



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:44 PM UTC

PDB ID : 4V4H / pdb_00004v4h
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with the antibiotic kasugamyin at 3.5Å resolution.
Authors : Schuwirth, B.S.; Vila-Sanjurjo, A.; Cate, J.H.D.
Deposited on : 2006-08-04
Resolution : 3.46 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

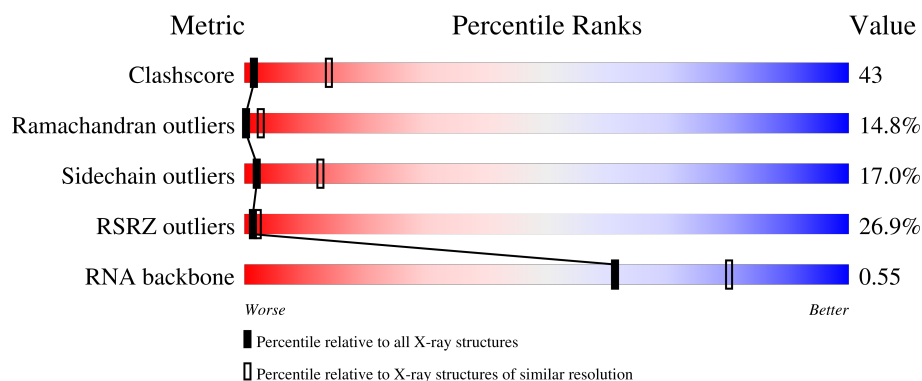
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

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	17% 23% 62% 13% ..
1	CA	1542	9% 22% 64% 11% ..
2	AC	233	21% 25% 52% 10% 12%
2	CC	233	13% 28% 47% 12% 12%
3	AD	206	38% 28% 54% 16% .

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Mol	Chain	Length	Quality of chain
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	

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Mol	Chain	Length	Quality of chain
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AB	241	
20	CB	241	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	
28	BF	179	

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Mol	Chain	Length	Quality of chain
28	DF	179	
29	BG	177	
29	DG	177	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	

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Mol	Chain	Length	Quality of chain
41	BT	100	
41	DT	100	
42	BU	104	
42	DU	104	
43	BW	85	
43	DW	85	
44	BX	63	
44	DX	63	
45	BY	59	
45	DY	59	
46	BZ	70	
46	DZ	70	
47	B0	57	
47	D0	57	
48	B1	55	
48	D1	55	
49	B2	46	
49	D2	46	
50	B3	65	
50	D3	65	
51	B4	38	
51	D4	38	
52	BI	142	
52	DI	142	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DB	3093	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 284160 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	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
			716	440	146	129	1			
14	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	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 RIBOSOMAL RNA.

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 RIBOSOMAL RNA.

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 L25.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			
25	DC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	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 L4.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			
31	DJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
33	DL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
35	DN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
36	DO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			
41	DT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0
43	DW	84	Total	C	N	O	S			
			634	391	129	113	1	0	0	0

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0
46	DZ	70	Total	C	N	O	S			
			549	339	104	100	6	0	0	0

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	54	Total	C	N	O	0	0	0
			441	284	81	76			
48	D1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

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

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

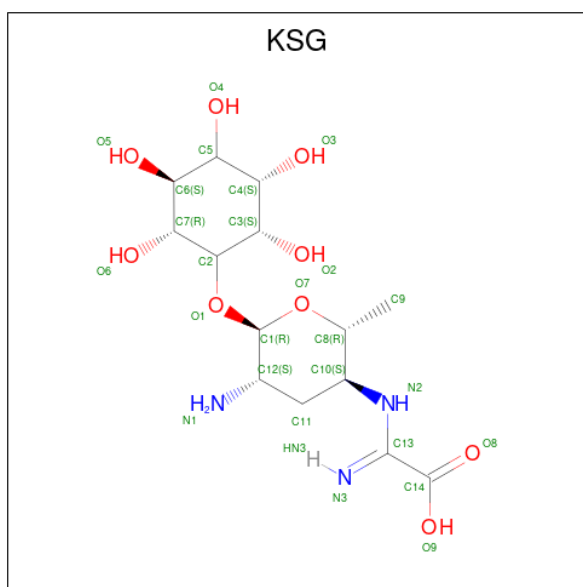
- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 53 is (1S,2R,3S,4R,5S,6S)-2,3,4,5,6-PENTAHYDROXYCYCLOHEXYL 2-AMINO-4-{{[CARBOXY(IMINO)METHYL]AMINO}}-2,3,4,6-TETRADEOXY-ALPHA-D-ARABINO-HEXOPYRANOSIDE (CCD ID: KSG) (formula: C₁₄H₂₅N₃O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
53	AA	1	Total	C	N	O	0	0
			26	14	3	9		
53	CA	1	Total	C	N	O	0	0
			26	14	3	9		

- 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	CA	62	Total	Mg	0	0
			62	62		
54	DB	109	Total	Mg	0	0
			109	109		
54	DE	1	Total	Mg	0	0
			1	1		
54	DN	1	Total	Mg	0	0
			1	1		

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	289	Total	O	0	0
			289	289		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	AE	3	Total O 3 3	0	0
55	AK	2	Total O 2 2	0	0
55	AN	3	Total O 3 3	0	0
55	AP	2	Total O 2 2	0	0
55	AT	1	Total O 1 1	0	0
55	BB	497	Total O 497 497	0	0
55	BC	1	Total O 1 1	0	0
55	BE	5	Total O 5 5	0	0
55	BH	1	Total O 1 1	0	0
55	BL	2	Total O 2 2	0	0
55	BN	1	Total O 1 1	0	0
55	CA	293	Total O 293 293	0	0
55	CE	3	Total O 3 3	0	0
55	CK	1	Total O 1 1	0	0
55	CL	4	Total O 4 4	0	0
55	CN	3	Total O 3 3	0	0
55	CP	1	Total O 1 1	0	0
55	CT	3	Total O 3 3	0	0
55	DB	501	Total O 501 501	0	0
55	DC	1	Total O 1 1	0	0
55	DD	1	Total O 1 1	0	0

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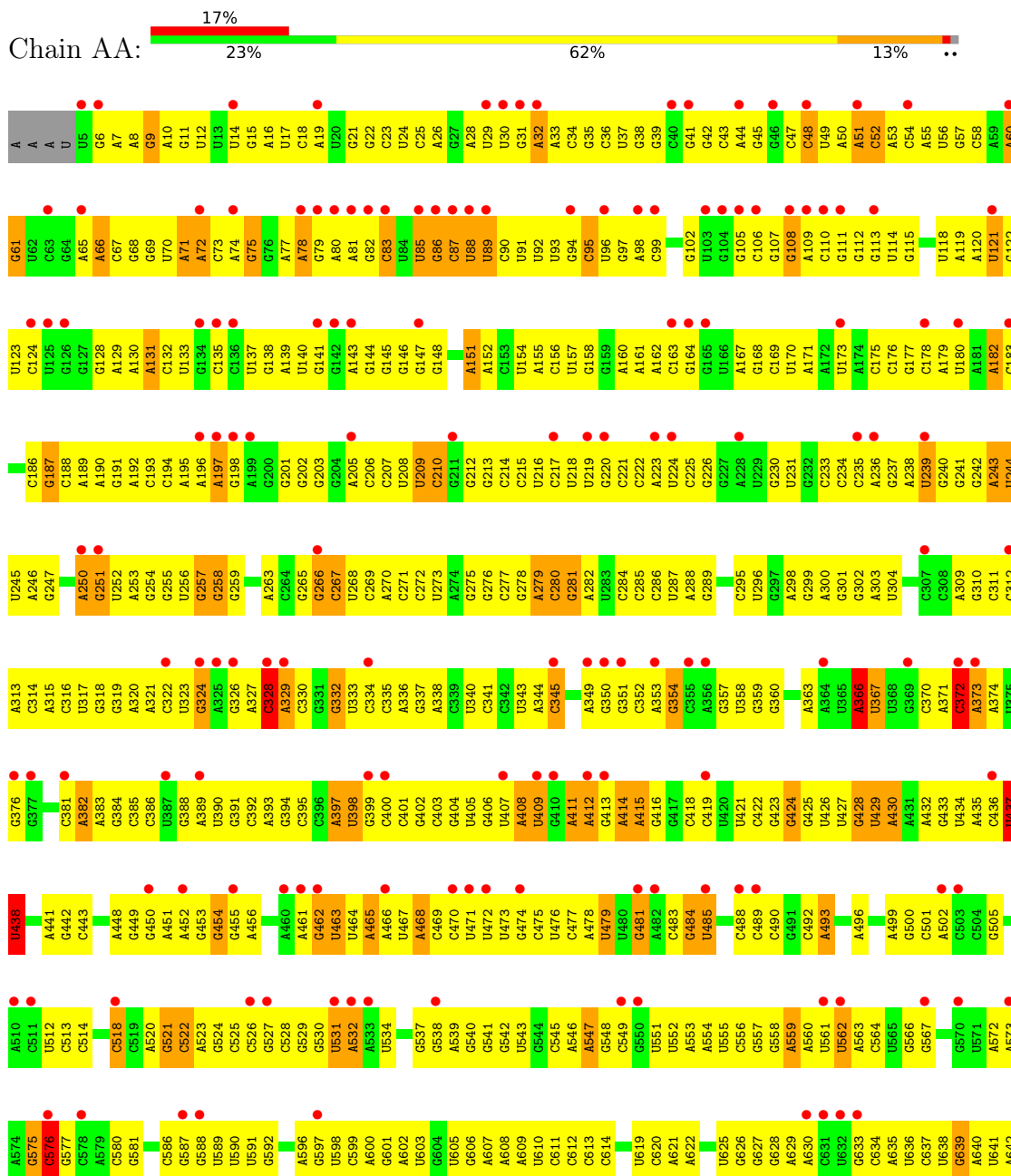
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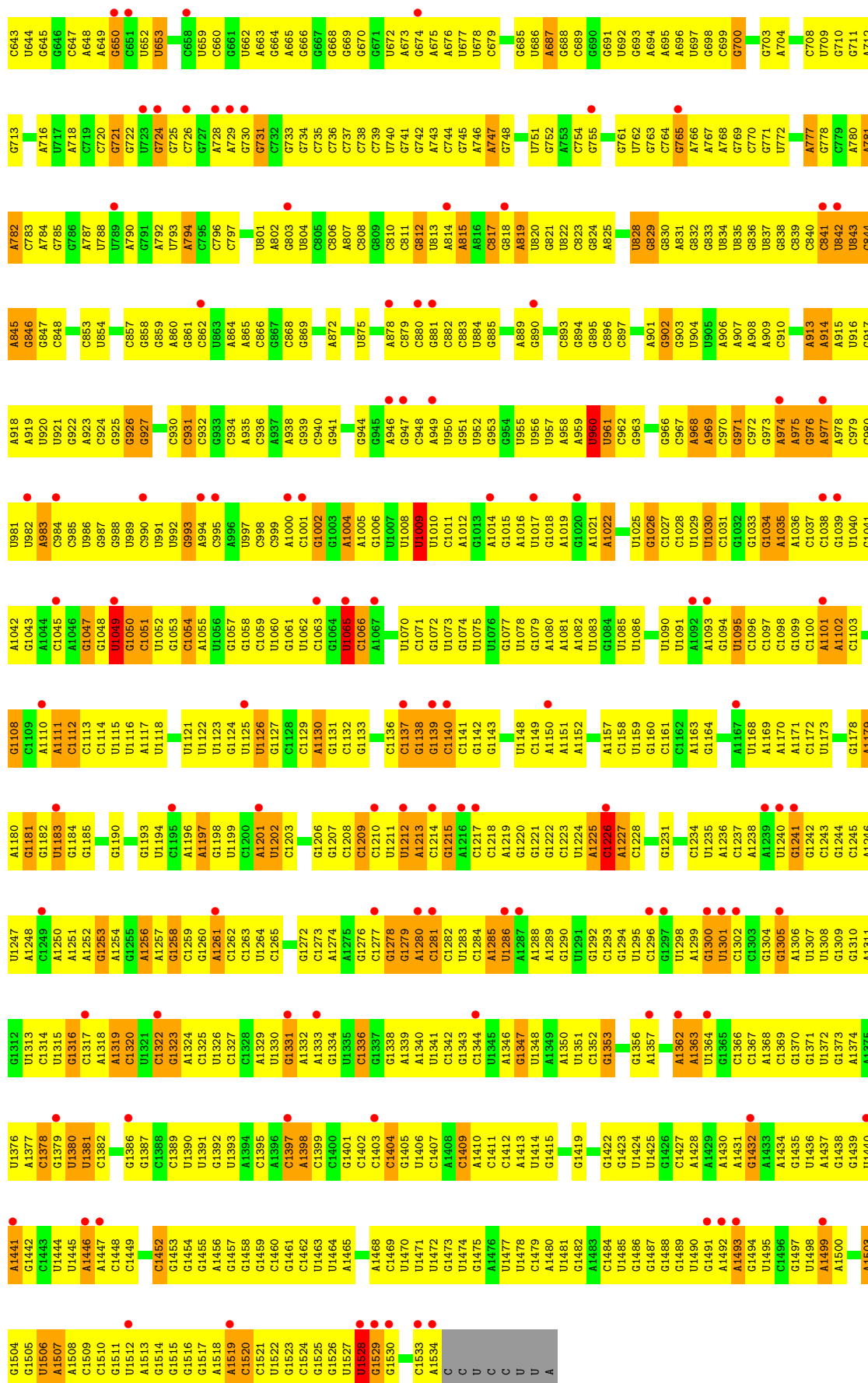
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DE	3	Total 3	O 3	0	0
55	DL	1	Total 1	O 1	0	0
55	DN	2	Total 2	O 2	0	0
55	DT	1	Total 1	O 1	0	0
55	D2	2	Total 2	O 2	0	0

3 Residue-property plots

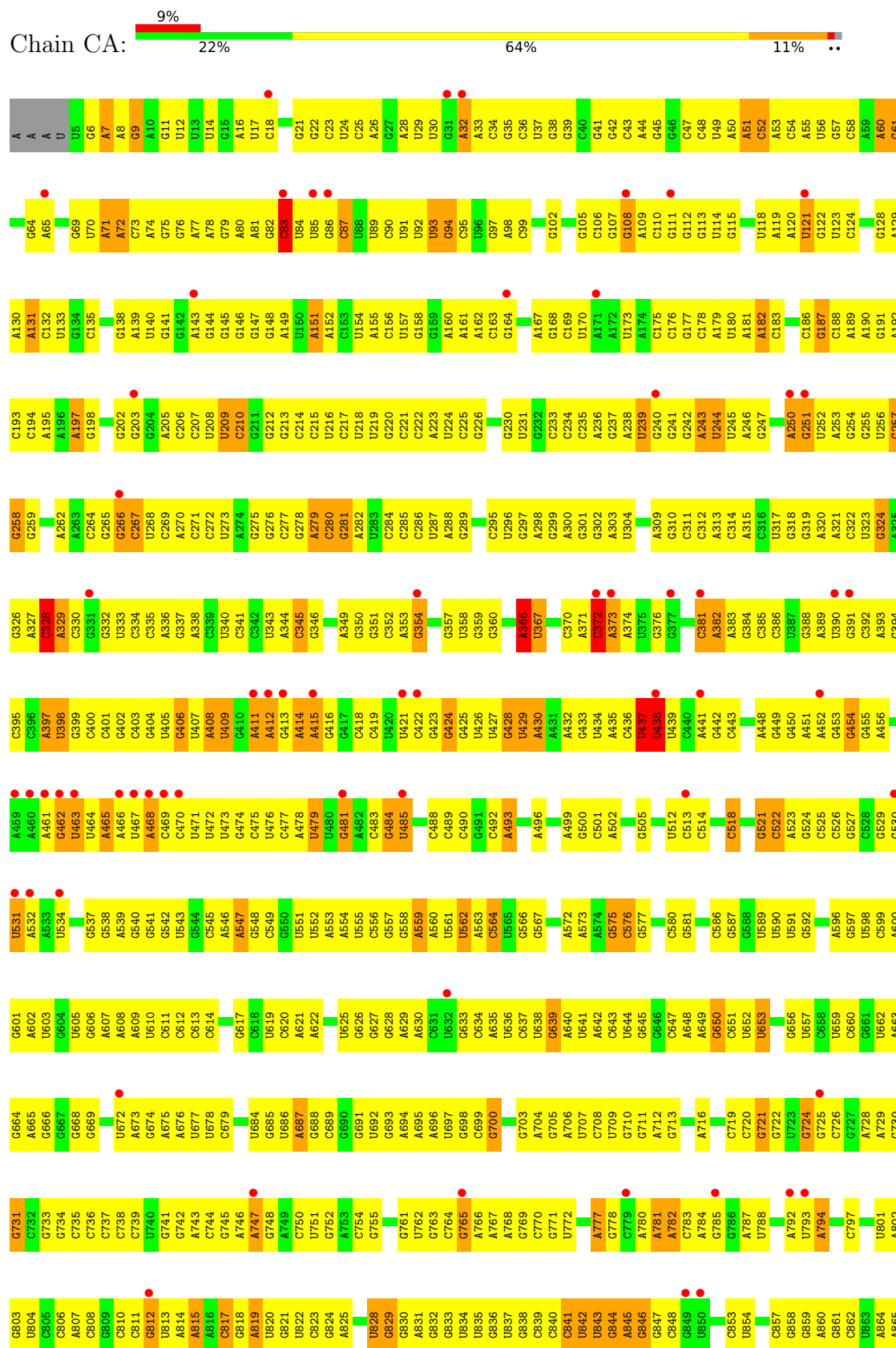
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

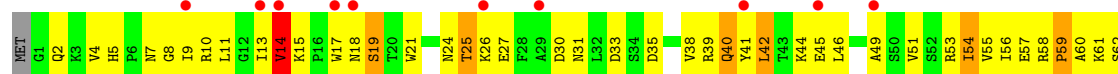
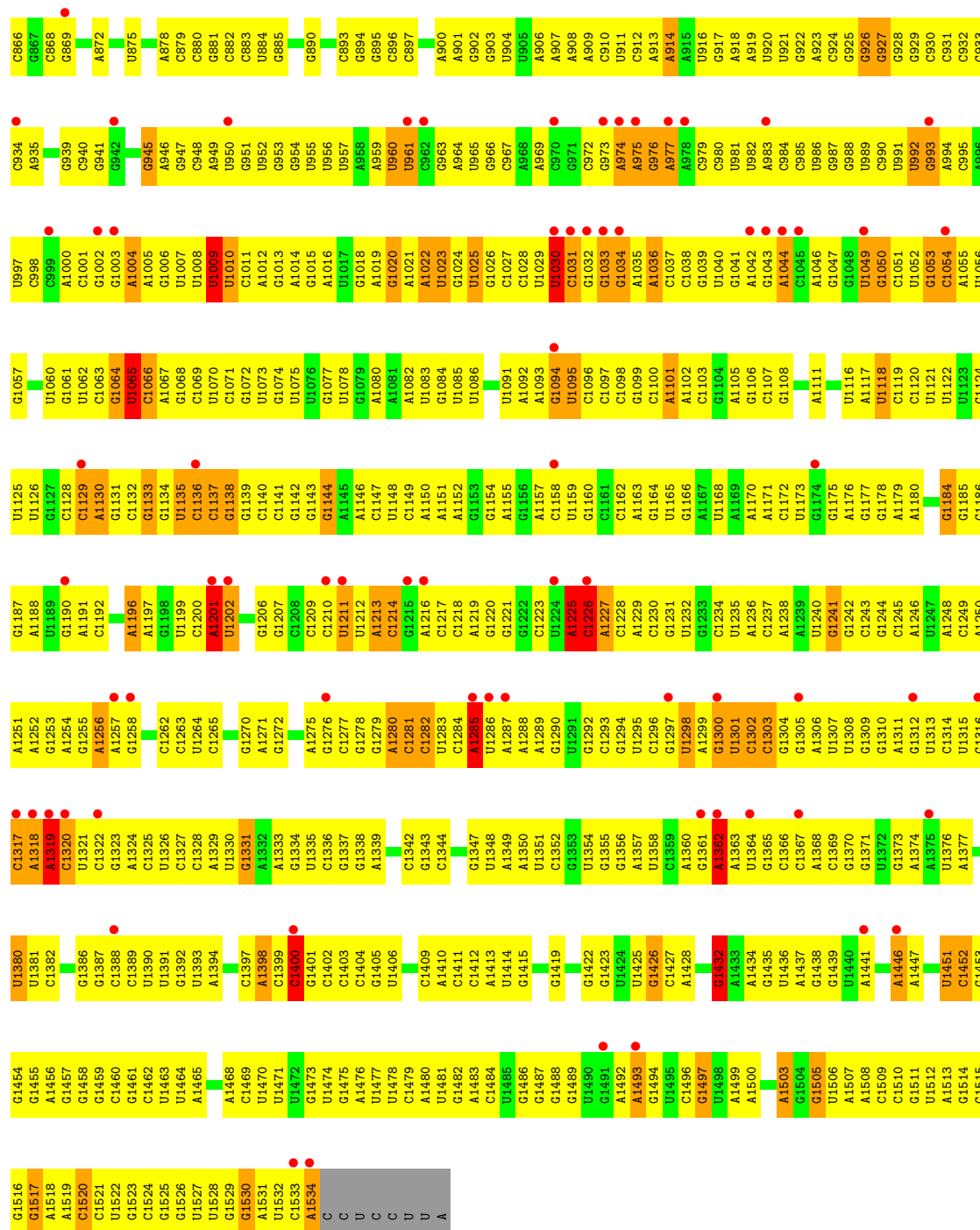
• Molecule 1: 16S RIBOSOMAL RNA

