wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 01:35 AM EDT

PDB ID	:	4V9D
Title	:	Structures of the bacterial ribosome in classical and hybrid states of tRNA binding
Authors	:	Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.
Deposited on	:	2012-07-31
Resolution	:	3.00 Å(reported)

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

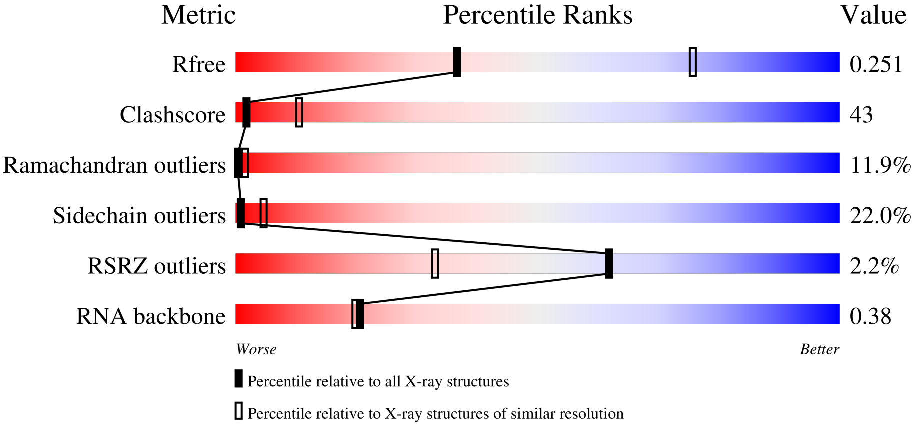
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

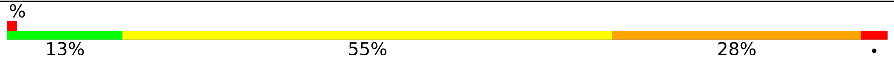
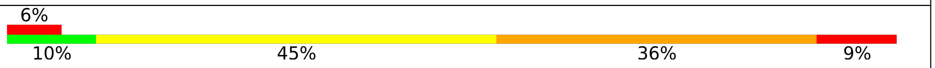
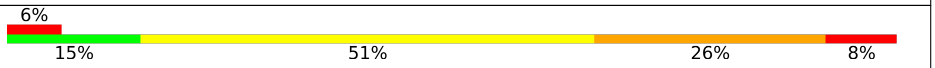
The reported resolution of this entry is 3.00 Å.

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	
1	BA	1539	
2	AB	218	
2	BB	218	

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Mol	Chain	Length	Quality of chain
3	AC	206	23% 51% 21% 5%
3	BC	206	% 20% 49% 29% •
4	AD	205	2% 21% 46% 31% •
4	BD	205	20% 48% 29% •
5	AE	150	% 17% 54% 24% 5%
5	BE	150	23% 45% 31% •
6	AF	100	18% 52% 25% 5%
6	BF	100	9% 56% 28% 7%
7	AG	151	9% 26% 49% 25% •
7	BG	151	3% 16% 55% 25% •
8	AH	129	21% 58% 19% •
8	BH	129	% 32% 43% 22% •
9	AI	127	3% 13% 57% 28% •
9	BI	127	6% 14% 55% 27% •
10	AJ	98	5% 17% 45% 32% 6%
10	BJ	98	6% 19% 46% 29% 6%
11	AK	117	% 29% 43% 26% •
11	BK	117	24% 51% 21% •
12	AL	123	2% 36% 54% 8% •
12	BL	123	2% 30% 46% 20% •
13	AM	114	4% 18% 61% 16% •
13	BM	114	6% 16% 52% 29% •
14	AN	100	% 13% 52% 26% 5% •
14	BN	100	4% 12% 50% 30% • •
15	AO	88	% 31% 53% 15% •

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Mol	Chain	Length	Quality of chain
15	BO	88	% 26% 44% 27% •
16	AP	82	4% 21% 44% 28% 7%
16	BP	82	5% 22% 51% 23% •
17	AQ	80	% 21% 45% 31% •
17	BQ	80	% 20% 49% 28% •
18	AR	55	2% 18% 67% 9% 5%
18	BR	55	4% 18% 67% 13% •
19	AS	79	5% 24% 49% 27%
19	BS	79	11% 24% 52% 22% •
20	AT	85	4% 26% 40% 33% •
20	BT	85	2% 15% 54% 28% •
21	AU	51	10% 8% 41% 47% •
21	BU	51	6% 14% 31% 41% 14%
22	AV	76	% 22% 43% 30% •
22	BV	76	28% 54% 14% •
23	AX	16	6% 12% 50% 31% 6%
23	BX	16	6% 6% 69% 25%
24	AY	183	21% 44% 45% 9% •
25	CA	2903	% 18% 44% 30% 7%
25	DA	2903	% 16% 50% 30% 5%
26	CB	119	18% 52% 27% •
27	CC	271	31% 54% 15% •
27	DC	271	31% 50% 17% •
28	CD	209	47% 40% 12%
28	DD	209	41% 45% 12% •

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Mol	Chain	Length	Quality of chain
29	CE	201	36% 54% 9%
29	DE	201	32% 47% 19% •
30	CF	177	2% 23% 53% 21% •
30	DF	177	5% 21% 51% 26% •
31	CG	176	31% 53% 15% •
31	DG	176	% 26% 55% 19% •
32	CH	149	5% 22% 51% 26% •
32	DH	149	5% 20% 56% 20% •
33	CI	141	52% 17% 52% 26% 5%
33	DI	141	50% 16% 57% 26% •
34	CJ	142	56% 33% 10% •
34	DJ	142	37% 51% 11% •
35	CK	122	43% 40% 16% •
35	DK	122	40% 43% 17%
36	CL	143	34% 46% 17% •
36	DL	143	2% 27% 55% 14% •
37	CM	136	42% 40% 16% •
37	DM	136	% 29% 53% 16% •
38	CN	120	32% 55% 12% •
38	DN	120	26% 57% 18%
39	CO	116	31% 50% 16% •
39	DO	116	7% 22% 56% 22% •
40	CP	114	32% 56% 10% •
40	DP	114	26% 55% 15% •
41	CQ	117	46% 47% 6% •

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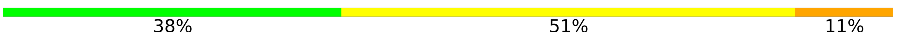
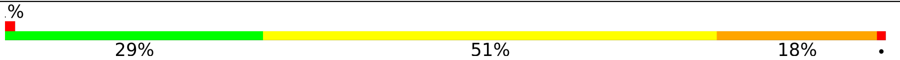
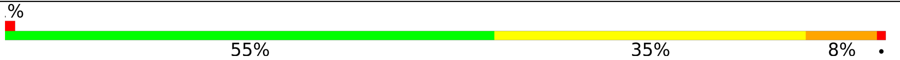
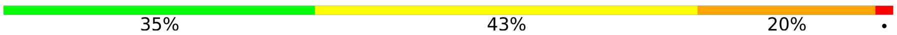
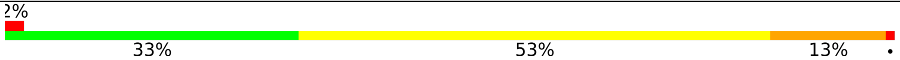
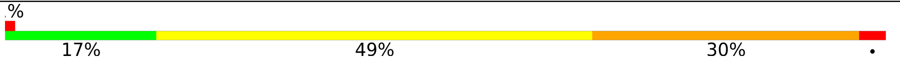
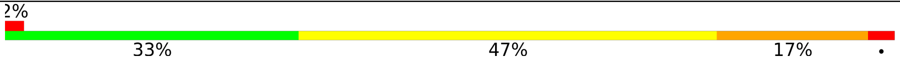
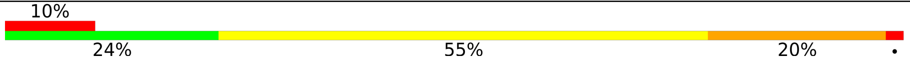
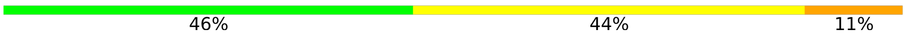
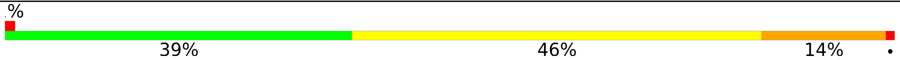
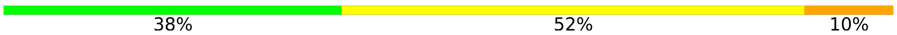
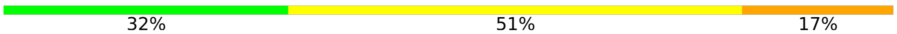
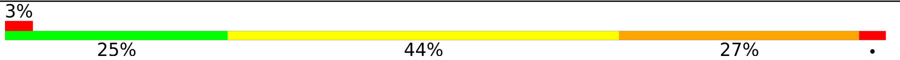
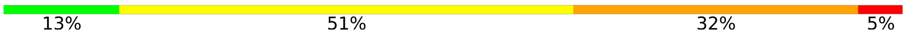
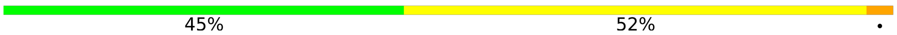
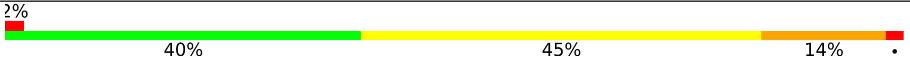
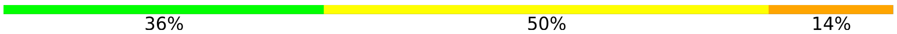
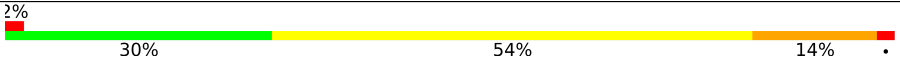
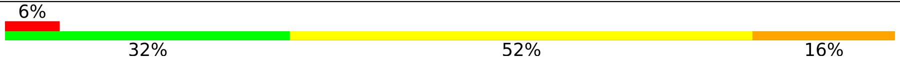
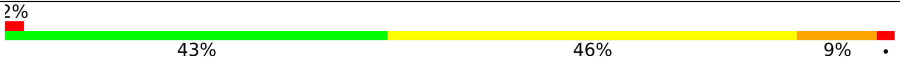
Mol	Chain	Length	Quality of chain
41	DQ	117	
42	CR	103	
42	DR	103	
43	CS	110	
43	DS	110	
44	CT	93	
44	DT	93	
45	CU	102	
45	DU	102	
46	CV	94	
46	DV	94	
47	CW	76	
48	CX	77	
48	DX	77	
49	CY	63	
49	DY	63	
50	CZ	58	
50	DZ	58	
51	C0	56	
51	D0	56	
52	C1	50	
52	D1	50	
53	C2	46	
53	D2	46	
54	C3	64	

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Mol	Chain	Length	Quality of chain
54	D3	64	
55	C4	38	
55	D4	38	
56	DB	118	
57	DW	75	

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
58	MG	DA	3098	-	-	-	X

2 Entry composition ⓘ

There are 60 unique types of molecules in this entry. The entry contains 292354 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	1538	Total 32995	C 14716	N 6050	O 10691	P 1538	0	0	0
1	BA	1539	Total 33015	C 14725	N 6052	O 10699	P 1539	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total 1705	C 1081	N 305	O 312	S 7	0	0	0
2	BB	218	Total 1705	C 1081	N 305	O 312	S 7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total 1625	C 1028	N 305	O 289	S 3	0	0	0
3	BC	206	Total 1625	C 1028	N 305	O 289	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total 1643	C 1026	N 315	O 298	S 4	0	0	0
4	BD	205	Total 1643	C 1026	N 315	O 298	S 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	AE	150	Total C N O S 1106 687 211 202 6	0	0	0
5	BE	150	Total C N O S 1106 687 211 202 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	AF	100	Total C N O S 818 515 148 149 6	0	0	0
6	BF	100	Total C N O S 818 515 148 149 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	AG	151	Total C N O S 1182 735 227 216 4	0	0	0
7	BG	151	Total C N O S 1182 735 227 216 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AH	129	Total C N O S 979 616 173 184 6	0	0	0
8	BH	129	Total C N O S 979 616 173 184 6	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AI	127	Total C N O S 1022 634 206 179 3	0	0	0
9	BI	127	Total C N O S 1022 634 206 179 3	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	AJ	98	Total C N O S 787 493 150 143 1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	BJ	98	Total C N O S 787 493 150 143 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	AK	117	Total C N O S 877 540 174 160 3	0	0	0
11	BK	117	Total C N O S 877 540 174 160 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	AL	123	Total C N O S 955 590 196 165 4	0	0	0
12	BL	123	Total C N O S 955 590 196 165 4	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	AM	114	Total C N O S 884 546 178 157 3	0	0	0
13	BM	114	Total C N O S 884 546 178 157 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	AN	96	Total C N O S 774 483 160 128 3	0	0	0
14	BN	96	Total C N O S 774 483 160 128 3	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	AO	88	Total C N O S 714 439 144 130 1	0	0	0
15	BO	88	Total C N O S 714 439 144 130 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AP	82	649	406	128	114	1	0	0	0
16	BP	82	649	406	128	114	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AQ	80	649	411	121	114	3	0	0	0
17	BQ	80	649	411	121	114	3	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	AR	55	456	288	86	82	0	0	0
18	BR	55	456	288	86	82	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	79	638	408	120	108	2	0	0	0
19	BS	79	638	408	120	108	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AT	85	665	411	137	114	3	0	0	0
20	BT	85	665	411	137	114	3	0	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total 426	C 265	N 86	O 74	S 1	0	0	0
21	BU	51	Total 426	C 265	N 86	O 74	S 1	0	0	0

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total 1623	C 723	N 290	O 534	P 76	0	0	0
22	BV	76	Total 1623	C 723	N 290	O 534	P 76	0	0	0

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	15	Total 324	C 145	N 61	O 103	P 15	0	0	0
23	BX	16	Total 346	C 155	N 66	O 109	P 16	0	0	0

- Molecule 24 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	183	Total 1419	C 871	N 260	O 283	S 5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	2	GLY	-	expression tag	UNP P0A805

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CA	2897	Total 62195	C 27745	N 11446	O 20107	P 2897	0	0	0
25	DA	2896	Total 62173	C 27735	N 11441	O 20101	P 2896	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	CB	119	Total C N O P 2548 1135 466 829 118	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	CC	271	Total C N O S 2083 1288 423 365 7	0	0	0
27	DC	271	Total C N O S 2083 1288 423 365 7	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	CD	209	Total C N O S 1565 979 288 294 4	0	0	0
28	DD	209	Total C N O S 1565 979 288 294 4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	CE	201	Total C N O S 1552 974 283 290 5	0	0	0
29	DE	201	Total C N O S 1552 974 283 290 5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	CF	177	Total C N O S 1411 899 249 257 6	0	0	0
30	DF	177	Total C N O S 1411 899 249 257 6	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	CG	176	Total C N O S 1323 832 243 246 2	0	0	0
31	DG	176	Total C N O S 1323 832 243 246 2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CH	149	Total 1110	C 699	N 197	O 213	S 1	0	0	0
32	DH	149	Total 1110	C 699	N 197	O 213	S 1	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CI	141	Total 1032	C 651	N 179	O 196	S 6	0	0	0
33	DI	141	Total 1032	C 651	N 179	O 196	S 6	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CJ	142	Total 1129	C 714	N 212	O 199	S 4	0	0	0
34	DJ	142	Total 1129	C 714	N 212	O 199	S 4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CK	122	Total 939	C 587	N 180	O 166	S 6	0	0	0
35	DK	122	Total 939	C 587	N 180	O 166	S 6	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CL	143	Total 1045	C 649	N 206	O 189	S 1	0	0	0
36	DL	143	Total 1045	C 649	N 206	O 189	S 1	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	CM	136	Total C N O S 1074 686 205 177 6	0	0	0
37	DM	136	Total C N O S 1074 686 205 177 6	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	CN	120	Total C N O S 961 593 196 167 5	0	0	0
38	DN	120	Total C N O S 961 593 196 167 5	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	CO	116	Total C N O 892 552 178 162	0	0	0
39	DO	116	Total C N O 892 552 178 162	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	CP	114	Total C N O S 917 574 179 163 1	0	0	0
40	DP	114	Total C N O S 917 574 179 163 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	CQ	117	Total C N O 947 604 192 151	0	0	0
41	DQ	117	Total C N O 947 604 192 151	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	CR	103	Total C N O S 816 516 153 145 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DR	103	Total 816	C 516	N 153	O 145	S 2	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CS	110	Total 857	C 532	N 166	O 156	S 3	0	0	0
43	DS	110	Total 857	C 532	N 166	O 156	S 3	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CT	93	Total 739	C 466	N 139	O 132	S 2	0	0	0
44	DT	93	Total 739	C 466	N 139	O 132	S 2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	CU	102	Total 780	C 492	N 146	O 142	0	0	0
45	DU	102	Total 780	C 492	N 146	O 142	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CV	94	Total 753	C 479	N 137	O 134	S 3	0	0	0
46	DV	94	Total 753	C 479	N 137	O 134	S 3	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CW	76	Total 575	C 356	N 117	O 101	S 1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
48	CX	77	Total C N O S 625 388 129 106 2	0	0	0
48	DX	77	Total C N O S 625 388 129 106 2	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
49	CY	63	Total C N O S 509 313 99 95 2	0	0	0
49	DY	63	Total C N O S 509 313 99 95 2	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
50	CZ	58	Total C N O S 449 281 87 79 2	0	0	0
50	DZ	58	Total C N O S 449 281 87 79 2	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
51	C0	56	Total C N O S 444 269 94 80 1	0	0	0
51	D0	56	Total C N O S 444 269 94 80 1	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	C1	50	Total C N O 410 263 75 72	0	0	0
52	D1	50	Total C N O 410 263 75 72	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	C2	46	Total C N O S 377 228 90 57 2	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	D2	46	Total C N O S 377 228 90 57 2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
54	C3	64	Total C N O S 504 323 105 74 2	0	0	0
54	D3	64	Total C N O S 504 323 105 74 2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	C4	38	Total C N O S 302 185 65 48 4	0	0	0
55	D4	38	Total C N O S 302 185 65 48 4	0	0	0

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	DB	118	Total C N O P 2529 1126 464 821 118	0	0	0

- Molecule 57 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	DW	75	Total C N O S 564 350 113 100 1	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	72	Total Mg 72 72	0	0
58	BA	56	Total Mg 56 56	0	0
58	CA	194	Total Mg 194 194	0	0
58	CB	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	CQ	1	Total Mg 1 1	0	0
58	DA	166	Total Mg 166 166	0	0
58	DB	3	Total Mg 3 3	0	0
58	DL	1	Total Mg 1 1	0	0
58	DQ	1	Total Mg 1 1	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	C4	1	Total Zn 1 1	0	0
59	D4	1	Total Zn 1 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	197	Total O 197 197	0	0
60	AN	4	Total O 4 4	0	0
60	AT	1	Total O 1 1	0	0
60	AU	1	Total O 1 1	0	0
60	BA	190	Total O 190 190	0	0
60	BL	1	Total O 1 1	0	0
60	BN	5	Total O 5 5	0	0
60	BT	1	Total O 1 1	0	0
60	BU	1	Total O 1 1	0	0
60	CA	625	Total O 625 625	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	CB	13	Total O 13 13	0	0
60	CC	8	Total O 8 8	0	0
60	CD	2	Total O 2 2	0	0
60	CE	2	Total O 2 2	0	0
60	CF	1	Total O 1 1	0	0
60	CJ	1	Total O 1 1	0	0
60	CL	6	Total O 6 6	0	0
60	CN	4	Total O 4 4	0	0
60	CS	1	Total O 1 1	0	0
60	CV	1	Total O 1 1	0	0
60	C2	1	Total O 1 1	0	0
60	C3	1	Total O 1 1	0	0
60	C4	2	Total O 2 2	0	0
60	DA	622	Total O 622 622	0	0
60	DB	14	Total O 14 14	0	0
60	DC	4	Total O 4 4	0	0
60	DD	5	Total O 5 5	0	0
60	DE	2	Total O 2 2	0	0
60	DJ	1	Total O 1 1	0	0
60	DL	4	Total O 4 4	0	0
60	DN	1	Total O 1 1	0	0

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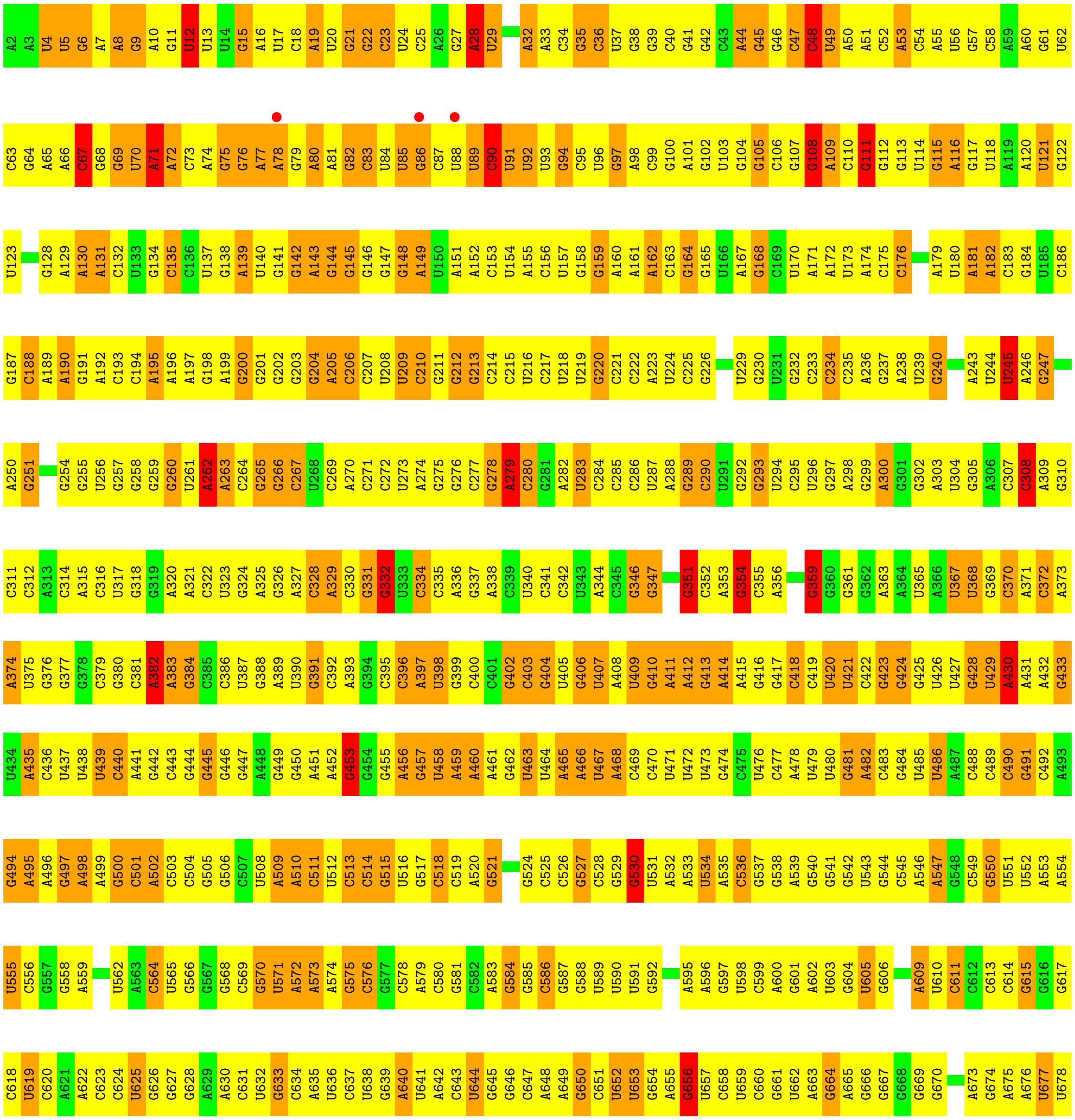
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	DR	1	Total O 1 1	0	0
60	D2	1	Total O 1 1	0	0
60	D3	2	Total O 2 2	0	0
60	D4	1	Total O 1 1	0	0

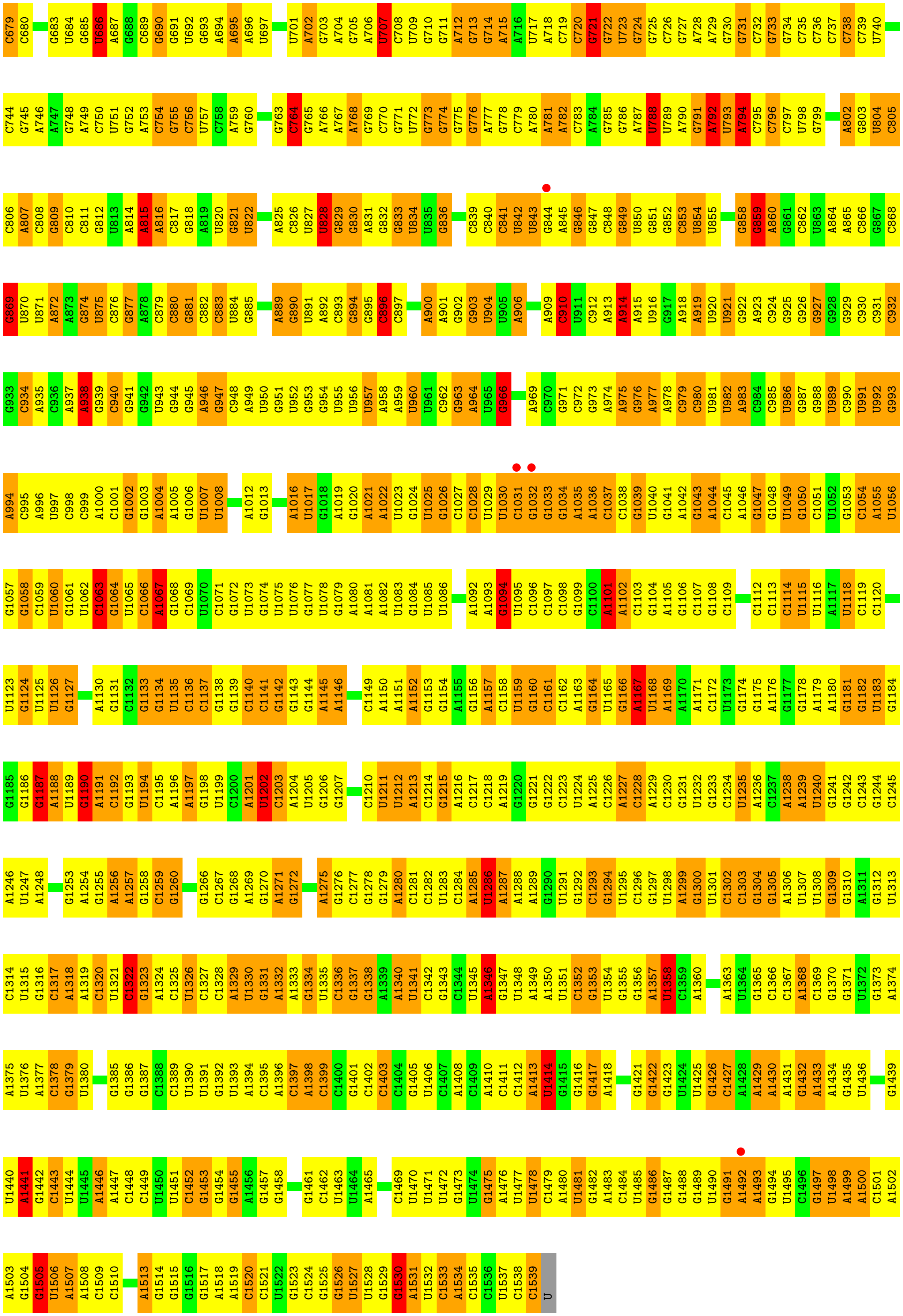
3 Residue-property plots ⓘ

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

- Molecule 1: 16S rRNA

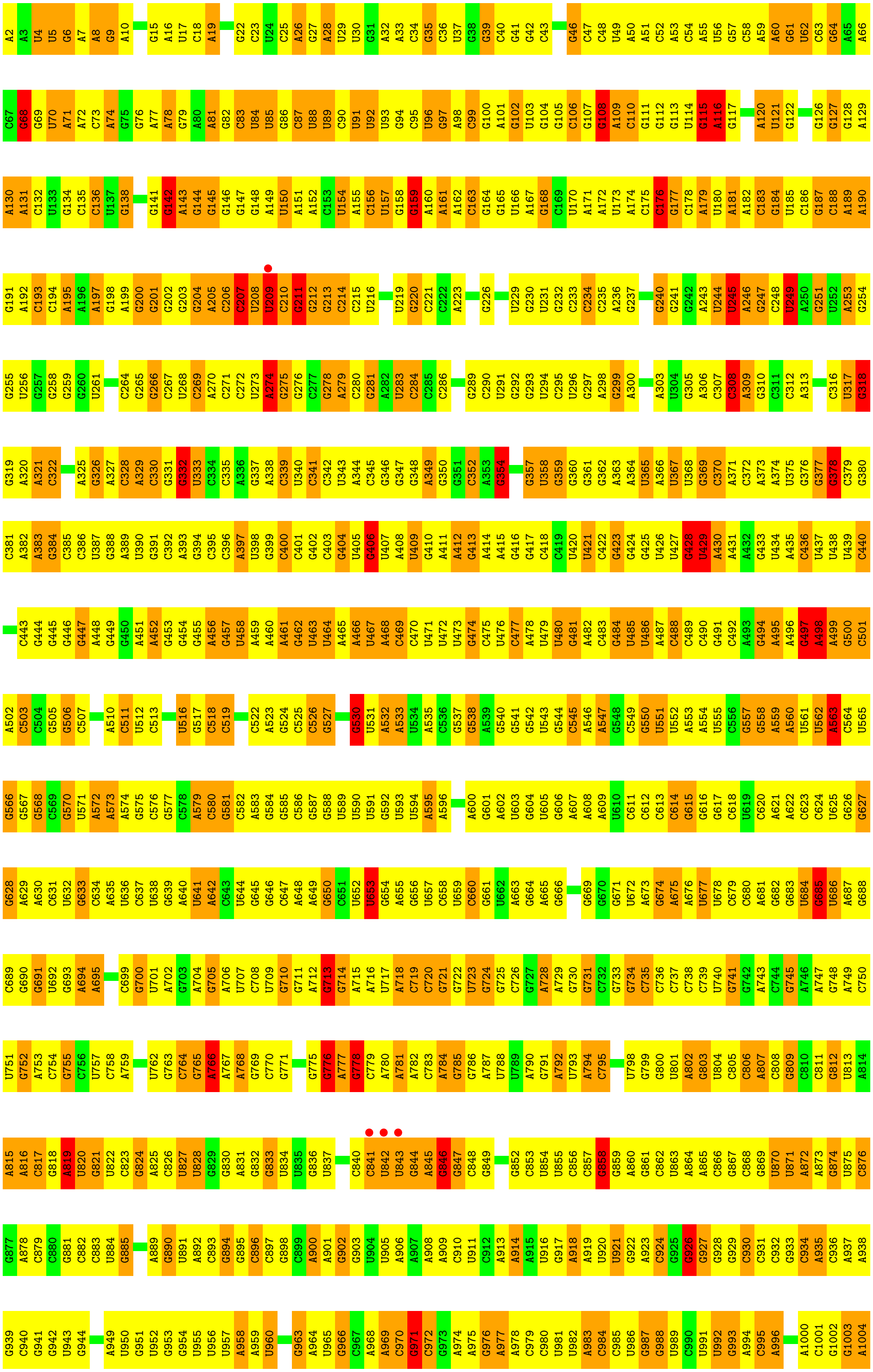
Chain AA:

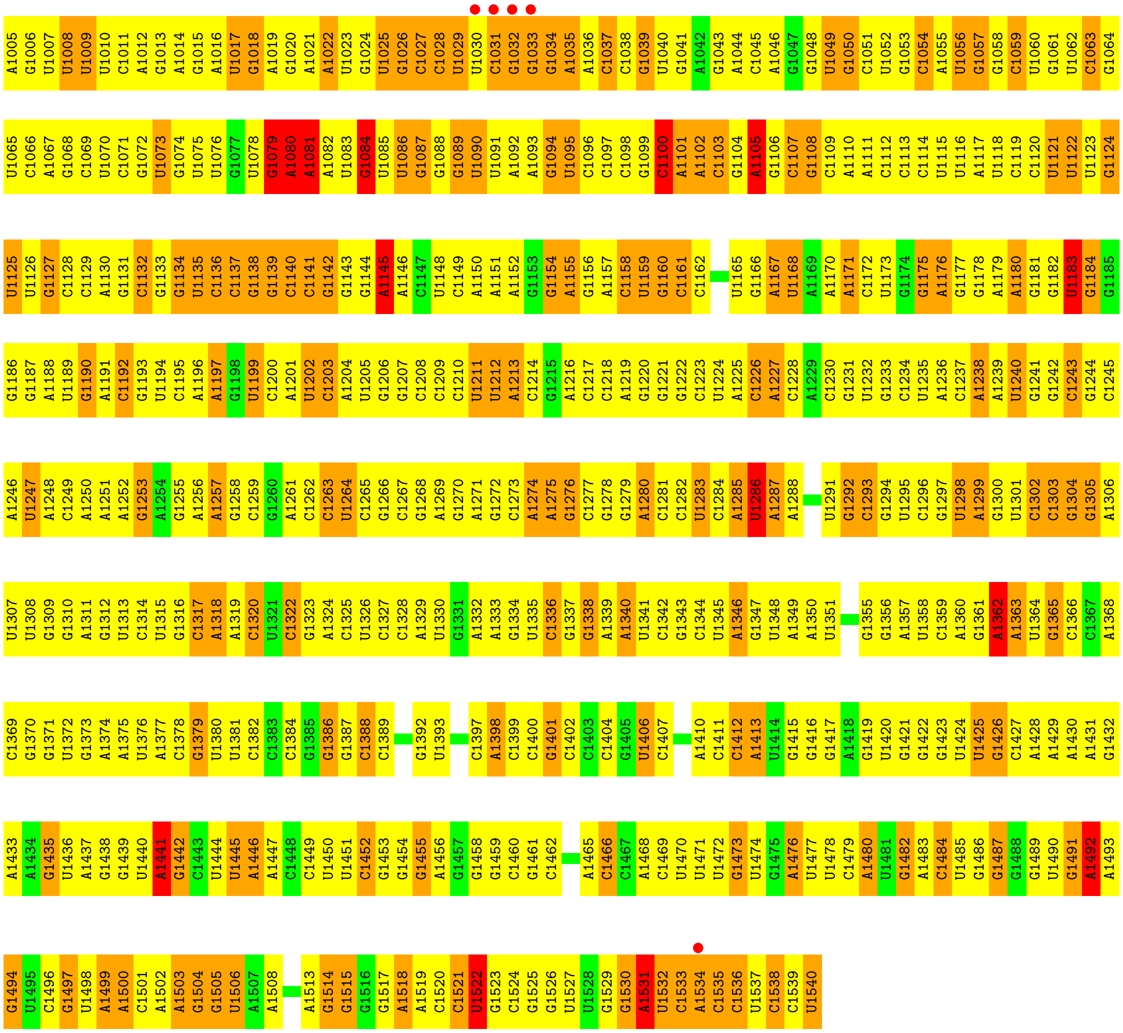




- Molecule 1: 16S rRNA

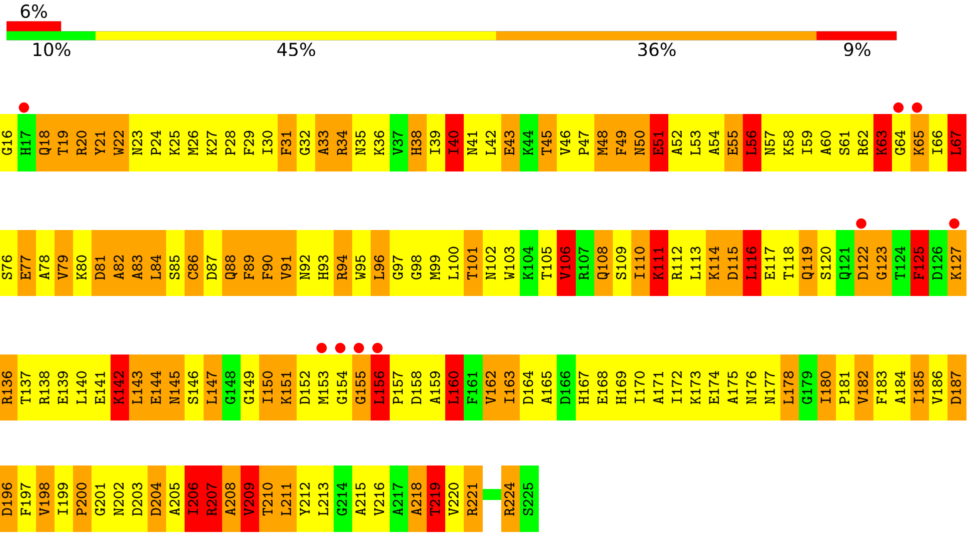
Chain BA:


A2 A3 U4 U5 G6 A7 A8 G9 A10 G15 A16 U17 C18 A19 G22 C23 U24 C25 A26 G27 A28 U29 U30 G31 A32 A33 C34 G35 C36 U37 G38 G39 C40 G41 G42 C43 G46 C47 C48 U49 A50 A51 C52 A53 C54 A55 U56 G57 C58 A59 A60 G61 U62 C63 G64 A65 A66
C67 G68 G69 U70 A71 A72 C73 A74 G75 G76 A77 A78 G79 A80 A81 G82 C83 U84 U85 G86 C87 U88 U89 C90 U91 U92 U93 G94 C95 U96 G97 A98 C99 G100 A101 G102 U103 G104 G105 C106 G107 G108 A109 C110 G111 G112 G113 U114 G115 A116 G117 A120 U121 G122 G126 G127 G128 A129
A130 A131 C132 U133 G134 C135 C136 U137 G138 G141 G142 A143 G144 G145 G146 G147 G148 A149 U150 A151 A152 C153 U154 A155 C156 U157 G158 G159 A160 A161 A162 C163 G164 G165 U166 A167 G168 C169 U170 A171 A172 U173 A174 C175 C176 G177 C178 A179 U180 A181 A182 C183 G184 U185 C186 G187 C188 A189 A190
G191 A192 C193 C194 A195 A196 A197 G198 A199 G200 G201 G202 G203 G204 A205 C206 C207 U208 U209 C210 G211 G212 G213 C214 C215 U216 U219 G220 C221 C222 A223 G226 U229 G230 U231 G232 C233 C234 C235 A236 G237 G240 G241 G242 A243 U244 U245 A246 G247 C248 U249 A250 G251 U252 A253 G254
G255 U256 G257 G258 G259 G260 U261 C264 G265 G266 C267 U268 C269 A270 C271 C272 U273 A274 G275 G276 C277 G278 A279 C280 G281 A282 U283 C284 C285 C286 G289 C290 U291 G292 G293 U294 C295 U296 G297 A298 G299 A300 A303 U304 G305 A306 C307 G308 A309 G310 C311 U312 A313 C316 U317 G318
G319 A320 A321 C322 A325 G326 A327 C328 A329 C330 G331 G332 U333 C334 C335 A336 G337 A338 C339 U340 C341 C342 U343 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 G357 U358 G359 G360 G361 G362 A363 A364 U365 A366 U367 U368 G369 C370 A371 C372 A373 A374 U375 G376 G377 G378 C379 G380
C381 A382 A383 G384 C385 C386 U387 G388 A389 U390 G391 C392 A393 G394 C395 C396 A397 U398 G399 C400 C401 G402 C403 G404 U405 G406 U407 A408 U409 G410 A411 A412 G413 A414 A415 G416 G417 C418 C419 U420 U421 C422 G423 G424 G425 U426 U427 G428 U429 A430 A431 A432 G433 U434 A435 C436 U437 U438 U439 C440
C443 G444 G445 G446 G447 A448 G449 G450 A451 A452 G453 G454 G455 A456 G457 U458 A459 A460 A461 G462 U463 U464 A465 A466 U467 A468 C469 C470 U471 U472 U473 G474 C475 U476 C477 A478 U479 U480 G481 A482 C483 G484 U485 U486 A487 C488 C489 C490 G491 C492 A493 G494 A495 A496 G497 A498 A499 G500 C501
A502 C503 C504 G505 G506 C507 A510 C511 U512 C513 U516 G517 C518 C519 C522 A523 G524 C525 C526 G527 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 G542 U543 G544 C545 A546 A547 G548 C549 G550 U551 U552 A553 U554 U555 C556 G557 G558 A559 A560 U561 U562 A563 C564 U565
G566 G567 G568 C569 G570 U571 A572 A573 A574 G575 C576 G577 C578 A579 C580 G581 C582 A583 G584 G585 C586 G587 G588 U589 U590 U591 G592 U593 U594 A595 A596 A600 G601 A602 U603 G604 U605 G606 A607 A608 A609 U610 C611 C612 C613 C614 G615 G616 G617 C618 U619 C620 A621 A622 C623 C624 U625 G626 G627
G628 A629 A630 C631 U632 G633 C634 A635 U636 C637 U638 G639 A640 U641 A642 C643 U644 G645 G646 C647 A648 A649 G650 C651 U652 U653 G654 A655 G656 U657 C658 U659 C660 G661 U662 A663 G664 A665 G666 G669 G670 G671 U672 A673 G674 A675 A676 U677 U678 C679 C680 A681 G682 G683 U684 G685 U686 A687 G688
C689 G690 G691 U692 G693 A694 A695 C699 G700 U701 A702 G703 A704 G705 A706 U707 C708 U709 G710 G711 A712 G713 G714 A715 A716 U717 A718 C719 C720 G721 G722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 G733 G734 C735 C736 C737 C738 C739 U740 G741 G742 A743 C744 G745 A746 A747 G748 A749 C750
U751 G752 A753 C754 G755 C756 U757 C758 A759 U762 G763 C764 G765 A766 A767 A768 G769 C770 G771 G775 G776 A777 G778 C779 A780 A781 A782 C783 A784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 U798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 G812 U813 A814
A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829 G830 A831 G832 G833 U834 U835 G836 U837 C840 C841 U842 U843 G844 A845 G846 G847 C848 G849 C852 C853 U854 U855 C856 C857 G858 G859 A860 G861 C862 U863 A864 A865 C866 C867 G868 C869 U870 U871 A872 A873 G874 U875 C876
G877 A878 C879 C880 G881 C882 C883 U884 G885 A889 G890 U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 G902 G903 U904 U905 A906 A907 A908 A909 C910 U911 C912 A913 A914 A915 U916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938
G939 C940 G941 G942 U943 G944 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 G963 A964 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 U986 G987 G988 U989 C990 U991 U992 G993 A994 C995 A996 A1000 C1001 G1002 G1003 A1004



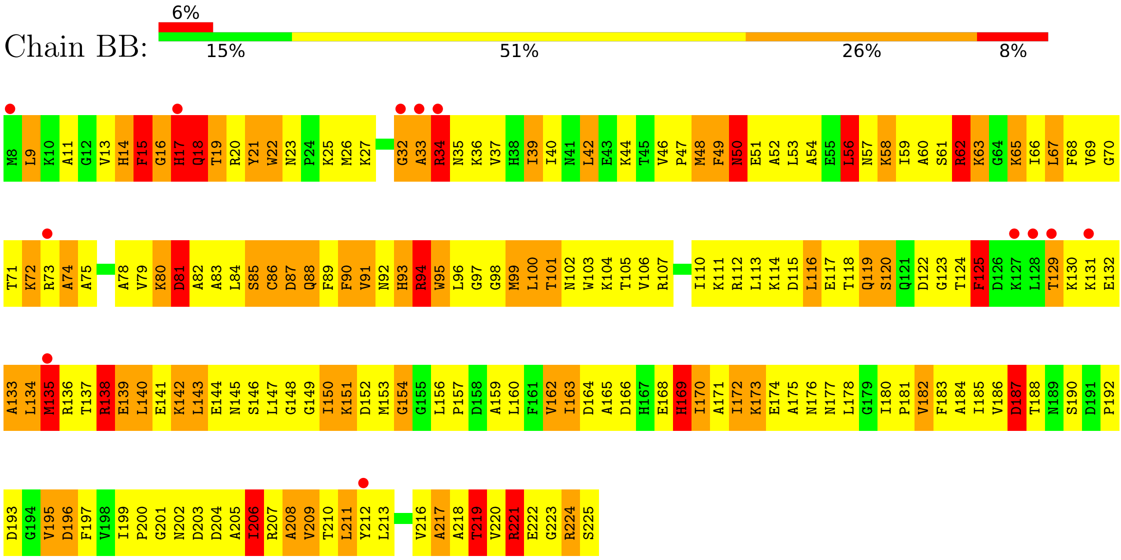
- Molecule 2: 30S ribosomal protein S2

Chain AB:



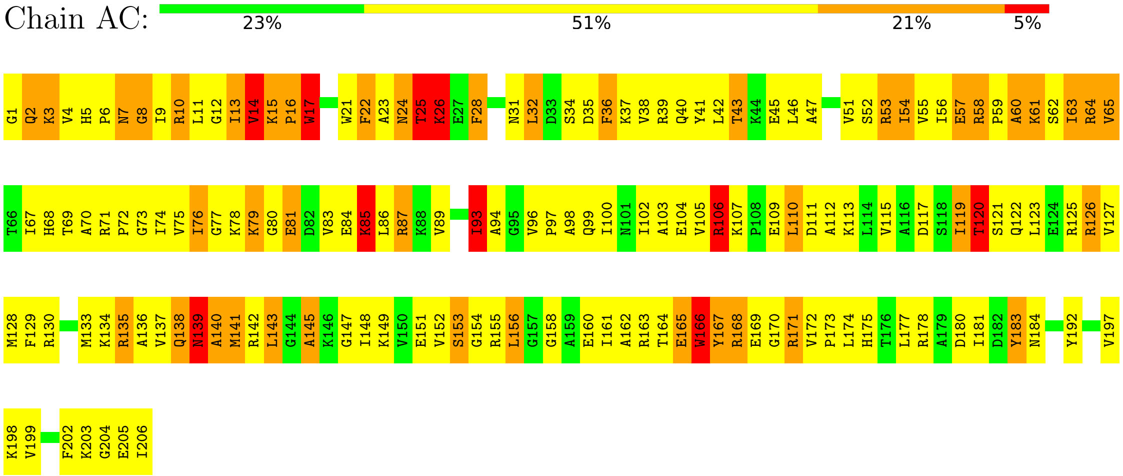
- Molecule 2: 30S ribosomal protein S2

Chain BB:



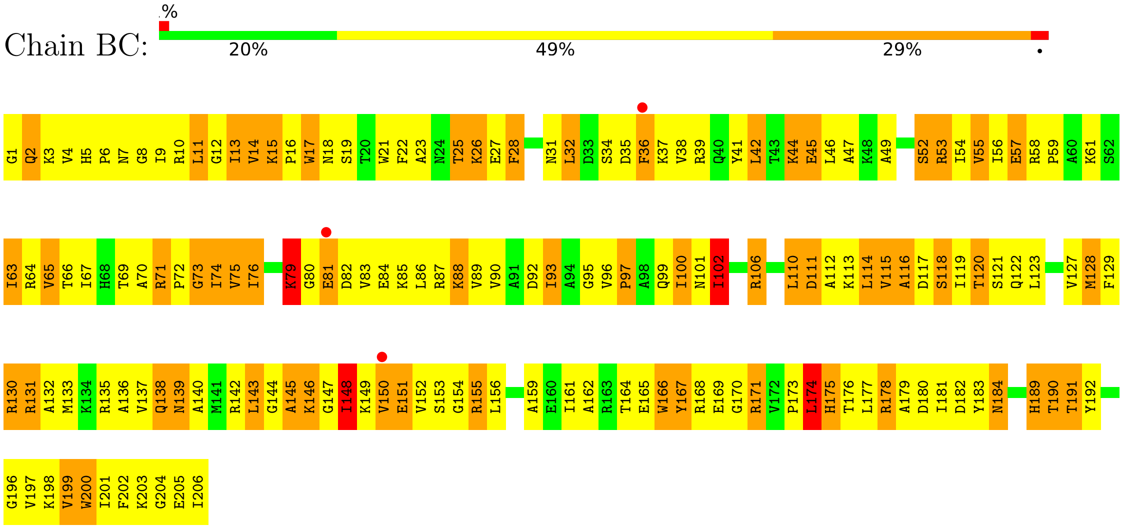
- Molecule 3: 30S ribosomal protein S3

Chain AC:

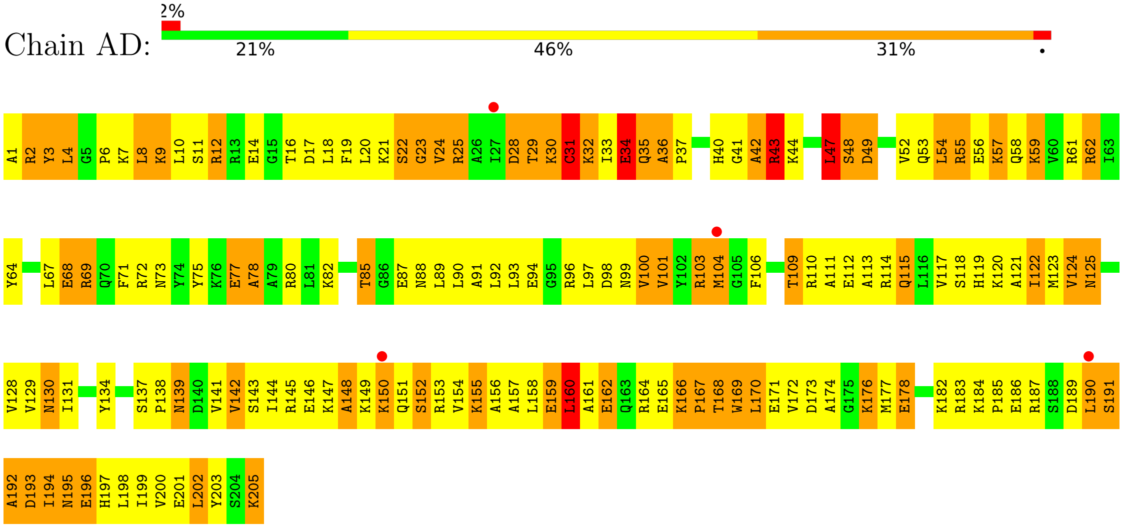


- Molecule 3: 30S ribosomal protein S3

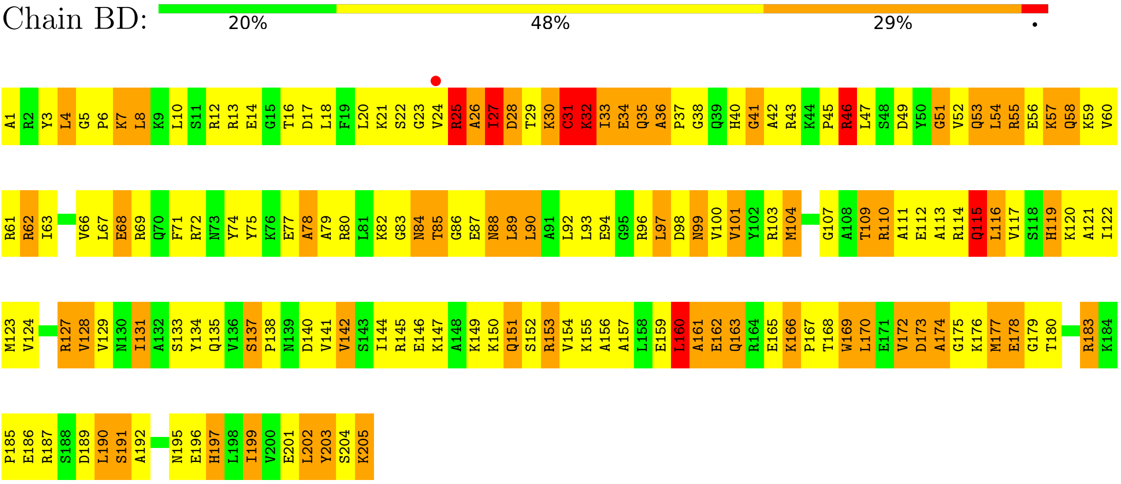
Chain BC:



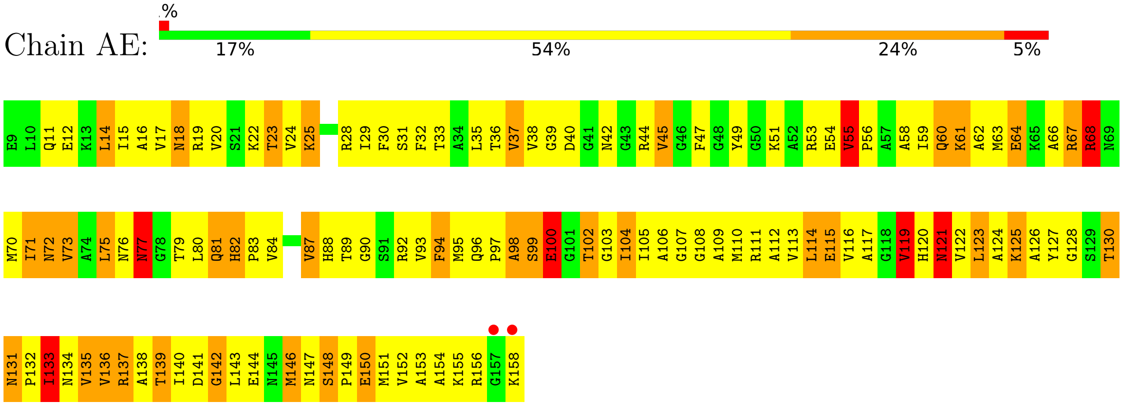
- Molecule 4: 30S ribosomal protein S4



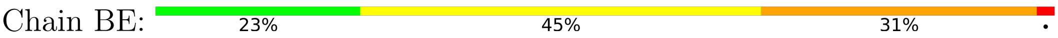
- Molecule 4: 30S ribosomal protein S4

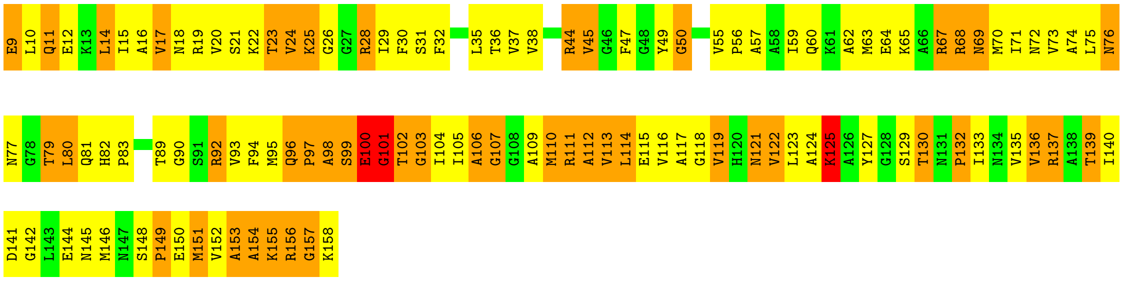


- Molecule 5: 30S ribosomal protein S5

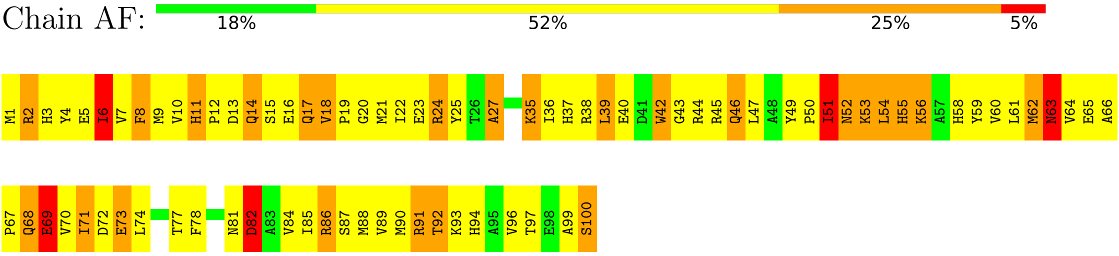


- Molecule 5: 30S ribosomal protein S5

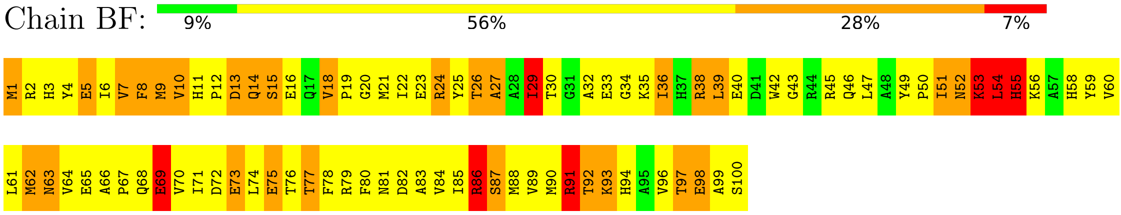




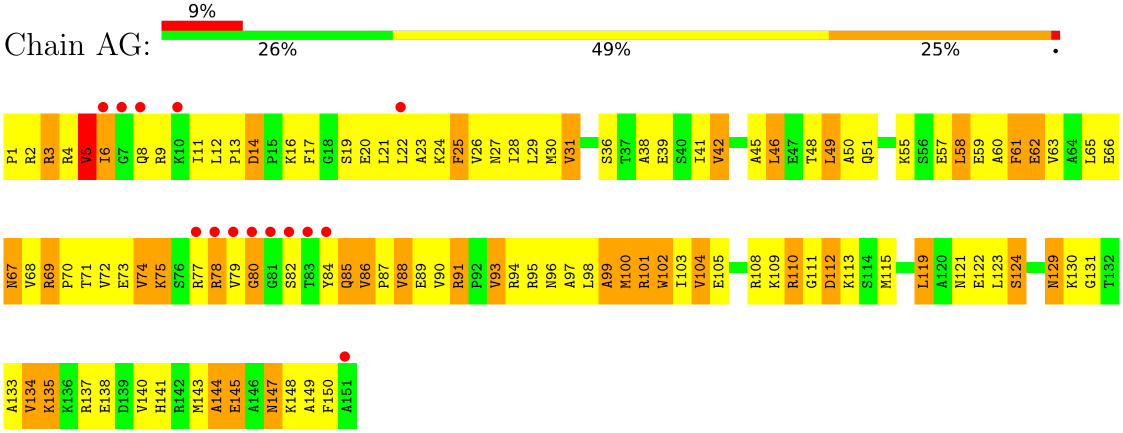
- Molecule 6: 30S ribosomal protein S6



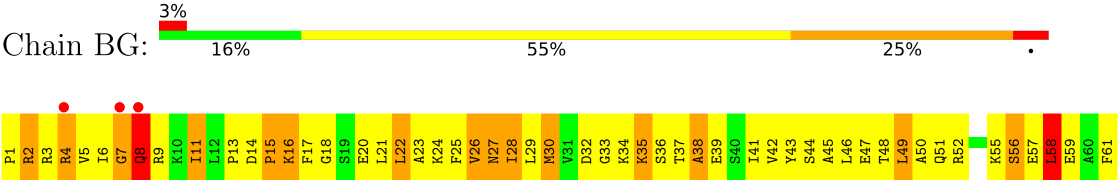
- Molecule 6: 30S ribosomal protein S6

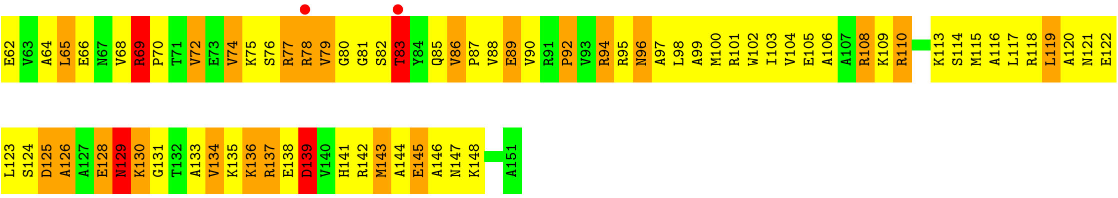


- Molecule 7: 30S ribosomal protein S7



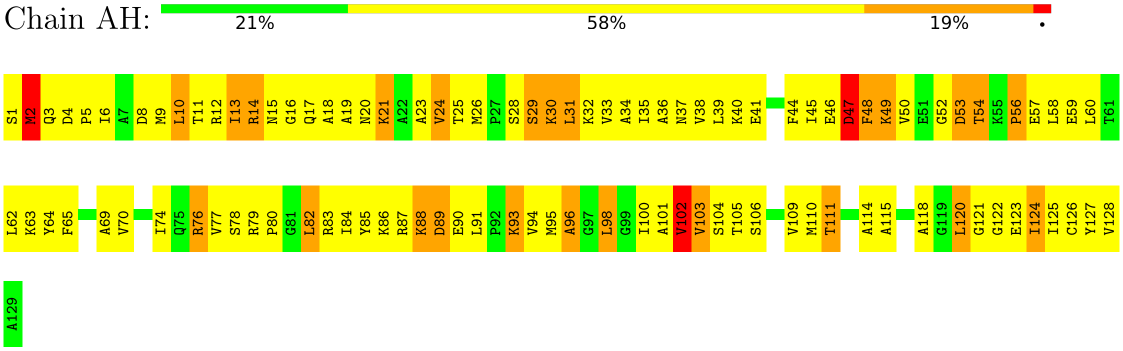
- Molecule 7: 30S ribosomal protein S7





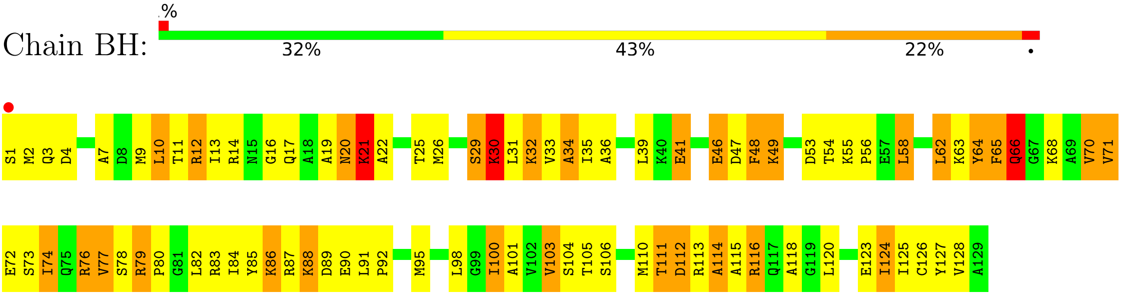
- Molecule 8: 30S ribosomal protein S8

Chain AH:



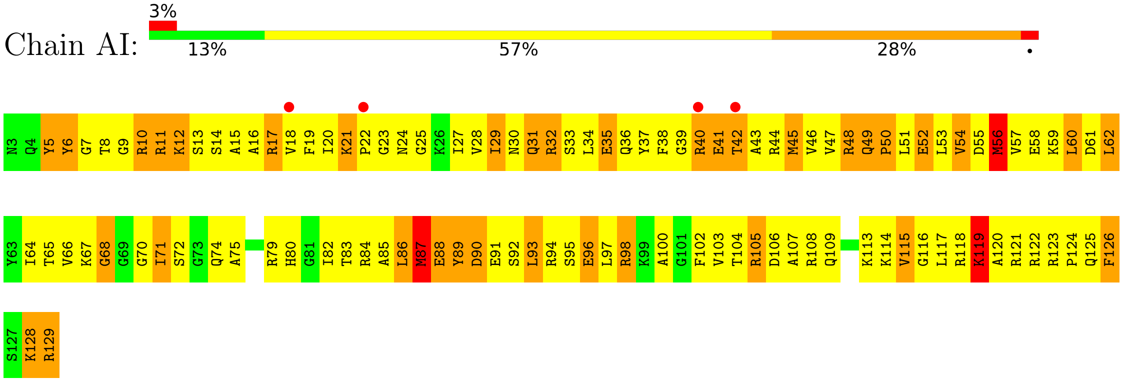
- Molecule 8: 30S ribosomal protein S8

Chain BH:



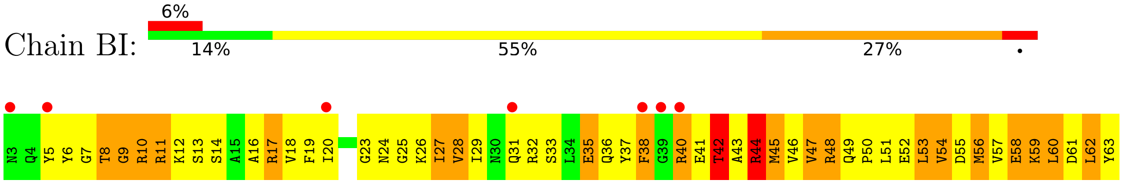
- Molecule 9: 30S ribosomal protein S9

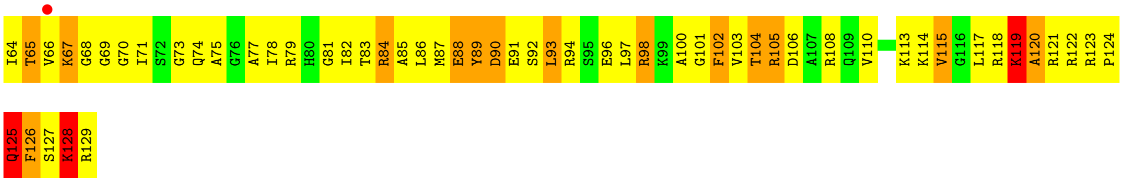
Chain AI:



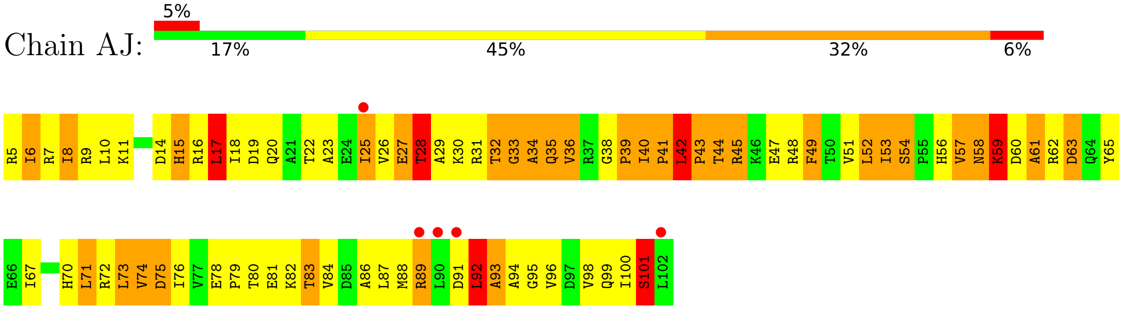
- Molecule 9: 30S ribosomal protein S9

Chain BI:

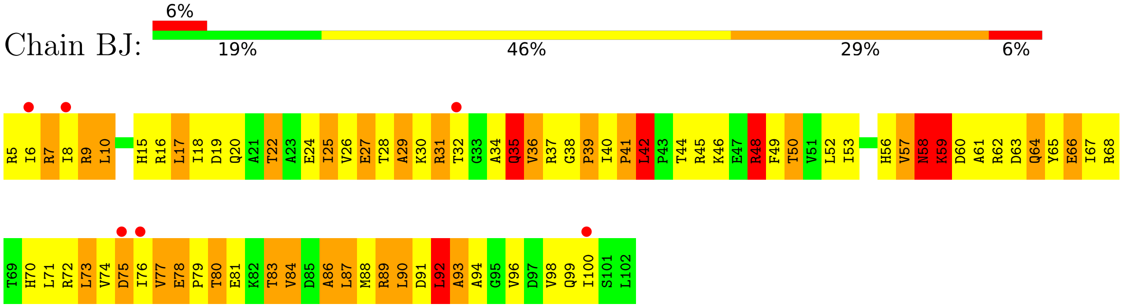




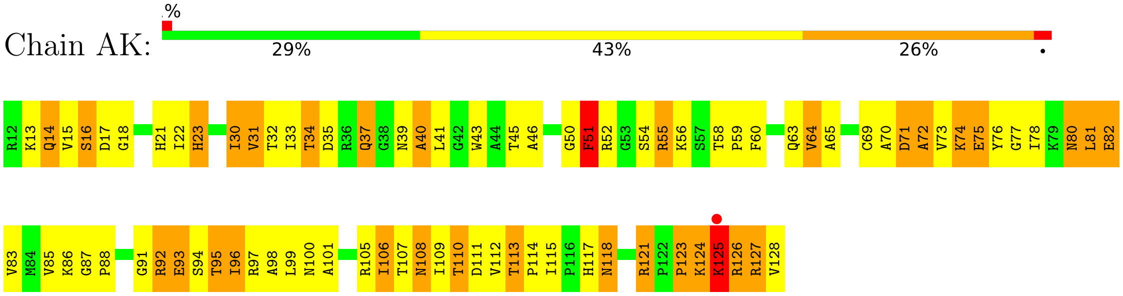
- Molecule 10: 30S ribosomal protein S10



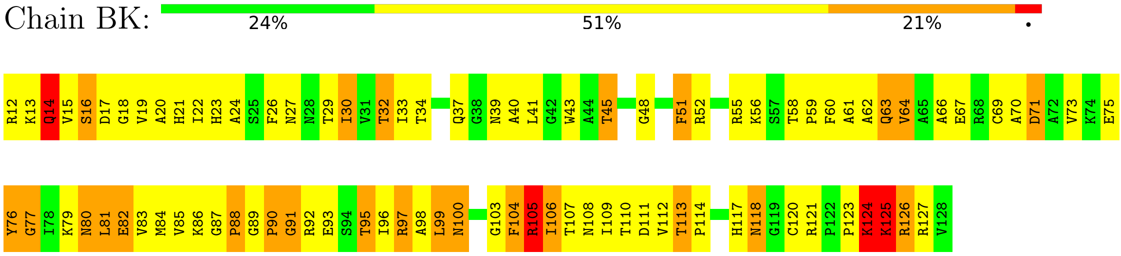
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11

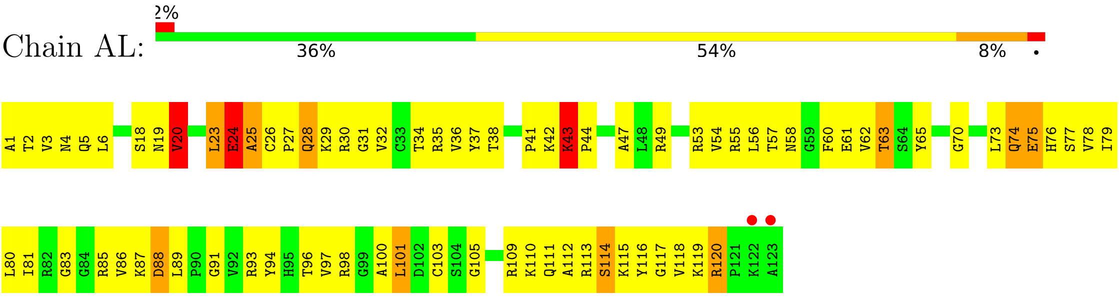


- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

Chain AL:



- Molecule 12: 30S ribosomal protein S12

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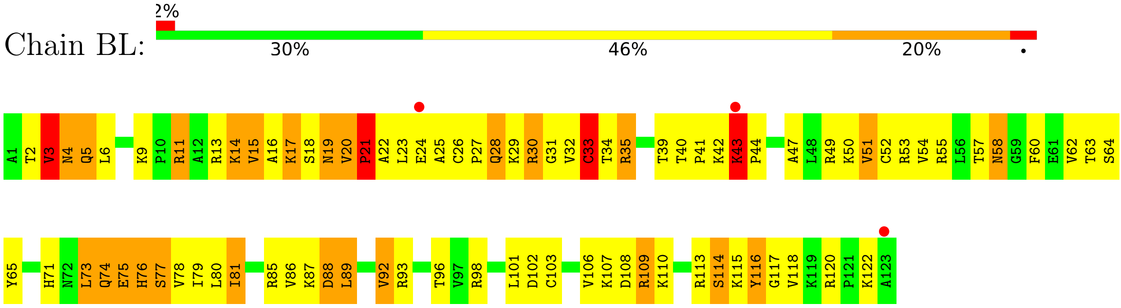
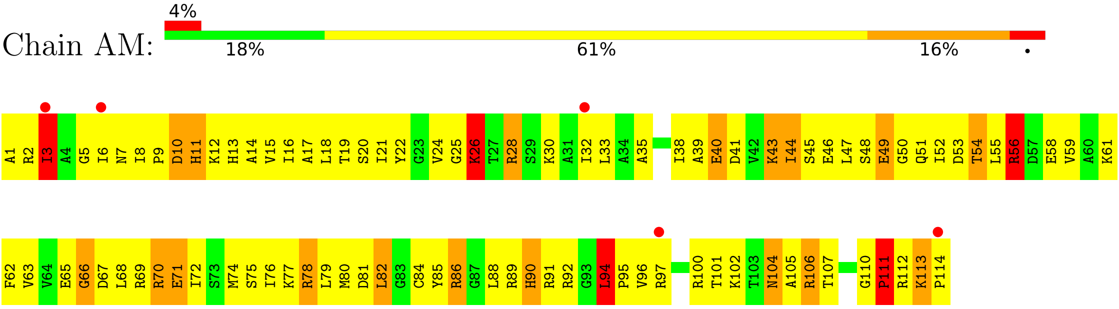


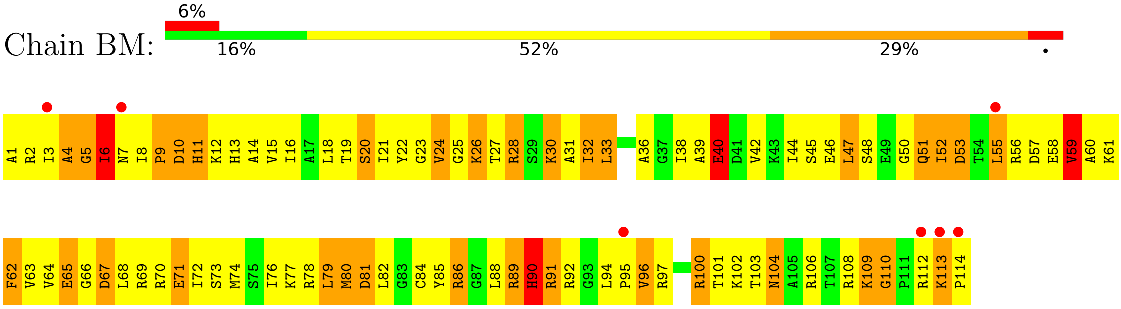
- Molecule 13: 30S ribosomal protein S13

Chain AM:



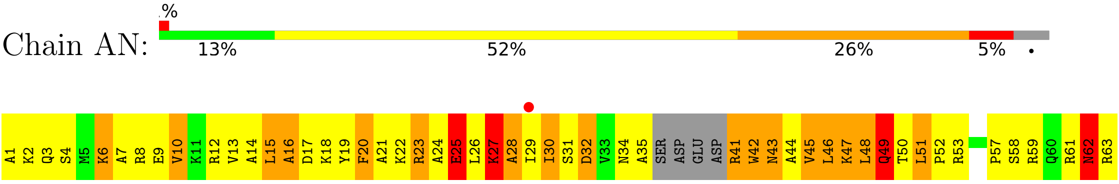
- Molecule 13: 30S ribosomal protein S13

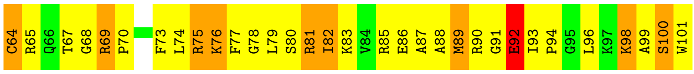
Chain BM:



- Molecule 14: 30S ribosomal protein S14

Chain AN:





- Molecule 14: 30S ribosomal protein S14

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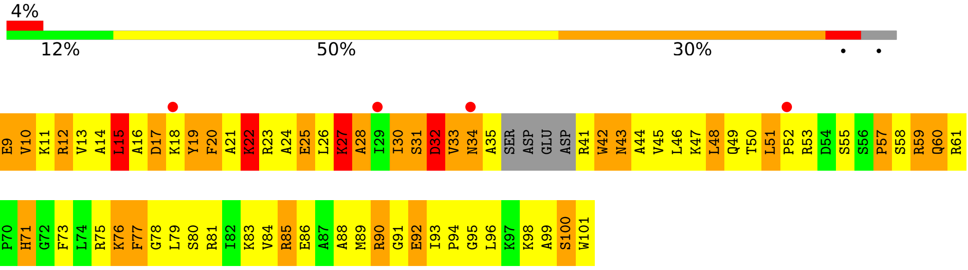

- Molecule 15: 30S ribosomal protein S15

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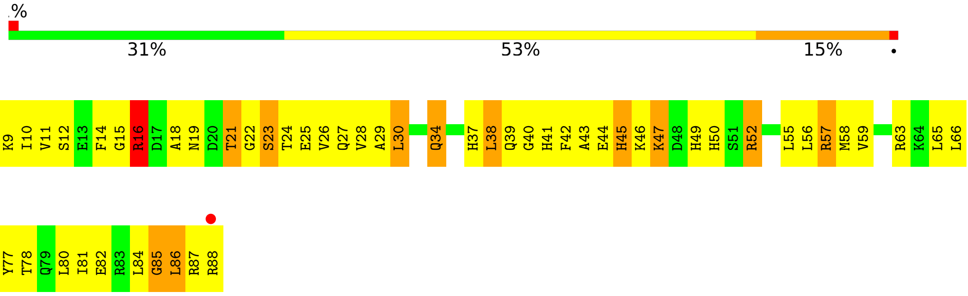

- Molecule 15: 30S ribosomal protein S15

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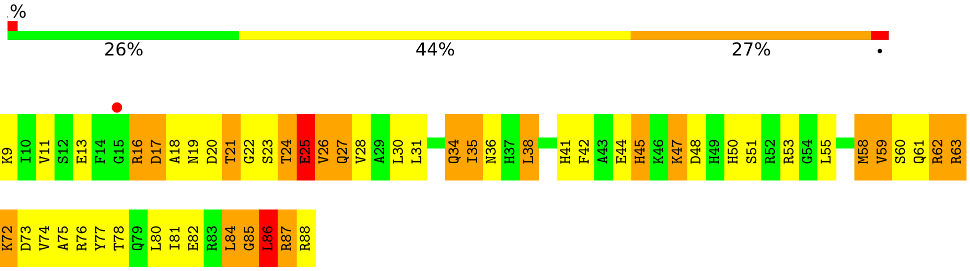
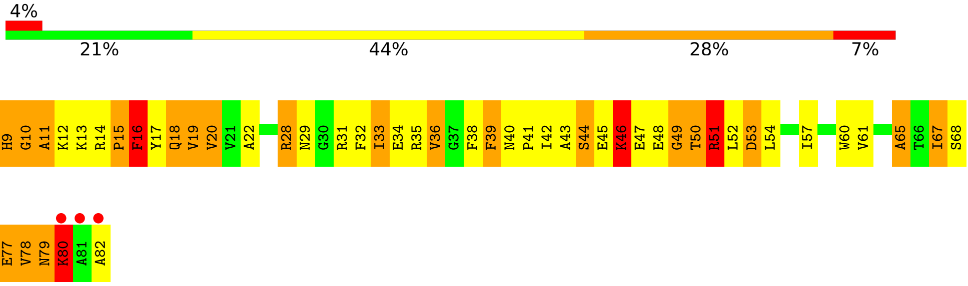


- Molecule 16: 30S ribosomal protein S16

Chain AP:



- Molecule 16: 30S ribosomal protein S16

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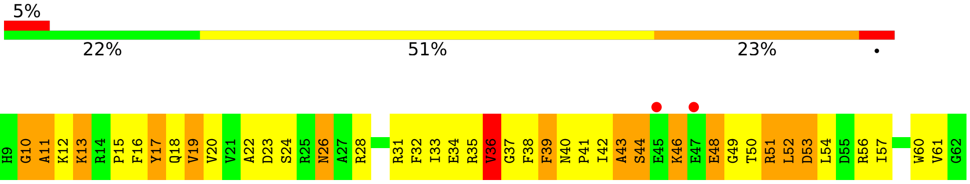
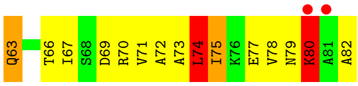
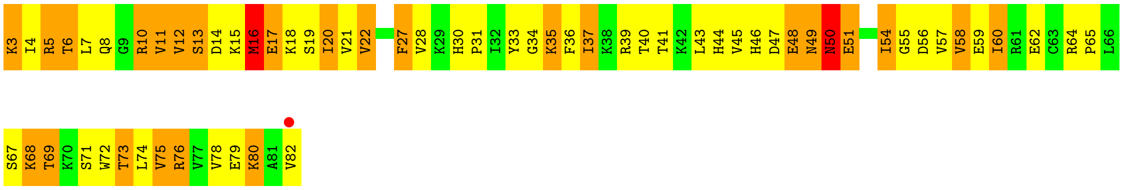




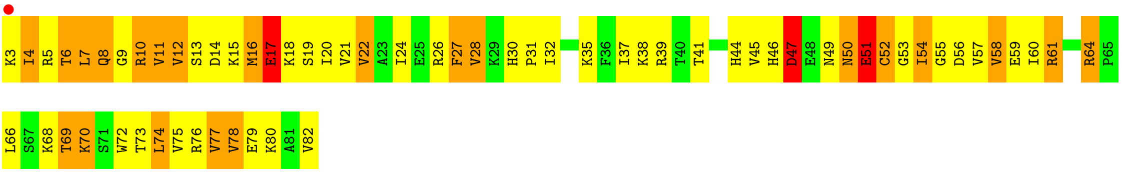
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

Chain BQ:



- Molecule 18: 30S ribosomal protein S18

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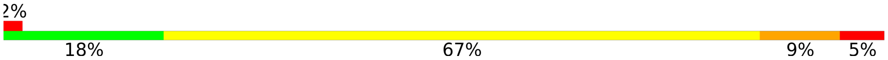
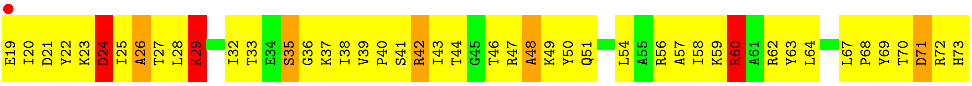
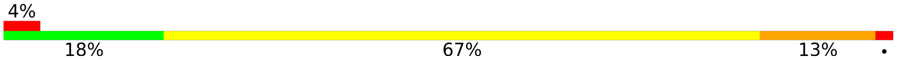
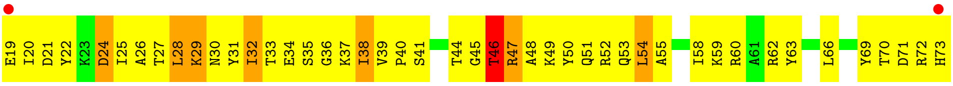




- Molecule 18: 30S ribosomal protein S18

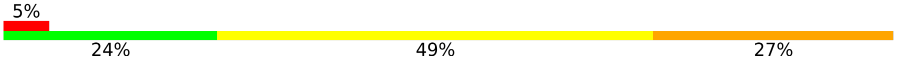
Chain BR:

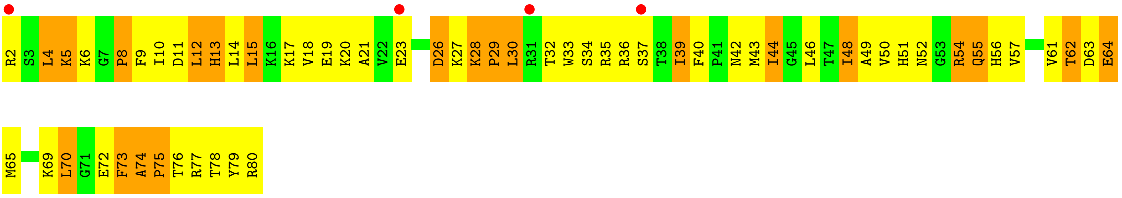




- Molecule 19: 30S ribosomal protein S19

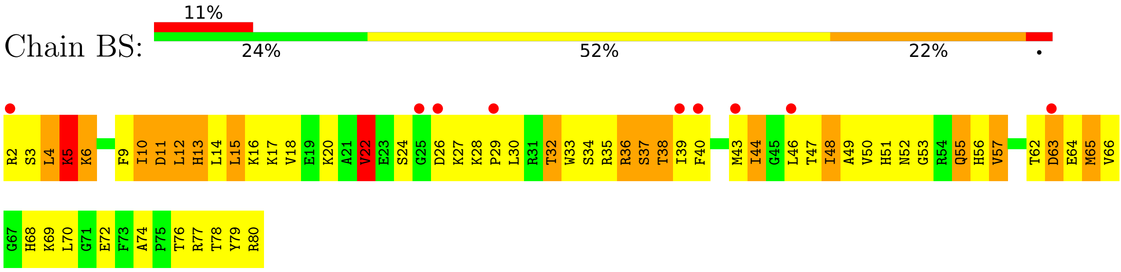
Chain AS:





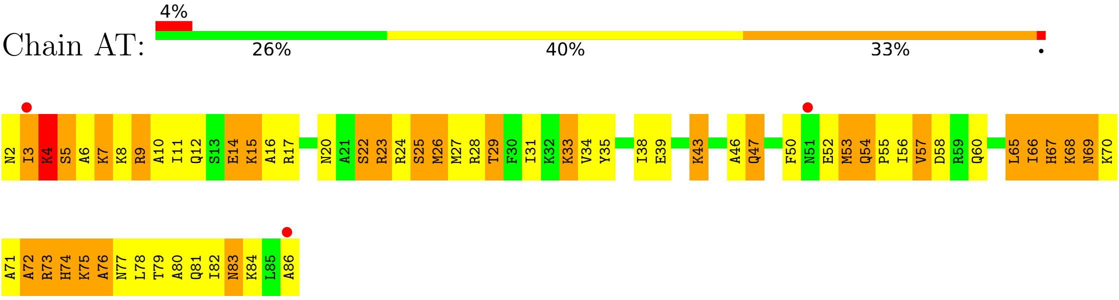
- Molecule 19: 30S ribosomal protein S19

Chain BS:



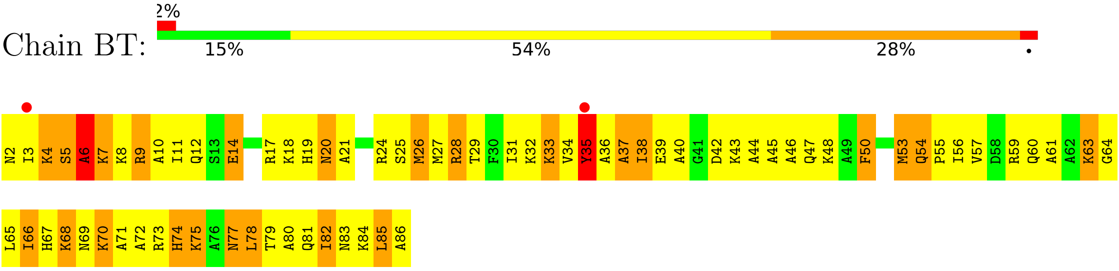
- Molecule 20: 30S ribosomal protein S20

Chain AT:



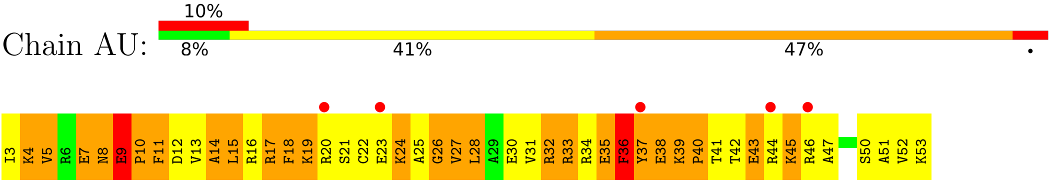
- Molecule 20: 30S ribosomal protein S20

Chain BT:



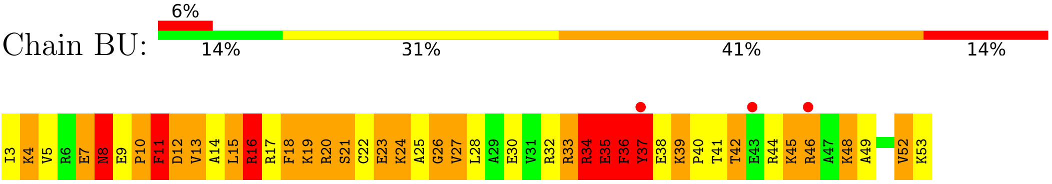
- Molecule 21: 30S ribosomal protein S21

Chain AU:



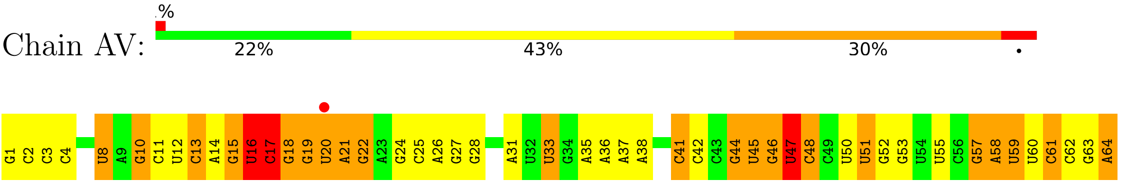
- Molecule 21: 30S ribosomal protein S21

Chain BU:



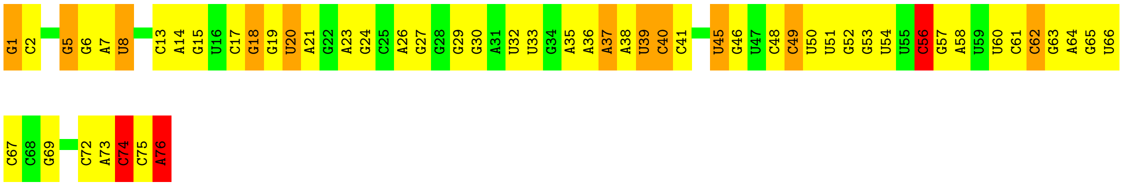
- Molecule 22: phenylalanine specific transfer RNA

Chain AV:



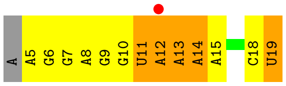
- Molecule 22: phenylalanine specific transfer RNA

Chain BV:



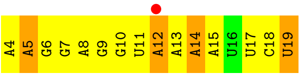
- Molecule 23: messenger RNA

Chain AX:



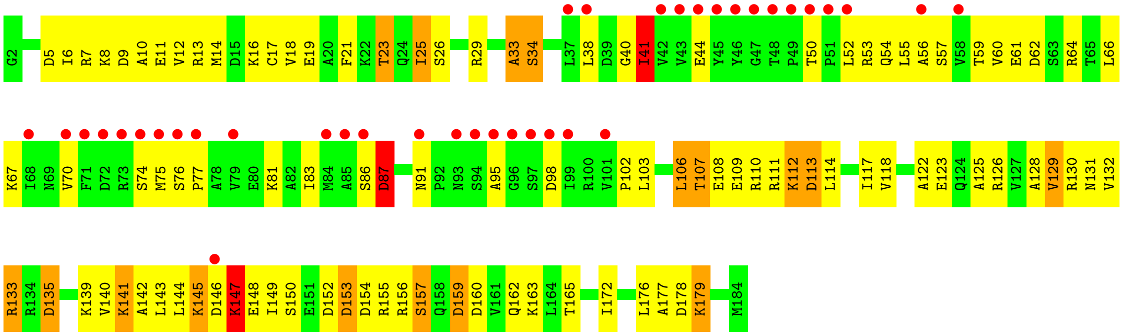
- Molecule 23: messenger RNA

Chain BX:



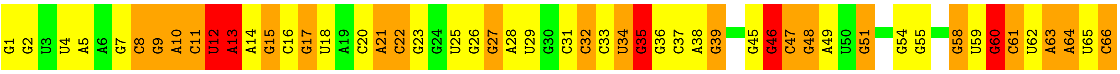
- Molecule 24: ribosome recycling factor

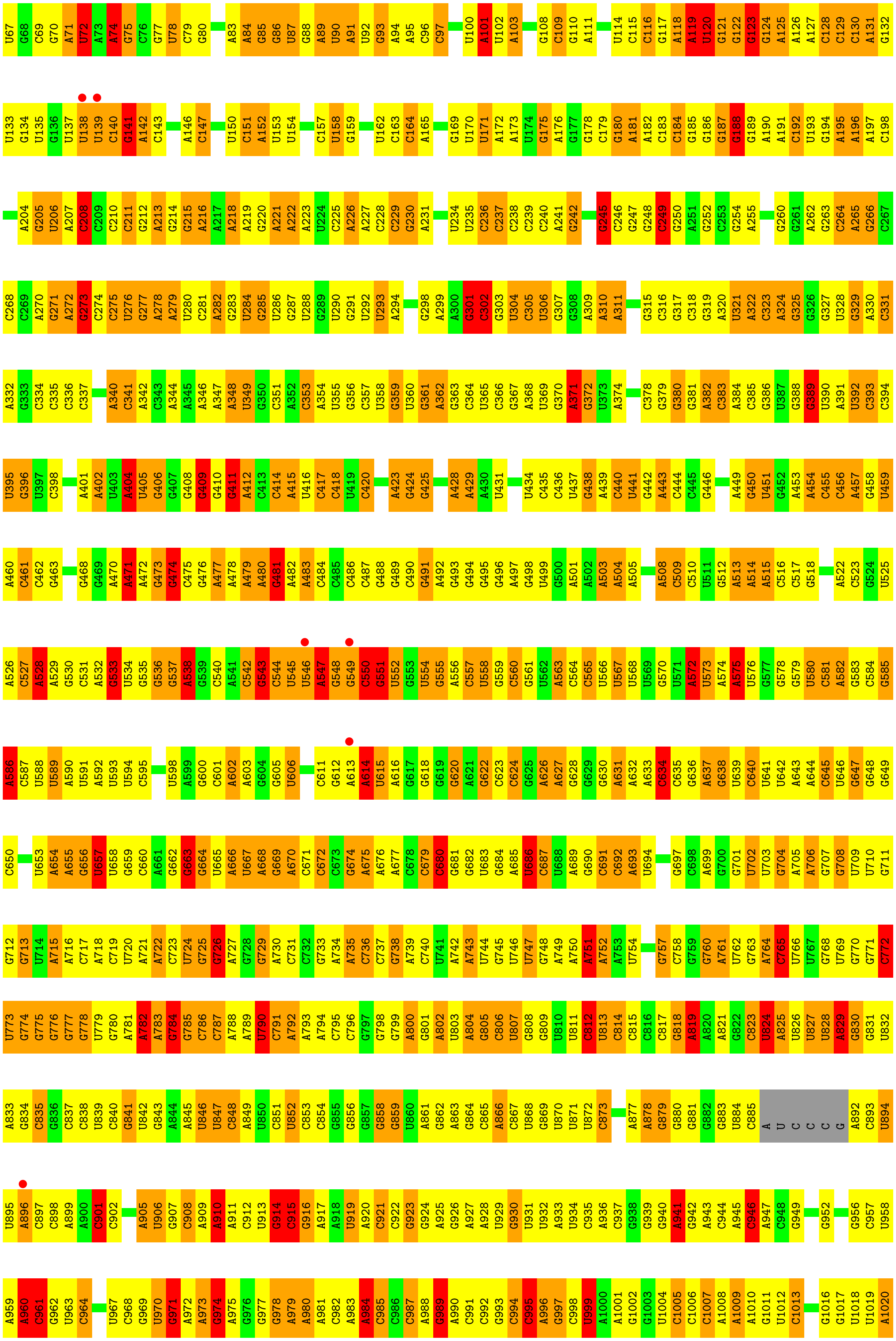
Chain AY:



- Molecule 25: 23S rRNA

Chain CA:

