG	BD	301	1/1	0.96	0.45	9.13	51,51,51,51	0
52	MG	DA	3268	1/1	0.68	0.58	9.11	72,72,72,72	0
52	MG	DA	3108	1/1	0.85	0.33	9.08	56,56,56,56	0
52	MG	CA	1621	1/1	0.78	0.47	9.00	78,78,78,78	0
52	MG	CA	1644	1/1	0.90	0.27	9.00	86,86,86,86	0
52	MG	DA	3015	1/1	0.96	0.47	8.93	40,40,40,40	0
52	MG	DA	3062	1/1	0.94	0.59	8.92	76,76,76,76	0
52	MG	DA	3006	1/1	0.95	0.52	8.86	40,40,40,40	0
52	MG	DA	3197	1/1	0.94	0.52	8.76	59,59,59,59	0
52	MG	BA	3034	1/1	0.90	0.40	8.69	69,69,69,69	0
52	MG	BA	3122	1/1	0.94	0.40	8.57	61,61,61,61	0
52	MG	DA	3020	1/1	0.96	0.54	8.56	74,74,74,74	0
52	MG	DA	3037	1/1	0.97	0.54	8.31	39,39,39,39	0
52	MG	BA	3066	1/1	0.98	0.34	8.27	36,36,36,36	0
52	MG	BA	3041	1/1	0.99	0.30	8.25	22,22,22,22	0
52	MG	BA	3061	1/1	0.96	0.43	8.15	36,36,36,36	0
52	MG	BA	3319	1/1	0.96	0.42	8.09	60,60,60,60	0
52	MG	DA	3314	1/1	0.82	0.69	7.95	54,54,54,54	0
52	MG	BA	3012	1/1	0.96	0.54	7.93	61,61,61,61	0
52	MG	BA	3028	1/1	0.96	0.34	7.88	30,30,30,30	0
52	MG	BA	3089	1/1	0.98	0.31	7.81	20,20,20,20	0
52	MG	DX	101	1/1	0.84	0.43	7.80	76,76,76,76	0
52	MG	DA	3259	1/1	0.90	0.48	7.63	60,60,60,60	0
52	MG	D5	101	1/1	0.98	0.57	7.59	51,51,51,51	0
52	MG	DA	3096	1/1	0.93	0.38	7.54	42,42,42,42	0
52	MG	BA	3075	1/1	0.91	0.47	7.50	56,56,56,56	0
52	MG	DA	3060	1/1	0.90	0.47	7.23	50,50,50,50	0
52	MG	BA	3055	1/1	0.98	0.39	7.20	31,31,31,31	0
52	MG	BA	3060	1/1	0.97	0.33	6.97	59,59,59,59	0
52	MG	BA	3016	1/1	0.98	0.36	6.68	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3124	1/1	0.99	0.37	6.67	12,12,12,12	0
52	MG	B5	101	1/1	0.96	0.33	6.63	54,54,54,54	0
52	MG	CA	1606	1/1	0.89	1.11	6.45	73,73,73,73	0
52	MG	DA	3278	1/1	0.92	0.86	6.41	83,83,83,83	0
52	MG	DA	3048	1/1	0.90	0.46	6.25	51,51,51,51	0
52	MG	DA	3008	1/1	0.97	0.37	6.23	50,50,50,50	0
52	MG	DA	3236	1/1	0.70	0.79	6.17	76,76,76,76	0
52	MG	DA	3161	1/1	0.95	0.29	6.10	72,72,72,72	0
52	MG	BA	3071	1/1	0.93	0.47	5.99	32,32,32,32	0
52	MG	DA	3155	1/1	0.71	0.23	5.98	59,59,59,59	0
52	MG	DA	3218	1/1	0.97	0.56	5.97	53,53,53,53	0
55	TEL	DA	3320	58/58	0.91	0.31	5.76	110,110,110,110	0
52	MG	BA	3052	1/1	0.95	0.34	5.76	17,17,17,17	0
52	MG	BA	3116	1/1	0.89	0.33	5.64	67,67,67,67	0
52	MG	BA	3051	1/1	0.97	0.32	5.62	22,22,22,22	0
52	MG	BA	3126	1/1	0.71	0.25	5.62	56,56,56,56	0
52	MG	BA	3176	1/1	0.84	0.95	5.49	68,68,68,68	0
52	MG	BA	3235	1/1	0.86	0.50	5.48	43,43,43,43	0
52	MG	BA	3021	1/1	0.96	0.36	5.42	30,30,30,30	0
52	MG	BA	3046	1/1	0.94	0.40	5.05	38,38,38,38	0
52	MG	DA	3056	1/1	0.97	0.41	4.99	51,51,51,51	0
52	MG	BA	3222	1/1	0.93	0.29	4.66	58,58,58,58	0
52	MG	BA	3321	1/1	0.76	0.35	4.64	69,69,69,69	0
52	MG	BA	3164	1/1	0.93	0.25	4.32	40,40,40,40	0
52	MG	BA	3109	1/1	0.95	0.29	4.22	36,36,36,36	0
55	TEL	BA	3362	58/58	0.91	0.32	4.20	110,110,110,110	0
52	MG	DR	201	1/1	0.98	0.61	4.09	45,45,45,45	0
52	MG	BA	3063	1/1	0.94	0.45	3.99	57,57,57,57	0
52	MG	BA	3118	1/1	0.97	0.34	3.96	44,44,44,44	0
52	MG	DA	3241	1/1	0.88	0.33	3.96	48,48,48,48	0
52	MG	DA	3070	1/1	0.97	0.43	3.96	52,52,52,52	0
52	MG	DA	3115	1/1	0.89	0.36	3.93	58,58,58,58	0
52	MG	BA	3141	1/1	0.95	0.34	3.92	19,19,19,19	0
52	MG	DA	3167	1/1	0.95	0.27	3.88	45,45,45,45	0
52	MG	DA	3223	1/1	0.95	0.28	3.77	62,62,62,62	0
52	MG	DA	3165	1/1	0.71	0.48	3.71	53,53,53,53	0
52	MG	AA	1609	1/1	0.92	0.28	3.68	65,65,65,65	0
52	MG	BA	3018	1/1	0.97	0.27	3.65	25,25,25,25	0
52	MG	DD	301	1/1	0.94	0.36	3.64	56,56,56,56	0
52	MG	DA	3120	1/1	0.89	0.37	3.63	84,84,84,84	0
52	MG	DA	3288	1/1	0.94	0.29	3.61	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3252	1/1	0.90	0.30	3.54	55,55,55,55	0
52	MG	BA	3174	1/1	0.94	0.34	3.53	51,51,51,51	0
52	MG	DA	3069	1/1	0.96	0.35	3.50	54,54,54,54	0
52	MG	BA	3247	1/1	0.83	0.51	3.48	77,77,77,77	0
52	MG	DA	3290	1/1	0.87	0.29	3.21	74,74,74,74	0
52	MG	AA	1623	1/1	0.90	0.41	3.17	50,50,50,50	0
52	MG	DA	3212	1/1	0.93	0.41	3.11	71,71,71,71	0
52	MG	BA	3317	1/1	0.91	0.41	3.07	49,49,49,49	0
52	MG	AA	1647	1/1	0.81	0.30	3.02	72,72,72,72	0
52	MG	DA	3256	1/1	0.92	0.27	2.99	77,77,77,77	0
52	MG	DA	3103	1/1	0.94	0.41	2.93	58,58,58,58	0
52	MG	DA	3274	1/1	0.83	0.20	2.91	68,68,68,68	0
52	MG	CA	1611	1/1	0.88	0.30	2.86	72,72,72,72	0