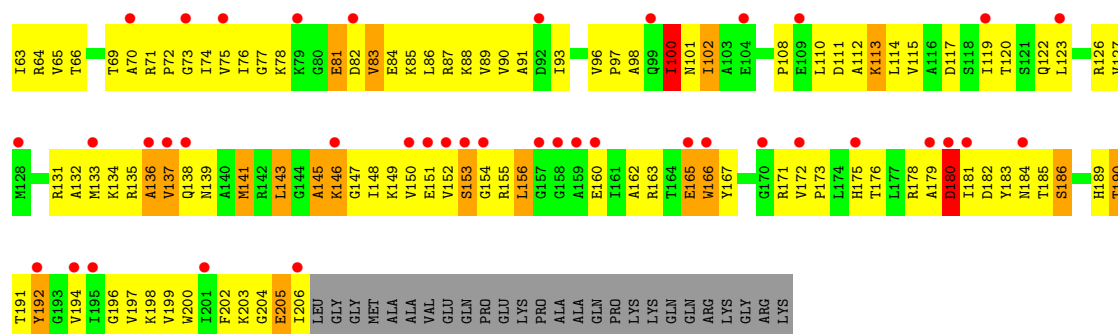




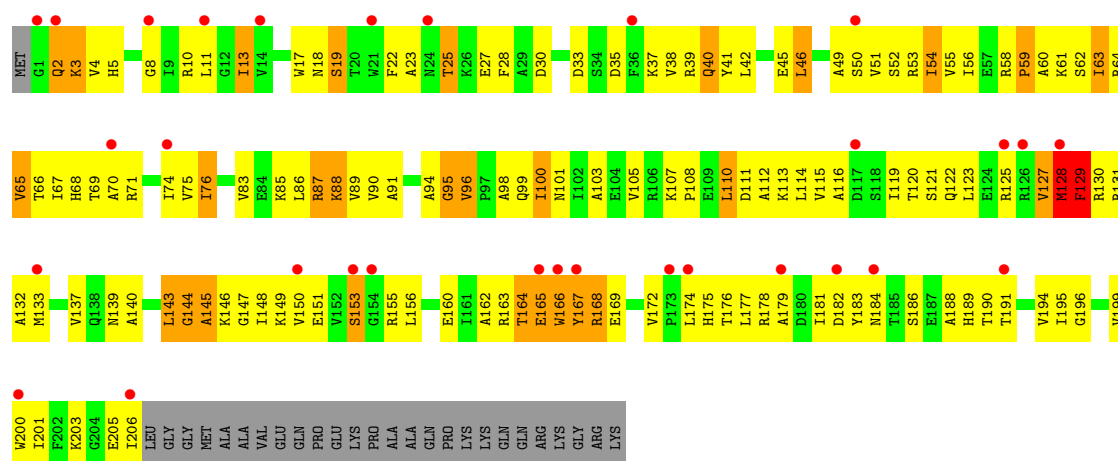
- Molecule 1: 16S RIBOSOMAL RNA



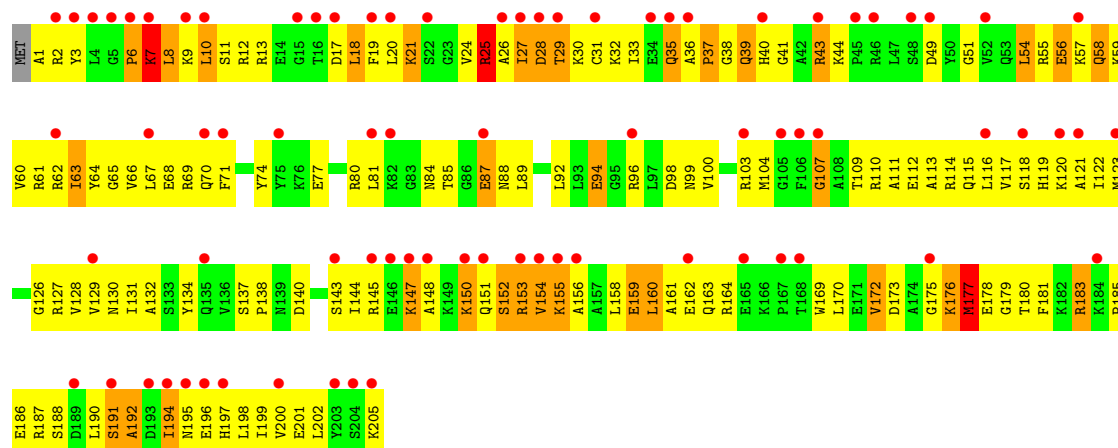




• Molecule 2: 30S RIBOSOMAL PROTEIN S3

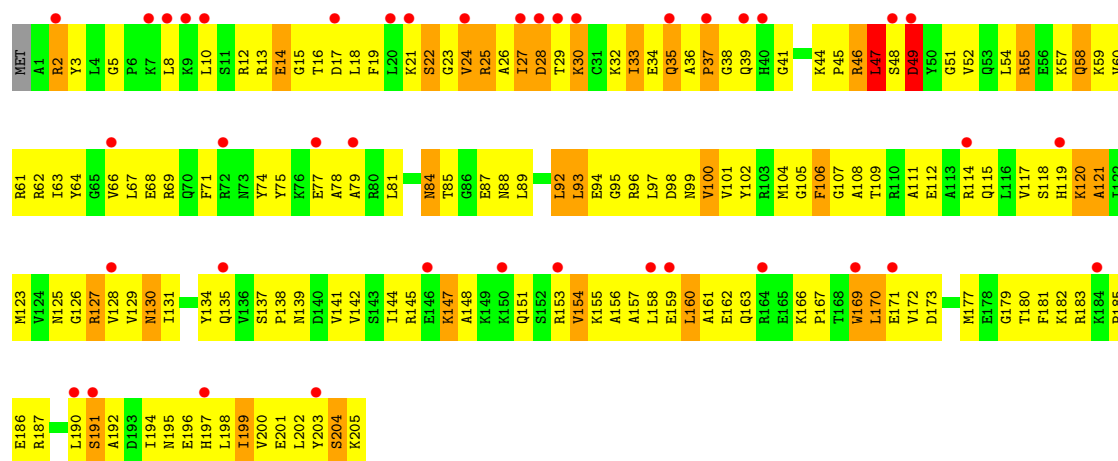


• Molecule 3: 30S RIBOSOMAL PROTEIN S4

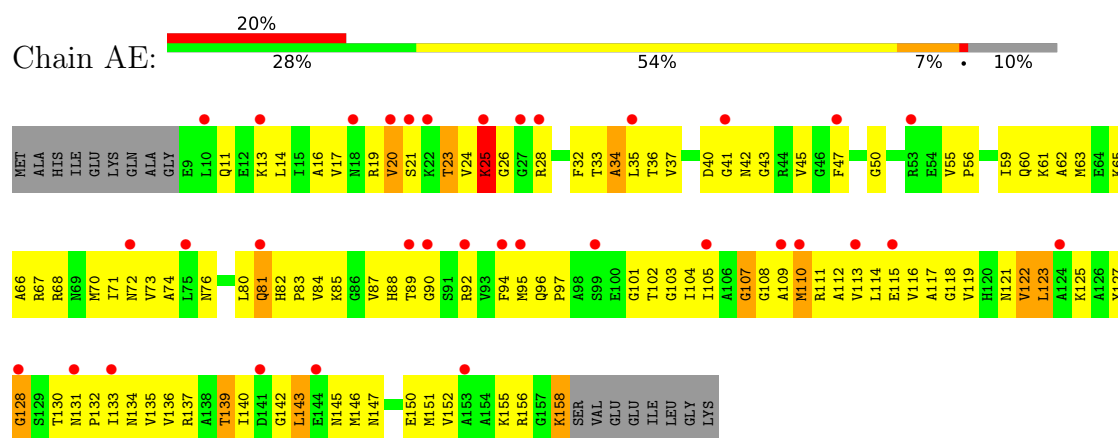


• Molecule 3: 30S RIBOSOMAL PROTEIN S4

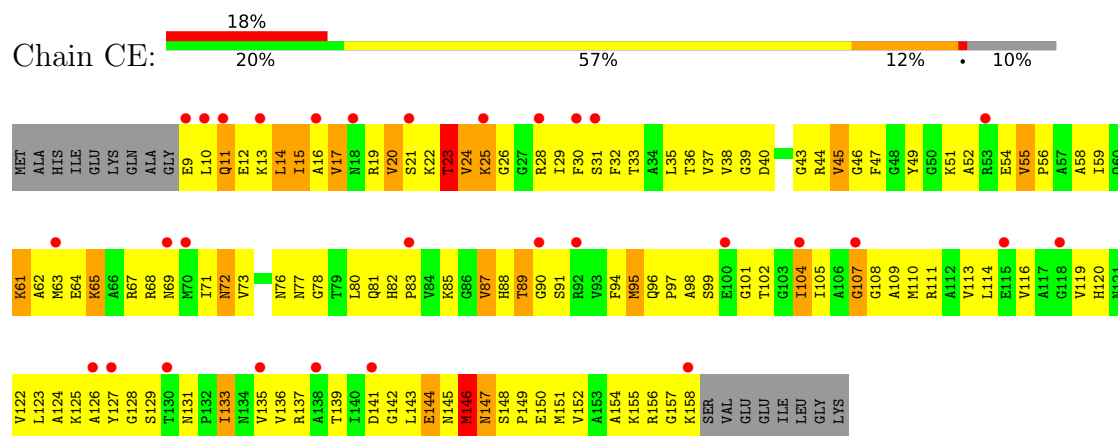




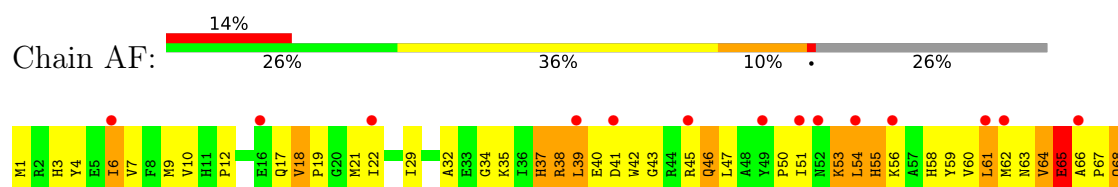
• Molecule 4: 30S RIBOSOMAL PROTEIN S5

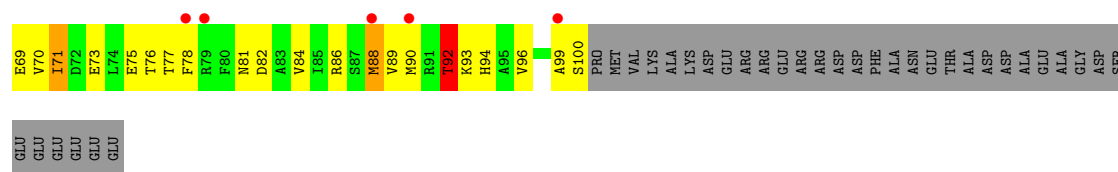


• Molecule 4: 30S RIBOSOMAL PROTEIN S5

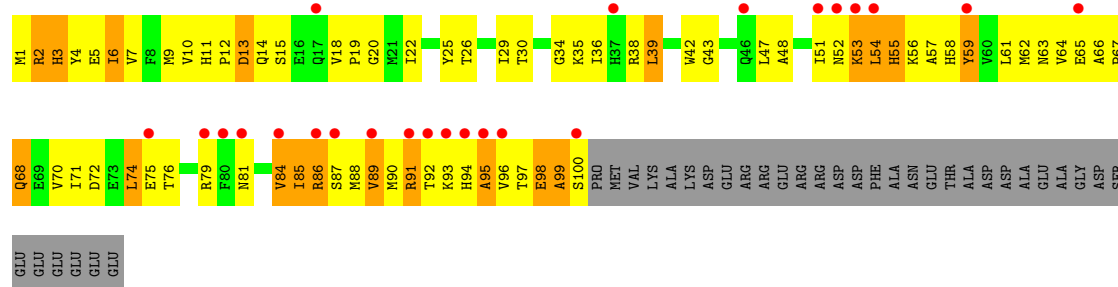
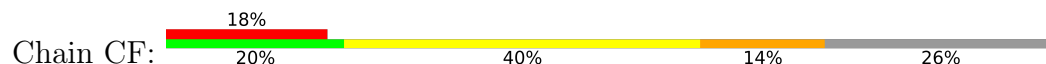


• Molecule 5: 30S RIBOSOMAL PROTEIN S6

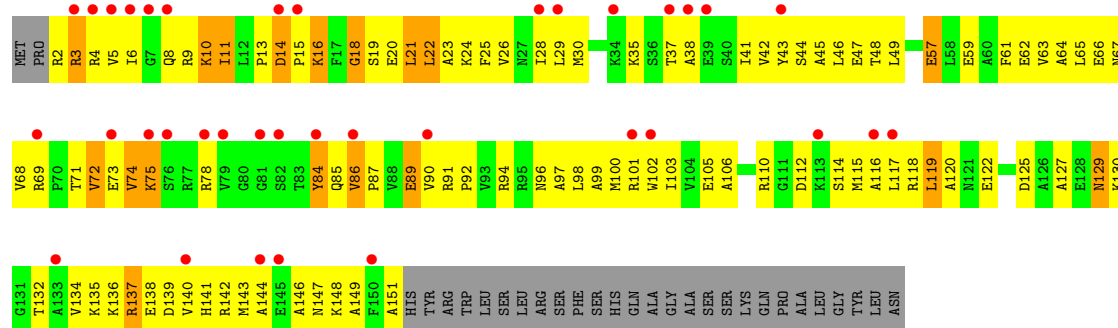




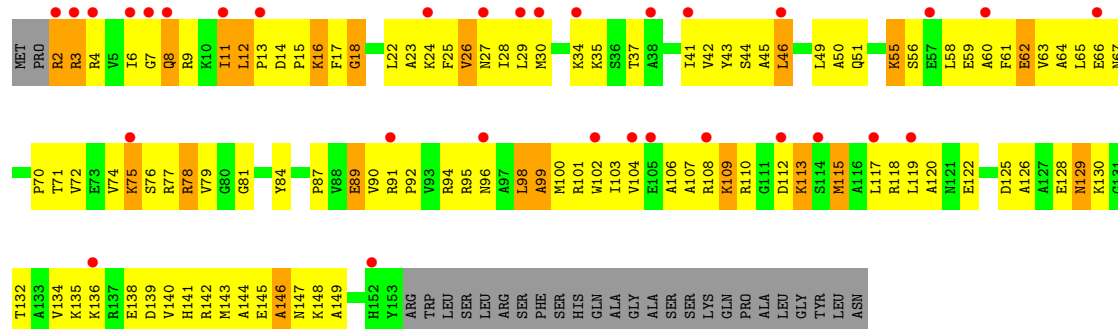
• Molecule 5: 30S RIBOSOMAL PROTEIN S6



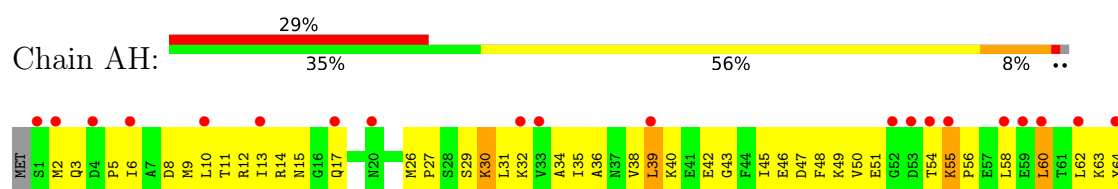
• Molecule 6: 30S RIBOSOMAL PROTEIN S7



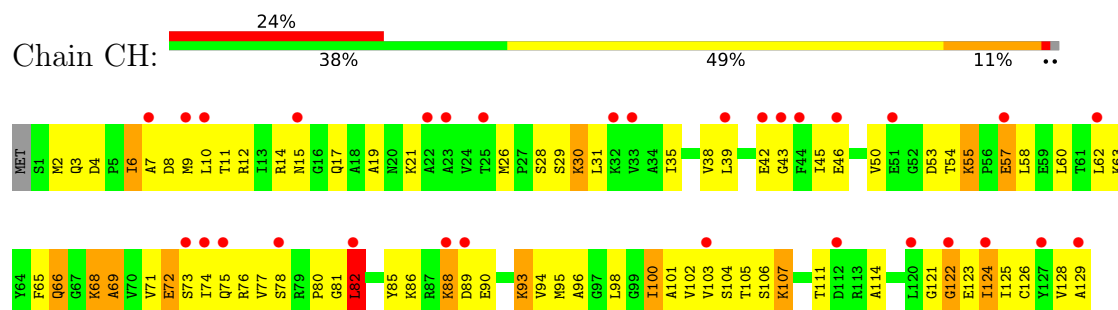
• Molecule 6: 30S RIBOSOMAL PROTEIN S7



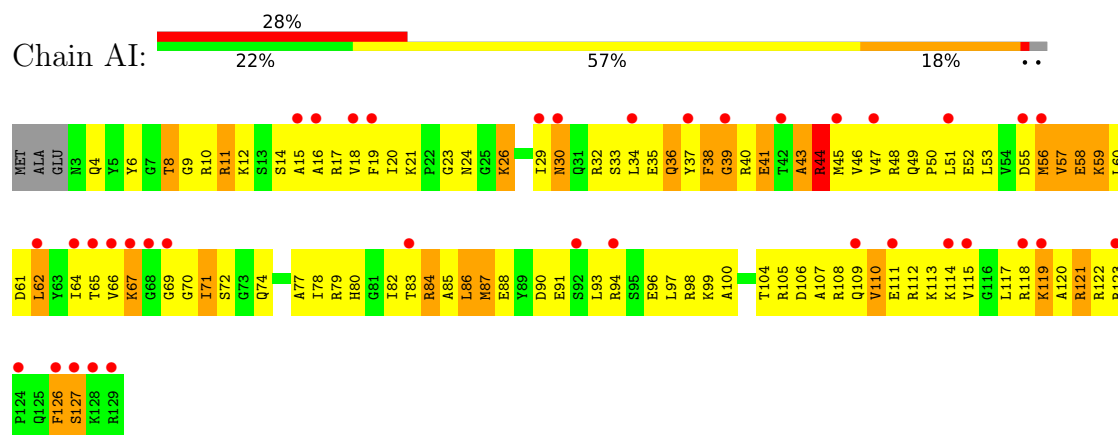
• Molecule 7: 30S RIBOSOMAL PROTEIN S8



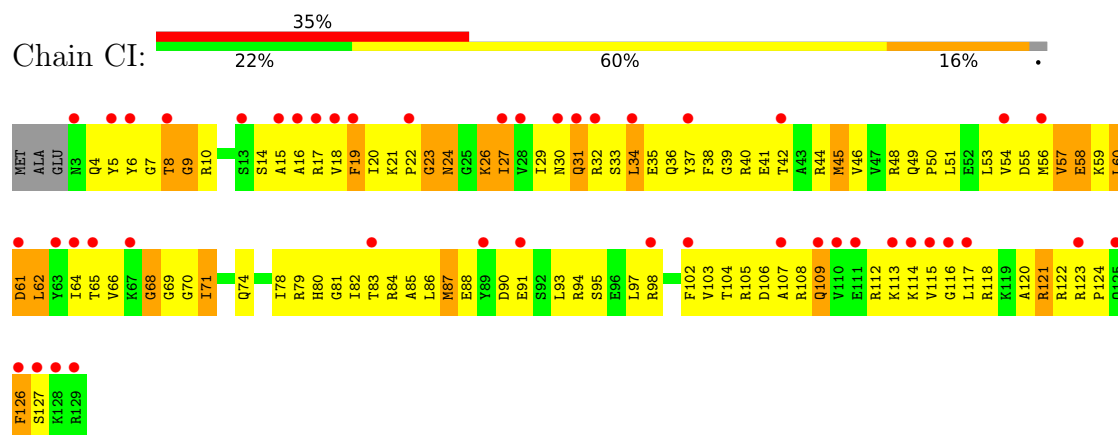
• Molecule 7: 30S RIBOSOMAL PROTEIN S8



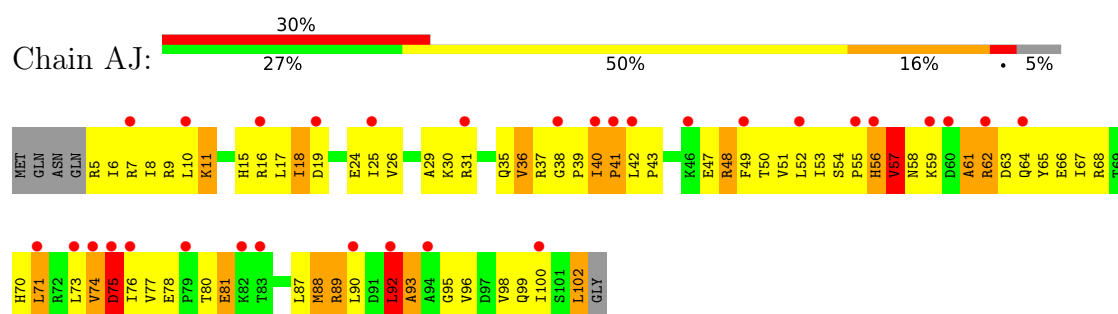
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



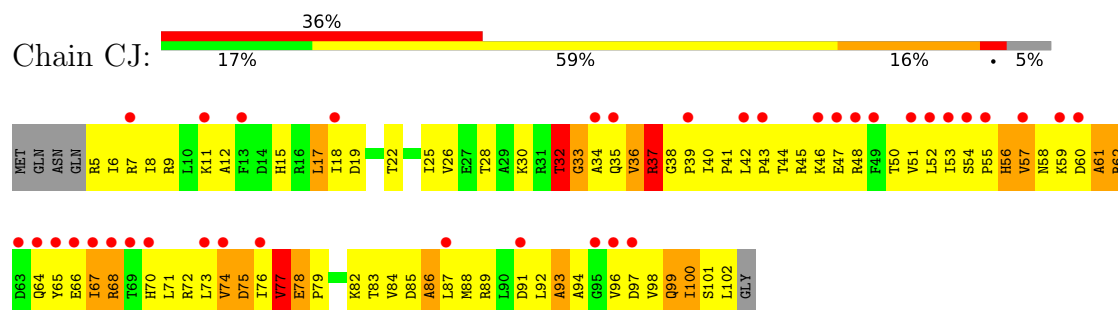
• Molecule 8: 30S RIBOSOMAL PROTEIN S9



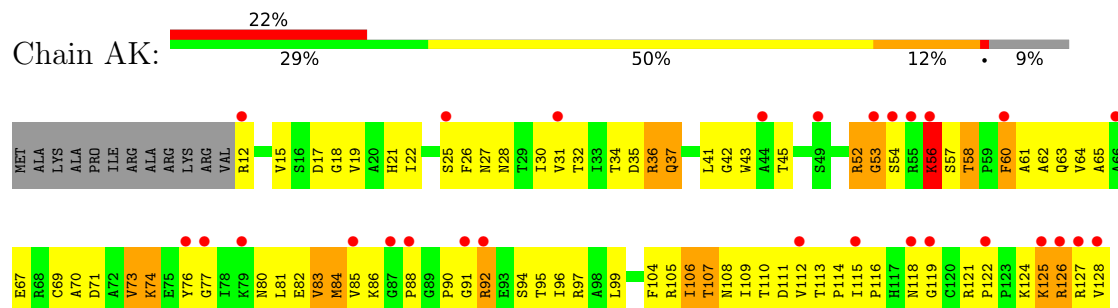
• Molecule 9: 30S RIBOSOMAL PROTEIN S10



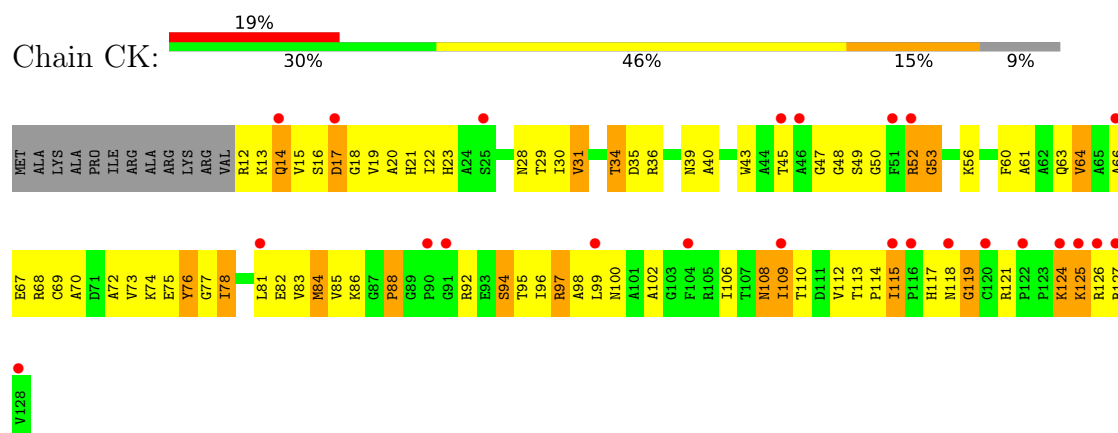
- Molecule 9: 30S RIBOSOMAL PROTEIN S10



- Molecule 10: 30S RIBOSOMAL PROTEIN S11

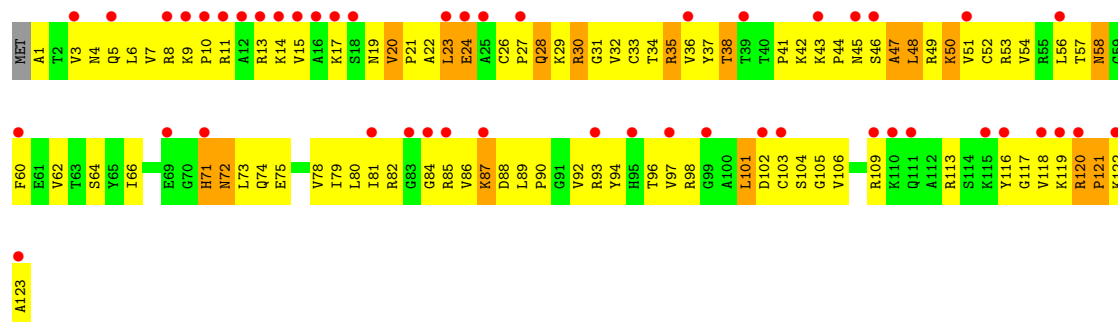


- Molecule 10: 30S RIBOSOMAL PROTEIN S11

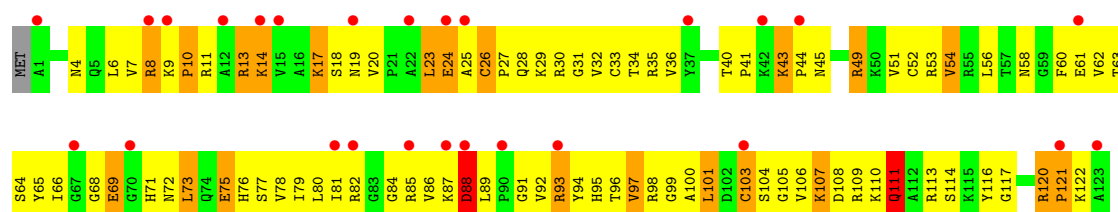


- Molecule 11: 30S RIBOSOMAL PROTEIN S12

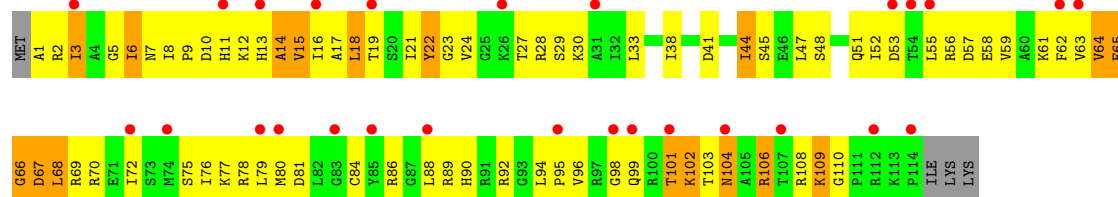




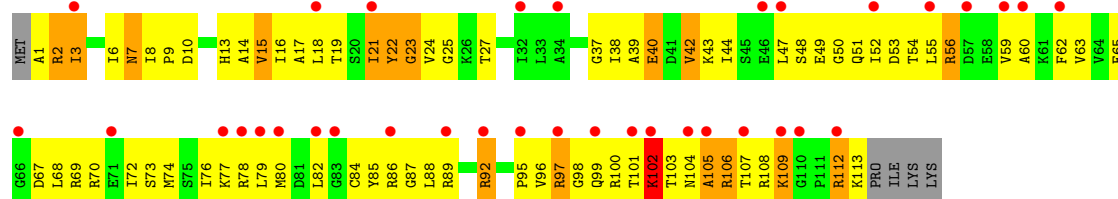
• Molecule 11: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S13

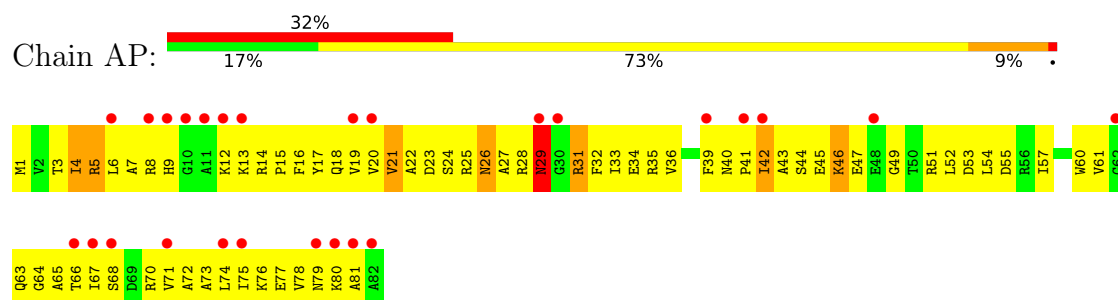
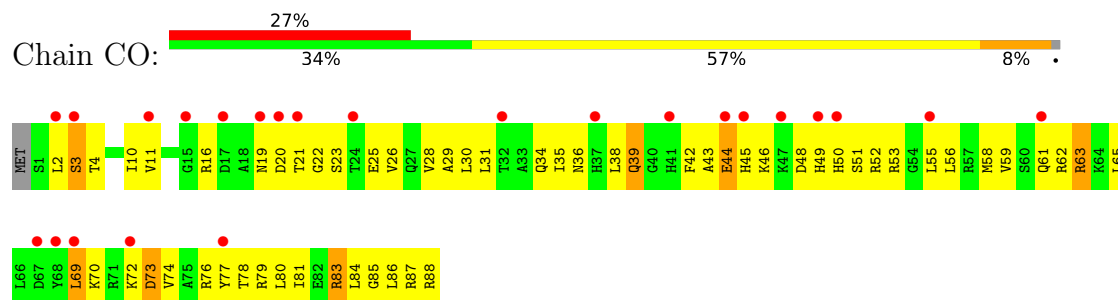
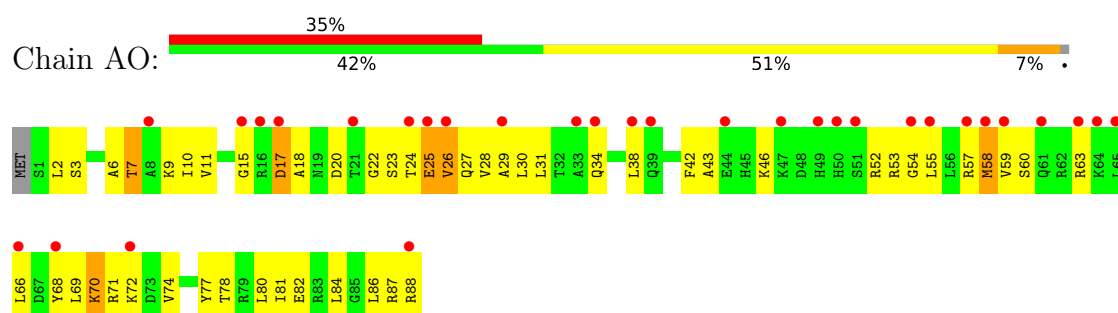
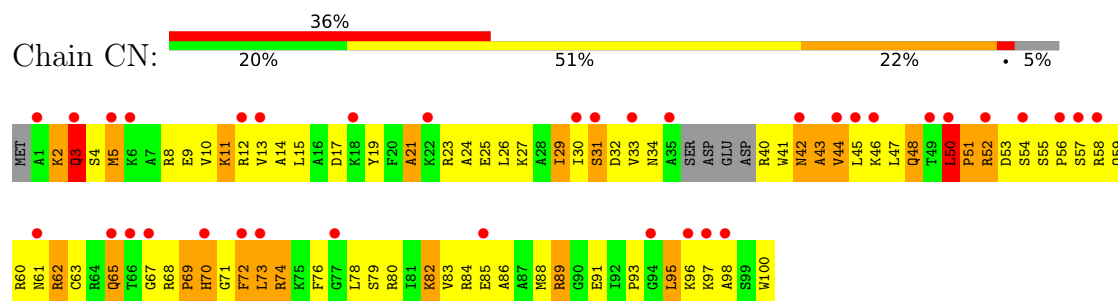
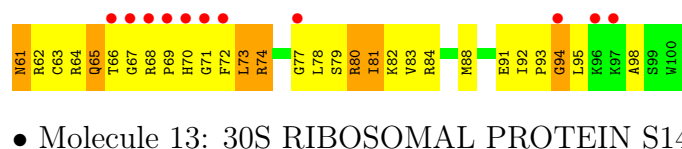


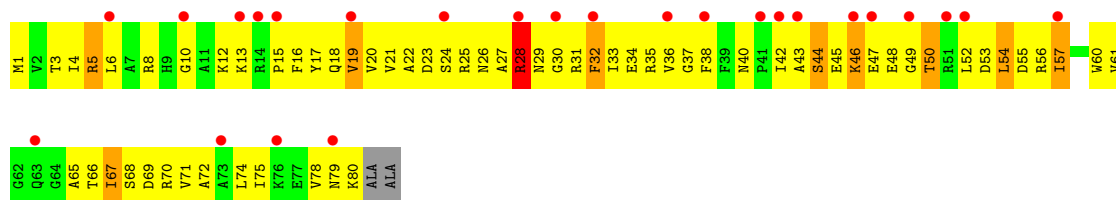
• Molecule 12: 30S RIBOSOMAL PROTEIN S13



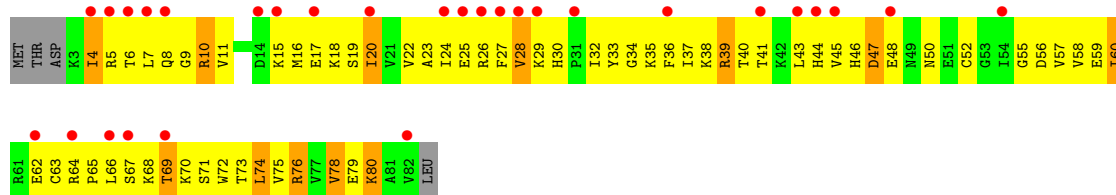
• Molecule 13: 30S RIBOSOMAL PROTEIN S14



