



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 12:24 PM UTC

PDB ID : 4V54 / pdb_00004v54
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-16
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

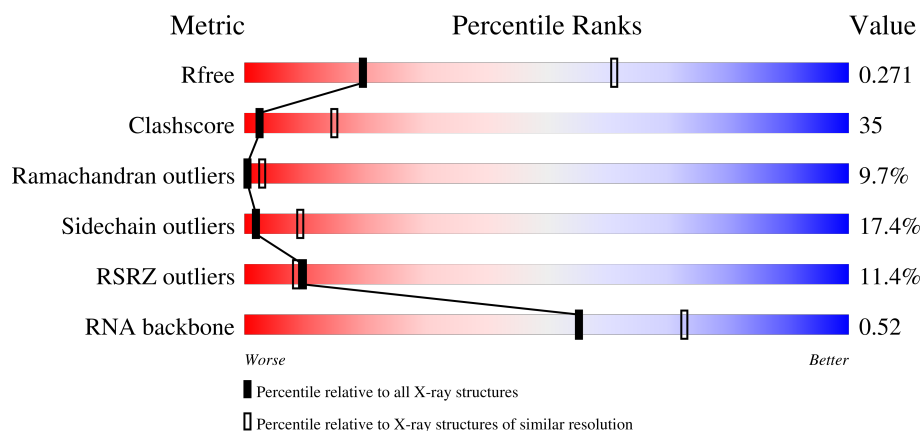
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	3% 26% 59% 13% ..
1	CA	1542	3% 26% 60% 12% ..
2	AC	232	5% 28% 48% 11% 11%
2	CC	232	7% 30% 46% 11% 11%

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Mol	Chain	Length	Quality of chain
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	

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Mol	Chain	Length	Quality of chain
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	

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Mol	Chain	Length	Quality of chain
53	B6	185	
53	D6	185	

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
54	MG	AA	2059	-	-	-	X
54	MG	DB	3058	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286960 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	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
15	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
20	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
30	DY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
31	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
32	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
33	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
34	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
36	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
39	DX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
40	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BU	102	Total	C	N	O		0	0	0
			779	492	146	141				
46	DU	102	Total	C	N	O		0	0	0
			779	492	146	141				

- Molecule 47 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
47	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
50	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
52	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 53 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	AA	60	Total	Mg	0	0
			60	60		
54	BB	110	Total	Mg	0	0
			110	110		
54	CE	1	Total	Mg	0	0
			1	1		
54	CA	61	Total	Mg	0	0
			61	61		
54	DB	111	Total	Mg	0	0
			111	111		

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B4	1	Total	Zn	0	0
			1	1		
55	D4	1	Total	Zn	0	0
			1	1		

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	289	Total	O	0	0
			289	289		
56	AE	4	Total	O	0	0
			4	4		
56	AK	1	Total	O	0	0
			1	1		
56	AL	1	Total	O	0	0
			1	1		
56	AN	3	Total	O	0	0
			3	3		
56	AP	1	Total	O	0	0
			1	1		

Continued on next page...

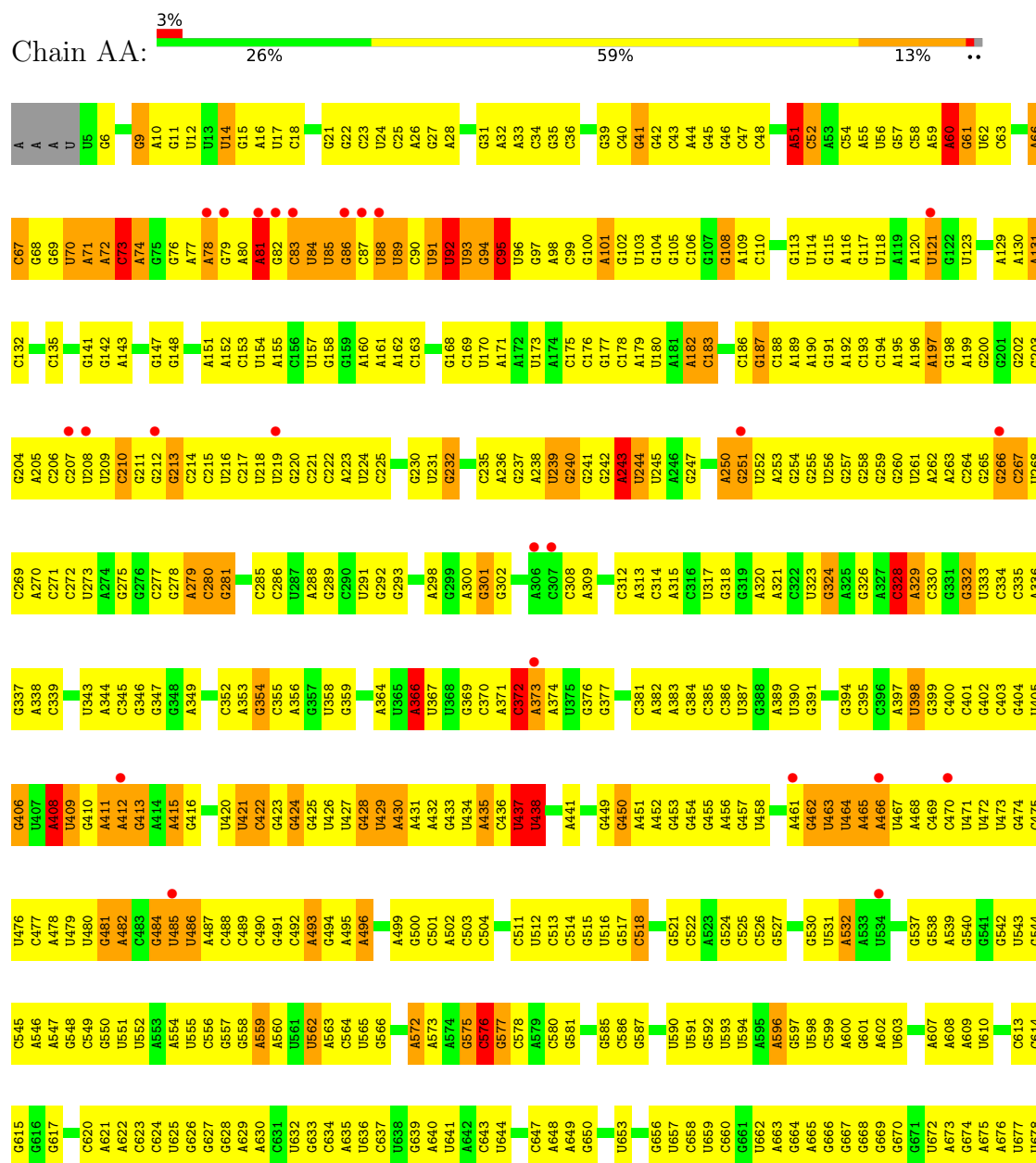
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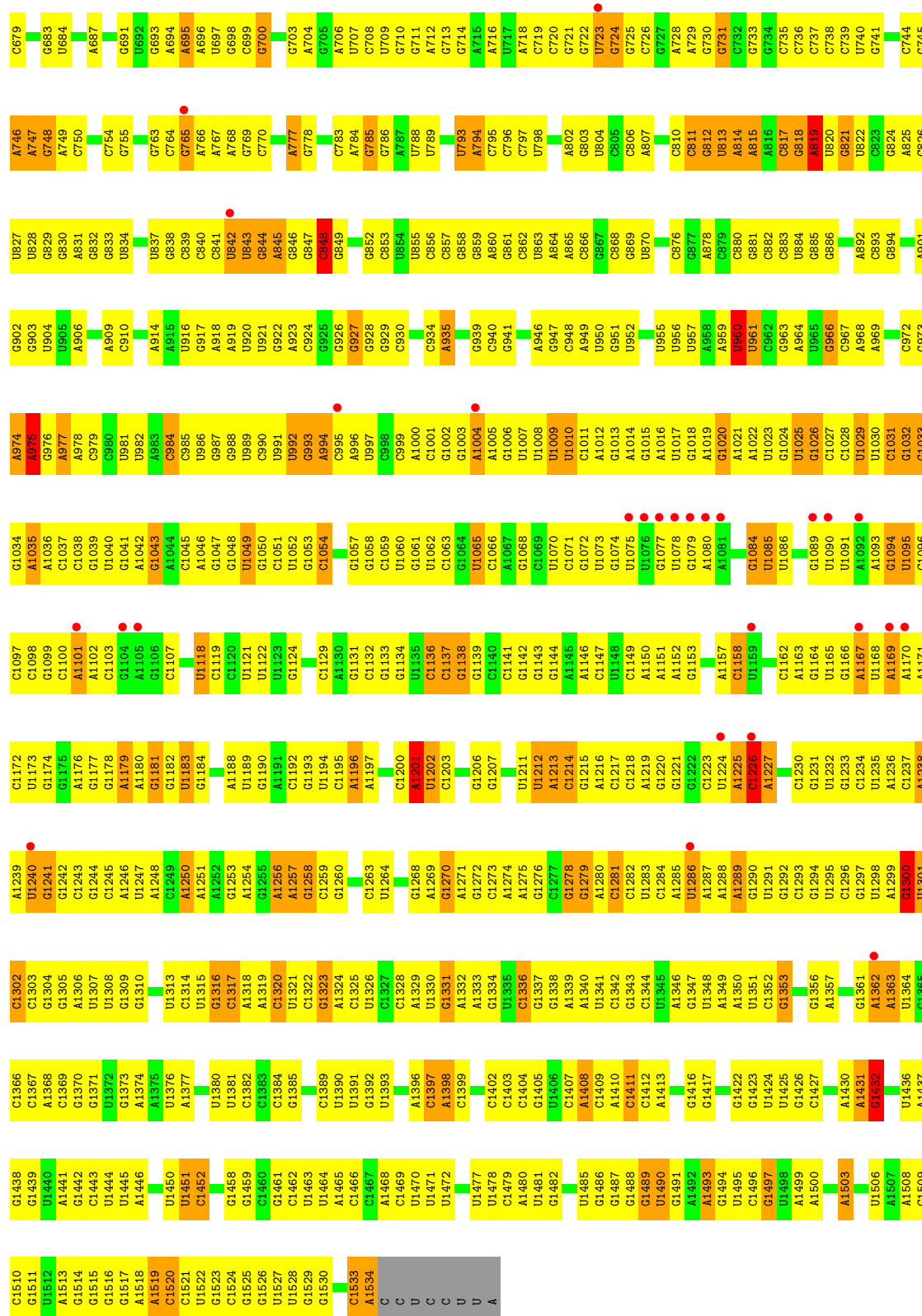
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	BB	495	Total 495	O 495	0	0
56	BC	4	Total 4	O 4	0	0
56	BD	1	Total 1	O 1	0	0
56	BE	3	Total 3	O 3	0	0
56	B2	1	Total 1	O 1	0	0
56	BL	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	4	Total 4	O 4	0	0
56	CT	1	Total 1	O 1	0	0
56	CA	300	Total 300	O 300	0	0
56	DB	505	Total 505	O 505	0	0
56	DC	4	Total 4	O 4	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	2	Total 2	O 2	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.

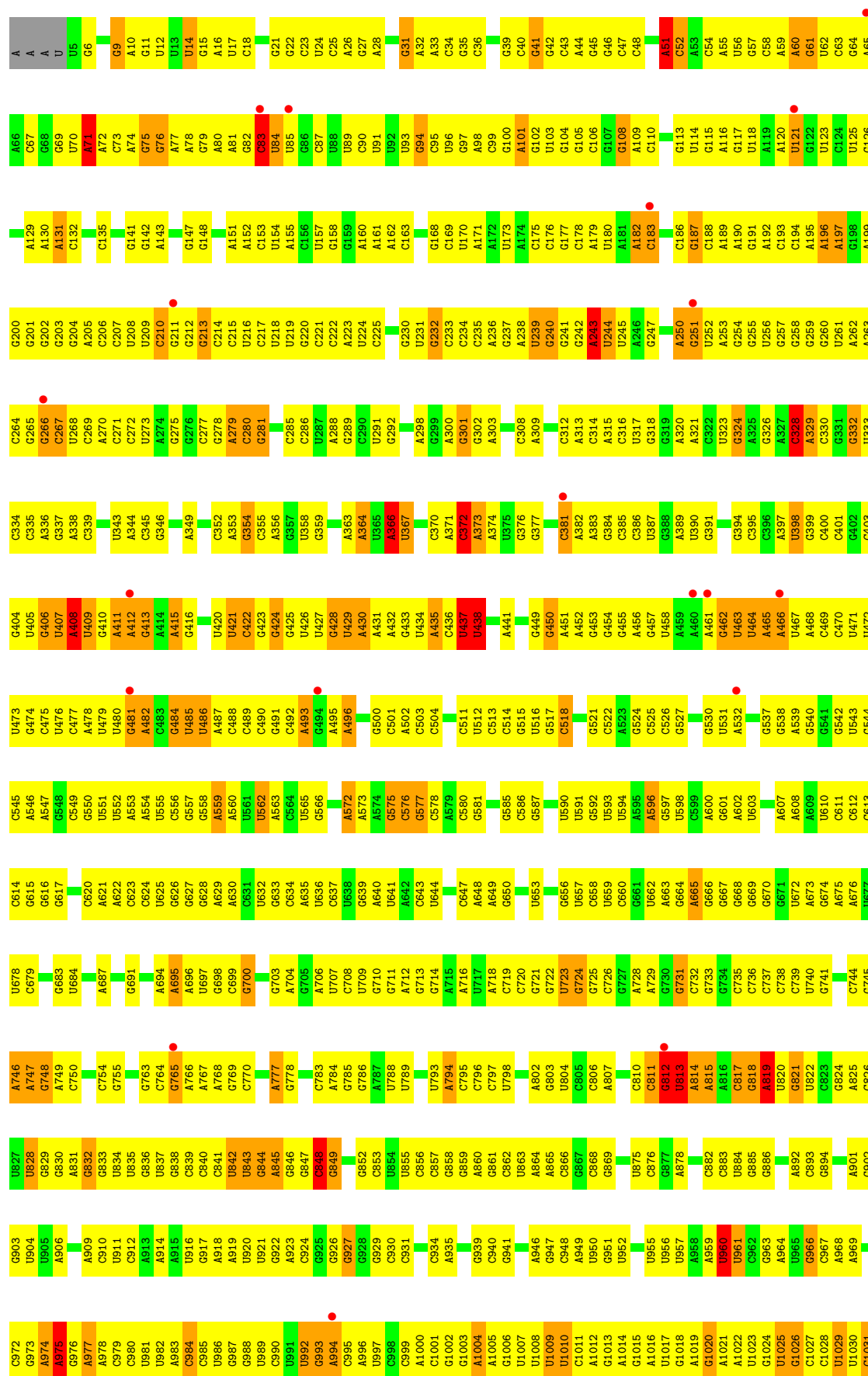
• Molecule 1: 16S rRNA

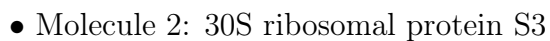


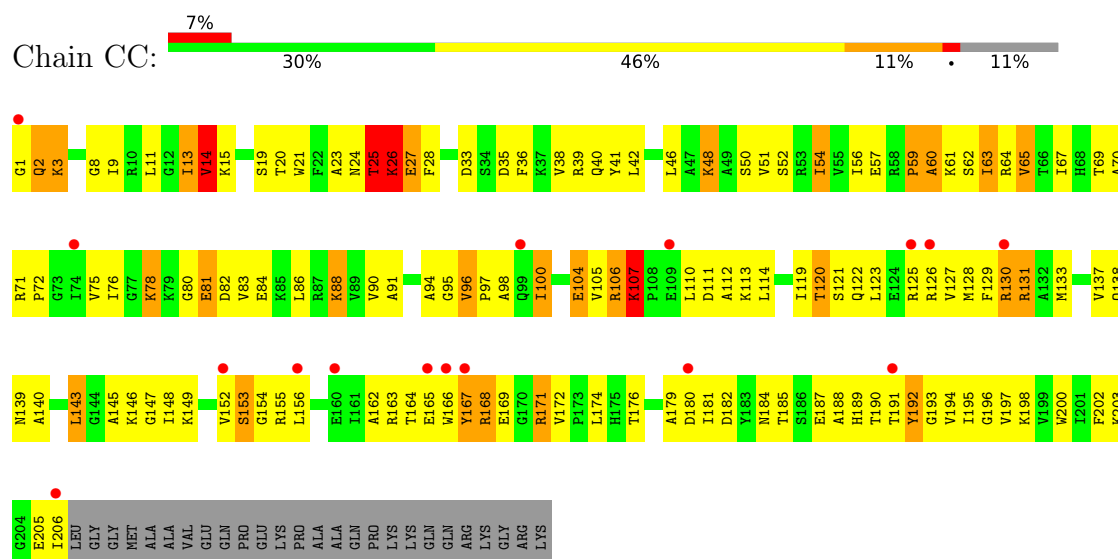


- Molecule 1: 16S rRNA

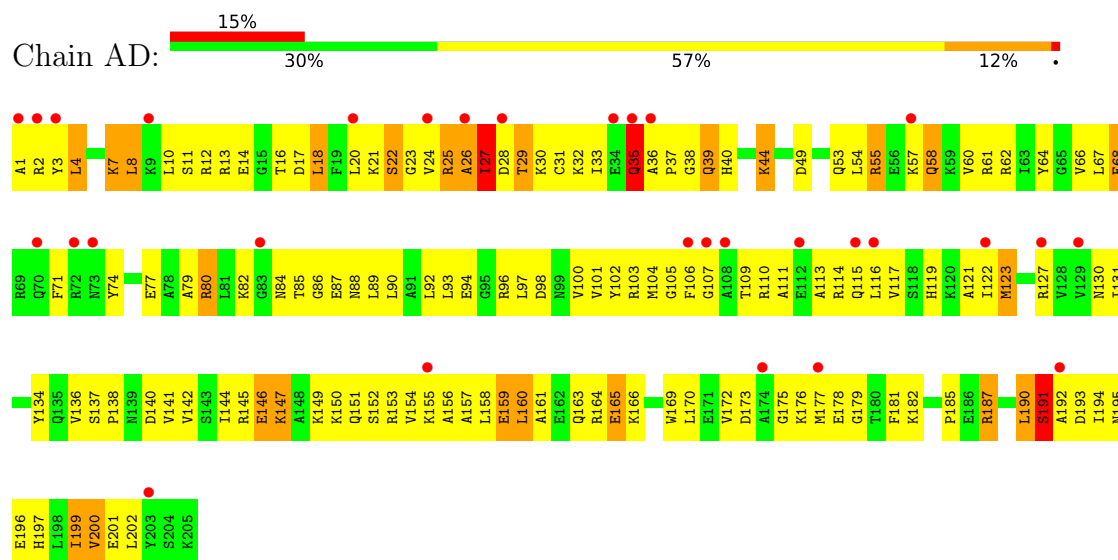




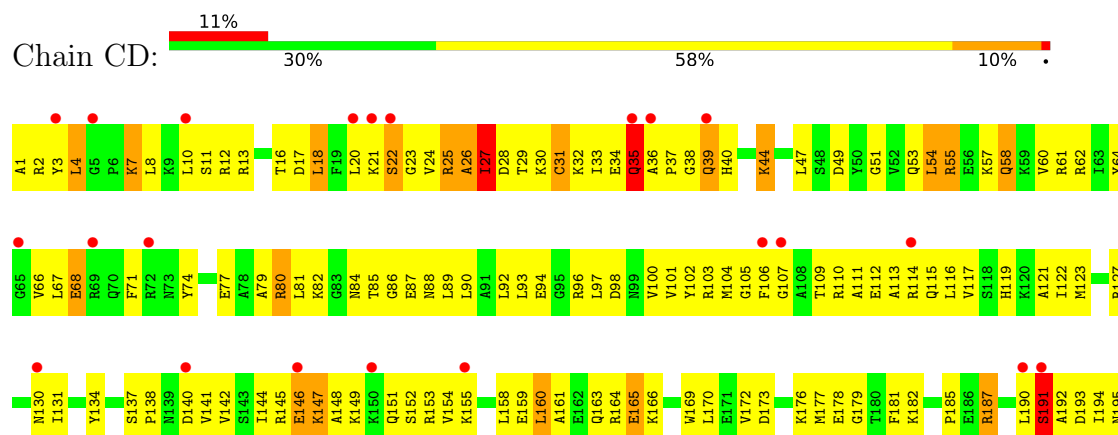


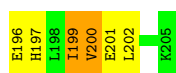


• Molecule 3: 30S ribosomal protein S4

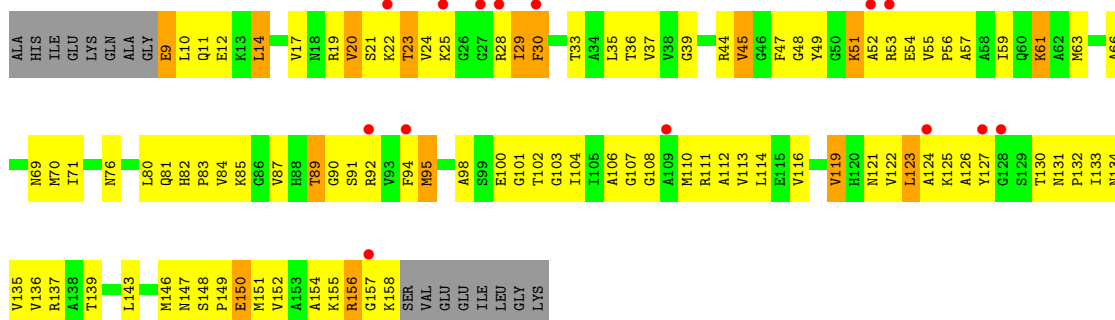


• Molecule 3: 30S ribosomal protein S4

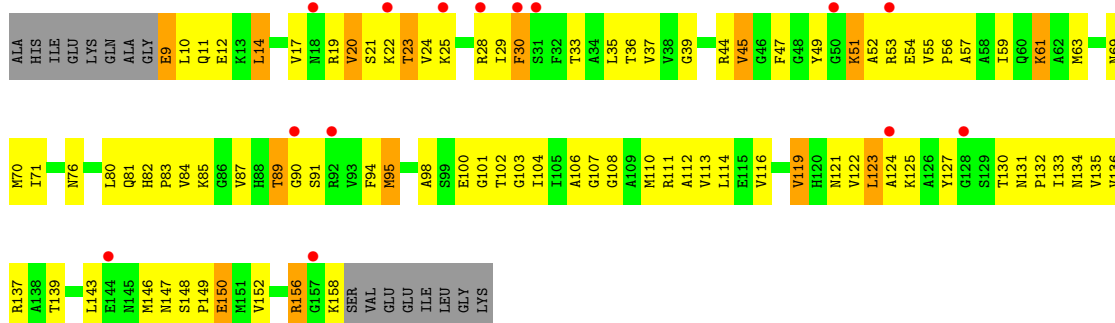




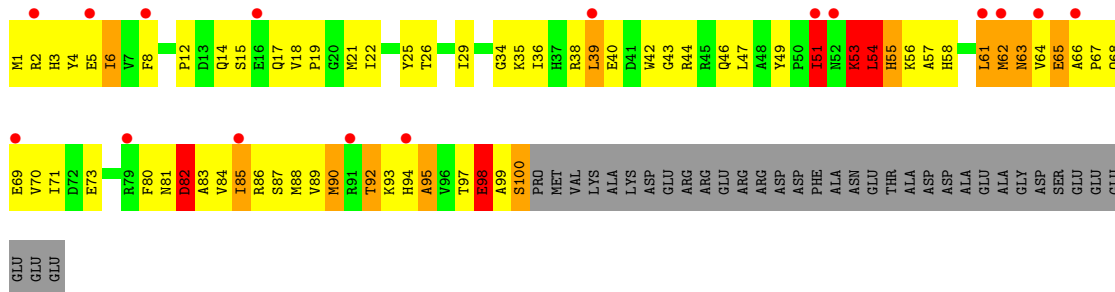
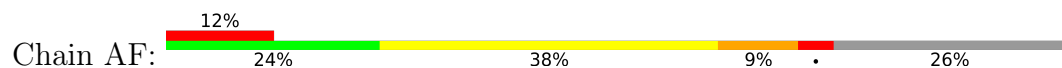
• Molecule 4: 30S ribosomal protein S5