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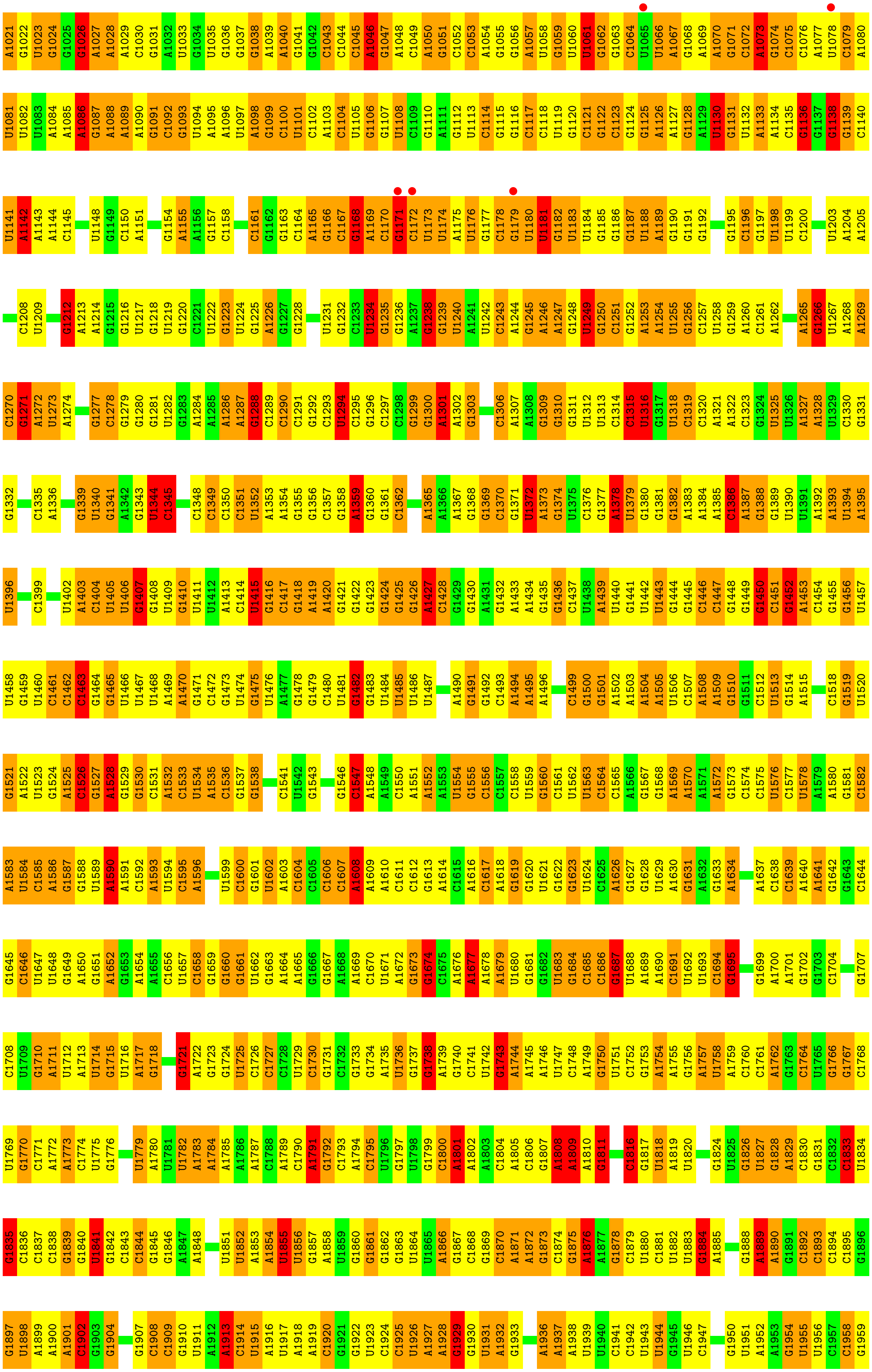
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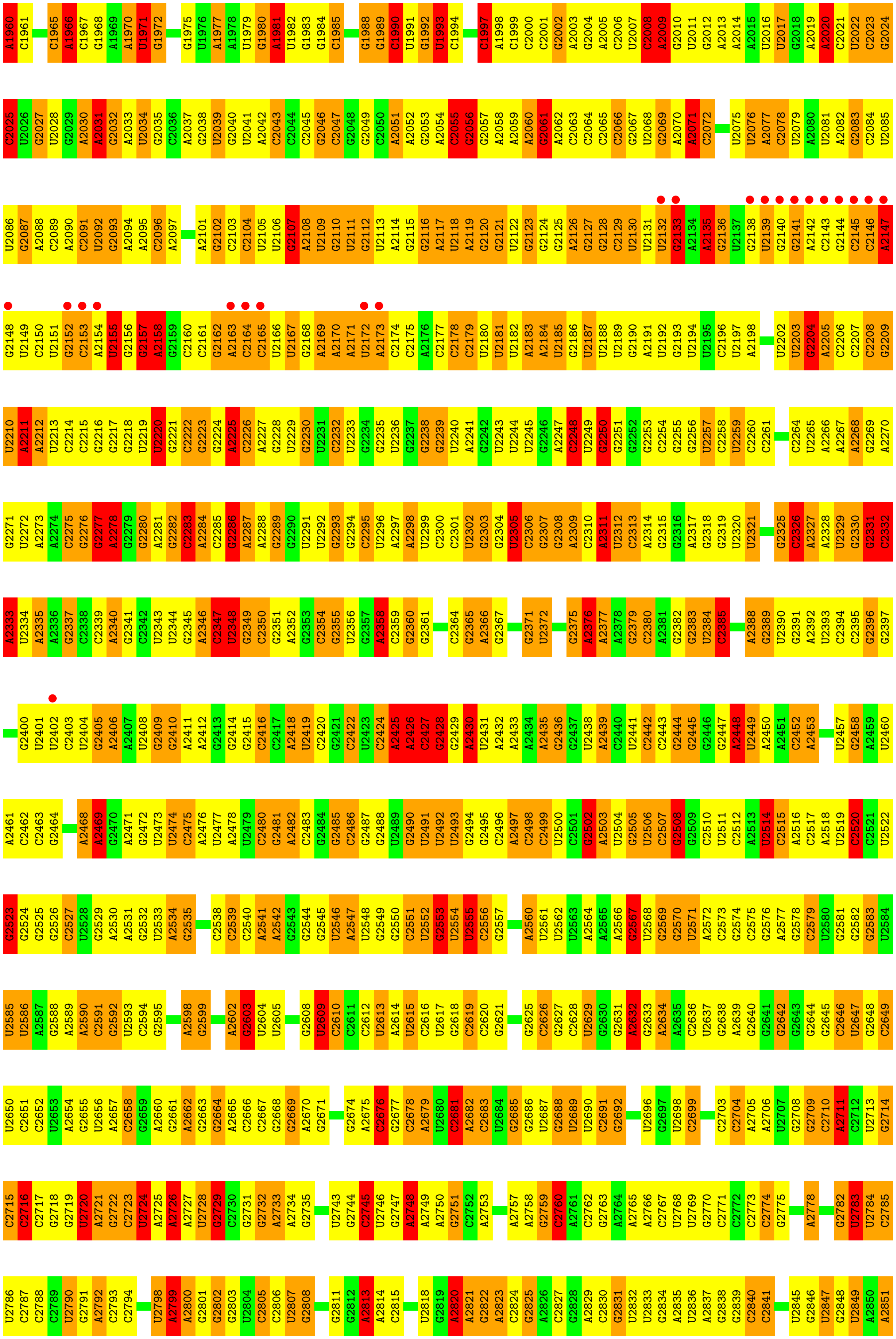

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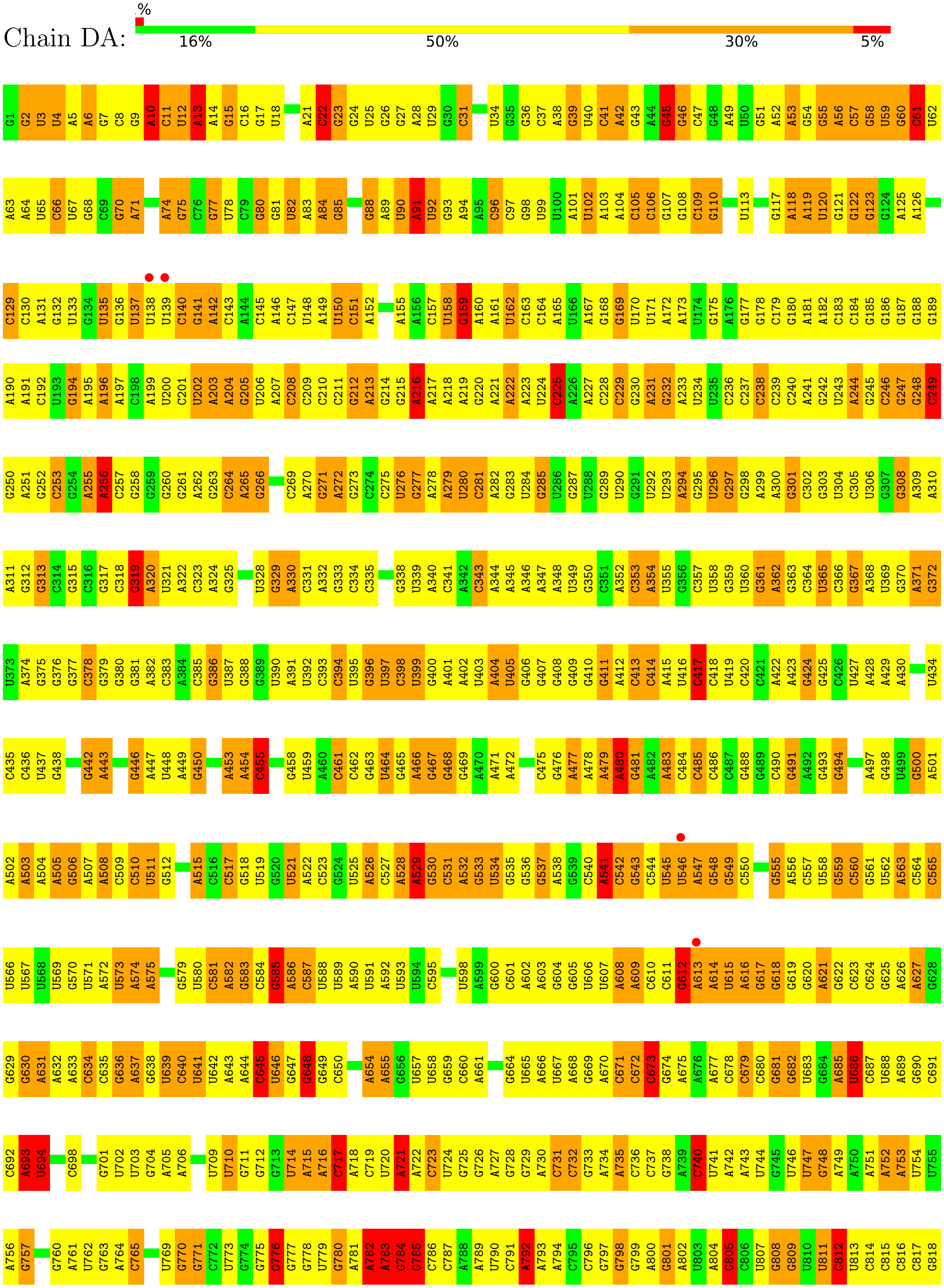

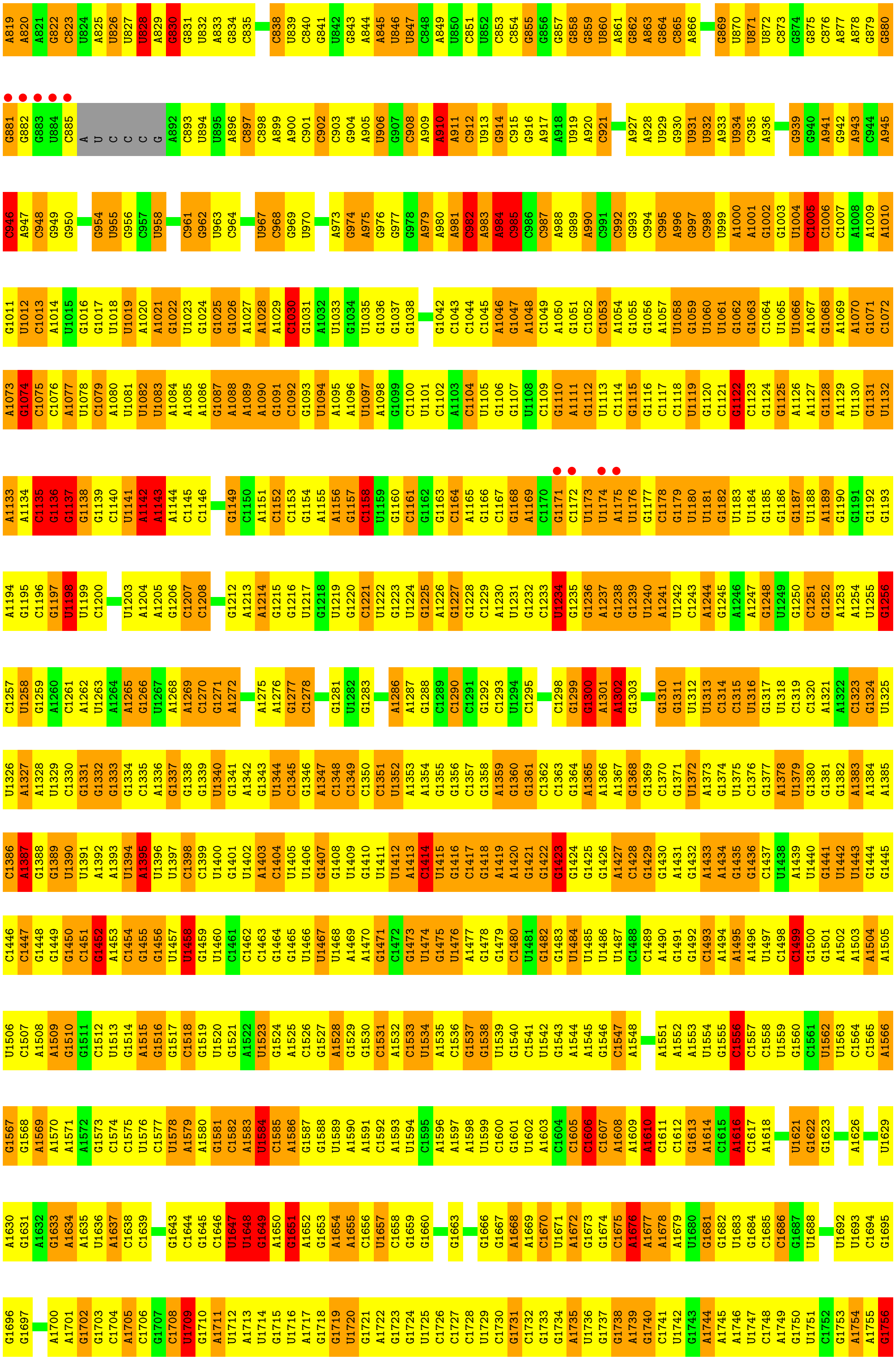
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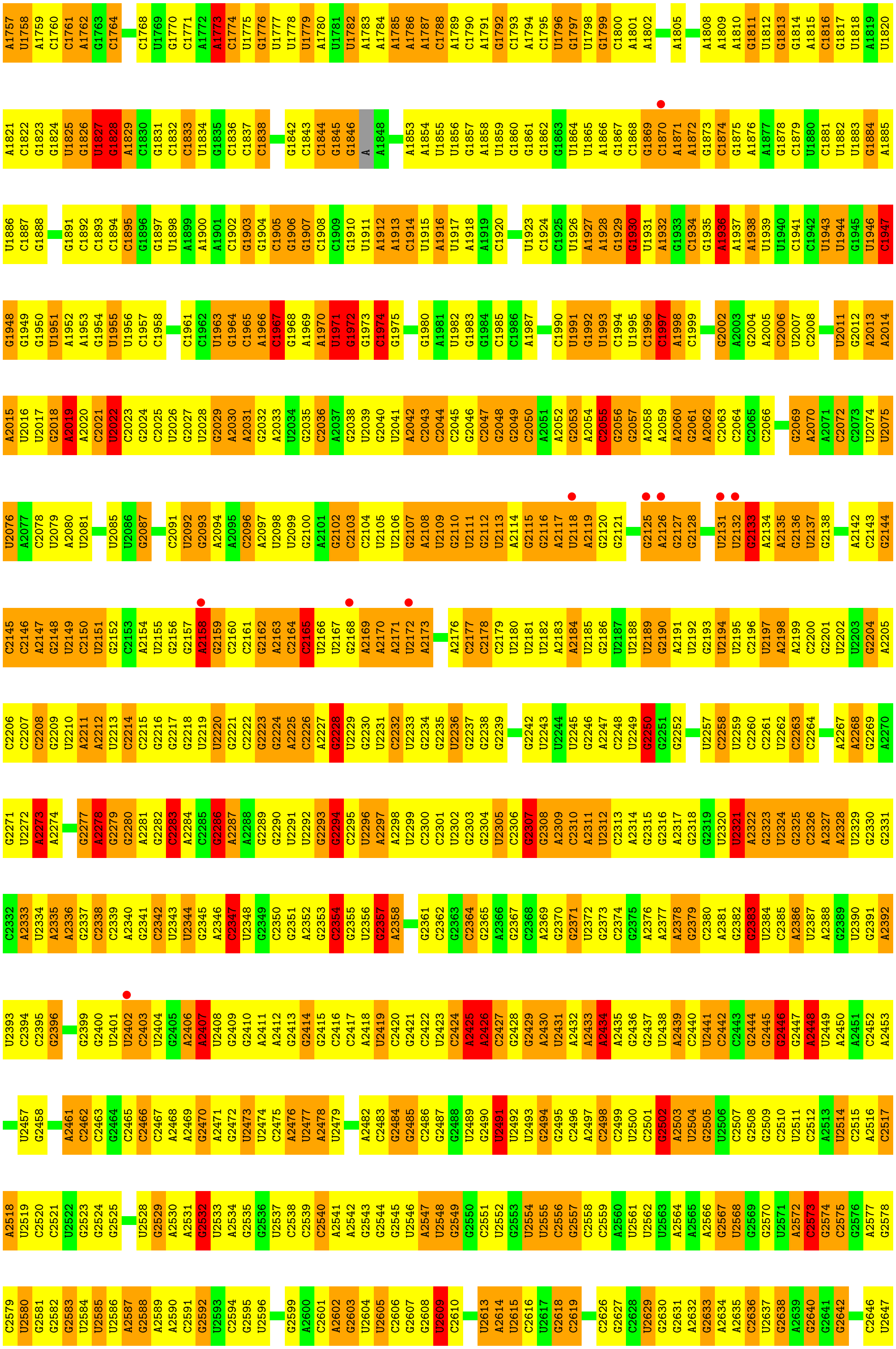
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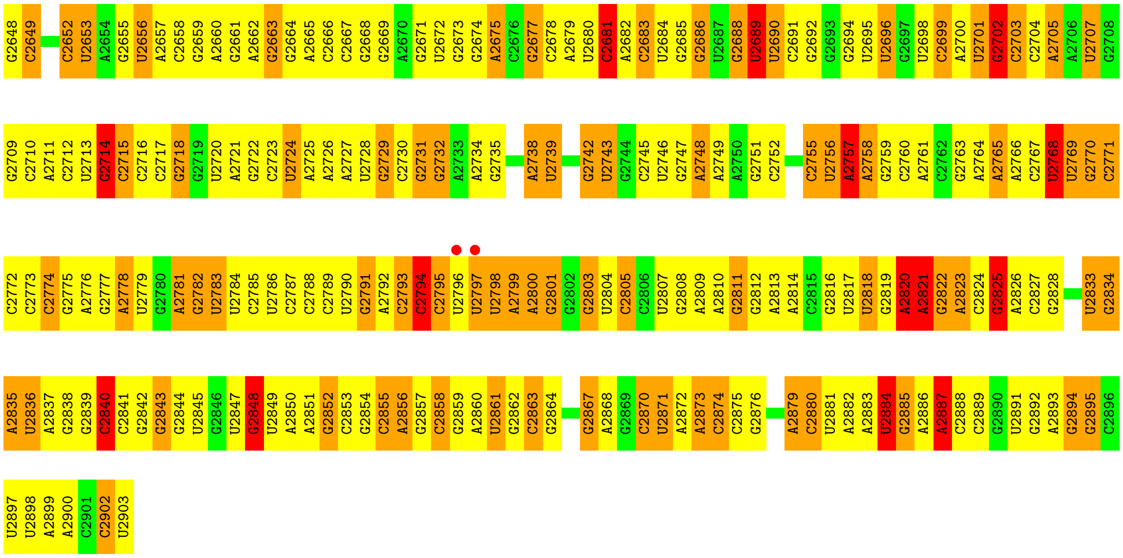
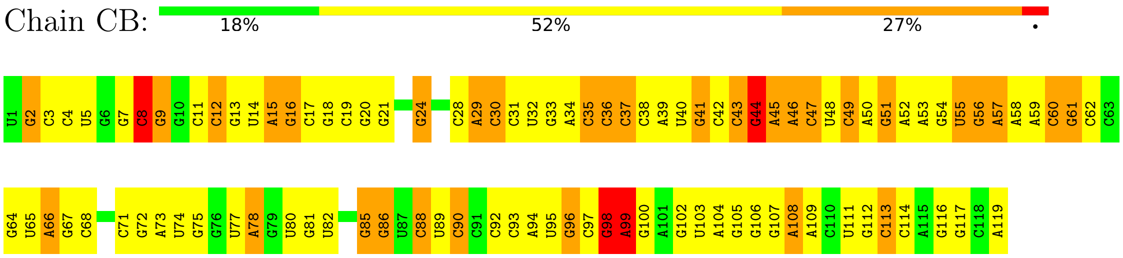
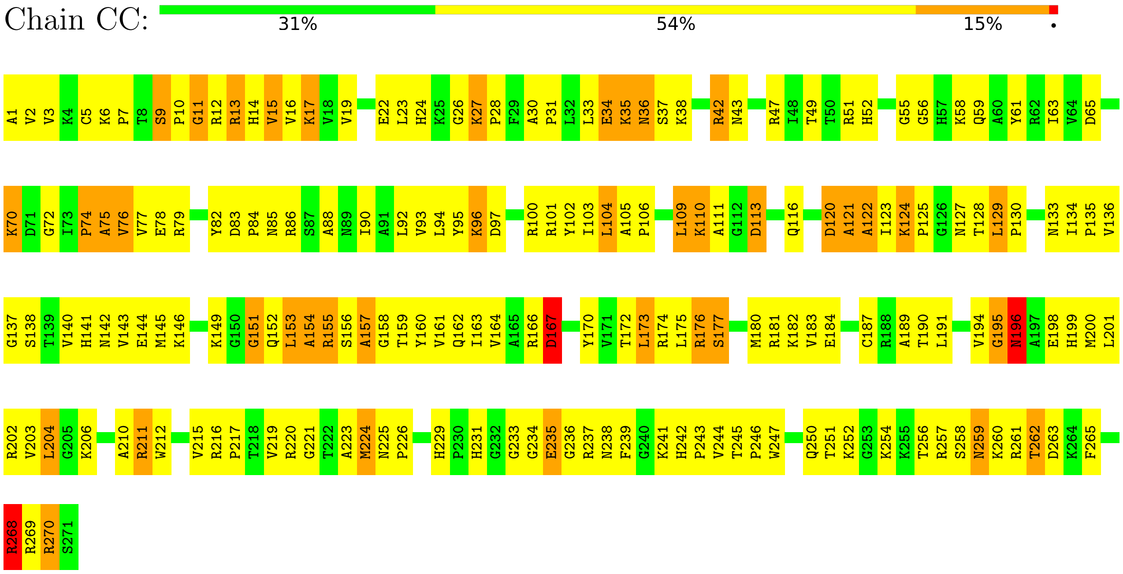


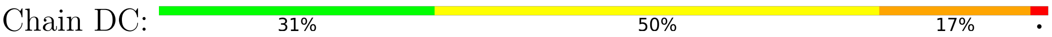
- Molecule 26: 5S rRNA

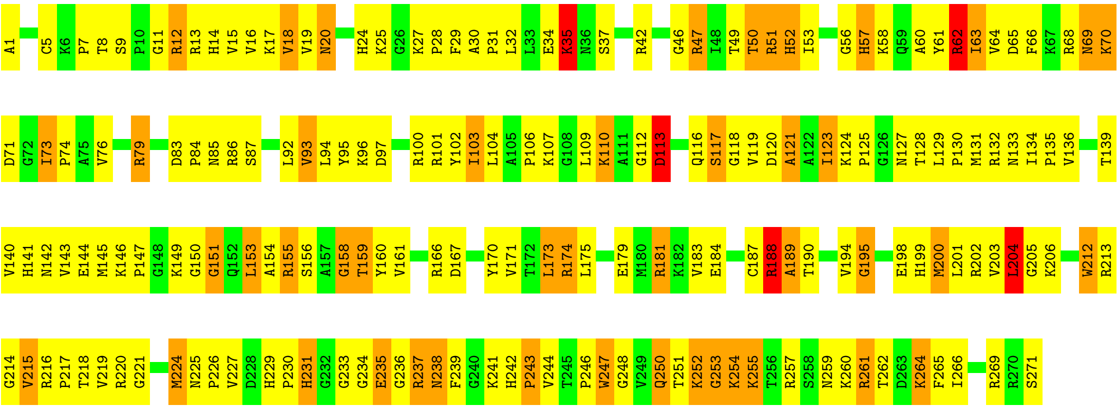


- Molecule 27: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L2





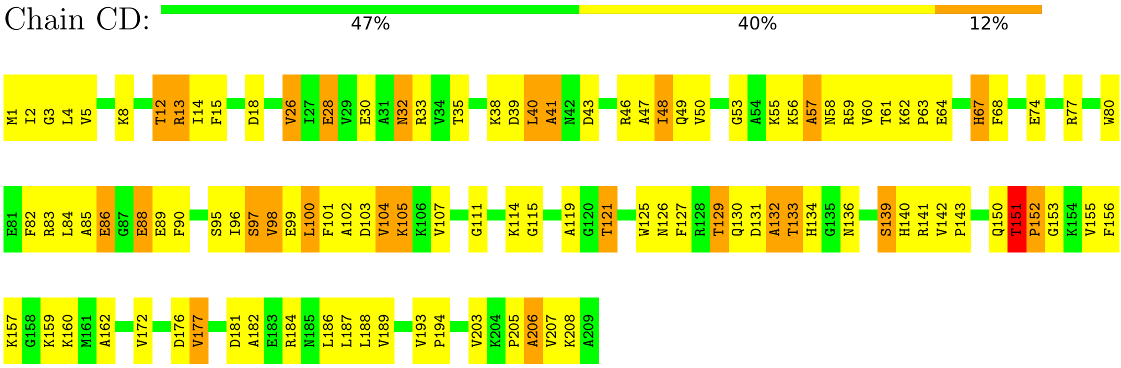
A1 C5 K6 P7 T8 S9 P10 G11 R12 R13 H14 V15 V16 K17 V18 V19 N20 H24 K25 G26 K27 P28 F29 A30 P31 L32 L33 E34 K35 N36 S37 R42 G46 R47 I48 T49 T50 R51 H52 I53 G56 H57 K58 Q59 A60 Y61 R62 I63 V64 D65 F66 K67 R68 N69 K70

D71 G72 I73 P74 A75 V76 R79 D83 P84 N85 R86 S87 L92 V93 L94 Y95 K96 D97 R100 R101 Y102 I103 L104 A105 P106 K107 G108 L109 K110 A111 G112 D113 Q116 S117 G118 V119 D120 A121 A122 I123 K124 P125 G126 N127 T128 L129 P130 M131 R132 N133 I134 P135 V136 T139

V140 H141 N142 V143 E144 M145 K146 P147 G148 K149 G150 G151 Q152 L153 A154 R155 S156 A157 G158 T159 Y160 V161 R166 D167 Y170 V171 T172 L173 R174 L175 E179 M180 R181 K182 V183 E184 C187 R188 A189 T190 V194 G195 E198 H199 M200 L201 R202 V203 L204 G205 K206 W212 R213

G214 V215 R216 P217 T218 V219 R220 G221 M224 N225 P226 V227 D228 H229 P230 H231 G232 G233 G234 E235 G236 R237 N238 F239 G240 K241 H242 P243 V244 T245 P246 W247 G248 V249 Q250 T251 K252 G253 K254 K255 T256 R257 S258 N259 K260 R261 T262 D263 K264 F265 I266 R269 R270 S271

- Molecule 28: 50S ribosomal protein L3



Chain CD:

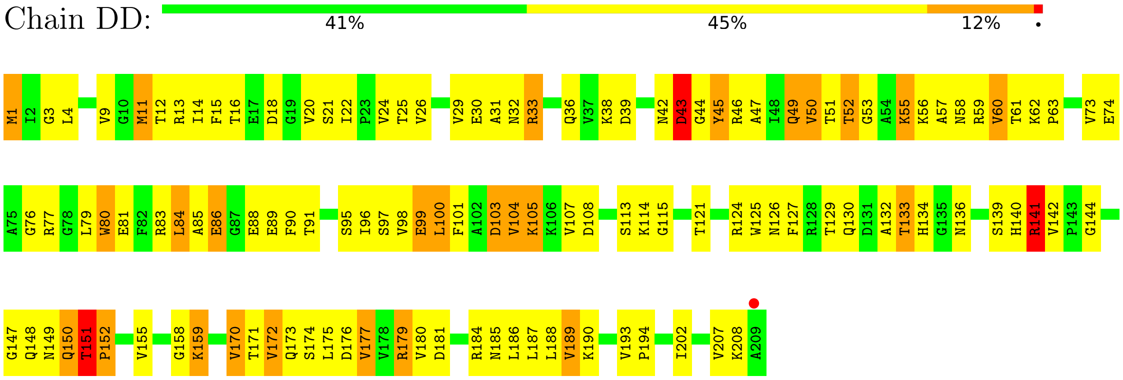
47% 40% 12%

M1 I2 G3 L4 V5 K8 T12 R13 I14 F15 D18 V26 I27 E28 V29 E30 A31 N32 R33 V34 T35 K38 D39 L40 A41 N42 D43 R46 A47 I48 Q49 V50 G53 A54 K55 K56 A57 N58 R59 V60 T61 K62 P63 E64 H67 F68 E74 R77 W80

E81 F82 R83 L84 A85 E86 G87 E88 E89 F90 S95 I96 S97 V98 E99 L100 F101 A102 D103 V104 K105 K106 V107 G111 K114 G115 A119 G120 T121 W125 N126 F127 R128 T129 Q130 D131 A132 T133 H134 G135 N136 S139 H140 R141 V142 P143 Q150 T151 P152 G153 K154 V155 F156

K157 G158 K159 K160 M161 A162 V172 D176 V177 D181 A182 E183 R184 N185 L186 L187 L188 V189 V193 P194 V203 K204 P205 A206 V207 K208 A209

- Molecule 28: 50S ribosomal protein L3



Chain DD:

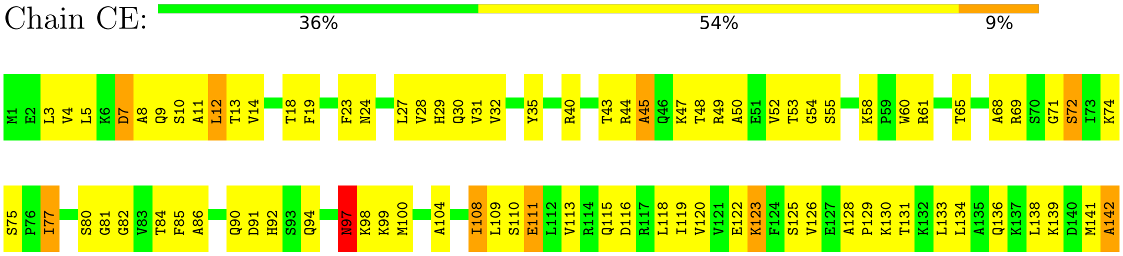
41% 45% 12% •

M1 I2 G3 L4 V9 G10 M11 T12 R13 I14 F15 T16 E17 D18 G19 V20 S21 I22 P23 V24 T25 V26 V29 E30 A31 N32 R33 Q36 V37 K38 D39 N42 D43 G44 Y45 R46 A47 I48 Q49 V50 T51 T52 G53 A54 K55 K56 A57 N58 R59 V60 T61 K62 P63 V73 E74

A75 G76 R77 G78 L79 W80 E81 F82 R83 L84 A85 E86 G87 E88 E89 F90 T91 S95 I96 S97 V98 E99 L100 F101 A102 D103 V104 K105 K106 V107 D108 S113 K114 G115 T121 R124 W125 N126 F127 R128 T129 Q130 D131 A132 T133 H134 G135 N136 S139 H140 R141 V142 P143 G144

G147 Q148 N149 Q150 T151 P152 V155 G158 K159 V170 T171 V172 Q173 S174 L175 D176 V177 V178 R179 V180 D181 R184 N185 L186 L187 L188 V189 K190 V193 P194 I202 V207 K208 A209

- Molecule 29: 50S ribosomal protein L4



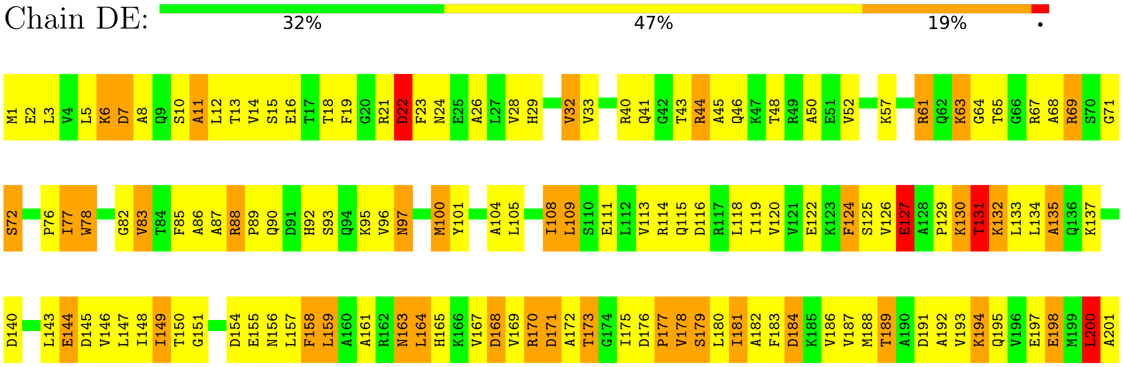
Chain CE:

36% 54% 9%

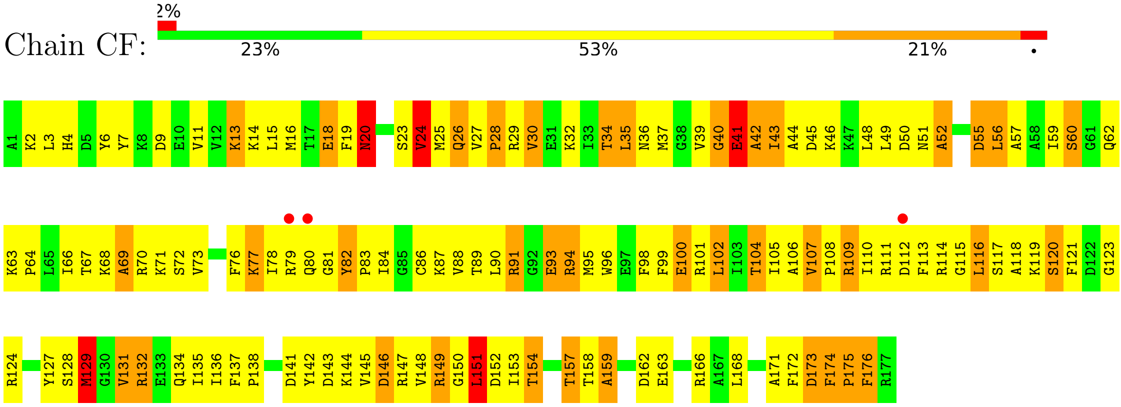
M1 E2 L3 V4 L5 K6 D7 A8 Q9 S10 A11 L12 T13 V14 T18 F19 F23 N24 L27 V28 H29 Q30 V31 V32 Y35 R40 T43 R44 A45 Q46 K47 T48 R49 A50 E51 V52 T53 G54 S55 K58 P59 W60 R61 T65 A68 R69 S70 G71 S72 I73 K74

S75 P76 I77 S80 G81 G82 V83 T84 F85 A86 Q90 D91 H92 S93 Q94 N97 K98 K99 M100 A104 I108 L109 S110 E111 L112 V113 R114 Q115 D116 R117 L118 I119 V120 V121 E122 K123 F124 S125 V126 E127 A128 P129 K130 T131 K132 L133 L134 A135 Q136 K137 L138 K139 D140 M141 A142

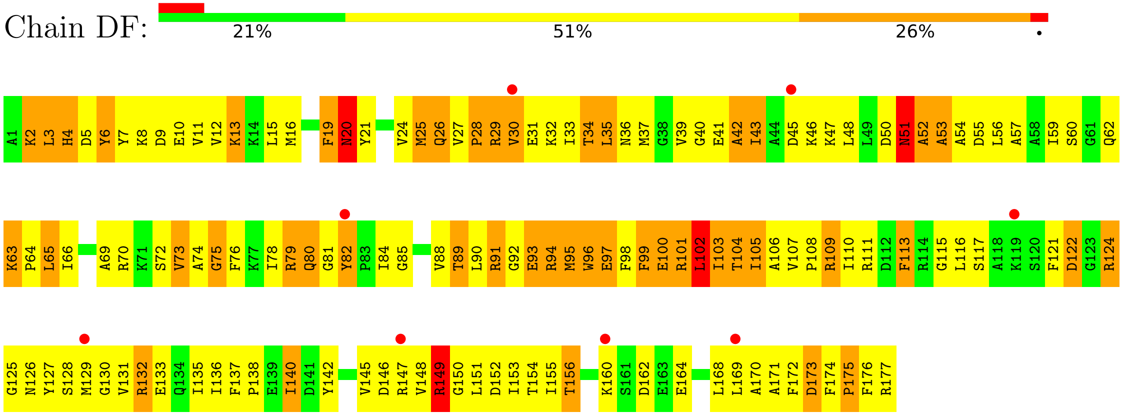
- Molecule 29: 50S ribosomal protein L4



- Molecule 30: 50S ribosomal protein L5

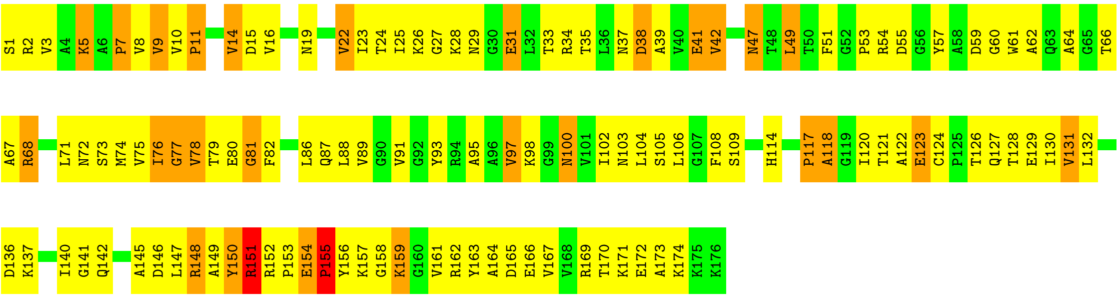


- Molecule 30: 50S ribosomal protein L5

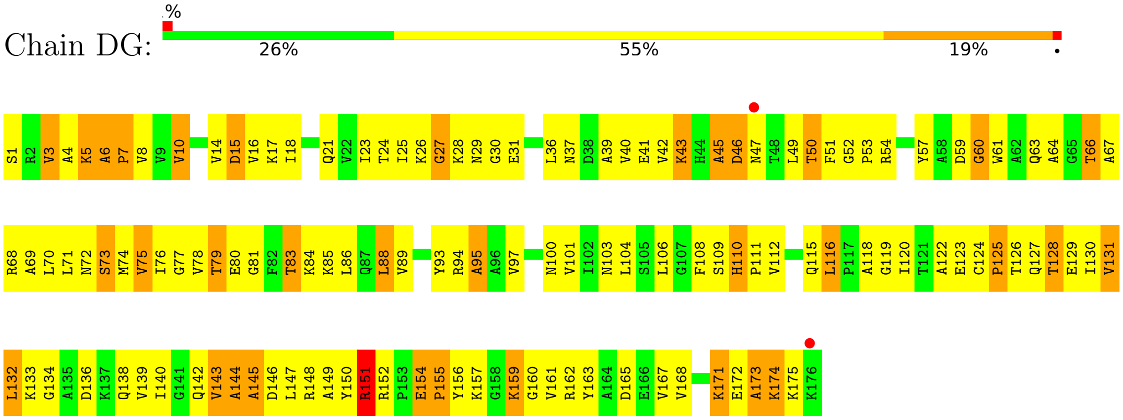


- Molecule 31: 50S ribosomal protein L6

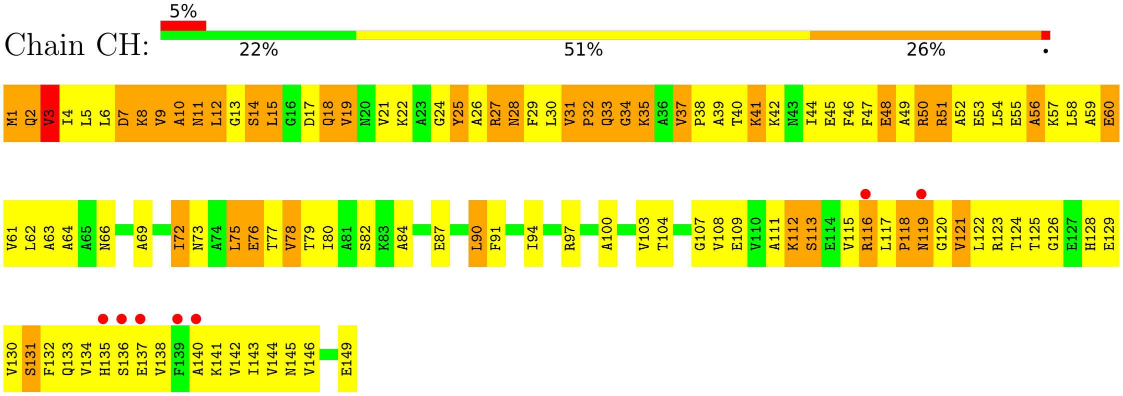
Chain CG:



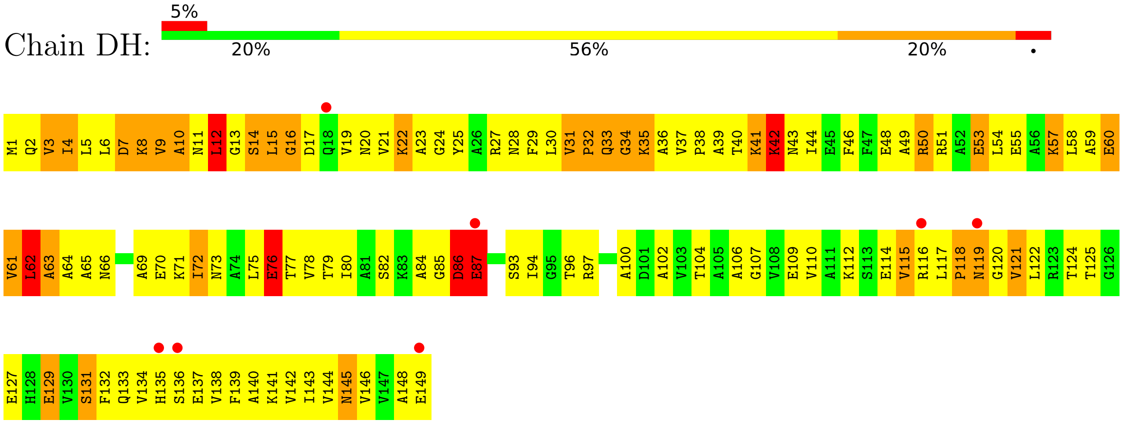
- Molecule 31: 50S ribosomal protein L6



- Molecule 32: 50S ribosomal protein L9

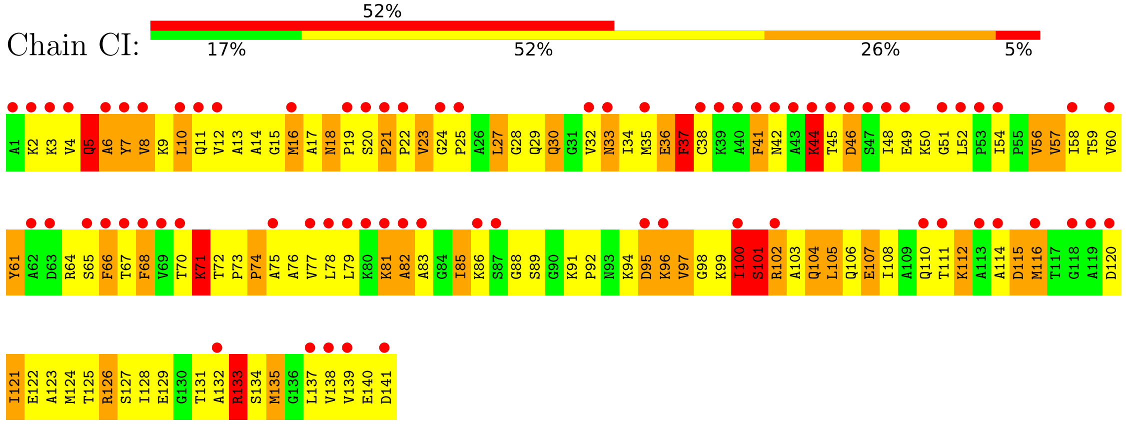


- Molecule 32: 50S ribosomal protein L9



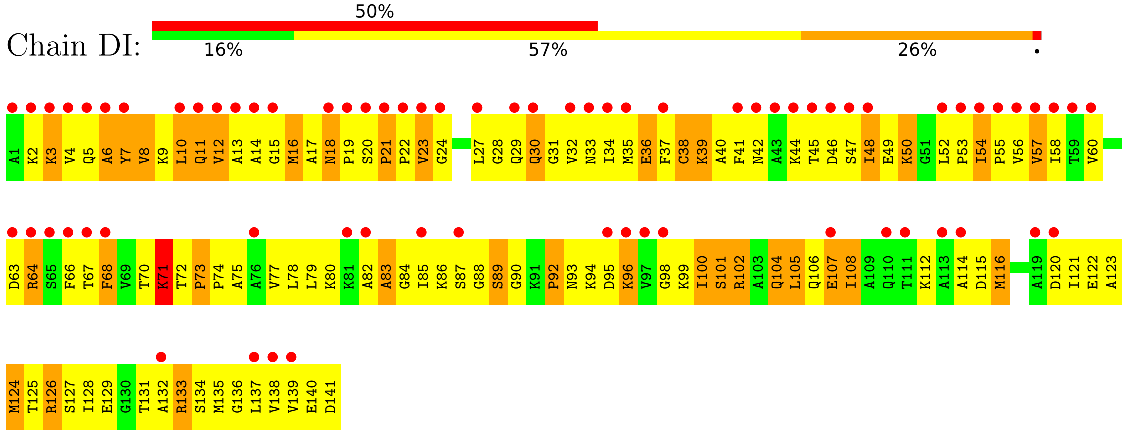
- Molecule 33: 50S ribosomal protein L11

Chain CI:



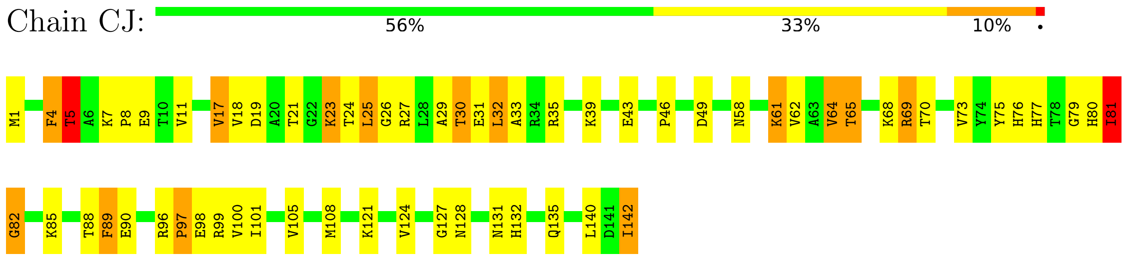
- Molecule 33: 50S ribosomal protein L11

Chain DI:



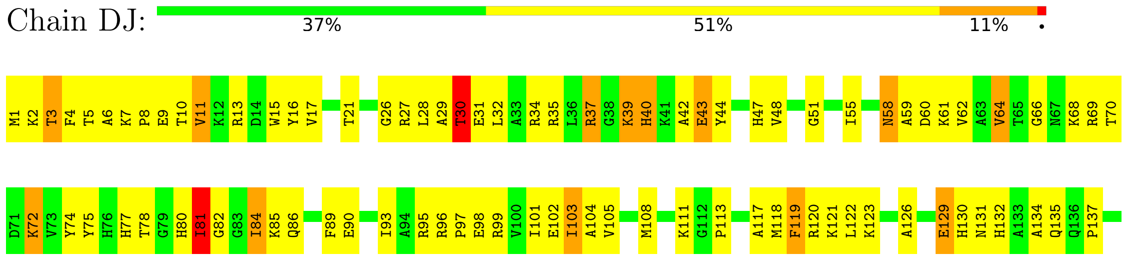
- Molecule 34: 50S ribosomal protein L13

Chain CJ:



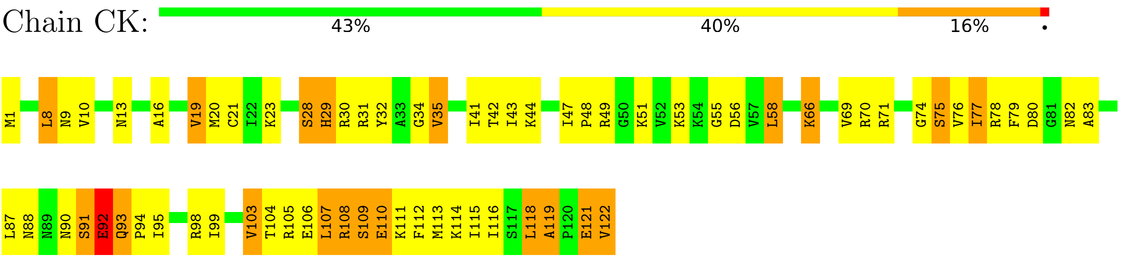
- Molecule 34: 50S ribosomal protein L13

Chain DJ:



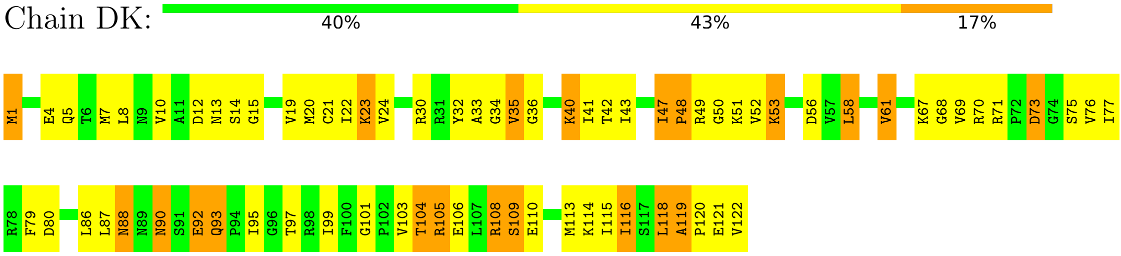
- Molecule 35: 50S ribosomal protein L14

Chain CK:



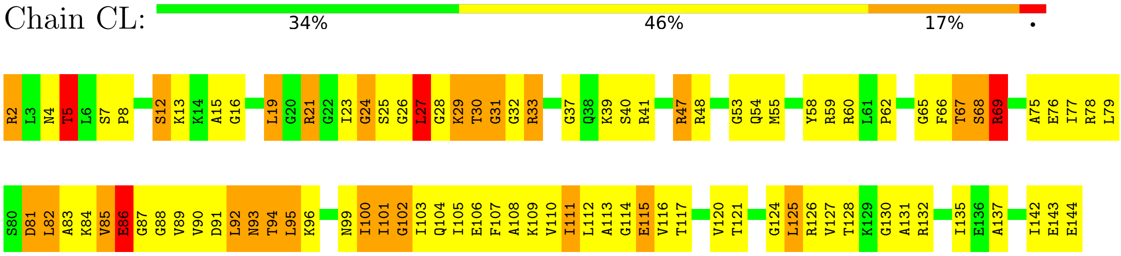
- Molecule 35: 50S ribosomal protein L14

Chain DK:



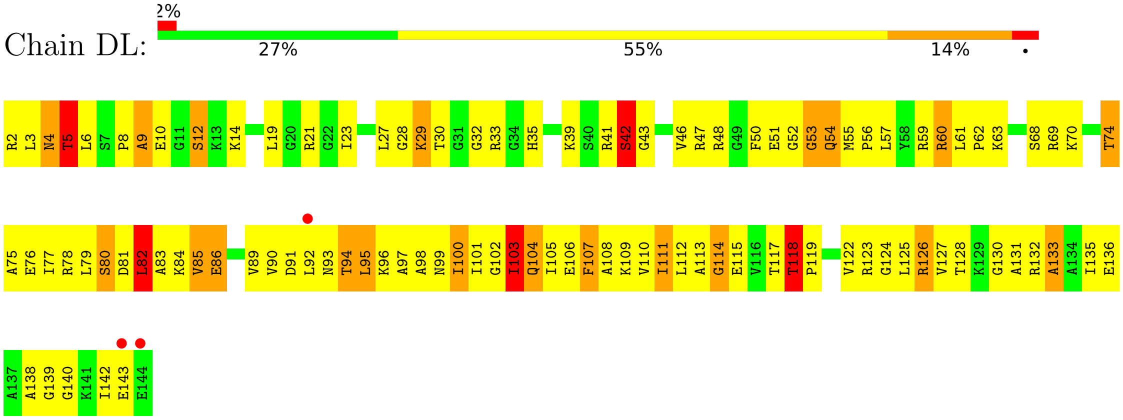
- Molecule 36: 50S ribosomal protein L15

Chain CL:



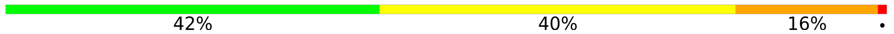
- Molecule 36: 50S ribosomal protein L15

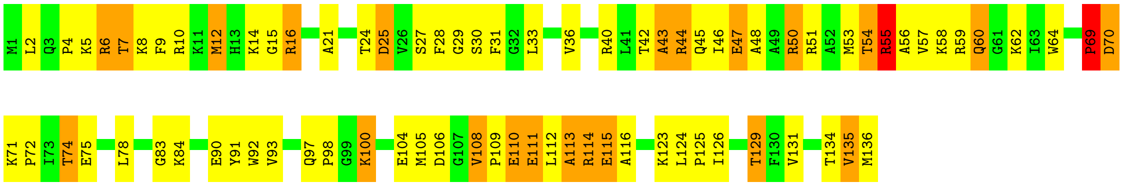
Chain DL:



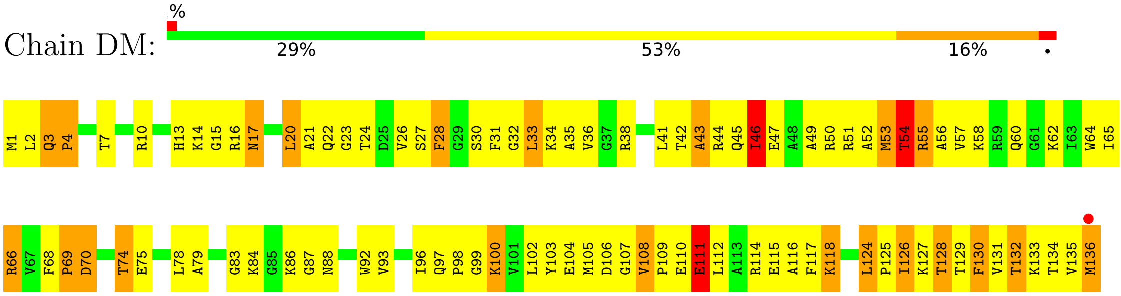
- Molecule 37: 50S ribosomal protein L16

Chain CM:

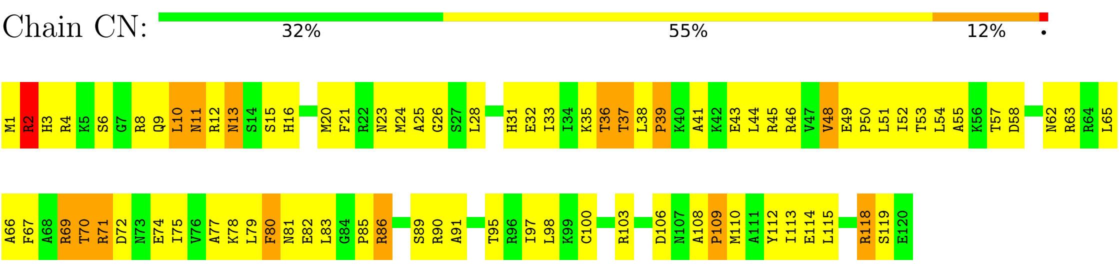




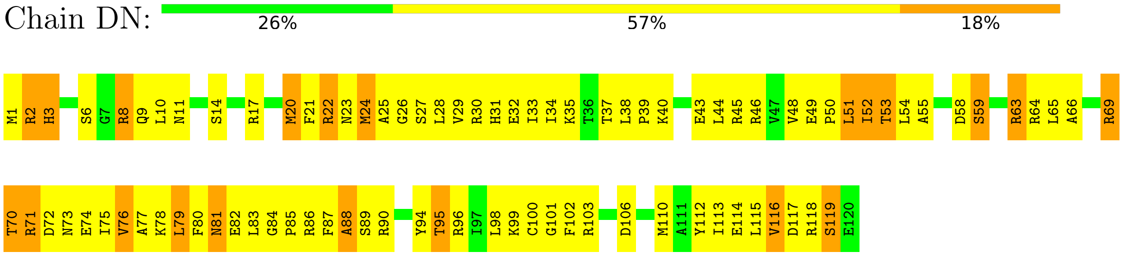
- Molecule 37: 50S ribosomal protein L16



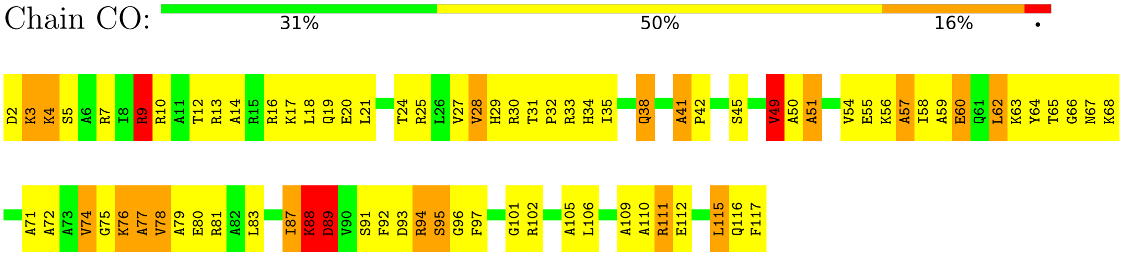
- Molecule 38: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L17

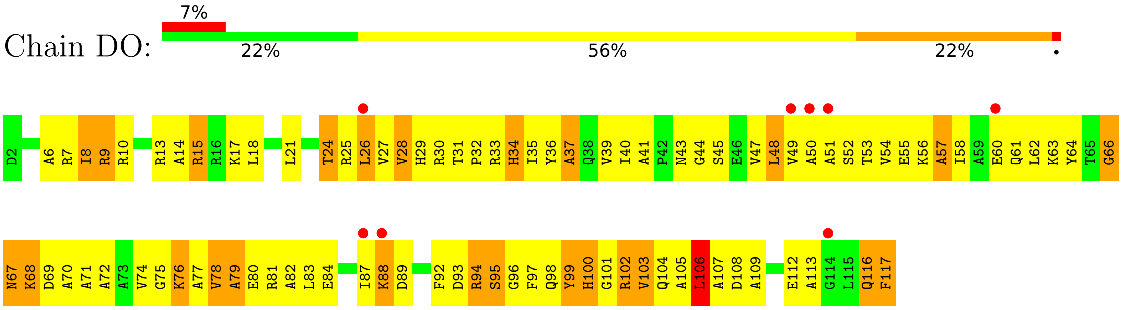


- Molecule 39: 50S ribosomal protein L18



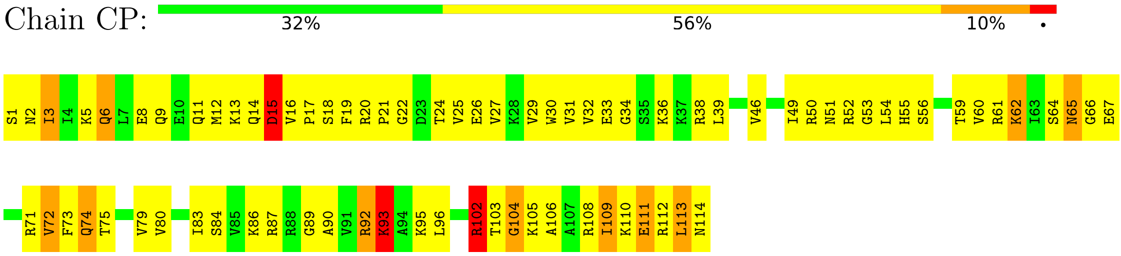
- Molecule 39: 50S ribosomal protein L18

Chain DO:



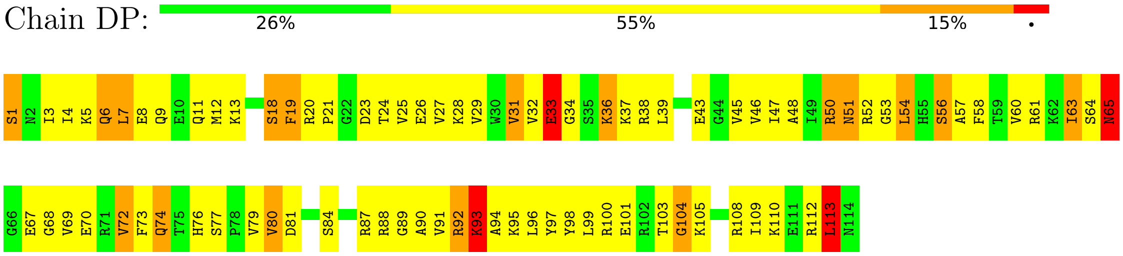
- Molecule 40: 50S ribosomal protein L19

Chain CP:



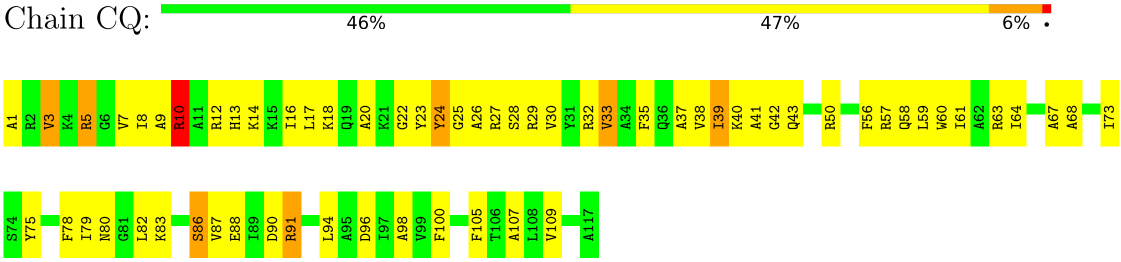
- Molecule 40: 50S ribosomal protein L19

Chain DP:



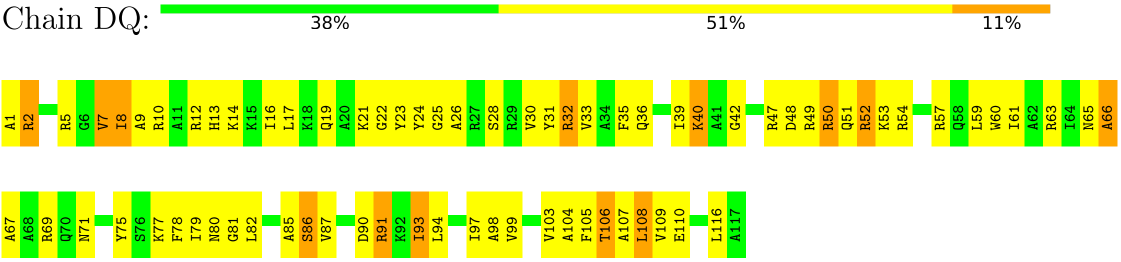
- Molecule 41: 50S ribosomal protein L20

Chain CQ:

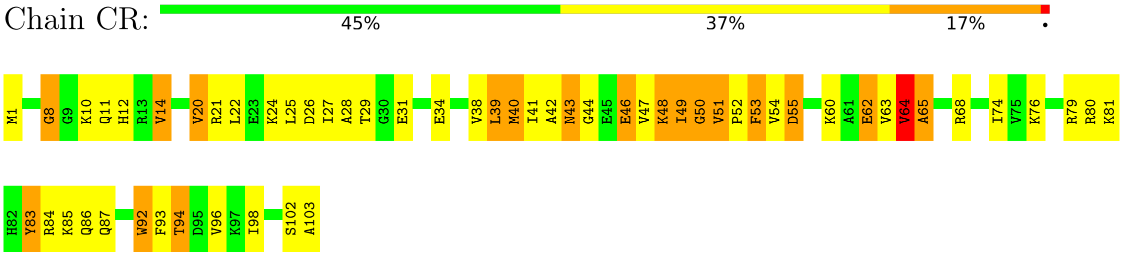


- Molecule 41: 50S ribosomal protein L20

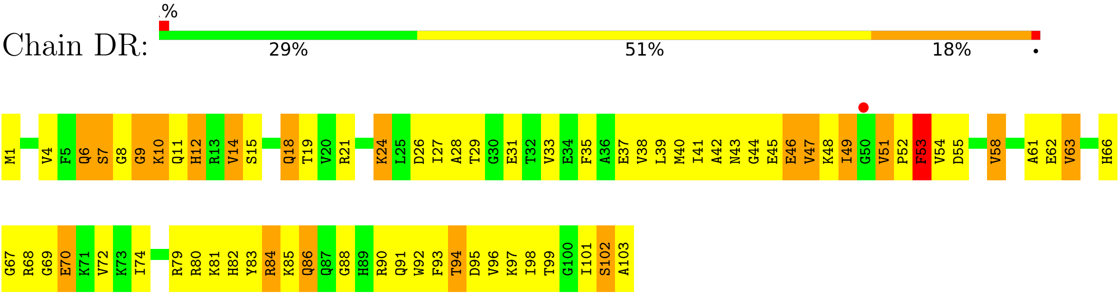
Chain DQ:



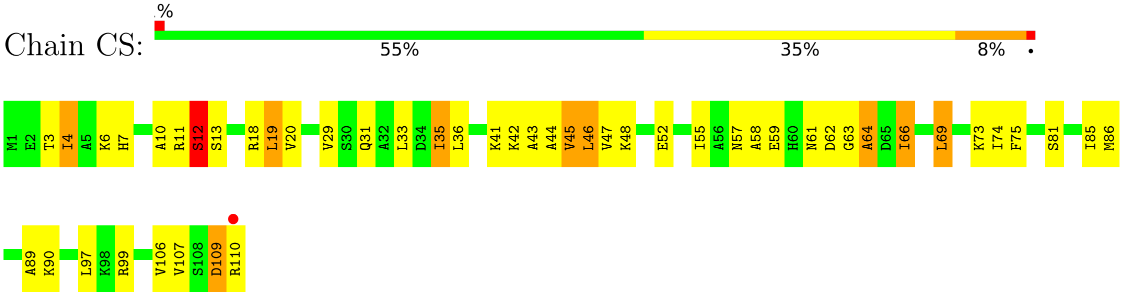
- Molecule 42: 50S ribosomal protein L21



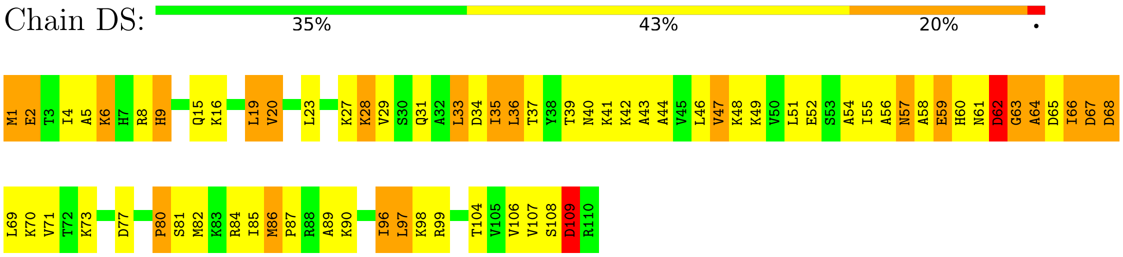
- Molecule 42: 50S ribosomal protein L21



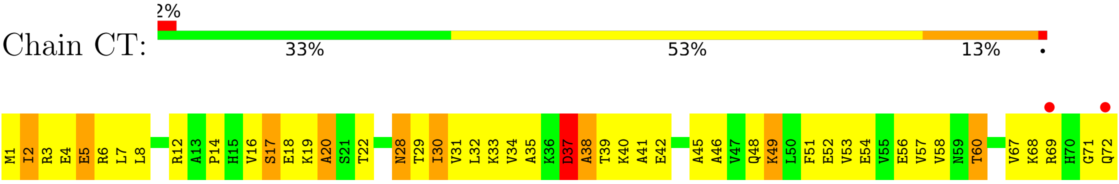
- Molecule 43: 50S ribosomal protein L22

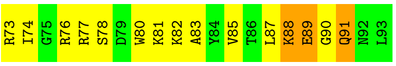


- Molecule 43: 50S ribosomal protein L22



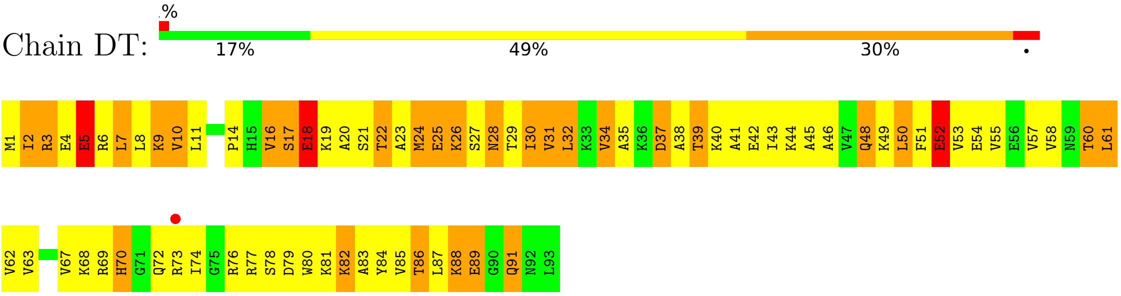
- Molecule 44: 50S ribosomal protein L23





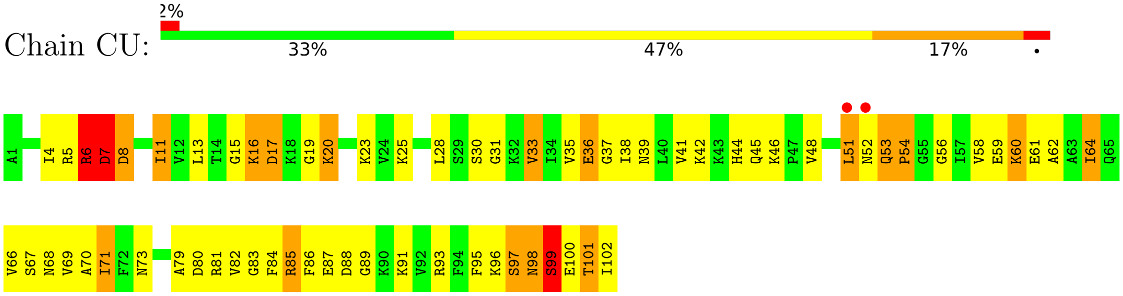
- Molecule 44: 50S ribosomal protein L23

Chain DT:



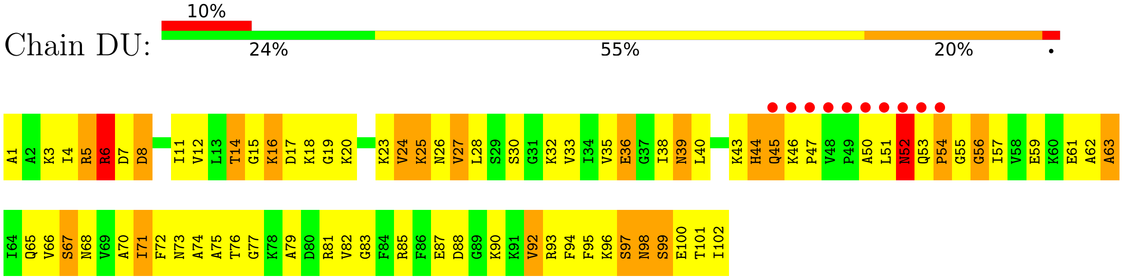
- Molecule 45: 50S ribosomal protein L24

Chain CU:



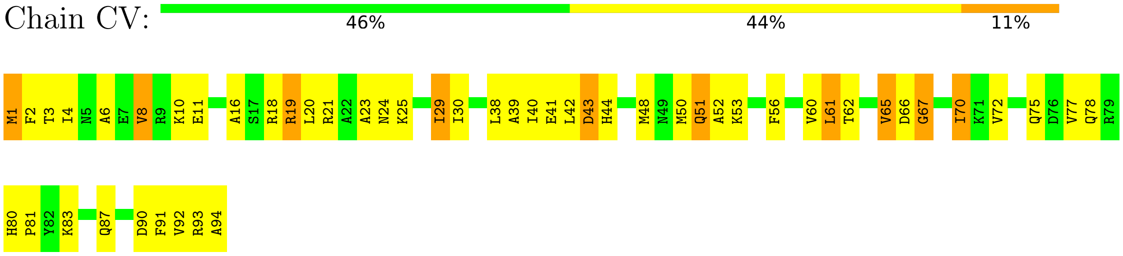
- Molecule 45: 50S ribosomal protein L24

Chain DU:



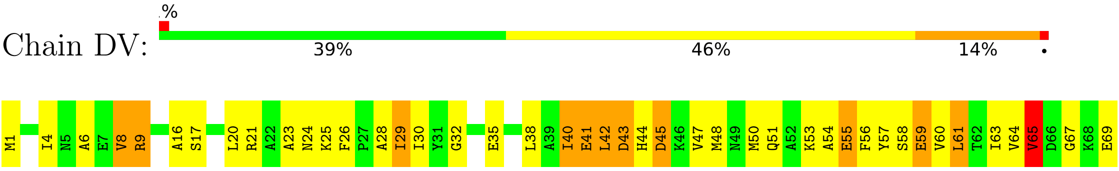
- Molecule 46: 50S ribosomal protein L25

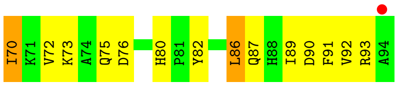
Chain CV:



- Molecule 46: 50S ribosomal protein L25

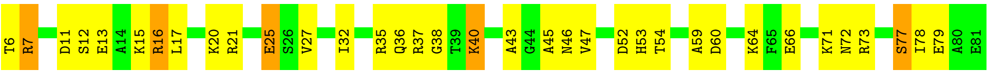
Chain DV:





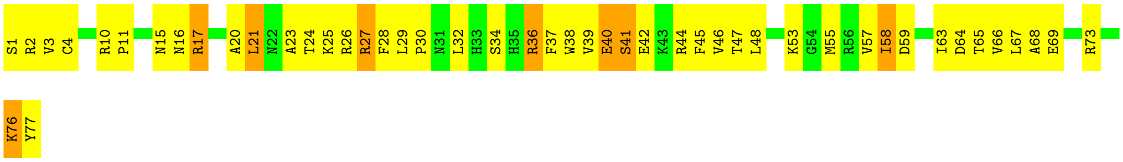
- Molecule 47: 50S ribosomal protein L27

Chain CW:



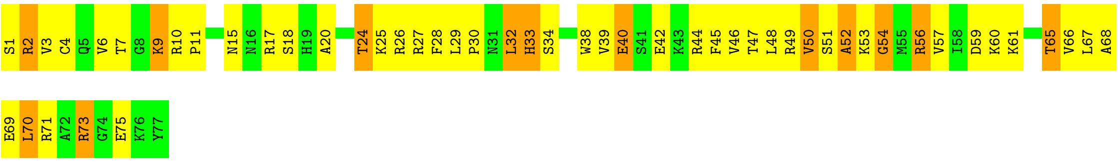
- Molecule 48: 50S ribosomal protein L28

Chain CX:



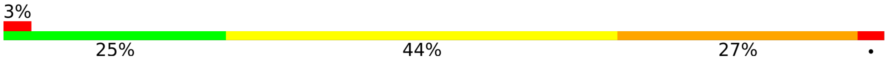
- Molecule 48: 50S ribosomal protein L28

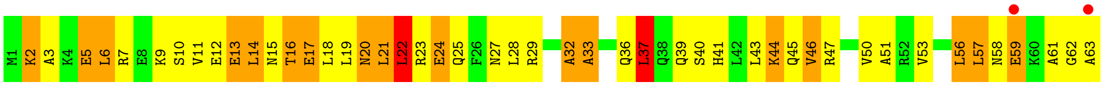
Chain DX:



- Molecule 49: 50S ribosomal protein L29

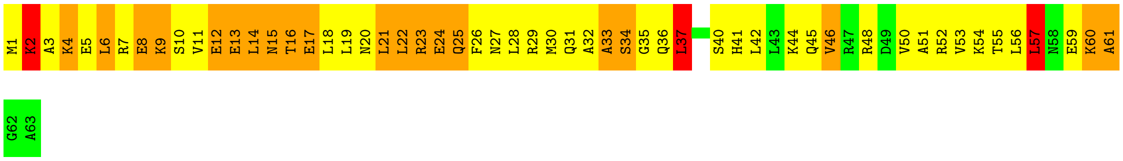
Chain CY:





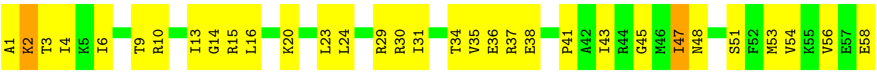
- Molecule 49: 50S ribosomal protein L29

Chain DY:



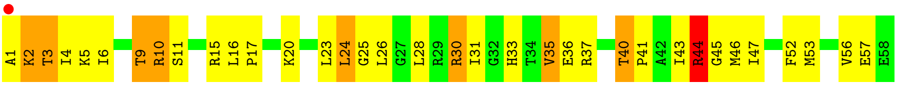
- Molecule 50: 50S ribosomal protein L30

Chain CZ:



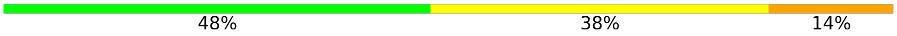
- Molecule 50: 50S ribosomal protein L30

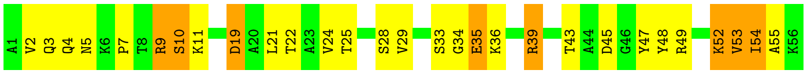
Chain DZ:



- Molecule 51: 50S ribosomal protein L32

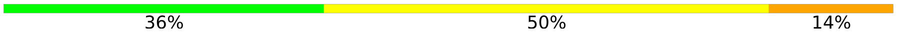
Chain C0:

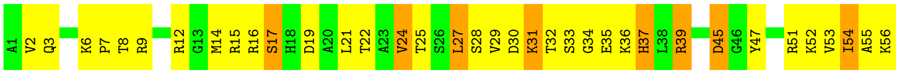




- Molecule 51: 50S ribosomal protein L32

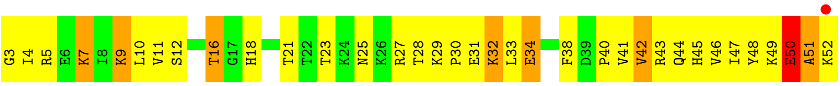
Chain D0:





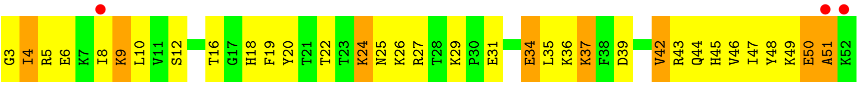
- Molecule 52: 50S ribosomal protein L33

Chain C1:



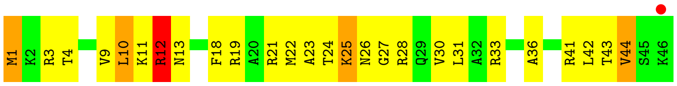
- Molecule 52: 50S ribosomal protein L33

Chain D1:



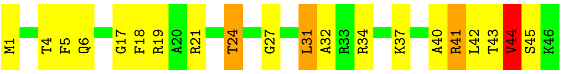
- Molecule 53: 50S ribosomal protein L34

Chain C2:

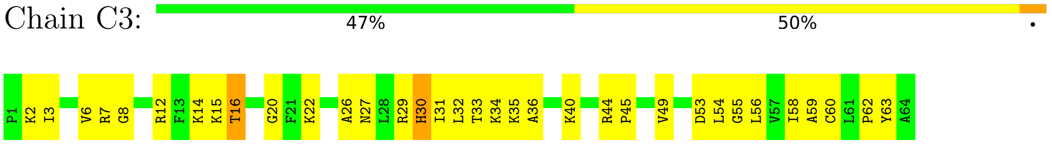


- Molecule 53: 50S ribosomal protein L34

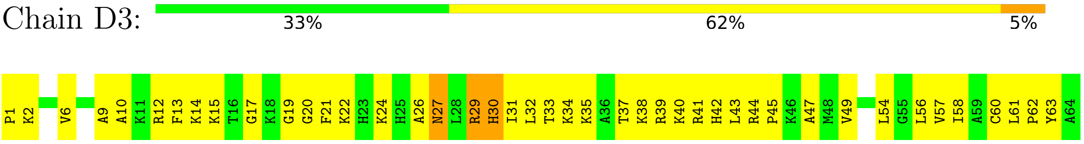
Chain D2:



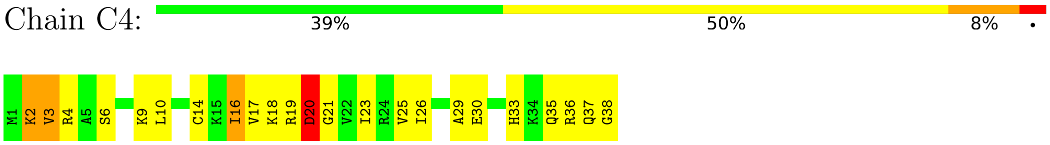
- Molecule 54: 50S ribosomal protein L35



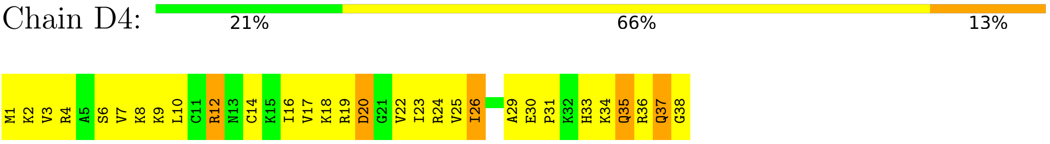
- Molecule 54: 50S ribosomal protein L35



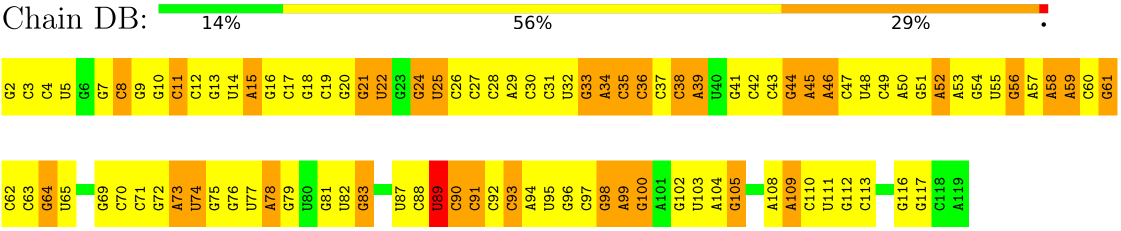
- Molecule 55: 50S ribosomal protein L36



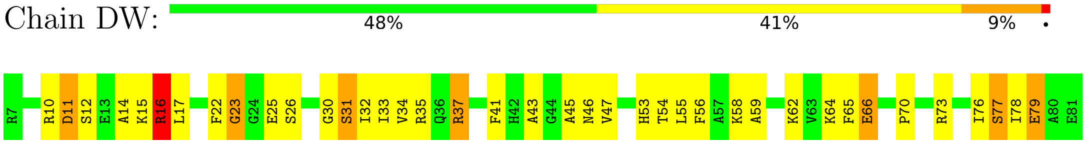
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 5S rRNA



- Molecule 57: 50S ribosomal protein L27



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.67Å 438.07Å 613.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 69.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 83.5 (69.21-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.260 0.196 , 0.251	Depositor DCC
R_{free} test set	19022 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 22.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	292354	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.87	8/36944 (0.0%)	1.28	318/57632 (0.6%)
1	BA	0.86	8/36966 (0.0%)	1.30	335/57666 (0.6%)
2	AB	0.60	0/1736	0.79	0/2338
2	BB	0.54	0/1736	0.72	0/2338
3	AC	0.56	0/1652	0.72	0/2225
3	BC	0.51	0/1652	0.72	1/2225 (0.0%)
4	AD	0.59	0/1665	0.74	1/2227 (0.0%)
4	BD	0.65	0/1665	0.80	1/2227 (0.0%)
5	AE	0.62	0/1119	0.85	0/1504
5	BE	0.62	0/1119	0.85	0/1504
6	AF	0.65	0/836	0.82	1/1128 (0.1%)
6	BF	0.55	0/836	0.80	1/1128 (0.1%)
7	AG	0.50	0/1196	0.67	0/1602
7	BG	0.48	0/1196	0.67	0/1602
8	AH	0.60	0/989	0.77	0/1326
8	BH	0.58	0/989	0.74	0/1326
9	AI	0.48	0/1034	0.71	0/1375
9	BI	0.53	0/1034	0.75	0/1375
10	AJ	0.57	0/797	0.74	0/1077
10	BJ	0.52	0/797	0.76	1/1077 (0.1%)
11	AK	0.67	0/893	0.82	0/1205
11	BK	0.59	0/893	0.75	0/1205
12	AL	0.61	0/969	0.81	0/1300
12	BL	0.72	0/969	0.92	0/1300
13	AM	0.52	0/893	0.74	0/1193
13	BM	0.50	0/893	0.71	0/1193
14	AN	0.55	0/785	0.76	0/1043
14	BN	0.51	0/785	0.65	0/1043
15	AO	0.55	0/722	0.73	0/964
15	BO	0.53	0/722	0.73	0/964
16	AP	0.54	0/659	0.82	1/884 (0.1%)
16	BP	0.61	0/659	0.79	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.57	0/658	0.74	0/881
17	BQ	0.62	0/658	0.76	0/881
18	AR	0.61	0/463	0.69	0/621
18	BR	0.54	0/463	0.68	0/621
19	AS	0.48	0/653	0.73	0/877
19	BS	0.55	0/653	0.67	0/877
20	AT	0.54	0/671	0.69	0/888
20	BT	0.57	0/671	0.73	0/888
21	AU	0.93	0/431	0.96	0/570
21	BU	0.78	0/431	0.85	0/570
22	AV	0.76	1/1813 (0.1%)	1.22	14/2823 (0.5%)
22	BV	0.74	1/1813 (0.1%)	1.22	10/2823 (0.4%)
23	AX	0.86	0/363	1.11	0/564
23	BX	0.73	0/388	1.09	0/603
24	AY	0.65	0/1430	0.74	0/1924
25	CA	1.60	600/69659 (0.9%)	1.67	2062/108672 (1.9%)
25	DA	1.07	82/69633 (0.1%)	1.48	1284/108629 (1.2%)
26	CB	1.33	5/2847 (0.2%)	1.58	77/4440 (1.7%)
27	CC	0.80	0/2122	0.90	1/2852 (0.0%)
27	DC	0.68	1/2122 (0.0%)	0.86	1/2852 (0.0%)
28	CD	0.96	0/1586	0.92	1/2134 (0.0%)
28	DD	0.70	0/1586	0.87	2/2134 (0.1%)
29	CE	0.91	0/1571	0.89	1/2113 (0.0%)
29	DE	0.67	0/1571	0.81	0/2113
30	CF	0.64	0/1435	0.74	0/1926
30	DF	0.51	0/1435	0.67	0/1926
31	CG	0.75	0/1343	0.85	1/1816 (0.1%)
31	DG	0.51	0/1343	0.69	0/1816
32	CH	0.68	1/1121 (0.1%)	0.77	0/1515
32	DH	0.66	1/1121 (0.1%)	0.80	1/1515 (0.1%)
33	CI	0.72	0/1046	0.74	0/1410
33	DI	0.67	0/1046	0.72	0/1410
34	CJ	1.01	0/1152	0.84	1/1551 (0.1%)
34	DJ	0.77	0/1152	0.82	0/1551
35	CK	0.91	3/948 (0.3%)	0.94	1/1268 (0.1%)
35	DK	0.68	0/948	0.84	0/1268
36	CL	0.94	0/1054	1.01	0/1403
36	DL	0.65	0/1054	0.85	0/1403
37	CM	0.94	0/1093	0.96	0/1460
37	DM	0.64	0/1093	0.80	0/1460
38	CN	0.91	0/974	0.96	1/1301 (0.1%)
38	DN	0.67	0/974	0.82	0/1301
39	CO	0.76	0/902	0.87	1/1209 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	DO	0.50	0/902	0.66	0/1209
40	CP	0.89	0/929	0.88	1/1242 (0.1%)
40	DP	0.71	0/929	0.82	0/1242
41	CQ	1.14	0/960	0.96	1/1278 (0.1%)
41	DQ	0.80	0/960	0.79	0/1278
42	CR	1.01	1/829 (0.1%)	0.98	0/1107
42	DR	0.79	0/829	0.90	1/1107 (0.1%)
43	CS	1.08	1/864 (0.1%)	0.97	1/1156 (0.1%)
43	DS	0.71	0/864	0.89	1/1156 (0.1%)
44	CT	0.82	0/745	0.86	0/994
44	DT	0.59	0/745	0.74	0/994
45	CU	0.91	0/788	0.90	0/1051
45	DU	0.66	0/788	0.76	0/1051
46	CV	0.79	0/766	0.81	0/1025
46	DV	0.53	0/766	0.69	0/1025
47	CW	1.02	0/582	0.97	0/769
48	CX	0.78	0/635	0.84	0/848
48	DX	0.61	0/635	0.77	0/848
49	CY	0.76	0/510	0.96	1/677 (0.1%)
49	DY	0.56	0/510	0.77	0/677
50	CZ	1.04	0/453	0.94	0/605
50	DZ	0.58	0/453	0.78	0/605
51	C0	0.95	0/450	0.98	2/599 (0.3%)
51	D0	0.71	0/450	0.89	1/599 (0.2%)
52	C1	0.74	0/417	0.76	0/554
52	D1	0.50	0/417	0.66	0/554
53	C2	1.03	0/380	0.99	2/498 (0.4%)
53	D2	0.70	0/380	0.84	0/498
54	C3	0.94	0/513	0.85	0/676
54	D3	0.60	0/513	0.78	1/676 (0.1%)
55	C4	0.92	0/303	0.99	0/397
55	D4	0.68	0/303	0.76	0/397
56	DB	0.75	0/2828	1.23	18/4410 (0.4%)
57	DW	0.60	0/571	0.72	0/755
All	All	1.08	713/315257 (0.2%)	1.34	4150/471496 (0.9%)

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
4	AD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	BD	0	1
5	AE	0	1
5	BE	0	2
6	BF	0	1
9	AI	0	1
11	AK	0	1
11	BK	0	2
12	BL	0	2
13	AM	0	1
14	AN	0	1
20	BT	0	1
21	AU	0	2
21	BU	0	1
27	CC	0	1
27	DC	0	1
28	CD	0	2
28	DD	0	1
32	DH	0	2
33	CI	0	1
34	DJ	0	1
39	DO	0	1
42	CR	0	1
45	CU	0	1
50	CZ	0	1
All	All	0	31

The worst 5 of 713 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CA	1142	A	N9-C4	-18.22	1.26	1.37
25	CA	984	A	N9-C4	-13.29	1.29	1.37
25	DA	984	A	N9-C4	-10.51	1.31	1.37
25	CA	984	A	C5-C6	-10.44	1.31	1.41
25	CA	528	A	N7-C5	-10.29	1.33	1.39

The worst 5 of 4150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	CA	984	A	C2-N3-C4	-18.86	101.17	110.60
25	CA	2250	G	N3-C4-C5	17.23	137.22	128.60
25	CA	1638	C	N1-C2-O2	-16.64	108.92	118.90
25	CA	1142	A	C2-N3-C4	-16.61	102.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	1142	A	N3-C4-C5	16.11	138.07	126.80

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	47	LEU	Peptide
5	AE	100	GLU	Peptide
9	AI	5	TYR	Peptide
11	AK	125	LYS	Peptide
13	AM	111	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	2052	0
1	BA	33015	0	16617	2194	0
2	AB	1705	0	1732	374	0
2	BB	1705	0	1732	298	0
3	AC	1625	0	1699	235	0
3	BC	1625	0	1699	237	0
4	AD	1643	0	1710	291	0
4	BD	1643	0	1710	228	0
5	AE	1106	0	1148	214	0
5	BE	1106	0	1148	211	0
6	AF	818	0	808	116	0
6	BF	818	0	808	156	0
7	AG	1182	0	1240	116	0
7	BG	1182	0	1240	166	0
8	AH	979	0	1034	161	0
8	BH	979	0	1034	119	0
9	AI	1022	0	1070	189	0
9	BI	1022	0	1070	186	0
10	AJ	787	0	828	178	0
10	BJ	787	0	828	142	0
11	AK	877	0	887	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BK	877	0	887	136	0
12	AL	955	0	1019	94	0
12	BL	955	0	1019	118	0
13	AM	884	0	944	163	0
13	BM	884	0	944	144	0
14	AN	774	0	827	130	0
14	BN	774	0	827	131	0
15	AO	714	0	737	61	0
15	BO	714	0	737	87	0
16	AP	649	0	666	106	0
16	BP	649	0	666	87	0
17	AQ	649	0	691	118	0
17	BQ	649	0	691	103	0
18	AR	456	0	478	46	0
18	BR	456	0	478	57	0
19	AS	638	0	665	88	0
19	BS	638	0	665	96	0
20	AT	665	0	714	84	0
20	BT	665	0	714	129	0
21	AU	426	0	449	139	0
21	BU	426	0	449	119	0
22	AV	1623	0	821	88	0
22	BV	1623	0	821	47	0
23	AX	324	0	162	19	0
23	BX	346	0	173	24	0
24	AY	1419	0	1467	97	0
25	CA	62195	0	31271	2445	0
25	DA	62173	0	31270	3398	0
26	CB	2548	0	1292	98	0
27	CC	2083	0	2157	227	0
27	DC	2083	0	2157	213	0
28	CD	1565	0	1616	129	0
28	DD	1565	0	1616	114	0
29	CE	1552	0	1619	143	0
29	DE	1552	0	1619	163	0
30	CF	1411	0	1447	202	0
30	DF	1411	0	1447	197	0
31	CG	1323	0	1374	146	0
31	DG	1323	0	1374	177	0
32	CH	1110	0	1148	145	0
32	DH	1110	0	1148	210	0
33	CI	1032	0	1088	246	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DI	1032	0	1088	180	0
34	CJ	1129	0	1162	57	0
34	DJ	1129	0	1162	96	0
35	CK	939	0	1012	75	0
35	DK	939	0	1012	79	0
36	CL	1045	0	1117	130	0
36	DL	1045	0	1117	168	0
37	CM	1074	0	1157	96	0
37	DM	1074	0	1157	127	0
38	CN	961	0	1000	94	0
38	DN	961	0	1000	124	0
39	CO	892	0	923	84	0
39	DO	892	0	923	141	0
40	CP	917	0	965	93	0
40	DP	917	0	965	107	0
41	CQ	947	0	1022	63	0
41	DQ	947	0	1022	83	0
42	CR	816	0	839	84	0
42	DR	816	0	839	99	0
43	CS	857	0	922	42	0
43	DS	857	0	922	82	0
44	CT	739	0	807	71	0
44	DT	739	0	807	114	0
45	CU	780	0	834	66	0
45	DU	780	0	834	111	0
46	CV	753	0	780	59	0
46	DV	753	0	780	71	0
47	CW	575	0	589	27	0
48	CX	625	0	655	41	0
48	DX	625	0	655	58	0
49	CY	509	0	543	88	0
49	DY	509	0	543	109	0
50	CZ	449	0	491	26	0
50	DZ	449	0	491	47	0
51	C0	444	0	461	35	0
51	D0	444	0	461	41	0
52	C1	410	0	440	37	0
52	D1	410	0	440	45	0
53	C2	377	0	418	26	0
53	D2	377	0	418	18	0
54	C3	504	0	574	40	0
54	D3	504	0	574	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	C4	302	0	340	23	0
55	D4	302	0	340	34	0
56	DB	2529	0	1281	163	0
57	DW	564	0	576	36	0
58	AA	72	0	0	0	0
58	BA	56	0	0	0	0
58	CA	194	0	0	0	0
58	CB	4	0	0	0	0
58	CQ	1	0	0	0	0
58	DA	166	0	0	0	0
58	DB	3	0	0	0	0
58	DL	1	0	0	0	0
58	DQ	1	0	0	0	0
59	C4	1	0	0	0	0
59	D4	1	0	0	0	0
60	AA	197	0	0	11	0
60	AN	4	0	0	0	0
60	AT	1	0	0	0	0
60	AU	1	0	0	0	0
60	BA	190	0	0	12	0
60	BL	1	0	0	0	0
60	BN	5	0	0	1	0
60	BT	1	0	0	0	0
60	BU	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	625	0	0	62	0
60	CB	13	0	0	0	0
60	CC	8	0	0	0	0
60	CD	2	0	0	0	0
60	CE	2	0	0	0	0
60	CF	1	0	0	0	0
60	CJ	1	0	0	0	0
60	CL	6	0	0	2	0
60	CN	4	0	0	0	0
60	CS	1	0	0	0	0
60	CV	1	0	0	0	0
60	D2	1	0	0	0	0
60	D3	2	0	0	0	0
60	D4	1	0	0	0	0
60	DA	622	0	0	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DB	14	0	0	0	0
60	DC	4	0	0	0	0
60	DD	5	0	0	2	0
60	DE	2	0	0	0	0
60	DJ	1	0	0	0	0
60	DL	4	0	0	1	0
60	DN	1	0	0	0	0
60	DR	1	0	0	0	0
All	All	292354	0	195461	20868	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