52	MG	BX	101	1/1	0.93	0.33	2.85	58,58,58,58	0
52	MG	BA	3117	1/1	0.82	0.26	2.84	58,58,58,58	0
52	MG	DA	3208	1/1	0.98	0.41	2.82	43,43,43,43	0
52	MG	DU	201	1/1	0.92	0.42	2.77	75,75,75,75	0
52	MG	DA	3009	1/1	0.97	0.31	2.71	52,52,52,52	0
52	MG	CA	1607	1/1	0.88	0.45	2.71	74,74,74,74	0
52	MG	DA	3027	1/1	0.96	0.31	2.71	43,43,43,43	0
52	MG	BA	3070	1/1	0.94	0.31	2.70	25,25,25,25	0
52	MG	BA	3284	1/1	0.92	0.34	2.67	34,34,34,34	0
52	MG	BA	3280	1/1	0.90	0.26	2.67	80,80,80,80	0
52	MG	BA	3332	1/1	0.83	0.25	2.60	65,65,65,65	0
52	MG	DA	3017	1/1	0.94	0.25	2.59	55,55,55,55	0
52	MG	DA	3011	1/1	0.95	0.33	2.59	43,43,43,43	0
52	MG	DA	3239	1/1	0.92	0.21	2.58	65,65,65,65	0
52	MG	DA	3109	1/1	0.83	0.44	2.48	60,60,60,60	0
52	MG	BA	3091	1/1	0.88	0.27	2.46	44,44,44,44	0
52	MG	BA	3341	1/1	0.88	0.26	2.38	67,67,67,67	0
52	MG	DA	3117	1/1	0.95	0.33	2.33	59,59,59,59	0
52	MG	D7	101	1/1	0.79	0.42	2.25	58,58,58,58	0
52	MG	DA	3004	1/1	0.92	0.27	2.24	39,39,39,39	0
52	MG	BA	3278	1/1	0.73	0.25	2.21	62,62,62,62	0
52	MG	AA	1627	1/1	0.86	0.23	2.15	71,71,71,71	0
52	MG	DA	3076	1/1	0.98	0.26	2.03	56,56,56,56	0
52	MG	CA	1631	1/1	0.68	0.22	2.00	95,95,95,95	0
52	MG	DA	3057	1/1	0.99	0.24	1.92	60,60,60,60	0
52	MG	DA	3195	1/1	0.96	0.23	1.86	62,62,62,62	0
52	MG	BA	3258	1/1	0.78	0.19	1.85	57,57,57,57	0
52	MG	DA	3095	1/1	0.86	0.19	1.74	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	AA	1622	1/1	0.90	0.34	1.67	64,64,64,64	0
52	MG	DA	3064	1/1	0.94	0.26	1.64	46,46,46,46	0
52	MG	BA	3274	1/1	0.98	0.23	1.59	36,36,36,36	0
52	MG	BA	3020	1/1	0.94	0.33	1.58	24,24,24,24	0
52	MG	CA	1610	1/1	0.99	0.18	1.57	106,106,106,106	0
52	MG	DA	3141	1/1	0.90	0.24	1.56	65,65,65,65	0
52	MG	BA	3261	1/1	0.94	0.29	1.50	34,34,34,34	0
52	MG	BA	3213	1/1	0.89	0.23	1.47	34,34,34,34	0
52	MG	BA	3009	1/1	0.94	0.35	1.46	44,44,44,44	0
52	MG	DA	3086	1/1	0.95	0.24	1.39	61,61,61,61	0
52	MG	BA	3143	1/1	0.94	0.40	1.37	34,34,34,34	0
52	MG	BA	3178	1/1	0.98	0.26	1.32	25,25,25,25	0
52	MG	DA	3181	1/1	0.95	0.30	1.28	62,62,62,62	0
52	MG	BU	201	1/1	0.97	0.30	1.24	29,29,29,29	0
52	MG	AA	1625	1/1	0.89	0.22	1.24	73,73,73,73	0
52	MG	DA	3303	1/1	0.96	0.25	1.19	57,57,57,57	0
52	MG	BA	3345	1/1	0.91	0.25	1.19	70,70,70,70	0
52	MG	BA	3194	1/1	0.96	0.27	1.11	27,27,27,27	0
52	MG	DA	3089	1/1	0.93	0.22	1.04	54,54,54,54	0
52	MG	AA	1633	1/1	0.59	0.22	0.88	90,90,90,90	0
52	MG	DA	3123	1/1	0.54	0.26	0.88	67,67,67,67	0
52	MG	DA	3107	1/1	0.98	0.30	0.83	42,42,42,42	0
52	MG	BD	302	1/1	0.91	0.36	0.82	47,47,47,47	0
52	MG	AA	1606	1/1	0.92	0.46	0.79	63,63,63,63	0
52	MG	BP	201	1/1	0.97	0.32	0.76	17,17,17,17	0
52	MG	BA	3057	1/1	0.94	0.24	0.66	40,40,40,40	0
52	MG	DA	3298	1/1	0.97	0.23	0.61	46,46,46,46	0
52	MG	BF	301	1/1	0.78	0.28	0.53	59,59,59,59	0
52	MG	DA	3196	1/1	0.83	0.20	0.52	41,41,41,41	0
52	MG	DA	3119	1/1	0.87	0.22	0.46	56,56,56,56	0
52	MG	CA	1650	1/1	0.93	0.22	0.39	66,66,66,66	0
52	MG	DA	3164	1/1	0.98	0.28	0.26	50,50,50,50	0
52	MG	BQ	202	1/1	0.94	0.23	0.25	49,49,49,49	0
52	MG	CA	1649	1/1	0.94	0.17	0.20	80,80,80,80	0
52	MG	BA	3120	1/1	0.94	0.30	0.17	65,65,65,65	0
52	MG	CA	1605	1/1	0.90	0.27	0.16	102,102,102,102	0
52	MG	DA	3179	1/1	0.93	0.21	0.10	67,67,67,67	0
52	MG	DA	3240	1/1	0.95	0.17	0.06	47,47,47,47	0
52	MG	DA	3042	1/1	0.98	0.22	0.04	48,48,48,48	0
52	MG	BA	3086	1/1	0.97	0.21	0.03	28,28,28,28	0
52	MG	BA	3058	1/1	0.98	0.22	-0.11	47,47,47,47	0
52	MG	DA	3145	1/1	0.89	0.18	-0.14	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3061	1/1	0.99	0.17	-0.18	40,40,40,40	0
52	MG	DD	302	1/1	0.94	0.24	-0.19	38,38,38,38	0
52	MG	BA	3112	1/1	0.91	0.20	-0.19	43,43,43,43	0
52	MG	AA	1651	1/1	0.97	0.21	-0.19	81,81,81,81	0
52	MG	DA	3153	1/1	0.98	0.20	-0.20	80,80,80,80	0
52	MG	BA	3111	1/1	0.93	0.23	-0.20	19,19,19,19	0
52	MG	CA	1620	1/1	0.96	0.22	-0.20	70,70,70,70	0
52	MG	BA	3249	1/1	0.95	0.16	-0.21	56,56,56,56	0
52	MG	BA	3320	1/1	0.93	0.19	-0.24	48,48,48,48	0
52	MG	BA	3322	1/1	0.93	0.21	-0.25	44,44,44,44	0
52	MG	AA	1607	1/1	0.98	0.29	-0.28	81,81,81,81	0
52	MG	DA	3277	1/1	0.97	0.19	-0.30	66,66,66,66	0
52	MG	DA	3122	1/1	0.89	0.16	-0.31	61,61,61,61	0