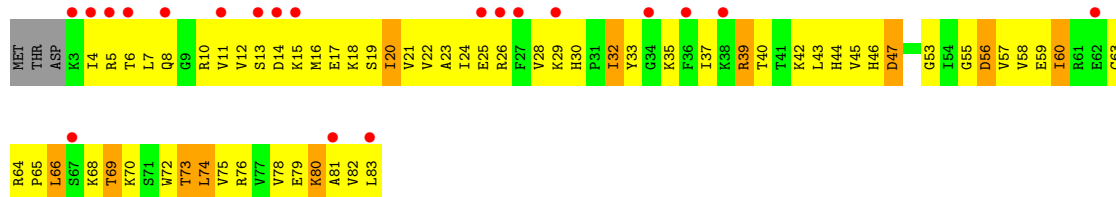




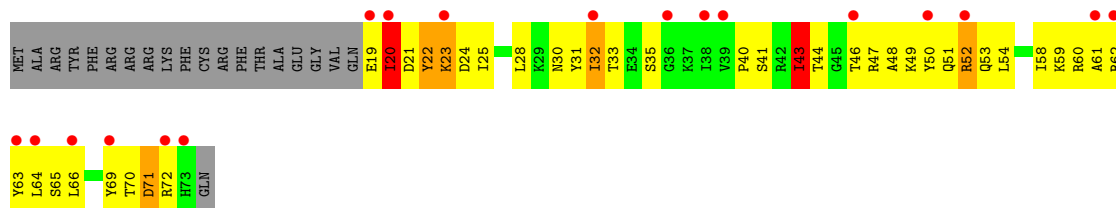
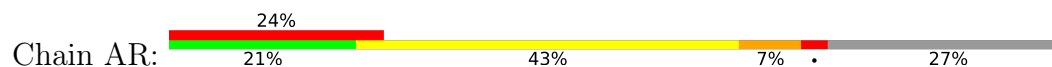
• Molecule 16: 30S RIBOSOMAL PROTEIN S17



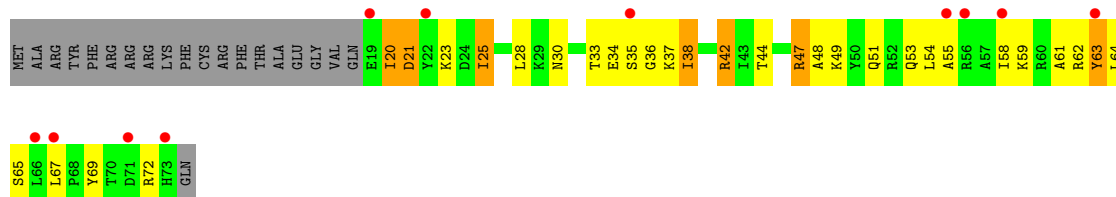
• Molecule 16: 30S RIBOSOMAL PROTEIN S17



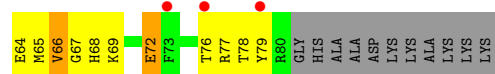
• Molecule 17: 30S RIBOSOMAL PROTEIN S18



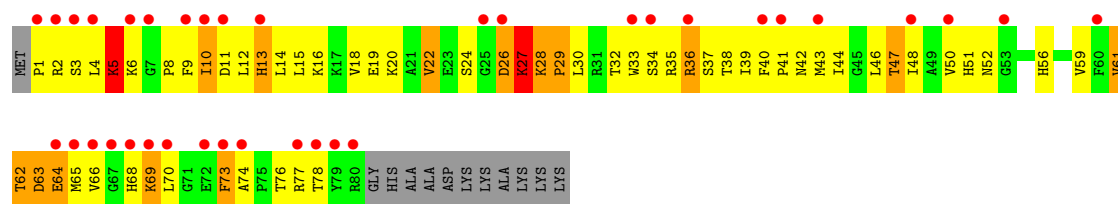
• Molecule 17: 30S RIBOSOMAL PROTEIN S18



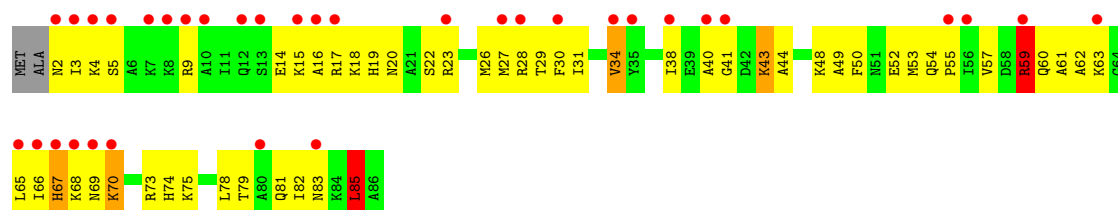
• Molecule 18: 30S RIBOSOMAL PROTEIN S19



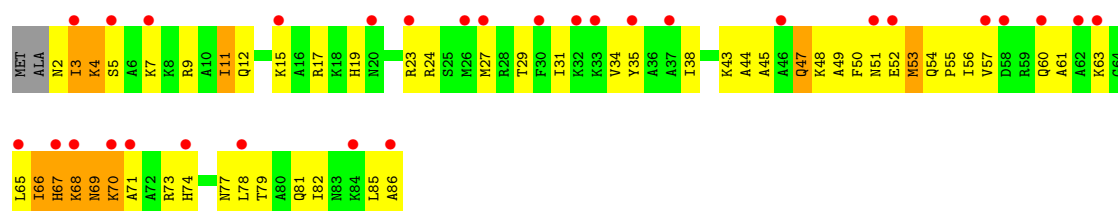
Chain CS:



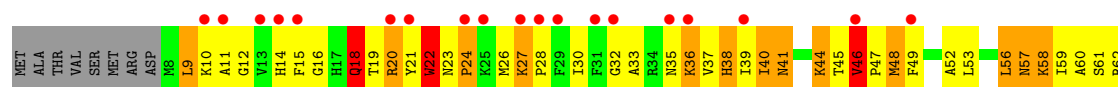
Chain AT: 39% 36% 55% 5%

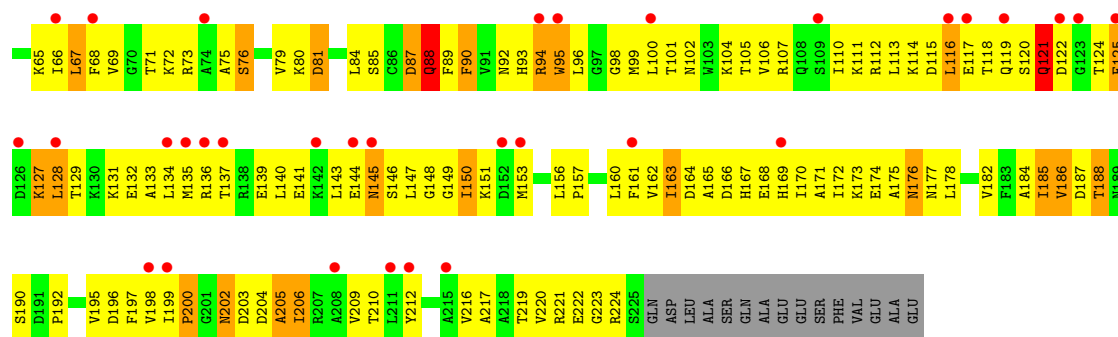


Chain CT:

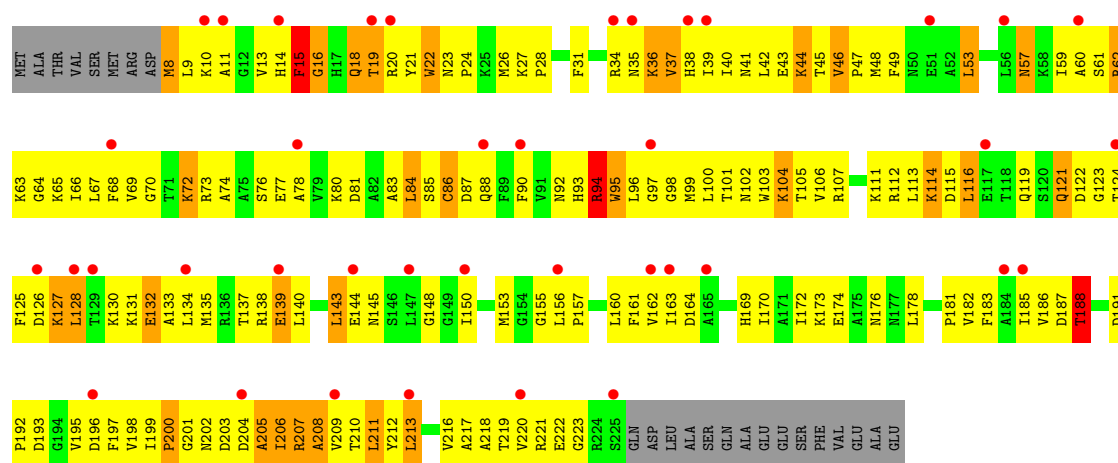


Chain AB:

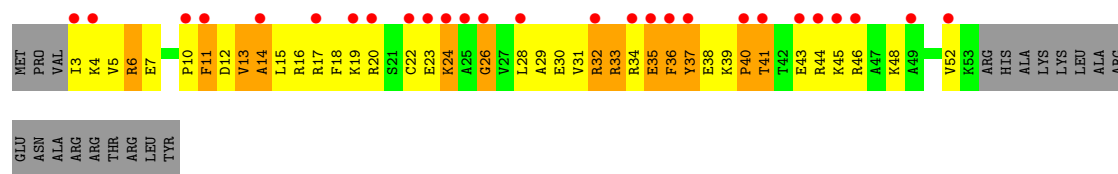




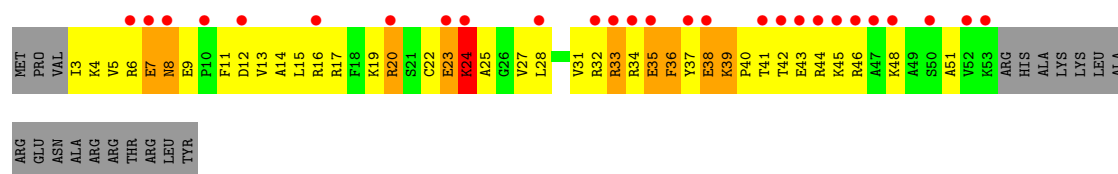
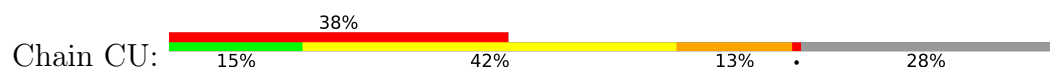
• Molecule 20: 30S RIBOSOMAL PROTEIN S2



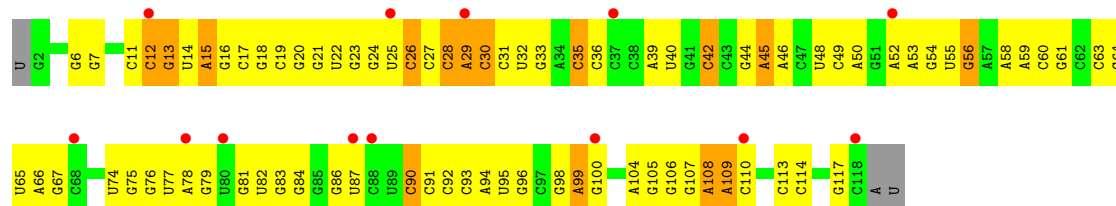
• Molecule 21: 30S RIBOSOMAL PROTEIN S21



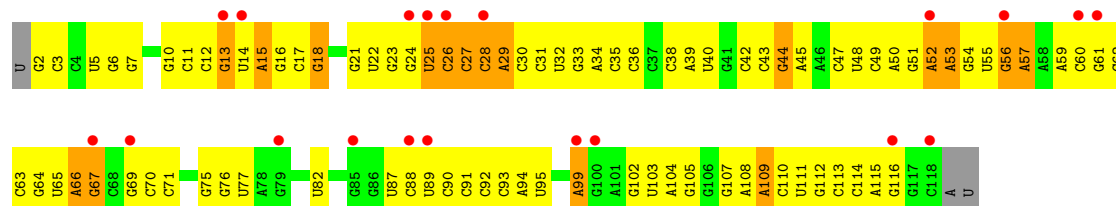
• Molecule 21: 30S RIBOSOMAL PROTEIN S21



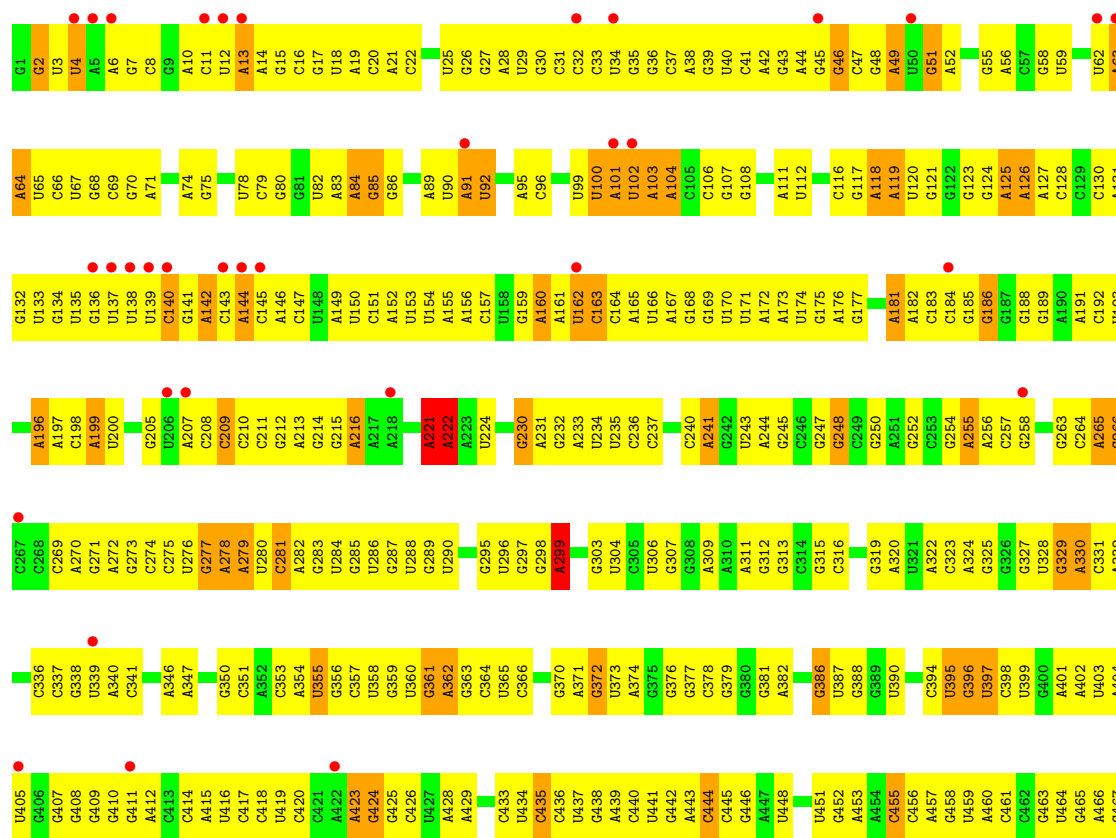
• Molecule 22: 5S RIBOSOMAL RNA

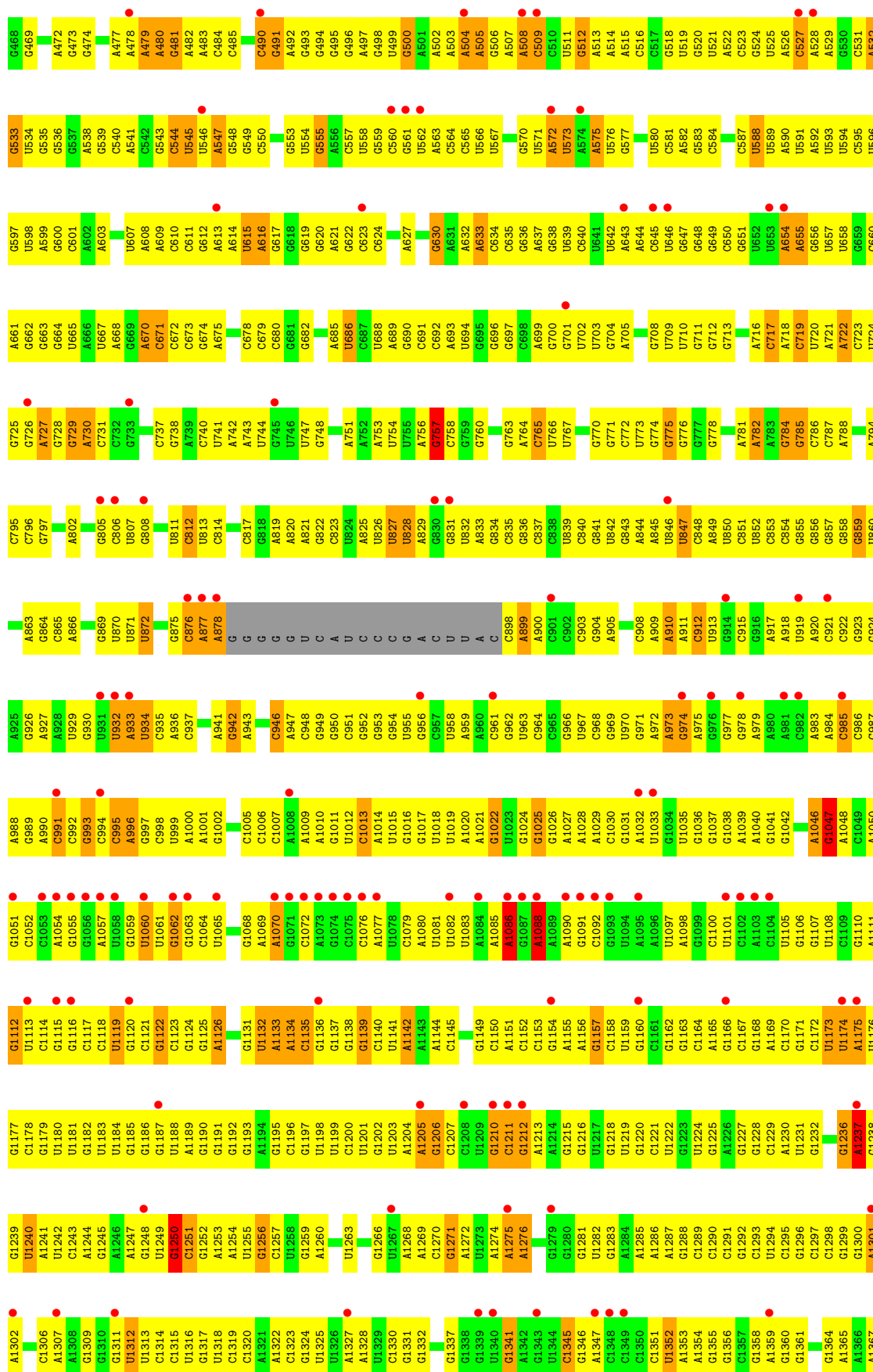


• Molecule 22: 5S RIBOSOMAL RNA

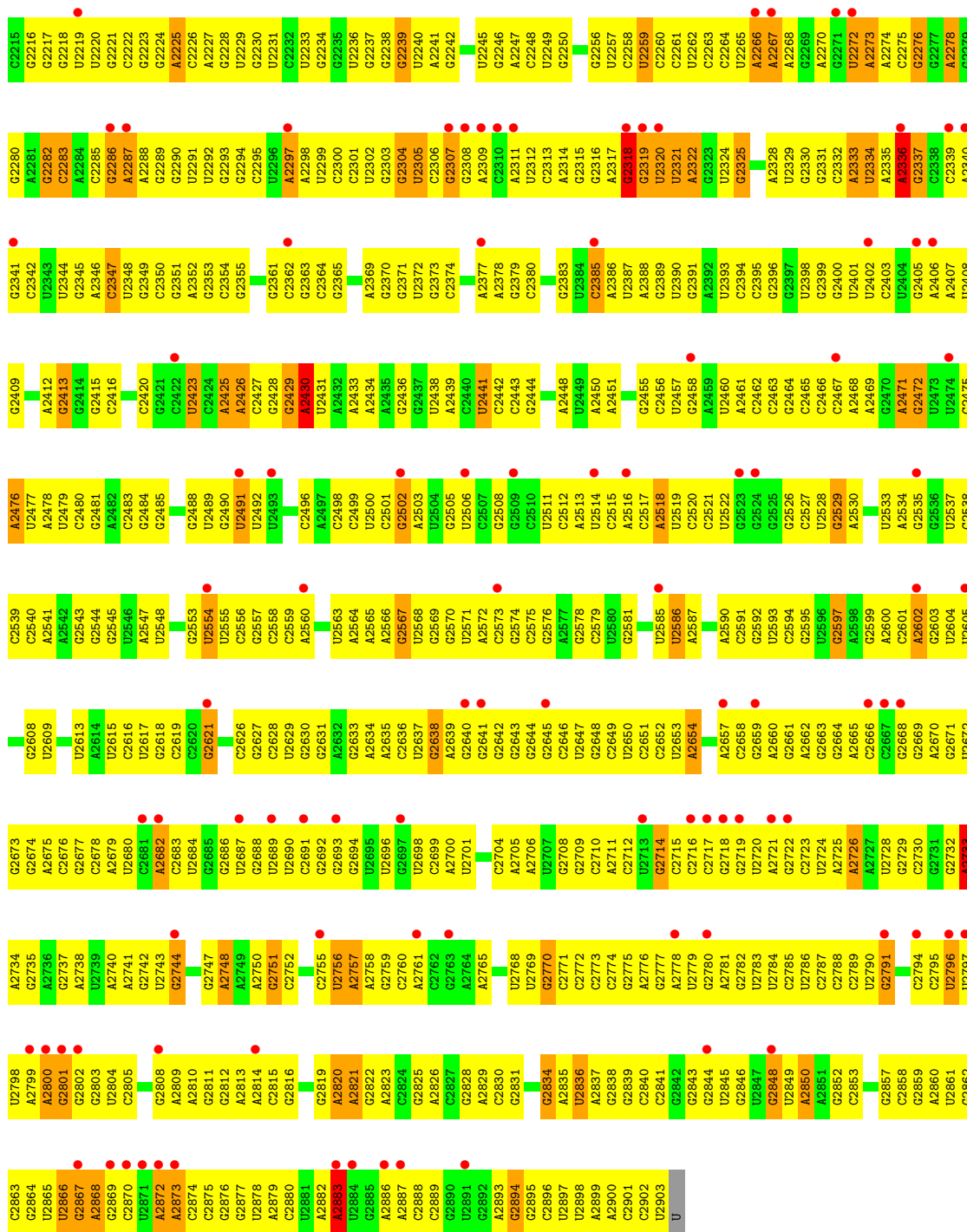


• Molecule 23: 23S RIBOSOMAL RNA



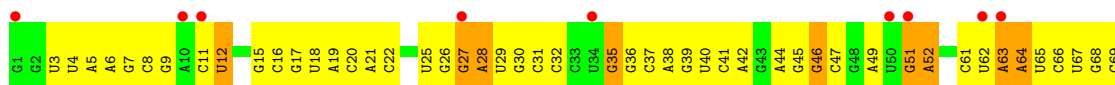


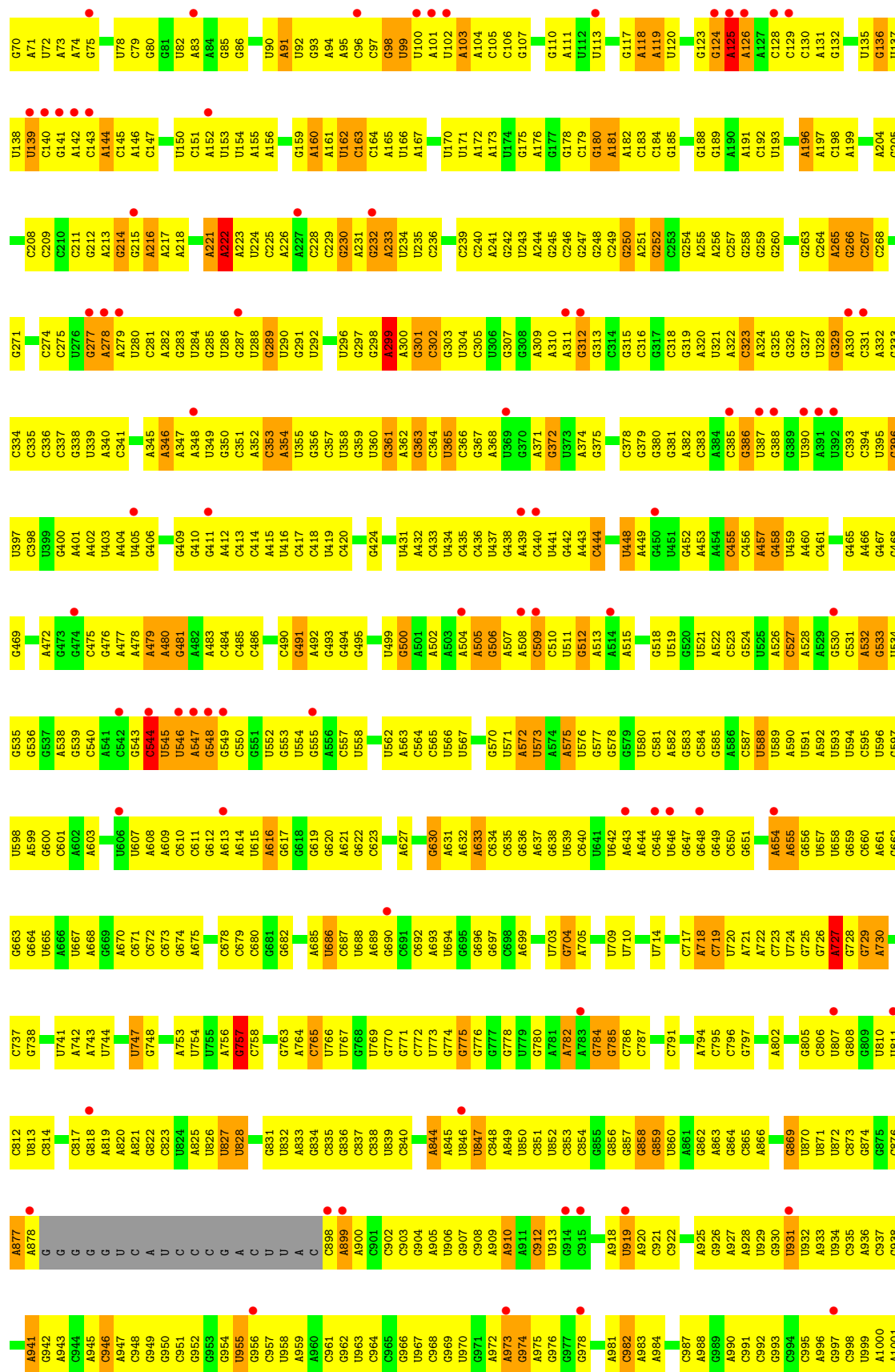
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U2155	A2095	A2033	A1966	A1901	G1826	C1761	U1636	U1561	A1496	A1433	G1370
G2156	C2096	U2034	C1967	G1904	U1827	A1762	C1637	U1562	U1497	A1434	G1371
A	A2097	C2036	G1967	G1905	G1829	G1764	C1638	U1563	C1498	U1372	U1372
C	U2098	A2037	A1970	C1906	A1830	U1765	A1640	C1565	C1499	A1374	A1373
C	U2099	A2037	U1971	G1906	C1833	G1766	A1641	A1566	U1438	G1374	G1374
C	G2100	U2038	U1972	C1909	C1833	G1770	G1642	A1567	A1439	U1375	U1375
C	A2101	U2039	G1973	C1909	C1838	C1771	G1645	G1568	U1440	U1379	U1379
G	G2102	U2040	C1974	U1910	C1844	C1771	U1646	A1569	G1441	G1390	G1390
A	C2103	U2041	C1974	U1911	G1845	A1772	U1647	A1570	U1442	G1381	G1381
C	C2104	A2042	G1975	U1912	G1846	A1773	U1648	A1571	U1443	G1382	G1382
C	U2105	C2043	U1976	A1913	A1847	C1774	U1649	A1572	G1445	A1383	A1383
U	U2106	C2044	G1979	A1914	C1843	U1775	A1650	U1578	C1446	A1384	A1384
U	G2107	C2045	U1979	U1915	C1843	U1776	A1651	A1579	C1447	A1385	A1385
G	U2108	G2046	G1980	U1916	C1844	U1777	A1652	A1580	G1448	A1386	A1386
A	U2109	A1981	A1981	U1917	G1845	U1778	A1653	G1581	U1449	A1387	A1387
A	A	C2047	U1917	U1917	G1846	U1778	G1654	C1582	G1450	G1388	G1388
A	U	G2049	A1918	A1918	A1847	U1779	G1655	C1583	C1451	G1389	G1389
U	G	C2050	A1919	A1919	A1848	A1780	A1654	U1583	G1452	U1390	U1390
A	A	A2051	A1987	C1920	U1885	U1781	A1655	U1584	A1453	U1391	U1391
C	A	A2052	G1988	G1921	U1886	U1782	U1656	C1585	C1454	A1392	A1392
C	C	G2053	G1989	G1922	U1887	A1783	U1657	U1585	G1455	A1393	A1393
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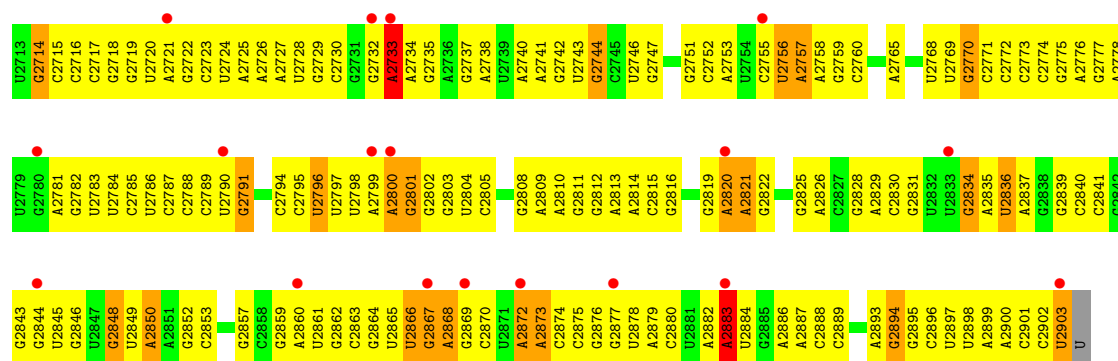
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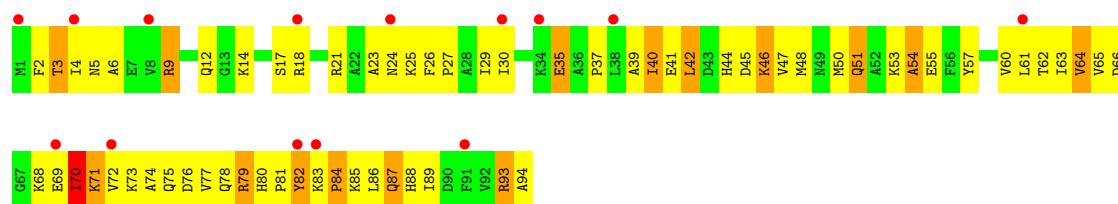