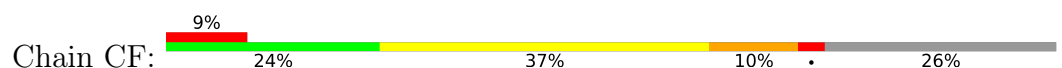
• Molecule 4: 30S ribosomal protein S5

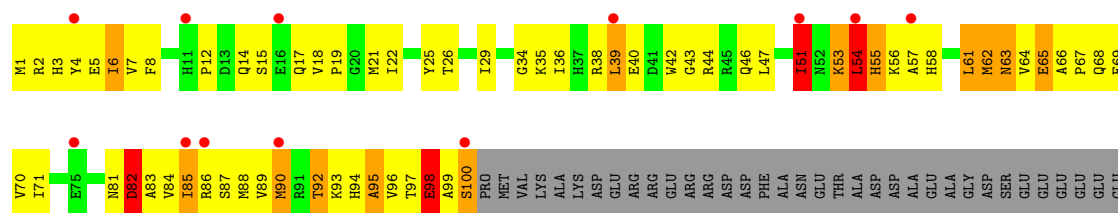


• Molecule 5: 30S ribosomal protein S6

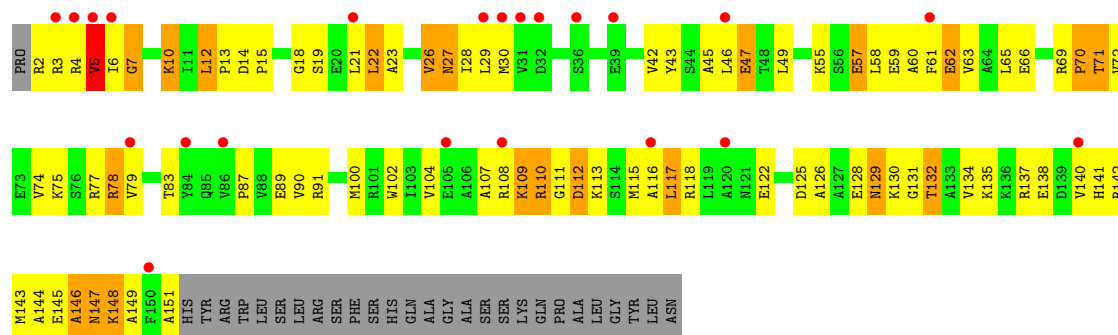


• Molecule 5: 30S ribosomal protein S6

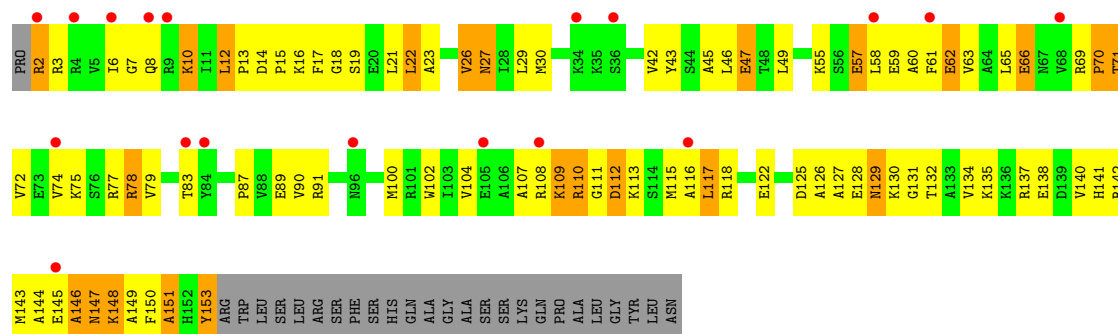




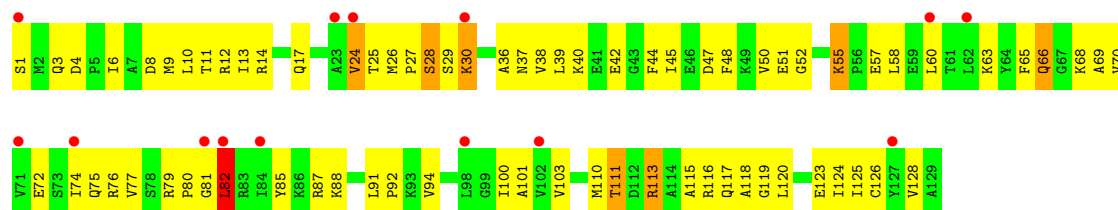
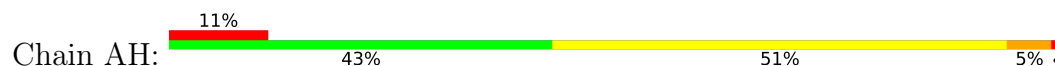
• Molecule 6: 30S ribosomal protein S7



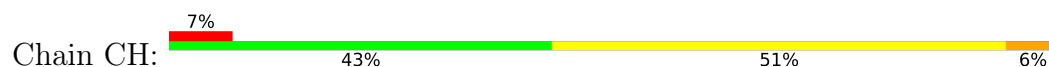
• Molecule 6: 30S ribosomal protein S7

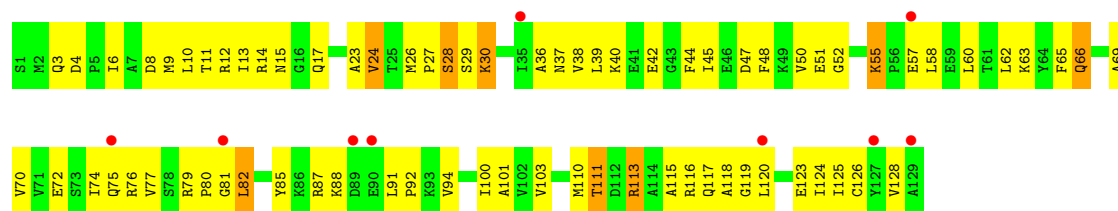


• Molecule 7: 30S ribosomal protein S8

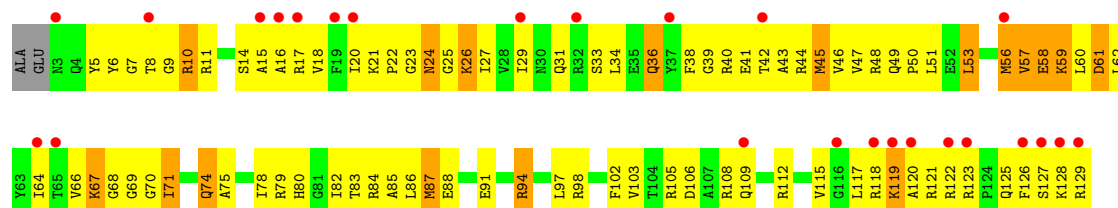


• Molecule 7: 30S ribosomal protein S8

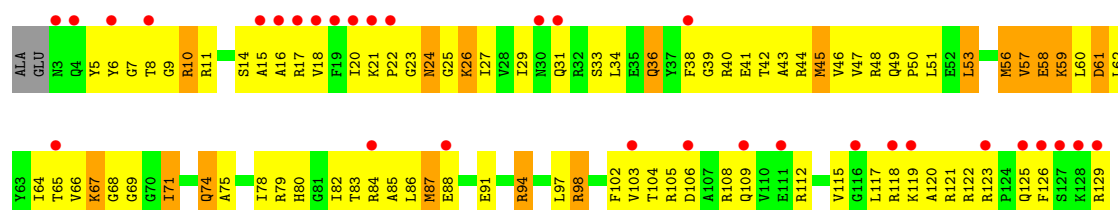




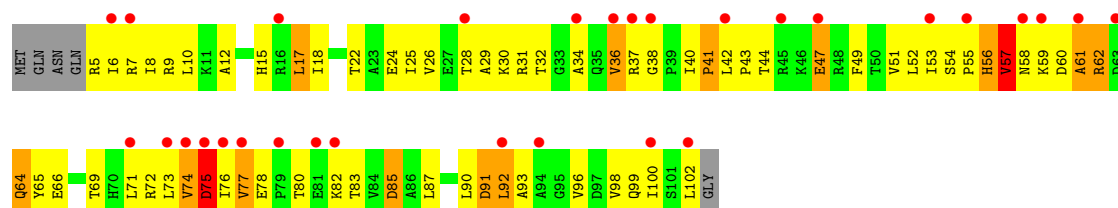
• Molecule 8: 30S ribosomal protein S9



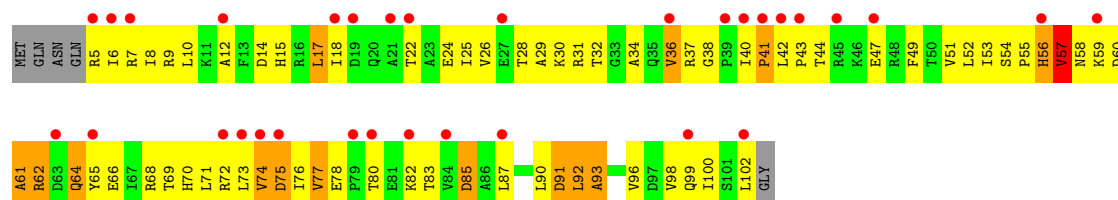
• Molecule 8: 30S ribosomal protein S9



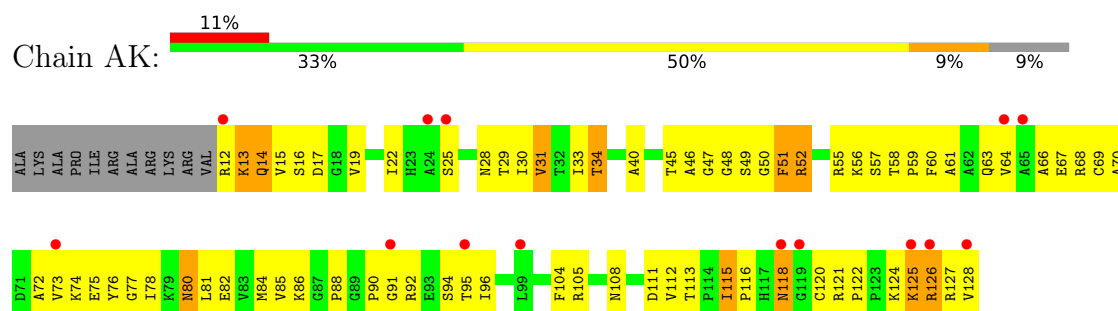
• Molecule 9: 30S ribosomal protein S10



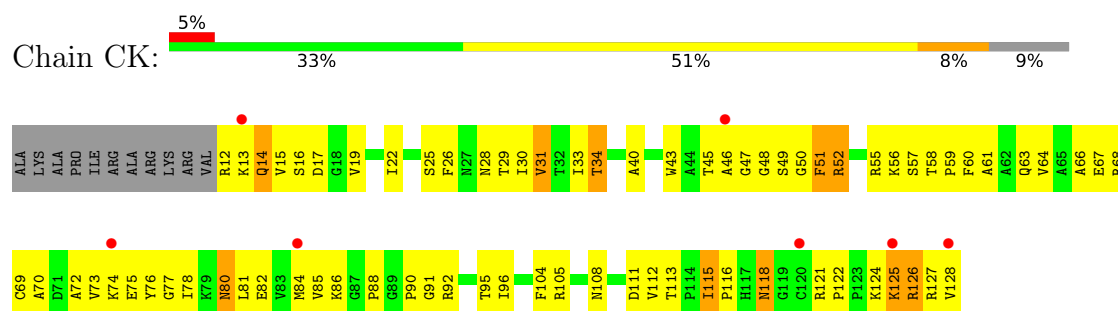
• Molecule 9: 30S ribosomal protein S10



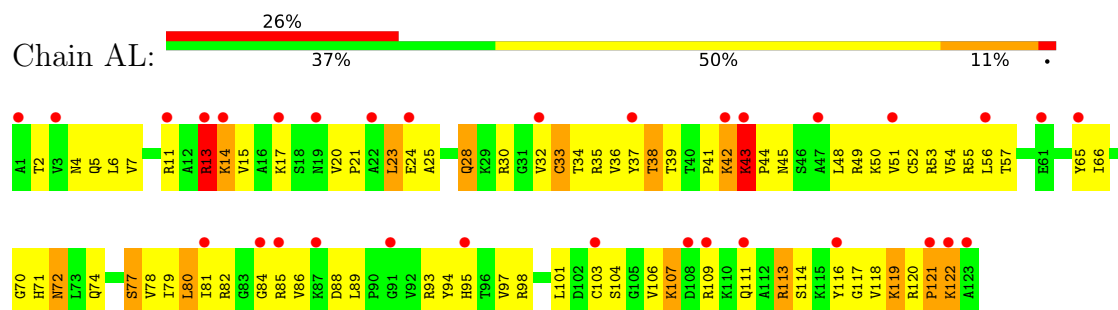
- Molecule 10: 30S ribosomal protein S11



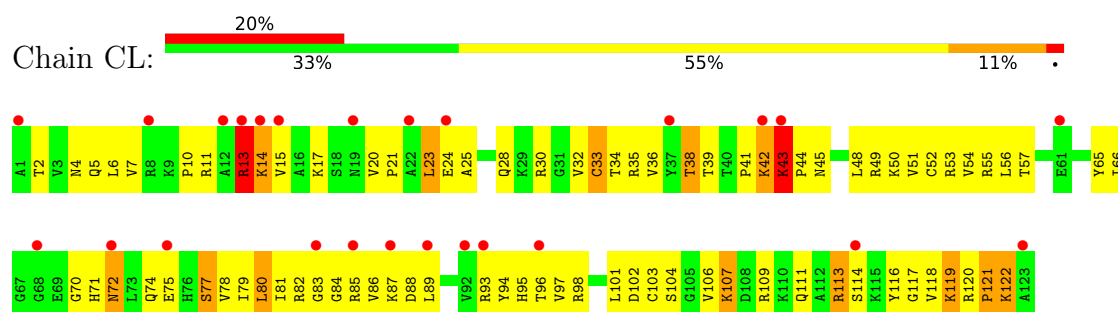
- Molecule 10: 30S ribosomal protein S11



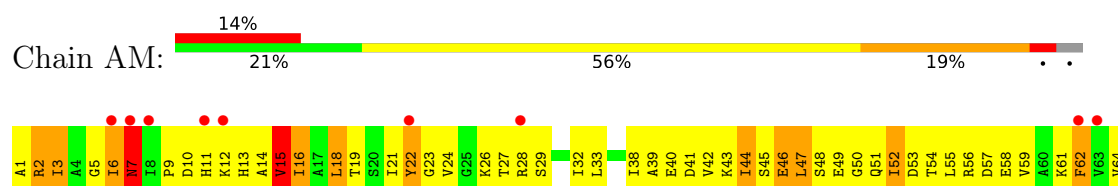
- Molecule 11: 30S ribosomal protein S12



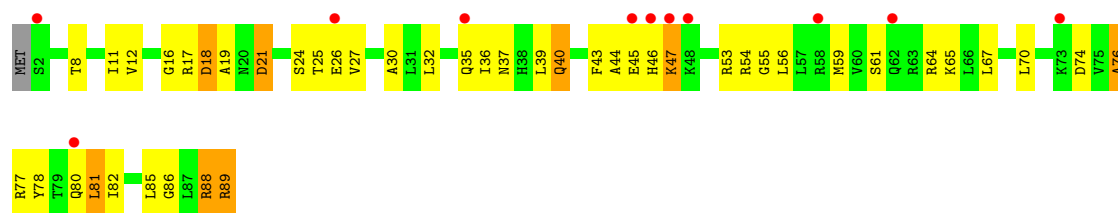
- Molecule 11: 30S ribosomal protein S12



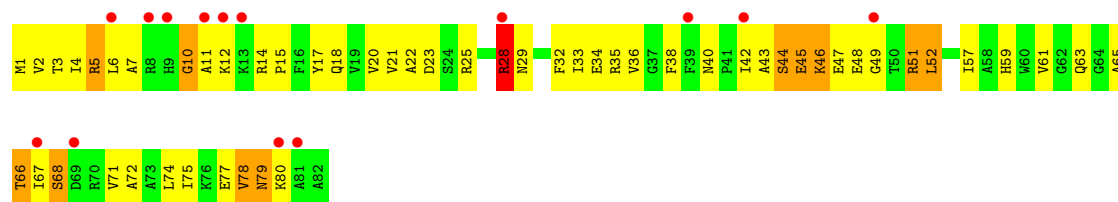
- Molecule 12: 30S ribosomal protein S13



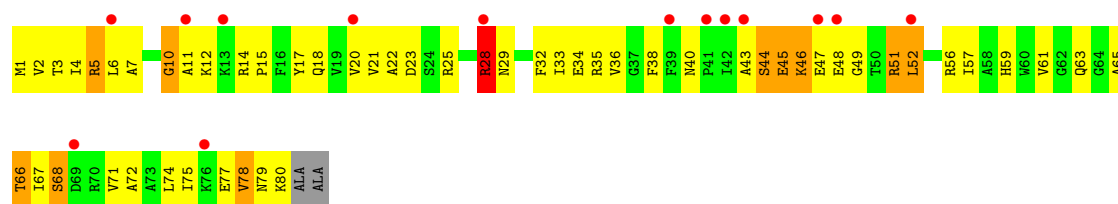




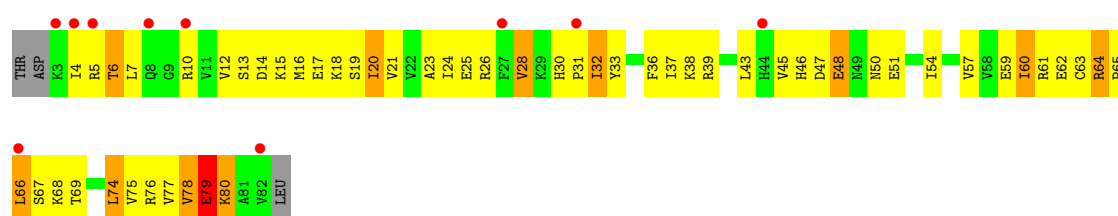
• Molecule 15: 30S ribosomal protein S16



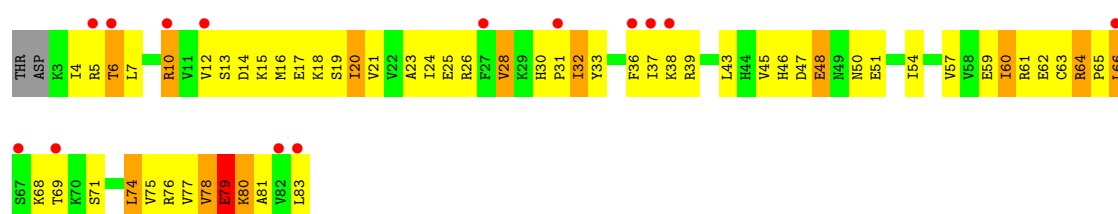
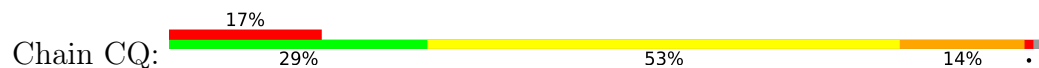
• Molecule 15: 30S ribosomal protein S16



• Molecule 16: 30S ribosomal protein S17



• Molecule 16: 30S ribosomal protein S17



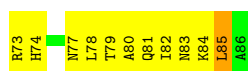
- Chain AR:
-
- | Amino Acid | Percentage |
|------------|------------|
| ALA | 14% |
| ARG | |
| ARG | |
| TYR | |
| PHE | |
| ARG | |
| ARG | |
| ARG | |
| LYS | |
| PHE | |
| CYS | |
| ARG | |
| PHE | |
| THR | |
| ALA | |
| GLU | |
| GLY | |
| VAL | |
| GLN | |
| E19 | 38% |
| I20 | |
| D21 | |
| Y22 | |
| K23 | |
| L28 | |
| Y31 | |
| I32 | |
| T33 | |
| F34 | |
| S35 | 34% |
| G36 | |
| K37 | |
| I38 | |
| V39 | |
| P40 | |
| I43 | |
| T46 | |
| R47 | |
| Y50 | |
| Q53 | 26% |
| L54 | |
| A55 | |
| R56 | |
| A57 | |
| I58 | |
| K59 | |
| R60 | |
| A61 | |
| R62 | |
| Y63 | |

- Chain CR:
-
- | Amino Acid | Category |
|------------|----------|
| ALA | Grey |
| ARG | Grey |
| TYR | Grey |
| PHE | Grey |
| ARG | Grey |
| ARG | Grey |
| ARG | Grey |
| LYS | Grey |
| PHE | Grey |
| CYS | Grey |
| ARG | Grey |
| PHE | Grey |
| THR | Grey |
| ALA | Grey |
| GLU | Grey |
| GLY | Grey |
| VAL | Grey |
| GLN | Grey |
| E19 | Red |
| I20 | Red |
| D21 | Orange |
| Y22 | Yellow |
| K23 | Yellow |
| D24 | Green |
| I25 | Yellow |
| A26 | Yellow |
| Y31 | Yellow |
| I32 | Yellow |
| T33 | Orange |
| E34 | Green |
| S35 | Yellow |
| G36 | Green |
| K37 | Yellow |
| I38 | Orange |
| V39 | Yellow |
| P40 | Yellow |
| I43 | Yellow |
| T44 | Yellow |
| G45 | Green |
| T46 | Orange |
| R47 | Yellow |
| Y50 | Yellow |
| Q53 | Yellow |
| L54 | Yellow |
| A55 | Green |
| R56 | Yellow |
| A57 | Yellow |
| I58 | Yellow |
| K59 | Yellow |
| R60 | Yellow |
| A61 | Green |
| R62 | Yellow |
| Y63 | Yellow |
| L64 | Yellow |
| S65 | Green |
| T66 | Green |
| D71 | Yellow |
| R72 | Yellow |
| H73 | Yellow |
| GLN | Grey |

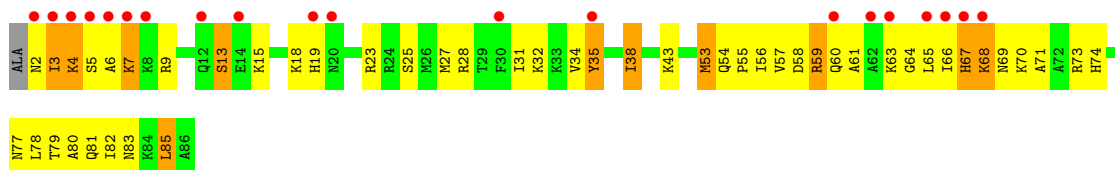
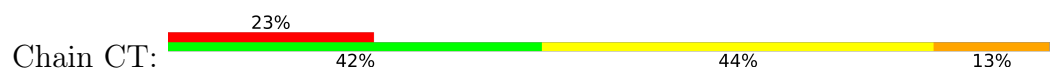
- Chain AS:
-
- | Country | Percentage |
|----------------|------------|
| United States | 18% |
| Germany | 14% |
| France | 51% |
| United Kingdom | 19% |
| Other | 13% |

- Chain CS:
-
- | Amino Acid | Percentage |
|------------|------------|
| P1 | 21% |
| R2 | 16% |
| S3 | 48% |
| L4 | 20% |
| K5 | 12% |
| K6 | |
| G7 | |
| P8 | |
| F9 | |
| I10 | |
| D11 | |
| L12 | |
| H13 | |
| L14 | |
| L15 | |
| V18 | |
| E19 | |
| K20 | |
| A21 | |
| V22 | |
| E23 | |
| S24 | |
| G25 | |
| D26 | |
| K28 | |
| P29 | |
| L30 | |
| L31 | |
| R32 | |
| S35 | |
| R36 | |
| S37 | |
| T38 | |
| I39 | |
| F40 | |
| P41 | |
| M42 | |
| M43 | |
| I44 | |
| G45 | |
| L46 | |
| T47 | |
| I48 | |
| A49 | |
| V50 | |
| H51 | |
| N52 | |
| G53 | |
| R54 | |
| Q55 | |
| H56 | |
| V57 | |
| P58 | |
| V59 | |
| F60 | |
| V61 | |
| T62 | |

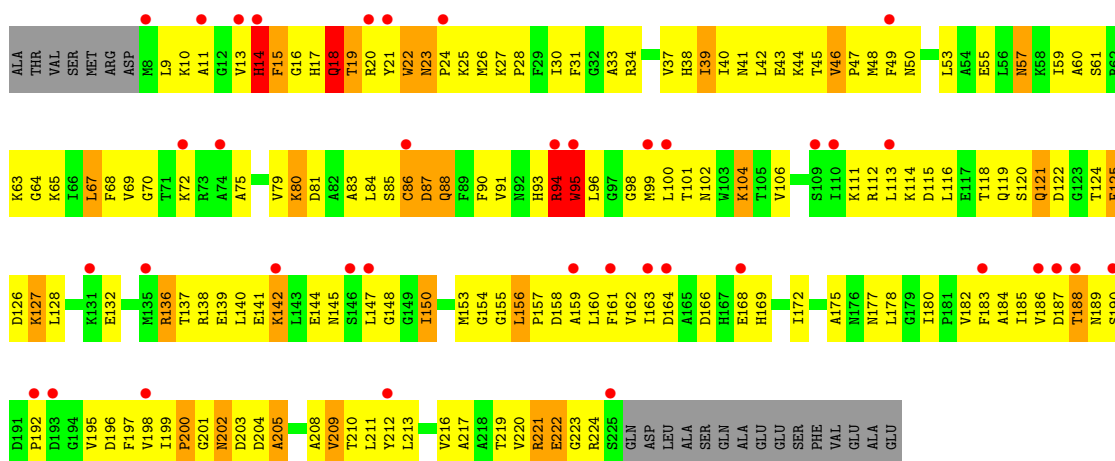
- Chain AT:
-
- 30% 43% 44% 12%
- ALA I2 M3 I3 K4 S5 A6 K7 K8 K8 R9 Q12 I12 S13 E14 K15 A16 R17 K18 H19 N20 A21 R22 R23 R24 S25 P26 M27 R28 T29 F30 I31 K32 K33 V34 Y35 I38 K43 E52 M53 Q54 P55 I56 V57 D58 R59 Q60 A61 K62 K63 G64 L65 I66 H67 K68 M69 K70 A71 P72