52	MG	DF	301	1/1	0.72	0.24	-0.38	83,83,83,83	0
52	MG	BA	3152	1/1	0.85	0.16	-0.38	58,58,58,58	0
52	MG	DA	3302	1/1	0.91	0.27	-0.47	64,64,64,64	0
52	MG	BA	3180	1/1	0.94	0.17	-0.62	68,68,68,68	0
53	ZN	AD	301	1/1	0.99	0.28	-0.68	110,110,110,110	0
52	MG	CA	1637	1/1	0.96	0.14	-0.69	85,85,85,85	0
52	MG	B1	101	1/1	0.98	0.16	-0.70	41,41,41,41	0
52	MG	DA	3267	1/1	0.96	0.24	-0.74	57,57,57,57	0
53	ZN	AN	101	1/1	0.90	0.15	-0.76	181,181,181,181	0
52	MG	CA	1612	1/1	0.73	0.18	-0.77	70,70,70,70	0
53	ZN	CD	301	1/1	0.98	0.21	-0.81	105,105,105,105	0
52	MG	BA	3289	1/1	0.86	0.16	-0.82	66,66,66,66	0
52	MG	CA	1623	1/1	0.96	0.15	-0.86	79,79,79,79	0
52	MG	BA	3300	1/1	0.98	0.15	-0.93	56,56,56,56	0
52	MG	DA	3114	1/1	0.82	0.18	-0.93	75,75,75,75	0
52	MG	BA	3043	1/1	0.96	0.20	-0.98	39,39,39,39	0
53	ZN	CN	101	1/1	0.95	0.14	-1.02	164,164,164,164	0
52	MG	DA	3112	1/1	0.97	0.13	-1.06	76,76,76,76	0
52	MG	DA	3059	1/1	0.97	0.16	-1.11	55,55,55,55	0
52	MG	BA	3128	1/1	0.95	0.18	-1.43	63,63,63,63	0
52	MG	DA	3315	1/1	0.95	0.14	-1.45	69,69,69,69	0
52	MG	BA	3281	1/1	0.93	0.17	-1.56	45,45,45,45	0
54	K	DA	3319	1/1	0.94	0.17	-1.58	82,82,82,82	0
52	MG	BA	3195	1/1	0.97	0.17	-1.61	40,40,40,40	0
52	MG	BA	3062	1/1	0.96	0.16	-1.78	38,38,38,38	0
52	MG	DA	3304	1/1	0.96	0.13	-1.91	67,67,67,67	0
52	MG	BA	3115	1/1	0.83	0.15	-1.92	71,71,71,71	0
52	MG	BB	207	1/1	0.96	0.27	-1.97	80,80,80,80	0
52	MG	BA	3259	1/1	0.90	0.14	-2.03	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3129	1/1	0.89	0.11	-2.04	55,55,55,55	0
52	MG	BA	3316	1/1	0.97	0.11	-2.11	43,43,43,43	0
52	MG	AA	1642	1/1	0.94	0.14	-2.34	58,58,58,58	0
52	MG	BB	203	1/1	0.90	0.12	-2.36	82,82,82,82	0
52	MG	AA	1652	1/1	0.95	0.14	-2.51	83,83,83,83	0
52	MG	BA	3149	1/1	0.98	0.14	-2.56	24,24,24,24	0
52	MG	BB	205	1/1	0.84	0.10	-2.57	90,90,90,90	0
52	MG	BA	3125	1/1	0.96	0.12	-2.87	53,53,53,53	0
52	MG	DA	3124	1/1	0.98	0.14	-2.97	63,63,63,63	0
52	MG	BA	3293	1/1	0.99	0.07	-3.35	51,51,51,51	0
52	MG	DA	3166	1/1	0.90	0.10	-3.39	55,55,55,55	0
52	MG	DA	3233	1/1	0.99	0.07	-3.40	57,57,57,57	0
52	MG	BA	3212	1/1	0.99	0.12	-3.50	29,29,29,29	0
52	MG	BA	3229	1/1	0.96	0.06	-3.88	30,30,30,30	0
52	MG	BA	3260	1/1	0.97	0.15	-4.13	46,46,46,46	0
52	MG	BA	3056	1/1	0.94	0.12	-4.19	31,31,31,31	0
52	MG	BA	3344	1/1	0.96	0.17	-4.68	43,43,43,43	0
52	MG	BA	3087	1/1	0.99	0.09	-5.08	18,18,18,18	0
52	MG	BA	3253	1/1	0.98	0.07	-5.49	42,42,42,42	0
52	MG	BA	3254	1/1	0.99	0.09	-6.05	58,58,58,58	0
52	MG	DA	3125	1/1	0.94	0.11	-9.65	54,54,54,54	0
52	MG	BA	3248	1/1	0.96	0.08	-18.35	57,57,57,57	0
52	MG	BA	3223	1/1	0.92	0.67	-	45,45,45,45	0
52	MG	BA	3277	1/1	0.95	0.26	-	49,49,49,49	0
52	MG	DA	3097	1/1	0.96	0.40	-	51,51,51,51	0
52	MG	DA	3135	1/1	0.95	0.40	-	74,74,74,74	0
52	MG	BA	3335	1/1	0.82	0.58	-	55,55,55,55	0
52	MG	AA	1644	1/1	0.92	1.24	-	94,94,94,94	0
52	MG	DA	3257	1/1	0.93	0.23	-	72,72,72,72	0
52	MG	DA	3317	1/1	0.86	0.12	-	60,60,60,60	0
52	MG	DA	3204	1/1	0.94	0.17	-	48,48,48,48	0
52	MG	BA	3333	1/1	0.94	0.24	-	48,48,48,48	0
52	MG	CA	1604	1/1	0.92	0.24	-	98,98,98,98	0
52	MG	DA	3187	1/1	0.98	0.65	-	53,53,53,53	0
52	MG	DA	3028	1/1	0.97	0.33	-	68,68,68,68	0
52	MG	BA	3294	1/1	0.93	0.28	-	40,40,40,40	0
52	MG	CA	1615	1/1	0.95	0.38	-	69,69,69,69	0
52	MG	AA	1650	1/1	0.63	1.51	-	86,86,86,86	0
52	MG	DA	3316	1/1	0.89	0.37	-	75,75,75,75	0
52	MG	BA	3331	1/1	0.79	0.41	-	52,52,52,52	0
52	MG	DA	3082	1/1	0.81	0.37	-	50,50,50,50	0
52	MG	BA	3169	1/1	0.95	0.74	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3137	1/1	0.97	0.27	-	16,16,16,16	0
52	MG	DA	3221	1/1	0.85	0.49	-	62,62,62,62	0
52	MG	DA	3130	1/1	0.85	0.18	-	83,83,83,83	0
52	MG	DE	301	1/1	0.99	0.18	-	34,34,34,34	0
52	MG	DA	3194	1/1	0.84	0.59	-	56,56,56,56	0
52	MG	BA	3123	1/1	0.93	0.39	-	48,48,48,48	0
52	MG	BA	3216	1/1	0.96	0.23	-	46,46,46,46	0
52	MG	DA	3203	1/1	0.87	0.69	-	55,55,55,55	0
52	MG	BB	202	1/1	0.96	0.45	-	44,44,44,44	0
52	MG	CA	1617	1/1	0.82	0.59	-	74,74,74,74	0
52	MG	DA	3024	1/1	0.93	0.41	-	54,54,54,54	0
52	MG	BA	3236	1/1	0.97	0.57	-	38,38,38,38	0
52	MG	DA	3136	1/1	0.85	0.15	-	81,81,81,81	0
52	MG	DA	3294	1/1	0.96	0.30	-	50,50,50,50	0
52	MG	DA	3049	1/1	0.96	0.20	-	54,54,54,54	0
