wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2023 – 02:43 AM EDT

PDB ID	:	4V52
Title	:	Crystal structure of the bacterial ribosome from Escherichia coli in complex with neomycin.
Authors	:	Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on	:	2007-06-15
Resolution	:	3.21 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 (i) 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 (i)) were used in the production of this report:

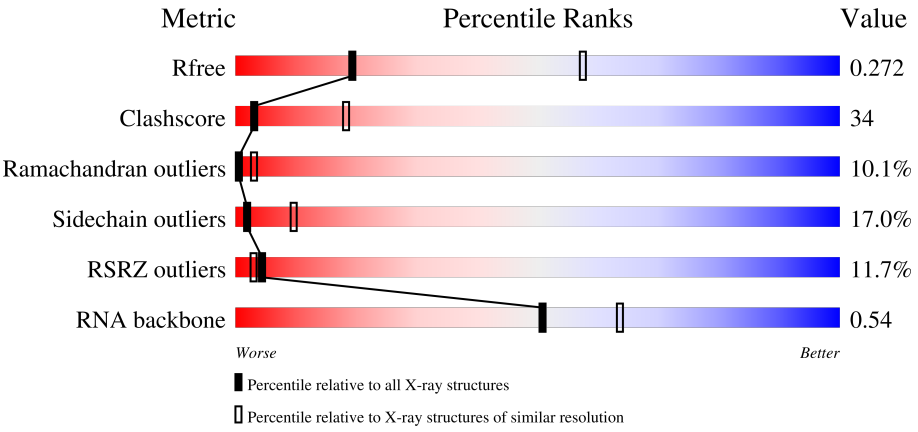
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1542	28% 60% 12%
1	CA	1542	28% 60% 11%
2	AC	232	15% 32% 44% 13% 11%

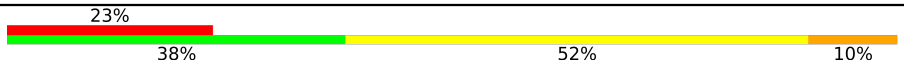
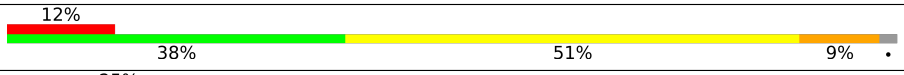
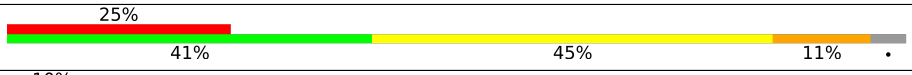
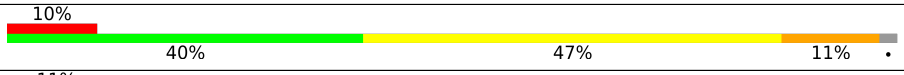
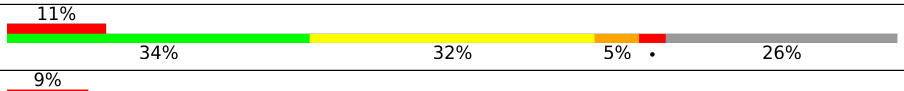
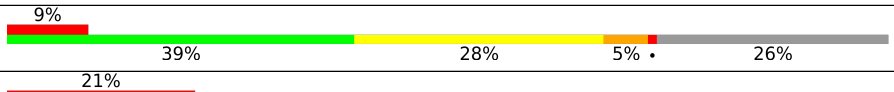
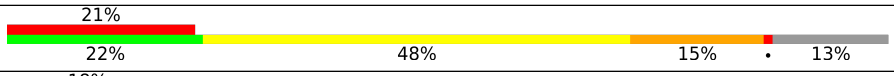
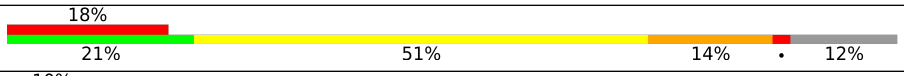
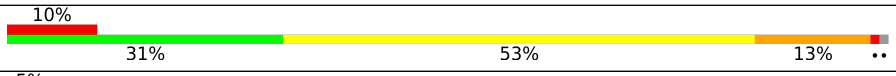
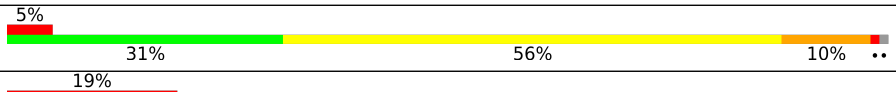
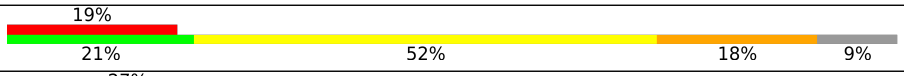
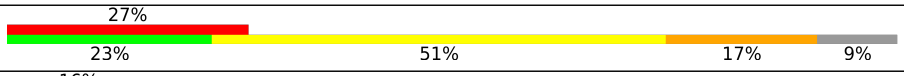
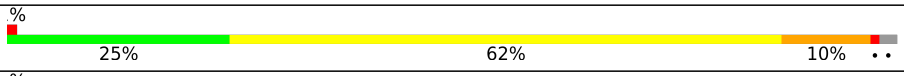
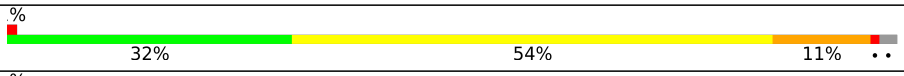
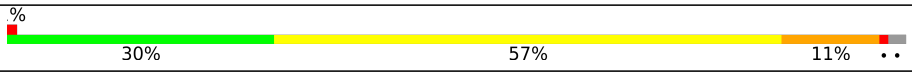
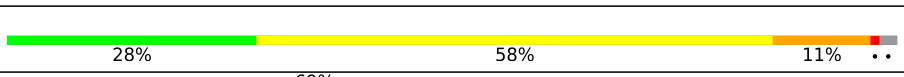
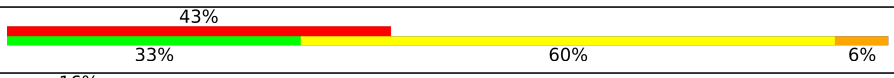
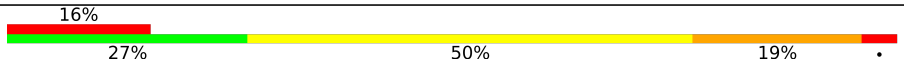
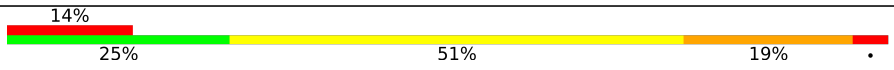
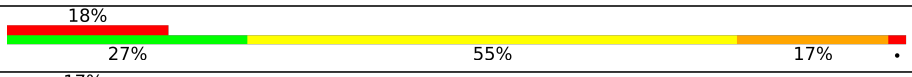
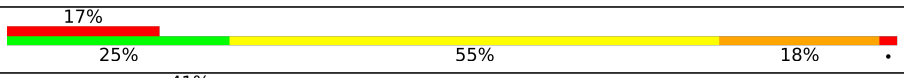
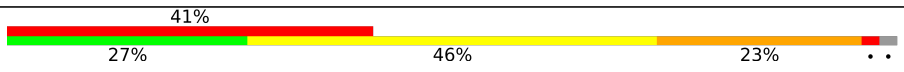
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	CC	232	12% 31% 46% 12% 11%
3	AD	205	25% 36% 50% 13%
3	CD	205	14% 39% 47% 13%
4	AE	166	9% 33% 50% 7% 10%
4	CE	166	20% 32% 51% 8% 10%
5	AF	135	23% 24% 39% 9% 26%
5	CF	135	11% 24% 39% 9% 26%
6	AG	178	13% 32% 43% 8% 16%
6	CG	178	5% 29% 48% 8% 15%
7	AH	129	31% 38% 53% 9%
7	CH	129	13% 38% 54% 8%
8	AI	129	19% 29% 53% 15%
8	CI	129	12% 33% 51% 14%
9	AJ	103	18% 26% 50% 18% 5%
9	CJ	103	21% 26% 50% 18% 5%
10	AK	128	5% 32% 50% 8% 9%
10	CK	128	2% 32% 48% 9% 9%
11	AL	123	15% 45% 43% 12%
11	CL	123	5% 45% 43% 12%
12	AM	117	14% 24% 56% 17%
12	CM	117	14% 22% 58% 16%
13	AN	100	8% 26% 52% 18%
13	CN	100	12% 25% 50% 21%
14	AO	89	24% 43% 48% 8%
14	CO	89	3% 42% 49% 8%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	DK	123	21% 24% 48% 24%
28	BP	114	46% 25% 54% 18%
28	DP	114	11% 25% 54% 18%
29	BE	201	32% 29% 56% 13%
29	DE	201	18% 31% 54% 13%
30	BY	58	19% 28% 53% 17%
30	DY	58	16% 28% 53% 17%
31	B0	56	14% 45% 38% 16%
31	D0	56	7% 41% 39% 16%
32	B4	38	16% 32% 42% 24%
32	D4	38	32% 39% 26%
33	B1	54	37% 15% 63% 13% 7%
33	D1	54	20% 19% 61% 11% 7%
34	B3	64	23% 30% 58% 12%
34	D3	64	14% 31% 56% 12%
35	BV	94	19% 31% 56% 13%
35	DV	94	24% 26% 62% 13%
36	B2	46	7% 39% 46% 15%
36	D2	46	4% 35% 50% 15%
37	BL	144	18% 25% 54% 20%
37	DL	144	26% 26% 53% 20%
38	BM	136	14% 27% 54% 18%
38	DM	136	10% 29% 54% 17%
39	BX	63	40% 21% 56% 24%
39	DX	63	8% 17% 59% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	BH	149	70% 13% 50% 29% 8%
40	DH	149	42% 24% 50% 21% 5%
41	BJ	142	23% 21% 63% 13%
41	DJ	142	9% 20% 63% 15%
42	BN	127	18% 17% 67% 8% 6%
42	DN	127	4% 17% 65% 10% 6%
43	BO	117	24% 36% 50% 13%
43	DO	117	6% 35% 49% 15%
44	BQ	117	7% 30% 57% 9%
44	DQ	117	10% 30% 56% 10%
45	BS	110	36% 27% 54% 17%
45	DS	110	29% 27% 55% 16%
46	BU	103	31% 17% 56% 22%
46	DU	103	8% 18% 55% 22%
47	BF	178	29% 20% 52% 26%
47	DF	178	34% 20% 53% 25%
48	BG	176	30% 23% 56% 18%
48	DG	176	24% 22% 57% 19%
49	BR	103	13% 26% 57% 17%
49	DR	103	21% 25% 59% 16%
50	BT	100	17% 21% 52% 18% 7%
50	DT	100	25% 21% 51% 19% 7%
51	BZ	78	19% 21% 63% 12%
51	DZ	78	9% 22% 60% 13%
52	BW	84	30% 8% 57% 25% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	DW	84	13% 11% 54% 26% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	NMY	BB	3001	-	-	-	X
53	NMY	DB	3001	-	-	-	X
54	MG	DB	3059	-	-	-	X