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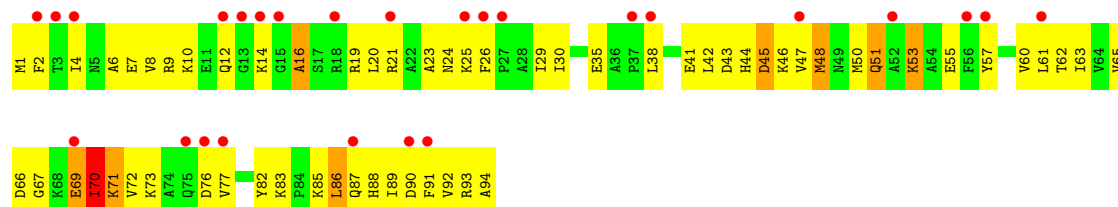
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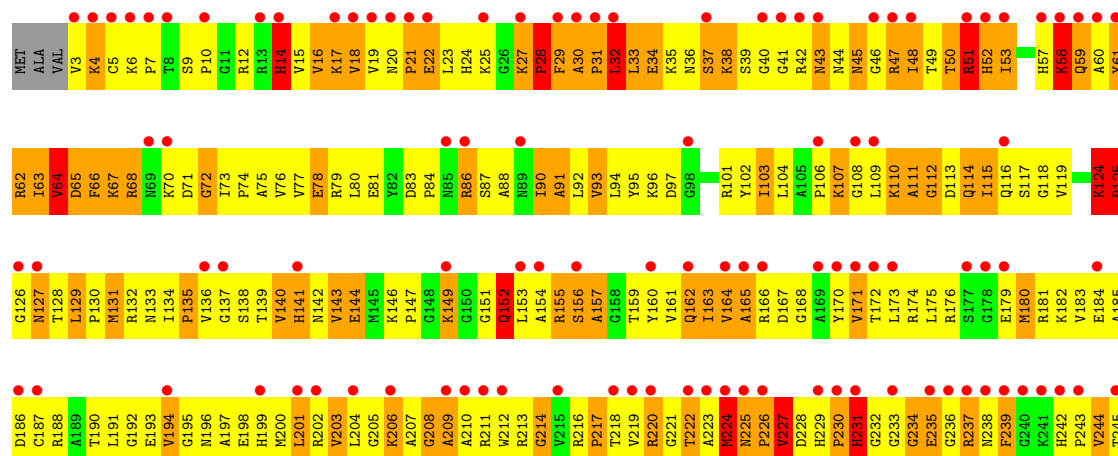
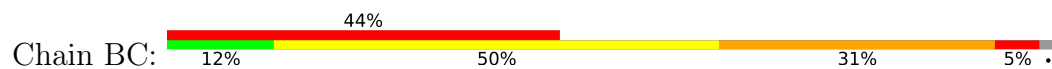
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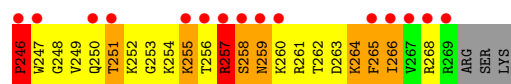


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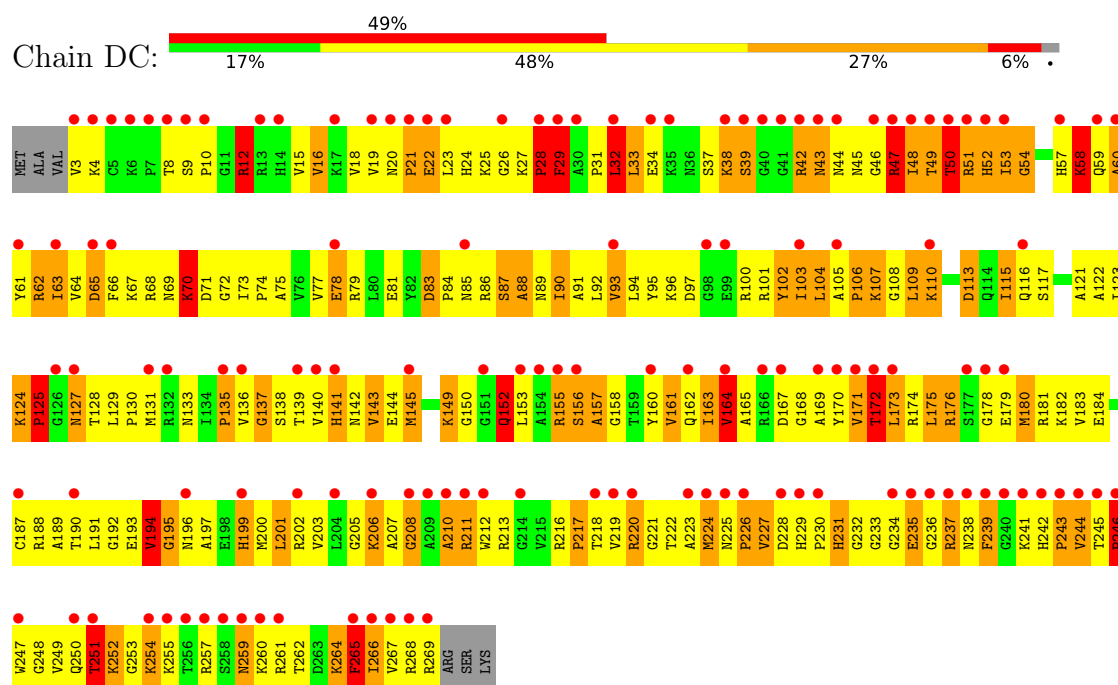


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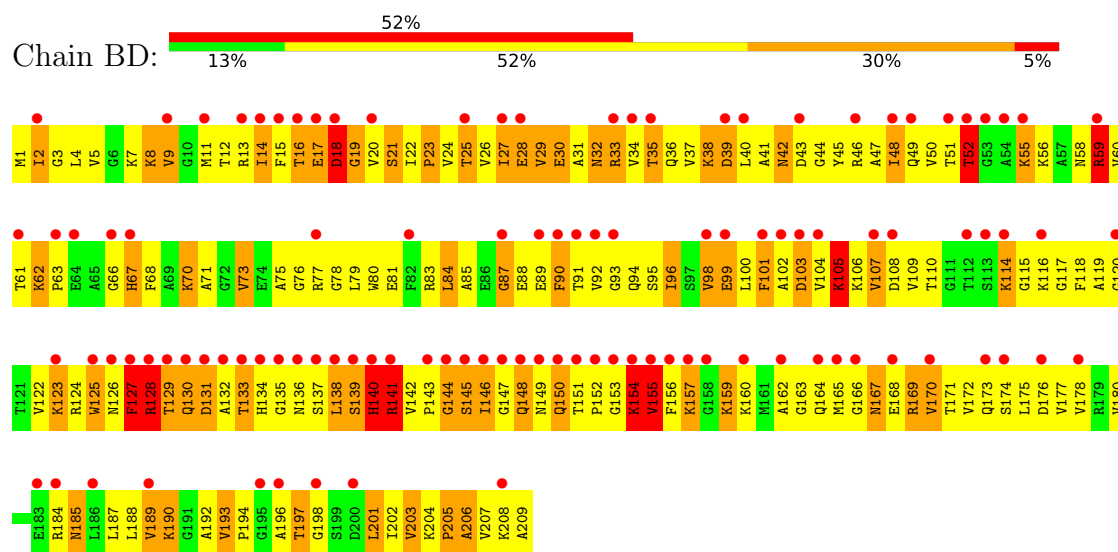




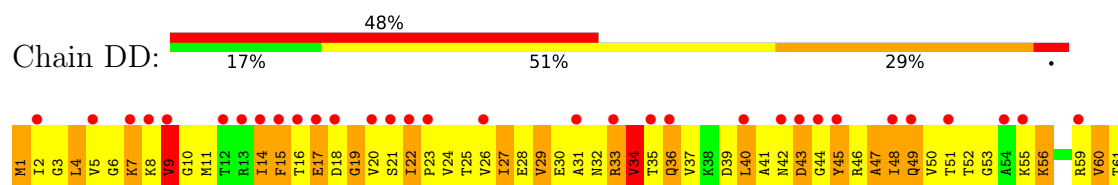
• Molecule 25: 50S RIBOSOMAL PROTEIN L2

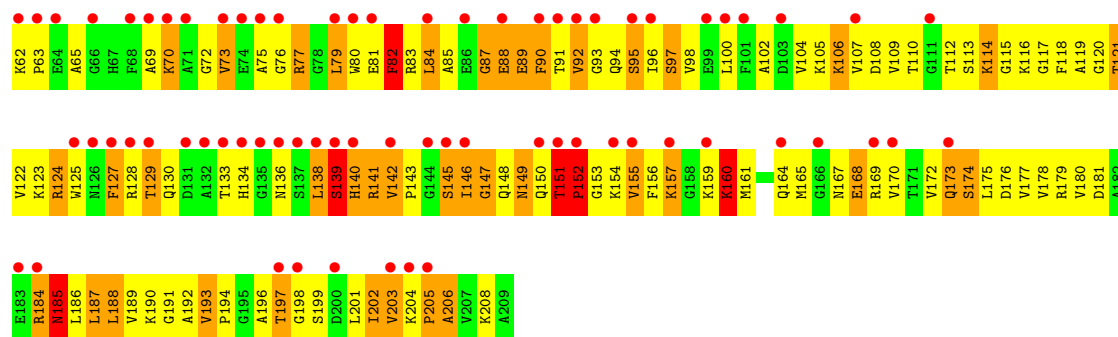


• Molecule 26: 50S RIBOSOMAL PROTEIN L3

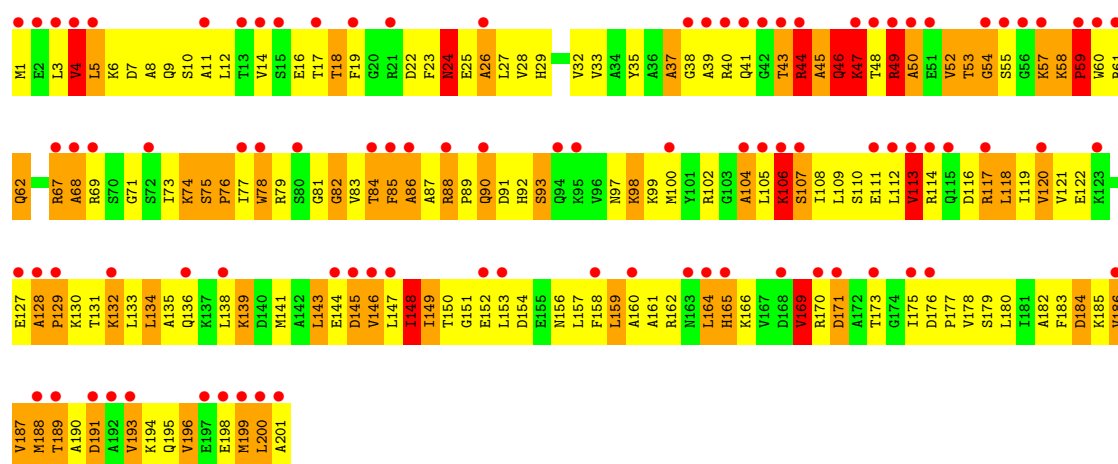
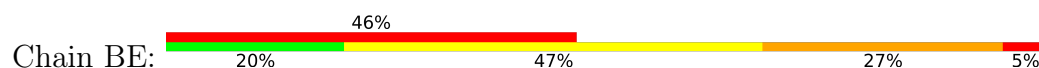


• Molecule 26: 50S RIBOSOMAL PROTEIN L3

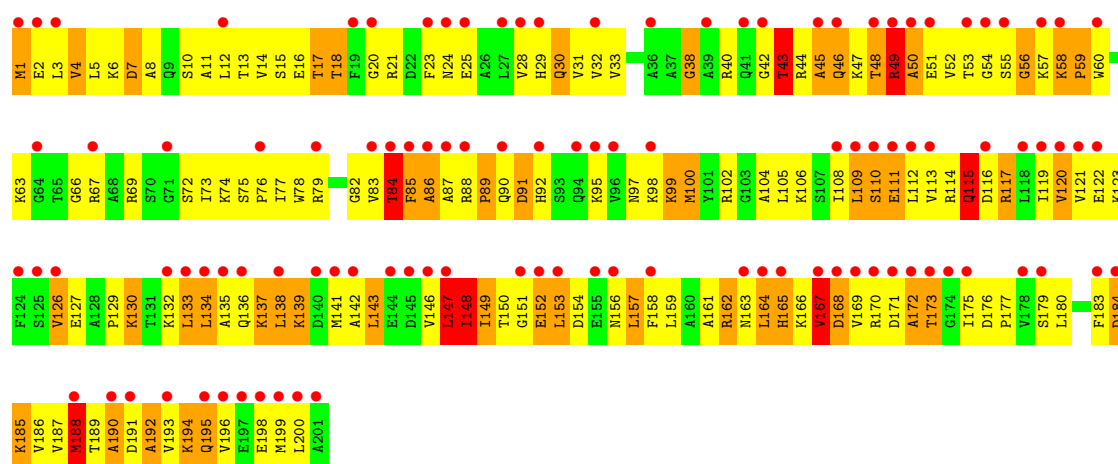




• Molecule 27: 50S RIBOSOMAL PROTEIN L4

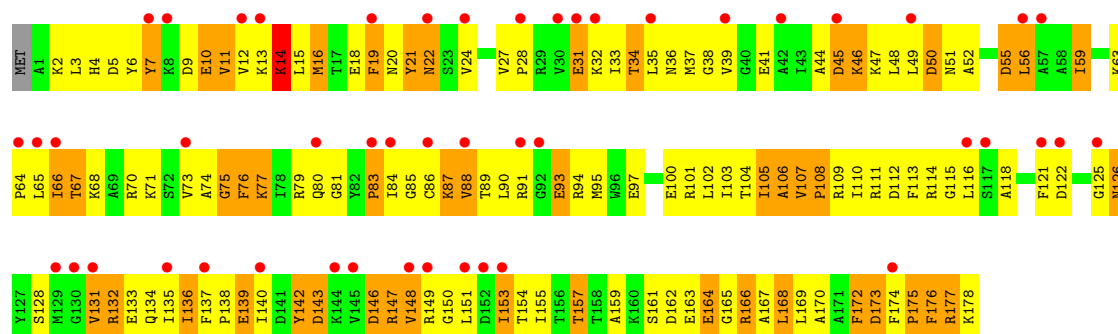


• Molecule 27: 50S RIBOSOMAL PROTEIN L4

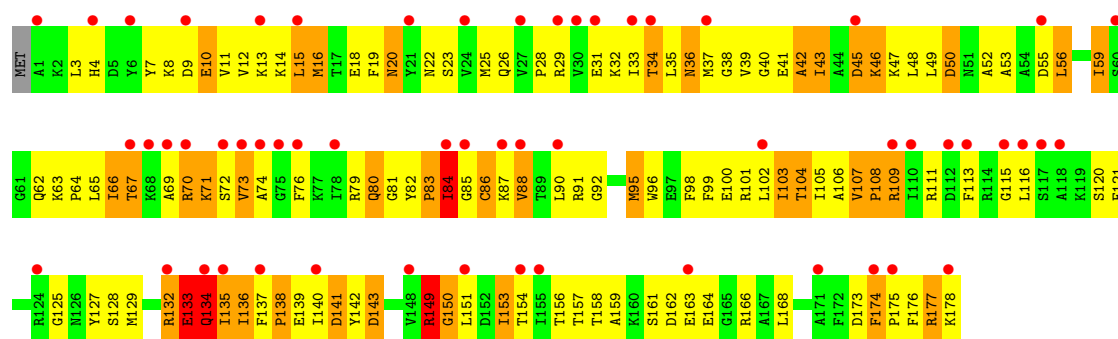


• Molecule 28: 50S RIBOSOMAL PROTEIN L5

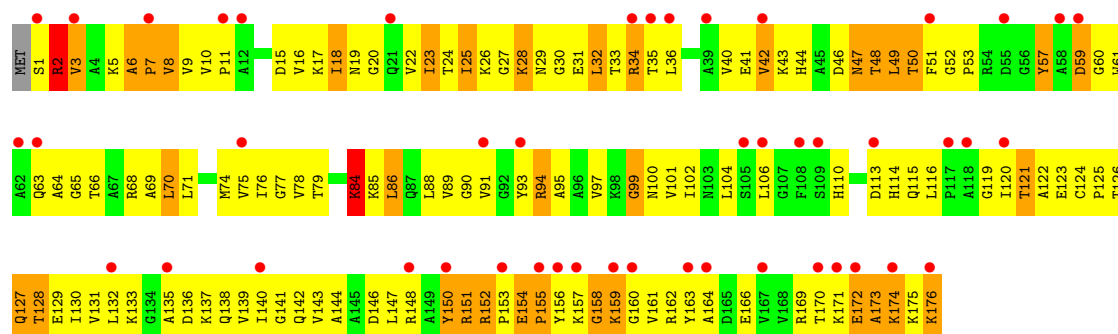




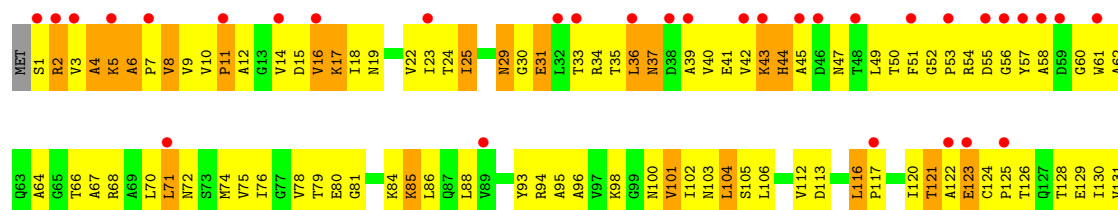
• Molecule 28: 50S RIBOSOMAL PROTEIN L5

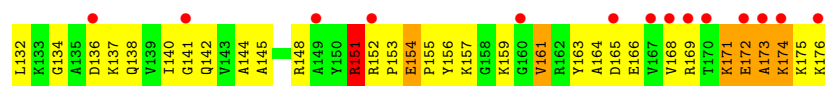


• Molecule 29: 50S RIBOSOMAL PROTEIN L6

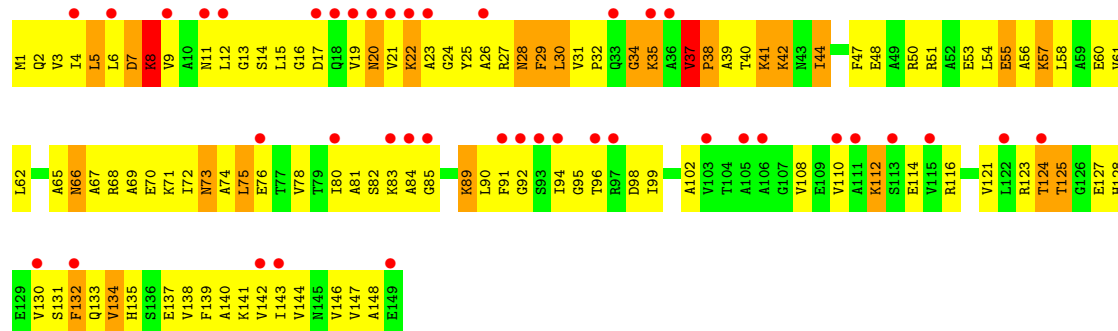


• Molecule 29: 50S RIBOSOMAL PROTEIN L6

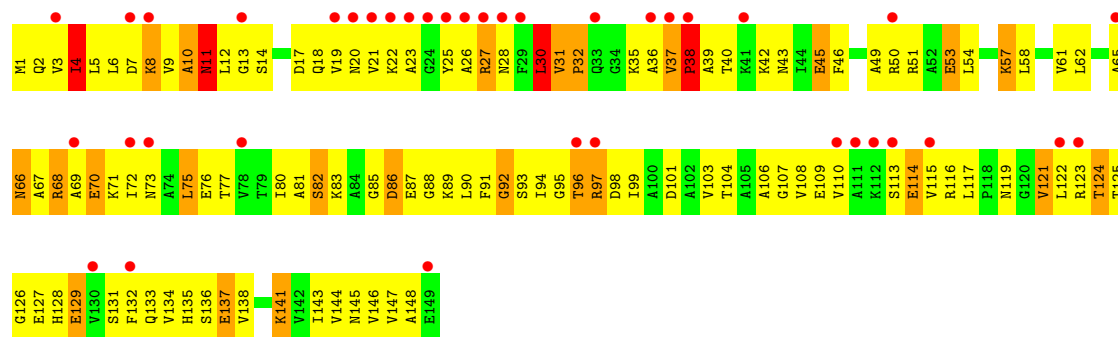




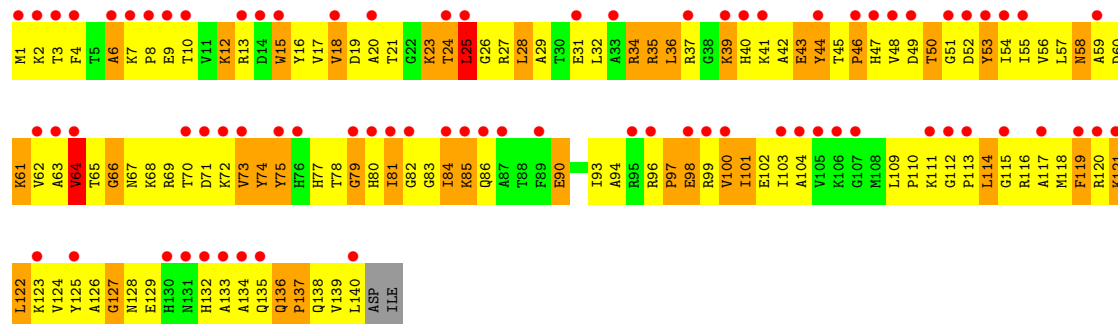
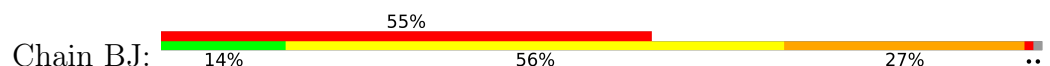
• Molecule 30: 50S RIBOSOMAL PROTEIN L9



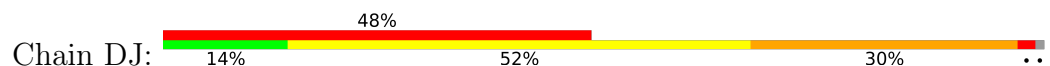
• Molecule 30: 50S RIBOSOMAL PROTEIN L9

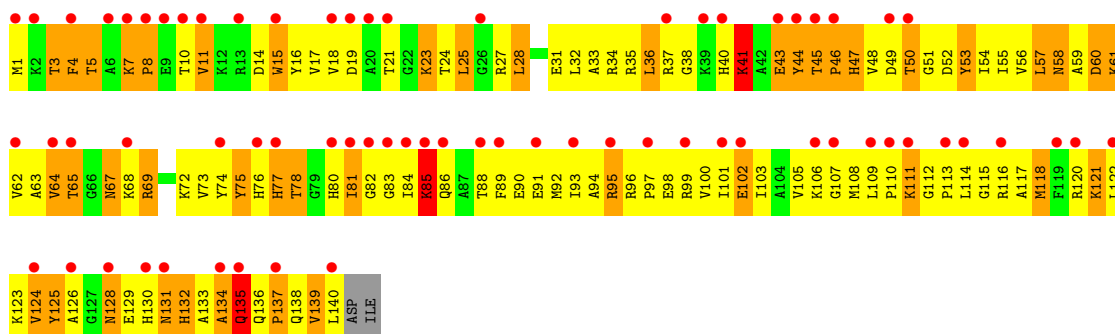


• Molecule 31: 50S RIBOSOMAL PROTEIN L13

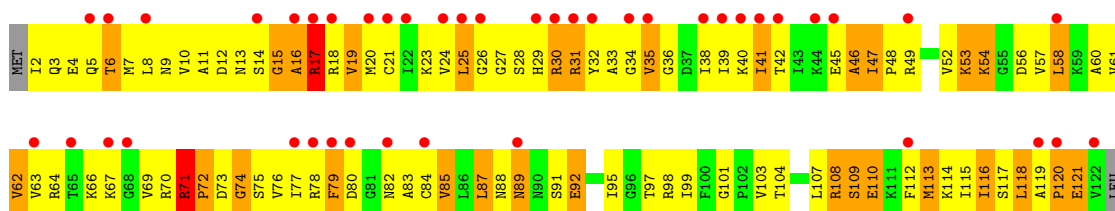
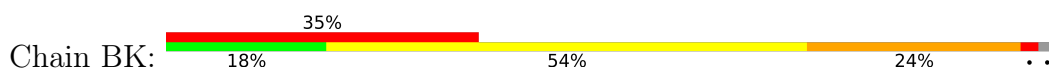