52	MG	BA	3353	1/1	0.89	0.31	-	73,73,73,73	0
52	MG	CA	1635	1/1	0.90	1.22	-	80,80,80,80	0
52	MG	BA	3275	1/1	0.89	0.13	-	47,47,47,47	0
52	MG	BA	3231	1/1	0.96	0.25	-	31,31,31,31	0
52	MG	CA	1638	1/1	0.86	0.28	-	62,62,62,62	0
52	MG	CA	1648	1/1	0.62	0.88	-	69,69,69,69	0
52	MG	BA	3308	1/1	0.92	0.24	-	55,55,55,55	0
52	MG	BA	3288	1/1	0.90	0.10	-	55,55,55,55	0
52	MG	BA	3140	1/1	0.89	0.21	-	78,78,78,78	0
52	MG	DA	3224	1/1	0.96	0.59	-	47,47,47,47	0
52	MG	BA	3304	1/1	0.90	0.39	-	41,41,41,41	0
52	MG	AA	1645	1/1	0.84	0.46	-	104,104,104,104	0
52	MG	AA	1602	1/1	0.91	0.68	-	50,50,50,50	0
52	MG	BA	3172	1/1	0.92	0.22	-	50,50,50,50	0
52	MG	CA	1640	1/1	0.96	0.33	-	74,74,74,74	0
52	MG	BA	3238	1/1	0.94	0.35	-	70,70,70,70	0
52	MG	BA	3163	1/1	0.96	0.36	-	45,45,45,45	0
52	MG	BR	201	1/1	0.93	0.56	-	27,27,27,27	0
52	MG	BA	3358	1/1	0.96	0.07	-	34,34,34,34	0
52	MG	BA	3268	1/1	0.86	0.14	-	60,60,60,60	0
52	MG	DA	3034	1/1	0.97	0.60	-	51,51,51,51	0
52	MG	BA	3338	1/1	0.95	0.25	-	61,61,61,61	0
52	MG	BA	3301	1/1	0.92	0.42	-	52,52,52,52	0
52	MG	DA	3132	1/1	0.93	0.14	-	72,72,72,72	0
52	MG	BA	3287	1/1	0.97	0.34	-	59,59,59,59	0
52	MG	DA	3213	1/1	0.97	0.45	-	44,44,44,44	0
52	MG	BA	3306	1/1	0.92	0.65	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3162	1/1	0.94	0.49	-	69,69,69,69	0
52	MG	DA	3238	1/1	0.90	0.15	-	80,80,80,80	0
52	MG	DA	3083	1/1	0.92	0.45	-	43,43,43,43	0
52	MG	BA	3024	1/1	0.99	0.18	-	37,37,37,37	0
52	MG	BA	3346	1/1	0.98	0.16	-	61,61,61,61	0
52	MG	BA	3357	1/1	0.92	0.19	-	66,66,66,66	0
52	MG	BA	3342	1/1	0.96	0.20	-	39,39,39,39	0
52	MG	BA	3187	1/1	0.92	0.78	-	60,60,60,60	0
52	MG	DA	3229	1/1	0.73	0.47	-	78,78,78,78	0
52	MG	BA	3103	1/1	0.97	0.25	-	31,31,31,31	0
52	MG	BA	3105	1/1	0.98	0.40	-	32,32,32,32	0
52	MG	DA	3128	1/1	0.94	0.56	-	62,62,62,62	0
52	MG	DA	3080	1/1	0.95	0.63	-	59,59,59,59	0
52	MG	DA	3193	1/1	0.98	0.47	-	54,54,54,54	0
52	MG	DA	3285	1/1	0.66	0.56	-	70,70,70,70	0
52	MG	CA	1602	1/1	0.76	0.91	-	73,73,73,73	0
52	MG	DA	3127	1/1	0.96	0.33	-	40,40,40,40	0
52	MG	BA	3170	1/1	0.96	0.86	-	44,44,44,44	0
52	MG	DA	3003	1/1	0.89	0.79	-	61,61,61,61	0
52	MG	DA	3113	1/1	0.90	0.29	-	75,75,75,75	0
52	MG	DA	3225	1/1	0.53	0.61	-	81,81,81,81	0
52	MG	DA	3201	1/1	0.93	0.78	-	46,46,46,46	0
52	MG	DA	3230	1/1	0.92	0.22	-	69,69,69,69	0
52	MG	DA	3198	1/1	0.93	0.38	-	53,53,53,53	0
52	MG	AA	1638	1/1	0.84	0.37	-	91,91,91,91	0
52	MG	BA	3351	1/1	0.94	0.63	-	53,53,53,53	0
52	MG	CA	1616	1/1	0.84	0.27	-	74,74,74,74	0
52	MG	BA	3197	1/1	0.96	0.48	-	46,46,46,46	0
52	MG	DA	3105	1/1	0.95	0.45	-	74,74,74,74	0
52	MG	BA	3114	1/1	0.89	0.49	-	49,49,49,49	0
52	MG	BA	3242	1/1	0.78	0.55	-	71,71,71,71	0
52	MG	BA	3266	1/1	0.97	0.67	-	63,63,63,63	0
52	MG	CA	1628	1/1	0.84	0.76	-	92,92,92,92	0
52	MG	BA	3265	1/1	0.92	0.55	-	51,51,51,51	0
52	MG	BA	3209	1/1	0.93	0.23	-	51,51,51,51	0
52	MG	DA	3188	1/1	0.79	0.73	-	81,81,81,81	0
52	MG	BA	3224	1/1	0.84	0.16	-	43,43,43,43	0
52	MG	CA	1626	1/1	0.97	0.62	-	70,70,70,70	0
52	MG	BA	3014	1/1	0.96	0.47	-	46,46,46,46	0
54	K	BA	3361	1/1	0.98	0.10	-	69,69,69,69	0
52	MG	BA	3203	1/1	0.92	0.41	-	53,53,53,53	0
52	MG	DA	3163	1/1	0.85	0.13	-	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3279	1/1	0.86	0.27	-	55,55,55,55	0
52	MG	BA	3136	1/1	0.92	0.34	-	51,51,51,51	0
52	MG	BA	3347	1/1	0.79	0.37	-	58,58,58,58	0
52	MG	DA	3309	1/1	0.94	0.05	-	76,76,76,76	0
52	MG	BA	3154	1/1	0.92	0.24	-	73,73,73,73	0
52	MG	DA	3067	1/1	0.97	0.64	-	57,57,57,57	0
52	MG	DA	3041	1/1	0.89	0.33	-	55,55,55,55	0
52	MG	DA	3258	1/1	0.89	0.46	-	70,70,70,70	0
52	MG	BA	3004	1/1	0.95	0.28	-	31,31,31,31	0
52	MG	BA	3183	1/1	0.84	0.46	-	55,55,55,55	0
52	MG	BA	3033	1/1	0.94	0.26	-	27,27,27,27	0
52	MG	DQ	201	1/1	0.92	0.24	-	63,63,63,63	0
52	MG	CA	1624	1/1	0.84	0.24	-	69,69,69,69	0
52	MG	CA	1647	1/1	0.93	0.41	-	78,78,78,78	0
52	MG	DA	3084	1/1	0.94	0.34	-	27,27,27,27	0
52	MG	BA	3360	1/1	0.90	0.06	-	68,68,68,68	0
52	MG	DA	3246	1/1	0.97	0.15	-	70,70,70,70	0
52	MG	BA	3279	1/1	0.92	0.91	-	62,62,62,62	0
52	MG	BA	3292	1/1	0.91	0.29	-	67,67,67,67	0
52	MG	BA	3255	1/1	0.75	0.34	-	46,46,46,46	0