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 284172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

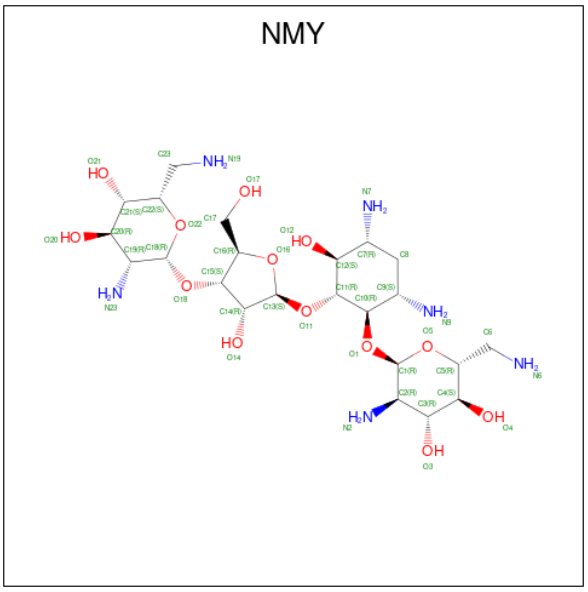
- Molecule 51 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 53 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	AA	1	Total C N O 42 23 6 13	0	0
53	BB	1	Total C N O 42 23 6 13	0	0
53	CA	1	Total C N O 42 23 6 13	0	0
53	DB	1	Total C N O 42 23 6 13	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	291	Total O 291 291	0	0
56	AL	4	Total O 4 4	0	0
56	AN	4	Total O 4 4	0	0
56	AT	1	Total O 1 1	0	0
56	BB	497	Total O 497 497	0	0
56	BC	5	Total O 5 5	0	0
56	BE	1	Total O 1 1	0	0
56	BL	1	Total O 1 1	0	0
56	BN	1	Total O 1 1	0	0
56	BR	1	Total O 1 1	0	0
56	CA	298	Total O 298 298	0	0
56	CE	3	Total O 3 3	0	0
56	CL	2	Total O 2 2	0	0
56	CN	4	Total O 4 4	0	0
56	CP	1	Total O 1 1	0	0
56	CT	1	Total O 1 1	0	0
56	DB	502	Total O 502 502	0	0
56	DC	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

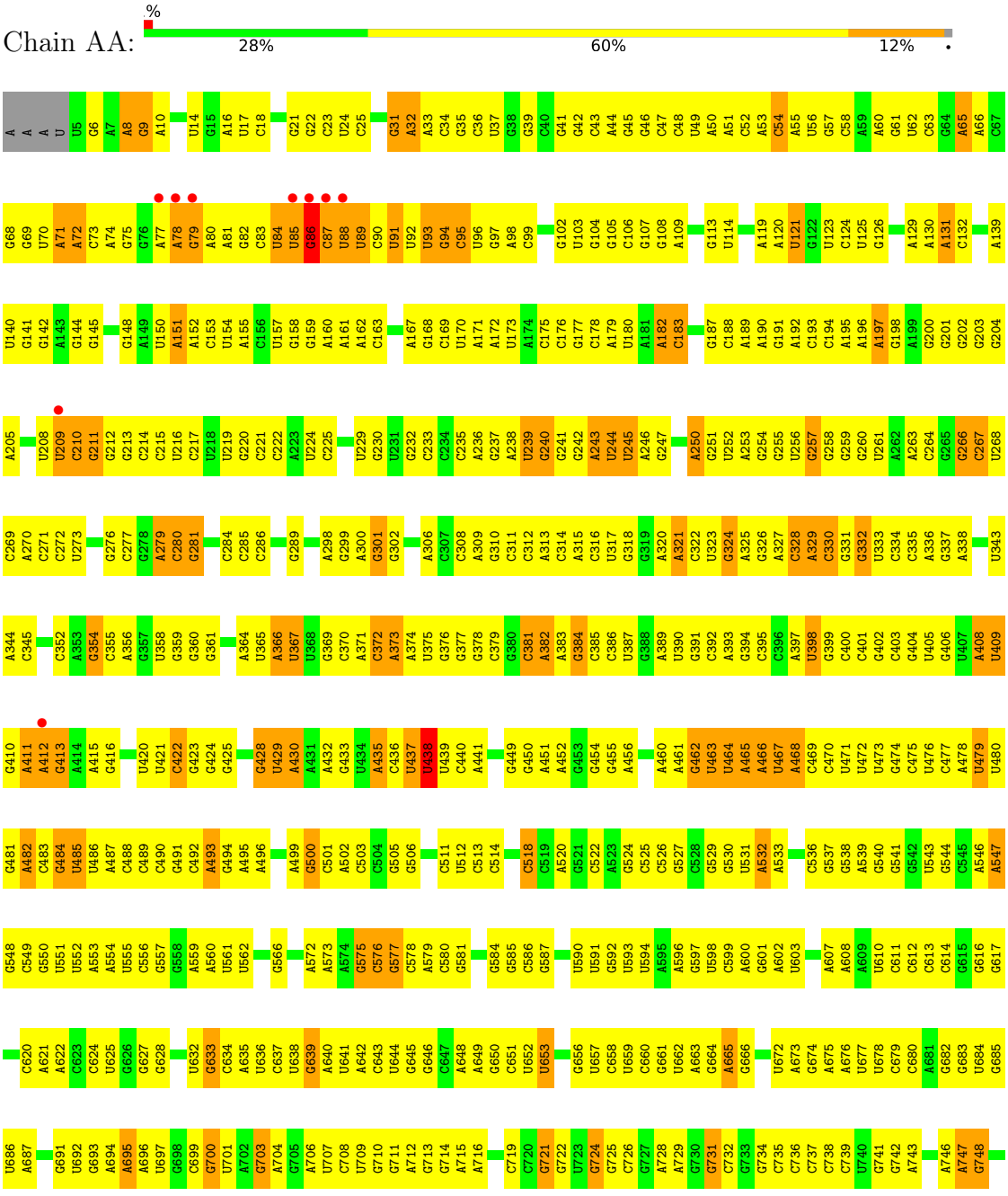
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DE	1	Total O 1 1	0	0
56	DL	2	Total O 2 2	0	0
56	DR	1	Total O 1 1	0	0