The worst 5 of 20868 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)
32:DH:93:SER:OG	32:DH:121:VAL:HG12	1.46	1.15
1:BA:1053:G:H4’	1:BA:1054:C:H5’	1.29	1.11
32:DH:93:SER:OG	32:DH:121:VAL:CG1	2.03	1.06
25:DA:1153:C:OP2	60:DA:3363:HOH:O	1.78	1.01
12:BL:33:CYS:HA	12:BL:54:VAL:HA	1.44	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	109 (50%)	49 (23%)	58 (27%)	0	0
2	BB	216/218 (99%)	112 (52%)	49 (23%)	55 (26%)	0	0
3	AC	204/206 (99%)	125 (61%)	49 (24%)	30 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BC	204/206 (99%)	126 (62%)	47 (23%)	31 (15%)	0	1
4	AD	203/205 (99%)	123 (61%)	41 (20%)	39 (19%)	0	0
4	BD	203/205 (99%)	136 (67%)	36 (18%)	31 (15%)	0	1
5	AE	148/150 (99%)	87 (59%)	38 (26%)	23 (16%)	0	1
5	BE	148/150 (99%)	90 (61%)	31 (21%)	27 (18%)	0	0
6	AF	98/100 (98%)	62 (63%)	21 (21%)	15 (15%)	0	1
6	BF	98/100 (98%)	54 (55%)	23 (24%)	21 (21%)	0	0
7	AG	149/151 (99%)	86 (58%)	41 (28%)	22 (15%)	0	1
7	BG	149/151 (99%)	79 (53%)	46 (31%)	24 (16%)	0	1
8	AH	127/129 (98%)	79 (62%)	37 (29%)	11 (9%)	1	3
8	BH	127/129 (98%)	82 (65%)	32 (25%)	13 (10%)	0	2
9	AI	125/127 (98%)	76 (61%)	34 (27%)	15 (12%)	0	1
9	BI	125/127 (98%)	77 (62%)	33 (26%)	15 (12%)	0	1
10	AJ	96/98 (98%)	60 (62%)	14 (15%)	22 (23%)	0	0
10	BJ	96/98 (98%)	64 (67%)	14 (15%)	18 (19%)	0	0
11	AK	115/117 (98%)	84 (73%)	17 (15%)	14 (12%)	0	1
11	BK	115/117 (98%)	81 (70%)	19 (16%)	15 (13%)	0	1
12	AL	121/123 (98%)	85 (70%)	29 (24%)	7 (6%)	1	10
12	BL	121/123 (98%)	91 (75%)	16 (13%)	14 (12%)	0	1
13	AM	112/114 (98%)	78 (70%)	22 (20%)	12 (11%)	0	2
13	BM	112/114 (98%)	65 (58%)	24 (21%)	23 (20%)	0	0
14	AN	92/100 (92%)	47 (51%)	27 (29%)	18 (20%)	0	0
14	BN	92/100 (92%)	39 (42%)	30 (33%)	23 (25%)	0	0
15	AO	86/88 (98%)	57 (66%)	22 (26%)	7 (8%)	1	4
15	BO	86/88 (98%)	52 (60%)	17 (20%)	17 (20%)	0	0
16	AP	80/82 (98%)	48 (60%)	11 (14%)	21 (26%)	0	0
16	BP	80/82 (98%)	47 (59%)	22 (28%)	11 (14%)	0	1
17	AQ	78/80 (98%)	47 (60%)	18 (23%)	13 (17%)	0	0
17	BQ	78/80 (98%)	48 (62%)	18 (23%)	12 (15%)	0	1
18	AR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	0	2
18	BR	53/55 (96%)	31 (58%)	19 (36%)	3 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AS	77/79 (98%)	36 (47%)	29 (38%)	12 (16%)	0	1
19	BS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	3
20	AT	83/85 (98%)	37 (45%)	31 (37%)	15 (18%)	0	0
20	BT	83/85 (98%)	46 (55%)	23 (28%)	14 (17%)	0	0
21	AU	49/51 (96%)	20 (41%)	15 (31%)	14 (29%)	0	0
21	BU	49/51 (96%)	22 (45%)	10 (20%)	17 (35%)	0	0
24	AY	181/183 (99%)	135 (75%)	35 (19%)	11 (6%)	1	8
27	CC	269/271 (99%)	216 (80%)	32 (12%)	21 (8%)	1	4
27	DC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	0	2
28	CD	207/209 (99%)	166 (80%)	30 (14%)	11 (5%)	2	11
28	DD	207/209 (99%)	162 (78%)	35 (17%)	10 (5%)	2	13
29	CE	199/201 (99%)	158 (79%)	32 (16%)	9 (4%)	2	14
29	DE	199/201 (99%)	142 (71%)	38 (19%)	19 (10%)	0	3
30	CF	175/177 (99%)	118 (67%)	38 (22%)	19 (11%)	0	2
30	DF	175/177 (99%)	113 (65%)	34 (19%)	28 (16%)	0	1
31	CG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1	3
31	DG	174/176 (99%)	106 (61%)	43 (25%)	25 (14%)	0	1
32	CH	147/149 (99%)	95 (65%)	29 (20%)	23 (16%)	0	1
32	DH	147/149 (99%)	95 (65%)	27 (18%)	25 (17%)	0	0
33	CI	139/141 (99%)	65 (47%)	47 (34%)	27 (19%)	0	0
33	DI	139/141 (99%)	71 (51%)	46 (33%)	22 (16%)	0	1
34	CJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	15
34	DJ	140/142 (99%)	112 (80%)	24 (17%)	4 (3%)	4	24
35	CK	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	1	6
35	DK	120/122 (98%)	87 (72%)	21 (18%)	12 (10%)	0	2
36	CL	141/143 (99%)	99 (70%)	21 (15%)	21 (15%)	0	1
36	DL	141/143 (99%)	88 (62%)	36 (26%)	17 (12%)	0	1
37	CM	134/136 (98%)	110 (82%)	15 (11%)	9 (7%)	1	6
37	DM	134/136 (98%)	97 (72%)	23 (17%)	14 (10%)	0	2
38	CN	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	2	12
38	DN	118/120 (98%)	82 (70%)	28 (24%)	8 (7%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CO	114/116 (98%)	83 (73%)	17 (15%)	14 (12%)	0	1
39	DO	114/116 (98%)	77 (68%)	25 (22%)	12 (10%)	0	2
40	CP	112/114 (98%)	96 (86%)	12 (11%)	4 (4%)	3	19
40	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	1	7
41	CQ	115/117 (98%)	100 (87%)	13 (11%)	2 (2%)	9	39
41	DQ	115/117 (98%)	95 (83%)	18 (16%)	2 (2%)	9	39
42	CR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	4
42	DR	101/103 (98%)	78 (77%)	14 (14%)	9 (9%)	1	3
43	CS	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	10
43	DS	108/110 (98%)	78 (72%)	19 (18%)	11 (10%)	0	2
44	CT	91/93 (98%)	67 (74%)	13 (14%)	11 (12%)	0	1
44	DT	91/93 (98%)	59 (65%)	20 (22%)	12 (13%)	0	1
45	CU	100/102 (98%)	74 (74%)	14 (14%)	12 (12%)	0	1
45	DU	100/102 (98%)	73 (73%)	14 (14%)	13 (13%)	0	1
46	CV	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	6	31
46	DV	92/94 (98%)	71 (77%)	15 (16%)	6 (6%)	1	7
47	CW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	5	26
48	CX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	5	26
48	DX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	4
49	CY	61/63 (97%)	34 (56%)	13 (21%)	14 (23%)	0	0
49	DY	61/63 (97%)	28 (46%)	16 (26%)	17 (28%)	0	0
50	CZ	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
50	DZ	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	3	19
51	C0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	3	19
51	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0	3
52	C1	48/50 (96%)	32 (67%)	12 (25%)	4 (8%)	1	4
52	D1	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	3	16
53	C2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	6	30
53	D2	44/46 (96%)	31 (70%)	8 (18%)	5 (11%)	0	2
54	C3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
54	D3	62/64 (97%)	49 (79%)	11 (18%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	C4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	25
55	D4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	25
57	DW	73/75 (97%)	57 (78%)	12 (16%)	4 (6%)	2	10
All	All	11416/11626 (98%)	7804 (68%)	2248 (20%)	1364 (12%)	0	1

5 of 1364 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	21	TYR
2	AB	33	ALA
2	AB	63	LYS
2	AB	67	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	114 (63%)	66 (37%)	0	1
2	BB	180/180 (100%)	131 (73%)	49 (27%)	0	2
3	AC	170/170 (100%)	127 (75%)	43 (25%)	0	3
3	BC	170/170 (100%)	123 (72%)	47 (28%)	0	2
4	AD	172/172 (100%)	132 (77%)	40 (23%)	1	4
4	BD	172/172 (100%)	123 (72%)	49 (28%)	0	2
5	AE	113/113 (100%)	80 (71%)	33 (29%)	0	2
5	BE	113/113 (100%)	87 (77%)	26 (23%)	1	4
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	1
6	BF	87/87 (100%)	61 (70%)	26 (30%)	0	1
7	AG	124/124 (100%)	90 (73%)	34 (27%)	0	2
7	BG	124/124 (100%)	85 (68%)	39 (32%)	0	1
8	AH	104/104 (100%)	78 (75%)	26 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	BH	104/104 (100%)	78 (75%)	26 (25%)	0	3
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	1
9	BI	105/105 (100%)	67 (64%)	38 (36%)	0	1
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	0	2
10	BJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
11	AK	90/90 (100%)	66 (73%)	24 (27%)	0	2
11	BK	90/90 (100%)	67 (74%)	23 (26%)	0	3
12	AL	103/103 (100%)	86 (84%)	17 (16%)	2	11
12	BL	103/103 (100%)	75 (73%)	28 (27%)	0	2
13	AM	92/92 (100%)	73 (79%)	19 (21%)	1	6
13	BM	92/92 (100%)	71 (77%)	21 (23%)	1	4
14	AN	79/83 (95%)	56 (71%)	23 (29%)	0	2
14	BN	79/83 (95%)	60 (76%)	19 (24%)	0	3
15	AO	76/76 (100%)	61 (80%)	15 (20%)	1	7
15	BO	76/76 (100%)	60 (79%)	16 (21%)	1	5
16	AP	65/65 (100%)	45 (69%)	20 (31%)	0	1
16	BP	65/65 (100%)	48 (74%)	17 (26%)	0	2
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	0	2
17	BQ	74/74 (100%)	47 (64%)	27 (36%)	0	1
18	AR	48/48 (100%)	40 (83%)	8 (17%)	2	11
18	BR	48/48 (100%)	40 (83%)	8 (17%)	2	11
19	AS	70/70 (100%)	56 (80%)	14 (20%)	1	7
19	BS	70/70 (100%)	53 (76%)	17 (24%)	0	3
20	AT	65/65 (100%)	45 (69%)	20 (31%)	0	1
20	BT	65/65 (100%)	47 (72%)	18 (28%)	0	2
21	AU	44/44 (100%)	23 (52%)	21 (48%)	0	0
21	BU	44/44 (100%)	26 (59%)	18 (41%)	0	0
24	AY	157/157 (100%)	139 (88%)	18 (12%)	5	24
27	CC	216/216 (100%)	182 (84%)	34 (16%)	2	13
27	DC	216/216 (100%)	173 (80%)	43 (20%)	1	7
28	CD	164/164 (100%)	143 (87%)	21 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DD	164/164 (100%)	135 (82%)	29 (18%)	2	9
29	CE	165/165 (100%)	143 (87%)	22 (13%)	4	17
29	DE	165/165 (100%)	126 (76%)	39 (24%)	1	3
30	CF	148/148 (100%)	112 (76%)	36 (24%)	0	3
30	DF	148/148 (100%)	114 (77%)	34 (23%)	1	4
31	CG	137/137 (100%)	114 (83%)	23 (17%)	2	11
31	DG	137/137 (100%)	119 (87%)	18 (13%)	4	18
32	CH	114/114 (100%)	89 (78%)	25 (22%)	1	5
32	DH	114/114 (100%)	92 (81%)	22 (19%)	1	8
33	CI	109/109 (100%)	78 (72%)	31 (28%)	0	2
33	DI	109/109 (100%)	83 (76%)	26 (24%)	0	3
34	CJ	116/116 (100%)	97 (84%)	19 (16%)	2	11
34	DJ	116/116 (100%)	95 (82%)	21 (18%)	1	9
35	CK	103/103 (100%)	85 (82%)	18 (18%)	2	10
35	DK	103/103 (100%)	85 (82%)	18 (18%)	2	10
36	CL	102/102 (100%)	81 (79%)	21 (21%)	1	6
36	DL	102/102 (100%)	81 (79%)	21 (21%)	1	6
37	CM	109/109 (100%)	87 (80%)	22 (20%)	1	6
37	DM	109/109 (100%)	87 (80%)	22 (20%)	1	6
38	CN	100/100 (100%)	83 (83%)	17 (17%)	2	10
38	DN	100/100 (100%)	80 (80%)	20 (20%)	1	7
39	CO	86/86 (100%)	68 (79%)	18 (21%)	1	5
39	DO	86/86 (100%)	66 (77%)	20 (23%)	1	4
40	CP	99/99 (100%)	78 (79%)	21 (21%)	1	5
40	DP	99/99 (100%)	76 (77%)	23 (23%)	1	4
41	CQ	89/89 (100%)	76 (85%)	13 (15%)	3	15
41	DQ	89/89 (100%)	74 (83%)	15 (17%)	2	11
42	CR	84/84 (100%)	70 (83%)	14 (17%)	2	11
42	DR	84/84 (100%)	66 (79%)	18 (21%)	1	5
43	CS	93/93 (100%)	83 (89%)	10 (11%)	6	26
43	DS	93/93 (100%)	71 (76%)	22 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	CT	80/80 (100%)	69 (86%)	11 (14%)	3	17
44	DT	80/80 (100%)	57 (71%)	23 (29%)	0	2
45	CU	83/83 (100%)	64 (77%)	19 (23%)	1	4
45	DU	83/83 (100%)	63 (76%)	20 (24%)	0	3
46	CV	78/78 (100%)	63 (81%)	15 (19%)	1	8
46	DV	78/78 (100%)	63 (81%)	15 (19%)	1	8
47	CW	56/58 (97%)	50 (89%)	6 (11%)	6	26
48	CX	67/67 (100%)	56 (84%)	11 (16%)	2	11
48	DX	67/67 (100%)	56 (84%)	11 (16%)	2	11
49	CY	55/55 (100%)	46 (84%)	9 (16%)	2	11
49	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
50	CZ	48/48 (100%)	40 (83%)	8 (17%)	2	11
50	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	5
51	C0	47/47 (100%)	41 (87%)	6 (13%)	4	19
51	D0	47/47 (100%)	41 (87%)	6 (13%)	4	19
52	C1	45/45 (100%)	38 (84%)	7 (16%)	2	13
52	D1	45/45 (100%)	37 (82%)	8 (18%)	2	9
53	C2	38/38 (100%)	32 (84%)	6 (16%)	2	12
53	D2	38/38 (100%)	33 (87%)	5 (13%)	4	18
54	C3	51/51 (100%)	48 (94%)	3 (6%)	19	54
54	D3	51/51 (100%)	48 (94%)	3 (6%)	19	54
55	C4	34/34 (100%)	28 (82%)	6 (18%)	2	10
55	D4	34/34 (100%)	27 (79%)	7 (21%)	1	6
57	DW	55/57 (96%)	47 (86%)	8 (14%)	3	15
All	All	9482/9494 (100%)	7392 (78%)	2090 (22%)	1	4

5 of 2090 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	DN	63	ARG
41	DQ	2	ARG
38	DN	34	ILE
54	D3	13	PHE
7	BG	145	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
32	CH	135	HIS
45	CU	68	ASN
46	DV	87	GLN
34	CJ	77	HIS
38	CN	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	441 (28%)	28 (1%)
1	BA	1538/1539 (99%)	445 (28%)	20 (1%)
22	AV	75/76 (98%)	29 (38%)	1 (1%)
22	BV	75/76 (98%)	15 (20%)	1 (1%)
23	AX	14/16 (87%)	5 (35%)	0
23	BX	15/16 (93%)	4 (26%)	0
25	CA	2895/2903 (99%)	747 (25%)	53 (1%)
25	DA	2893/2903 (99%)	764 (26%)	48 (1%)
26	CB	118/119 (99%)	24 (20%)	1 (0%)
56	DB	117/118 (99%)	34 (29%)	3 (2%)
All	All	9277/9305 (99%)	2508 (27%)	155 (1%)

5 of 2508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	9	G
1	AA	12	U

5 of 155 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	614	A
25	DA	2311	A
25	DA	945	A
25	DA	1738	G
25	DA	2800	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1538/1539 (99%)	-0.64	7 (0%) 91 75	0, 31, 105, 170	0
1	BA	1539/1539 (100%)	-0.58	9 (0%) 89 72	0, 33, 101, 147	0
2	AB	218/218 (100%)	0.58	13 (5%) 21 7	12, 52, 84, 115	0
2	BB	218/218 (100%)	0.41	12 (5%) 25 9	19, 59, 88, 113	0
3	AC	206/206 (100%)	-0.32	0 100 100	0, 35, 69, 93	0
3	BC	206/206 (100%)	0.23	3 (1%) 73 46	9, 46, 75, 92	0
4	AD	205/205 (100%)	0.09	4 (1%) 65 36	14, 42, 73, 98	0
4	BD	205/205 (100%)	-0.26	1 (0%) 91 75	0, 24, 64, 82	0
5	AE	150/150 (100%)	-0.15	2 (1%) 77 51	0, 32, 68, 105	0
5	BE	150/150 (100%)	-0.38	0 100 100	0, 31, 68, 98	0
6	AF	100/100 (100%)	-0.37	0 100 100	0, 33, 68, 86	0
6	BF	100/100 (100%)	-0.01	0 100 100	17, 54, 80, 93	0
7	AG	151/151 (100%)	0.50	14 (9%) 8 3	12, 56, 86, 111	0
7	BG	151/151 (100%)	0.01	5 (3%) 46 20	20, 54, 81, 94	0
8	AH	129/129 (100%)	-0.48	0 100 100	0, 32, 60, 71	0
8	BH	129/129 (100%)	-0.25	1 (0%) 86 65	4, 34, 58, 82	0
9	AI	127/127 (100%)	0.18	4 (3%) 49 21	6, 54, 79, 108	0
9	BI	127/127 (100%)	0.36	8 (6%) 20 6	20, 55, 85, 117	0
10	AJ	98/98 (100%)	0.42	5 (5%) 28 10	8, 55, 89, 104	0
10	BJ	98/98 (100%)	0.38	6 (6%) 21 7	25, 58, 82, 113	0
11	AK	117/117 (100%)	-0.37	1 (0%) 84 63	0, 19, 50, 87	0
11	BK	117/117 (100%)	-0.24	0 100 100	0, 32, 66, 79	0
12	AL	123/123 (100%)	-0.32	2 (1%) 72 44	0, 22, 67, 93	0
12	BL	123/123 (100%)	-0.27	3 (2%) 59 30	0, 17, 58, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($\AA^2$)	Q<0.9
13	AM	114/114 (100%)	0.08	5 (4%) 34 13	9, 53, 87, 100	0
13	BM	114/114 (100%)	0.73	7 (6%) 21 7	26, 63, 87, 97	0
14	AN	96/100 (96%)	-0.03	1 (1%) 82 59	12, 45, 84, 107	0
14	BN	96/100 (96%)	0.26	4 (4%) 36 14	10, 56, 84, 98	0
15	AO	88/88 (100%)	-0.40	1 (1%) 80 56	0, 28, 55, 93	0
15	BO	88/88 (100%)	-0.08	1 (1%) 80 56	1, 33, 66, 89	0
16	AP	82/82 (100%)	0.13	3 (3%) 41 17	5, 30, 73, 86	0
16	BP	82/82 (100%)	-0.12	4 (4%) 29 11	0, 24, 67, 91	0
17	AQ	80/80 (100%)	0.03	1 (1%) 77 51	8, 42, 75, 96	0
17	BQ	80/80 (100%)	-0.10	1 (1%) 77 51	7, 44, 79, 94	0
18	AR	55/55 (100%)	-0.37	1 (1%) 68 40	0, 25, 59, 93	0
18	BR	55/55 (100%)	-0.10	2 (3%) 42 17	5, 38, 80, 101	0
19	AS	79/79 (100%)	0.51	4 (5%) 28 10	21, 52, 83, 98	0
19	BS	79/79 (100%)	0.78	9 (11%) 5 1	37, 65, 83, 95	0
20	AT	85/85 (100%)	0.19	3 (3%) 44 18	7, 37, 67, 80	0
20	BT	85/85 (100%)	0.20	2 (2%) 59 30	8, 38, 69, 96	0
21	AU	51/51 (100%)	0.20	5 (9%) 7 2	7, 39, 74, 77	0
21	BU	51/51 (100%)	0.27	3 (5%) 22 7	8, 47, 74, 80	0
22	AV	76/76 (100%)	-0.23	1 (1%) 77 51	0, 70, 127, 154	0
22	BV	76/76 (100%)	-0.33	0 100 100	22, 43, 72, 119	0
23	AX	15/16 (93%)	0.40	1 (6%) 17 5	6, 76, 115, 133	0
23	BX	16/16 (100%)	0.19	1 (6%) 20 6	16, 77, 102, 124	0
24	AY	183/183 (100%)	0.71	38 (20%) 1 0	0, 50, 96, 117	0
25	CA	2897/2903 (99%)	-0.52	33 (1%) 80 56	0, 0, 103, 162	0
25	DA	2896/2903 (99%)	-0.60	25 (0%) 84 63	0, 15, 109, 162	0
26	CB	119/119 (100%)	-0.84	0 100 100	0, 7, 32, 85	0
27	CC	271/271 (100%)	-0.62	0 100 100	0, 1, 29, 56	0
27	DC	271/271 (100%)	-0.53	0 100 100	0, 19, 46, 77	0
28	CD	209/209 (100%)	-0.63	0 100 100	0, 0, 19, 61	0
28	DD	209/209 (100%)	-0.55	1 (0%) 91 75	0, 10, 52, 66	0
29	CE	201/201 (100%)	-0.53	0 100 100	0, 0, 39, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
29	DE	201/201 (100%)	-0.39	0 100 100	0, 21, 60, 89	0
30	CF	177/177 (100%)	0.06	3 (1%) 70 41	0, 35, 82, 91	0
30	DF	177/177 (100%)	0.41	8 (4%) 33 12	12, 58, 84, 95	0
31	CG	176/176 (100%)	-0.37	0 100 100	0, 15, 48, 88	0
31	DG	176/176 (100%)	0.19	2 (1%) 80 56	15, 48, 73, 93	0
32	CH	149/149 (100%)	0.10	7 (4%) 31 11	0, 52, 87, 100	0
32	DH	149/149 (100%)	0.60	7 (4%) 31 11	8, 58, 92, 107	0
33	CI	141/141 (100%)	2.32	73 (51%) 0 0	44, 79, 102, 124	0
33	DI	141/141 (100%)	2.45	71 (50%) 0 0	54, 82, 104, 118	0
34	CJ	142/142 (100%)	-0.61	0 100 100	0, 0, 21, 56	0
34	DJ	142/142 (100%)	-0.44	0 100 100	0, 8, 37, 65	0
35	CK	122/122 (100%)	-0.64	0 100 100	0, 0, 27, 73	0
35	DK	122/122 (100%)	-0.45	0 100 100	0, 15, 50, 71	0
36	CL	143/143 (100%)	-0.54	0 100 100	0, 0, 27, 68	0
36	DL	143/143 (100%)	-0.30	3 (2%) 63 34	0, 18, 56, 82	0
37	CM	136/136 (100%)	-0.61	0 100 100	0, 0, 21, 83	0
37	DM	136/136 (100%)	-0.17	1 (0%) 87 69	0, 21, 55, 88	0
38	CN	120/120 (100%)	-0.57	0 100 100	0, 0, 14, 68	0
38	DN	120/120 (100%)	-0.50	0 100 100	0, 12, 44, 78	0
39	CO	116/116 (100%)	-0.55	0 100 100	0, 11, 39, 49	0
39	DO	116/116 (100%)	0.33	8 (6%) 16 5	5, 49, 78, 98	0
40	CP	114/114 (100%)	-0.61	0 100 100	0, 0, 47, 70	0
40	DP	114/114 (100%)	-0.46	0 100 100	0, 21, 51, 81	0
41	CQ	117/117 (100%)	-0.60	0 100 100	0, 0, 7, 63	0
41	DQ	117/117 (100%)	-0.70	0 100 100	0, 2, 27, 45	0
42	CR	103/103 (100%)	-0.57	0 100 100	0, 0, 35, 57	0
42	DR	103/103 (100%)	-0.61	1 (0%) 82 59	0, 10, 46, 78	0
43	CS	110/110 (100%)	-0.46	1 (0%) 84 63	0, 0, 22, 98	0
43	DS	110/110 (100%)	-0.63	0 100 100	0, 8, 40, 77	0
44	CT	93/93 (100%)	-0.27	2 (2%) 62 33	0, 6, 68, 78	0
44	DT	93/93 (100%)	0.13	1 (1%) 80 56	0, 35, 71, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB($Å^2$)	Q<0.9
45	CU	102/102 (100%)	-0.49	2 (1%) 65 36	0, 5, 42, 79	0
45	DU	102/102 (100%)	0.36	10 (9%) 7 2	0, 34, 74, 100	0
46	CV	94/94 (100%)	-0.55	0 100 100	0, 6, 42, 62	0
46	DV	94/94 (100%)	-0.10	1 (1%) 80 56	11, 43, 68, 82	0
47	CW	76/76 (100%)	-0.54	0 100 100	0, 1, 31, 69	0
48	CX	77/77 (100%)	-0.47	0 100 100	0, 1, 47, 74	0
48	DX	77/77 (100%)	-0.42	0 100 100	0, 23, 55, 67	0
49	CY	63/63 (100%)	-0.32	2 (3%) 47 20	0, 14, 56, 97	0
49	DY	63/63 (100%)	-0.18	0 100 100	8, 43, 70, 111	0
50	CZ	58/58 (100%)	-0.53	0 100 100	0, 0, 13, 50	0
50	DZ	58/58 (100%)	-0.39	1 (1%) 70 41	0, 20, 52, 72	0
51	C0	56/56 (100%)	-0.60	0 100 100	0, 0, 25, 69	0
51	D0	56/56 (100%)	-0.54	0 100 100	0, 10, 53, 94	0
52	C1	50/50 (100%)	-0.03	1 (2%) 65 36	0, 8, 51, 93	0
52	D1	50/50 (100%)	0.47	3 (6%) 21 7	21, 38, 70, 88	0
53	C2	46/46 (100%)	-0.50	1 (2%) 62 33	0, 0, 15, 101	0
53	D2	46/46 (100%)	-0.64	0 100 100	0, 10, 26, 94	0
54	C3	64/64 (100%)	-0.61	0 100 100	0, 0, 11, 38	0
54	D3	64/64 (100%)	-0.42	0 100 100	0, 15, 35, 52	0
55	C4	38/38 (100%)	-0.38	0 100 100	0, 1, 32, 72	0
55	D4	38/38 (100%)	-0.12	0 100 100	3, 26, 59, 65	0
56	DB	118/118 (100%)	-0.71	0 100 100	6, 58, 86, 106	0
57	DW	75/75 (100%)	-0.16	0 100 100	0, 27, 54, 94	0
All	All	20908/20931 (99%)	-0.31	466 (2%) 62 33	0, 23, 86, 170	0