52	MG	DA	3014	1/1	0.92	0.53	-	76,76,76,76	0
52	MG	DA	3106	1/1	0.97	0.65	-	50,50,50,50	0
52	MG	BA	3029	1/1	0.98	0.27	-	30,30,30,30	0
52	MG	BA	3325	1/1	0.91	0.48	-	49,49,49,49	0
52	MG	DA	3146	1/1	0.87	0.48	-	59,59,59,59	0
52	MG	DA	3180	1/1	0.94	0.56	-	56,56,56,56	0
52	MG	BA	3314	1/1	0.89	0.52	-	63,63,63,63	0
52	MG	BA	3065	1/1	0.93	0.23	-	37,37,37,37	0
52	MG	DA	3209	1/1	0.83	0.57	-	58,58,58,58	0
52	MG	DA	3254	1/1	0.84	0.23	-	61,61,61,61	0
52	MG	BA	3025	1/1	0.96	0.42	-	64,64,64,64	0
52	MG	BA	3078	1/1	0.97	0.46	-	39,39,39,39	0
52	MG	BA	3017	1/1	0.98	0.52	-	46,46,46,46	0
52	MG	BA	3276	1/1	0.95	0.54	-	76,76,76,76	0
52	MG	BA	3098	1/1	0.87	0.23	-	76,76,76,76	0
52	MG	CA	1608	1/1	0.87	0.42	-	90,90,90,90	0
52	MG	DA	3190	1/1	0.93	0.29	-	49,49,49,49	0
52	MG	BA	3171	1/1	0.96	0.57	-	45,45,45,45	0
52	MG	DA	3310	1/1	0.94	0.47	-	54,54,54,54	0
52	MG	AA	1643	1/1	0.77	0.57	-	85,85,85,85	0
52	MG	BA	3185	1/1	0.92	0.55	-	61,61,61,61	0
52	MG	BA	3207	1/1	0.88	0.44	-	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3152	1/1	0.91	0.44	-	66,66,66,66	0
52	MG	DA	3058	1/1	0.98	0.55	-	42,42,42,42	0
52	MG	BA	3334	1/1	0.86	0.11	-	61,61,61,61	0
52	MG	BA	3147	1/1	0.90	0.78	-	55,55,55,55	0
52	MG	BA	3298	1/1	0.82	0.87	-	65,65,65,65	0
52	MG	BA	3177	1/1	0.96	0.33	-	57,57,57,57	0
52	MG	DA	3099	1/1	0.98	0.41	-	56,56,56,56	0
52	MG	BA	3157	1/1	0.95	0.19	-	24,24,24,24	0
52	MG	DA	3044	1/1	0.96	0.40	-	39,39,39,39	0
52	MG	BA	3159	1/1	0.94	0.73	-	58,58,58,58	0
52	MG	DA	3005	1/1	0.91	0.12	-	69,69,69,69	0
52	MG	BA	3343	1/1	0.74	0.53	-	51,51,51,51	0
52	MG	DA	3311	1/1	0.73	0.80	-	86,86,86,86	0
52	MG	BA	3273	1/1	0.96	0.35	-	44,44,44,44	0
52	MG	BA	3155	1/1	0.98	0.47	-	42,42,42,42	0
52	MG	BA	3134	1/1	0.95	0.19	-	52,52,52,52	0
52	MG	BA	3267	1/1	0.95	0.41	-	40,40,40,40	0
52	MG	CA	1643	1/1	0.86	1.15	-	93,93,93,93	0
52	MG	BA	3219	1/1	0.69	0.42	-	75,75,75,75	0
52	MG	BA	3153	1/1	0.95	0.31	-	62,62,62,62	0
52	MG	BA	3019	1/1	0.89	0.50	-	26,26,26,26	0
52	MG	BA	3210	1/1	0.96	0.59	-	46,46,46,46	0
52	MG	DA	3140	1/1	0.97	0.62	-	46,46,46,46	0
52	MG	DA	3047	1/1	0.97	0.25	-	28,28,28,28	0
52	MG	BA	3307	1/1	0.96	1.20	-	70,70,70,70	0
52	MG	DA	3247	1/1	0.92	0.38	-	61,61,61,61	0
52	MG	DA	3269	1/1	0.73	0.83	-	64,64,64,64	0
52	MG	DA	3175	1/1	0.97	0.58	-	68,68,68,68	0
52	MG	DA	3151	1/1	0.96	0.20	-	66,66,66,66	0
52	MG	DA	3202	1/1	0.89	0.45	-	73,73,73,73	0
52	MG	AA	1630	1/1	0.85	0.76	-	75,75,75,75	0
52	MG	BA	3230	1/1	0.97	0.38	-	44,44,44,44	0
52	MG	DA	3210	1/1	0.94	0.18	-	49,49,49,49	0
52	MG	BA	3233	1/1	0.90	0.56	-	54,54,54,54	0
52	MG	BA	3206	1/1	0.97	0.37	-	36,36,36,36	0
52	MG	CA	1614	1/1	0.91	0.14	-	80,80,80,80	0
52	MG	BA	3168	1/1	0.96	0.35	-	59,59,59,59	0
52	MG	DA	3149	1/1	0.98	0.49	-	51,51,51,51	0
52	MG	DA	3030	1/1	0.98	0.21	-	66,66,66,66	0
52	MG	BA	3323	1/1	0.85	0.26	-	51,51,51,51	0
52	MG	CA	1636	1/1	0.75	0.45	-	74,74,74,74	0
52	MG	CA	1622	1/1	0.93	0.41	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3302	1/1	0.80	0.23	-	67,67,67,67	0
52	MG	CA	1603	1/1	0.96	0.34	-	57,57,57,57	0
52	MG	BA	3015	1/1	0.98	0.18	-	46,46,46,46	0
52	MG	BA	3312	1/1	0.89	0.18	-	55,55,55,55	0
52	MG	DA	3235	1/1	0.83	0.16	-	48,48,48,48	0
52	MG	AA	1611	1/1	0.97	0.57	-	50,50,50,50	0
52	MG	BA	3192	1/1	0.97	0.71	-	42,42,42,42	0
52	MG	DA	3251	1/1	0.95	0.43	-	91,91,91,91	0
52	MG	DA	3075	1/1	0.96	0.26	-	50,50,50,50	0
52	MG	BA	3011	1/1	0.93	0.52	-	22,22,22,22	0
52	MG	BA	3221	1/1	0.95	0.48	-	47,47,47,47	0
52	MG	BA	3059	1/1	0.99	0.39	-	46,46,46,46	0
52	MG	AA	1616	1/1	0.98	0.18	-	68,68,68,68	0
52	MG	DA	3142	1/1	0.92	0.56	-	69,69,69,69	0
52	MG	DA	3299	1/1	0.82	0.34	-	64,64,64,64	0
52	MG	AA	1639	1/1	0.90	1.18	-	77,77,77,77	0
52	MG	BA	3013	1/1	0.97	0.59	-	33,33,33,33	0
52	MG	BA	3264	1/1	0.97	0.23	-	58,58,58,58	0
52	MG	DA	3318	1/1	0.78	0.07	-	83,83,83,83	0
52	MG	DA	3280	1/1	0.98	0.27	-	67,67,67,67	0
52	MG	AA	1620	1/1	0.93	0.70	-	95,95,95,95	0
52	MG	BA	3133	1/1	0.92	0.26	-	38,38,38,38	0
52	MG	B5	102	1/1	0.87	0.43	-	80,80,80,80	0
52	MG	DA	3296	1/1	0.77	0.28	-	104,104,104,104	0
52	MG	DA	3253	1/1	0.95	0.14	-	51,51,51,51	0
52	MG	AA	1637	1/1	0.90	0.28	-	54,54,54,54	0