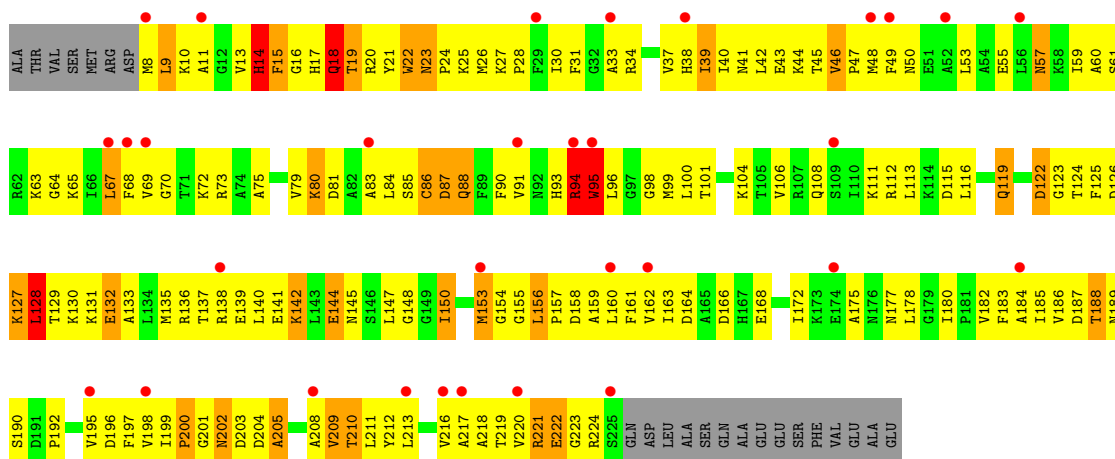
• Molecule 19: 30S ribosomal protein S20



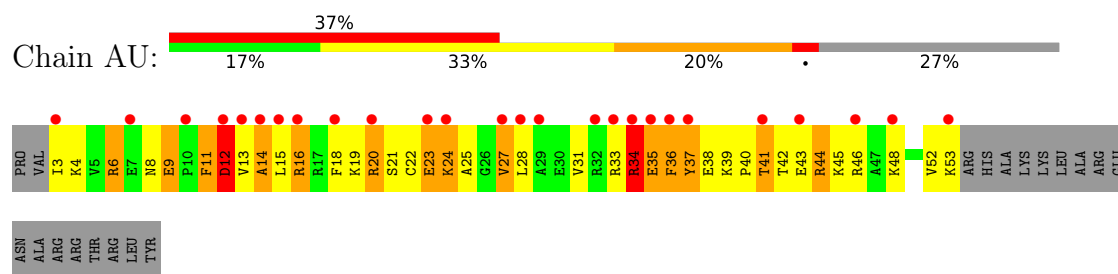
• Molecule 20: 30S ribosomal protein S2



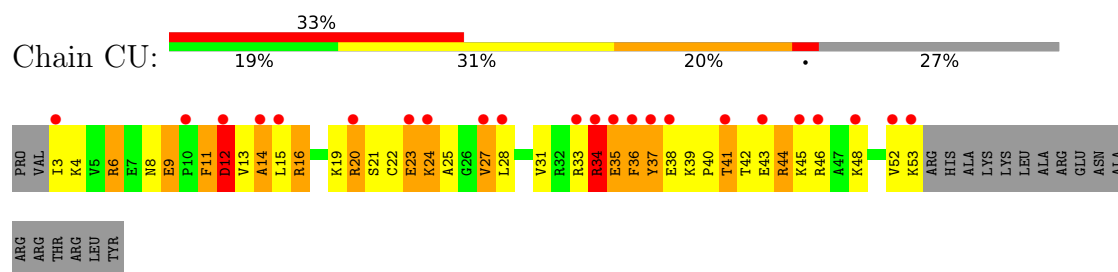
• Molecule 20: 30S ribosomal protein S2



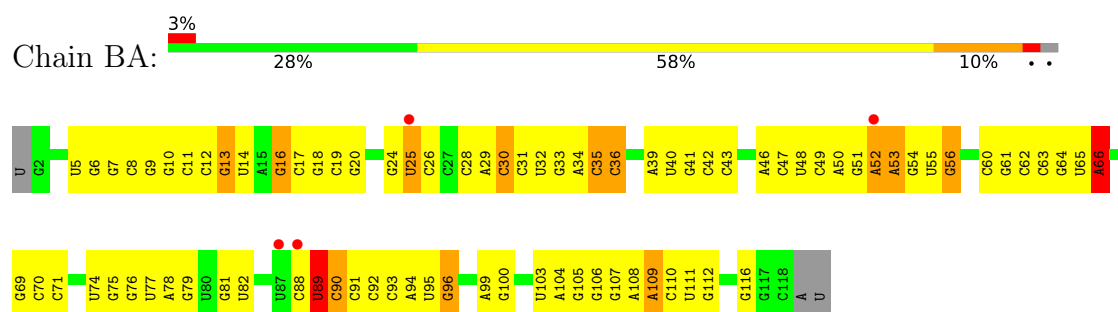
• Molecule 21: 30S ribosomal protein S21



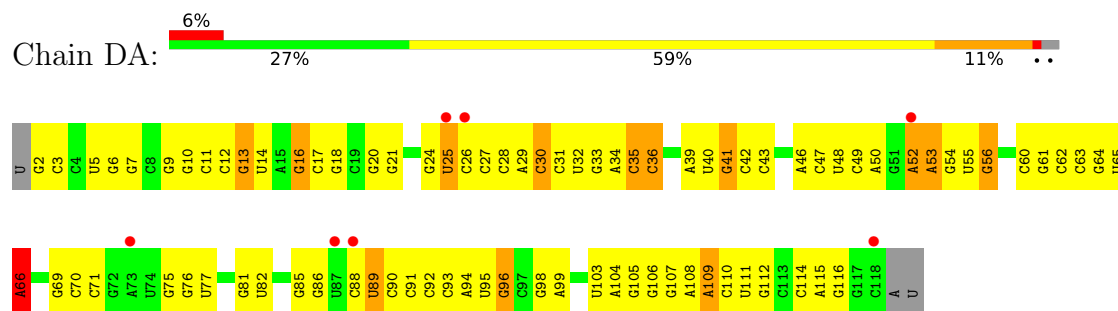
- Molecule 21: 30S ribosomal protein S21