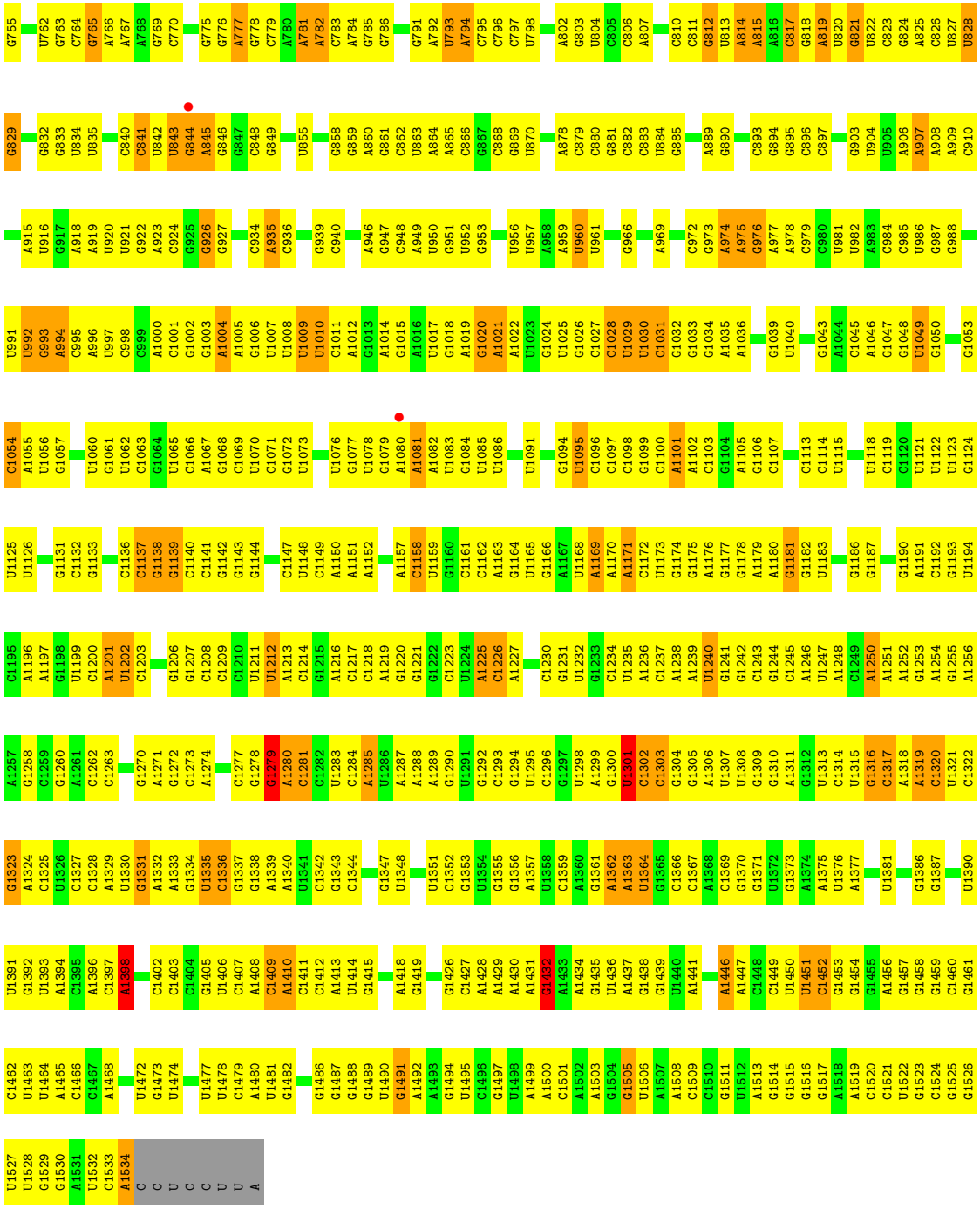
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

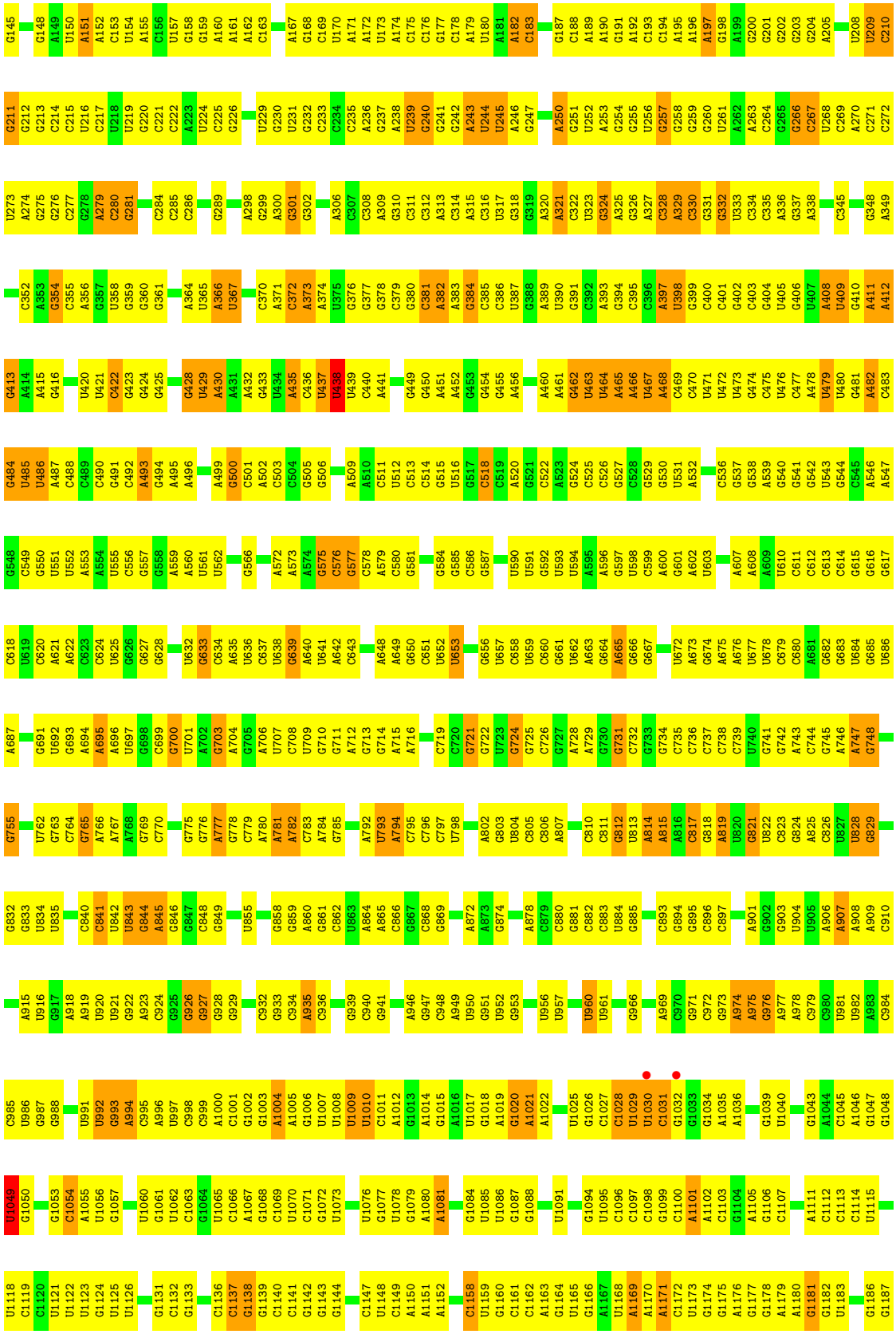
Chain AA:

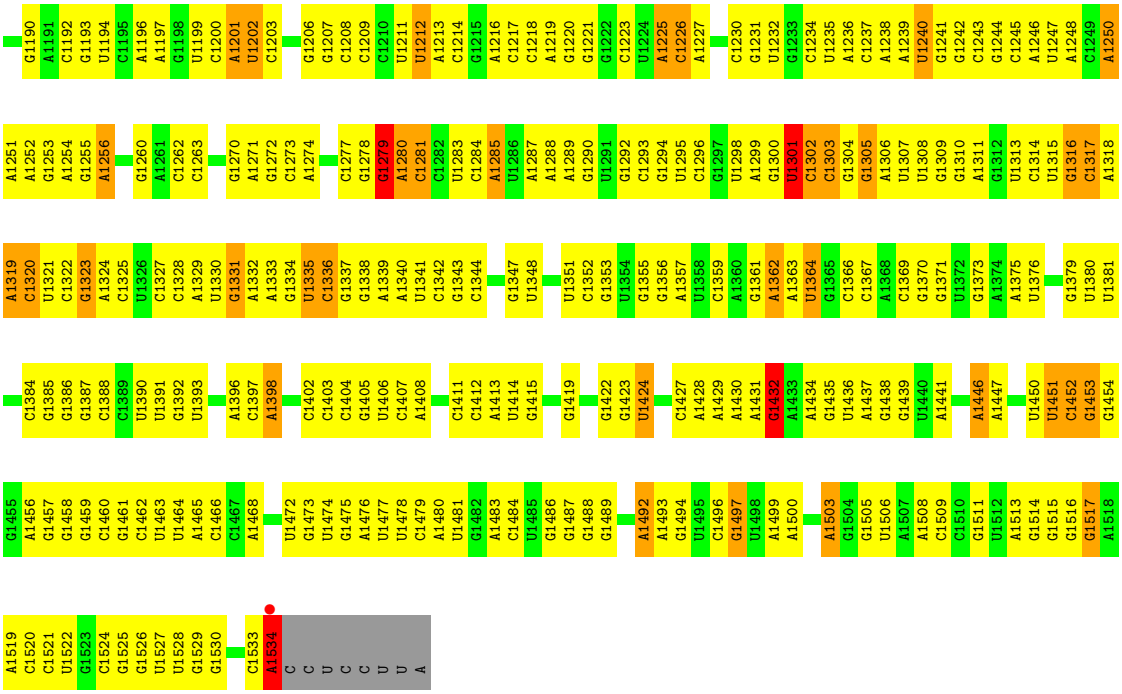




• Molecule 1: 16S rRNA

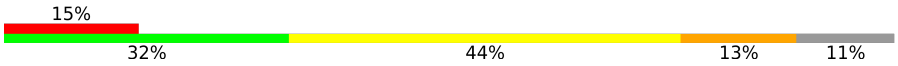
Chain CA:

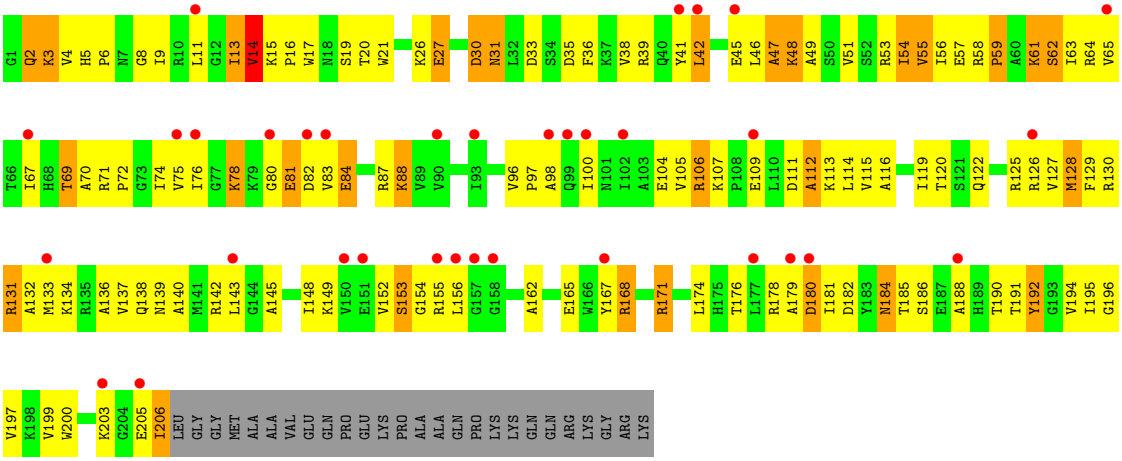




• Molecule 2: 30S ribosomal protein S3

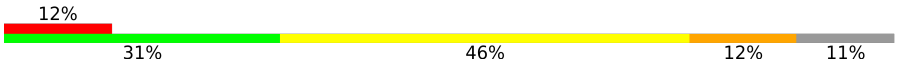
Chain AC:

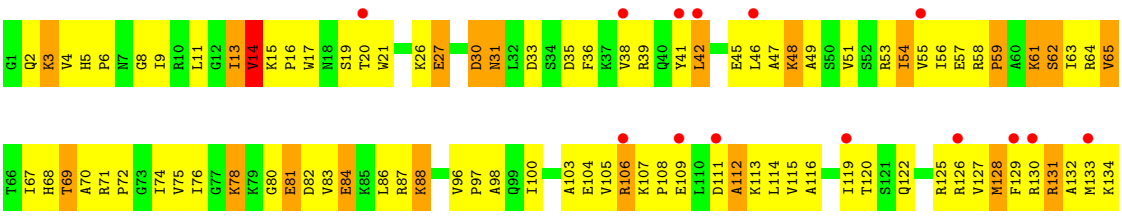


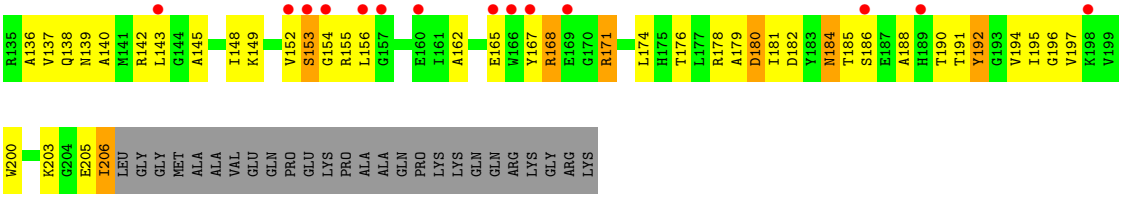


• Molecule 2: 30S ribosomal protein S3

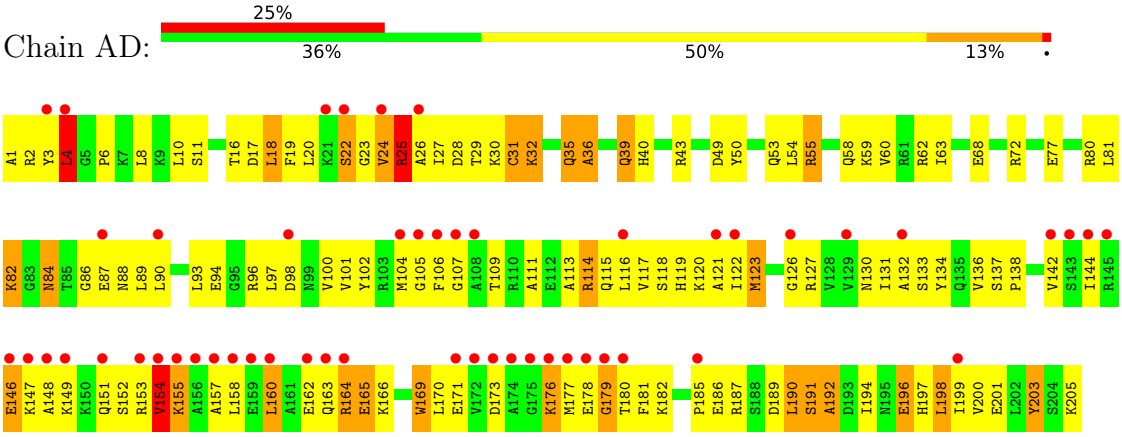
Chain CC:



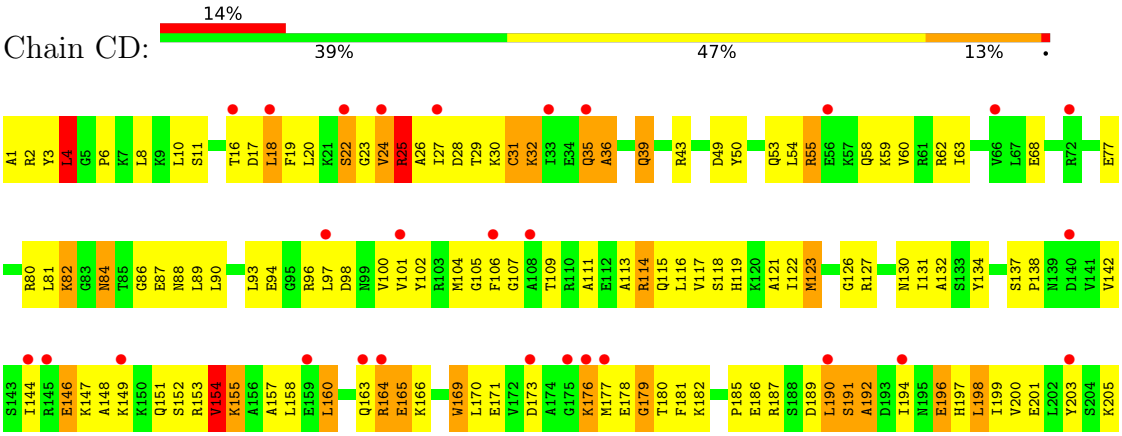




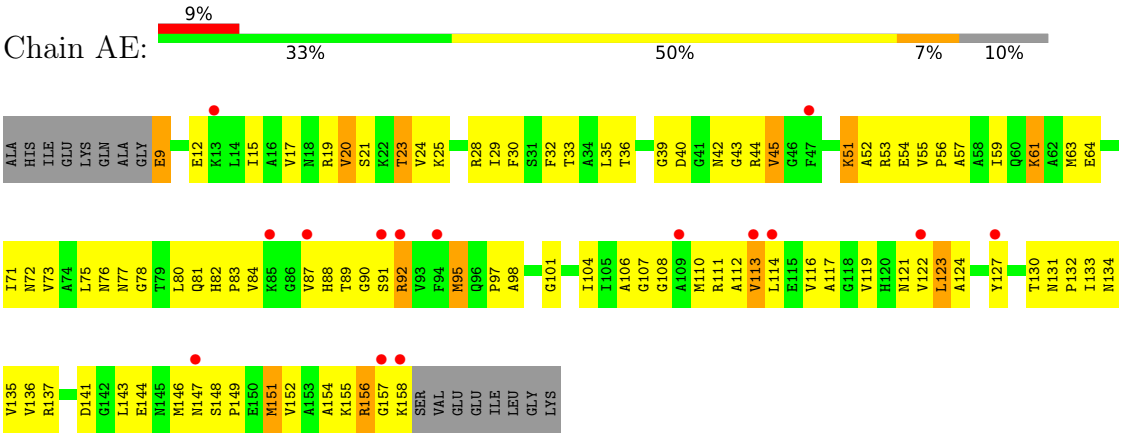
• Molecule 3: 30S ribosomal protein S4



• Molecule 3: 30S ribosomal protein S4

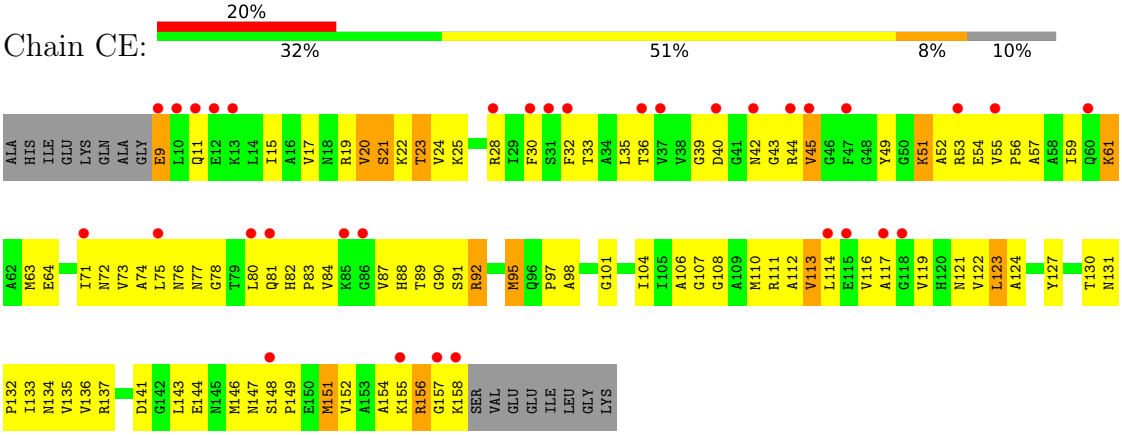


• Molecule 4: 30S ribosomal protein S5



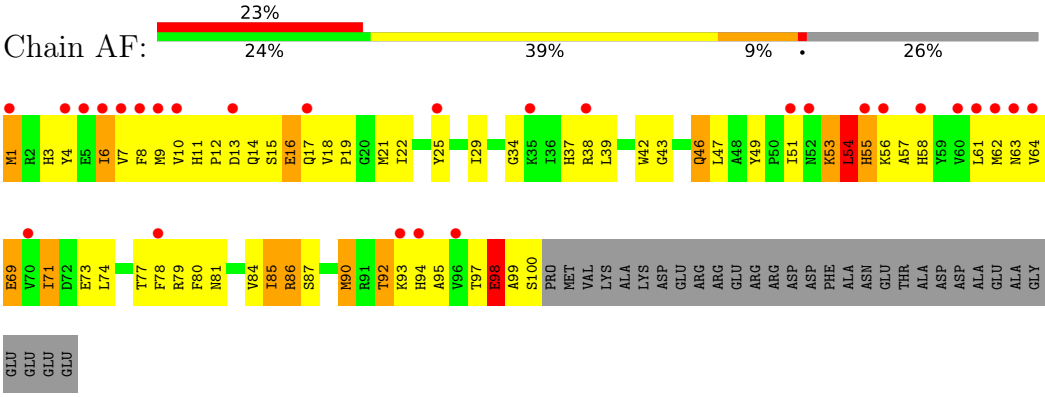
• Molecule 4: 30S ribosomal protein S5

Chain CE:



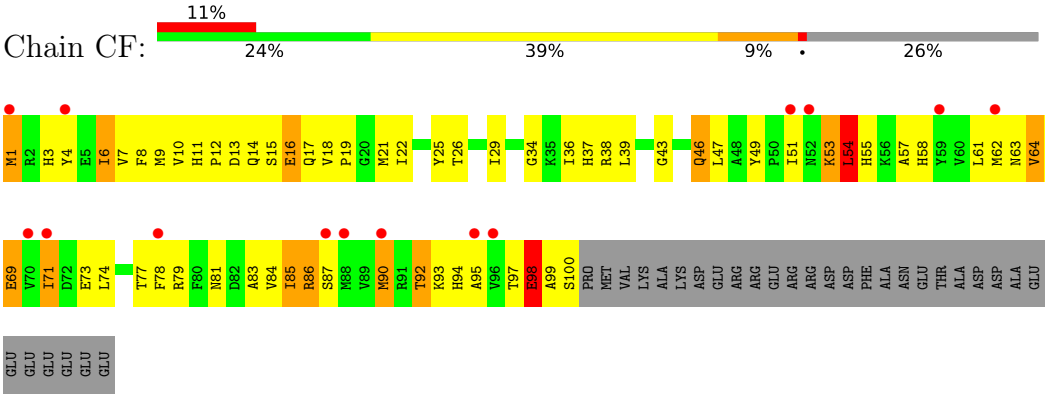
• Molecule 5: 30S ribosomal protein S6

Chain AF:



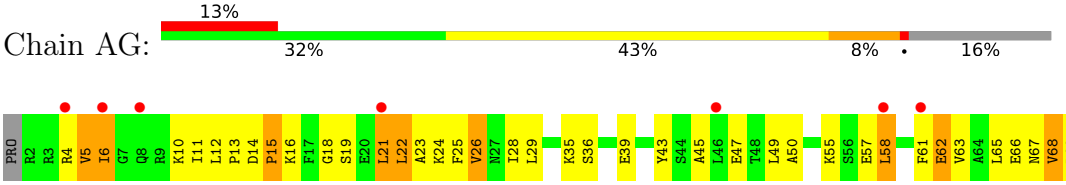
• Molecule 5: 30S ribosomal protein S6

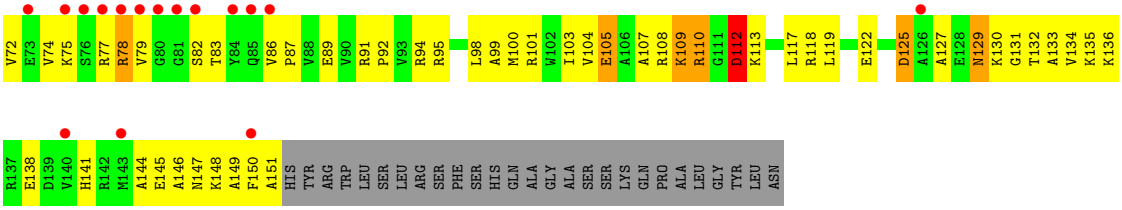
Chain CF:



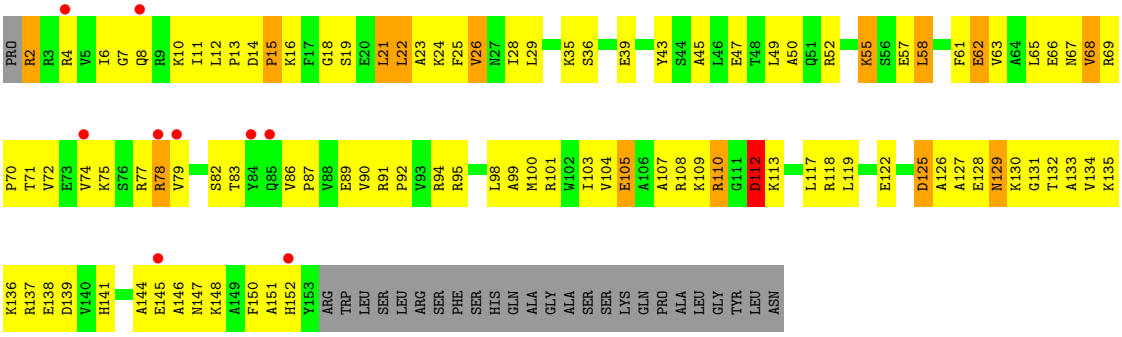
• Molecule 6: 30S ribosomal protein S7

Chain AG:

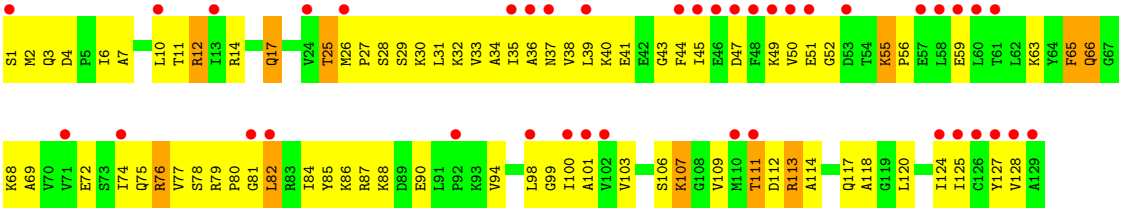




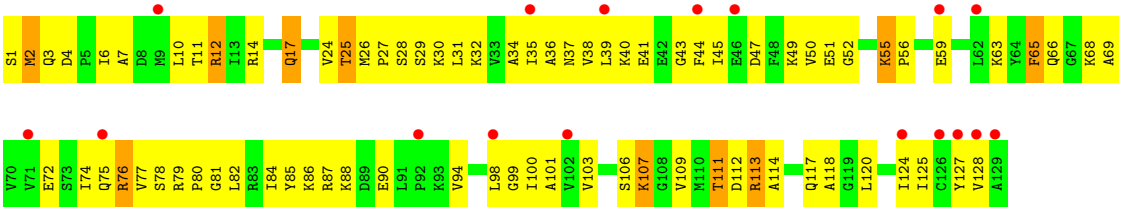
• Molecule 6: 30S ribosomal protein S7



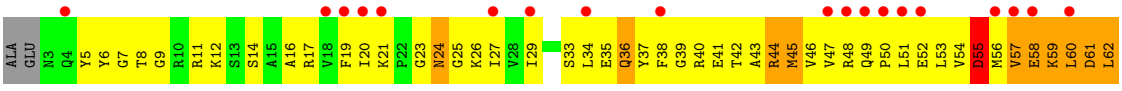
• Molecule 7: 30S ribosomal protein S8

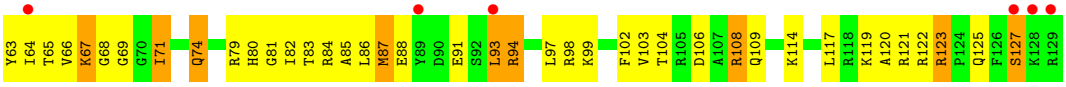


• Molecule 7: 30S ribosomal protein S8

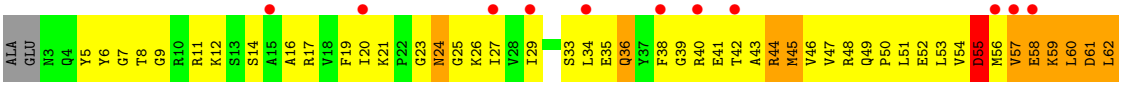


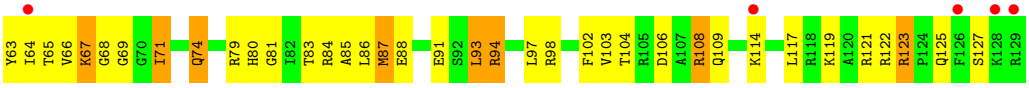
• Molecule 8: 30S ribosomal protein S9



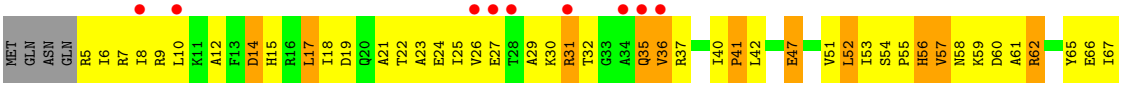


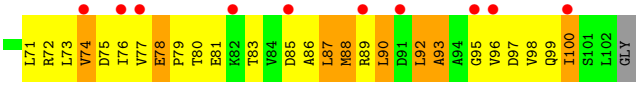
• Molecule 8: 30S ribosomal protein S9



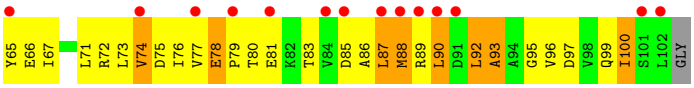


• Molecule 9: 30S ribosomal protein S10

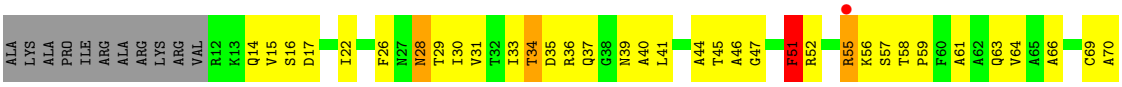


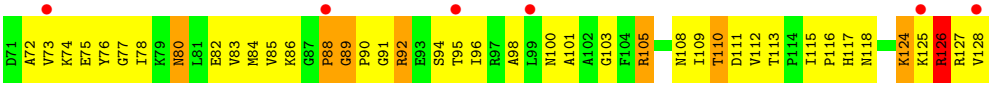


• Molecule 9: 30S ribosomal protein S10

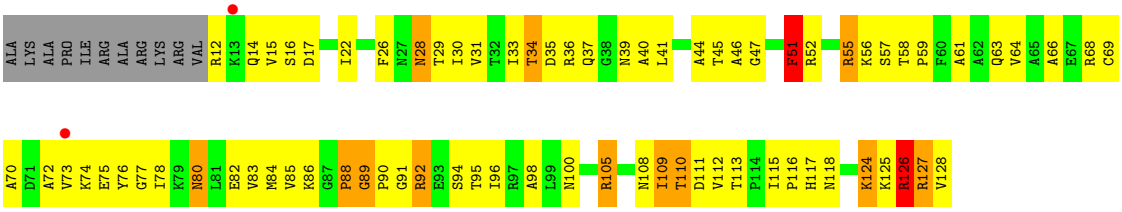


• Molecule 10: 30S ribosomal protein S11



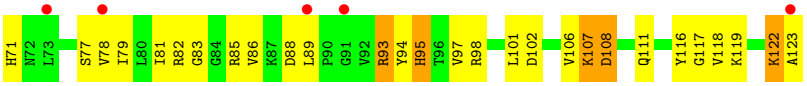


• Molecule 10: 30S ribosomal protein S11



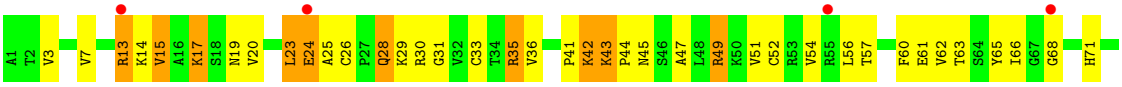
• Molecule 11: 30S ribosomal protein S12

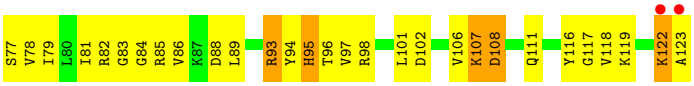
Chain AL:



• Molecule 11: 30S ribosomal protein S12

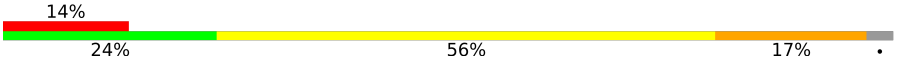
Chain CL:

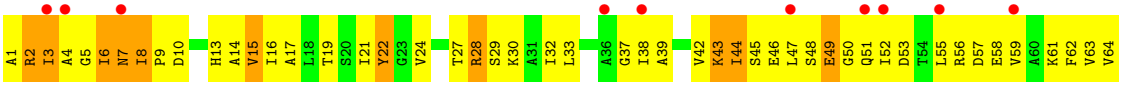


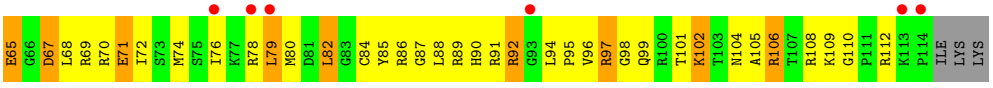


• Molecule 12: 30S ribosomal protein S13

Chain AM:

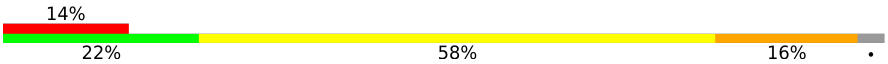


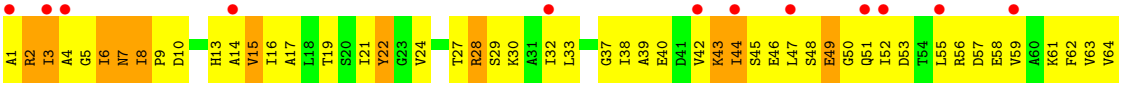


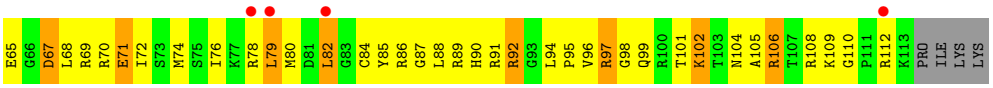


• Molecule 12: 30S ribosomal protein S13

Chain CM:

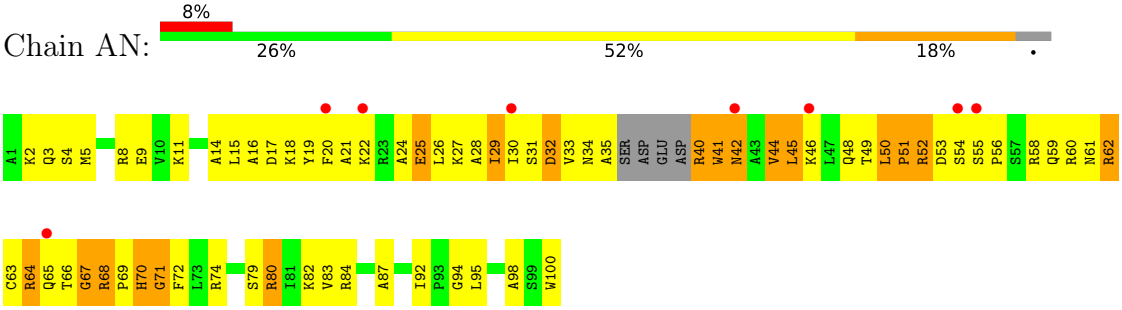






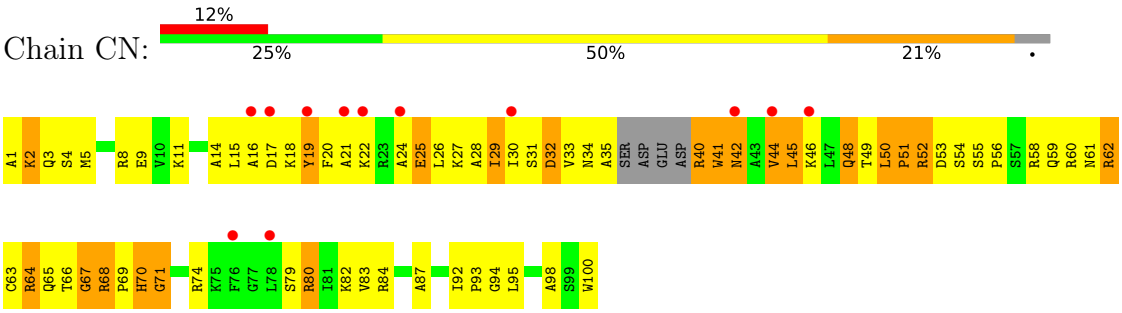
• Molecule 13: 30S ribosomal protein S14

Chain AN:



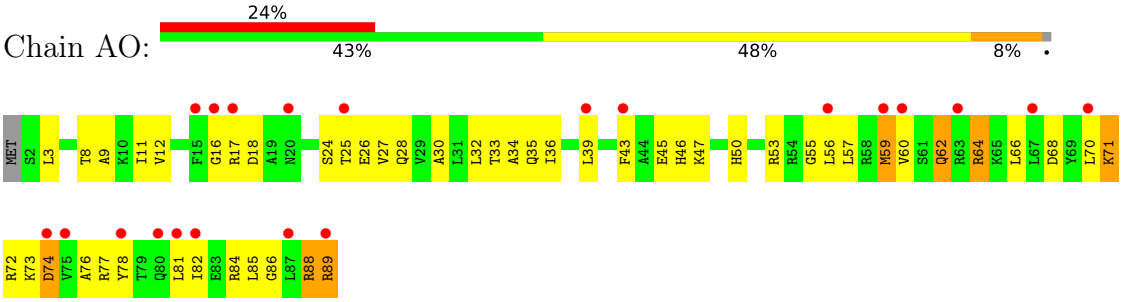
• Molecule 13: 30S ribosomal protein S14

Chain CN:



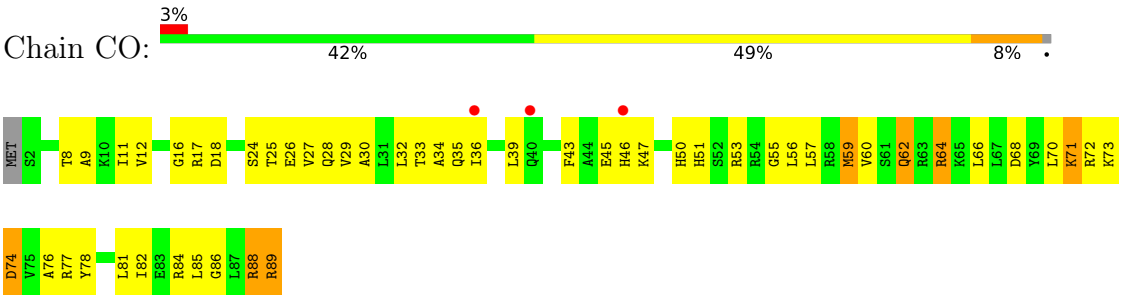
• Molecule 14: 30S ribosomal protein S15

Chain AO:



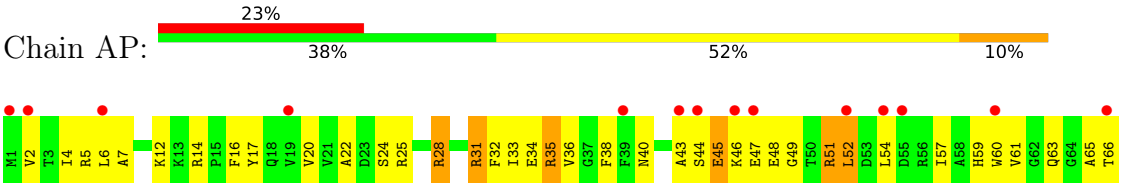
• Molecule 14: 30S ribosomal protein S15

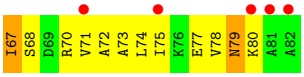
Chain CO:



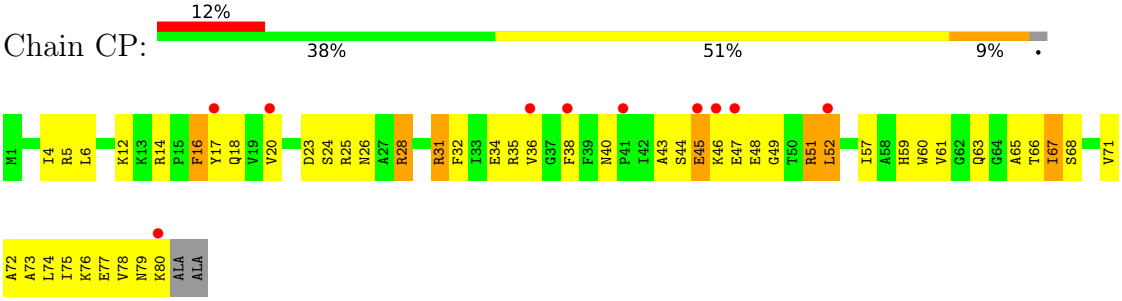
• Molecule 15: 30S ribosomal protein S16

Chain AP:

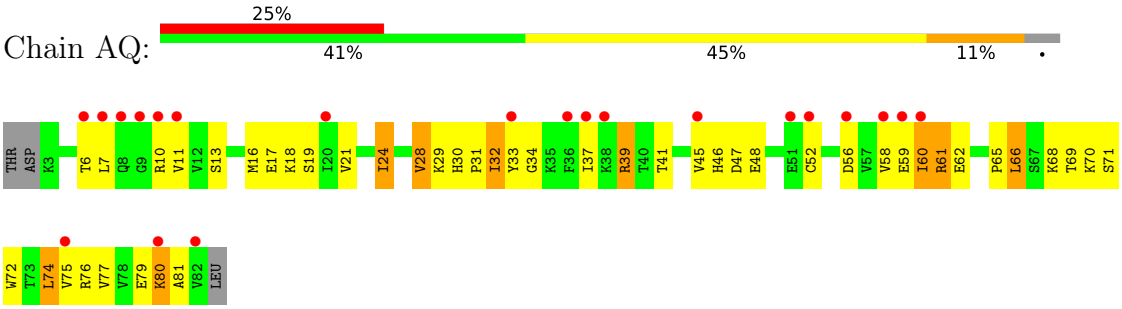




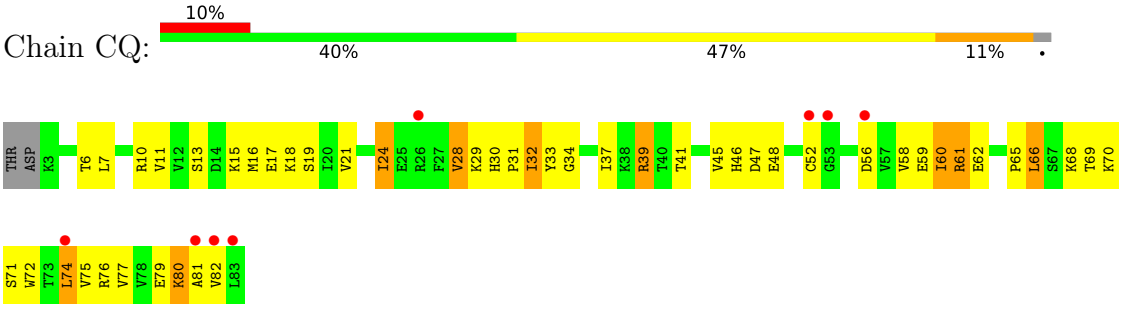
• Molecule 15: 30S ribosomal protein S16