52	MG	BA	3186	1/1	0.96	0.45	-	44,44,44,44	0
52	MG	DA	3154	1/1	0.94	0.54	-	66,66,66,66	0
52	MG	BA	3135	1/1	0.95	0.52	-	30,30,30,30	0
52	MG	DA	3066	1/1	0.93	0.24	-	52,52,52,52	0
52	MG	DA	3169	1/1	0.93	0.64	-	49,49,49,49	0
52	MG	DA	3226	1/1	0.90	0.70	-	73,73,73,73	0
52	MG	CA	1646	1/1	0.89	0.45	-	68,68,68,68	0
52	MG	DA	3170	1/1	0.92	0.78	-	76,76,76,76	0
52	MG	DA	3263	1/1	0.94	0.67	-	55,55,55,55	0
52	MG	DA	3248	1/1	0.68	0.62	-	72,72,72,72	0
52	MG	DA	3133	1/1	0.96	0.33	-	31,31,31,31	0
52	MG	DA	3116	1/1	0.71	0.40	-	65,65,65,65	0
52	MG	DA	3148	1/1	0.96	0.69	-	61,61,61,61	0
52	MG	DA	3172	1/1	0.91	0.68	-	59,59,59,59	0
52	MG	AA	1605	1/1	0.90	0.28	-	106,106,106,106	0
52	MG	DA	3293	1/1	0.85	0.41	-	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3295	1/1	0.82	0.36	-	65,65,65,65	0
52	MG	DA	3138	1/1	0.97	0.52	-	35,35,35,35	0
52	MG	BA	3256	1/1	0.95	0.40	-	43,43,43,43	0
52	MG	BA	3350	1/1	0.83	0.67	-	64,64,64,64	0
52	MG	AA	1618	1/1	0.91	0.86	-	81,81,81,81	0
52	MG	BA	3026	1/1	0.92	0.34	-	58,58,58,58	0
52	MG	BA	3303	1/1	0.76	0.47	-	36,36,36,36	0
52	MG	CA	1618	1/1	0.98	0.68	-	84,84,84,84	0
52	MG	DA	3185	1/1	0.93	0.33	-	65,65,65,65	0
52	MG	DA	3214	1/1	0.96	0.32	-	33,33,33,33	0
52	MG	BA	3076	1/1	0.98	0.15	-	29,29,29,29	0
52	MG	BA	3201	1/1	0.88	0.16	-	52,52,52,52	0
52	MG	BA	3290	1/1	0.54	0.56	-	87,87,87,87	0
52	MG	BA	3349	1/1	0.98	0.40	-	51,51,51,51	0
52	MG	BA	3188	1/1	0.92	0.17	-	80,80,80,80	0
52	MG	BA	3189	1/1	0.95	0.46	-	40,40,40,40	0
52	MG	BA	3240	1/1	0.95	0.43	-	39,39,39,39	0
52	MG	BA	3191	1/1	0.97	0.59	-	59,59,59,59	0
52	MG	BA	3286	1/1	0.95	0.22	-	72,72,72,72	0
52	MG	DA	3012	1/1	0.91	0.53	-	29,29,29,29	0
52	MG	BA	3243	1/1	0.92	0.47	-	39,39,39,39	0
52	MG	DA	3102	1/1	0.71	0.88	-	54,54,54,54	0
52	MG	BA	3082	1/1	0.96	0.43	-	37,37,37,37	0
52	MG	BA	3035	1/1	0.97	0.37	-	23,23,23,23	0
52	MG	BA	3330	1/1	0.84	0.58	-	64,64,64,64	0
52	MG	DA	3068	1/1	0.94	0.25	-	80,80,80,80	0
52	MG	CA	1630	1/1	0.72	0.62	-	74,74,74,74	0
52	MG	BA	3048	1/1	0.99	0.37	-	20,20,20,20	0
52	MG	DA	3177	1/1	0.87	0.57	-	48,48,48,48	0
52	MG	BA	3340	1/1	0.85	0.10	-	83,83,83,83	0
52	MG	DA	3078	1/1	0.99	0.14	-	62,62,62,62	0
52	MG	DA	3100	1/1	0.94	0.22	-	59,59,59,59	0
52	MG	BQ	201	1/1	0.95	0.21	-	32,32,32,32	0
52	MG	BA	3202	1/1	0.88	0.28	-	49,49,49,49	0
52	MG	DA	3271	1/1	0.80	0.33	-	67,67,67,67	0
52	MG	BA	3262	1/1	0.88	0.40	-	68,68,68,68	0
52	MG	BA	3165	1/1	0.86	0.15	-	57,57,57,57	0
52	MG	DA	3065	1/1	0.97	0.41	-	70,70,70,70	0
52	MG	BA	3204	1/1	0.96	0.60	-	49,49,49,49	0
52	MG	BA	3355	1/1	0.80	0.20	-	78,78,78,78	0
52	MG	BA	3068	1/1	0.95	0.58	-	47,47,47,47	0
52	MG	AA	1646	1/1	0.91	0.56	-	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	AA	1641	1/1	0.86	0.28	-	57,57,57,57	0
52	MG	BA	3139	1/1	0.91	0.45	-	60,60,60,60	0
52	MG	DA	3077	1/1	0.97	0.40	-	46,46,46,46	0
52	MG	DA	3242	1/1	0.67	0.15	-	84,84,84,84	0
52	MG	DA	3255	1/1	0.46	0.48	-	91,91,91,91	0
52	MG	DA	3273	1/1	0.50	1.75	-	80,80,80,80	0
52	MG	DA	3158	1/1	0.89	0.72	-	71,71,71,71	0
52	MG	BA	3193	1/1	0.93	0.50	-	51,51,51,51	0
52	MG	CA	1642	1/1	0.79	0.27	-	80,80,80,80	0
52	MG	DA	3260	1/1	0.89	0.87	-	73,73,73,73	0
52	MG	DA	3206	1/1	0.81	0.99	-	74,74,74,74	0
52	MG	DA	3160	1/1	0.96	0.57	-	51,51,51,51	0
52	MG	BA	3271	1/1	0.82	0.55	-	57,57,57,57	0
52	MG	DA	3052	1/1	0.94	0.49	-	44,44,44,44	0
52	MG	BA	3104	1/1	0.96	0.18	-	45,45,45,45	0
52	MG	BA	3218	1/1	0.96	0.89	-	38,38,38,38	0
52	MG	AA	1601	1/1	0.97	0.08	-	68,68,68,68	0
52	MG	BA	3272	1/1	0.97	0.51	-	38,38,38,38	0
52	MG	DA	3207	1/1	0.91	0.16	-	53,53,53,53	0
52	MG	BA	3145	1/1	0.97	0.54	-	54,54,54,54	0
52	MG	BA	3099	1/1	0.97	0.25	-	45,45,45,45	0
52	MG	DA	3281	1/1	0.89	0.84	-	87,87,87,87	0
52	MG	DA	3276	1/1	0.76	1.23	-	87,87,87,87	0
52	MG	DA	3087	1/1	0.92	0.51	-	53,53,53,53	0
52	MG	DA	3297	1/1	0.85	0.23	-	93,93,93,93	0
52	MG	BA	3326	1/1	0.80	0.44	-	60,60,60,60	0
52	MG	BA	3095	1/1	0.91	0.35	-	43,43,43,43	0
52	MG	BA	3199	1/1	0.91	0.62	-	39,39,39,39	0
52	MG	DA	3249	1/1	0.88	0.44	-	69,69,69,69	0
52	MG	DA	3307	1/1	0.89	0.65	-	65,65,65,65	0
52	MG	BA	3097	1/1	0.93	0.43	-	53,53,53,53	0