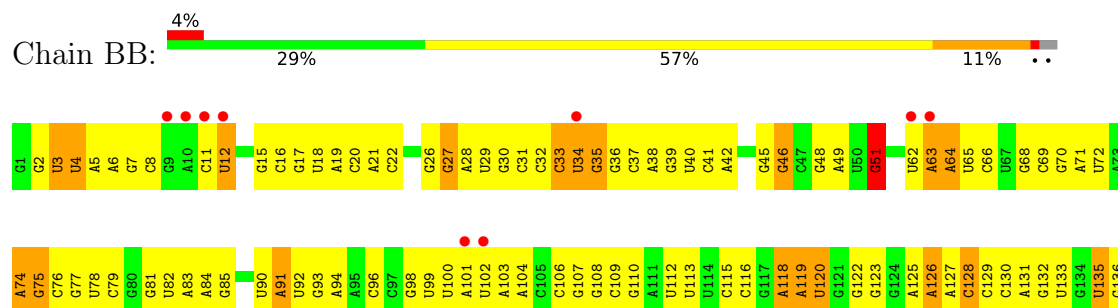
- Molecule 22: 5S rRNA

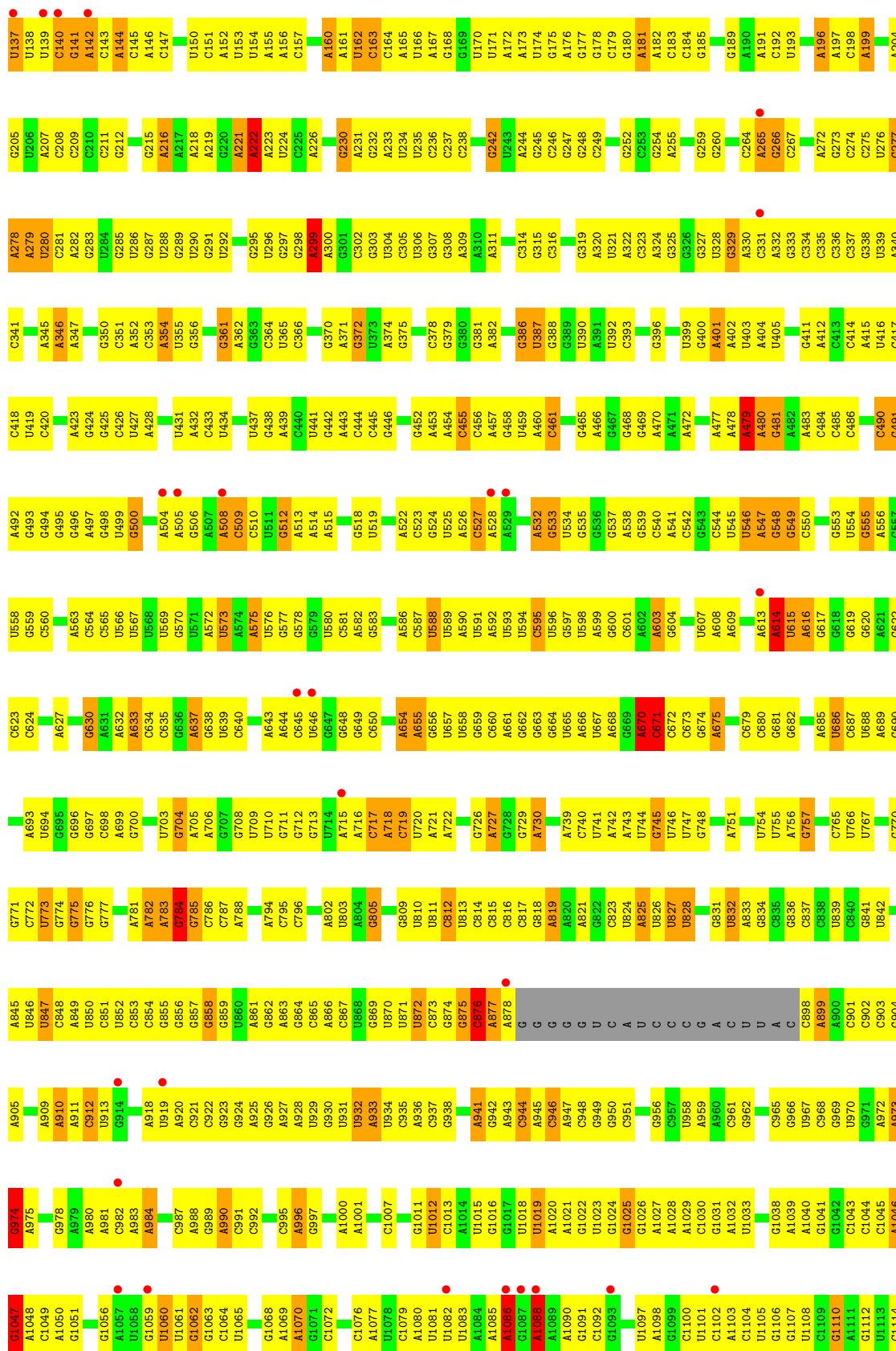


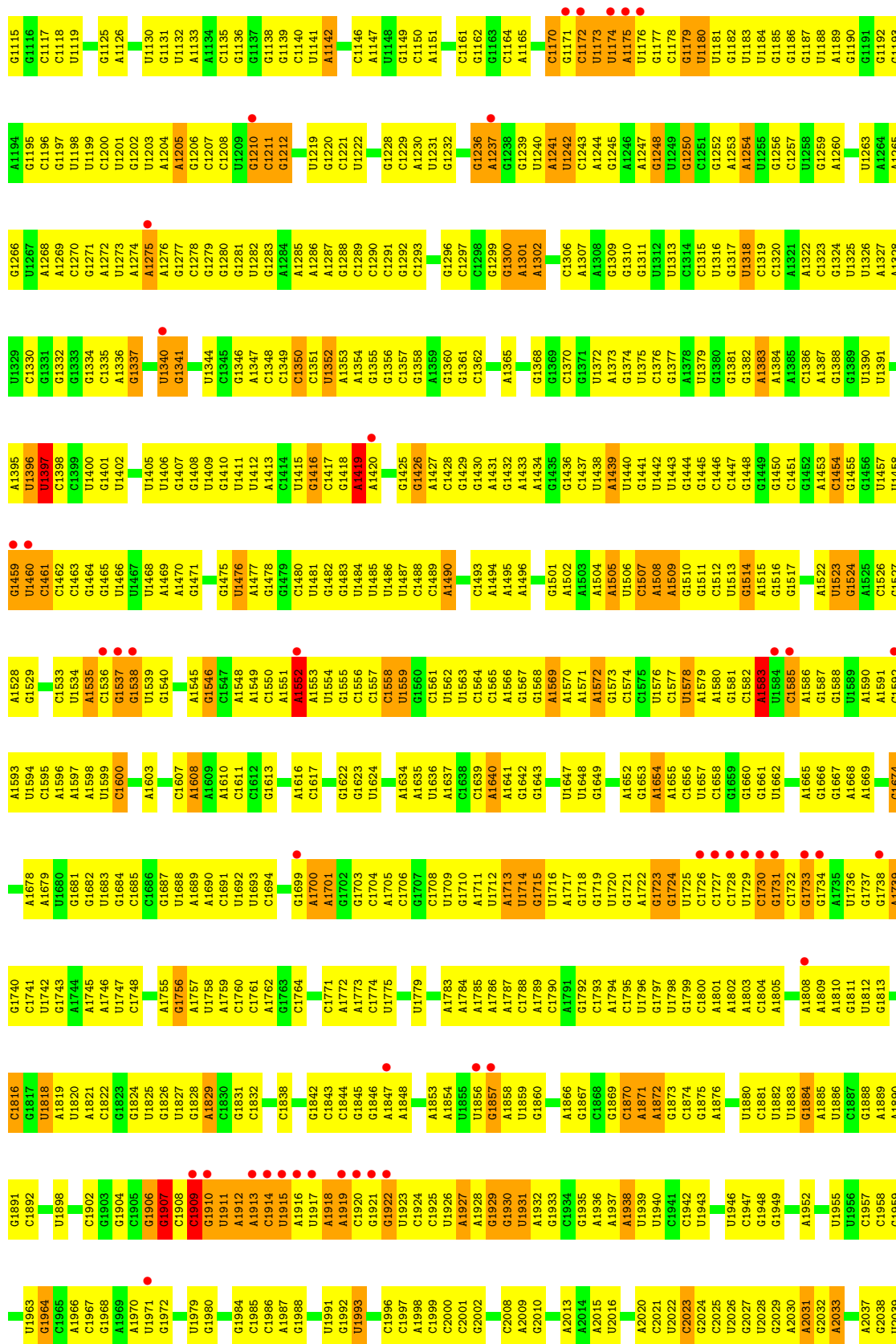
- Molecule 22: 5S rRNA

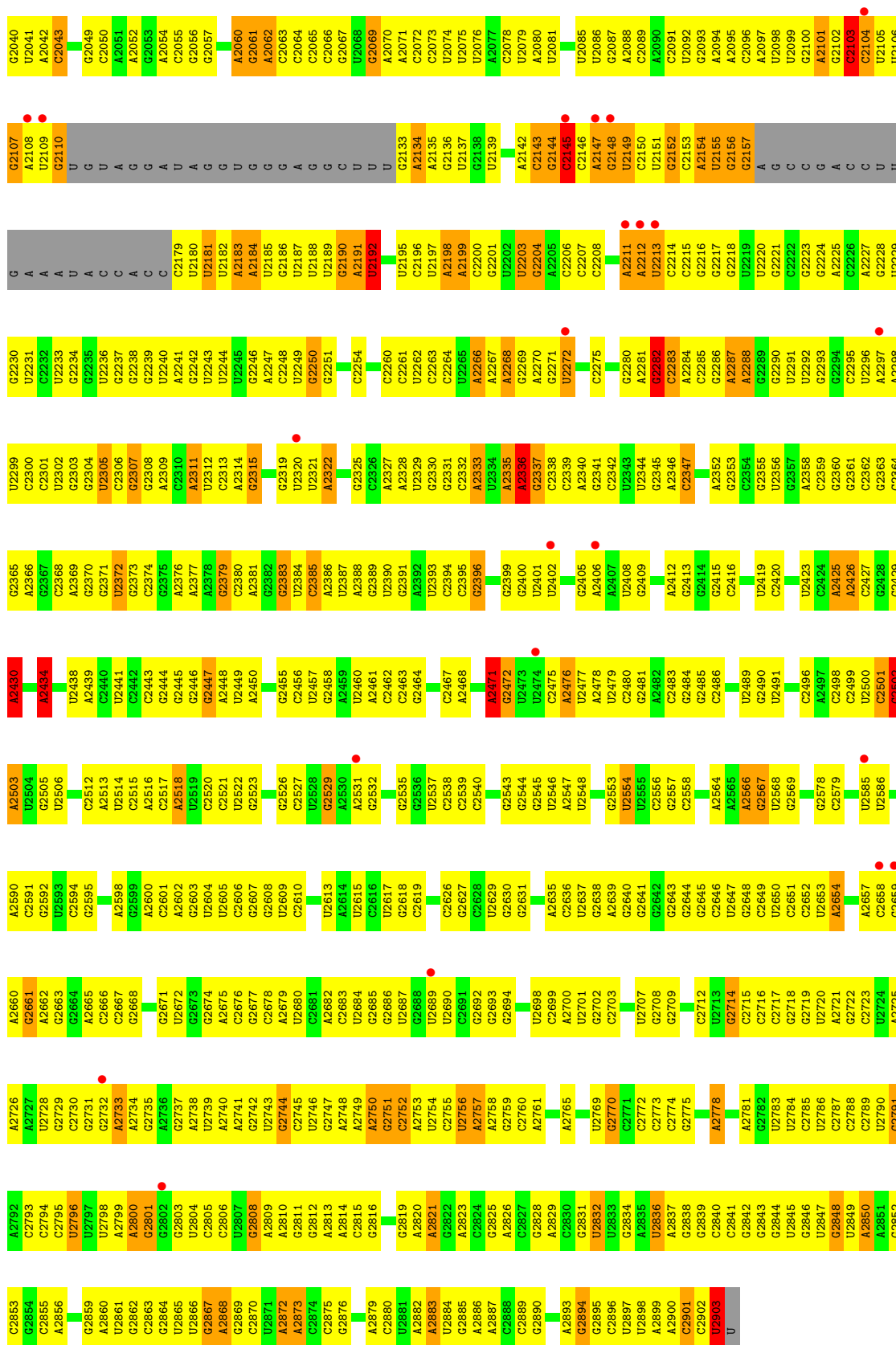


- Molecule 23: 23S rRNA

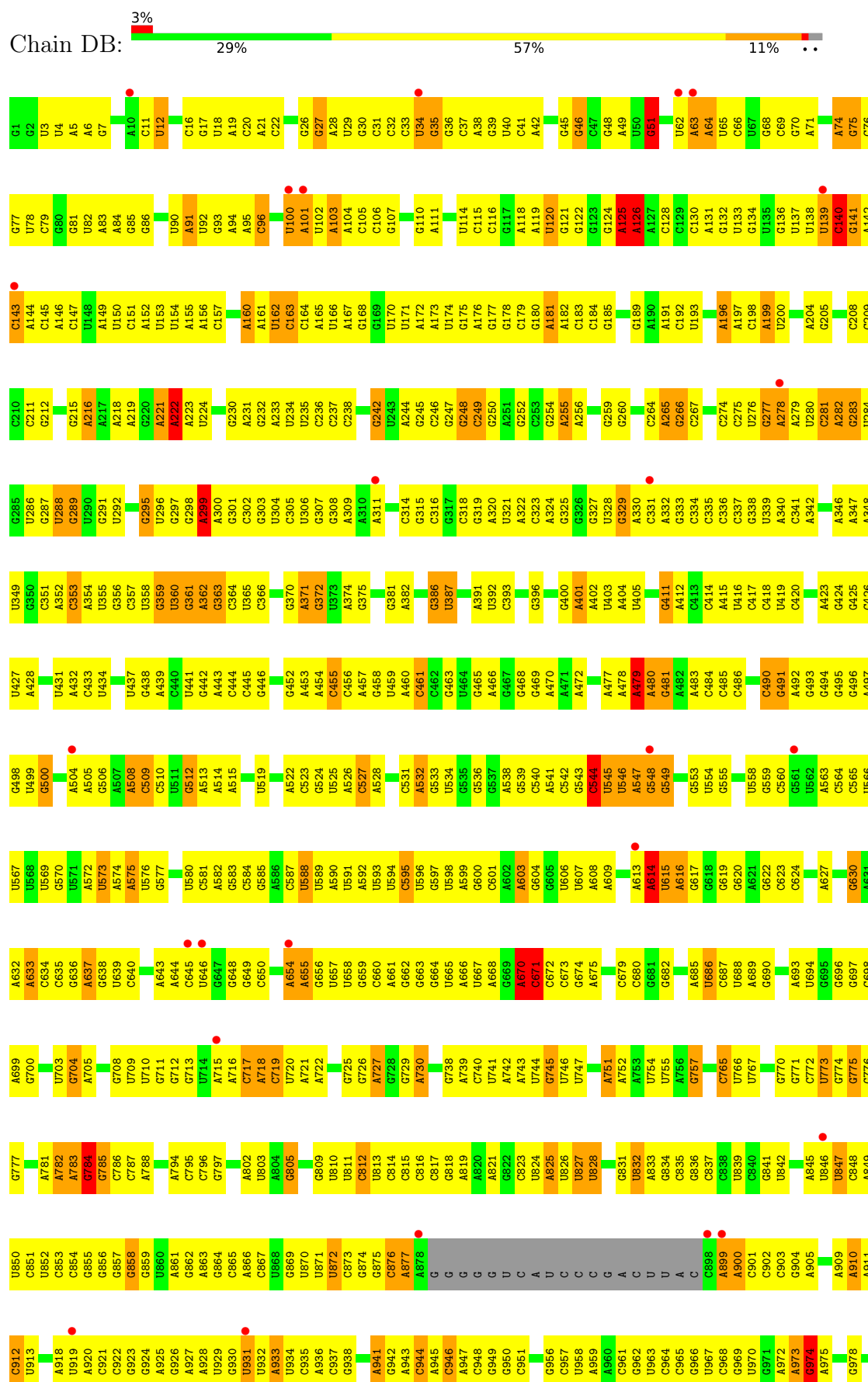








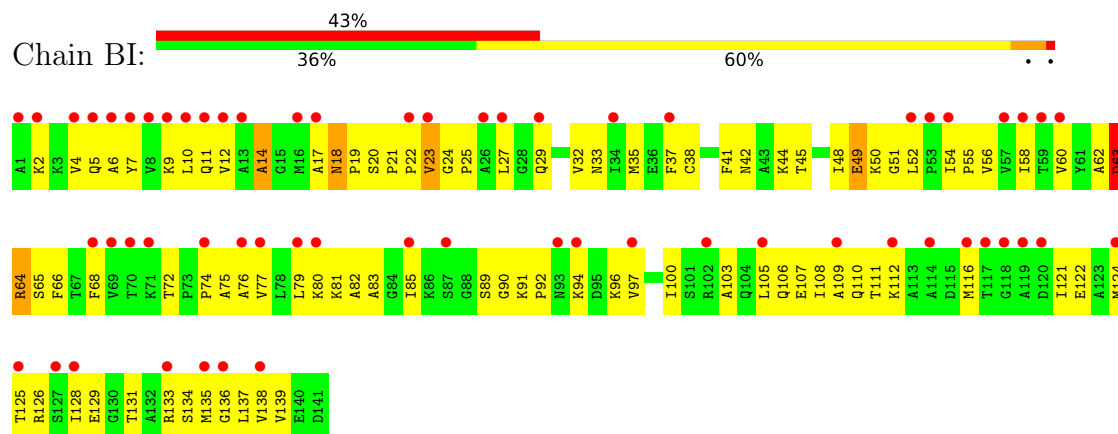
- Molecule 23: 23S rRNA



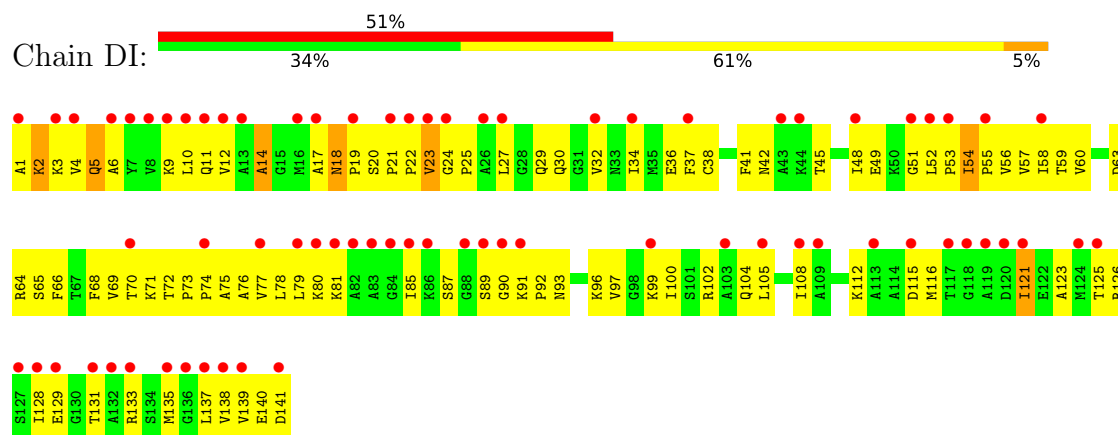
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U1886	A1809	U1736	A1668	G1587	A1453	C1386	A1321	U1255	U1183	U1113	G1051	C982
C1887	A1810	G1738	G1674	U1588	C1454	A1387	C1322	G1257	G1183	C1114	C1053	A983
A1888	G1811	G1737	A1675	U1589	U1457	G1388	C1323	C1257	G1115	A1054	A1054	A984
A1889	U1812	A1740	A1676	A1590	U1458	U1389	G1324	U1258	C1116	C1117	A1055	C985
A1890	G1813	C1741	A1677	A1591	G1459	U1390	U1325	G1259	C1118	C1118	G1056	C986
G1891	C1816	U1742	A1678	C1592	U1460	U1391	U1326	A1260	G1119	U1119	A1057	C987
C1892	G1817	G1743	A1679	A1593	C1461	A1327	A1327	U1263	U1120	U1120	U1058	A988
U1898	G1818	G1744	U1680	C1595	C1462	U1395	U1329	U1264	G1121	G1121	U1060	A990
G1902	A1819	A1745	U1681	C1596	C1463	U1397	U1330	A1265	G1122	G1124	U1062	C991
G1903	U1820	U1746	U1682	A1597	G1464	G1391	G1331	G1266	G1125	G1125	U1061	C992
G1904	G1824	G1748	U1683	U1598	G1465	U1400	G1332	U1267	C1126	A1126	G1063	C993
C1905	U1825	A1755	C1685	G1600	U1468	G1401	G1333	A1268	U1130	U1130	G1064	C994
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G1907	U1827	A1757	U1687	U1602	A1470	U1406	C1335	C1270	C1132	C1132	U1066	A996
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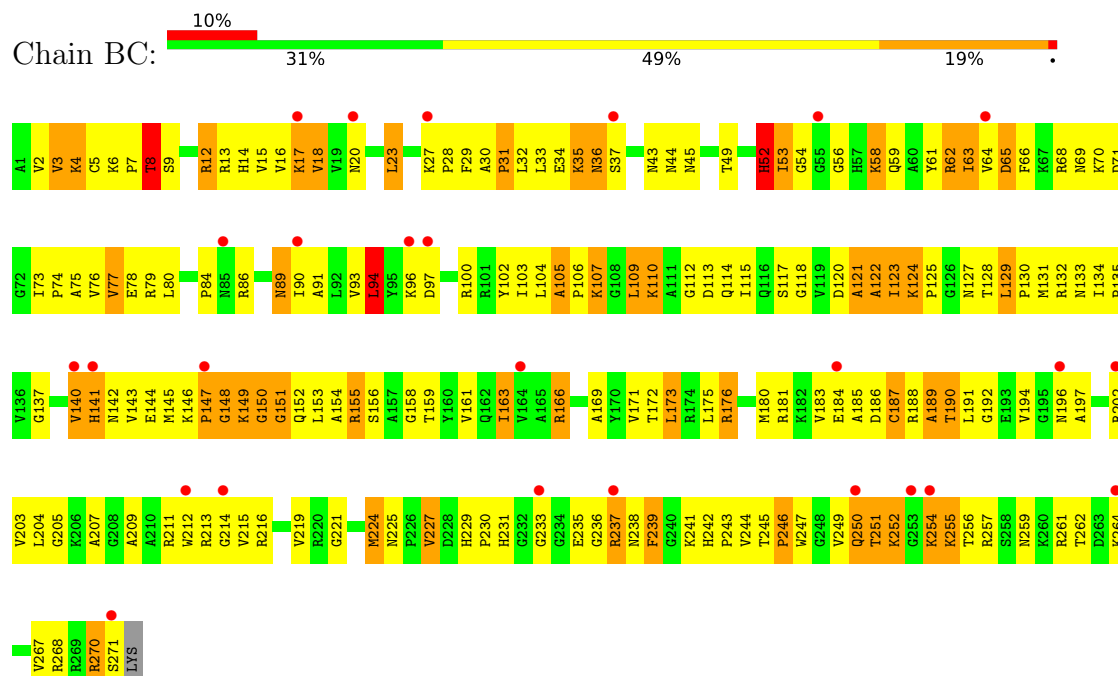
- Molecule 24: 50S ribosomal protein L11



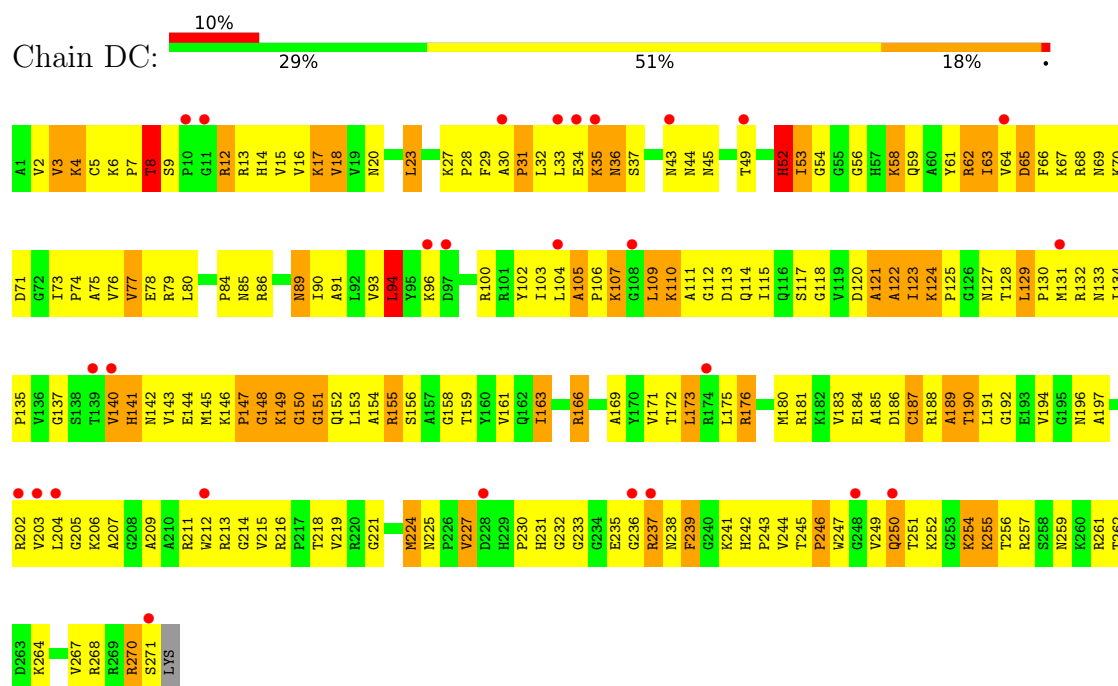
- Molecule 24: 50S ribosomal protein L11



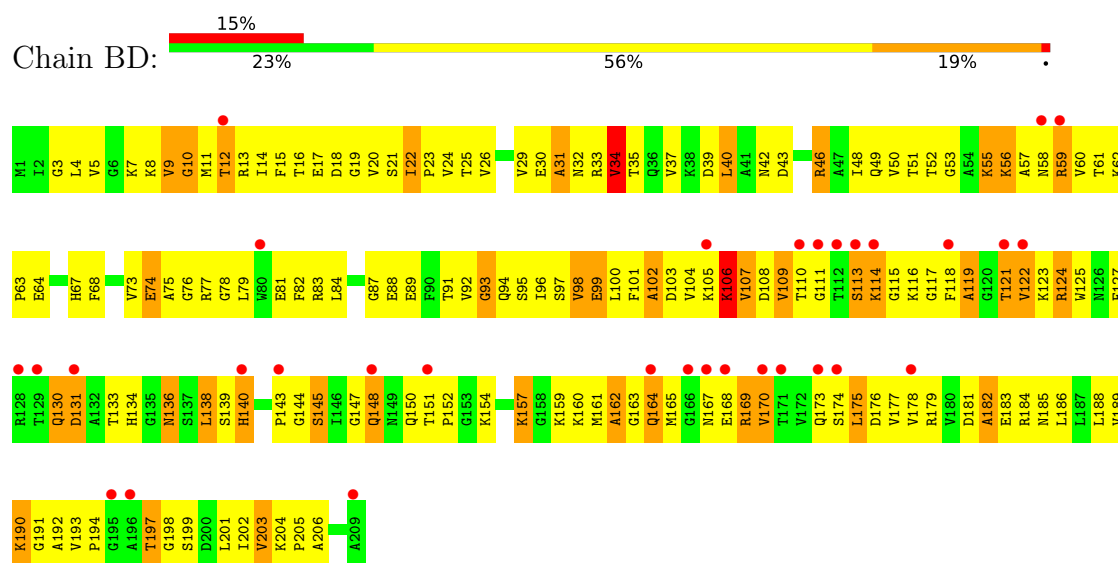
- Molecule 25: 50S ribosomal protein L2



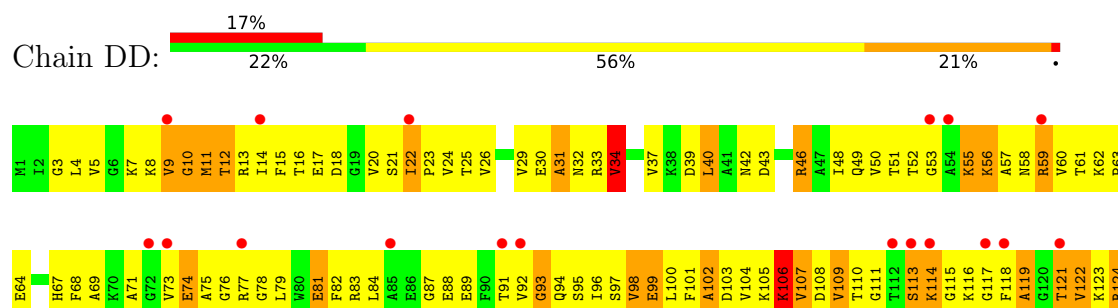
• Molecule 25: 50S ribosomal protein L2

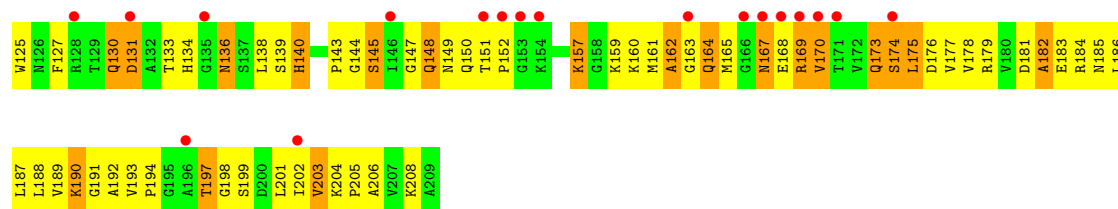


• Molecule 26: 50S ribosomal protein L3

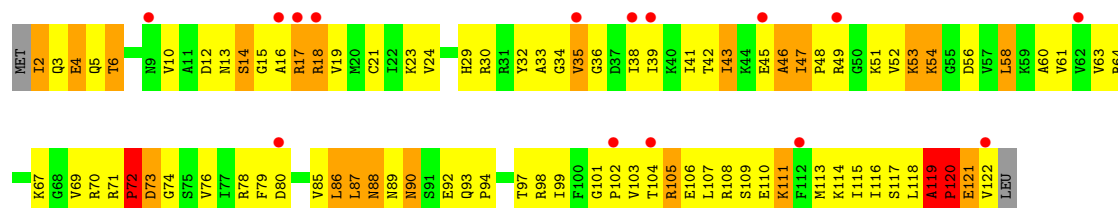


• Molecule 26: 50S ribosomal protein L3

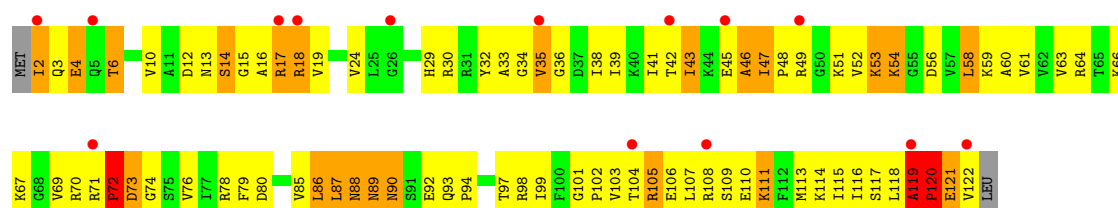




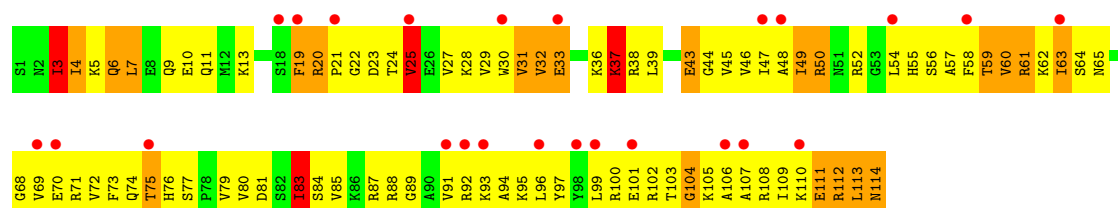
• Molecule 27: 50S ribosomal protein L14



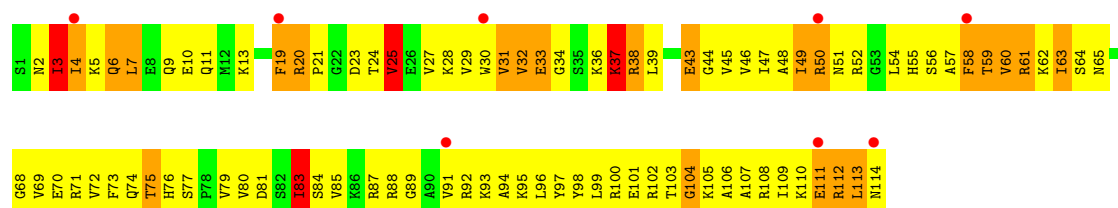
• Molecule 27: 50S ribosomal protein L14



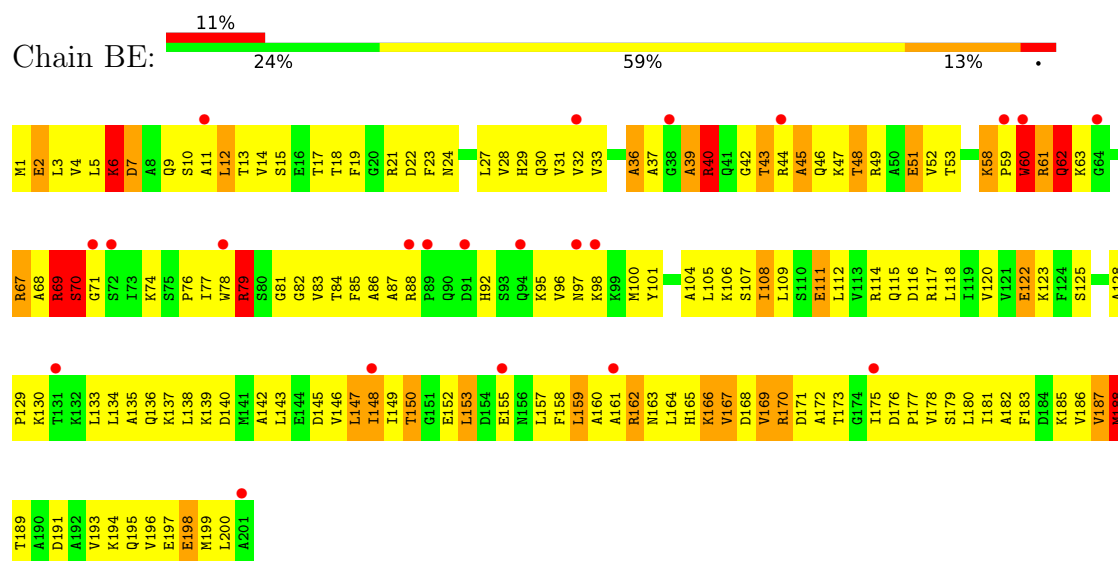
• Molecule 28: 50S ribosomal protein L19



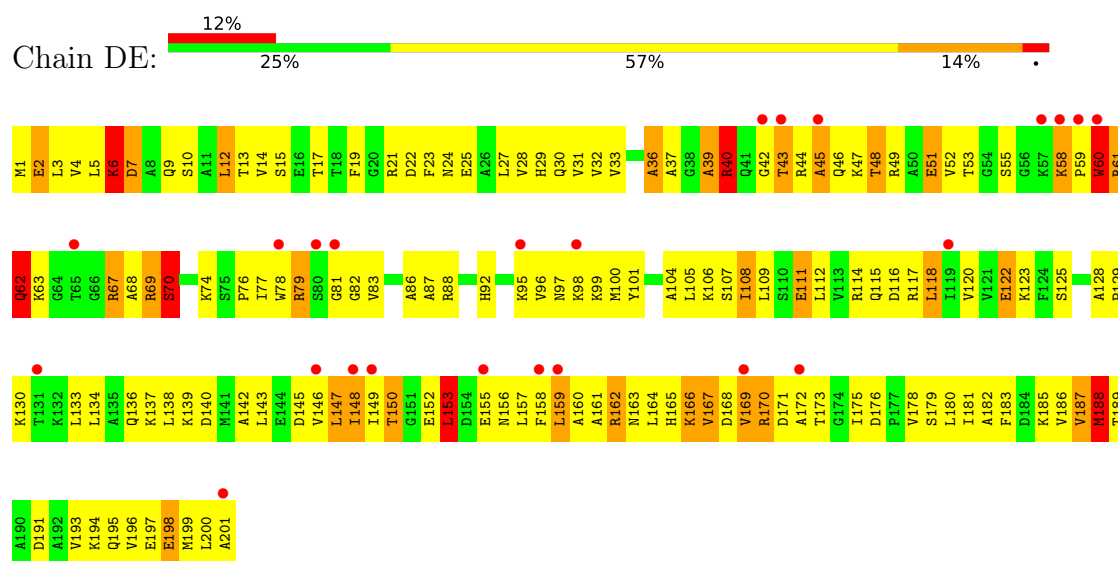
• Molecule 28: 50S ribosomal protein L19



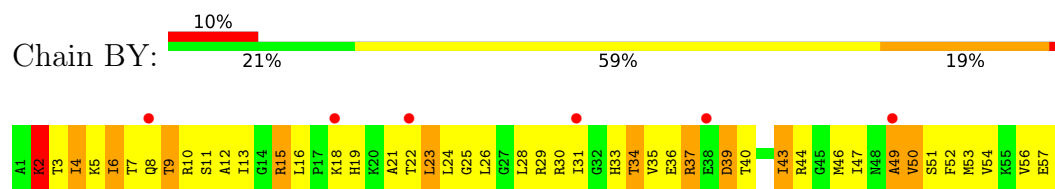
• Molecule 29: 50S ribosomal protein L4



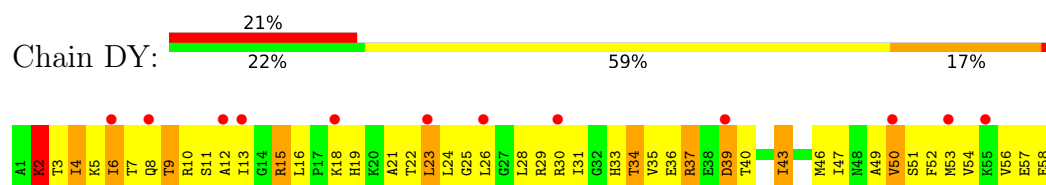
• Molecule 29: 50S ribosomal protein L4



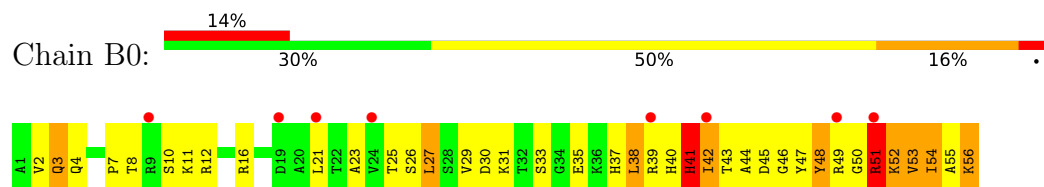
• Molecule 30: 50S ribosomal protein L30



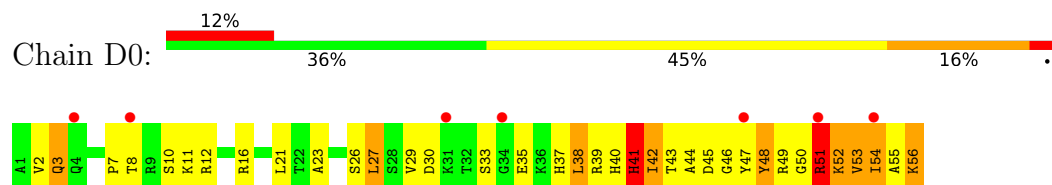
• Molecule 30: 50S ribosomal protein L30



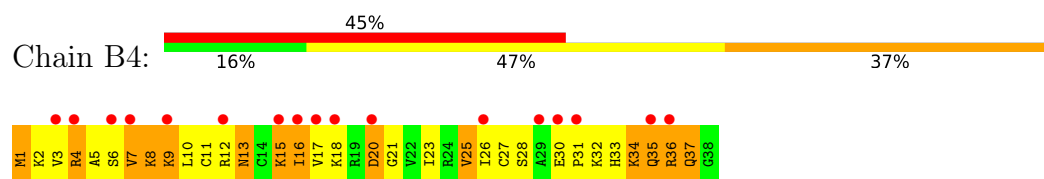
• Molecule 31: 50S ribosomal protein L32



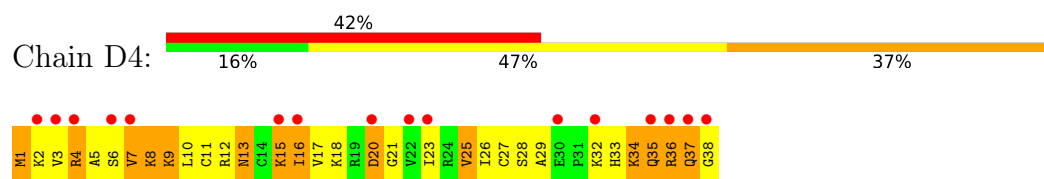
• Molecule 31: 50S ribosomal protein L32



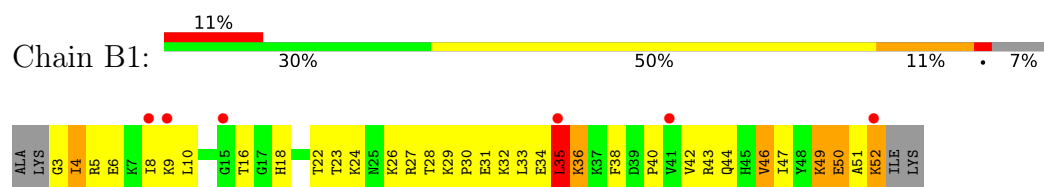
• Molecule 32: 50S ribosomal protein L36



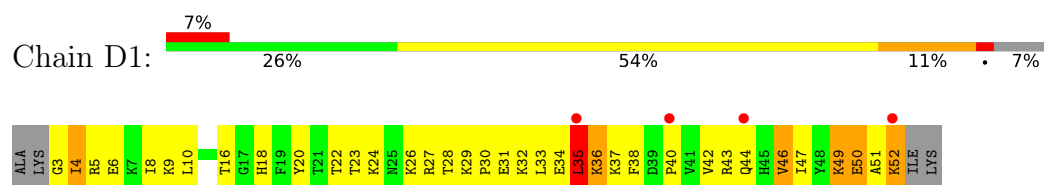
• Molecule 32: 50S ribosomal protein L36