• Molecule 31: 50S RIBOSOMAL PROTEIN L13

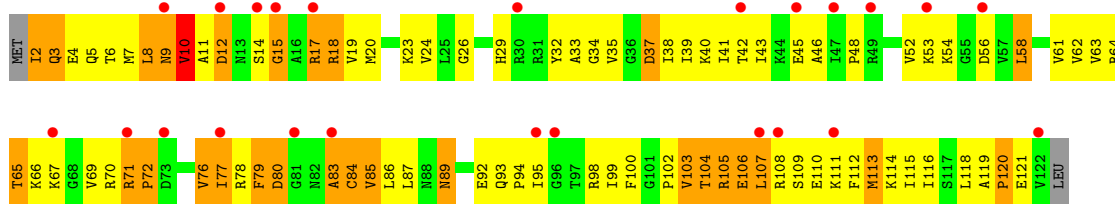




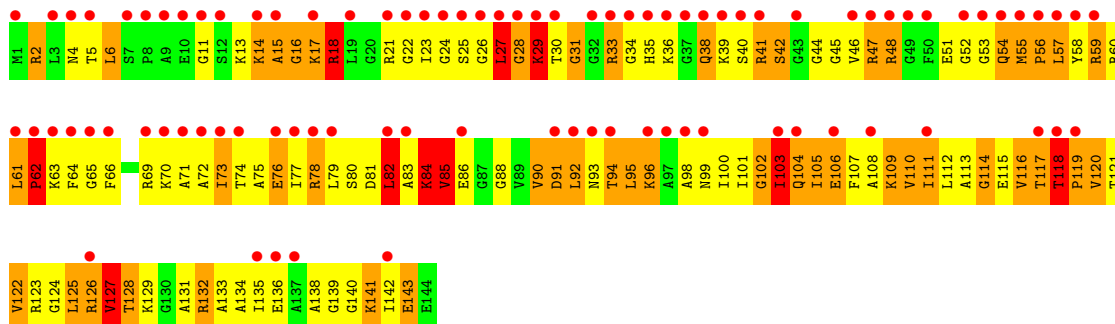
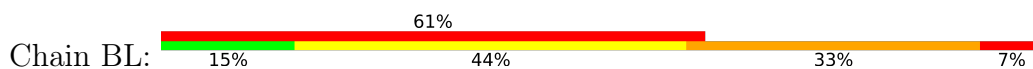
• Molecule 32: 50S RIBOSOMAL PROTEIN L14



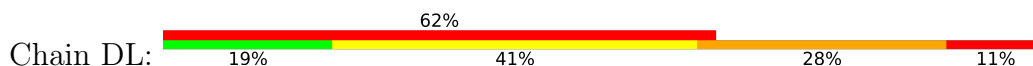
• Molecule 32: 50S RIBOSOMAL PROTEIN L14

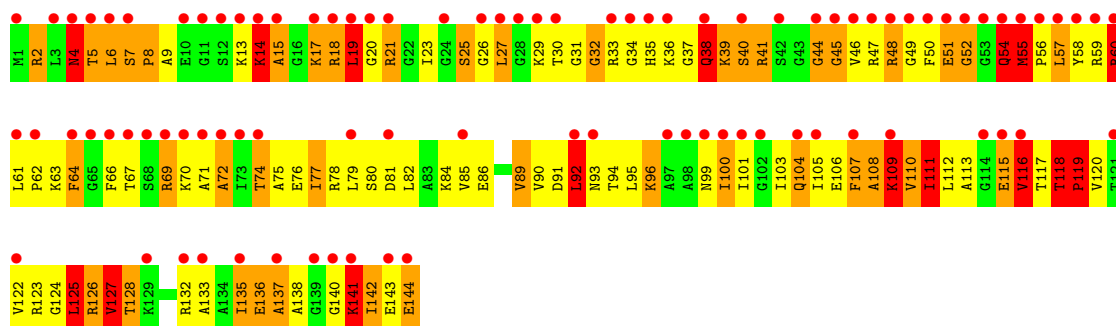


• Molecule 33: 50S RIBOSOMAL PROTEIN L15

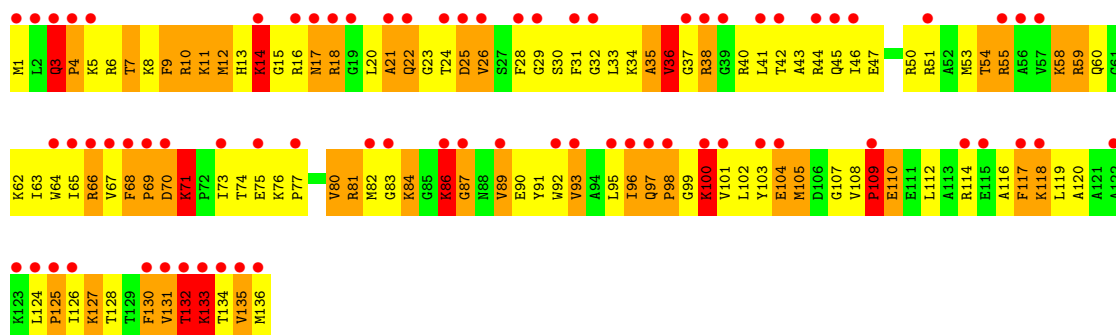
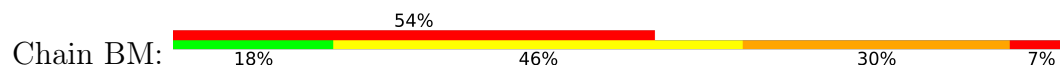


• Molecule 33: 50S RIBOSOMAL PROTEIN L15

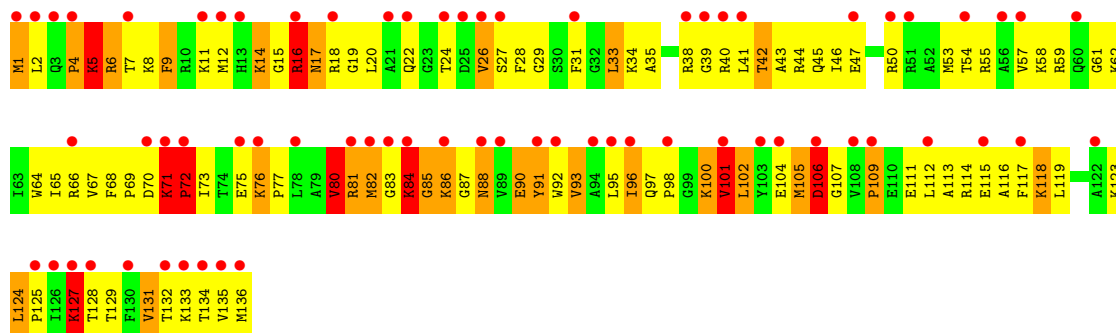




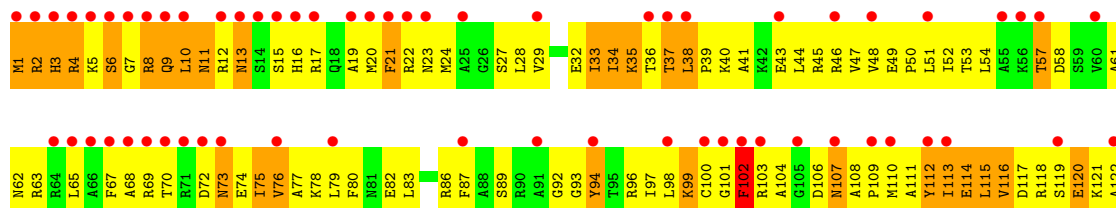
• Molecule 34: 50S RIBOSOMAL PROTEIN L16

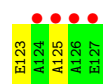


• Molecule 34: 50S RIBOSOMAL PROTEIN L16

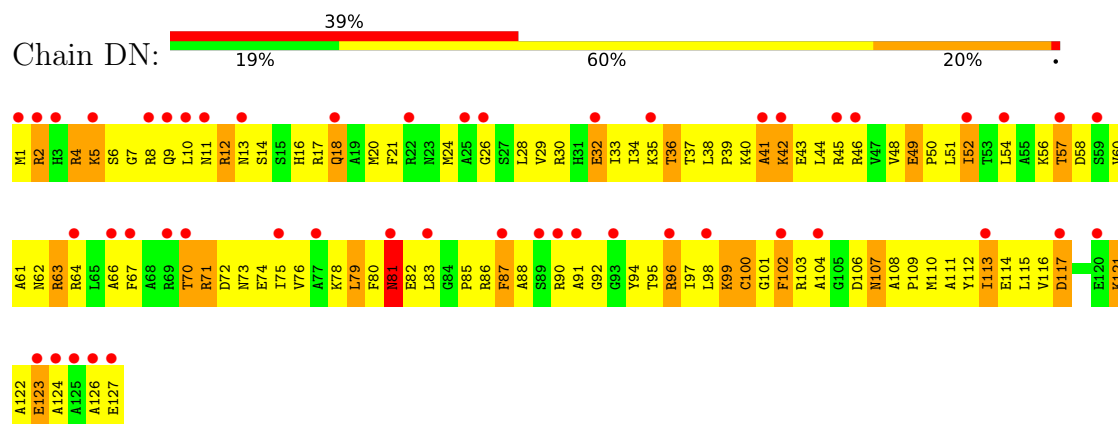


• Molecule 35: 50S RIBOSOMAL PROTEIN L17

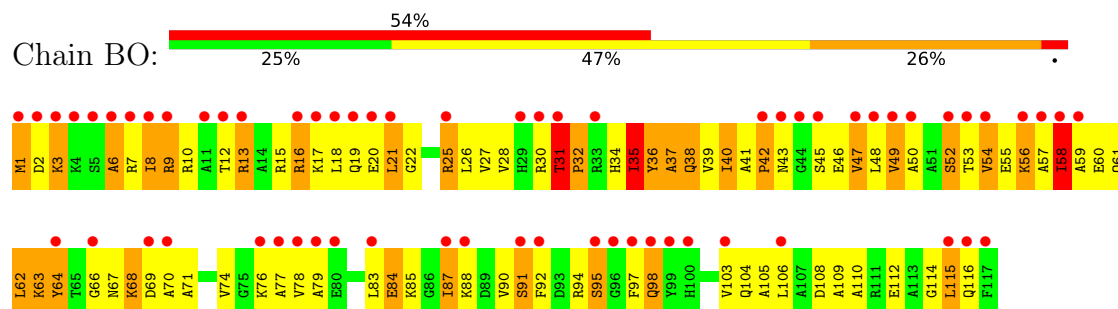




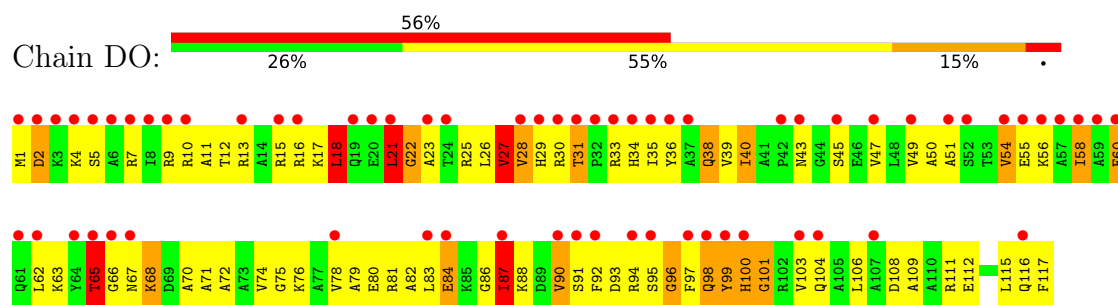
• Molecule 35: 50S RIBOSOMAL PROTEIN L17



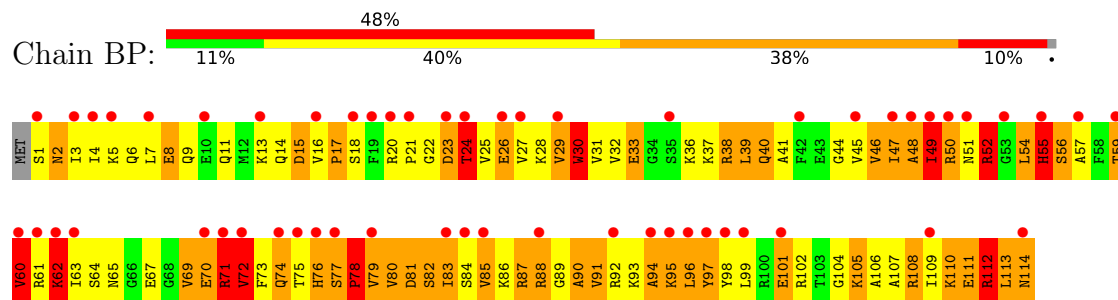
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



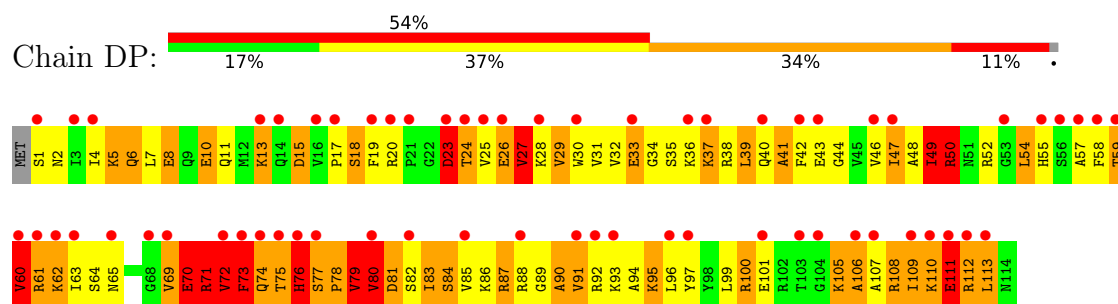
• Molecule 36: 50S RIBOSOMAL PROTEIN L18



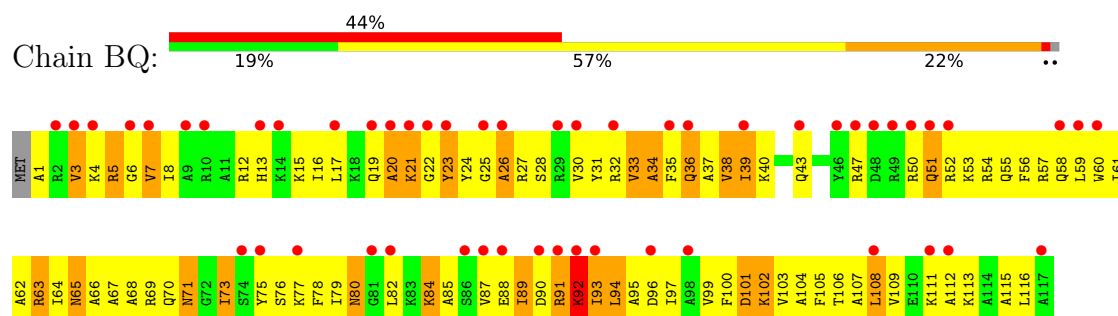
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



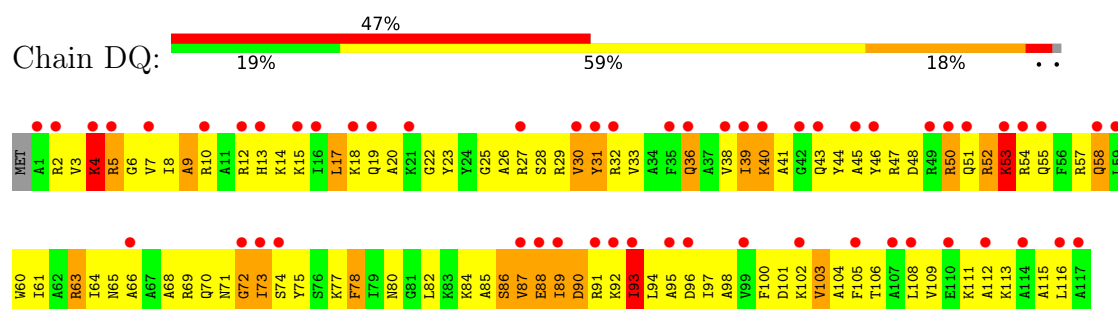
• Molecule 37: 50S RIBOSOMAL PROTEIN L19



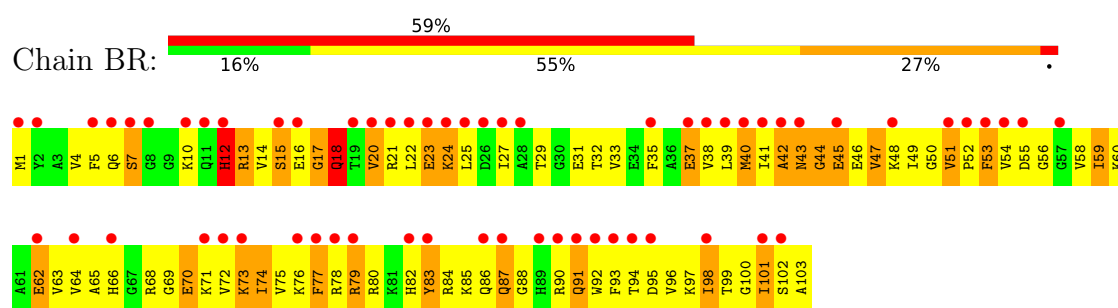
• Molecule 38: 50S RIBOSOMAL PROTEIN L20



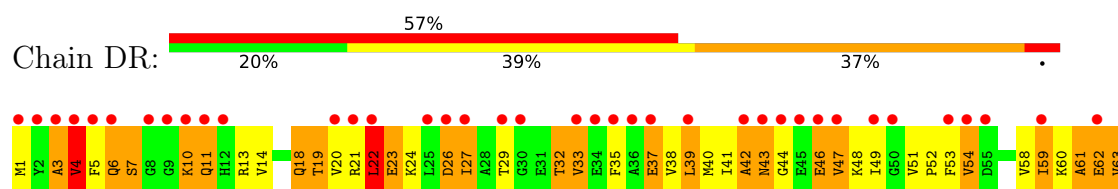
• Molecule 38: 50S RIBOSOMAL PROTEIN L20

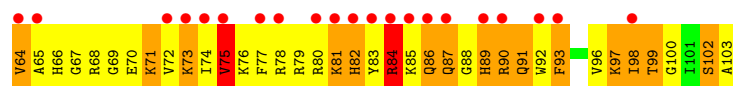


• Molecule 39: 50S RIBOSOMAL PROTEIN L21

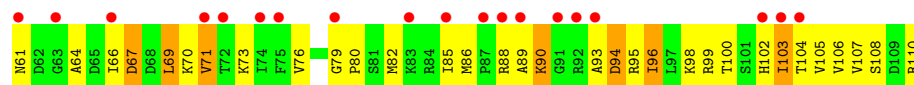
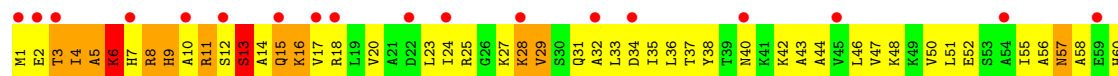


• Molecule 39: 50S RIBOSOMAL PROTEIN L21

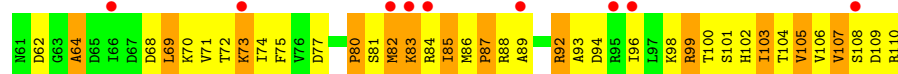
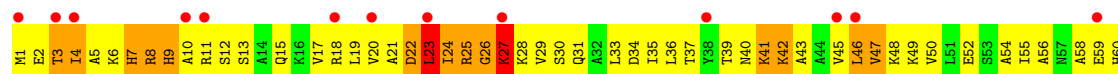




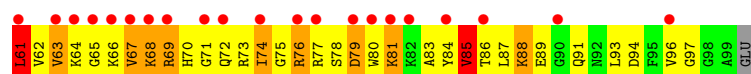
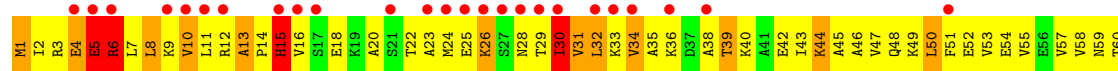
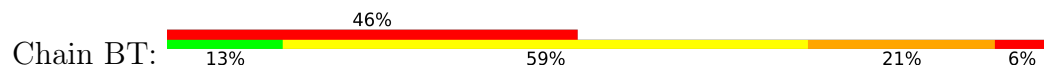
• Molecule 40: 50S RIBOSOMAL PROTEIN L22



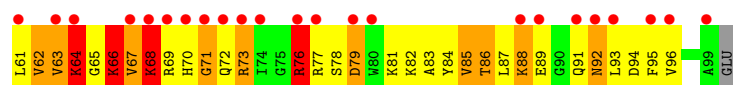
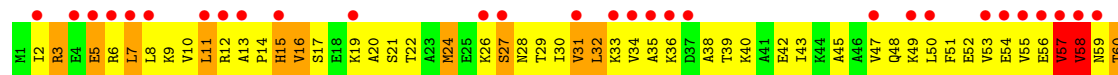
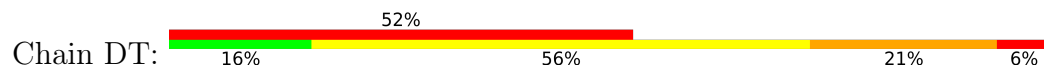
• Molecule 40: 50S RIBOSOMAL PROTEIN L22



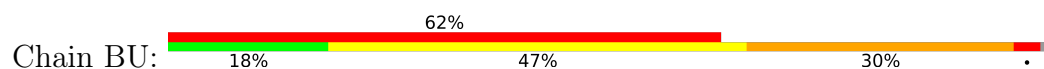
• Molecule 41: 50S RIBOSOMAL PROTEIN L23

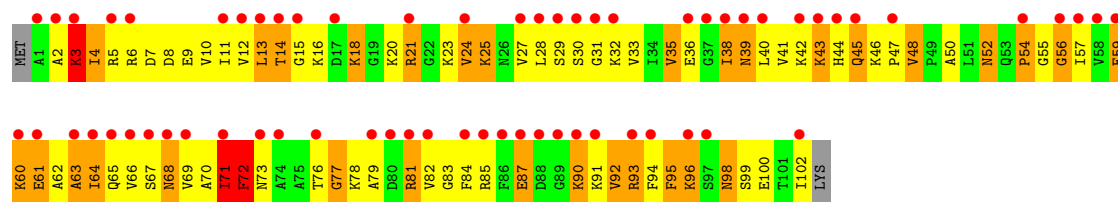


• Molecule 41: 50S RIBOSOMAL PROTEIN L23

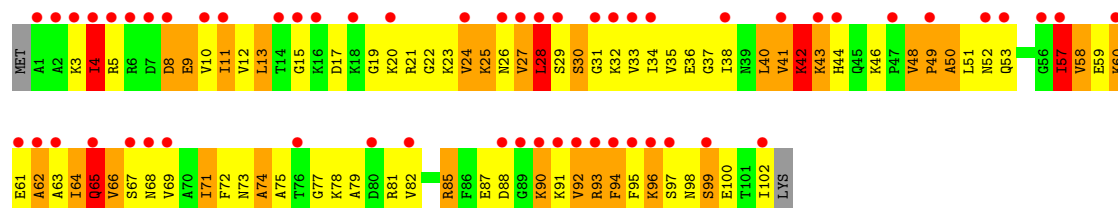
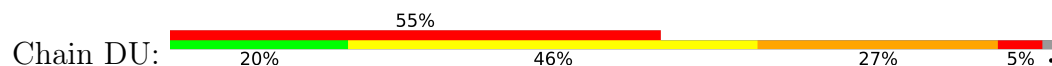


• Molecule 42: 50S RIBOSOMAL PROTEIN L24

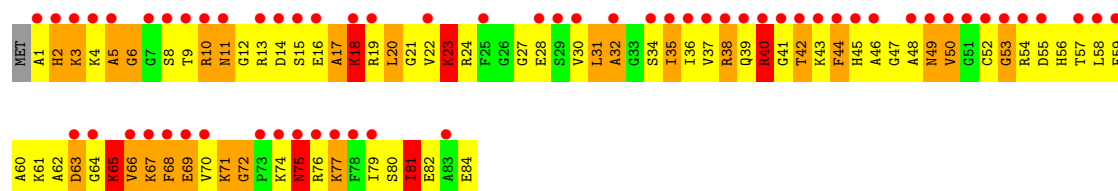
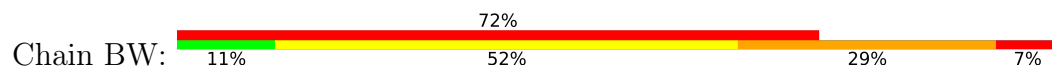




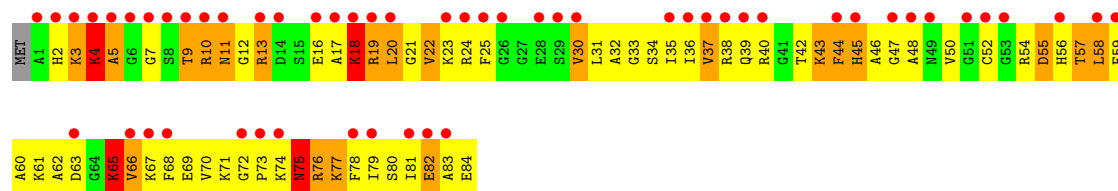
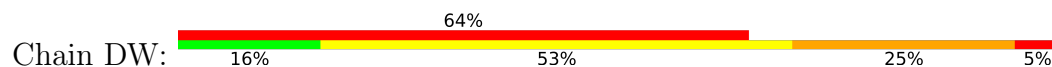
• Molecule 42: 50S RIBOSOMAL PROTEIN L24



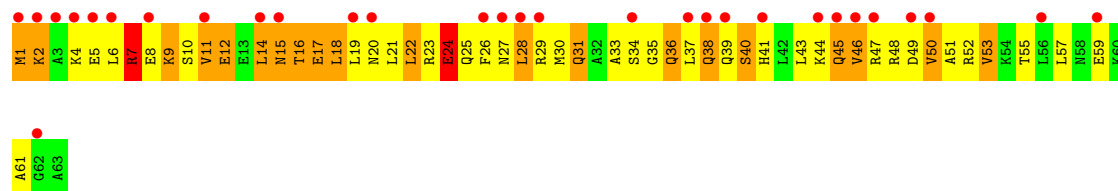
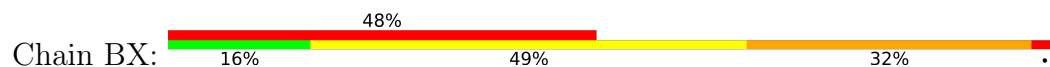
• Molecule 43: 50S RIBOSOMAL PROTEIN L27



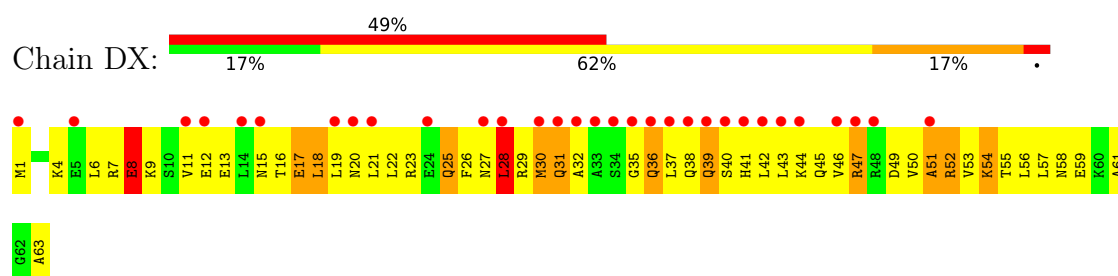
• Molecule 43: 50S RIBOSOMAL PROTEIN L27



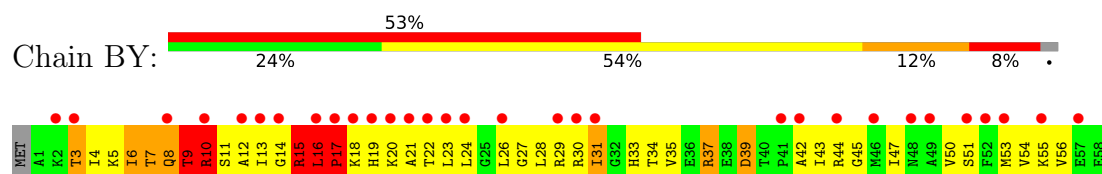
• Molecule 44: 50S RIBOSOMAL PROTEIN L29



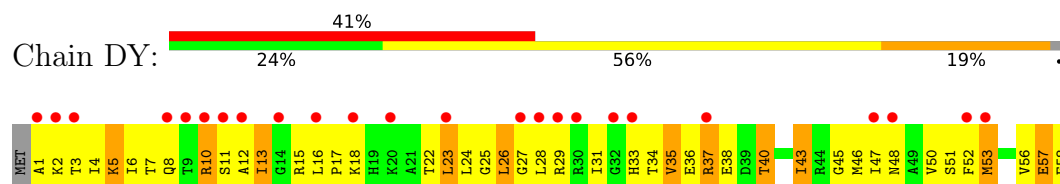
• Molecule 44: 50S RIBOSOMAL PROTEIN L29