52	MG	BA	3257	1/1	0.94	0.33	-	19,19,19,19	0
52	MG	AA	1624	1/1	0.96	0.43	-	55,55,55,55	0
52	MG	BA	3005	1/1	0.96	0.37	-	56,56,56,56	0
52	MG	DA	3176	1/1	0.98	0.83	-	41,41,41,41	0
52	MG	DA	3243	1/1	0.97	0.12	-	94,94,94,94	0
52	MG	BA	3269	1/1	0.92	0.45	-	45,45,45,45	0
52	MG	BA	3050	1/1	0.95	0.28	-	34,34,34,34	0
52	MG	BA	3241	1/1	0.93	0.58	-	69,69,69,69	0
52	MG	DA	3032	1/1	0.95	0.44	-	51,51,51,51	0
52	MG	DA	3144	1/1	0.85	0.55	-	65,65,65,65	0
52	MG	DA	3192	1/1	0.96	0.60	-	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3306	1/1	0.91	0.34	-	63,63,63,63	0
52	MG	DA	3013	1/1	0.90	0.43	-	77,77,77,77	0
52	MG	BA	3215	1/1	0.96	0.36	-	37,37,37,37	0
52	MG	BA	3084	1/1	0.98	0.40	-	25,25,25,25	0
52	MG	AA	1608	1/1	0.93	0.39	-	71,71,71,71	0
52	MG	DA	3301	1/1	0.68	0.88	-	67,67,67,67	0
52	MG	AA	1640	1/1	0.96	0.32	-	77,77,77,77	0
52	MG	DA	3232	1/1	0.69	0.81	-	56,56,56,56	0
52	MG	BA	3083	1/1	0.95	0.57	-	45,45,45,45	0
52	MG	DA	3104	1/1	0.74	0.44	-	85,85,85,85	0
52	MG	BA	3045	1/1	0.97	0.35	-	22,22,22,22	0
52	MG	CA	1634	1/1	0.41	0.31	-	88,88,88,88	0
52	MG	BA	3313	1/1	0.89	0.50	-	61,61,61,61	0
52	MG	BA	3297	1/1	0.83	0.54	-	68,68,68,68	0
52	MG	DA	3129	1/1	0.93	0.16	-	48,48,48,48	0
52	MG	DR	202	1/1	0.94	0.60	-	50,50,50,50	0
52	MG	DA	3262	1/1	0.90	0.52	-	55,55,55,55	0
52	MG	CA	1641	1/1	0.90	0.12	-	54,54,54,54	0
52	MG	CA	1601	1/1	0.91	0.21	-	85,85,85,85	0
52	MG	BA	3121	1/1	0.85	0.45	-	51,51,51,51	0
52	MG	DA	3289	1/1	0.90	0.27	-	71,71,71,71	0
52	MG	DA	3291	1/1	0.88	1.23	-	88,88,88,88	0
52	MG	DA	3072	1/1	0.98	0.28	-	42,42,42,42	0
52	MG	BA	3069	1/1	0.90	0.44	-	46,46,46,46	0
52	MG	BA	3113	1/1	0.97	0.46	-	28,28,28,28	0
52	MG	BP	202	1/1	0.97	0.85	-	66,66,66,66	0
52	MG	DA	3081	1/1	0.84	0.46	-	58,58,58,58	0
52	MG	BB	201	1/1	0.85	0.42	-	47,47,47,47	0
52	MG	BA	3085	1/1	0.97	0.12	-	0,0,0,0	0
52	MG	DA	3282	1/1	0.94	0.26	-	59,59,59,59	0
52	MG	BA	3354	1/1	0.96	0.21	-	71,71,71,71	0
52	MG	CA	1633	1/1	0.70	1.23	-	77,77,77,77	0
52	MG	BA	3036	1/1	0.97	0.25	-	0,0,0,0	0
52	MG	AA	1631	1/1	0.99	0.09	-	63,63,63,63	0
52	MG	BA	3245	1/1	0.94	0.33	-	48,48,48,48	0
52	MG	DA	3284	1/1	0.83	0.23	-	70,70,70,70	0
52	MG	CA	1629	1/1	0.98	0.11	-	69,69,69,69	0
52	MG	DA	3010	1/1	0.95	0.61	-	45,45,45,45	0
52	MG	DA	3101	1/1	0.98	0.61	-	57,57,57,57	0
52	MG	DA	3261	1/1	0.93	0.34	-	38,38,38,38	0
52	MG	AA	1617	1/1	0.81	0.40	-	55,55,55,55	0
52	MG	BA	3007	1/1	0.94	0.65	-	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DA	3023	1/1	0.97	0.24	-	39,39,39,39	0
52	MG	DA	3110	1/1	0.96	0.65	-	46,46,46,46	0
52	MG	BA	3030	1/1	0.97	0.17	-	26,26,26,26	0
52	MG	BA	3132	1/1	0.96	0.39	-	59,59,59,59	0
52	MG	DA	3264	1/1	0.89	0.46	-	87,87,87,87	0
52	MG	DA	3021	1/1	0.94	0.28	-	42,42,42,42	0
52	MG	BA	3182	1/1	0.99	0.47	-	54,54,54,54	0
52	MG	BA	3356	1/1	0.68	0.56	-	75,75,75,75	0
52	MG	CA	1609	1/1	0.91	0.18	-	48,48,48,48	0
52	MG	B0	101	1/1	0.94	0.11	-	48,48,48,48	0
52	MG	DA	3234	1/1	0.93	0.14	-	73,73,73,73	0
52	MG	BA	3079	1/1	0.98	0.20	-	48,48,48,48	0
52	MG	BA	3167	1/1	0.95	0.30	-	27,27,27,27	0
52	MG	BA	3131	1/1	0.96	0.16	-	17,17,17,17	0
52	MG	DA	3168	1/1	0.96	0.49	-	64,64,64,64	0
52	MG	DA	3182	1/1	0.79	0.67	-	54,54,54,54	0
52	MG	AA	1626	1/1	0.88	0.46	-	84,84,84,84	0
52	MG	BA	3175	1/1	0.93	0.28	-	50,50,50,50	0
52	MG	DA	3228	1/1	0.82	0.20	-	57,57,57,57	0
52	MG	DA	3025	1/1	0.81	0.65	-	61,61,61,61	0
52	MG	BA	3305	1/1	0.92	0.54	-	72,72,72,72	0
52	MG	BA	3283	1/1	0.90	0.62	-	70,70,70,70	0
52	MG	AA	1603	1/1	0.94	0.29	-	45,45,45,45	0
52	MG	BA	3329	1/1	0.84	0.59	-	65,65,65,65	0
52	MG	DA	3215	1/1	0.94	0.15	-	61,61,61,61	0
52	MG	BA	3296	1/1	0.85	0.27	-	54,54,54,54	0
52	MG	BA	3196	1/1	0.84	1.12	-	66,66,66,66	0
52	MG	BA	3110	1/1	0.94	0.40	-	23,23,23,23	0
52	MG	BA	3239	1/1	0.89	0.20	-	61,61,61,61	0
52	MG	DA	3092	1/1	0.94	0.30	-	61,61,61,61	0
52	MG	DA	3183	1/1	0.61	1.25	-	80,80,80,80	0
52	MG	DA	3220	1/1	0.77	0.25	-	68,68,68,68	0
52	MG	BA	3263	1/1	0.96	0.45	-	54,54,54,54	0
52	MG	BA	3027	1/1	0.94	0.49	-	19,19,19,19	0
52	MG	BA	3107	1/1	0.97	0.15	-	20,20,20,20	0
52	MG	BA	3324	1/1	0.96	0.42	-	64,64,64,64	0
52	MG	BA	3064	1/1	0.89	0.29	-	45,45,45,45	0