• Molecule 33: 50S ribosomal protein L33

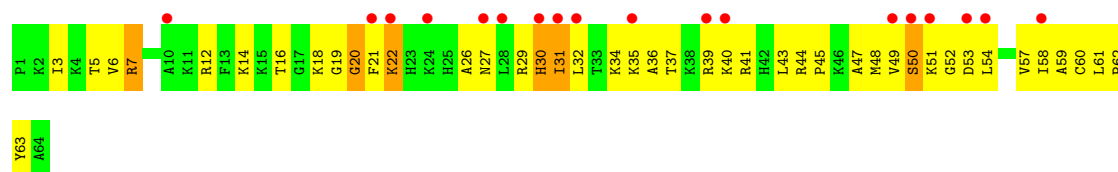


• Molecule 33: 50S ribosomal protein L33



• Molecule 34: 50S ribosomal protein L35





- Molecule 34: 50S ribosomal protein L35



- Molecule 35: 50S ribosomal protein L25



- Molecule 35: 50S ribosomal protein L25



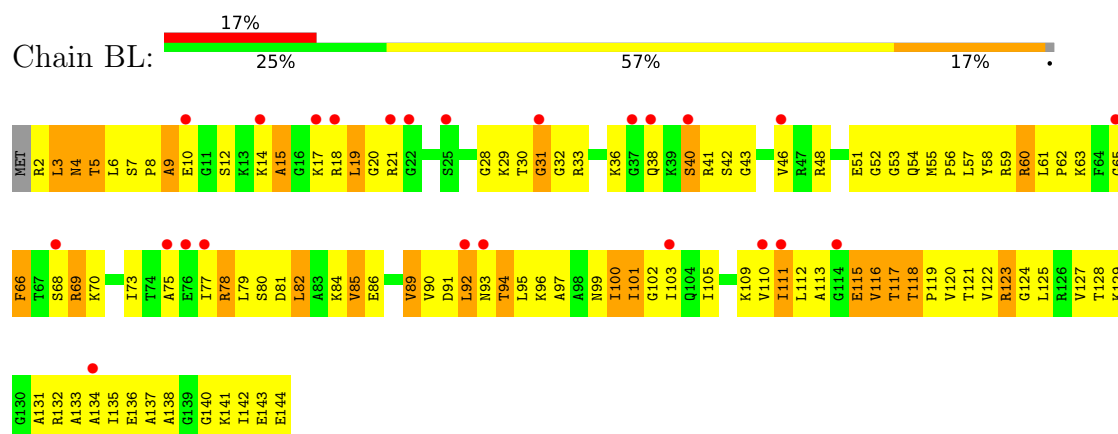
- Molecule 36: 50S ribosomal protein L34



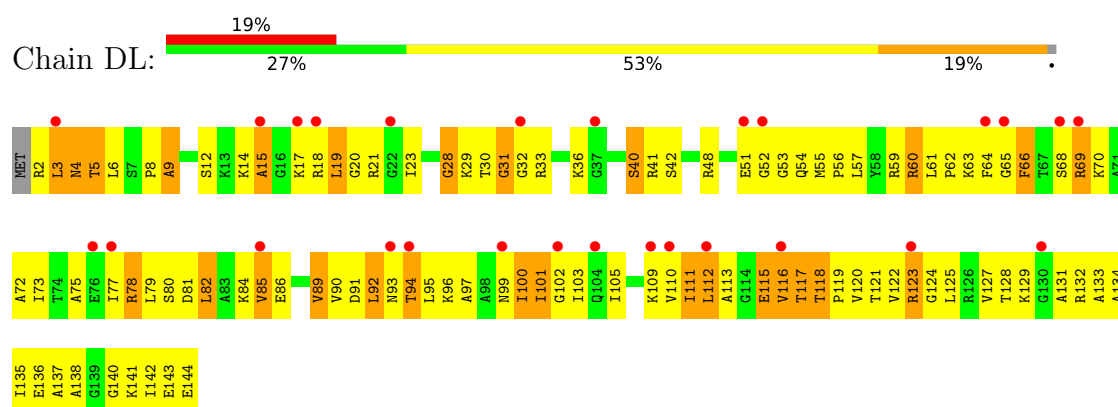
- Molecule 36: 50S ribosomal protein L34



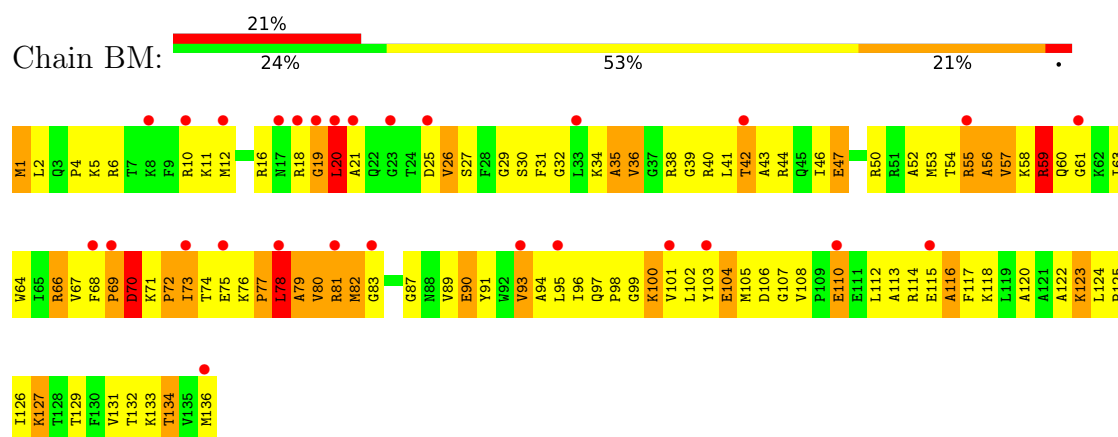
- Molecule 37: 50S ribosomal protein L15



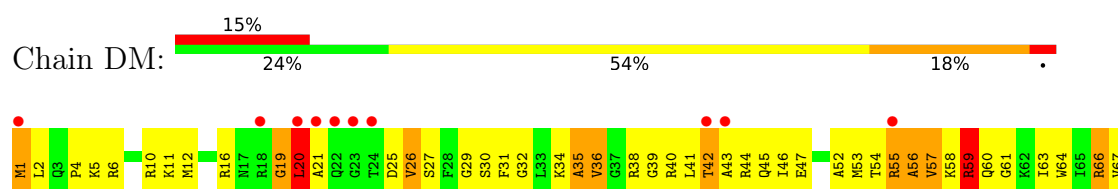
- Molecule 37: 50S ribosomal protein L15

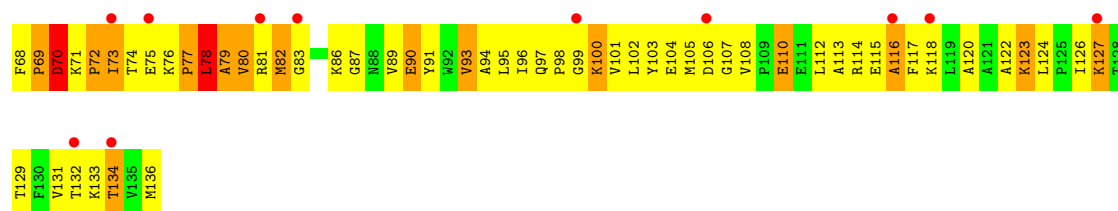


- Molecule 38: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L16





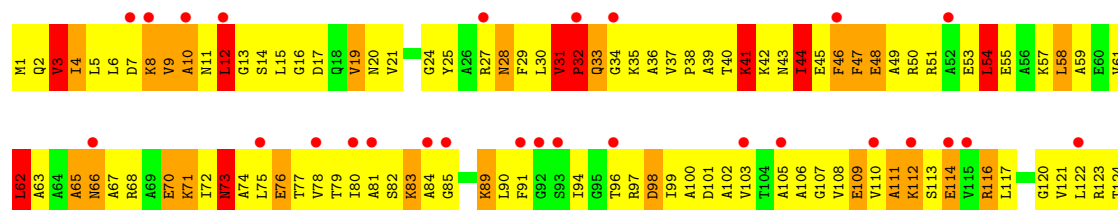
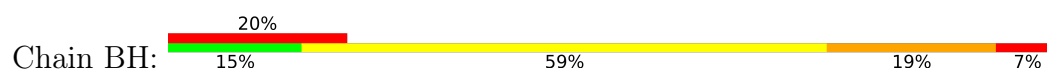
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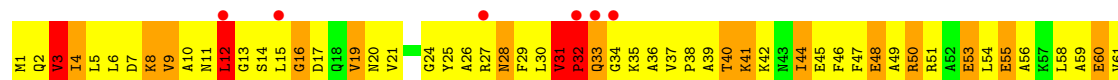
● Molecule 39: 50S ribosomal protein L29

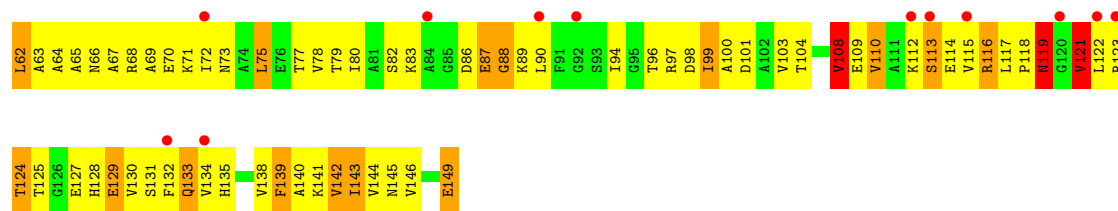


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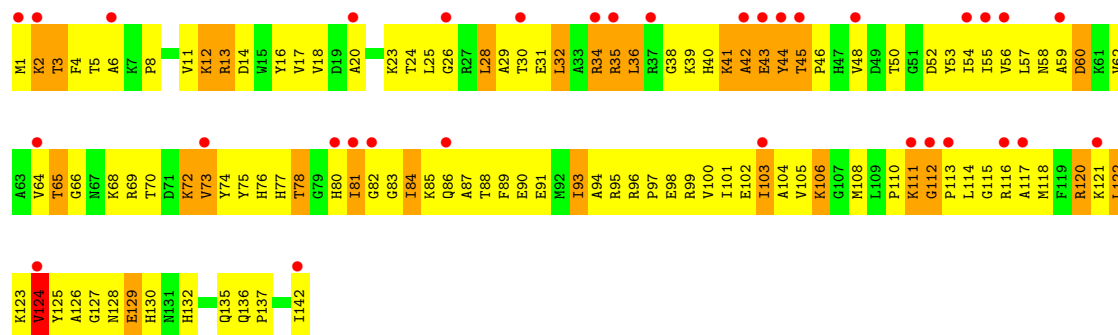


● Molecule 40: 50S ribosomal protein L9

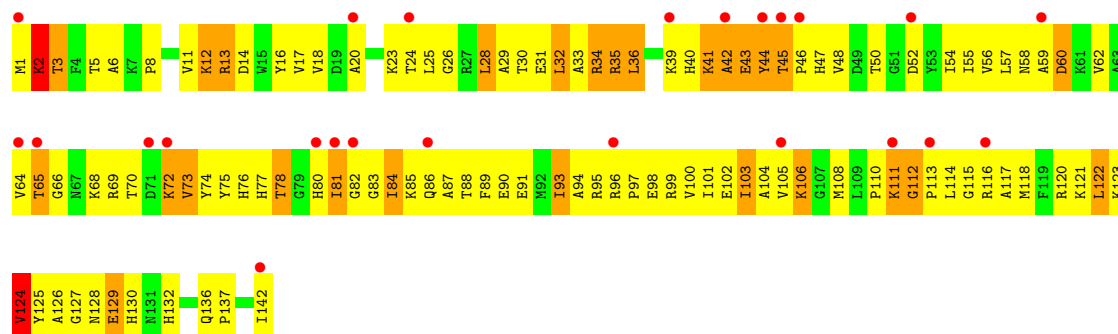




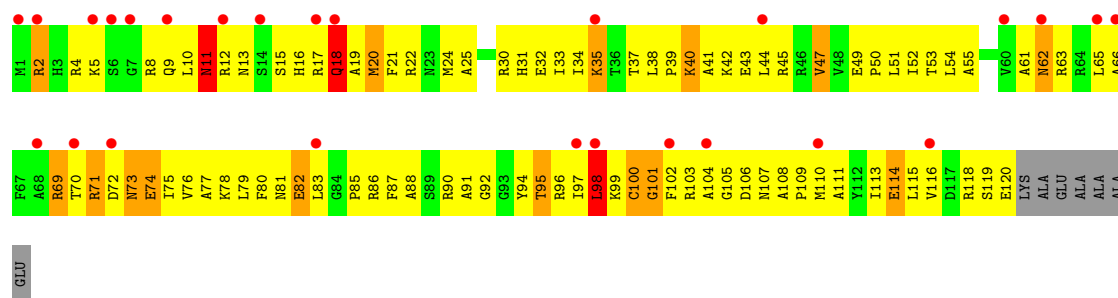
• Molecule 41: 50S ribosomal protein L13



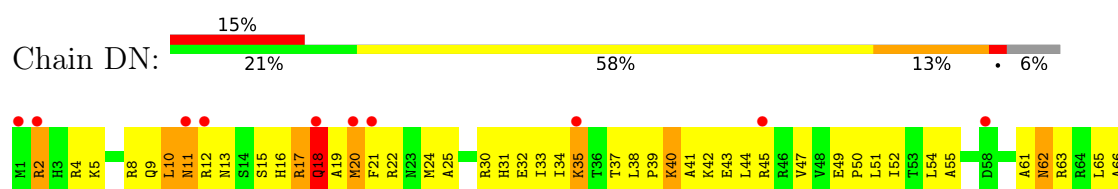
• Molecule 41: 50S ribosomal protein L13



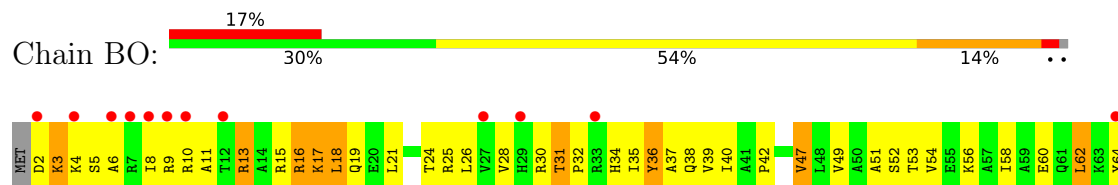
• Molecule 42: 50S ribosomal protein L17



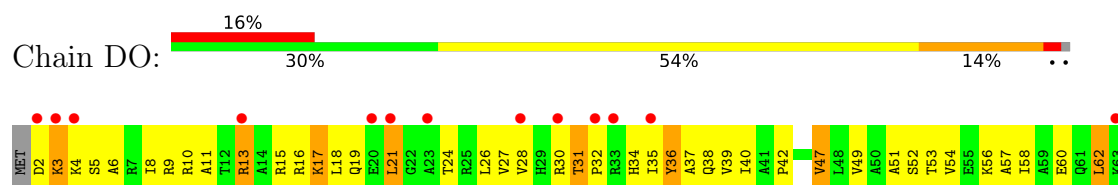
• Molecule 42: 50S ribosomal protein L17



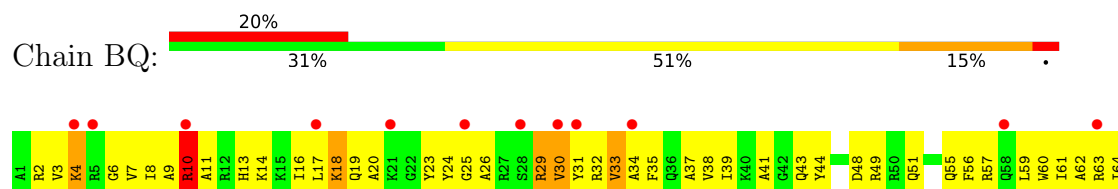
• Molecule 43: 50S ribosomal protein L18



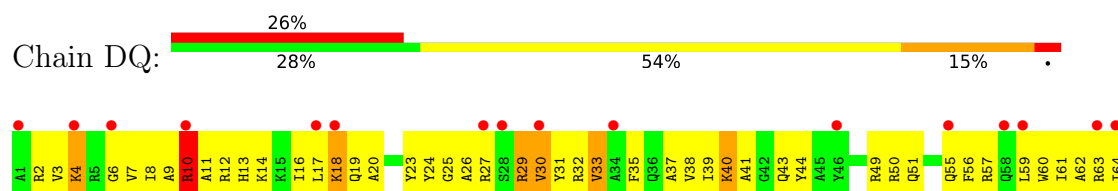
• Molecule 43: 50S ribosomal protein L18

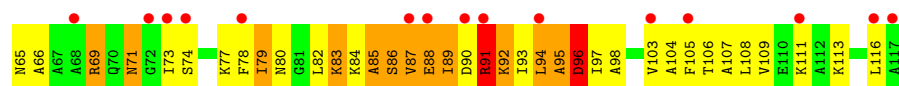


• Molecule 44: 50S ribosomal protein L20

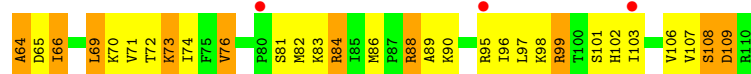
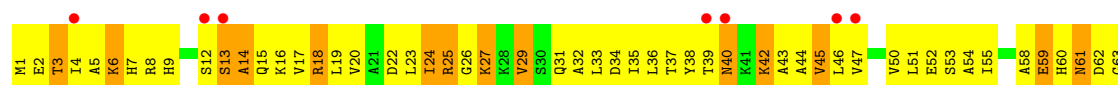


• Molecule 44: 50S ribosomal protein L20

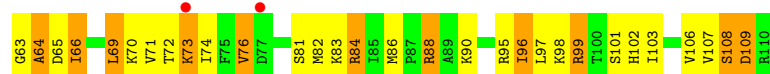
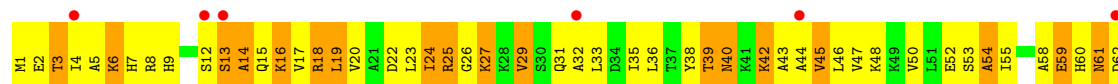




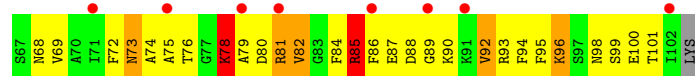
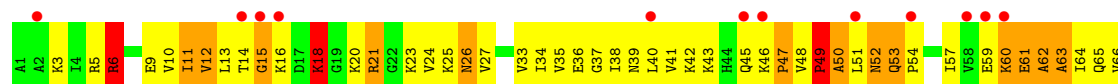
• Molecule 45: 50S ribosomal protein L22



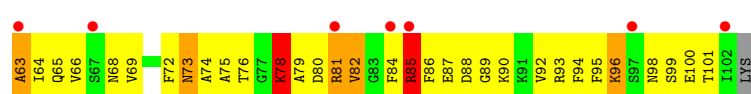
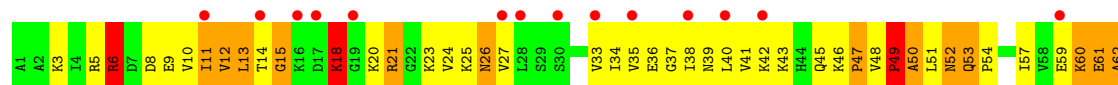
• Molecule 45: 50S ribosomal protein L22



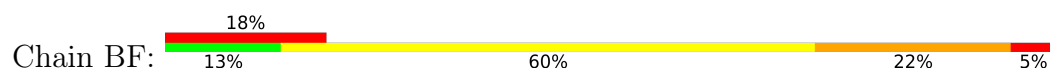
• Molecule 46: 50S ribosomal protein L24

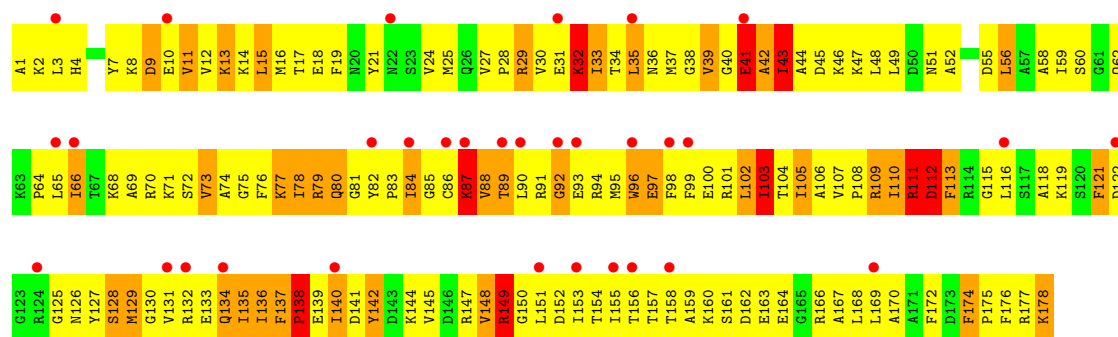


• Molecule 46: 50S ribosomal protein L24

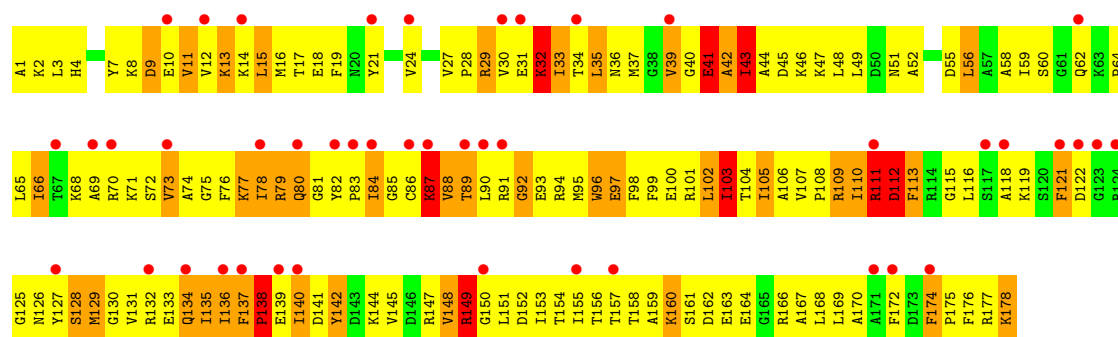
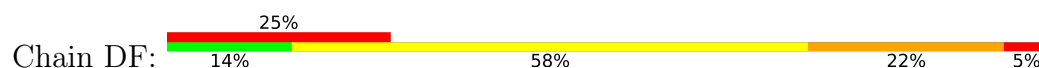


• Molecule 47: 50S ribosomal protein L5

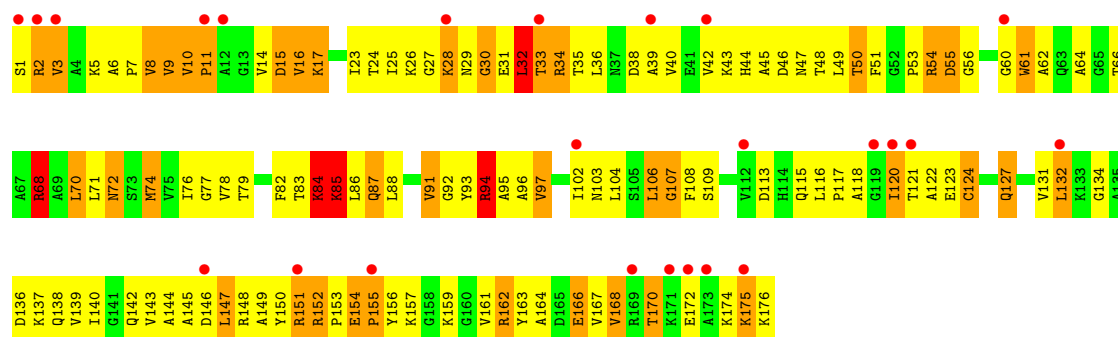




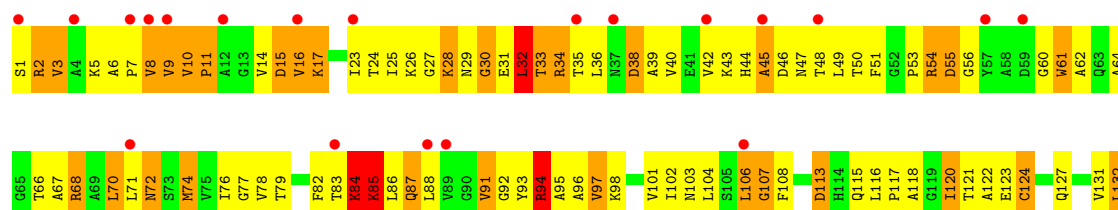
• Molecule 47: 50S ribosomal protein L5

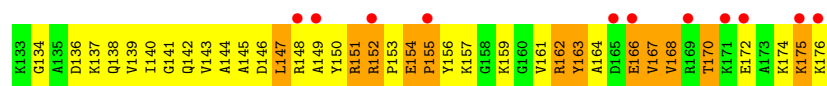


• Molecule 48: 50S ribosomal protein L6

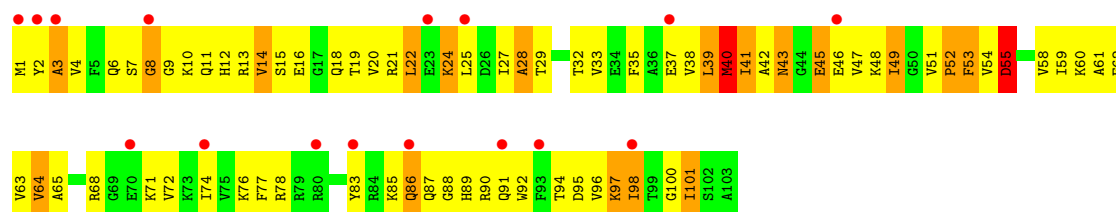


• Molecule 48: 50S ribosomal protein L6

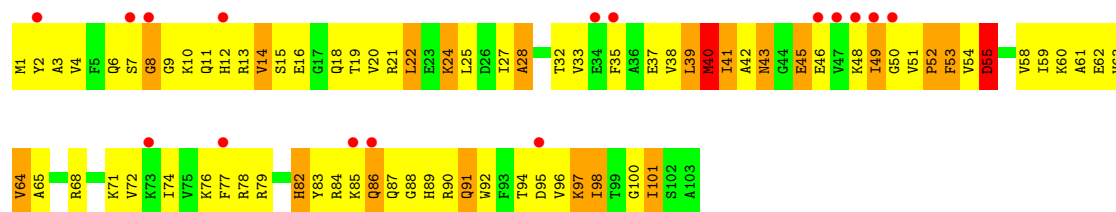




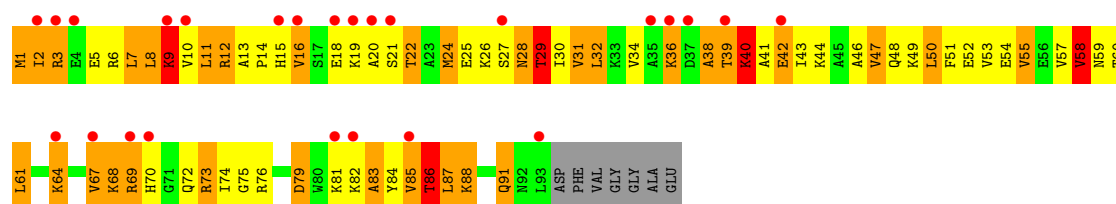
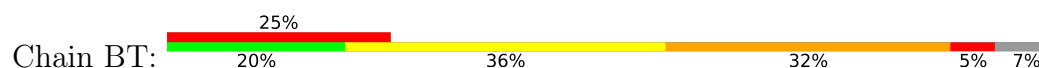
• Molecule 49: 50S ribosomal protein L21