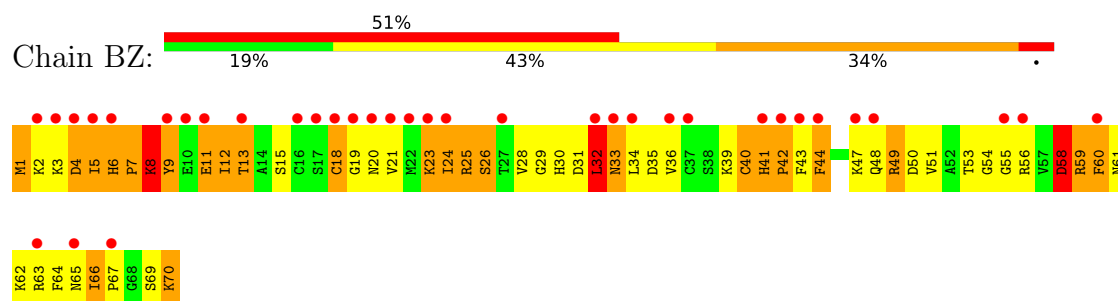
- Molecule 45: 50S RIBOSOMAL PROTEIN L30



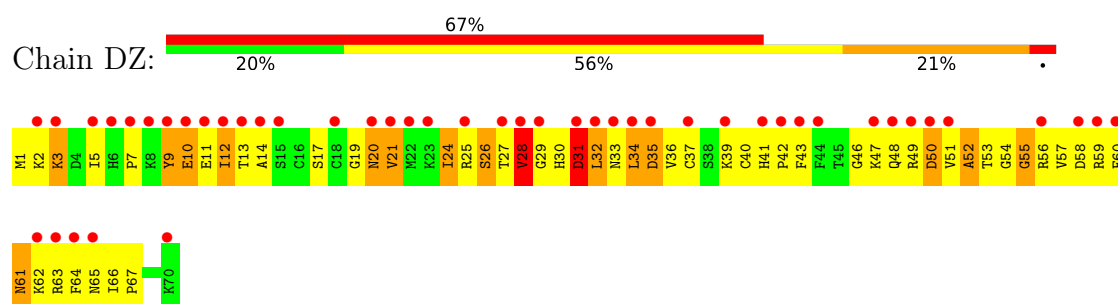
- Molecule 45: 50S RIBOSOMAL PROTEIN L30



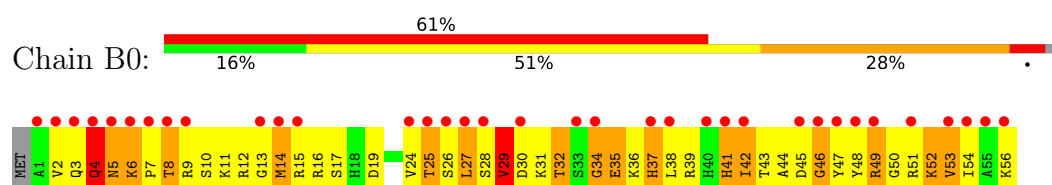
- Molecule 46: 50S RIBOSOMAL PROTEIN L31



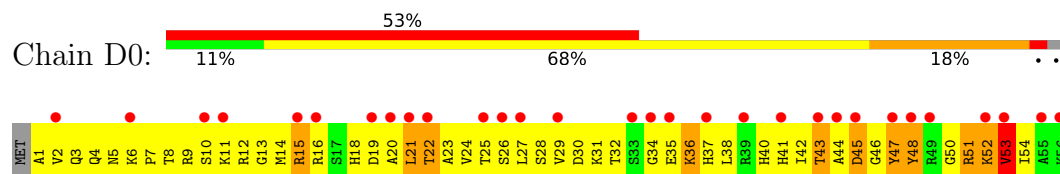
- Molecule 46: 50S RIBOSOMAL PROTEIN L31



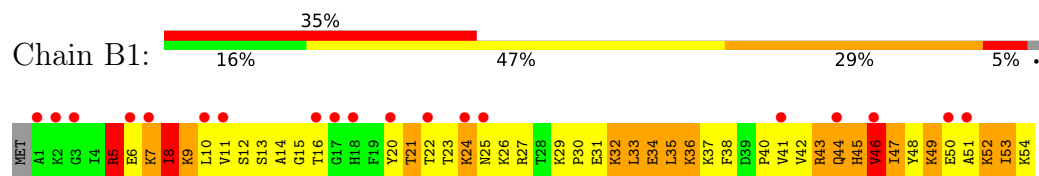
- Molecule 47: 50S RIBOSOMAL PROTEIN L32



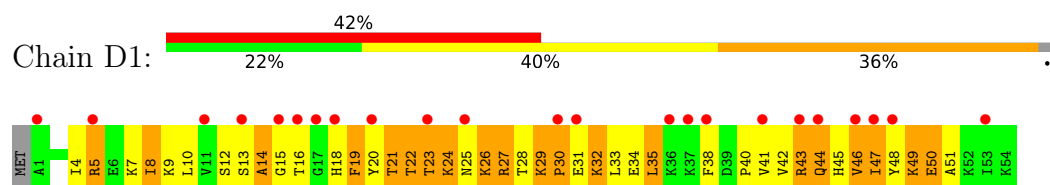
- Molecule 47: 50S RIBOSOMAL PROTEIN L32



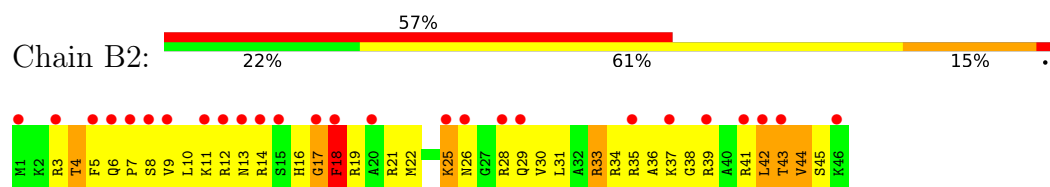
- Molecule 48: 50S RIBOSOMAL PROTEIN L33



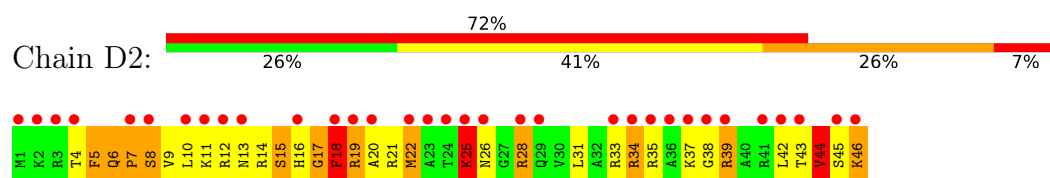
- Molecule 48: 50S RIBOSOMAL PROTEIN L33



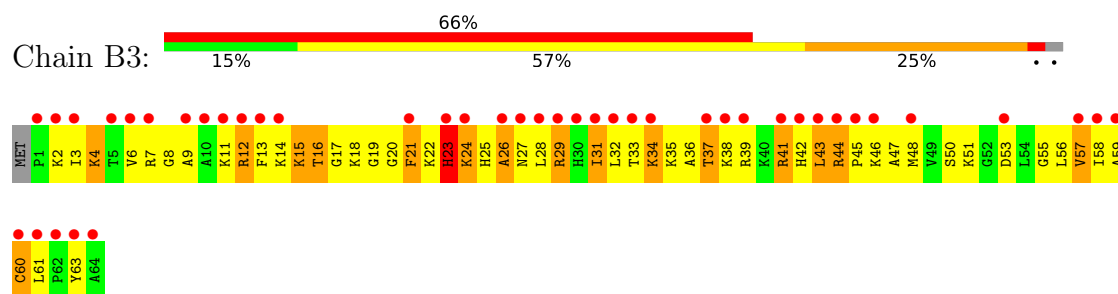
- Molecule 49: 50S RIBOSOMAL PROTEIN L34



- Molecule 49: 50S RIBOSOMAL PROTEIN L34



- Molecule 50: 50S RIBOSOMAL PROTEIN L35



- Molecule 50: 50S RIBOSOMAL PROTEIN L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 70.00 – 3.54	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 93.1 (70.00-3.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.331 0.286 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	83.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	284160	wwPDB-VP
Average B, all atoms (Å ²)	69.0	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: KSG, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.25	0/36762	0.55	14/57350 (0.0%)
1	CA	0.25	0/36762	0.56	18/57350 (0.0%)
2	AC	0.28	0/1651	0.72	1/2225 (0.0%)
2	CC	0.28	0/1651	0.75	0/2225
3	AD	0.26	0/1665	0.73	1/2227 (0.0%)
3	CD	0.27	0/1665	0.74	0/2227
4	AE	0.28	0/1118	0.75	0/1504
4	CE	0.30	0/1118	0.75	0/1504
5	AF	0.29	0/835	0.78	1/1128 (0.1%)
5	CF	0.28	0/835	0.71	0/1128
6	AG	0.27	0/1187	0.75	0/1591
6	CG	0.27	0/1211	0.78	1/1624 (0.1%)
7	AH	0.27	0/989	0.76	1/1326 (0.1%)
7	CH	0.30	0/989	0.76	0/1326
8	AI	0.27	0/1034	0.73	0/1375
8	CI	0.28	0/1034	0.71	0/1375
9	AJ	0.30	0/796	0.71	0/1077
9	CJ	0.28	0/796	0.73	0/1077
10	AK	0.28	0/893	0.75	0/1205
10	CK	0.31	0/893	0.80	2/1205 (0.2%)
11	AL	0.27	0/969	0.72	1/1300 (0.1%)
11	CL	0.28	0/969	0.73	2/1300 (0.2%)
12	AM	0.27	0/892	0.78	0/1193
12	CM	0.27	0/884	0.76	0/1181
13	AN	0.28	0/785	0.76	0/1043
13	CN	0.26	0/785	0.66	0/1043
14	AO	0.26	0/724	0.72	1/966 (0.1%)
14	CO	0.26	0/724	0.78	1/966 (0.1%)
15	AP	0.30	0/659	0.74	0/884
15	CP	0.29	0/648	0.70	0/870
16	AQ	0.26	0/657	0.67	0/881
16	CQ	0.28	0/666	0.72	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.30	0/462	0.75	0/621
17	CR	0.30	0/462	0.73	0/621
18	AS	0.26	0/652	0.71	0/877
18	CS	0.26	0/660	0.72	0/888
19	AT	0.29	0/671	0.79	0/888
19	CT	0.29	0/671	0.71	0/888
20	AB	0.31	1/1735 (0.1%)	0.77	1/2338 (0.0%)
20	CB	0.29	0/1735	0.76	1/2338 (0.0%)
21	AU	0.28	0/430	0.82	1/570 (0.2%)
21	CU	0.28	0/430	0.95	2/570 (0.4%)
22	BA	0.25	0/2803	0.53	0/4371
22	DA	0.26	0/2803	0.56	0/4371
23	BB	0.25	1/68314 (0.0%)	0.56	13/106569 (0.0%)
23	DB	0.25	1/68314 (0.0%)	0.56	19/106569 (0.0%)
24	BV	0.27	0/766	0.75	0/1025
24	DV	0.28	0/766	0.74	0/1025
25	BC	0.32	0/2092	0.90	7/2813 (0.2%)
25	DC	0.30	0/2092	0.89	4/2813 (0.1%)
26	BD	0.30	0/1586	0.79	3/2134 (0.1%)
26	DD	0.30	0/1586	0.83	6/2134 (0.3%)
27	BE	0.29	0/1571	0.86	6/2113 (0.3%)
27	DE	0.29	0/1571	0.81	3/2113 (0.1%)
28	BF	0.30	0/1444	0.99	8/1937 (0.4%)
28	DF	0.28	0/1444	0.94	8/1937 (0.4%)
29	BG	0.29	0/1343	0.80	1/1816 (0.1%)
29	DG	0.27	0/1343	0.78	1/1816 (0.1%)
30	BH	0.28	0/1122	0.77	2/1515 (0.1%)
30	DH	0.28	0/1122	0.76	1/1515 (0.1%)
31	BJ	0.29	0/1135	0.72	0/1529
31	DJ	0.29	0/1135	0.88	3/1529 (0.2%)
32	BK	0.29	0/939	0.95	3/1258 (0.2%)
32	DK	0.28	0/939	1.00	9/1258 (0.7%)
33	BL	0.33	0/1062	1.09	12/1413 (0.8%)
33	DL	0.34	0/1062	1.11	11/1413 (0.8%)
34	BM	0.33	0/1093	0.93	7/1460 (0.5%)
34	DM	0.29	0/1093	0.88	4/1460 (0.3%)
35	BN	0.30	0/1021	0.84	1/1364 (0.1%)
35	DN	0.28	0/1021	0.79	2/1364 (0.1%)
36	BO	0.28	0/910	0.83	5/1219 (0.4%)
36	DO	0.28	0/910	0.76	2/1219 (0.2%)
37	BP	0.31	0/929	1.21	11/1242 (0.9%)
37	DP	0.31	0/929	1.23	11/1242 (0.9%)
38	BQ	0.29	0/960	0.80	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.30	0/960	0.83	0/1278
39	BR	0.31	0/829	0.90	5/1107 (0.5%)
39	DR	0.29	0/829	0.82	4/1107 (0.4%)
40	BS	0.28	0/864	0.75	0/1156
40	DS	0.28	0/864	0.79	2/1156 (0.2%)
41	BT	0.29	0/784	0.74	2/1048 (0.2%)
41	DT	0.30	0/784	0.85	4/1048 (0.4%)
42	BU	0.27	0/787	0.77	0/1051
42	DU	0.28	0/787	0.98	5/1051 (0.5%)
43	BW	0.30	0/642	0.86	2/848 (0.2%)
43	DW	0.28	0/642	0.78	2/848 (0.2%)
44	BX	0.29	0/510	0.82	0/677
44	DX	0.27	0/510	0.88	1/677 (0.1%)
45	BY	0.30	0/453	0.68	0/605
45	DY	0.30	0/453	0.78	0/605
46	BZ	0.29	0/559	1.07	6/745 (0.8%)
46	DZ	0.30	0/559	0.99	4/745 (0.5%)
47	B0	0.34	0/450	0.85	2/599 (0.3%)
47	D0	0.31	0/450	0.92	1/599 (0.2%)
48	B1	0.30	0/448	0.74	0/594
48	D1	0.30	0/448	0.67	0/594
49	B2	0.30	0/380	0.78	1/498 (0.2%)
49	D2	0.30	0/380	0.74	0/498
50	B3	0.27	0/513	0.71	1/676 (0.1%)
50	D3	0.28	0/513	0.74	0/676
51	B4	0.29	0/303	0.86	0/397
51	D4	0.30	0/303	0.78	0/397
52	BI	0.32	0/1046	0.87	3/1410 (0.2%)
52	DI	0.38	1/1046 (0.1%)	0.91	2/1410 (0.1%)
All	All	0.26	4/306470 (0.0%)	0.64	260/458101 (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	16
23	BB	0	41
23	DB	1	41
47	D0	0	1
All	All	1	113

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-7.68	1.25	1.41
23	DB	1086	A	C5-C6	-7.66	1.25	1.41
52	DI	3	LYS	CA-C	5.67	1.58	1.53
20	AB	46	VAL	CA-CB	5.27	1.56	1.54

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	DU	49	PRO	N-CA-C	-11.92	98.96	113.86
37	DP	70	GLU	N-CA-C	10.38	124.67	108.79
23	DB	2790	U	OP2-P-O3'	10.08	138.25	108.00
23	BB	2790	U	OP1-P-O3'	10.00	138.01	108.00
27	BE	74	LYS	N-CA-C	-9.83	100.55	112.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	DB	2076	U	C3'

5 of 113 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	438	U	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	1328	0
1	CA	32831	0	16521	1388	0
2	AC	1624	0	1699	195	0
2	CC	1624	0	1699	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AD	1643	0	1710	190	0
3	CD	1643	0	1710	185	0
4	AE	1105	0	1148	111	0
4	CE	1105	0	1148	150	0
5	AF	817	0	808	79	0
5	CF	817	0	808	105	0
6	AG	1174	0	1230	110	0
6	CG	1196	0	1246	108	0
7	AH	979	0	1034	88	0
7	CH	979	0	1034	83	0
8	AI	1022	0	1070	159	0
8	CI	1022	0	1070	130	0
9	AJ	786	0	828	97	0
9	CJ	786	0	828	113	0
10	AK	877	0	887	108	0
10	CK	877	0	887	107	0
11	AL	955	0	1019	106	0
11	CL	955	0	1019	92	0
12	AM	883	0	944	92	0
12	CM	876	0	937	117	0
13	AN	774	0	827	113	0
13	CN	774	0	827	126	0
14	AO	716	0	742	56	0
14	CO	716	0	742	58	0
15	AP	649	0	666	82	0
15	CP	638	0	656	83	0
16	AQ	648	0	691	104	0
16	CQ	657	0	702	91	0
17	AR	455	0	478	49	0
17	CR	455	0	478	47	0
18	AS	637	0	665	89	0
18	CS	644	0	675	100	0
19	AT	665	0	714	65	0
19	CT	665	0	714	64	0
20	AB	1704	0	1732	202	0
20	CB	1704	0	1732	179	0
21	AU	425	0	449	71	0
21	CU	425	0	449	67	0
22	BA	2507	0	1270	83	0
22	DA	2507	0	1270	119	0
23	BB	60995	0	30678	2748	0
23	DB	60995	0	30677	2694	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BV	753	0	780	107	0
24	DV	753	0	780	72	0
25	BC	2053	0	2122	470	0
25	DC	2053	0	2122	396	0
26	BD	1565	0	1616	387	0
26	DD	1565	0	1616	323	0
27	BE	1552	0	1619	293	0
27	DE	1552	0	1619	274	0
28	BF	1420	0	1460	180	0
28	DF	1420	0	1460	166	0
29	BG	1323	0	1374	168	0
29	DG	1323	0	1374	168	0
30	BH	1111	0	1148	178	0
30	DH	1111	0	1148	172	0
31	BJ	1112	0	1147	222	0
31	DJ	1112	0	1147	217	0
32	BK	930	0	1000	130	0
32	DK	930	0	1000	127	0
33	BL	1053	0	1129	290	0
33	DL	1053	0	1129	253	0
34	BM	1074	0	1157	244	0
34	DM	1074	0	1157	183	0
35	BN	1008	0	1045	189	0
35	DN	1008	0	1045	163	0
36	BO	900	0	935	138	0
36	DO	900	0	935	147	0
37	BP	917	0	965	202	0
37	DP	917	0	965	200	0
38	BQ	947	0	1022	206	0
38	DQ	947	0	1022	182	0
39	BR	816	0	839	176	0
39	DR	816	0	839	170	0
40	BS	857	0	922	128	0
40	DS	857	0	922	125	0
41	BT	777	0	840	154	0
41	DT	777	0	840	138	0
42	BU	779	0	834	167	0
42	DU	779	0	834	127	0
43	BW	634	0	656	166	0
43	DW	634	0	656	174	0
44	BX	509	0	543	90	0
44	DX	509	0	543	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BY	449	0	491	62	0
45	DY	449	0	491	85	0
46	BZ	549	0	552	120	0
46	DZ	549	0	552	107	0
47	B0	444	0	461	80	0
47	D0	444	0	461	93	0
48	B1	441	0	485	83	0
48	D1	441	0	485	80	0
49	B2	377	0	418	62	0
49	D2	377	0	418	69	0
50	B3	504	0	574	118	0
50	D3	504	0	574	110	0
51	B4	302	0	343	62	0
51	D4	302	0	343	79	0
52	BI	1032	0	1088	127	0
52	DI	1032	0	1088	189	0
53	AA	26	0	23	3	0
53	CA	26	0	23	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	62	0	0	0	0
54	DB	109	0	0	0	0
54	DE	1	0	0	0	0
54	DN	1	0	0	0	0
55	AA	289	0	0	1	0
55	AE	3	0	0	0	0
55	AK	2	0	0	0	0
55	AN	3	0	0	0	0
55	AP	2	0	0	0	0
55	AT	1	0	0	0	0
55	BB	497	0	0	11	0
55	BC	1	0	0	0	0
55	BE	5	0	0	0	0
55	BH	1	0	0	0	0
55	BL	2	0	0	0	0
55	BN	1	0	0	0	0
55	CA	293	0	0	1	0
55	CE	3	0	0	0	0
55	CK	1	0	0	0	0
55	CL	4	0	0	0	0
55	CN	3	0	0	0	0
55	CP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CT	3	0	0	0	0
55	D2	2	0	0	0	0
55	DB	501	0	0	10	0
55	DC	1	0	0	0	0
55	DD	1	0	0	0	0
55	DE	3	0	0	0	0
55	DL	1	0	0	0	0
55	DN	2	0	0	0	0
55	DT	1	0	0	0	0
All	All	284160	0	190815	20206	0

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

The worst 5 of 20206 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:O5'	52:DI:4:VAL:N	1.71	1.23
32:DK:78:ARG:HG2	37:DP:72:VAL:HG21	1.24	1.15
23:DB:1098:A:H3'	52:DI:3:LYS:CA	1.76	1.15
23:DB:587:C:H3'	33:DL:29:LYS:HD2	1.20	1.14
48:D1:29:LYS:HB2	48:D1:30:PRO:HD3	1.30	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AC	204/233 (88%)	144 (71%)	44 (22%)	16 (8%)	1 8
2	CC	204/233 (88%)	138 (68%)	46 (22%)	20 (10%)	0 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	203/206 (98%)	133 (66%)	49 (24%)	21 (10%)	0	6
3	CD	203/206 (98%)	137 (68%)	49 (24%)	17 (8%)	0	7
4	AE	148/167 (89%)	110 (74%)	30 (20%)	8 (5%)	1	14
4	CE	148/167 (89%)	109 (74%)	30 (20%)	9 (6%)	1	12
5	AF	98/135 (73%)	68 (69%)	25 (26%)	5 (5%)	1	15
5	CF	98/135 (73%)	72 (74%)	18 (18%)	8 (8%)	0	8
6	AG	148/179 (83%)	105 (71%)	35 (24%)	8 (5%)	1	14
6	CG	150/179 (84%)	101 (67%)	37 (25%)	12 (8%)	1	8
7	AH	127/130 (98%)	108 (85%)	14 (11%)	5 (4%)	2	20
7	CH	127/130 (98%)	91 (72%)	29 (23%)	7 (6%)	1	14
8	AI	125/130 (96%)	84 (67%)	30 (24%)	11 (9%)	0	7
8	CI	125/130 (96%)	82 (66%)	30 (24%)	13 (10%)	0	6
9	AJ	96/103 (93%)	65 (68%)	20 (21%)	11 (12%)	0	5
9	CJ	96/103 (93%)	59 (62%)	18 (19%)	19 (20%)	0	1
10	AK	115/129 (89%)	75 (65%)	32 (28%)	8 (7%)	1	10
10	CK	115/129 (89%)	76 (66%)	30 (26%)	9 (8%)	1	8
11	AL	121/124 (98%)	73 (60%)	35 (29%)	13 (11%)	0	5
11	CL	121/124 (98%)	76 (63%)	28 (23%)	17 (14%)	0	3
12	AM	112/118 (95%)	89 (80%)	13 (12%)	10 (9%)	0	7
12	CM	111/118 (94%)	82 (74%)	17 (15%)	12 (11%)	0	5
13	AN	92/101 (91%)	64 (70%)	19 (21%)	9 (10%)	0	6
13	CN	92/101 (91%)	50 (54%)	26 (28%)	16 (17%)	0	2
14	AO	86/89 (97%)	66 (77%)	19 (22%)	1 (1%)	10	41
14	CO	86/89 (97%)	69 (80%)	15 (17%)	2 (2%)	5	30
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1	9
15	CP	78/82 (95%)	55 (70%)	14 (18%)	9 (12%)	0	5
16	AQ	78/84 (93%)	49 (63%)	25 (32%)	4 (5%)	1	15
16	CQ	79/84 (94%)	58 (73%)	15 (19%)	6 (8%)	1	8
17	AR	53/75 (71%)	31 (58%)	16 (30%)	6 (11%)	0	5
17	CR	53/75 (71%)	36 (68%)	13 (24%)	4 (8%)	1	9
18	AS	77/92 (84%)	54 (70%)	12 (16%)	11 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CS	78/92 (85%)	50 (64%)	17 (22%)	11 (14%)	0	3
19	AT	83/87 (95%)	68 (82%)	12 (14%)	3 (4%)	2	22
19	CT	83/87 (95%)	62 (75%)	16 (19%)	5 (6%)	1	12
20	AB	216/241 (90%)	148 (68%)	52 (24%)	16 (7%)	1	9
20	CB	216/241 (90%)	149 (69%)	41 (19%)	26 (12%)	0	4
21	AU	49/71 (69%)	23 (47%)	12 (24%)	14 (29%)	0	0
21	CU	49/71 (69%)	26 (53%)	18 (37%)	5 (10%)	0	6
24	BV	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	1	8
24	DV	92/94 (98%)	64 (70%)	23 (25%)	5 (5%)	1	14
25	BC	265/273 (97%)	94 (36%)	95 (36%)	76 (29%)	0	0
25	DC	265/273 (97%)	97 (37%)	101 (38%)	67 (25%)	0	0
26	BD	207/209 (99%)	87 (42%)	68 (33%)	52 (25%)	0	0
26	DD	207/209 (99%)	91 (44%)	72 (35%)	44 (21%)	0	1
27	BE	199/201 (99%)	101 (51%)	57 (29%)	41 (21%)	0	1
27	DE	199/201 (99%)	90 (45%)	63 (32%)	46 (23%)	0	1
28	BF	176/179 (98%)	99 (56%)	42 (24%)	35 (20%)	0	1
28	DF	176/179 (98%)	98 (56%)	49 (28%)	29 (16%)	0	2
29	BG	174/177 (98%)	112 (64%)	41 (24%)	21 (12%)	0	4
29	DG	174/177 (98%)	108 (62%)	51 (29%)	15 (9%)	0	7
30	BH	147/149 (99%)	83 (56%)	49 (33%)	15 (10%)	0	6
30	DH	147/149 (99%)	83 (56%)	46 (31%)	18 (12%)	0	4
31	BJ	138/142 (97%)	68 (49%)	43 (31%)	27 (20%)	0	1
31	DJ	138/142 (97%)	72 (52%)	36 (26%)	30 (22%)	0	1
32	BK	119/123 (97%)	73 (61%)	27 (23%)	19 (16%)	0	2
32	DK	119/123 (97%)	70 (59%)	30 (25%)	19 (16%)	0	2
33	BL	142/144 (99%)	56 (39%)	47 (33%)	39 (28%)	0	0
33	DL	142/144 (99%)	68 (48%)	35 (25%)	39 (28%)	0	0
34	BM	134/136 (98%)	64 (48%)	37 (28%)	33 (25%)	0	0
34	DM	134/136 (98%)	71 (53%)	43 (32%)	20 (15%)	0	2
35	BN	125/127 (98%)	68 (54%)	41 (33%)	16 (13%)	0	4
35	DN	125/127 (98%)	86 (69%)	29 (23%)	10 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BO	115/117 (98%)	61 (53%)	34 (30%)	20 (17%)	0	2
36	DO	115/117 (98%)	62 (54%)	33 (29%)	20 (17%)	0	2
37	BP	112/115 (97%)	37 (33%)	38 (34%)	37 (33%)	0	0
37	DP	112/115 (97%)	42 (38%)	37 (33%)	33 (30%)	0	0
38	BQ	115/118 (98%)	79 (69%)	23 (20%)	13 (11%)	0	5
38	DQ	115/118 (98%)	78 (68%)	21 (18%)	16 (14%)	0	3
39	BR	101/103 (98%)	39 (39%)	38 (38%)	24 (24%)	0	0
39	DR	101/103 (98%)	42 (42%)	30 (30%)	29 (29%)	0	0
40	BS	108/110 (98%)	58 (54%)	34 (32%)	16 (15%)	0	3
40	DS	108/110 (98%)	62 (57%)	26 (24%)	20 (18%)	0	1
41	BT	97/100 (97%)	38 (39%)	42 (43%)	17 (18%)	0	2
41	DT	97/100 (97%)	44 (45%)	28 (29%)	25 (26%)	0	0
42	BU	100/104 (96%)	36 (36%)	43 (43%)	21 (21%)	0	1
42	DU	100/104 (96%)	47 (47%)	34 (34%)	19 (19%)	0	1
43	BW	82/85 (96%)	35 (43%)	22 (27%)	25 (30%)	0	0
43	DW	82/85 (96%)	28 (34%)	31 (38%)	23 (28%)	0	0
44	BX	61/63 (97%)	20 (33%)	30 (49%)	11 (18%)	0	1
44	DX	61/63 (97%)	37 (61%)	15 (25%)	9 (15%)	0	3
45	BY	56/59 (95%)	29 (52%)	17 (30%)	10 (18%)	0	2
45	DY	56/59 (95%)	38 (68%)	15 (27%)	3 (5%)	1	14
46	BZ	68/70 (97%)	32 (47%)	23 (34%)	13 (19%)	0	1
46	DZ	68/70 (97%)	36 (53%)	22 (32%)	10 (15%)	0	3
47	B0	54/57 (95%)	27 (50%)	17 (32%)	10 (18%)	0	1
47	D0	54/57 (95%)	25 (46%)	20 (37%)	9 (17%)	0	2
48	B1	52/55 (94%)	22 (42%)	20 (38%)	10 (19%)	0	1
48	D1	52/55 (94%)	21 (40%)	18 (35%)	13 (25%)	0	0
49	B2	44/46 (96%)	22 (50%)	15 (34%)	7 (16%)	0	2
49	D2	44/46 (96%)	22 (50%)	10 (23%)	12 (27%)	0	0
50	B3	62/65 (95%)	26 (42%)	28 (45%)	8 (13%)	0	4
50	D3	62/65 (95%)	30 (48%)	21 (34%)	11 (18%)	0	2
51	B4	36/38 (95%)	17 (47%)	9 (25%)	10 (28%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D4	36/38 (95%)	13 (36%)	10 (28%)	13 (36%)	0	0
52	BI	139/142 (98%)	122 (88%)	12 (9%)	5 (4%)	2	22
52	DI	139/142 (98%)	119 (86%)	15 (11%)	5 (4%)	2	22
All	All	11263/11954 (94%)	6605 (59%)	2995 (27%)	1663 (15%)	0	3