The worst 5 of 466 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	CI	52	LEU	10.6
33	DI	2	LYS	9.5
33	DI	59	THR	9.0
33	DI	4	VAL	8.9
33	CI	48	ILE	8.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
58	MG	DA	3115	1/1	0.60	0.18	27,27,27,27	0
58	MG	DA	3083	1/1	0.64	0.22	31,31,31,31	0
58	MG	DA	3098	1/1	0.65	0.54	49,49,49,49	0
58	MG	DA	3055	1/1	0.71	0.13	28,28,28,28	0
58	MG	DA	3091	1/1	0.71	0.26	50,50,50,50	0
58	MG	DA	3088	1/1	0.74	0.11	12,12,12,12	0
58	MG	AA	1640	1/1	0.74	0.18	34,34,34,34	0
58	MG	BA	1631	1/1	0.78	0.13	35,35,35,35	0
58	MG	CA	3084	1/1	0.78	0.11	22,22,22,22	0
58	MG	CA	3015	1/1	0.79	0.25	36,36,36,36	0
58	MG	CA	3062	1/1	0.80	0.46	46,46,46,46	0
58	MG	BA	1630	1/1	0.80	0.07	41,41,41,41	0
58	MG	DA	3061	1/1	0.81	0.19	24,24,24,24	0
58	MG	BA	1602	1/1	0.82	0.08	21,21,21,21	0
58	MG	AA	1631	1/1	0.82	0.17	35,35,35,35	0
58	MG	DA	3078	1/1	0.82	0.09	15,15,15,15	0
58	MG	AA	1601	1/1	0.82	0.10	44,44,44,44	0
58	MG	AA	1620	1/1	0.83	0.07	10,10,10,10	0
58	MG	AA	1644	1/1	0.83	0.19	5,5,5,5	0
58	MG	CA	3105	1/1	0.84	0.16	0,0,0,0	0
58	MG	CA	3106	1/1	0.84	0.18	0,0,0,0	0
58	MG	DA	3116	1/1	0.84	0.14	13,13,13,13	0
58	MG	AA	1603	1/1	0.85	0.08	28,28,28,28	0
58	MG	DA	3080	1/1	0.85	0.09	1,1,1,1	0
58	MG	AA	1626	1/1	0.85	0.10	0,0,0,0	0
58	MG	AA	1611	1/1	0.85	0.09	0,0,0,0	0
58	MG	DA	3136	1/1	0.85	0.11	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	BA	1636	1/1	0.86	0.10	42,42,42,42	0
58	MG	CA	3082	1/1	0.86	0.12	0,0,0,0	0
58	MG	DA	3090	1/1	0.86	0.08	15,15,15,15	0
58	MG	AA	1639	1/1	0.86	0.10	22,22,22,22	0
58	MG	DA	3015	1/1	0.87	0.18	23,23,23,23	0
58	MG	AA	1662	1/1	0.87	0.10	8,8,8,8	0
58	MG	AA	1623	1/1	0.87	0.07	24,24,24,24	0
58	MG	BA	1618	1/1	0.87	0.19	4,4,4,4	0
58	MG	DA	3101	1/1	0.87	0.12	0,0,0,0	0
58	MG	AA	1658	1/1	0.87	0.19	16,16,16,16	0
58	MG	DA	3005	1/1	0.87	0.11	25,25,25,25	0
58	MG	DA	3084	1/1	0.87	0.12	32,32,32,32	0
58	MG	DA	3165	1/1	0.87	0.23	0,0,0,0	0
58	MG	CA	3099	1/1	0.88	0.85	53,53,53,53	0
58	MG	DA	3025	1/1	0.88	0.20	16,16,16,16	0
58	MG	BA	1641	1/1	0.88	0.09	20,20,20,20	0
58	MG	CA	3014	1/1	0.88	0.14	12,12,12,12	0
58	MG	DA	3064	1/1	0.88	0.10	0,0,0,0	0
58	MG	AA	1617	1/1	0.88	0.05	21,21,21,21	0
58	MG	DB	203	1/1	0.88	0.06	16,16,16,16	0
58	MG	BA	1624	1/1	0.89	0.07	1,1,1,1	0
58	MG	CA	3019	1/1	0.89	0.09	0,0,0,0	0
58	MG	DA	3050	1/1	0.89	0.06	0,0,0,0	0
58	MG	CA	3117	1/1	0.89	0.14	5,5,5,5	0
58	MG	DA	3057	1/1	0.89	0.14	14,14,14,14	0
58	MG	CA	3134	1/1	0.89	0.32	14,14,14,14	0
58	MG	AA	1645	1/1	0.89	0.24	8,8,8,8	0
58	MG	AA	1669	1/1	0.90	0.14	10,10,10,10	0
58	MG	BA	1627	1/1	0.90	0.12	35,35,35,35	0
58	MG	AA	1634	1/1	0.90	0.05	2,2,2,2	0
58	MG	BA	1609	1/1	0.90	0.09	26,26,26,26	0
58	MG	BA	1614	1/1	0.90	0.07	19,19,19,19	0
58	MG	DA	3102	1/1	0.90	0.09	12,12,12,12	0
58	MG	DA	3103	1/1	0.90	0.08	0,0,0,0	0
58	MG	AA	1666	1/1	0.90	0.16	13,13,13,13	0
58	MG	CA	3089	1/1	0.90	0.08	19,19,19,19	0
58	MG	DA	3131	1/1	0.90	0.59	55,55,55,55	0
58	MG	CA	3092	1/1	0.90	0.09	16,16,16,16	0
58	MG	DA	3036	1/1	0.90	0.08	21,21,21,21	0
58	MG	DA	3087	1/1	0.90	0.05	20,20,20,20	0
58	MG	AA	1635	1/1	0.91	0.09	18,18,18,18	0
58	MG	AA	1637	1/1	0.91	0.09	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	BA	1653	1/1	0.91	0.08	7,7,7,7	0
58	MG	BA	1655	1/1	0.91	0.11	9,9,9,9	0
58	MG	AA	1606	1/1	0.91	0.06	6,6,6,6	0
58	MG	AA	1660	1/1	0.91	0.12	15,15,15,15	0
58	MG	DA	3047	1/1	0.91	0.05	28,28,28,28	0
58	MG	DA	3133	1/1	0.91	0.17	16,16,16,16	0
58	MG	AA	1604	1/1	0.91	0.18	22,22,22,22	0
58	MG	DA	3160	1/1	0.91	0.12	0,0,0,0	0
58	MG	CA	3026	1/1	0.91	0.33	30,30,30,30	0
58	MG	CA	3114	1/1	0.91	0.10	0,0,0,0	0
58	MG	AA	1655	1/1	0.92	0.15	0,0,0,0	0
58	MG	AA	1670	1/1	0.92	0.27	11,11,11,11	0
58	MG	DA	3063	1/1	0.92	0.15	0,0,0,0	0
58	MG	CA	3091	1/1	0.92	0.08	3,3,3,3	0
58	MG	DA	3070	1/1	0.92	0.08	0,0,0,0	0
58	MG	DA	3071	1/1	0.92	0.08	0,0,0,0	0
58	MG	BA	1635	1/1	0.92	0.08	21,21,21,21	0
58	MG	DA	3079	1/1	0.92	0.08	27,27,27,27	0
58	MG	AA	1630	1/1	0.92	0.09	16,16,16,16	0
58	MG	CA	3102	1/1	0.92	0.15	0,0,0,0	0
58	MG	BA	1605	1/1	0.92	0.06	21,21,21,21	0
58	MG	BA	1649	1/1	0.92	0.15	11,11,11,11	0
58	MG	BA	1608	1/1	0.92	0.15	18,18,18,18	0
58	MG	AA	1659	1/1	0.92	0.08	12,12,12,12	0
58	MG	BA	1611	1/1	0.92	0.11	13,13,13,13	0
58	MG	DA	3092	1/1	0.92	0.25	34,34,34,34	0
58	MG	DA	3095	1/1	0.92	0.11	10,10,10,10	0
58	MG	CA	3138	1/1	0.92	0.43	0,0,0,0	0
58	MG	CA	3164	1/1	0.92	0.24	0,0,0,0	0
58	MG	AA	1613	1/1	0.92	0.06	2,2,2,2	0
58	MG	DA	3006	1/1	0.92	0.05	10,10,10,10	0
58	MG	AA	1636	1/1	0.92	0.08	0,0,0,0	0
58	MG	DA	3019	1/1	0.92	0.11	0,0,0,0	0
58	MG	AA	1632	1/1	0.92	0.07	15,15,15,15	0
58	MG	DA	3030	1/1	0.92	0.12	0,0,0,0	0
58	MG	CA	3028	1/1	0.92	0.14	21,21,21,21	0
58	MG	DA	3138	1/1	0.92	0.45	0,0,0,0	0
58	MG	DA	3152	1/1	0.92	0.17	6,6,6,6	0
58	MG	CA	3048	1/1	0.92	0.09	13,13,13,13	0
58	MG	AA	1667	1/1	0.92	0.26	13,13,13,13	0
58	MG	BA	1629	1/1	0.92	0.06	17,17,17,17	0
58	MG	CA	3187	1/1	0.93	0.16	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3024	1/1	0.93	0.11	0,0,0,0	0
58	MG	CA	3025	1/1	0.93	0.17	0,0,0,0	0
58	MG	DA	3014	1/1	0.93	0.11	12,12,12,12	0
58	MG	BA	1625	1/1	0.93	0.06	0,0,0,0	0
58	MG	DA	3016	1/1	0.93	0.08	1,1,1,1	0
58	MG	BA	1634	1/1	0.93	0.05	10,10,10,10	0
58	MG	AA	1654	1/1	0.93	0.16	5,5,5,5	0
58	MG	CA	3002	1/1	0.93	0.07	0,0,0,0	0
58	MG	CA	3112	1/1	0.93	0.10	4,4,4,4	0
58	MG	DA	3038	1/1	0.93	0.12	0,0,0,0	0
58	MG	CA	3076	1/1	0.93	0.15	0,0,0,0	0
58	MG	CA	3116	1/1	0.93	0.22	10,10,10,10	0
58	MG	CA	3080	1/1	0.93	0.07	1,1,1,1	0
58	MG	CA	3129	1/1	0.93	0.12	0,0,0,0	0
58	MG	CA	3132	1/1	0.93	0.40	24,24,24,24	0
58	MG	DA	3062	1/1	0.93	0.09	0,0,0,0	0
58	MG	AA	1627	1/1	0.93	0.14	19,19,19,19	0
58	MG	AA	1641	1/1	0.93	0.09	0,0,0,0	0
58	MG	DA	3065	1/1	0.93	0.08	0,0,0,0	0
58	MG	CA	3154	1/1	0.93	0.29	0,0,0,0	0
58	MG	BA	1645	1/1	0.93	0.08	8,8,8,8	0
58	MG	DA	3161	1/1	0.93	0.09	15,15,15,15	0
58	MG	DA	3075	1/1	0.93	0.12	8,8,8,8	0
58	MG	CA	3185	1/1	0.93	0.28	0,0,0,0	0
58	MG	DL	201	1/1	0.93	0.05	10,10,10,10	0
58	MG	AA	1616	1/1	0.94	0.09	11,11,11,11	0
58	MG	CA	3135	1/1	0.94	0.12	0,0,0,0	0
58	MG	AA	1607	1/1	0.94	0.08	10,10,10,10	0
58	MG	BA	1626	1/1	0.94	0.06	14,14,14,14	0
58	MG	CA	3160	1/1	0.94	0.32	0,0,0,0	0
58	MG	AA	1625	1/1	0.94	0.07	6,6,6,6	0
58	MG	CA	3178	1/1	0.94	0.13	0,0,0,0	0
58	MG	AA	1671	1/1	0.94	0.17	6,6,6,6	0
58	MG	DA	3077	1/1	0.94	0.05	12,12,12,12	0
58	MG	CA	3006	1/1	0.94	0.07	1,1,1,1	0
58	MG	CA	3191	1/1	0.94	0.20	0,0,0,0	0
58	MG	CA	3194	1/1	0.94	0.19	0,0,0,0	0
58	MG	CB	201	1/1	0.94	0.05	0,0,0,0	0
58	MG	DA	3003	1/1	0.94	0.07	8,8,8,8	0
58	MG	DA	3085	1/1	0.94	0.20	0,0,0,0	0
58	MG	DA	3004	1/1	0.94	0.10	30,30,30,30	0
58	MG	BA	1612	1/1	0.94	0.05	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	AA	1619	1/1	0.94	0.16	32,32,32,32	0
58	MG	DA	3009	1/1	0.94	0.09	4,4,4,4	0
58	MG	DA	3010	1/1	0.94	0.09	7,7,7,7	0
58	MG	BA	1632	1/1	0.94	0.04	18,18,18,18	0
58	MG	CA	3100	1/1	0.94	0.10	0,0,0,0	0
58	MG	BA	1633	1/1	0.94	0.12	11,11,11,11	0
58	MG	BA	1615	1/1	0.94	0.18	9,9,9,9	0
58	MG	BA	1617	1/1	0.94	0.06	13,13,13,13	0
58	MG	DA	3109	1/1	0.94	0.13	2,2,2,2	0
58	MG	DA	3110	1/1	0.94	0.05	18,18,18,18	0
58	MG	DA	3112	1/1	0.94	0.09	5,5,5,5	0
58	MG	DA	3114	1/1	0.94	0.08	14,14,14,14	0
58	MG	DA	3026	1/1	0.94	0.09	0,0,0,0	0
58	MG	BA	1603	1/1	0.94	0.09	13,13,13,13	0
58	MG	DA	3119	1/1	0.94	0.15	44,44,44,44	0
58	MG	DA	3120	1/1	0.94	0.11	8,8,8,8	0
58	MG	DA	3124	1/1	0.94	0.05	0,0,0,0	0
58	MG	DA	3126	1/1	0.94	0.14	0,0,0,0	0
58	MG	DA	3033	1/1	0.94	0.12	0,0,0,0	0
58	MG	DA	3034	1/1	0.94	0.06	11,11,11,11	0
58	MG	DA	3135	1/1	0.94	0.08	11,11,11,11	0
58	MG	CA	3030	1/1	0.94	0.11	0,0,0,0	0
58	MG	CA	3035	1/1	0.94	0.07	1,1,1,1	0
58	MG	DA	3044	1/1	0.94	0.05	11,11,11,11	0
58	MG	DA	3156	1/1	0.94	0.23	3,3,3,3	0
58	MG	CA	3040	1/1	0.94	0.16	0,0,0,0	0
58	MG	CA	3120	1/1	0.94	0.12	2,2,2,2	0
58	MG	DA	3162	1/1	0.94	0.20	4,4,4,4	0
58	MG	BA	1622	1/1	0.94	0.05	4,4,4,4	0
58	MG	CA	3056	1/1	0.94	0.08	10,10,10,10	0
58	MG	DA	3059	1/1	0.94	0.11	6,6,6,6	0
58	MG	CA	3061	1/1	0.95	0.12	9,9,9,9	0
58	MG	CA	3009	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3063	1/1	0.95	0.12	0,0,0,0	0
58	MG	DA	3066	1/1	0.95	0.05	0,0,0,0	0
58	MG	CA	3168	1/1	0.95	0.20	0,0,0,0	0
58	MG	CA	3169	1/1	0.95	0.22	7,7,7,7	0
58	MG	CA	3171	1/1	0.95	0.14	0,0,0,0	0
58	MG	DA	3076	1/1	0.95	0.09	5,5,5,5	0
58	MG	CA	3173	1/1	0.95	0.25	0,0,0,0	0
58	MG	CA	3175	1/1	0.95	0.17	0,0,0,0	0
58	MG	BA	1637	1/1	0.95	0.16	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3180	1/1	0.95	0.19	6,6,6,6	0
58	MG	DA	3082	1/1	0.95	0.05	7,7,7,7	0
58	MG	BA	1639	1/1	0.95	0.06	0,0,0,0	0
58	MG	CA	3081	1/1	0.95	0.07	0,0,0,0	0
58	MG	AA	1602	1/1	0.95	0.11	17,17,17,17	0
58	MG	AA	1608	1/1	0.95	0.20	0,0,0,0	0
58	MG	CA	3085	1/1	0.95	0.21	12,12,12,12	0
58	MG	BA	1646	1/1	0.95	0.14	10,10,10,10	0
58	MG	BA	1613	1/1	0.95	0.13	0,0,0,0	0
58	MG	CA	3027	1/1	0.95	0.14	0,0,0,0	0
58	MG	CA	3098	1/1	0.95	0.14	0,0,0,0	0
58	MG	DA	3096	1/1	0.95	0.06	13,13,13,13	0
58	MG	BA	1652	1/1	0.95	0.10	1,1,1,1	0
58	MG	DA	3099	1/1	0.95	0.07	0,0,0,0	0
58	MG	AA	1653	1/1	0.95	0.15	1,1,1,1	0
58	MG	CA	3101	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3032	1/1	0.95	0.07	0,0,0,0	0
58	MG	CA	3034	1/1	0.95	0.20	0,0,0,0	0
58	MG	AA	1663	1/1	0.95	0.10	6,6,6,6	0
58	MG	DA	3111	1/1	0.95	0.08	1,1,1,1	0
58	MG	DA	3021	1/1	0.95	0.08	3,3,3,3	0
58	MG	DA	3113	1/1	0.95	0.12	0,0,0,0	0
58	MG	CA	3109	1/1	0.95	0.15	0,0,0,0	0
58	MG	CA	3001	1/1	0.95	0.10	0,0,0,0	0
58	MG	DA	3027	1/1	0.95	0.10	14,14,14,14	0
58	MG	DA	3117	1/1	0.95	0.05	5,5,5,5	0
58	MG	DA	3118	1/1	0.95	0.10	7,7,7,7	0
58	MG	DA	3028	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3041	1/1	0.95	0.16	0,0,0,0	0
58	MG	DA	3122	1/1	0.95	0.15	0,0,0,0	0
58	MG	CA	3044	1/1	0.95	0.06	0,0,0,0	0
58	MG	CA	3045	1/1	0.95	0.10	0,0,0,0	0
58	MG	CA	3046	1/1	0.95	0.06	0,0,0,0	0
58	MG	DA	3037	1/1	0.95	0.18	0,0,0,0	0
58	MG	CA	3121	1/1	0.95	0.19	0,0,0,0	0
58	MG	CA	3126	1/1	0.95	0.13	0,0,0,0	0
58	MG	DA	3045	1/1	0.95	0.09	0,0,0,0	0
58	MG	DA	3145	1/1	0.95	0.11	0,0,0,0	0
58	MG	DA	3149	1/1	0.95	0.18	0,0,0,0	0
58	MG	CA	3127	1/1	0.95	0.11	0,0,0,0	0
58	MG	BA	1616	1/1	0.95	0.11	0,0,0,0	0
58	MG	CA	3051	1/1	0.95	0.09	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	AA	1665	1/1	0.95	0.08	0,0,0,0	0
58	MG	CA	3058	1/1	0.95	0.10	10,10,10,10	0
58	MG	DA	3060	1/1	0.95	0.13	5,5,5,5	0
58	MG	DB	201	1/1	0.95	0.05	24,24,24,24	0
58	MG	CA	3059	1/1	0.95	0.07	4,4,4,4	0
58	MG	CA	3153	1/1	0.95	0.29	0,0,0,0	0
58	MG	BA	1643	1/1	0.96	0.14	3,3,3,3	0
58	MG	CA	3090	1/1	0.96	0.08	1,1,1,1	0
58	MG	CA	3172	1/1	0.96	0.17	0,0,0,0	0
58	MG	AA	1656	1/1	0.96	0.13	14,14,14,14	0
58	MG	AA	1657	1/1	0.96	0.18	2,2,2,2	0
58	MG	DA	3073	1/1	0.96	0.11	6,6,6,6	0
58	MG	CA	3177	1/1	0.96	0.13	0,0,0,0	0
58	MG	CA	3093	1/1	0.96	0.12	11,11,11,11	0
58	MG	CA	3179	1/1	0.96	0.15	0,0,0,0	0
58	MG	CA	3094	1/1	0.96	0.06	3,3,3,3	0
58	MG	CA	3181	1/1	0.96	0.15	0,0,0,0	0
58	MG	BA	1648	1/1	0.96	0.17	0,0,0,0	0
58	MG	AA	1643	1/1	0.96	0.27	0,0,0,0	0
58	MG	CA	3188	1/1	0.96	0.15	2,2,2,2	0
58	MG	AA	1612	1/1	0.96	0.05	0,0,0,0	0
58	MG	CA	3193	1/1	0.96	0.25	0,0,0,0	0
58	MG	AA	1614	1/1	0.96	0.05	12,12,12,12	0
58	MG	BA	1654	1/1	0.96	0.10	22,22,22,22	0
58	MG	CB	202	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3001	1/1	0.96	0.05	0,0,0,0	0
58	MG	DA	3002	1/1	0.96	0.06	1,1,1,1	0
58	MG	DA	3093	1/1	0.96	0.08	2,2,2,2	0
58	MG	DA	3094	1/1	0.96	0.08	43,43,43,43	0
58	MG	AA	1646	1/1	0.96	0.17	0,0,0,0	0
58	MG	BA	1656	1/1	0.96	0.19	9,9,9,9	0
58	MG	AA	1647	1/1	0.96	0.23	1,1,1,1	0
58	MG	CA	3111	1/1	0.96	0.04	6,6,6,6	0
58	MG	DA	3100	1/1	0.96	0.06	4,4,4,4	0
58	MG	AA	1648	1/1	0.96	0.12	4,4,4,4	0
58	MG	CA	3003	1/1	0.96	0.06	0,0,0,0	0
58	MG	DA	3012	1/1	0.96	0.11	0,0,0,0	0
58	MG	DA	3105	1/1	0.96	0.11	0,0,0,0	0
58	MG	DA	3013	1/1	0.96	0.14	0,0,0,0	0
58	MG	AA	1649	1/1	0.96	0.23	0,0,0,0	0
58	MG	CA	3007	1/1	0.96	0.04	0,0,0,0	0
58	MG	AA	1651	1/1	0.96	0.24	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	DA	3018	1/1	0.96	0.07	6,6,6,6	0
58	MG	AA	1633	1/1	0.96	0.04	3,3,3,3	0
58	MG	CA	3124	1/1	0.96	0.09	0,0,0,0	0
58	MG	CA	3125	1/1	0.96	0.08	0,0,0,0	0
58	MG	AA	1622	1/1	0.96	0.17	0,0,0,0	0
58	MG	CA	3067	1/1	0.96	0.13	0,0,0,0	0
58	MG	CA	3070	1/1	0.96	0.12	25,25,25,25	0
58	MG	CA	3071	1/1	0.96	0.07	0,0,0,0	0
58	MG	DA	3121	1/1	0.96	0.07	7,7,7,7	0
58	MG	CA	3075	1/1	0.96	0.07	0,0,0,0	0
58	MG	AA	1618	1/1	0.96	0.07	21,21,21,21	0
58	MG	CA	3136	1/1	0.96	0.09	0,0,0,0	0
58	MG	CA	3137	1/1	0.96	0.09	4,4,4,4	0
58	MG	DA	3132	1/1	0.96	0.05	6,6,6,6	0
58	MG	CA	3021	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3040	1/1	0.96	0.14	5,5,5,5	0
58	MG	DA	3042	1/1	0.96	0.06	5,5,5,5	0
58	MG	CA	3140	1/1	0.96	0.52	0,0,0,0	0
58	MG	DA	3139	1/1	0.96	0.28	0,0,0,0	0
58	MG	CA	3146	1/1	0.96	0.33	0,0,0,0	0
58	MG	DA	3046	1/1	0.96	0.07	1,1,1,1	0
58	MG	DA	3150	1/1	0.96	0.15	0,0,0,0	0
58	MG	CA	3150	1/1	0.96	0.10	0,0,0,0	0
58	MG	DA	3154	1/1	0.96	0.17	0,0,0,0	0
58	MG	BA	1638	1/1	0.96	0.09	27,27,27,27	0
58	MG	BA	1620	1/1	0.96	0.07	19,19,19,19	0
58	MG	CA	3155	1/1	0.96	0.37	0,0,0,0	0
58	MG	AA	1672	1/1	0.96	0.21	3,3,3,3	0
58	MG	BA	1642	1/1	0.96	0.23	6,6,6,6	0
58	MG	DA	3166	1/1	0.96	0.20	9,9,9,9	0
58	MG	CA	3165	1/1	0.96	0.20	0,0,0,0	0
58	MG	DB	202	1/1	0.96	0.04	9,9,9,9	0
58	MG	CA	3166	1/1	0.96	0.14	0,0,0,0	0
58	MG	CA	3086	1/1	0.96	0.16	0,0,0,0	0
58	MG	CA	3052	1/1	0.97	0.12	0,0,0,0	0
58	MG	CA	3053	1/1	0.97	0.08	0,0,0,0	0
58	MG	BA	1651	1/1	0.97	0.14	7,7,7,7	0
58	MG	CA	3157	1/1	0.97	0.21	0,0,0,0	0
58	MG	CA	3158	1/1	0.97	0.33	0,0,0,0	0
58	MG	AA	1650	1/1	0.97	0.11	0,0,0,0	0
58	MG	DA	3023	1/1	0.97	0.06	0,0,0,0	0
58	MG	CA	3163	1/1	0.97	0.20	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3023	1/1	0.97	0.13	0,0,0,0	0
58	MG	CA	3103	1/1	0.97	0.09	0,0,0,0	0
58	MG	DA	3097	1/1	0.97	0.08	13,13,13,13	0
58	MG	CA	3104	1/1	0.97	0.06	0,0,0,0	0
58	MG	CA	3167	1/1	0.97	0.30	0,0,0,0	0
58	MG	DA	3031	1/1	0.97	0.11	0,0,0,0	0
58	MG	CA	3060	1/1	0.97	0.04	4,4,4,4	0
58	MG	BA	1623	1/1	0.97	0.08	3,3,3,3	0
58	MG	CA	3170	1/1	0.97	0.07	0,0,0,0	0
58	MG	DA	3104	1/1	0.97	0.09	0,0,0,0	0
58	MG	CA	3108	1/1	0.97	0.10	0,0,0,0	0
58	MG	BA	1610	1/1	0.97	0.03	0,0,0,0	0
58	MG	CA	3110	1/1	0.97	0.17	0,0,0,0	0
58	MG	AA	1615	1/1	0.97	0.08	9,9,9,9	0
58	MG	DA	3043	1/1	0.97	0.05	6,6,6,6	0
58	MG	CA	3176	1/1	0.97	0.14	10,10,10,10	0
58	MG	CA	3065	1/1	0.97	0.09	0,0,0,0	0
58	MG	CA	3113	1/1	0.97	0.12	0,0,0,0	0
58	MG	AA	1610	1/1	0.97	0.07	32,32,32,32	0
58	MG	CA	3115	1/1	0.97	0.06	0,0,0,0	0
58	MG	DA	3051	1/1	0.97	0.07	0,0,0,0	0
58	MG	AA	1624	1/1	0.97	0.06	10,10,10,10	0
58	MG	DA	3056	1/1	0.97	0.05	5,5,5,5	0
58	MG	CA	3183	1/1	0.97	0.18	0,0,0,0	0
58	MG	CA	3184	1/1	0.97	0.22	0,0,0,0	0
58	MG	DA	3123	1/1	0.97	0.05	6,6,6,6	0
58	MG	AA	1621	1/1	0.97	0.03	10,10,10,10	0
58	MG	CA	3074	1/1	0.97	0.15	0,0,0,0	0
58	MG	DA	3128	1/1	0.97	0.11	0,0,0,0	0
58	MG	CA	3031	1/1	0.97	0.22	0,0,0,0	0
58	MG	BA	1604	1/1	0.97	0.07	13,13,13,13	0
58	MG	CA	3079	1/1	0.97	0.05	3,3,3,3	0
58	MG	CA	3004	1/1	0.97	0.05	11,11,11,11	0
58	MG	BA	1644	1/1	0.97	0.09	0,0,0,0	0
58	MG	DA	3137	1/1	0.97	0.47	0,0,0,0	0
58	MG	DA	3067	1/1	0.97	0.07	0,0,0,0	0
58	MG	DA	3068	1/1	0.97	0.06	6,6,6,6	0
58	MG	DA	3140	1/1	0.97	0.28	0,0,0,0	0
58	MG	DA	3144	1/1	0.97	0.07	0,0,0,0	0
58	MG	DA	3069	1/1	0.97	0.09	41,41,41,41	0
58	MG	DA	3146	1/1	0.97	0.18	0,0,0,0	0
58	MG	DA	3147	1/1	0.97	0.19	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
58	MG	CA	3037	1/1	0.97	0.06	11,11,11,11	0
58	MG	CQ	201	1/1	0.97	0.31	0,0,0,0	0
58	MG	DA	3072	1/1	0.97	0.09	0,0,0,0	0
58	MG	AA	1668	1/1	0.97	0.09	0,0,0,0	0
58	MG	CA	3008	1/1	0.97	0.09	0,0,0,0	0
58	MG	DA	3157	1/1	0.97	0.22	0,0,0,0	0
58	MG	CA	3042	1/1	0.97	0.10	0,0,0,0	0
58	MG	BA	1606	1/1	0.97	0.12	24,24,24,24	0
58	MG	CA	3011	1/1	0.97	0.20	0,0,0,0	0
58	MG	DA	3164	1/1	0.97	0.15	0,0,0,0	0
58	MG	CA	3013	1/1	0.97	0.15	0,0,0,0	0
58	MG	BA	1607	1/1	0.97	0.06	1,1,1,1	0
58	MG	DA	3081	1/1	0.97	0.06	0,0,0,0	0
58	MG	CA	3145	1/1	0.97	0.13	0,0,0,0	0
58	MG	CA	3049	1/1	0.97	0.07	0,0,0,0	0
58	MG	AA	1661	1/1	0.97	0.15	15,15,15,15	0
58	MG	DQ	801	1/1	0.97	0.26	0,0,0,0	0
58	MG	CA	3088	1/1	0.98	0.10	0,0,0,0	0
58	MG	CA	3029	1/1	0.98	0.13	0,0,0,0	0
58	MG	CA	3054	1/1	0.98	0.14	0,0,0,0	0
58	MG	CA	3055	1/1	0.98	0.10	6,6,6,6	0
58	MG	CA	3010	1/1	0.98	0.11	0,0,0,0	0
58	MG	CA	3057	1/1	0.98	0.04	0,0,0,0	0
58	MG	CA	3141	1/1	0.98	0.27	0,0,0,0	0
58	MG	DA	3008	1/1	0.98	0.11	0,0,0,0	0
58	MG	DA	3086	1/1	0.98	0.15	0,0,0,0	0
58	MG	CA	3144	1/1	0.98	0.33	0,0,0,0	0
58	MG	BA	1621	1/1	0.98	0.05	12,12,12,12	0
58	MG	DA	3089	1/1	0.98	0.08	24,24,24,24	0
58	MG	DA	3011	1/1	0.98	0.08	0,0,0,0	0
58	MG	CA	3095	1/1	0.98	0.16	17,17,17,17	0
58	MG	CA	3147	1/1	0.98	0.27	0,0,0,0	0
58	MG	CA	3148	1/1	0.98	0.47	0,0,0,0	0
58	MG	CA	3149	1/1	0.98	0.32	0,0,0,0	0
58	MG	CA	3096	1/1	0.98	0.07	0,0,0,0	0
58	MG	DA	3017	1/1	0.98	0.13	0,0,0,0	0
58	MG	CA	3152	1/1	0.98	0.17	0,0,0,0	0
58	MG	CA	3097	1/1	0.98	0.12	0,0,0,0	0
58	MG	DA	3020	1/1	0.98	0.06	0,0,0,0	0
58	MG	CA	3012	1/1	0.98	0.18	0,0,0,0	0
58	MG	DA	3022	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3033	1/1	0.98	0.14	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	3024	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3156	1/1	0.98	0.30	0,0,0,0	0
58	MG	AA	1638	1/1	0.98	0.06	12,12,12,12	0
58	MG	DA	3106	1/1	0.98	0.17	0,0,0,0	0
58	MG	DA	3107	1/1	0.98	0.09	9,9,9,9	0
58	MG	AA	1642	1/1	0.98	0.06	1,1,1,1	0
58	MG	CA	3159	1/1	0.98	0.26	0,0,0,0	0
58	MG	CA	3036	1/1	0.98	0.16	0,0,0,0	0
58	MG	CA	3161	1/1	0.98	0.19	0,0,0,0	0
58	MG	DA	3032	1/1	0.98	0.08	0,0,0,0	0
58	MG	CA	3162	1/1	0.98	0.28	0,0,0,0	0
58	MG	CA	3064	1/1	0.98	0.18	0,0,0,0	0
58	MG	DA	3035	1/1	0.98	0.10	0,0,0,0	0
58	MG	BA	1601	1/1	0.98	0.08	2,2,2,2	0
58	MG	CA	3066	1/1	0.98	0.21	0,0,0,0	0
58	MG	CA	3039	1/1	0.98	0.11	0,0,0,0	0
58	MG	DA	3039	1/1	0.98	0.09	3,3,3,3	0
58	MG	CA	3107	1/1	0.98	0.17	0,0,0,0	0
58	MG	DA	3041	1/1	0.98	0.04	6,6,6,6	0
58	MG	CA	3069	1/1	0.98	0.14	0,0,0,0	0
58	MG	CA	3017	1/1	0.98	0.16	0,0,0,0	0
58	MG	DA	3125	1/1	0.98	0.07	0,0,0,0	0
58	MG	AA	1609	1/1	0.98	0.05	0,0,0,0	0
58	MG	DA	3127	1/1	0.98	0.05	0,0,0,0	0
58	MG	CA	3072	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3073	1/1	0.98	0.12	0,0,0,0	0
58	MG	CA	3020	1/1	0.98	0.12	0,0,0,0	0
58	MG	DA	3048	1/1	0.98	0.06	0,0,0,0	0
58	MG	DA	3049	1/1	0.98	0.05	0,0,0,0	0
58	MG	CA	3174	1/1	0.98	0.31	0,0,0,0	0
58	MG	CA	3043	1/1	0.98	0.07	0,0,0,0	0
58	MG	DA	3052	1/1	0.98	0.05	0,0,0,0	0
58	MG	DA	3054	1/1	0.98	0.09	0,0,0,0	0
58	MG	AA	1652	1/1	0.98	0.12	13,13,13,13	0
58	MG	DA	3142	1/1	0.98	0.16	0,0,0,0	0
58	MG	DA	3143	1/1	0.98	0.21	0,0,0,0	0
58	MG	CA	3077	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3078	1/1	0.98	0.07	0,0,0,0	0
58	MG	DA	3058	1/1	0.98	0.07	6,6,6,6	0
58	MG	CA	3118	1/1	0.98	0.08	0,0,0,0	0
58	MG	BA	1647	1/1	0.98	0.06	0,0,0,0	0
58	MG	AA	1628	1/1	0.98	0.04	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3123	1/1	0.98	0.20	0,0,0,0	0
58	MG	CA	3047	1/1	0.98	0.09	0,0,0,0	0
58	MG	DA	3155	1/1	0.98	0.18	1,1,1,1	0
58	MG	BA	1619	1/1	0.98	0.07	0,0,0,0	0
58	MG	CA	3186	1/1	0.98	0.27	0,0,0,0	0
58	MG	DA	3159	1/1	0.98	0.26	3,3,3,3	0
58	MG	CA	3083	1/1	0.98	0.04	10,10,10,10	0
58	MG	BA	1650	1/1	0.98	0.21	5,5,5,5	0
58	MG	CA	3189	1/1	0.98	0.14	0,0,0,0	0
58	MG	DA	3163	1/1	0.98	0.09	0,0,0,0	0
58	MG	CA	3128	1/1	0.98	0.14	0,0,0,0	0
58	MG	CA	3192	1/1	0.98	0.11	0,0,0,0	0
58	MG	AA	1664	1/1	0.98	0.11	4,4,4,4	0
58	MG	CA	3130	1/1	0.98	0.18	0,0,0,0	0
58	MG	CA	3131	1/1	0.98	0.15	0,0,0,0	0
58	MG	BA	1640	1/1	0.98	0.14	0,0,0,0	0
58	MG	CB	203	1/1	0.98	0.04	5,5,5,5	0
58	MG	CB	204	1/1	0.98	0.39	0,0,0,0	0
58	MG	DA	3141	1/1	0.99	0.23	0,0,0,0	0
58	MG	DA	3029	1/1	0.99	0.05	0,0,0,0	0
58	MG	CA	3190	1/1	0.99	0.23	0,0,0,0	0
58	MG	CA	3068	1/1	0.99	0.12	0,0,0,0	0
58	MG	CA	3142	1/1	0.99	0.41	0,0,0,0	0
58	MG	DA	3074	1/1	0.99	0.13	0,0,0,0	0
58	MG	DA	3053	1/1	0.99	0.06	0,0,0,0	0
58	MG	DA	3148	1/1	0.99	0.27	0,0,0,0	0
58	MG	CA	3143	1/1	0.99	0.29	0,0,0,0	0
58	MG	CA	3087	1/1	0.99	0.13	0,0,0,0	0
58	MG	DA	3151	1/1	0.99	0.15	11,11,11,11	0
58	MG	AA	1605	1/1	0.99	0.07	0,0,0,0	0
58	MG	DA	3153	1/1	0.99	0.10	11,11,11,11	0
58	MG	CA	3119	1/1	0.99	0.02	8,8,8,8	0
58	MG	CA	3022	1/1	0.99	0.14	0,0,0,0	0
58	MG	CA	3133	1/1	0.99	0.05	0,0,0,0	0
58	MG	CA	3016	1/1	0.99	0.12	0,0,0,0	0
58	MG	DA	3158	1/1	0.99	0.14	0,0,0,0	0
58	MG	CA	3182	1/1	0.99	0.30	0,0,0,0	0
58	MG	DA	3129	1/1	0.99	0.08	0,0,0,0	0
58	MG	DA	3130	1/1	0.99	0.11	0,0,0,0	0
58	MG	CA	3038	1/1	0.99	0.20	0,0,0,0	0
58	MG	CA	3151	1/1	0.99	0.32	0,0,0,0	0
58	MG	DA	3108	1/1	0.99	0.17	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
58	MG	DA	3134	1/1	0.99	0.07	0,0,0,0	0
58	MG	AA	1629	1/1	0.99	0.07	0,0,0,0	0
58	MG	CA	3018	1/1	0.99	0.18	0,0,0,0	0
58	MG	CA	3005	1/1	0.99	0.05	14,14,14,14	0
58	MG	DA	3007	1/1	0.99	0.19	26,26,26,26	0
58	MG	CA	3139	1/1	0.99	0.42	0,0,0,0	0
58	MG	BA	1628	1/1	0.99	0.08	25,25,25,25	0
59	ZN	C4	101	1/1	0.99	0.07	0,0,0,0	0
59	ZN	D4	101	1/1	0.99	0.06	41,41,41,41	0
58	MG	CA	3050	1/1	1.00	0.15	0,0,0,0	0
58	MG	CA	3122	1/1	1.00	0.11	0,0,0,0	0

6.5 Other polymers ⓘ

There are no such residues in this entry.