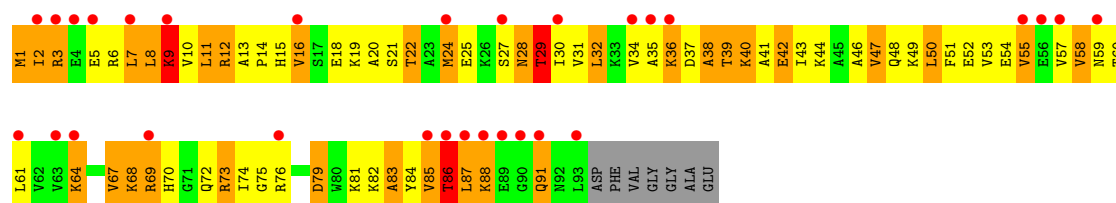
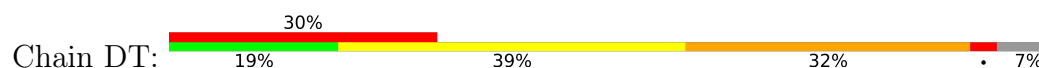
• Molecule 49: 50S ribosomal protein L21



• Molecule 50: 50S ribosomal protein L23

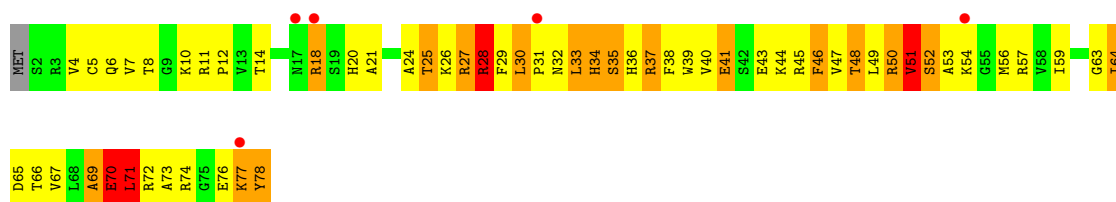


• Molecule 50: 50S ribosomal protein L23

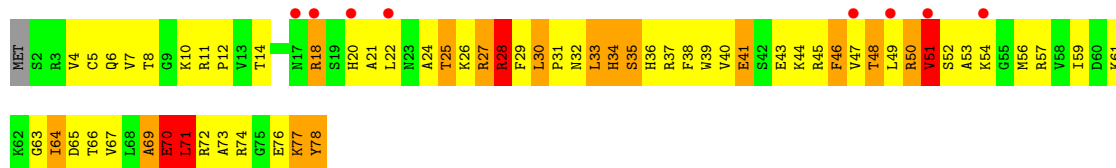


• Molecule 51: 50S ribosomal protein L28

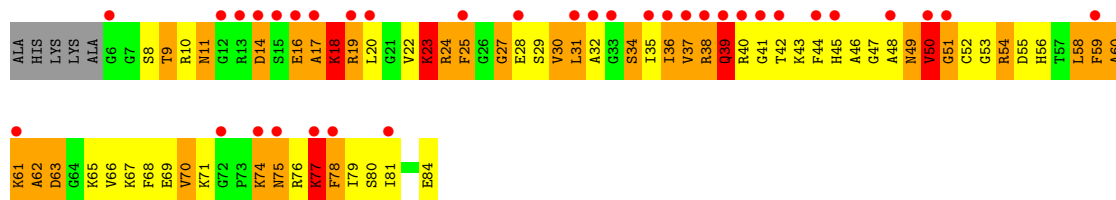
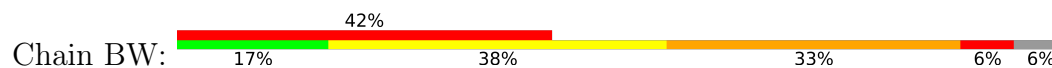




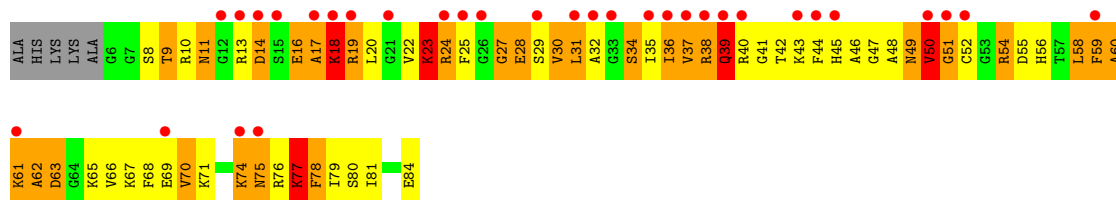
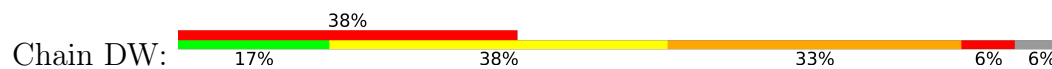
• Molecule 51: 50S ribosomal protein L28



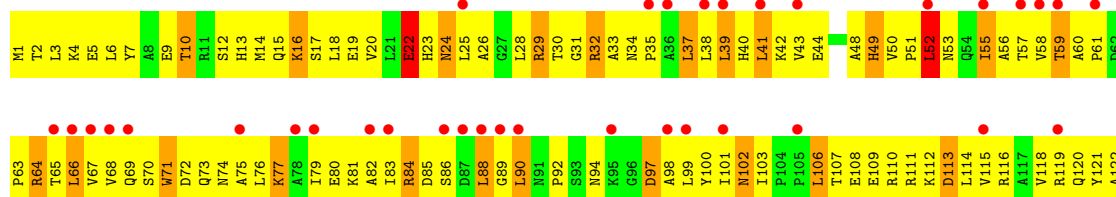
• Molecule 52: 50S ribosomal protein L27

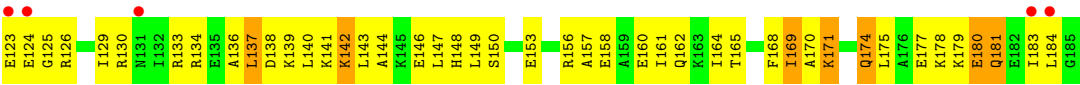


• Molecule 52: 50S ribosomal protein L27

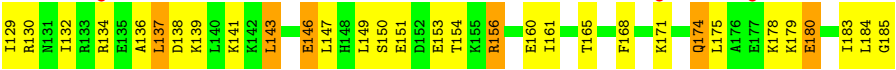
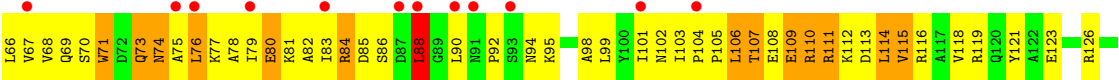
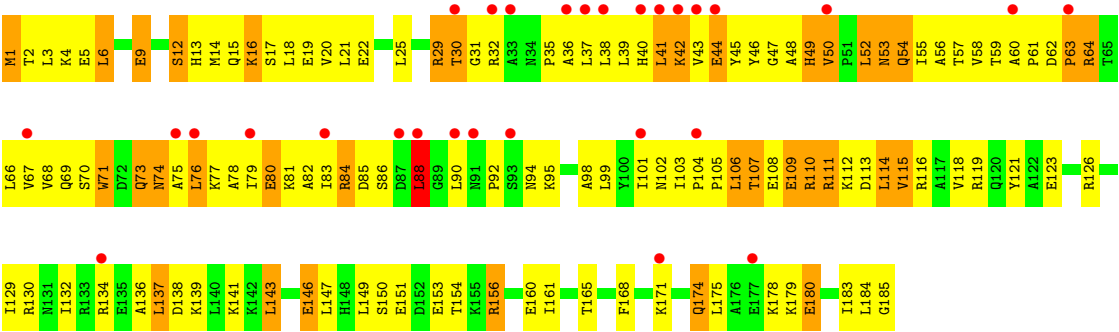


• Molecule 53: ribosome recycling factor





● Molecule 53: ribosome recycling factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.90Å 378.20Å 736.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 40.00 – 3.32	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.00-3.30) 87.1 (40.00-3.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.304 0.247 , 0.271	Depositor DCC
R_{free} test set	35399 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	286960	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.27	0/36762	0.63	51/57350 (0.1%)
1	CA	0.28	0/36762	0.64	56/57350 (0.1%)
2	AC	0.28	0/1651	0.71	0/2225
2	CC	0.28	0/1651	0.72	0/2225
3	AD	0.27	0/1665	0.72	0/2227
3	CD	0.27	0/1665	0.71	0/2227
4	AE	0.28	0/1118	0.77	1/1504 (0.1%)
4	CE	0.28	0/1118	0.77	1/1504 (0.1%)
5	AF	0.29	0/835	0.72	0/1128
5	CF	0.29	0/835	0.72	0/1128
6	AG	0.27	0/1187	0.75	2/1591 (0.1%)
6	CG	0.27	0/1211	0.76	2/1624 (0.1%)
7	AH	0.28	0/989	0.73	0/1326
7	CH	0.28	0/989	0.73	0/1326
8	AI	0.27	0/1034	0.70	0/1375
8	CI	0.27	0/1034	0.70	0/1375
9	AJ	0.29	0/796	0.75	0/1077
9	CJ	0.30	0/796	0.76	0/1077
10	AK	0.30	0/893	0.79	1/1205 (0.1%)
10	CK	0.30	0/893	0.79	1/1205 (0.1%)
11	AL	0.28	0/969	0.79	1/1300 (0.1%)
11	CL	0.28	0/969	0.78	1/1300 (0.1%)
12	AM	0.26	0/892	0.72	0/1193
12	CM	0.26	0/884	0.71	0/1181
13	AN	0.28	0/785	0.78	0/1043
13	CN	0.28	0/785	0.78	0/1043
14	AO	0.26	0/722	0.79	3/964 (0.3%)
14	CO	0.26	0/722	0.79	3/964 (0.3%)
15	AP	0.30	0/659	0.76	1/884 (0.1%)
15	CP	0.29	0/648	0.75	1/870 (0.1%)
16	AQ	0.25	0/657	0.73	0/881
16	CQ	0.25	0/666	0.74	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.30	0/462	0.77	0/621
17	CR	0.30	0/462	0.77	0/621
18	AS	0.28	0/652	0.74	1/877 (0.1%)
18	CS	0.28	0/660	0.76	1/888 (0.1%)
19	AT	0.28	0/671	0.70	0/888
19	CT	0.28	0/671	0.70	0/888
20	AB	0.30	0/1735	0.74	0/2338
20	CB	0.30	0/1735	0.76	1/2338 (0.0%)
21	AU	0.29	0/430	0.83	1/570 (0.2%)
21	CU	0.29	0/430	0.83	1/570 (0.2%)
22	BA	0.28	0/2803	0.66	4/4371 (0.1%)
22	DA	0.29	0/2803	0.66	5/4371 (0.1%)
23	BB	0.28	1/68314 (0.0%)	0.65	91/106569 (0.1%)
23	DB	0.28	1/68314 (0.0%)	0.65	88/106569 (0.1%)
24	BI	0.31	0/1046	0.82	1/1410 (0.1%)
24	DI	0.35	0/1046	0.85	0/1410
25	BC	0.28	0/2121	0.75	0/2852
25	DC	0.28	0/2121	0.75	0/2852
26	BD	0.28	0/1586	0.79	4/2134 (0.2%)
26	DD	0.28	0/1586	0.79	4/2134 (0.2%)
27	BK	0.29	0/939	0.85	2/1258 (0.2%)
27	DK	0.30	0/939	0.85	2/1258 (0.2%)
28	BP	0.28	0/929	0.86	3/1242 (0.2%)
28	DP	0.28	0/929	0.86	3/1242 (0.2%)
29	BE	0.27	0/1571	0.90	6/2113 (0.3%)
29	DE	0.27	0/1571	0.90	6/2113 (0.3%)
30	BY	0.28	0/453	0.81	0/605
30	DY	0.29	0/453	0.81	0/605
31	B0	0.27	0/450	0.81	1/599 (0.2%)
31	D0	0.27	0/450	0.81	1/599 (0.2%)
32	B4	0.28	0/303	0.73	1/397 (0.3%)
32	D4	0.28	0/303	0.74	1/397 (0.3%)
33	B1	0.30	0/416	0.76	0/554
33	D1	0.29	0/416	0.75	0/554
34	B3	0.27	0/513	0.74	0/676
34	D3	0.27	0/513	0.74	0/676
35	BV	0.27	0/766	0.73	0/1025
35	DV	0.27	0/766	0.73	0/1025
36	B2	0.29	0/380	0.93	2/498 (0.4%)
36	D2	0.29	0/380	0.93	2/498 (0.4%)
37	BL	0.28	0/1054	0.82	0/1403
37	DL	0.28	0/1054	0.81	0/1403
38	BM	0.29	0/1093	0.77	1/1460 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.28	0/1093	0.76	1/1460 (0.1%)
39	BX	0.26	0/510	0.88	2/677 (0.3%)
39	DX	0.26	0/510	0.88	2/677 (0.3%)
40	BH	0.29	0/1122	0.73	0/1515
40	DH	0.29	0/1122	0.76	1/1515 (0.1%)
41	BJ	0.28	0/1152	0.75	2/1551 (0.1%)
41	DJ	0.28	0/1152	0.76	2/1551 (0.1%)
42	BN	0.27	0/973	0.89	2/1301 (0.2%)
42	DN	0.27	0/973	0.88	2/1301 (0.2%)
43	BO	0.26	0/902	0.90	4/1209 (0.3%)
43	DO	0.26	0/902	0.89	3/1209 (0.2%)
44	BQ	0.28	0/960	0.90	5/1278 (0.4%)
44	DQ	0.28	0/960	0.89	4/1278 (0.3%)
45	BS	0.27	0/864	0.84	1/1156 (0.1%)
45	DS	0.27	0/864	0.86	3/1156 (0.3%)
46	BU	0.27	0/787	0.75	1/1051 (0.1%)
46	DU	0.28	0/787	0.75	1/1051 (0.1%)
47	BF	0.28	0/1444	0.82	2/1937 (0.1%)
47	DF	0.28	0/1444	0.83	2/1937 (0.1%)
48	BG	0.27	0/1343	0.79	2/1816 (0.1%)
48	DG	0.27	0/1343	0.79	2/1816 (0.1%)
49	BR	0.26	0/829	0.68	0/1107
49	DR	0.26	0/829	0.69	0/1107
50	BT	0.26	0/744	0.90	3/994 (0.3%)
50	DT	0.26	0/744	0.92	4/994 (0.4%)
51	BZ	0.28	0/635	0.88	1/848 (0.1%)
51	DZ	0.27	0/635	0.88	1/848 (0.1%)
52	BW	0.29	0/603	0.81	1/797 (0.1%)
52	DW	0.29	0/603	0.81	1/797 (0.1%)
53	B6	0.31	0/1497	0.80	1/2017 (0.0%)
53	D6	0.27	0/1497	0.76	1/2017 (0.0%)
All	All	0.28	2/309354 (0.0%)	0.69	415/462003 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	14
1	CA	0	13
23	BB	0	29

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	29
All	All	0	85

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-7.38	1.26	1.41
23	DB	1086	A	C5-C6	-7.33	1.26	1.41

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BE	60	TRP	N-CA-C	15.30	121.33	108.78
29	DE	60	TRP	N-CA-C	15.25	121.29	108.78
23	BB	508	A	C4'-C3'-O3'	-11.30	96.05	113.00
23	DB	508	A	C4'-C3'-O3'	-11.15	96.27	113.00
23	DB	2204	G	O5'-P-OP1	-10.82	75.55	108.00

There are no chirality outliers.

5 of 85 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	81	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1173	0
1	CA	32831	0	16521	1152	0
2	AC	1624	0	1699	147	0
2	CC	1624	0	1699	142	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AD	1643	0	1710	155	0
3	CD	1643	0	1710	161	0
4	AE	1105	0	1148	111	0
4	CE	1105	0	1148	105	0
5	AF	817	0	808	92	0
5	CF	817	0	808	87	0
6	AG	1174	0	1230	104	0
6	CG	1196	0	1246	95	0
7	AH	979	0	1034	64	0
7	CH	979	0	1034	65	0
8	AI	1022	0	1070	130	0
8	CI	1022	0	1070	131	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	77	0
10	AK	877	0	887	88	0
10	CK	877	0	887	76	0
11	AL	955	0	1019	87	0
11	CL	955	0	1019	94	0
12	AM	883	0	944	107	0
12	CM	876	0	937	112	0
13	AN	774	0	827	105	0
13	CN	774	0	827	104	0
14	AO	714	0	734	51	0
14	CO	714	0	734	55	0
15	AP	649	0	666	61	0
15	CP	638	0	656	62	0
16	AQ	648	0	691	64	0
16	CQ	657	0	702	64	0
17	AR	455	0	478	38	0
17	CR	455	0	478	39	0
18	AS	637	0	665	91	0
18	CS	644	0	675	93	0
19	AT	665	0	714	47	0
19	CT	665	0	714	47	0
20	AB	1704	0	1732	203	0
20	CB	1704	0	1732	208	0
21	AU	425	0	449	73	0
21	CU	425	0	449	71	0
22	BA	2507	0	1270	90	0
22	DA	2507	0	1270	83	0
23	BB	60995	0	30679	2162	0
23	DB	60995	0	30677	2182	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BI	1032	0	1088	121	0
24	DI	1032	0	1088	188	0
25	BC	2082	0	2157	243	0
25	DC	2082	0	2157	245	0
26	BD	1565	0	1616	197	0
26	DD	1565	0	1616	200	0
27	BK	930	0	1000	117	0
27	DK	930	0	1000	119	0
28	BP	917	0	965	143	0
28	DP	917	0	965	151	0
29	BE	1552	0	1619	196	0
29	DE	1552	0	1619	196	0
30	BY	449	0	491	53	0
30	DY	449	0	491	53	0
31	B0	444	0	461	40	0
31	D0	444	0	461	33	0
32	B4	302	0	340	49	0
32	D4	302	0	340	52	0
33	B1	409	0	440	53	0
33	D1	409	0	440	45	0
34	B3	504	0	574	56	0
34	D3	504	0	574	59	0
35	BV	753	0	780	89	0
35	DV	753	0	780	90	0
36	B2	377	0	418	36	0
36	D2	377	0	418	32	0
37	BL	1045	0	1117	146	0
37	DL	1045	0	1117	149	0
38	BM	1074	0	1157	125	0
38	DM	1074	0	1157	122	0
39	BX	509	0	543	61	0
39	DX	509	0	543	66	0
40	BH	1111	0	1148	224	0
40	DH	1111	0	1148	167	0
41	BJ	1129	0	1162	161	0
41	DJ	1129	0	1162	165	0
42	BN	960	0	1000	115	0
42	DN	960	0	1000	113	0
43	BO	892	0	923	79	0
43	DO	892	0	923	85	0
44	BQ	947	0	1022	130	0
44	DQ	947	0	1022	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BS	857	0	922	100	0
45	DS	857	0	922	99	0
46	BU	779	0	834	115	0
46	DU	779	0	834	114	0
47	BF	1420	0	1460	254	0
47	DF	1420	0	1460	245	0
48	BG	1323	0	1374	168	0
48	DG	1323	0	1374	166	0
49	BR	816	0	839	91	0
49	DR	816	0	839	104	0
50	BT	738	0	807	122	0
50	DT	738	0	807	122	0
51	BZ	625	0	652	70	0
51	DZ	625	0	652	65	0
52	BW	596	0	610	141	0
52	DW	596	0	610	156	0
53	B6	1478	0	1526	210	0
53	D6	1478	0	1526	184	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	289	0	0	1	0
56	AE	4	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	3	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	B2	1	0	0	0	0
56	BB	495	0	0	5	0
56	BC	4	0	0	0	0
56	BD	1	0	0	0	0
56	BE	3	0	0	0	0
56	BL	1	0	0	0	0
56	BT	1	0	0	0	0
56	CA	300	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CL	1	0	0	0	0
56	CN	4	0	0	0	0
56	CT	1	0	0	0	0
56	DB	505	0	0	7	0
56	DC	4	0	0	1	0
56	DD	1	0	0	0	0
56	DE	2	0	0	0	0
All	All	286960	0	193714	16653	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 35.