5 of 1663 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	2	GLN
2	AC	81	GLU
2	AC	91	ALA
3	AD	18	LEU
3	AD	25	ARG

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	170/190 (90%)	152 (89%)	18 (11%)	6	27
2	CC	170/190 (90%)	151 (89%)	19 (11%)	6	26
3	AD	172/173 (99%)	145 (84%)	27 (16%)	2	15
3	CD	172/173 (99%)	146 (85%)	26 (15%)	3	17
4	AE	113/126 (90%)	99 (88%)	14 (12%)	4	23
4	CE	113/126 (90%)	92 (81%)	21 (19%)	1	9
5	AF	87/116 (75%)	69 (79%)	18 (21%)	1	6
5	CF	87/116 (75%)	75 (86%)	12 (14%)	3	19
6	AG	123/147 (84%)	108 (88%)	15 (12%)	5	23
6	CG	125/147 (85%)	112 (90%)	13 (10%)	7	28
7	AH	104/105 (99%)	94 (90%)	10 (10%)	8	31
7	CH	104/105 (99%)	90 (86%)	14 (14%)	4	20
8	AI	105/107 (98%)	87 (83%)	18 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/107 (98%)	93 (89%)	12 (11%)	5	25
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	17
9	CJ	86/90 (96%)	78 (91%)	8 (9%)	8	32
10	AK	90/99 (91%)	75 (83%)	15 (17%)	2	13
10	CK	90/99 (91%)	79 (88%)	11 (12%)	5	23
11	AL	103/104 (99%)	91 (88%)	12 (12%)	5	25
11	CL	103/104 (99%)	83 (81%)	20 (19%)	1	8
12	AM	92/96 (96%)	78 (85%)	14 (15%)	3	16
12	CM	91/96 (95%)	80 (88%)	11 (12%)	5	23
13	AN	79/84 (94%)	68 (86%)	11 (14%)	3	19
13	CN	79/84 (94%)	68 (86%)	11 (14%)	3	19
14	AO	76/77 (99%)	70 (92%)	6 (8%)	11	37
14	CO	76/77 (99%)	66 (87%)	10 (13%)	4	21
15	AP	65/65 (100%)	54 (83%)	11 (17%)	2	13
15	CP	65/65 (100%)	57 (88%)	8 (12%)	4	23
16	AQ	74/78 (95%)	63 (85%)	11 (15%)	3	17
16	CQ	75/78 (96%)	67 (89%)	8 (11%)	6	27
17	AR	48/65 (74%)	43 (90%)	5 (10%)	7	28
17	CR	48/65 (74%)	43 (90%)	5 (10%)	7	28
18	AS	70/79 (89%)	64 (91%)	6 (9%)	10	34
18	CS	71/79 (90%)	59 (83%)	12 (17%)	2	13
19	AT	65/66 (98%)	56 (86%)	9 (14%)	3	19
19	CT	65/66 (98%)	54 (83%)	11 (17%)	2	13
20	AB	180/199 (90%)	149 (83%)	31 (17%)	2	12
20	CB	180/199 (90%)	155 (86%)	25 (14%)	3	19
21	AU	44/61 (72%)	41 (93%)	3 (7%)	14	41
21	CU	44/61 (72%)	35 (80%)	9 (20%)	1	7
24	BV	78/78 (100%)	66 (85%)	12 (15%)	2	16
24	DV	78/78 (100%)	71 (91%)	7 (9%)	9	33
25	BC	213/218 (98%)	161 (76%)	52 (24%)	1	4
25	DC	213/218 (98%)	163 (76%)	50 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	122 (74%)	42 (26%)	0	3
26	DD	164/164 (100%)	126 (77%)	38 (23%)	1	5
27	BE	165/165 (100%)	127 (77%)	38 (23%)	1	5
27	DE	165/165 (100%)	138 (84%)	27 (16%)	2	14
28	BF	149/150 (99%)	130 (87%)	19 (13%)	4	22
28	DF	149/150 (99%)	126 (85%)	23 (15%)	2	16
29	BG	137/138 (99%)	114 (83%)	23 (17%)	2	13
29	DG	137/138 (99%)	115 (84%)	22 (16%)	2	14
30	BH	114/114 (100%)	97 (85%)	17 (15%)	3	17
30	DH	114/114 (100%)	95 (83%)	19 (17%)	2	13
31	BJ	114/116 (98%)	95 (83%)	19 (17%)	2	13
31	DJ	114/116 (98%)	91 (80%)	23 (20%)	1	7
32	BK	102/104 (98%)	82 (80%)	20 (20%)	1	8
32	DK	102/104 (98%)	90 (88%)	12 (12%)	5	24
33	BL	103/103 (100%)	75 (73%)	28 (27%)	0	3
33	DL	103/103 (100%)	69 (67%)	34 (33%)	0	2
34	BM	109/109 (100%)	83 (76%)	26 (24%)	1	4
34	DM	109/109 (100%)	78 (72%)	31 (28%)	0	3
35	BN	103/103 (100%)	86 (84%)	17 (16%)	2	14
35	DN	103/103 (100%)	84 (82%)	19 (18%)	1	9
36	BO	87/87 (100%)	70 (80%)	17 (20%)	1	8
36	DO	87/87 (100%)	75 (86%)	12 (14%)	3	19
37	BP	99/100 (99%)	75 (76%)	24 (24%)	1	4
37	DP	99/100 (99%)	69 (70%)	30 (30%)	0	2
38	BQ	89/90 (99%)	71 (80%)	18 (20%)	1	7
38	DQ	89/90 (99%)	72 (81%)	17 (19%)	1	8
39	BR	84/84 (100%)	73 (87%)	11 (13%)	4	21
39	DR	84/84 (100%)	67 (80%)	17 (20%)	1	7
40	BS	93/93 (100%)	83 (89%)	10 (11%)	6	27
40	DS	93/93 (100%)	80 (86%)	13 (14%)	3	19
41	BT	83/84 (99%)	66 (80%)	17 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DT	83/84 (99%)	69 (83%)	14 (17%)	2	13
42	BU	83/85 (98%)	65 (78%)	18 (22%)	1	6
42	DU	83/85 (98%)	64 (77%)	19 (23%)	1	5
43	BW	62/63 (98%)	50 (81%)	12 (19%)	1	8
43	DW	62/63 (98%)	49 (79%)	13 (21%)	1	6
44	BX	55/55 (100%)	40 (73%)	15 (27%)	0	3
44	DX	55/55 (100%)	45 (82%)	10 (18%)	2	10
45	BY	48/49 (98%)	37 (77%)	11 (23%)	1	5
45	DY	48/49 (98%)	38 (79%)	10 (21%)	1	6
46	BZ	62/62 (100%)	45 (73%)	17 (27%)	0	3
46	DZ	62/62 (100%)	54 (87%)	8 (13%)	4	21
47	B0	47/48 (98%)	38 (81%)	9 (19%)	1	8
47	D0	47/48 (98%)	38 (81%)	9 (19%)	1	8
48	B1	48/49 (98%)	33 (69%)	15 (31%)	0	2
48	D1	48/49 (98%)	38 (79%)	10 (21%)	1	6
49	B2	38/38 (100%)	33 (87%)	5 (13%)	4	21
49	D2	38/38 (100%)	29 (76%)	9 (24%)	1	4
50	B3	51/52 (98%)	39 (76%)	12 (24%)	1	4
50	D3	51/52 (98%)	41 (80%)	10 (20%)	1	8
51	B4	34/34 (100%)	25 (74%)	9 (26%)	0	3
51	D4	34/34 (100%)	21 (62%)	13 (38%)	0	1
52	BI	109/110 (99%)	108 (99%)	1 (1%)	70	76
52	DI	109/110 (99%)	105 (96%)	4 (4%)	30	57
All	All	9341/9744 (96%)	7751 (83%)	1590 (17%)	2	12

5 of 1590 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	CK	31	VAL
26	DD	114	LYS
11	CL	107	LYS
9	CJ	99	GLN
20	CB	57	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 349 such sidechains are listed below:

Mol	Chain	Res	Type
16	CQ	50	ASN
29	DG	127	GLN
19	CT	12	GLN
25	DC	57	HIS
34	DM	45	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	256 (16%)	24 (1%)
1	CA	1529/1542 (99%)	232 (15%)	24 (1%)
22	BA	116/120 (96%)	23 (19%)	0
22	DA	116/120 (96%)	22 (18%)	0
23	BB	2837/2904 (97%)	424 (14%)	13 (0%)
23	DB	2837/2904 (97%)	438 (15%)	18 (0%)
All	All	8964/9132 (98%)	1395 (15%)	79 (0%)

5 of 1395 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1301	U
23	DB	1211	C
1	CA	1397	C
23	DB	301	G
23	DB	2286	G

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 345 ligands modelled in this entry, 343 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	KSG	AA	1601	-	26,27,27	1.49	4 (15%)	31,40,40	1.06	3 (9%)
53	KSG	CA	1601	-	26,27,27	1.59	3 (11%)	31,40,40	0.97	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	KSG	AA	1601	-	-	2/10/52/52	0/2/2/2
53	KSG	CA	1601	-	-	2/10/52/52	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AA	1601	KSG	C1-C12	2.66	1.57	1.52
53	CA	1601	KSG	C1-C12	2.61	1.57	1.52
53	CA	1601	KSG	O7-C1	2.56	1.48	1.41
53	CA	1601	KSG	O1-C1	2.31	1.48	1.41
53	AA	1601	KSG	O7-C1	2.20	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	KSG	C1-O1-C2	-2.33	112.46	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	AA	1601	KSG	C4-C3-C2	2.20	114.68	109.68
53	AA	1601	KSG	C5-C4-C3	2.07	114.47	110.83
53	CA	1601	KSG	C6-C7-C2	2.02	114.26	109.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

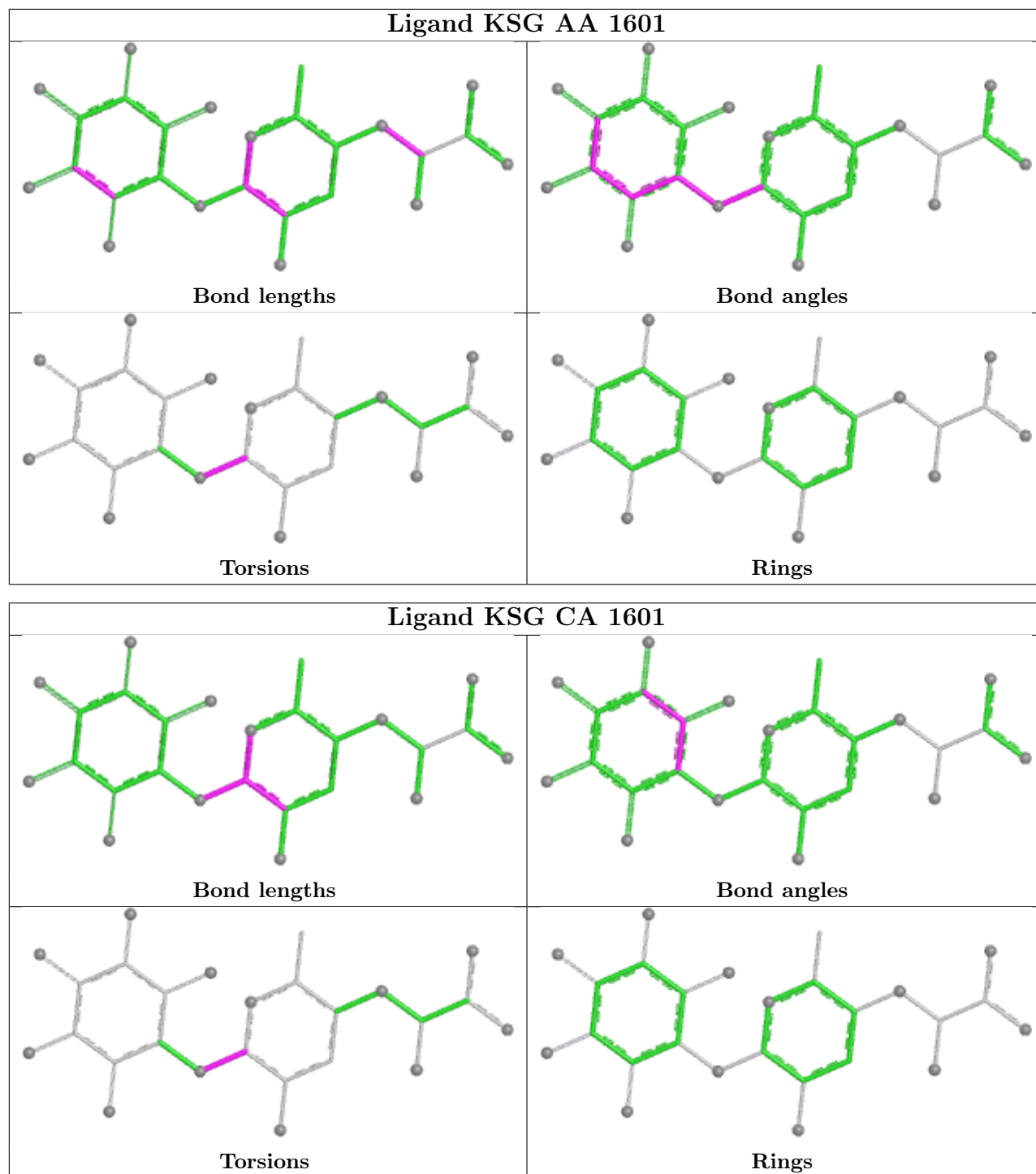
Mol	Chain	Res	Type	Atoms
53	AA	1601	KSG	C12-C1-O1-C2
53	CA	1601	KSG	C12-C1-O1-C2
53	CA	1601	KSG	O7-C1-O1-C2
53	AA	1601	KSG	O7-C1-O1-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	AA	1601	KSG	3	0
53	CA	1601	KSG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	1.21	265 (17%) 4 4	15, 73, 149, 180	0
1	CA	1530/1542 (99%)	0.86	135 (8%) 15 11	7, 52, 134, 180	0
2	AC	206/233 (88%)	1.22	50 (24%) 2 2	7, 68, 138, 180	0
2	CC	206/233 (88%)	1.05	30 (14%) 6 5	6, 74, 126, 169	0
3	AD	205/206 (99%)	1.75	78 (38%) 1 1	27, 79, 147, 180	0
3	CD	205/206 (99%)	1.20	40 (19%) 3 3	5, 55, 113, 165	0
4	AE	150/167 (89%)	1.22	34 (22%) 2 3	15, 62, 120, 162	0
4	CE	150/167 (89%)	1.13	30 (20%) 3 3	6, 55, 112, 180	0
5	AF	100/135 (74%)	1.22	19 (19%) 3 4	18, 72, 133, 166	0
5	CF	100/135 (74%)	1.30	24 (24%) 2 2	12, 71, 132, 165	0
6	AG	150/179 (83%)	1.35	36 (24%) 2 2	22, 89, 143, 180	0
6	CG	152/179 (84%)	1.20	32 (21%) 2 3	19, 86, 147, 180	0
7	AH	129/130 (99%)	1.53	38 (29%) 1 2	14, 70, 141, 176	0
7	CH	129/130 (99%)	1.33	31 (24%) 2 2	5, 54, 114, 160	0
8	AI	127/130 (97%)	1.46	37 (29%) 1 2	18, 90, 146, 180	0
8	CI	127/130 (97%)	1.78	46 (36%) 1 1	23, 92, 156, 180	0
9	AJ	98/103 (95%)	1.50	31 (31%) 1 1	20, 82, 157, 180	0
9	CJ	98/103 (95%)	1.63	37 (37%) 1 1	34, 79, 135, 151	0
10	AK	117/129 (90%)	1.42	28 (23%) 2 2	7, 55, 138, 160	0
10	CK	117/129 (90%)	1.21	24 (20%) 2 3	11, 50, 105, 142	0
11	AL	123/124 (99%)	1.89	48 (39%) 1 1	21, 61, 128, 178	0
11	CL	123/124 (99%)	1.21	26 (21%) 2 3	5, 39, 119, 160	0
12	AM	114/118 (96%)	1.37	27 (23%) 2 2	44, 106, 159, 173	0
12	CM	113/118 (95%)	1.49	35 (30%) 1 2	26, 100, 157, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	1.89	43 (44%)	0	1	15, 84, 151, 180	0
13	CN	96/101 (95%)	1.78	36 (37%)	1	1	21, 82, 139, 161	0
14	AO	88/89 (98%)	1.56	31 (35%)	1	1	18, 70, 114, 180	0
14	CO	88/89 (98%)	1.39	24 (27%)	1	2	14, 51, 112, 150	0
15	AP	82/82 (100%)	1.70	26 (31%)	1	1	27, 89, 142, 180	0
15	CP	80/82 (97%)	1.73	25 (31%)	1	1	5, 46, 145, 180	0
16	AQ	80/84 (95%)	1.81	29 (36%)	1	1	37, 91, 140, 180	0
16	CQ	81/84 (96%)	1.39	20 (24%)	2	2	12, 57, 119, 154	0
17	AR	55/75 (73%)	1.77	18 (32%)	1	1	18, 69, 147, 164	0
17	CR	55/75 (73%)	1.16	11 (20%)	3	3	13, 53, 126, 175	0
18	AS	79/92 (85%)	1.74	27 (34%)	1	1	59, 112, 174, 180	0
18	CS	80/92 (86%)	2.12	36 (45%)	0	1	48, 109, 172, 180	0
19	AT	85/87 (97%)	2.06	34 (40%)	1	1	36, 94, 142, 170	0
19	CT	85/87 (97%)	1.78	30 (35%)	1	1	17, 55, 118, 179	0
20	AB	218/241 (90%)	1.25	51 (23%)	2	3	28, 92, 142, 180	0
20	CB	218/241 (90%)	1.11	39 (17%)	3	4	26, 96, 157, 180	0
21	AU	51/71 (71%)	2.33	27 (52%)	0	1	26, 94, 153, 174	0
21	CU	51/71 (71%)	2.44	27 (52%)	0	1	29, 82, 163, 180	0
22	BA	117/120 (97%)	1.12	13 (11%)	10	8	39, 67, 125, 171	0
22	DA	117/120 (97%)	1.25	20 (17%)	4	4	34, 73, 116, 180	0
23	BB	2841/2904 (97%)	1.02	350 (12%)	8	7	9, 53, 144, 180	0
23	DB	2841/2904 (97%)	0.93	278 (9%)	13	9	5, 45, 143, 180	0
24	BV	94/94 (100%)	1.04	14 (14%)	5	5	26, 78, 134, 155	0
24	DV	94/94 (100%)	1.56	26 (27%)	1	2	34, 83, 139, 162	0
25	BC	267/273 (97%)	2.38	120 (44%)	0	1	5, 53, 143, 180	0
25	DC	267/273 (97%)	2.56	134 (50%)	0	1	5, 52, 158, 180	0
26	BD	209/209 (100%)	2.58	108 (51%)	0	1	8, 82, 157, 180	0
26	DD	209/209 (100%)	2.34	101 (48%)	0	1	5, 57, 142, 180	0
27	BE	201/201 (100%)	2.13	93 (46%)	0	1	5, 85, 162, 180	0
27	DE	201/201 (100%)	2.45	107 (53%)	0	1	6, 82, 170, 180	0
28	BF	178/179 (99%)	1.51	48 (26%)	1	2	39, 105, 168, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DF	178/179 (99%)	1.55	57 (32%)	1	1	29, 96, 154, 180	0
29	BG	176/177 (99%)	1.48	47 (26%)	1	2	34, 100, 164, 180	0
29	DG	176/177 (99%)	1.54	47 (26%)	1	2	23, 88, 156, 180	0
30	BH	149/149 (100%)	1.61	41 (27%)	1	2	22, 126, 180, 180	0
30	DH	149/149 (100%)	1.50	38 (25%)	1	2	30, 106, 167, 180	0
31	BJ	140/142 (98%)	2.61	78 (55%)	0	1	11, 88, 153, 180	0
31	DJ	140/142 (98%)	2.30	68 (48%)	0	1	7, 66, 148, 176	0
32	BK	121/123 (98%)	1.69	43 (35%)	1	1	13, 60, 118, 152	0
32	DK	121/123 (98%)	1.25	24 (19%)	3	3	5, 36, 92, 134	0
33	BL	144/144 (100%)	3.52	88 (61%)	0	1	15, 86, 167, 180	0
33	DL	144/144 (100%)	2.99	90 (62%)	0	1	5, 81, 156, 180	0
34	BM	136/136 (100%)	2.52	73 (53%)	0	1	13, 71, 175, 180	0
34	DM	136/136 (100%)	2.20	68 (50%)	0	1	11, 70, 164, 180	0
35	BN	127/127 (100%)	2.81	66 (51%)	0	1	17, 78, 168, 180	0
35	DN	127/127 (100%)	1.95	49 (38%)	1	1	5, 48, 159, 180	0
36	BO	117/117 (100%)	2.66	63 (53%)	0	1	26, 91, 167, 180	0
36	DO	117/117 (100%)	2.71	65 (55%)	0	1	5, 91, 172, 180	0
37	BP	114/115 (99%)	2.34	55 (48%)	0	1	18, 98, 172, 180	0
37	DP	114/115 (99%)	2.51	62 (54%)	0	1	7, 65, 166, 180	0
38	BQ	117/118 (99%)	2.18	52 (44%)	0	1	13, 66, 146, 174	0
38	DQ	117/118 (99%)	2.43	56 (47%)	0	1	6, 57, 158, 180	0
39	BR	103/103 (100%)	2.59	61 (59%)	0	1	24, 105, 167, 180	0
39	DR	103/103 (100%)	3.04	59 (57%)	0	1	25, 92, 157, 180	0
40	BS	110/110 (100%)	2.06	37 (33%)	1	1	9, 63, 133, 180	0
40	DS	110/110 (100%)	1.36	22 (20%)	3	3	5, 46, 137, 180	0
41	BT	99/100 (99%)	2.25	46 (46%)	0	1	25, 81, 162, 180	0
41	DT	99/100 (99%)	2.53	52 (52%)	0	1	15, 86, 168, 180	0
42	BU	102/104 (98%)	3.09	64 (62%)	0	1	17, 91, 169, 180	0
42	DU	102/104 (98%)	2.86	57 (55%)	0	1	30, 110, 171, 180	0
43	BW	84/85 (98%)	3.28	61 (72%)	0	0	10, 86, 159, 180	0
43	DW	84/85 (98%)	3.57	54 (64%)	0	0	16, 86, 168, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	1.93	30 (47%)	0	1	20, 97, 160, 180	0
44	DX	63/63 (100%)	2.56	31 (49%)	0	1	38, 110, 169, 180	0
45	BY	58/59 (98%)	2.45	31 (53%)	0	1	13, 86, 157, 180	0
45	DY	58/59 (98%)	2.23	24 (41%)	0	1	5, 79, 136, 150	0
46	BZ	70/70 (100%)	2.73	36 (51%)	0	1	19, 66, 145, 180	0
46	DZ	70/70 (100%)	3.23	47 (67%)	0	0	5, 68, 141, 180	0
47	B0	56/57 (98%)	2.67	35 (62%)	0	1	26, 95, 180, 180	0
47	D0	56/57 (98%)	2.46	30 (53%)	0	1	10, 70, 159, 177	0
48	B1	54/55 (98%)	1.74	19 (35%)	1	1	24, 97, 160, 180	0
48	D1	54/55 (98%)	1.88	23 (42%)	0	1	8, 82, 158, 180	0
49	B2	46/46 (100%)	2.95	26 (56%)	0	1	6, 51, 154, 174	0
49	D2	46/46 (100%)	3.07	33 (71%)	0	0	9, 55, 131, 150	0
50	B3	64/65 (98%)	3.45	43 (67%)	0	0	19, 61, 155, 180	0
50	D3	64/65 (98%)	3.25	41 (64%)	0	0	5, 61, 138, 178	0
51	B4	38/38 (100%)	3.86	28 (73%)	0	0	30, 102, 170, 180	0
51	D4	38/38 (100%)	4.23	30 (78%)	0	0	14, 111, 175, 180	0
52	BI	141/142 (99%)	2.08	65 (46%)	0	1	52, 152, 180, 180	0
52	DI	141/142 (99%)	1.79	53 (37%)	1	1	83, 160, 180, 180	0
All	All	20439/21086 (96%)	1.54	5495 (26%)	1	2	5, 67, 155, 180	0

The worst 5 of 5495 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	DB	2133	G	16.0
43	BW	45	HIS	15.2
33	DL	55	MET	13.9
36	DO	59	ALA	13.5
40	BS	93	ALA	13.1