52	MG	DA	3150	1/1	0.89	1.00	-	80,80,80,80	0
52	MG	BA	3151	1/1	0.85	0.59	-	68,68,68,68	0
52	MG	BA	3348	1/1	0.91	0.50	-	73,73,73,73	0
52	MG	BB	206	1/1	0.76	0.82	-	66,66,66,66	0
52	MG	DA	3157	1/1	0.83	0.27	-	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	DB	203	1/1	0.95	0.46	-	47,47,47,47	0
52	MG	DA	3245	1/1	0.97	0.54	-	44,44,44,44	0
52	MG	BA	3227	1/1	0.98	0.24	-	21,21,21,21	0
52	MG	DA	3300	1/1	0.87	0.75	-	58,58,58,58	0
52	MG	DA	3219	1/1	0.93	0.54	-	49,49,49,49	0
52	MG	DB	202	1/1	0.91	0.35	-	80,80,80,80	0
52	MG	BA	3054	1/1	0.89	0.22	-	50,50,50,50	0
52	MG	DA	3312	1/1	0.93	0.41	-	53,53,53,53	0
52	MG	BA	3246	1/1	0.80	0.41	-	68,68,68,68	0
52	MG	BA	3158	1/1	0.95	0.37	-	32,32,32,32	0
52	MG	BA	3119	1/1	0.94	0.26	-	47,47,47,47	0
52	MG	DA	3063	1/1	0.94	0.77	-	72,72,72,72	0
52	MG	DA	3199	1/1	0.92	0.22	-	74,74,74,74	0
52	MG	BA	3327	1/1	0.68	0.81	-	70,70,70,70	0
52	MG	BA	3359	1/1	0.30	0.17	-	81,81,81,81	0
52	MG	BA	3160	1/1	0.76	1.01	-	78,78,78,78	0
52	MG	DA	3222	1/1	0.96	0.23	-	72,72,72,72	0
52	MG	CA	1639	1/1	0.82	1.03	-	87,87,87,87	0
52	MG	AA	1632	1/1	0.81	0.69	-	70,70,70,70	0
52	MG	BA	3252	1/1	0.86	0.28	-	72,72,72,72	0
52	MG	AA	1604	1/1	0.88	0.46	-	100,100,100,100	0
52	MG	AA	1636	1/1	0.88	0.35	-	88,88,88,88	0
52	MG	DA	3118	1/1	0.92	0.49	-	72,72,72,72	0
52	MG	CA	1613	1/1	0.73	0.82	-	87,87,87,87	0
52	MG	BA	3179	1/1	0.96	0.68	-	55,55,55,55	0
52	MG	DA	3126	1/1	0.92	0.43	-	57,57,57,57	0
52	MG	DA	3171	1/1	0.84	0.14	-	73,73,73,73	0
52	MG	DA	3237	1/1	0.94	0.40	-	56,56,56,56	0
52	MG	DA	3305	1/1	0.98	0.06	-	80,80,80,80	0
52	MG	BA	3022	1/1	0.94	0.33	-	45,45,45,45	0
52	MG	BA	3339	1/1	0.82	0.32	-	74,74,74,74	0
52	MG	BA	3042	1/1	0.92	0.28	-	31,31,31,31	0
52	MG	DA	3283	1/1	0.77	0.56	-	57,57,57,57	0
52	MG	BB	204	1/1	0.97	0.48	-	47,47,47,47	0
52	MG	DA	3189	1/1	0.98	0.28	-	45,45,45,45	0
52	MG	DA	3085	1/1	0.93	0.31	-	62,62,62,62	0
52	MG	BA	3328	1/1	0.92	0.29	-	41,41,41,41	0
52	MG	BA	3031	1/1	0.98	0.32	-	66,66,66,66	0
52	MG	DA	3200	1/1	0.89	0.60	-	47,47,47,47	0
52	MG	BA	3003	1/1	0.96	0.56	-	34,34,34,34	0
52	MG	BA	3208	1/1	0.97	0.53	-	36,36,36,36	0
52	MG	AA	1619	1/1	0.79	0.54	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
52	MG	BA	3311	1/1	0.97	1.08	-	69,69,69,69	0
52	MG	DA	3184	1/1	0.94	0.24	-	96,96,96,96	0
52	MG	BA	3250	1/1	0.95	0.23	-	40,40,40,40	0
52	MG	DP	201	1/1	0.97	0.18	-	42,42,42,42	0
52	MG	BA	3067	1/1	0.88	0.48	-	38,38,38,38	0
52	MG	BA	3198	1/1	0.97	0.38	-	24,24,24,24	0
52	MG	BA	3285	1/1	0.74	0.90	-	56,56,56,56	0
52	MG	BA	3251	1/1	0.83	0.75	-	44,44,44,44	0
52	MG	BA	3081	1/1	0.98	0.44	-	39,39,39,39	0
52	MG	BA	3073	1/1	0.96	0.37	-	24,24,24,24	0
52	MG	DA	3287	1/1	0.90	0.28	-	64,64,64,64	0
52	MG	BA	3299	1/1	0.96	0.79	-	43,43,43,43	0
52	MG	DA	3131	1/1	0.83	0.68	-	66,66,66,66	0
52	MG	BA	3318	1/1	0.76	0.35	-	55,55,55,55	0
52	MG	BA	3108	1/1	0.87	0.30	-	43,43,43,43	0
52	MG	BA	3184	1/1	0.96	0.21	-	62,62,62,62	0
52	MG	BA	3053	1/1	0.95	0.57	-	33,33,33,33	0
52	MG	BA	3270	1/1	0.98	0.21	-	24,24,24,24	0
52	MG	AA	1615	1/1	0.92	0.63	-	72,72,72,72	0
52	MG	AA	1635	1/1	0.96	0.70	-	50,50,50,50	0
52	MG	DA	3266	1/1	0.86	1.05	-	55,55,55,55	0
52	MG	DA	3244	1/1	0.90	0.51	-	69,69,69,69	0
52	MG	BA	3220	1/1	0.95	0.53	-	36,36,36,36	0
52	MG	BP	203	1/1	0.94	0.30	-	29,29,29,29	0
52	MG	DB	201	1/1	0.82	0.49	-	59,59,59,59	0
52	MG	AA	1612	1/1	0.69	0.25	-	84,84,84,84	0
52	MG	CA	1619	1/1	0.90	0.44	-	61,61,61,61	0
52	MG	BA	3077	1/1	0.94	0.21	-	40,40,40,40	0
52	MG	BA	3142	1/1	0.97	0.71	-	47,47,47,47	0
52	MG	D8	101	1/1	0.88	0.64	-	66,66,66,66	0
52	MG	BA	3217	1/1	0.99	0.59	-	34,34,34,34	0
52	MG	BA	3200	1/1	0.96	0.82	-	55,55,55,55	0
52	MG	AA	1628	1/1	0.77	0.54	-	65,65,65,65	0
52	MG	BA	3130	1/1	0.90	0.70	-	65,65,65,65	0
52	MG	DA	3029	1/1	0.99	0.24	-	36,36,36,36	0
52	MG	DA	3174	1/1	0.96	0.48	-	35,35,35,35	0
52	MG	DA	3265	1/1	0.86	0.44	-	61,61,61,61	0
52	MG	BA	3106	1/1	0.85	0.91	-	43,43,43,43	0
52	MG	BA	3291	1/1	0.90	0.36	-	45,45,45,45	0
52	MG	DA	3250	1/1	0.91	0.31	-	62,62,62,62	0
52	MG	DA	3186	1/1	0.90	0.39	-	58,58,58,58	0
52	MG	DA	3231	1/1	0.93	0.20	-	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.