The worst 5 of 16653 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)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.39	1.17
13:CN:63:CYS:HB3	13:CN:67:GLY:H	1.09	1.16
13:AN:63:CYS:HB3	13:AN:67:GLY:H	1.05	1.15
10:AK:124:LYS:HA	21:AU:34:ARG:HB3	1.27	1.14
29:DE:21:ARG:HD2	29:DE:107:SER:HB3	1.30	1.13

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	AC	204/232 (88%)	152 (74%)	36 (18%)	16 (8%)	1	5
2	CC	204/232 (88%)	151 (74%)	37 (18%)	16 (8%)	1	5
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	1	8
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	6	27
4	CE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	6	27
5	AF	98/135 (73%)	71 (72%)	18 (18%)	9 (9%)	0	3
5	CF	98/135 (73%)	69 (70%)	21 (21%)	8 (8%)	0	5
6	AG	148/178 (83%)	114 (77%)	28 (19%)	6 (4%)	2	15
6	CG	150/178 (84%)	118 (79%)	25 (17%)	7 (5%)	2	12
7	AH	127/129 (98%)	106 (84%)	17 (13%)	4 (3%)	3	20
7	CH	127/129 (98%)	105 (83%)	18 (14%)	4 (3%)	3	20
8	AI	125/129 (97%)	92 (74%)	28 (22%)	5 (4%)	2	15
8	CI	125/129 (97%)	93 (74%)	28 (22%)	4 (3%)	3	19
9	AJ	96/103 (93%)	73 (76%)	13 (14%)	10 (10%)	0	2
9	CJ	96/103 (93%)	74 (77%)	12 (12%)	10 (10%)	0	2
10	AK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	2	14
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	1	11
11	AL	121/123 (98%)	84 (69%)	28 (23%)	9 (7%)	1	6
11	CL	121/123 (98%)	86 (71%)	25 (21%)	10 (8%)	0	5
12	AM	112/117 (96%)	85 (76%)	16 (14%)	11 (10%)	0	3
12	CM	111/117 (95%)	83 (75%)	17 (15%)	11 (10%)	0	3
13	AN	92/100 (92%)	65 (71%)	19 (21%)	8 (9%)	0	4
13	CN	92/100 (92%)	66 (72%)	18 (20%)	8 (9%)	0	4
14	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	3	18
14	CO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	5	25
15	AP	80/82 (98%)	62 (78%)	10 (12%)	8 (10%)	0	3
15	CP	78/82 (95%)	61 (78%)	11 (14%)	6 (8%)	1	5
16	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	1	11
16	CQ	79/83 (95%)	60 (76%)	15 (19%)	4 (5%)	1	11
17	AR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
17	CR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
18	AS	77/91 (85%)	59 (77%)	12 (16%)	6 (8%)	1	5
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	5
19	AT	83/86 (96%)	64 (77%)	15 (18%)	4 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CT	83/86 (96%)	65 (78%)	14 (17%)	4 (5%)	2	12
20	AB	216/240 (90%)	153 (71%)	48 (22%)	15 (7%)	1	7
20	CB	216/240 (90%)	150 (69%)	49 (23%)	17 (8%)	1	5
21	AU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
21	CU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	2	17
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	3	21
25	BC	269/272 (99%)	176 (65%)	61 (23%)	32 (12%)	0	1
25	DC	269/272 (99%)	177 (66%)	59 (22%)	33 (12%)	0	1
26	BD	207/209 (99%)	123 (59%)	56 (27%)	28 (14%)	0	1
26	DD	207/209 (99%)	122 (59%)	55 (27%)	30 (14%)	0	1
27	BK	119/123 (97%)	80 (67%)	25 (21%)	14 (12%)	0	1
27	DK	119/123 (97%)	81 (68%)	24 (20%)	14 (12%)	0	1
28	BP	112/114 (98%)	68 (61%)	29 (26%)	15 (13%)	0	1
28	DP	112/114 (98%)	69 (62%)	28 (25%)	15 (13%)	0	1
29	BE	199/201 (99%)	126 (63%)	54 (27%)	19 (10%)	0	3
29	DE	199/201 (99%)	127 (64%)	52 (26%)	20 (10%)	0	3
30	BY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	2
30	DY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	0	2
31	B0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
31	D0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
32	B4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
32	D4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	6 (12%)	5 (10%)	0	2
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	0	2
34	B3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	0	3
34	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	0	3
35	BV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	3	19
35	DV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	3	19
36	B2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	5	25
36	D2	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	141/144 (98%)	92 (65%)	31 (22%)	18 (13%)	0	1
37	DL	141/144 (98%)	94 (67%)	28 (20%)	19 (14%)	0	1
38	BM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	1
38	DM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	1
39	BX	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	1	7
39	DX	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	7
40	BH	147/149 (99%)	74 (50%)	50 (34%)	23 (16%)	0	1
40	DH	147/149 (99%)	92 (63%)	38 (26%)	17 (12%)	0	2
41	BJ	140/142 (99%)	96 (69%)	31 (22%)	13 (9%)	0	3
41	DJ	140/142 (99%)	95 (68%)	32 (23%)	13 (9%)	0	3
42	BN	118/127 (93%)	84 (71%)	25 (21%)	9 (8%)	1	6
42	DN	118/127 (93%)	82 (70%)	25 (21%)	11 (9%)	0	3
43	BO	114/117 (97%)	87 (76%)	21 (18%)	6 (5%)	1	10
43	DO	114/117 (97%)	86 (75%)	21 (18%)	7 (6%)	1	9
44	BQ	115/117 (98%)	81 (70%)	21 (18%)	13 (11%)	0	2
44	DQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	2
45	BS	108/110 (98%)	72 (67%)	21 (19%)	15 (14%)	0	1
45	DS	108/110 (98%)	73 (68%)	20 (18%)	15 (14%)	0	1
46	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
46	DU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	1
47	BF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	0
47	DF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	0
48	BG	174/176 (99%)	108 (62%)	41 (24%)	25 (14%)	0	1
48	DG	174/176 (99%)	109 (63%)	39 (22%)	26 (15%)	0	1
49	BR	101/103 (98%)	74 (73%)	16 (16%)	11 (11%)	0	2
49	DR	101/103 (98%)	73 (72%)	17 (17%)	11 (11%)	0	2
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	0
50	DT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	1
51	BZ	75/78 (96%)	50 (67%)	16 (21%)	9 (12%)	0	1
51	DZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	0	2
52	BW	77/84 (92%)	32 (42%)	20 (26%)	25 (32%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	DW	77/84 (92%)	33 (43%)	18 (23%)	26 (34%)	0	0
53	B6	183/185 (99%)	140 (76%)	36 (20%)	7 (4%)	2	16
53	D6	183/185 (99%)	146 (80%)	28 (15%)	9 (5%)	1	12
All	All	11607/12284 (94%)	8146 (70%)	2335 (20%)	1126 (10%)	0	3

5 of 1126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	100	ILE
2	AC	104	GLU

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	AC	170/189 (90%)	145 (85%)	25 (15%)	3	14
2	CC	170/189 (90%)	145 (85%)	25 (15%)	3	14
3	AD	172/172 (100%)	140 (81%)	32 (19%)	1	7
3	CD	172/172 (100%)	141 (82%)	31 (18%)	2	8
4	AE	113/125 (90%)	96 (85%)	17 (15%)	3	13
4	CE	113/125 (90%)	97 (86%)	16 (14%)	3	14
5	AF	87/116 (75%)	71 (82%)	16 (18%)	1	7
5	CF	87/116 (75%)	71 (82%)	16 (18%)	1	7
6	AG	123/146 (84%)	101 (82%)	22 (18%)	2	8
6	CG	125/146 (86%)	102 (82%)	23 (18%)	1	7
7	AH	104/104 (100%)	93 (89%)	11 (11%)	6	24
7	CH	104/104 (100%)	95 (91%)	9 (9%)	9	32
8	AI	105/106 (99%)	87 (83%)	18 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	86 (82%)	19 (18%)	2	8
9	AJ	86/90 (96%)	77 (90%)	9 (10%)	6	25
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	6	25
10	AK	90/98 (92%)	77 (86%)	13 (14%)	3	14
10	CK	90/98 (92%)	77 (86%)	13 (14%)	3	14
11	AL	103/103 (100%)	89 (86%)	14 (14%)	3	16
11	CL	103/103 (100%)	89 (86%)	14 (14%)	3	16
12	AM	92/95 (97%)	69 (75%)	23 (25%)	0	3
12	CM	91/95 (96%)	69 (76%)	22 (24%)	1	3
13	AN	79/83 (95%)	71 (90%)	8 (10%)	7	26
13	CN	79/83 (95%)	71 (90%)	8 (10%)	7	26
14	AO	76/77 (99%)	69 (91%)	7 (9%)	8	30
14	CO	76/77 (99%)	69 (91%)	7 (9%)	8	30
15	AP	65/65 (100%)	56 (86%)	9 (14%)	3	15
15	CP	65/65 (100%)	55 (85%)	10 (15%)	2	12
16	AQ	74/77 (96%)	63 (85%)	11 (15%)	3	13
16	CQ	75/77 (97%)	63 (84%)	12 (16%)	2	11
17	AR	48/64 (75%)	45 (94%)	3 (6%)	16	44
17	CR	48/64 (75%)	44 (92%)	4 (8%)	10	34
18	AS	70/78 (90%)	51 (73%)	19 (27%)	0	2
18	CS	71/78 (91%)	51 (72%)	20 (28%)	0	2
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2	10
19	CT	65/65 (100%)	54 (83%)	11 (17%)	2	10
20	AB	180/198 (91%)	146 (81%)	34 (19%)	1	7
20	CB	180/198 (91%)	144 (80%)	36 (20%)	1	6
21	AU	44/60 (73%)	31 (70%)	13 (30%)	0	2
21	CU	44/60 (73%)	31 (70%)	13 (30%)	0	2
24	BI	109/109 (100%)	108 (99%)	1 (1%)	70	78
24	DI	109/109 (100%)	105 (96%)	4 (4%)	30	58
25	BC	216/217 (100%)	185 (86%)	31 (14%)	3	14
25	DC	216/217 (100%)	185 (86%)	31 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	141 (86%)	23 (14%)	3	15
26	DD	164/164 (100%)	141 (86%)	23 (14%)	3	15
27	BK	102/104 (98%)	84 (82%)	18 (18%)	2	9
27	DK	102/104 (98%)	85 (83%)	17 (17%)	2	11
28	BP	99/99 (100%)	80 (81%)	19 (19%)	1	7
28	DP	99/99 (100%)	80 (81%)	19 (19%)	1	7
29	BE	165/165 (100%)	134 (81%)	31 (19%)	1	7
29	DE	165/165 (100%)	135 (82%)	30 (18%)	2	8
30	BY	48/48 (100%)	41 (85%)	7 (15%)	3	14
30	DY	48/48 (100%)	41 (85%)	7 (15%)	3	14
31	B0	47/47 (100%)	37 (79%)	10 (21%)	1	5
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	5
32	B4	34/34 (100%)	26 (76%)	8 (24%)	1	4
32	D4	34/34 (100%)	26 (76%)	8 (24%)	1	4
33	B1	45/48 (94%)	39 (87%)	6 (13%)	4	17
33	D1	45/48 (94%)	39 (87%)	6 (13%)	4	17
34	B3	51/51 (100%)	49 (96%)	2 (4%)	28	56
34	D3	51/51 (100%)	49 (96%)	2 (4%)	28	56
35	BV	78/78 (100%)	58 (74%)	20 (26%)	0	2
35	DV	78/78 (100%)	58 (74%)	20 (26%)	0	2
36	B2	38/38 (100%)	30 (79%)	8 (21%)	1	5
36	D2	38/38 (100%)	30 (79%)	8 (21%)	1	5
37	BL	102/103 (99%)	91 (89%)	11 (11%)	6	23
37	DL	102/103 (99%)	91 (89%)	11 (11%)	6	23
38	BM	109/109 (100%)	86 (79%)	23 (21%)	1	5
38	DM	109/109 (100%)	87 (80%)	22 (20%)	1	6
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	5
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	5
40	BH	114/114 (100%)	80 (70%)	34 (30%)	0	1
40	DH	114/114 (100%)	84 (74%)	30 (26%)	0	2
41	BJ	116/116 (100%)	96 (83%)	20 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	97 (84%)	19 (16%)	2	11
42	BN	100/103 (97%)	85 (85%)	15 (15%)	3	13
42	DN	100/103 (97%)	83 (83%)	17 (17%)	2	10
43	BO	86/87 (99%)	70 (81%)	16 (19%)	1	7
43	DO	86/87 (99%)	69 (80%)	17 (20%)	1	6
44	BQ	89/89 (100%)	76 (85%)	13 (15%)	3	14
44	DQ	89/89 (100%)	75 (84%)	14 (16%)	2	12
45	BS	93/93 (100%)	79 (85%)	14 (15%)	3	13
45	DS	93/93 (100%)	78 (84%)	15 (16%)	2	12
46	BU	83/84 (99%)	69 (83%)	14 (17%)	2	10
46	DU	83/84 (99%)	69 (83%)	14 (17%)	2	10
47	BF	149/149 (100%)	116 (78%)	33 (22%)	1	5
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	5
48	BG	137/137 (100%)	106 (77%)	31 (23%)	1	5
48	DG	137/137 (100%)	106 (77%)	31 (23%)	1	5
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	12
49	DR	84/84 (100%)	70 (83%)	14 (17%)	2	11
50	BT	80/84 (95%)	52 (65%)	28 (35%)	0	1
50	DT	80/84 (95%)	54 (68%)	26 (32%)	0	1
51	BZ	67/68 (98%)	51 (76%)	16 (24%)	1	4
51	DZ	67/68 (98%)	51 (76%)	16 (24%)	1	4
52	BW	59/62 (95%)	46 (78%)	13 (22%)	1	5
52	DW	59/62 (95%)	46 (78%)	13 (22%)	1	5
53	B6	157/157 (100%)	124 (79%)	33 (21%)	1	5
53	D6	157/157 (100%)	120 (76%)	37 (24%)	1	4
All	All	9647/10014 (96%)	7965 (83%)	1682 (17%)	2	9

5 of 1682 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	CG	2	ARG
21	CU	12	ASP
50	DT	22	THR

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Mol	Chain	Res	Type
7	CH	57	GLU
5	CF	100	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 394 such sidechains are listed below:

Mol	Chain	Res	Type
7	CH	66	GLN
25	DC	133	ASN
8	CI	80	HIS
15	CP	40	ASN
28	DP	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	248 (16%)	28 (1%)
1	CA	1529/1542 (99%)	239 (15%)	25 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	19 (16%)	0
23	BB	2837/2904 (97%)	451 (15%)	20 (0%)
23	DB	2837/2904 (97%)	435 (15%)	19 (0%)
All	All	8964/9132 (98%)	1410 (15%)	92 (1%)

5 of 1410 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	429	U
1	CA	1397	C
1	CA	484	G
1	CA	1065	U
23	DB	162	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 345 ligands modelled in this entry, 345 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	AA	1530/1542 (99%)	0.28	51 (3%)	49	33	20, 68, 149, 180	0
1	CA	1530/1542 (99%)	0.13	47 (3%)	51	35	10, 51, 126, 180	0
2	AC	206/232 (88%)	0.50	11 (5%)	32	22	24, 58, 114, 180	0
2	CC	206/232 (88%)	0.51	16 (7%)	19	14	28, 67, 117, 175	0
3	AD	205/205 (100%)	1.03	30 (14%)	6	5	22, 77, 137, 154	0
3	CD	205/205 (100%)	0.69	22 (10%)	11	9	15, 53, 129, 160	0
4	AE	150/166 (90%)	0.68	14 (9%)	14	11	16, 62, 116, 154	0
4	CE	150/166 (90%)	0.58	14 (9%)	14	11	20, 50, 105, 159	0
5	AF	100/135 (74%)	1.01	16 (16%)	5	4	33, 73, 126, 163	0
5	CF	100/135 (74%)	0.80	12 (12%)	9	7	20, 63, 115, 146	0
6	AG	150/178 (84%)	0.92	22 (14%)	6	5	40, 87, 140, 168	0
6	CG	152/178 (85%)	0.99	18 (11%)	9	8	21, 80, 132, 169	0
7	AH	129/129 (100%)	0.79	14 (10%)	10	9	34, 71, 116, 137	0
7	CH	129/129 (100%)	0.61	9 (6%)	22	15	18, 50, 96, 131	0
8	AI	127/129 (98%)	1.15	25 (19%)	3	3	23, 81, 151, 180	0
8	CI	127/129 (98%)	1.39	31 (24%)	2	1	26, 82, 135, 180	0
9	AJ	98/103 (95%)	1.27	30 (30%)	1	1	21, 74, 134, 180	0
9	CJ	98/103 (95%)	1.61	32 (32%)	1	1	34, 83, 136, 163	0
10	AK	117/128 (91%)	0.84	14 (11%)	9	7	19, 57, 100, 155	0
10	CK	117/128 (91%)	0.67	7 (5%)	27	19	18, 48, 100, 142	0
11	AL	123/123 (100%)	1.43	32 (26%)	1	1	29, 68, 124, 169	0
11	CL	123/123 (100%)	1.09	25 (20%)	3	2	10, 44, 107, 159	0
12	AM	114/117 (97%)	1.04	16 (14%)	6	5	48, 105, 157, 171	0
12	CM	113/117 (96%)	1.25	29 (25%)	1	1	44, 98, 149, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	1.43	23 (23%) 2 1	31, 77, 136, 171	0
13	CN	96/100 (96%)	1.41	24 (25%) 2 1	31, 78, 137, 161	0
14	AO	88/89 (98%)	0.66	7 (7%) 18 14	33, 67, 119, 173	0
14	CO	88/89 (98%)	0.78	11 (12%) 8 6	18, 53, 105, 133	0
15	AP	82/82 (100%)	1.12	14 (17%) 4 4	38, 78, 140, 157	0
15	CP	80/82 (97%)	1.00	14 (17%) 4 4	16, 44, 124, 180	0
16	AQ	80/83 (96%)	0.92	10 (12%) 8 6	47, 86, 139, 155	0
16	CQ	81/83 (97%)	0.90	14 (17%) 4 4	25, 56, 117, 151	0
17	AR	55/74 (74%)	1.17	10 (18%) 3 3	27, 66, 125, 149	0
17	CR	55/74 (74%)	1.26	11 (20%) 3 2	24, 51, 105, 154	0
18	AS	79/91 (86%)	1.38	16 (20%) 3 2	61, 116, 158, 179	0
18	CS	80/91 (87%)	1.26	19 (23%) 2 1	54, 107, 165, 177	0
19	AT	85/86 (98%)	1.46	26 (30%) 1 1	52, 92, 133, 180	0
19	CT	85/86 (98%)	1.31	20 (23%) 2 2	24, 52, 103, 156	0
20	AB	218/240 (90%)	1.06	38 (17%) 4 4	29, 88, 139, 180	0
20	CB	218/240 (90%)	1.01	31 (14%) 6 5	40, 92, 143, 161	0
21	AU	51/70 (72%)	2.06	26 (50%) 0 0	36, 90, 150, 153	0
21	CU	51/70 (72%)	2.07	23 (45%) 0 0	26, 74, 136, 174	0
22	BA	117/120 (97%)	0.32	4 (3%) 48 32	46, 80, 115, 168	0
22	DA	117/120 (97%)	0.43	7 (5%) 27 19	35, 69, 110, 178	0
23	BB	2841/2904 (97%)	0.22	103 (3%) 46 31	16, 56, 145, 180	0
23	DB	2841/2904 (97%)	0.16	101 (3%) 46 31	7, 44, 142, 180	0
24	BI	141/141 (100%)	1.98	60 (42%) 0 0	62, 152, 180, 180	0
24	DI	141/141 (100%)	2.21	72 (51%) 0 0	85, 155, 180, 180	0
25	BC	271/272 (99%)	0.84	26 (9%) 13 11	9, 45, 87, 170	0
25	DC	271/272 (99%)	0.84	27 (9%) 12 10	5, 37, 75, 125	0
26	BD	209/209 (100%)	1.11	32 (15%) 5 5	22, 66, 124, 167	0
26	DD	209/209 (100%)	0.98	36 (17%) 4 4	10, 44, 112, 139	0
27	BK	121/123 (98%)	1.01	15 (12%) 8 6	16, 67, 120, 154	0
27	DK	121/123 (98%)	0.72	14 (11%) 9 8	8, 39, 93, 152	0
28	BP	114/114 (100%)	1.14	24 (21%) 2 2	27, 77, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.75	8 (7%) 22 15	5, 42, 104, 160	0
29	BE	201/201 (100%)	0.88	22 (10%) 10 9	16, 67, 132, 148	0
29	DE	201/201 (100%)	0.93	24 (11%) 9 7	5, 65, 124, 156	0
30	BY	58/58 (100%)	0.90	6 (10%) 12 10	42, 73, 129, 143	0
30	DY	58/58 (100%)	1.19	12 (20%) 2 2	9, 58, 127, 150	0
31	B0	56/56 (100%)	1.01	8 (14%) 6 5	33, 71, 126, 141	0
31	D0	56/56 (100%)	0.82	7 (12%) 8 6	11, 45, 122, 170	0
32	B4	38/38 (100%)	1.95	17 (44%) 0 0	23, 75, 134, 149	0
32	D4	38/38 (100%)	1.82	16 (42%) 0 0	29, 54, 106, 125	0
33	B1	50/54 (92%)	0.66	6 (12%) 9 7	43, 79, 117, 132	0
33	D1	50/54 (92%)	0.65	4 (8%) 18 14	34, 66, 111, 135	0
34	B3	64/64 (100%)	1.31	18 (28%) 1 1	31, 51, 91, 115	0
34	D3	64/64 (100%)	1.07	8 (12%) 8 6	20, 40, 75, 110	0
35	BV	94/94 (100%)	0.81	10 (10%) 11 9	32, 90, 135, 169	0
35	DV	94/94 (100%)	0.55	5 (5%) 32 22	28, 74, 131, 167	0
36	B2	46/46 (100%)	1.19	11 (23%) 2 1	13, 40, 87, 121	0
36	D2	46/46 (100%)	0.98	6 (13%) 7 6	10, 32, 67, 131	0
37	BL	143/144 (99%)	1.10	24 (16%) 4 4	13, 64, 117, 161	0
37	DL	143/144 (99%)	1.08	27 (18%) 3 3	13, 54, 108, 133	0
38	BM	136/136 (100%)	1.08	28 (20%) 2 2	24, 68, 124, 174	0
38	DM	136/136 (100%)	1.04	21 (15%) 5 4	13, 46, 109, 131	0
39	BX	63/63 (100%)	1.08	10 (15%) 5 4	20, 86, 141, 171	0
39	DX	63/63 (100%)	0.94	11 (17%) 4 4	38, 84, 134, 172	0
40	BH	149/149 (100%)	1.21	30 (20%) 3 2	37, 121, 160, 180	0
40	DH	149/149 (100%)	0.93	18 (12%) 8 7	20, 108, 147, 180	0
41	BJ	142/142 (100%)	1.33	33 (23%) 2 2	25, 73, 126, 137	0
41	DJ	142/142 (100%)	1.13	24 (16%) 4 4	19, 55, 104, 167	0
42	BN	120/127 (94%)	1.19	26 (21%) 2 2	20, 65, 117, 173	0
42	DN	120/127 (94%)	0.88	19 (15%) 5 4	8, 40, 80, 125	0
43	BO	116/117 (99%)	1.12	20 (17%) 4 4	27, 82, 128, 179	0
43	DO	116/117 (99%)	1.09	19 (16%) 4 4	19, 68, 119, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	1.23	23 (19%) 3 3	5, 64, 111, 163	0
44	DQ	117/117 (100%)	1.33	31 (26%) 1 1	14, 48, 96, 180	0
45	BS	110/110 (100%)	0.82	10 (9%) 15 11	15, 58, 112, 161	0
45	DS	110/110 (100%)	0.67	8 (7%) 21 15	8, 42, 101, 132	0
46	BU	102/103 (99%)	1.20	20 (19%) 3 3	26, 75, 130, 171	0
46	DU	102/103 (99%)	1.18	21 (20%) 2 2	26, 83, 143, 180	0
47	BF	178/178 (100%)	1.17	32 (17%) 3 3	42, 113, 160, 180	0
47	DF	178/178 (100%)	1.34	44 (24%) 2 1	38, 97, 155, 180	0
48	BG	176/176 (100%)	1.00	24 (13%) 7 6	51, 103, 141, 162	0
48	DG	176/176 (100%)	1.04	31 (17%) 4 4	34, 91, 142, 169	0
49	BR	103/103 (100%)	1.15	16 (15%) 5 4	27, 86, 128, 157	0
49	DR	103/103 (100%)	1.26	16 (15%) 5 4	18, 76, 122, 148	0
50	BT	93/100 (93%)	1.40	25 (26%) 1 1	31, 70, 134, 164	0
50	DT	93/100 (93%)	1.62	30 (32%) 1 1	21, 66, 136, 173	0
51	BZ	77/78 (98%)	0.84	5 (6%) 25 17	22, 50, 93, 129	0
51	DZ	77/78 (98%)	0.73	8 (10%) 11 9	17, 46, 95, 130	0
52	BW	79/84 (94%)	2.05	35 (44%) 0 0	29, 81, 126, 153	0
52	DW	79/84 (94%)	1.87	32 (40%) 0 0	20, 59, 119, 135	0
53	B6	185/185 (100%)	1.17	40 (21%) 2 2	33, 116, 167, 180	0
53	D6	185/185 (100%)	0.86	29 (15%) 5 4	19, 88, 157, 180	0
All	All	20787/21416 (97%)	0.69	2373 (11%) 10 8	5, 63, 142, 180	0

The worst 5 of 2373 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	DB	2133	G	11.7
23	DB	2134	A	10.9
11	AL	24	GLU	9.8
8	CI	129	ARG	9.6
10	AK	125	LYS	9.2