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	AA	1626	1/1	-0.19	0.38	82,82,82,82	1
54	MG	DB	3093	1/1	-0.02	0.58	48,48,48,48	1
54	MG	AA	1650	1/1	0.50	0.18	133,133,133,133	0
54	MG	CA	1624	1/1	0.61	0.15	162,162,162,162	0
54	MG	AA	1631	1/1	0.62	0.19	143,143,143,143	0
54	MG	DB	3058	1/1	0.63	0.15	132,132,132,132	0
54	MG	BB	3082	1/1	0.66	0.25	63,63,63,63	0
54	MG	AA	1637	1/1	0.66	0.28	115,115,115,115	0
54	MG	CA	1616	1/1	0.67	0.17	153,153,153,153	0
53	KSG	AA	1601	26/26	0.74	0.21	53,53,53,53	0
54	MG	AA	1639	1/1	0.78	0.17	141,141,141,141	0
54	MG	CA	1649	1/1	0.79	0.20	86,86,86,86	0
54	MG	CA	1622	1/1	0.79	0.13	132,132,132,132	0
54	MG	BB	3100	1/1	0.79	0.26	37,37,37,37	1
54	MG	CA	1629	1/1	0.80	0.14	62,62,62,62	1
54	MG	DB	3064	1/1	0.80	0.42	66,66,66,66	1
53	KSG	CA	1601	26/26	0.80	0.24	53,53,53,53	0
54	MG	AA	1613	1/1	0.81	0.12	108,108,108,108	0
54	MG	BB	3041	1/1	0.81	0.12	47,47,47,47	0
54	MG	AA	1620	1/1	0.81	0.09	116,116,116,116	0
54	MG	AA	1609	1/1	0.81	0.14	119,119,119,119	0
54	MG	AA	1615	1/1	0.82	0.14	72,72,72,72	0
54	MG	AA	1621	1/1	0.82	0.11	96,96,96,96	0
54	MG	AA	1628	1/1	0.84	0.14	63,63,63,63	0
54	MG	CA	1640	1/1	0.84	0.09	139,139,139,139	0
54	MG	CA	1651	1/1	0.85	0.14	122,122,122,122	0
54	MG	BB	3047	1/1	0.85	0.24	128,128,128,128	0
54	MG	BB	3063	1/1	0.86	0.13	27,27,27,27	0
54	MG	CA	1637	1/1	0.86	0.10	107,107,107,107	0
54	MG	AA	1647	1/1	0.86	0.22	84,84,84,84	0
54	MG	BB	3028	1/1	0.86	0.21	66,66,66,66	0
54	MG	DB	3013	1/1	0.87	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3033	1/1	0.87	0.19	88,88,88,88	0
54	MG	AA	1616	1/1	0.87	0.08	86,86,86,86	0
54	MG	BB	3067	1/1	0.87	0.12	56,56,56,56	0
54	MG	BB	3034	1/1	0.87	0.13	42,42,42,42	0
54	MG	CA	1609	1/1	0.88	0.17	132,132,132,132	0
54	MG	AA	1642	1/1	0.88	0.17	107,107,107,107	0
54	MG	AA	1652	1/1	0.88	0.14	105,105,105,105	0
54	MG	DB	3081	1/1	0.88	0.16	110,110,110,110	0
54	MG	CA	1638	1/1	0.88	0.10	60,60,60,60	0
54	MG	DB	3106	1/1	0.88	0.07	7,7,7,7	0
54	MG	CA	1628	1/1	0.89	0.13	38,38,38,38	1
54	MG	BB	3008	1/1	0.89	0.12	82,82,82,82	0
54	MG	BB	3107	1/1	0.89	0.10	37,37,37,37	0
54	MG	DB	3059	1/1	0.89	0.11	75,75,75,75	0
54	MG	BB	3060	1/1	0.89	0.13	81,81,81,81	0
54	MG	AA	1625	1/1	0.89	0.15	81,81,81,81	0
54	MG	AA	1603	1/1	0.89	0.09	74,74,74,74	0
54	MG	AA	1633	1/1	0.89	0.11	92,92,92,92	0
54	MG	BB	3018	1/1	0.90	0.12	42,42,42,42	0
54	MG	BB	3007	1/1	0.90	0.10	57,57,57,57	0
54	MG	AA	1659	1/1	0.90	0.19	157,157,157,157	0
54	MG	DB	3060	1/1	0.91	0.11	105,105,105,105	0
54	MG	CA	1617	1/1	0.91	0.11	45,45,45,45	0
54	MG	AA	1624	1/1	0.91	0.23	25,25,25,25	1
54	MG	CA	1635	1/1	0.91	0.15	91,91,91,91	0
54	MG	AA	1649	1/1	0.91	0.09	102,102,102,102	0
54	MG	AA	1608	1/1	0.92	0.14	57,57,57,57	0
54	MG	CA	1627	1/1	0.92	0.17	114,114,114,114	0
54	MG	BB	3081	1/1	0.92	0.12	34,34,34,34	0
54	MG	AA	1658	1/1	0.92	0.12	113,113,113,113	0
54	MG	AA	1623	1/1	0.92	0.09	143,143,143,143	0
54	MG	DB	3082	1/1	0.92	0.21	61,61,61,61	0
54	MG	BB	3106	1/1	0.92	0.11	62,62,62,62	0
54	MG	DB	3049	1/1	0.92	0.07	79,79,79,79	0
54	MG	AA	1634	1/1	0.93	0.10	73,73,73,73	0
54	MG	BB	3092	1/1	0.93	0.10	56,56,56,56	0
54	MG	BB	3097	1/1	0.93	0.07	96,96,96,96	0
54	MG	AA	1636	1/1	0.93	0.13	83,83,83,83	0
54	MG	AA	1627	1/1	0.93	0.13	17,17,17,17	1
54	MG	AA	1618	1/1	0.93	0.10	102,102,102,102	0
54	MG	AA	1640	1/1	0.93	0.08	42,42,42,42	0
54	MG	DB	3075	1/1	0.93	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	AA	1654	1/1	0.93	0.08	81,81,81,81	0
54	MG	BB	3072	1/1	0.93	0.09	26,26,26,26	0
54	MG	BB	3033	1/1	0.93	0.12	113,113,113,113	0
54	MG	CA	1661	1/1	0.93	0.10	67,67,67,67	0
54	MG	DE	301	1/1	0.93	0.10	69,69,69,69	0
54	MG	BB	3109	1/1	0.94	0.09	33,33,33,33	0
54	MG	CA	1607	1/1	0.94	0.11	126,126,126,126	0
54	MG	BB	3089	1/1	0.94	0.12	82,82,82,82	0
54	MG	CA	1612	1/1	0.94	0.07	71,71,71,71	0
54	MG	AA	1657	1/1	0.94	0.12	83,83,83,83	0
54	MG	BB	3073	1/1	0.94	0.10	55,55,55,55	0
54	MG	DB	3076	1/1	0.94	0.10	69,69,69,69	0
54	MG	BB	3099	1/1	0.94	0.10	58,58,58,58	0
54	MG	BB	3064	1/1	0.94	0.10	71,71,71,71	0
54	MG	AA	1602	1/1	0.94	0.09	34,34,34,34	0
54	MG	DB	3015	1/1	0.94	0.12	69,69,69,69	0
54	MG	DB	3108	1/1	0.94	0.08	24,24,24,24	0
54	MG	BB	3087	1/1	0.94	0.08	53,53,53,53	0
54	MG	AA	1656	1/1	0.95	0.07	100,100,100,100	0
54	MG	DB	3034	1/1	0.95	0.09	84,84,84,84	0
54	MG	AA	1660	1/1	0.95	0.09	95,95,95,95	0
54	MG	DB	3052	1/1	0.95	0.16	42,42,42,42	0
54	MG	BB	3091	1/1	0.95	0.08	42,42,42,42	0
54	MG	AA	1646	1/1	0.95	0.10	103,103,103,103	0
54	MG	CA	1614	1/1	0.95	0.07	97,97,97,97	0
54	MG	AA	1655	1/1	0.95	0.08	67,67,67,67	0
54	MG	CA	1644	1/1	0.95	0.09	59,59,59,59	0
54	MG	BB	3010	1/1	0.95	0.15	74,74,74,74	0
54	MG	BB	3042	1/1	0.95	0.06	74,74,74,74	0
54	MG	CA	1659	1/1	0.95	0.10	88,88,88,88	0
54	MG	DB	3088	1/1	0.95	0.08	51,51,51,51	0
54	MG	CA	1623	1/1	0.95	0.07	77,77,77,77	0
54	MG	BB	3012	1/1	0.95	0.09	75,75,75,75	0
54	MG	BB	3048	1/1	0.95	0.08	39,39,39,39	0
54	MG	DB	3029	1/1	0.95	0.10	22,22,22,22	0
54	MG	DB	3027	1/1	0.96	0.07	37,37,37,37	0
54	MG	BB	3105	1/1	0.96	0.11	33,33,33,33	0
54	MG	BB	3051	1/1	0.96	0.06	74,74,74,74	0
54	MG	BB	3056	1/1	0.96	0.09	37,37,37,37	0
54	MG	DB	3035	1/1	0.96	0.08	24,24,24,24	0
54	MG	DB	3040	1/1	0.96	0.10	28,28,28,28	0
54	MG	CA	1631	1/1	0.96	0.07	21,21,21,21	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3086	1/1	0.96	0.20	94,94,94,94	0
54	MG	BB	3110	1/1	0.96	0.19	79,79,79,79	0
54	MG	AA	1645	1/1	0.96	0.07	97,97,97,97	0
54	MG	AA	1661	1/1	0.96	0.10	83,83,83,83	0
54	MG	DB	3061	1/1	0.96	0.08	48,48,48,48	0
54	MG	CA	1642	1/1	0.96	0.10	70,70,70,70	0
54	MG	DB	3071	1/1	0.96	0.08	27,27,27,27	0
54	MG	BB	3005	1/1	0.96	0.15	13,13,13,13	0
54	MG	CA	1646	1/1	0.96	0.07	94,94,94,94	0
54	MG	DB	3080	1/1	0.96	0.08	34,34,34,34	0
54	MG	BB	3043	1/1	0.96	0.10	63,63,63,63	0
54	MG	AA	1617	1/1	0.96	0.09	65,65,65,65	0
54	MG	DB	3083	1/1	0.96	0.07	18,18,18,18	0
54	MG	BB	3098	1/1	0.96	0.12	49,49,49,49	0
54	MG	DB	3090	1/1	0.96	0.08	106,106,106,106	0
54	MG	AA	1614	1/1	0.96	0.07	67,67,67,67	0
54	MG	DB	3094	1/1	0.96	0.14	33,33,33,33	0
54	MG	DB	3102	1/1	0.96	0.09	13,13,13,13	0
54	MG	DB	3103	1/1	0.96	0.12	61,61,61,61	0
54	MG	BB	3077	1/1	0.96	0.09	37,37,37,37	0
54	MG	BB	3102	1/1	0.96	0.06	34,34,34,34	0
54	MG	DB	3020	1/1	0.96	0.13	41,41,41,41	0
54	MG	DN	201	1/1	0.96	0.10	38,38,38,38	0
54	MG	DB	3024	1/1	0.97	0.06	27,27,27,27	0
54	MG	BB	3078	1/1	0.97	0.14	49,49,49,49	0
54	MG	BB	3014	1/1	0.97	0.07	33,33,33,33	0
54	MG	BB	3046	1/1	0.97	0.09	63,63,63,63	0
54	MG	BB	3017	1/1	0.97	0.09	54,54,54,54	0
54	MG	CA	1621	1/1	0.97	0.07	46,46,46,46	0
54	MG	AA	1622	1/1	0.97	0.03	16,16,16,16	0
54	MG	DB	3044	1/1	0.97	0.07	58,58,58,58	0
54	MG	BB	3019	1/1	0.97	0.10	22,22,22,22	0
54	MG	DB	3050	1/1	0.97	0.10	42,42,42,42	0
54	MG	BB	3090	1/1	0.97	0.06	65,65,65,65	0
54	MG	DB	3057	1/1	0.97	0.18	56,56,56,56	1
54	MG	BB	3053	1/1	0.97	0.06	36,36,36,36	0
54	MG	BB	3021	1/1	0.97	0.10	24,24,24,24	0
54	MG	BB	3096	1/1	0.97	0.05	39,39,39,39	0
54	MG	CA	1630	1/1	0.97	0.06	49,49,49,49	0
54	MG	DB	3062	1/1	0.97	0.09	24,24,24,24	0
54	MG	AA	1619	1/1	0.97	0.05	33,33,33,33	0
54	MG	DB	3069	1/1	0.97	0.05	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3062	1/1	0.97	0.11	34,34,34,34	0
54	MG	DB	3073	1/1	0.97	0.06	44,44,44,44	0
54	MG	BB	3030	1/1	0.97	0.06	45,45,45,45	0
54	MG	BB	3031	1/1	0.97	0.08	46,46,46,46	0
54	MG	BB	3065	1/1	0.97	0.08	47,47,47,47	0
54	MG	BB	3104	1/1	0.97	0.07	33,33,33,33	0
54	MG	BB	3066	1/1	0.97	0.07	42,42,42,42	0
54	MG	AA	1604	1/1	0.97	0.07	25,25,25,25	0
54	MG	CA	1648	1/1	0.97	0.06	39,39,39,39	0
54	MG	BB	3071	1/1	0.97	0.09	38,38,38,38	0
54	MG	BB	3108	1/1	0.97	0.07	22,22,22,22	0
54	MG	AA	1643	1/1	0.97	0.06	116,116,116,116	0
54	MG	AA	1644	1/1	0.97	0.11	81,81,81,81	0
54	MG	CA	1604	1/1	0.97	0.12	49,49,49,49	0
54	MG	BB	3076	1/1	0.97	0.06	43,43,43,43	0
54	MG	DB	3107	1/1	0.97	0.09	19,19,19,19	0
54	MG	DB	3016	1/1	0.97	0.08	25,25,25,25	0
54	MG	AA	1607	1/1	0.97	0.06	82,82,82,82	0
54	MG	DB	3023	1/1	0.97	0.06	44,44,44,44	0
54	MG	BB	3068	1/1	0.98	0.07	39,39,39,39	0
54	MG	DB	3014	1/1	0.98	0.06	28,28,28,28	0
54	MG	BB	3036	1/1	0.98	0.06	29,29,29,29	0
54	MG	BB	3038	1/1	0.98	0.03	82,82,82,82	0
54	MG	DB	3018	1/1	0.98	0.06	39,39,39,39	0
54	MG	BB	3039	1/1	0.98	0.07	26,26,26,26	0
54	MG	BB	3075	1/1	0.98	0.17	35,35,35,35	0
54	MG	BB	3013	1/1	0.98	0.07	36,36,36,36	0
54	MG	AA	1605	1/1	0.98	0.08	30,30,30,30	0
54	MG	DB	3028	1/1	0.98	0.09	29,29,29,29	0
54	MG	BB	3016	1/1	0.98	0.12	19,19,19,19	0
54	MG	CA	1613	1/1	0.98	0.08	63,63,63,63	0
54	MG	BB	3079	1/1	0.98	0.05	32,32,32,32	0
54	MG	BB	3080	1/1	0.98	0.05	42,42,42,42	0
54	MG	AA	1641	1/1	0.98	0.04	72,72,72,72	0
54	MG	AA	1611	1/1	0.98	0.05	57,57,57,57	0
54	MG	DB	3046	1/1	0.98	0.11	18,18,18,18	0
54	MG	DB	3047	1/1	0.98	0.06	29,29,29,29	0
54	MG	BB	3083	1/1	0.98	0.07	25,25,25,25	0
54	MG	BB	3084	1/1	0.98	0.06	19,19,19,19	0
54	MG	DB	3051	1/1	0.98	0.09	57,57,57,57	0
54	MG	BB	3001	1/1	0.98	0.06	28,28,28,28	0
54	MG	DB	3053	1/1	0.98	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	DB	3056	1/1	0.98	0.10	67,67,67,67	0
54	MG	BB	3004	1/1	0.98	0.05	39,39,39,39	0
54	MG	BB	3088	1/1	0.98	0.11	25,25,25,25	0
54	MG	BB	3052	1/1	0.98	0.05	27,27,27,27	0
54	MG	BB	3022	1/1	0.98	0.06	55,55,55,55	0
54	MG	BB	3054	1/1	0.98	0.10	77,77,77,77	0
54	MG	CA	1632	1/1	0.98	0.07	34,34,34,34	0
54	MG	CA	1634	1/1	0.98	0.07	46,46,46,46	0
54	MG	DB	3068	1/1	0.98	0.05	49,49,49,49	0
54	MG	BB	3055	1/1	0.98	0.08	19,19,19,19	0
54	MG	BB	3094	1/1	0.98	0.08	16,16,16,16	0
54	MG	BB	3023	1/1	0.98	0.07	27,27,27,27	0
54	MG	BB	3058	1/1	0.98	0.05	33,33,33,33	0
54	MG	BB	3024	1/1	0.98	0.09	22,22,22,22	0
54	MG	CA	1643	1/1	0.98	0.07	62,62,62,62	0
54	MG	BB	3026	1/1	0.98	0.05	25,25,25,25	0
54	MG	AA	1635	1/1	0.98	0.04	75,75,75,75	0
54	MG	CA	1647	1/1	0.98	0.08	40,40,40,40	0
54	MG	DB	3085	1/1	0.98	0.12	64,64,64,64	0
54	MG	DB	3087	1/1	0.98	0.09	40,40,40,40	0
54	MG	BB	3101	1/1	0.98	0.06	14,14,14,14	0
54	MG	AA	1612	1/1	0.98	0.07	52,52,52,52	0
54	MG	DB	3091	1/1	0.98	0.08	39,39,39,39	0
54	MG	CA	1650	1/1	0.98	0.09	67,67,67,67	0
54	MG	AA	1629	1/1	0.98	0.11	62,62,62,62	0
54	MG	DB	3095	1/1	0.98	0.07	44,44,44,44	0
54	MG	DB	3099	1/1	0.98	0.07	11,11,11,11	0
54	MG	DB	3101	1/1	0.98	0.04	30,30,30,30	0
54	MG	CA	1657	1/1	0.98	0.10	51,51,51,51	0
54	MG	AA	1638	1/1	0.98	0.11	88,88,88,88	0
54	MG	DB	3104	1/1	0.98	0.10	44,44,44,44	0
54	MG	CA	1660	1/1	0.98	0.12	27,27,27,27	0
54	MG	AA	1606	1/1	0.98	0.05	28,28,28,28	0
54	MG	CA	1663	1/1	0.98	0.07	20,20,20,20	0
54	MG	DB	3109	1/1	0.98	0.10	57,57,57,57	0
54	MG	DB	3002	1/1	0.98	0.06	20,20,20,20	0
54	MG	DB	3007	1/1	0.98	0.06	15,15,15,15	0
54	MG	AA	1632	1/1	0.99	0.07	44,44,44,44	0
54	MG	DB	3025	1/1	0.99	0.15	20,20,20,20	0
54	MG	DB	3026	1/1	0.99	0.11	30,30,30,30	0
54	MG	BB	3049	1/1	0.99	0.05	12,12,12,12	0
54	MG	BB	3050	1/1	0.99	0.03	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3006	1/1	0.99	0.05	20,20,20,20	0
54	MG	DB	3031	1/1	0.99	0.04	40,40,40,40	0
54	MG	DB	3032	1/1	0.99	0.08	29,29,29,29	0
54	MG	BB	3032	1/1	0.99	0.04	31,31,31,31	0
54	MG	AA	1630	1/1	0.99	0.04	20,20,20,20	0
54	MG	CA	1633	1/1	0.99	0.03	50,50,50,50	0
54	MG	DB	3036	1/1	0.99	0.09	25,25,25,25	0
54	MG	DB	3038	1/1	0.99	0.04	33,33,33,33	0
54	MG	AA	1651	1/1	0.99	0.05	64,64,64,64	0
54	MG	DB	3042	1/1	0.99	0.05	5,5,5,5	0
54	MG	BB	3009	1/1	0.99	0.04	35,35,35,35	0
54	MG	DB	3045	1/1	0.99	0.04	45,45,45,45	0
54	MG	CA	1636	1/1	0.99	0.08	13,13,13,13	0
54	MG	AA	1648	1/1	0.99	0.08	31,31,31,31	0
54	MG	BB	3057	1/1	0.99	0.10	19,19,19,19	0
54	MG	CA	1639	1/1	0.99	0.04	41,41,41,41	0
54	MG	BB	3002	1/1	0.99	0.05	9,9,9,9	0
54	MG	CA	1641	1/1	0.99	0.07	40,40,40,40	0
54	MG	BB	3040	1/1	0.99	0.07	18,18,18,18	0
54	MG	DB	3054	1/1	0.99	0.05	32,32,32,32	0
54	MG	BB	3061	1/1	0.99	0.04	33,33,33,33	0
54	MG	CA	1603	1/1	0.99	0.10	32,32,32,32	0
54	MG	CA	1645	1/1	0.99	0.05	28,28,28,28	0
54	MG	BB	3085	1/1	0.99	0.06	67,67,67,67	0
54	MG	CA	1605	1/1	0.99	0.05	37,37,37,37	0
54	MG	CA	1606	1/1	0.99	0.08	30,30,30,30	0
54	MG	BB	3003	1/1	0.99	0.04	23,23,23,23	0
54	MG	CA	1608	1/1	0.99	0.04	31,31,31,31	0
54	MG	DB	3065	1/1	0.99	0.06	25,25,25,25	0
54	MG	DB	3066	1/1	0.99	0.05	12,12,12,12	0
54	MG	DB	3067	1/1	0.99	0.17	11,11,11,11	0
54	MG	BB	3025	1/1	0.99	0.12	67,67,67,67	0
54	MG	CA	1652	1/1	0.99	0.10	20,20,20,20	0
54	MG	DB	3070	1/1	0.99	0.04	60,60,60,60	0
54	MG	CA	1653	1/1	0.99	0.03	48,48,48,48	0
54	MG	CA	1654	1/1	0.99	0.10	32,32,32,32	0
54	MG	CA	1655	1/1	0.99	0.05	26,26,26,26	0
54	MG	CA	1656	1/1	0.99	0.03	60,60,60,60	0
54	MG	DB	3077	1/1	0.99	0.05	41,41,41,41	0
54	MG	CA	1610	1/1	0.99	0.04	61,61,61,61	0
54	MG	CA	1658	1/1	0.99	0.04	18,18,18,18	0
54	MG	AA	1653	1/1	0.99	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	BB	3044	1/1	0.99	0.04	39,39,39,39	0
54	MG	BB	3045	1/1	0.99	0.03	40,40,40,40	0
54	MG	DB	3086	1/1	0.99	0.10	25,25,25,25	0
54	MG	CA	1662	1/1	0.99	0.03	38,38,38,38	0
54	MG	CA	1615	1/1	0.99	0.06	54,54,54,54	0
54	MG	DB	3089	1/1	0.99	0.14	28,28,28,28	0
54	MG	DB	3001	1/1	0.99	0.08	5,5,5,5	0
54	MG	BB	3027	1/1	0.99	0.04	29,29,29,29	0
54	MG	DB	3092	1/1	0.99	0.03	16,16,16,16	0
54	MG	DB	3003	1/1	0.99	0.06	8,8,8,8	0
54	MG	DB	3004	1/1	0.99	0.12	38,38,38,38	0
54	MG	BB	3015	1/1	0.99	0.04	23,23,23,23	0
54	MG	DB	3097	1/1	0.99	0.08	19,19,19,19	0
54	MG	DB	3098	1/1	0.99	0.05	9,9,9,9	0
54	MG	DB	3009	1/1	0.99	0.03	10,10,10,10	0
54	MG	DB	3100	1/1	0.99	0.07	6,6,6,6	0
54	MG	DB	3012	1/1	0.99	0.10	6,6,6,6	0
54	MG	CA	1620	1/1	0.99	0.11	32,32,32,32	0
54	MG	BB	3093	1/1	0.99	0.16	5,5,5,5	1
54	MG	BB	3069	1/1	0.99	0.04	8,8,8,8	0
54	MG	DB	3105	1/1	0.99	0.05	24,24,24,24	0
54	MG	BB	3095	1/1	0.99	0.04	48,48,48,48	0
54	MG	DB	3017	1/1	0.99	0.10	22,22,22,22	0
54	MG	BB	3070	1/1	0.99	0.07	55,55,55,55	0
54	MG	CA	1625	1/1	0.99	0.04	24,24,24,24	0
54	MG	DB	3021	1/1	0.99	0.06	25,25,25,25	0
54	MG	CA	1626	1/1	0.99	0.05	17,17,17,17	0
54	MG	DB	3078	1/1	1.00	0.02	5,5,5,5	0
54	MG	DB	3079	1/1	1.00	0.03	7,7,7,7	0
54	MG	DB	3048	1/1	1.00	0.02	7,7,7,7	0
54	MG	BB	3011	1/1	1.00	0.05	9,9,9,9	0
54	MG	BB	3103	1/1	1.00	0.07	11,11,11,11	0
54	MG	DB	3005	1/1	1.00	0.03	6,6,6,6	0
54	MG	DB	3084	1/1	1.00	0.03	18,18,18,18	0
54	MG	DB	3006	1/1	1.00	0.02	16,16,16,16	0
54	MG	BB	3029	1/1	1.00	0.02	7,7,7,7	0
54	MG	DB	3008	1/1	1.00	0.10	39,39,39,39	0
54	MG	DB	3055	1/1	1.00	0.08	20,20,20,20	0
54	MG	BB	3020	1/1	1.00	0.03	38,38,38,38	0
54	MG	DB	3030	1/1	1.00	0.06	11,11,11,11	0
54	MG	DB	3010	1/1	1.00	0.03	8,8,8,8	0
54	MG	DB	3011	1/1	1.00	0.09	23,23,23,23	0

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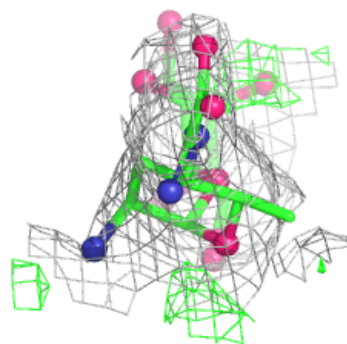
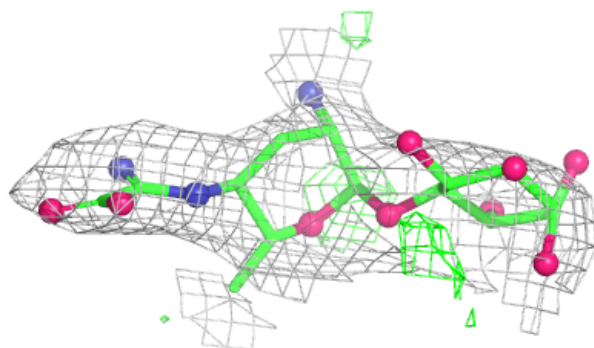
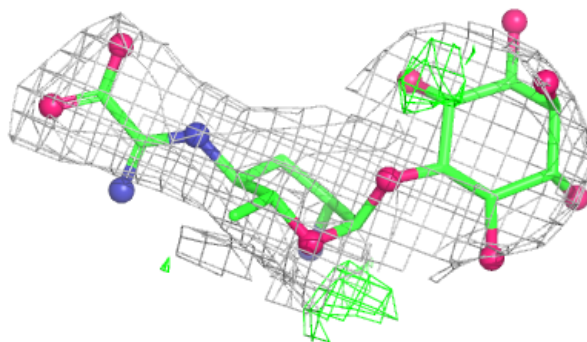
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	CA	1618	1/1	1.00	0.04	26,26,26,26	0
54	MG	CA	1619	1/1	1.00	0.03	9,9,9,9	0
54	MG	BB	3059	1/1	1.00	0.03	16,16,16,16	0
54	MG	DB	3096	1/1	1.00	0.10	31,31,31,31	0
54	MG	DB	3063	1/1	1.00	0.03	42,42,42,42	0
54	MG	BB	3074	1/1	1.00	0.05	7,7,7,7	0
54	MG	DB	3037	1/1	1.00	0.02	8,8,8,8	0
54	MG	BB	3035	1/1	1.00	0.06	25,25,25,25	0
54	MG	DB	3039	1/1	1.00	0.06	5,5,5,5	0
54	MG	AA	1610	1/1	1.00	0.09	10,10,10,10	0
54	MG	DB	3041	1/1	1.00	0.05	29,29,29,29	0
54	MG	CA	1611	1/1	1.00	0.02	43,43,43,43	0
54	MG	DB	3043	1/1	1.00	0.03	7,7,7,7	0
54	MG	DB	3072	1/1	1.00	0.06	5,5,5,5	0
54	MG	DB	3019	1/1	1.00	0.03	8,8,8,8	0
54	MG	DB	3074	1/1	1.00	0.05	12,12,12,12	0
54	MG	BB	3037	1/1	1.00	0.07	21,21,21,21	0
54	MG	CA	1602	1/1	1.00	0.06	8,8,8,8	0
54	MG	DB	3022	1/1	1.00	0.03	5,5,5,5	0

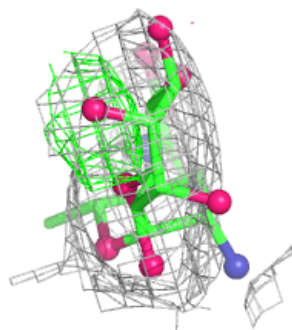
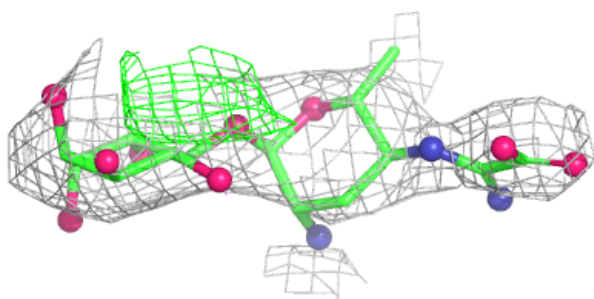
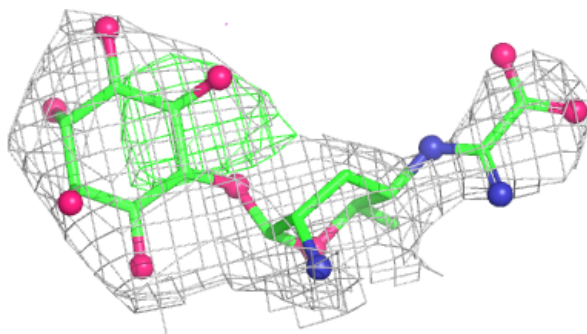
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KSG AA 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around KSG CA 1601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.