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	DB	3058	1/1	0.26	0.51	145,145,145,145	0
54	MG	AA	2025	1/1	0.29	0.19	54,54,54,54	1
54	MG	AA	2059	1/1	0.38	0.41	127,127,127,127	0
54	MG	DB	3095	1/1	0.53	0.35	19,19,19,19	1
54	MG	AA	2037	1/1	0.55	0.32	139,139,139,139	0
54	MG	BB	3008	1/1	0.68	0.19	93,93,93,93	0
54	MG	DB	3059	1/1	0.71	0.13	65,65,65,65	1
54	MG	CA	1626	1/1	0.72	0.37	42,42,42,42	1
54	MG	BB	3010	1/1	0.73	0.16	70,70,70,70	0
54	MG	DB	3030	1/1	0.74	0.17	47,47,47,47	0
54	MG	BB	3100	1/1	0.77	0.28	75,75,75,75	1
54	MG	AA	2023	1/1	0.78	0.31	32,32,32,32	1
54	MG	DB	3052	1/1	0.80	0.12	114,114,114,114	0
54	MG	DB	3066	1/1	0.81	0.35	63,63,63,63	1
54	MG	BB	3093	1/1	0.81	0.15	38,38,38,38	1
54	MG	BB	3042	1/1	0.82	0.09	123,123,123,123	0
54	MG	CE	201	1/1	0.83	0.14	102,102,102,102	0
54	MG	AA	2047	1/1	0.83	0.17	126,126,126,126	0
54	MG	CA	1615	1/1	0.84	0.11	121,121,121,121	0
54	MG	AA	2030	1/1	0.86	0.11	102,102,102,102	0
54	MG	DB	3077	1/1	0.86	0.13	51,51,51,51	0
54	MG	DB	3013	1/1	0.86	0.15	47,47,47,47	0
54	MG	AA	2032	1/1	0.87	0.22	64,64,64,64	0
54	MG	AA	2039	1/1	0.87	0.12	108,108,108,108	0
54	MG	DB	3034	1/1	0.87	0.10	82,82,82,82	0
54	MG	DB	3110	1/1	0.87	0.16	40,40,40,40	0
54	MG	AA	2014	1/1	0.88	0.10	101,101,101,101	0
54	MG	DB	3060	1/1	0.88	0.07	89,89,89,89	0
54	MG	AA	2019	1/1	0.89	0.09	120,120,120,120	0
54	MG	BB	3028	1/1	0.89	0.09	46,46,46,46	0
54	MG	BB	3097	1/1	0.89	0.08	101,101,101,101	0
54	MG	CA	1641	1/1	0.90	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3046	1/1	0.90	0.10	69,69,69,69	0
54	MG	BB	3063	1/1	0.90	0.11	52,52,52,52	0
54	MG	AA	2057	1/1	0.90	0.23	93,93,93,93	0
54	MG	AA	2002	1/1	0.90	0.11	85,85,85,85	0
54	MG	CA	1627	1/1	0.90	0.09	5,5,5,5	1
54	MG	CA	1621	1/1	0.91	0.11	110,110,110,110	0
54	MG	BB	3081	1/1	0.91	0.10	35,35,35,35	0
54	MG	AA	2008	1/1	0.91	0.10	94,94,94,94	0
54	MG	BB	3033	1/1	0.92	0.09	94,94,94,94	0
54	MG	AA	2027	1/1	0.92	0.10	62,62,62,62	0
54	MG	DB	3022	1/1	0.92	0.09	32,32,32,32	0
54	MG	DB	3029	1/1	0.92	0.09	67,67,67,67	0
54	MG	CA	1623	1/1	0.92	0.12	101,101,101,101	0
54	MG	BB	3009	1/1	0.92	0.10	87,87,87,87	0
54	MG	CA	1608	1/1	0.92	0.08	106,106,106,106	0
55	ZN	B4	101	1/1	0.92	0.07	55,55,55,55	0
54	MG	BB	3017	1/1	0.93	0.09	59,59,59,59	0
54	MG	BB	3090	1/1	0.93	0.07	78,78,78,78	0
54	MG	DB	3015	1/1	0.93	0.09	60,60,60,60	0
54	MG	BB	3073	1/1	0.93	0.09	70,70,70,70	0
54	MG	BB	3049	1/1	0.94	0.08	26,26,26,26	0
54	MG	AA	2043	1/1	0.94	0.08	42,42,42,42	0
54	MG	CA	1654	1/1	0.94	0.13	52,52,52,52	0
54	MG	AA	2035	1/1	0.94	0.07	102,102,102,102	0
54	MG	AA	2042	1/1	0.94	0.07	32,32,32,32	0
54	MG	BB	3087	1/1	0.94	0.16	100,100,100,100	0
54	MG	AA	2038	1/1	0.95	0.06	63,63,63,63	0
54	MG	BB	3102	1/1	0.95	0.06	38,38,38,38	0
54	MG	BB	3047	1/1	0.95	0.09	70,70,70,70	0
54	MG	AA	2015	1/1	0.95	0.06	86,86,86,86	0
54	MG	AA	2020	1/1	0.95	0.07	84,84,84,84	0
54	MG	AA	2022	1/1	0.95	0.17	77,77,77,77	0
54	MG	AA	2017	1/1	0.95	0.11	75,75,75,75	0
54	MG	AA	2050	1/1	0.95	0.05	101,101,101,101	0
54	MG	AA	2053	1/1	0.95	0.08	46,46,46,46	0
54	MG	CA	1634	1/1	0.95	0.06	32,32,32,32	0
54	MG	CA	1636	1/1	0.95	0.06	63,63,63,63	0
54	MG	BB	3040	1/1	0.95	0.12	60,60,60,60	0
54	MG	CA	1648	1/1	0.95	0.09	47,47,47,47	0
54	MG	AA	2018	1/1	0.95	0.06	78,78,78,78	0
54	MG	DB	3010	1/1	0.95	0.03	19,19,19,19	0
54	MG	BB	3031	1/1	0.96	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	2028	1/1	0.96	0.06	66,66,66,66	0
54	MG	CA	1611	1/1	0.96	0.06	81,81,81,81	0
54	MG	DB	3020	1/1	0.96	0.10	14,14,14,14	0
54	MG	BB	3079	1/1	0.96	0.06	63,63,63,63	0
54	MG	AA	2051	1/1	0.96	0.06	80,80,80,80	0
54	MG	BB	3007	1/1	0.96	0.06	74,74,74,74	0
54	MG	BB	3044	1/1	0.96	0.07	70,70,70,70	0
54	MG	DB	3048	1/1	0.96	0.07	41,41,41,41	0
54	MG	DB	3050	1/1	0.96	0.05	70,70,70,70	0
54	MG	BB	3024	1/1	0.96	0.07	47,47,47,47	0
54	MG	CA	1633	1/1	0.96	0.06	42,42,42,42	0
54	MG	BB	3094	1/1	0.96	0.06	21,21,21,21	0
54	MG	AA	2012	1/1	0.96	0.05	63,63,63,63	0
54	MG	DB	3064	1/1	0.96	0.06	37,37,37,37	0
54	MG	BB	3099	1/1	0.96	0.07	51,51,51,51	0
54	MG	DB	3070	1/1	0.96	0.04	26,26,26,26	0
54	MG	BB	3029	1/1	0.96	0.05	28,28,28,28	0
54	MG	DB	3083	1/1	0.96	0.06	72,72,72,72	0
54	MG	DB	3090	1/1	0.96	0.08	49,49,49,49	0
54	MG	BB	3053	1/1	0.96	0.05	61,61,61,61	0
54	MG	DB	3100	1/1	0.96	0.06	17,17,17,17	0
54	MG	DB	3109	1/1	0.96	0.10	35,35,35,35	0
54	MG	CA	1657	1/1	0.96	0.07	62,62,62,62	0
54	MG	CA	1659	1/1	0.96	0.06	64,64,64,64	0
54	MG	CA	1644	1/1	0.97	0.06	52,52,52,52	0
54	MG	CA	1647	1/1	0.97	0.06	102,102,102,102	0
54	MG	BB	3002	1/1	0.97	0.07	12,12,12,12	0
54	MG	BB	3021	1/1	0.97	0.07	43,43,43,43	0
54	MG	AA	2004	1/1	0.97	0.08	36,36,36,36	0
54	MG	CA	1658	1/1	0.97	0.21	33,33,33,33	0
54	MG	BB	3025	1/1	0.97	0.09	49,49,49,49	0
54	MG	CA	1660	1/1	0.97	0.06	96,96,96,96	0
54	MG	DB	3003	1/1	0.97	0.07	29,29,29,29	0
54	MG	AA	2056	1/1	0.97	0.14	46,46,46,46	0
54	MG	AA	2026	1/1	0.97	0.08	5,5,5,5	1
54	MG	BB	3101	1/1	0.97	0.07	22,22,22,22	0
54	MG	BB	3051	1/1	0.97	0.05	35,35,35,35	0
54	MG	BB	3108	1/1	0.97	0.06	37,37,37,37	0
54	MG	DB	3024	1/1	0.97	0.10	30,30,30,30	0
54	MG	BB	3110	1/1	0.97	0.07	56,56,56,56	0
54	MG	AA	2045	1/1	0.97	0.05	63,63,63,63	0
54	MG	CA	1605	1/1	0.97	0.05	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3037	1/1	0.97	0.07	45,45,45,45	0
54	MG	DB	3045	1/1	0.97	0.05	61,61,61,61	0
54	MG	BB	3054	1/1	0.97	0.07	57,57,57,57	0
54	MG	BB	3057	1/1	0.97	0.16	37,37,37,37	0
54	MG	CA	1614	1/1	0.97	0.12	58,58,58,58	0
54	MG	DB	3057	1/1	0.97	0.06	40,40,40,40	0
54	MG	BB	3059	1/1	0.97	0.07	32,32,32,32	0
54	MG	CA	1616	1/1	0.97	0.05	42,42,42,42	0
54	MG	CA	1619	1/1	0.97	0.08	51,51,51,51	0
54	MG	DB	3062	1/1	0.97	0.05	41,41,41,41	0
54	MG	DB	3063	1/1	0.97	0.06	28,28,28,28	0
54	MG	CA	1620	1/1	0.97	0.05	58,58,58,58	0
54	MG	BB	3014	1/1	0.97	0.05	58,58,58,58	0
54	MG	BB	3034	1/1	0.97	0.07	35,35,35,35	0
54	MG	BB	3078	1/1	0.97	0.09	47,47,47,47	0
54	MG	DB	3078	1/1	0.97	0.05	45,45,45,45	0
54	MG	DB	3080	1/1	0.97	0.07	29,29,29,29	0
54	MG	BB	3037	1/1	0.97	0.07	23,23,23,23	0
54	MG	DB	3088	1/1	0.97	0.05	28,28,28,28	0
54	MG	BB	3038	1/1	0.97	0.04	98,98,98,98	0
54	MG	DB	3092	1/1	0.97	0.05	65,65,65,65	0
54	MG	BB	3084	1/1	0.97	0.05	38,38,38,38	0
54	MG	DB	3099	1/1	0.97	0.06	15,15,15,15	0
54	MG	CA	1635	1/1	0.97	0.06	55,55,55,55	0
54	MG	BB	3039	1/1	0.97	0.05	43,43,43,43	0
54	MG	CA	1638	1/1	0.97	0.07	90,90,90,90	0
54	MG	BB	3089	1/1	0.97	0.04	38,38,38,38	0
55	ZN	D4	101	1/1	0.97	0.04	55,55,55,55	0
54	MG	CA	1643	1/1	0.98	0.04	20,20,20,20	0
54	MG	BB	3080	1/1	0.98	0.08	57,57,57,57	0
54	MG	CA	1646	1/1	0.98	0.07	46,46,46,46	0
54	MG	BB	3032	1/1	0.98	0.05	34,34,34,34	0
54	MG	BB	3004	1/1	0.98	0.06	52,52,52,52	0
54	MG	CA	1650	1/1	0.98	0.06	41,41,41,41	0
54	MG	CA	1652	1/1	0.98	0.06	54,54,54,54	0
54	MG	BB	3085	1/1	0.98	0.08	56,56,56,56	0
54	MG	BB	3005	1/1	0.98	0.05	24,24,24,24	0
54	MG	BB	3006	1/1	0.98	0.04	28,28,28,28	0
54	MG	AA	2049	1/1	0.98	0.05	90,90,90,90	0
54	MG	AA	2006	1/1	0.98	0.04	71,71,71,71	0
54	MG	AA	2034	1/1	0.98	0.04	40,40,40,40	0
54	MG	DB	3004	1/1	0.98	0.03	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3006	1/1	0.98	0.05	26,26,26,26	0
54	MG	DB	3008	1/1	0.98	0.05	33,33,33,33	0
54	MG	BB	3095	1/1	0.98	0.08	25,25,25,25	0
54	MG	DB	3011	1/1	0.98	0.05	16,16,16,16	0
54	MG	DB	3012	1/1	0.98	0.07	23,23,23,23	0
54	MG	AA	2052	1/1	0.98	0.08	50,50,50,50	0
54	MG	BB	3013	1/1	0.98	0.07	36,36,36,36	0
54	MG	DB	3018	1/1	0.98	0.05	23,23,23,23	0
54	MG	BB	3045	1/1	0.98	0.05	41,41,41,41	0
54	MG	AA	2013	1/1	0.98	0.06	85,85,85,85	0
54	MG	BB	3015	1/1	0.98	0.05	40,40,40,40	0
54	MG	DB	3025	1/1	0.98	0.04	28,28,28,28	0
54	MG	BB	3104	1/1	0.98	0.04	20,20,20,20	0
54	MG	BB	3106	1/1	0.98	0.05	36,36,36,36	0
54	MG	DB	3032	1/1	0.98	0.08	33,33,33,33	0
54	MG	BB	3048	1/1	0.98	0.07	30,30,30,30	0
54	MG	BB	3109	1/1	0.98	0.04	42,42,42,42	0
54	MG	DB	3039	1/1	0.98	0.06	34,34,34,34	0
54	MG	DB	3041	1/1	0.98	0.04	36,36,36,36	0
54	MG	BB	3016	1/1	0.98	0.13	34,34,34,34	0
54	MG	BB	3050	1/1	0.98	0.04	28,28,28,28	0
54	MG	AA	2044	1/1	0.98	0.05	47,47,47,47	0
54	MG	CA	1606	1/1	0.98	0.06	59,59,59,59	0
54	MG	DB	3053	1/1	0.98	0.07	28,28,28,28	0
54	MG	DB	3055	1/1	0.98	0.05	17,17,17,17	0
54	MG	CA	1607	1/1	0.98	0.05	37,37,37,37	0
54	MG	BB	3052	1/1	0.98	0.11	25,25,25,25	0
54	MG	CA	1610	1/1	0.98	0.04	56,56,56,56	0
54	MG	BB	3019	1/1	0.98	0.04	37,37,37,37	0
54	MG	DB	3061	1/1	0.98	0.05	51,51,51,51	0
54	MG	CA	1612	1/1	0.98	0.05	46,46,46,46	0
54	MG	CA	1613	1/1	0.98	0.04	39,39,39,39	0
54	MG	BB	3020	1/1	0.98	0.06	20,20,20,20	0
54	MG	AA	2024	1/1	0.98	0.09	61,61,61,61	0
54	MG	DB	3068	1/1	0.98	0.06	8,8,8,8	0
54	MG	AA	2058	1/1	0.98	0.04	88,88,88,88	0
54	MG	DB	3071	1/1	0.98	0.07	57,57,57,57	0
54	MG	DB	3074	1/1	0.98	0.04	30,30,30,30	0
54	MG	BB	3061	1/1	0.98	0.04	38,38,38,38	0
54	MG	AA	2046	1/1	0.98	0.07	46,46,46,46	0
54	MG	BB	3067	1/1	0.98	0.05	45,45,45,45	0
54	MG	CA	1622	1/1	0.98	0.05	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3085	1/1	0.98	0.06	5,5,5,5	0
54	MG	BB	3068	1/1	0.98	0.05	43,43,43,43	0
54	MG	DB	3089	1/1	0.98	0.08	50,50,50,50	0
54	MG	BB	3070	1/1	0.98	0.05	35,35,35,35	0
54	MG	DB	3091	1/1	0.98	0.04	29,29,29,29	0
54	MG	BB	3072	1/1	0.98	0.05	44,44,44,44	0
54	MG	AA	2060	1/1	0.98	0.04	75,75,75,75	0
54	MG	DB	3097	1/1	0.98	0.07	32,32,32,32	0
54	MG	BB	3074	1/1	0.98	0.06	21,21,21,21	0
54	MG	BB	3076	1/1	0.98	0.06	43,43,43,43	0
54	MG	DB	3106	1/1	0.98	0.06	9,9,9,9	0
54	MG	BB	3077	1/1	0.98	0.05	36,36,36,36	0
54	MG	AA	2021	1/1	0.98	0.05	52,52,52,52	0
54	MG	DB	3111	1/1	0.98	0.10	51,51,51,51	0
54	MG	BB	3003	1/1	0.98	0.05	47,47,47,47	0
54	MG	CA	1642	1/1	0.98	0.03	63,63,63,63	0
54	MG	BB	3055	1/1	0.99	0.08	41,41,41,41	0
54	MG	BB	3056	1/1	0.99	0.04	31,31,31,31	0
54	MG	AA	2048	1/1	0.99	0.04	27,27,27,27	0
54	MG	BB	3103	1/1	0.99	0.06	20,20,20,20	0
54	MG	CA	1661	1/1	0.99	0.04	49,49,49,49	0
54	MG	BB	3058	1/1	0.99	0.04	33,33,33,33	0
54	MG	BB	3105	1/1	0.99	0.08	65,65,65,65	0
54	MG	DB	3005	1/1	0.99	0.04	56,56,56,56	0
54	MG	AA	2011	1/1	0.99	0.03	45,45,45,45	0
54	MG	DB	3007	1/1	0.99	0.04	30,30,30,30	0
54	MG	BB	3107	1/1	0.99	0.03	31,31,31,31	0
54	MG	BB	3060	1/1	0.99	0.02	47,47,47,47	0
54	MG	BB	3030	1/1	0.99	0.08	40,40,40,40	0
54	MG	BB	3062	1/1	0.99	0.03	41,41,41,41	0
54	MG	AA	2036	1/1	0.99	0.05	65,65,65,65	0
54	MG	CA	1601	1/1	0.99	0.04	9,9,9,9	0
54	MG	DB	3016	1/1	0.99	0.04	28,28,28,28	0
54	MG	DB	3017	1/1	0.99	0.04	18,18,18,18	0
54	MG	CA	1603	1/1	0.99	0.02	29,29,29,29	0
54	MG	DB	3019	1/1	0.99	0.05	21,21,21,21	0
54	MG	BB	3064	1/1	0.99	0.07	31,31,31,31	0
54	MG	BB	3066	1/1	0.99	0.04	21,21,21,21	0
54	MG	DB	3023	1/1	0.99	0.04	33,33,33,33	0
54	MG	AA	2005	1/1	0.99	0.03	36,36,36,36	0
54	MG	AA	2003	1/1	0.99	0.04	31,31,31,31	0
54	MG	DB	3026	1/1	0.99	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3028	1/1	0.99	0.13	29,29,29,29	0
54	MG	CA	1609	1/1	0.99	0.05	56,56,56,56	0
54	MG	BB	3069	1/1	0.99	0.04	17,17,17,17	0
54	MG	DB	3031	1/1	0.99	0.03	17,17,17,17	0
54	MG	AA	2007	1/1	0.99	0.03	42,42,42,42	0
54	MG	DB	3033	1/1	0.99	0.04	20,20,20,20	0
54	MG	BB	3071	1/1	0.99	0.09	25,25,25,25	0
54	MG	DB	3035	1/1	0.99	0.04	57,57,57,57	0
54	MG	BB	3035	1/1	0.99	0.03	41,41,41,41	0
54	MG	DB	3038	1/1	0.99	0.05	26,26,26,26	0
54	MG	BB	3011	1/1	0.99	0.04	30,30,30,30	0
54	MG	BB	3012	1/1	0.99	0.04	32,32,32,32	0
54	MG	DB	3042	1/1	0.99	0.04	45,45,45,45	0
54	MG	DB	3043	1/1	0.99	0.03	8,8,8,8	0
54	MG	AA	2055	1/1	0.99	0.11	54,54,54,54	0
54	MG	DB	3046	1/1	0.99	0.04	22,22,22,22	0
54	MG	CA	1617	1/1	0.99	0.04	21,21,21,21	0
54	MG	DB	3049	1/1	0.99	0.03	26,26,26,26	0
54	MG	AA	2040	1/1	0.99	0.06	56,56,56,56	0
54	MG	DB	3051	1/1	0.99	0.06	25,25,25,25	0
54	MG	BB	3041	1/1	0.99	0.03	22,22,22,22	0
54	MG	AA	2041	1/1	0.99	0.04	40,40,40,40	0
54	MG	DB	3054	1/1	0.99	0.04	25,25,25,25	0
54	MG	BB	3043	1/1	0.99	0.13	53,53,53,53	0
54	MG	AA	2029	1/1	0.99	0.03	40,40,40,40	0
54	MG	CA	1624	1/1	0.99	0.10	22,22,22,22	0
54	MG	CA	1625	1/1	0.99	0.09	19,19,19,19	0
54	MG	BB	3082	1/1	0.99	0.06	38,38,38,38	0
54	MG	AA	2001	1/1	0.99	0.03	29,29,29,29	0
54	MG	CA	1628	1/1	0.99	0.10	38,38,38,38	0
54	MG	CA	1629	1/1	0.99	0.10	20,20,20,20	1
54	MG	CA	1630	1/1	0.99	0.04	39,39,39,39	0
54	MG	CA	1631	1/1	0.99	0.04	38,38,38,38	0
54	MG	DB	3067	1/1	0.99	0.03	18,18,18,18	0
54	MG	CA	1632	1/1	0.99	0.04	41,41,41,41	0
54	MG	DB	3069	1/1	0.99	0.05	21,21,21,21	0
54	MG	BB	3018	1/1	0.99	0.04	45,45,45,45	0
54	MG	BB	3086	1/1	0.99	0.10	45,45,45,45	0
54	MG	DB	3072	1/1	0.99	0.04	23,23,23,23	0
54	MG	DB	3073	1/1	0.99	0.05	29,29,29,29	0
54	MG	AA	2031	1/1	0.99	0.03	51,51,51,51	0
54	MG	DB	3075	1/1	0.99	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3076	1/1	0.99	0.05	17,17,17,17	0
54	MG	BB	3088	1/1	0.99	0.06	75,75,75,75	0
54	MG	CA	1637	1/1	0.99	0.03	53,53,53,53	0
54	MG	DB	3079	1/1	0.99	0.04	34,34,34,34	0
54	MG	BB	3001	1/1	0.99	0.04	35,35,35,35	0
54	MG	DB	3082	1/1	0.99	0.04	21,21,21,21	0
54	MG	CA	1640	1/1	0.99	0.03	43,43,43,43	0
54	MG	DB	3084	1/1	0.99	0.08	34,34,34,34	0
54	MG	AA	2016	1/1	0.99	0.04	50,50,50,50	0
54	MG	BB	3091	1/1	0.99	0.04	31,31,31,31	0
54	MG	BB	3092	1/1	0.99	0.04	51,51,51,51	0
54	MG	BB	3022	1/1	0.99	0.03	44,44,44,44	0
54	MG	CA	1645	1/1	0.99	0.03	45,45,45,45	0
54	MG	AA	2033	1/1	0.99	0.03	40,40,40,40	0
54	MG	DB	3094	1/1	0.99	0.04	39,39,39,39	0
54	MG	AA	2010	1/1	0.99	0.03	36,36,36,36	0
54	MG	DB	3096	1/1	0.99	0.04	30,30,30,30	0
54	MG	BB	3096	1/1	0.99	0.05	37,37,37,37	0
54	MG	CA	1649	1/1	0.99	0.03	80,80,80,80	0
54	MG	BB	3026	1/1	0.99	0.03	28,28,28,28	0
54	MG	DB	3102	1/1	0.99	0.04	15,15,15,15	0
54	MG	DB	3104	1/1	0.99	0.03	28,28,28,28	0
54	MG	DB	3105	1/1	0.99	0.04	32,32,32,32	0
54	MG	CA	1651	1/1	0.99	0.04	50,50,50,50	0
54	MG	DB	3107	1/1	0.99	0.03	34,34,34,34	0
54	MG	DB	3108	1/1	0.99	0.04	11,11,11,11	0
54	MG	BB	3098	1/1	0.99	0.03	30,30,30,30	0
54	MG	CA	1653	1/1	0.99	0.03	55,55,55,55	0
54	MG	BB	3027	1/1	0.99	0.12	34,34,34,34	0
54	MG	CA	1655	1/1	0.99	0.03	28,28,28,28	0
54	MG	CA	1656	1/1	0.99	0.04	22,22,22,22	0
54	MG	CA	1602	1/1	1.00	0.07	34,34,34,34	0
54	MG	DB	3021	1/1	1.00	0.02	21,21,21,21	0
54	MG	DB	3086	1/1	1.00	0.07	26,26,26,26	0
54	MG	DB	3087	1/1	1.00	0.04	54,54,54,54	0
54	MG	DB	3040	1/1	1.00	0.01	9,9,9,9	0
54	MG	AA	2054	1/1	1.00	0.04	49,49,49,49	0
54	MG	CA	1604	1/1	1.00	0.04	36,36,36,36	0
54	MG	DB	3065	1/1	1.00	0.04	12,12,12,12	0
54	MG	BB	3023	1/1	1.00	0.05	23,23,23,23	0
54	MG	DB	3093	1/1	1.00	0.03	6,6,6,6	0
54	MG	DB	3044	1/1	1.00	0.11	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3009	1/1	1.00	0.02	17,17,17,17	0
54	MG	BB	3036	1/1	1.00	0.03	39,39,39,39	0
54	MG	DB	3047	1/1	1.00	0.07	13,13,13,13	0
54	MG	DB	3098	1/1	1.00	0.06	29,29,29,29	0
54	MG	DB	3027	1/1	1.00	0.06	27,27,27,27	0
54	MG	BB	3075	1/1	1.00	0.06	37,37,37,37	0
54	MG	DB	3101	1/1	1.00	0.03	5,5,5,5	0
54	MG	BB	3065	1/1	1.00	0.04	40,40,40,40	0
54	MG	DB	3103	1/1	1.00	0.02	26,26,26,26	0
54	MG	CA	1618	1/1	1.00	0.03	18,18,18,18	0
54	MG	DB	3014	1/1	1.00	0.05	21,21,21,21	0
54	MG	CA	1639	1/1	1.00	0.05	24,24,24,24	0
54	MG	DB	3001	1/1	1.00	0.05	9,9,9,9	0
54	MG	DB	3002	1/1	1.00	0.04	11,11,11,11	0
54	MG	DB	3056	1/1	1.00	0.03	11,11,11,11	0
54	MG	BB	3083	1/1	1.00	0.02	30,30,30,30	0
54	MG	DB	3081	1/1	1.00	0.03	17,17,17,17	0
54	MG	DB	3036	1/1	1.00	0.03	25,25,25,25	0
54	MG	AA	2009	1/1	1.00	0.05	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.