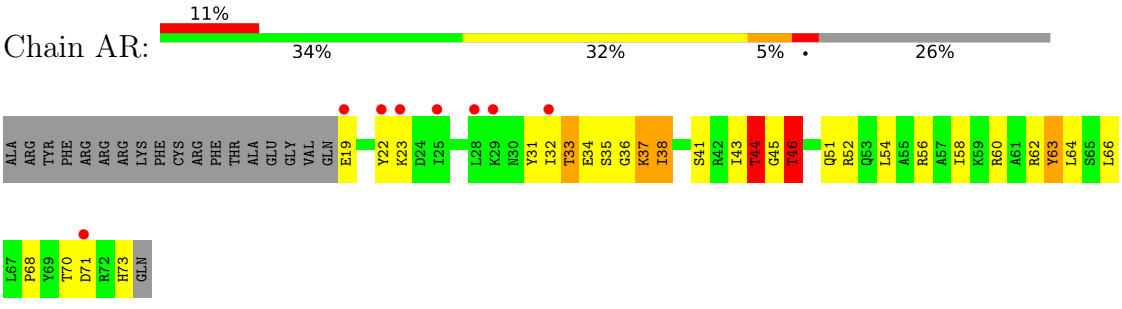
• Molecule 16: 30S ribosomal protein S17



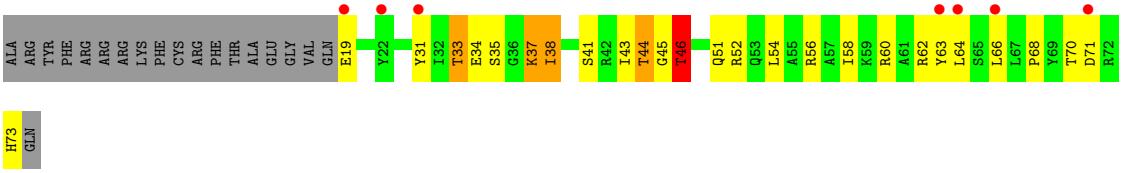
• Molecule 16: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S18

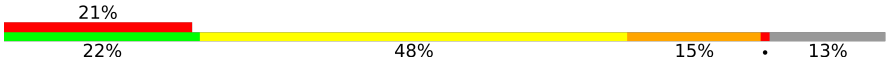


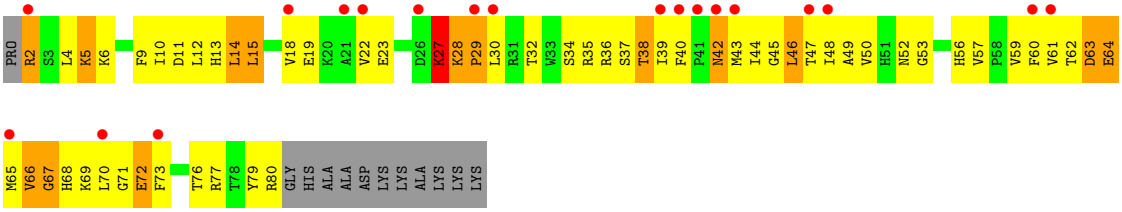
• Molecule 17: 30S ribosomal protein S18



• Molecule 18: 30S ribosomal protein S19

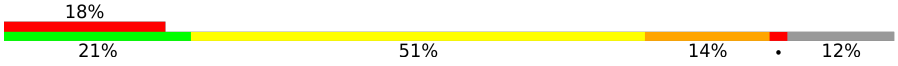
Chain AS:

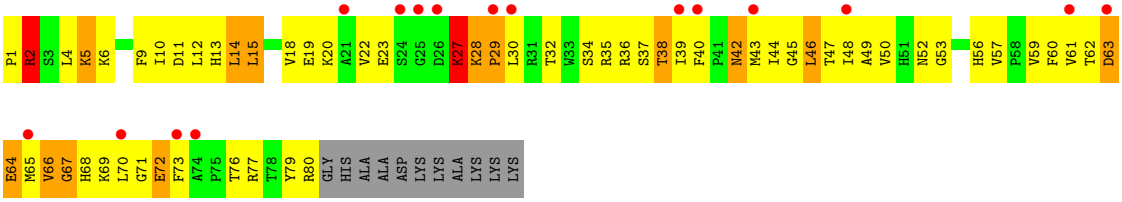




• Molecule 18: 30S ribosomal protein S19

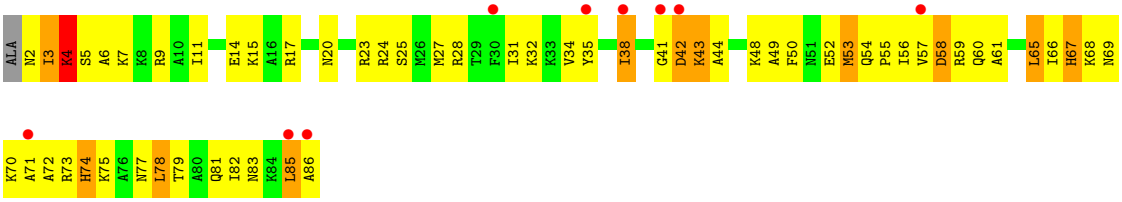
Chain CS:





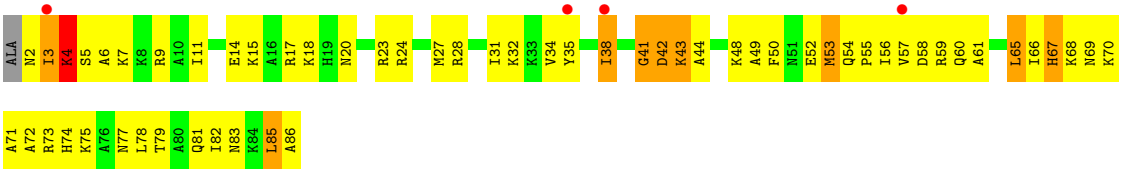
• Molecule 19: 30S ribosomal protein S20

Chain AT:



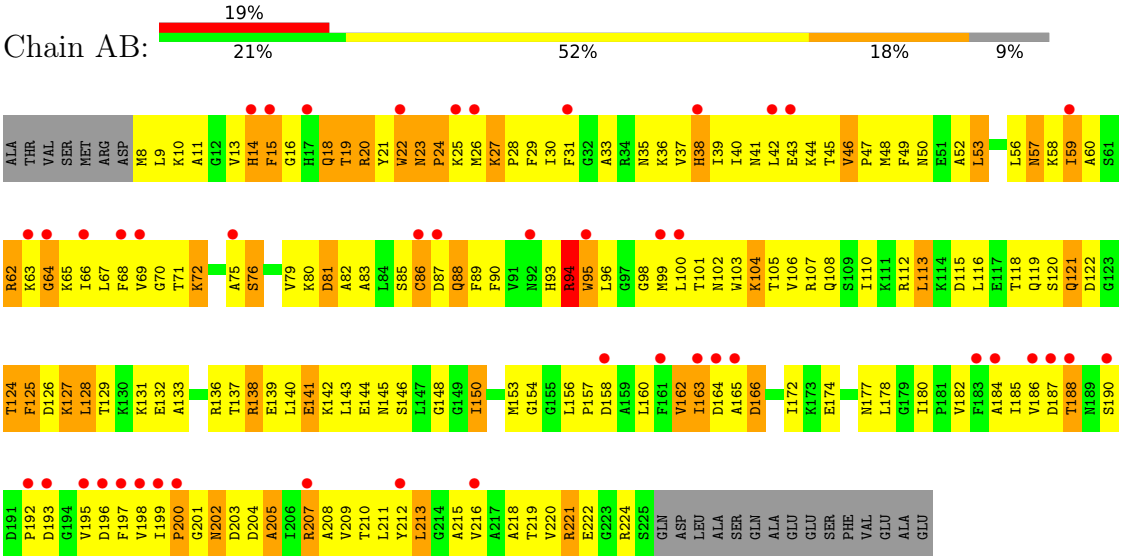
• Molecule 19: 30S ribosomal protein S20

Chain CT:



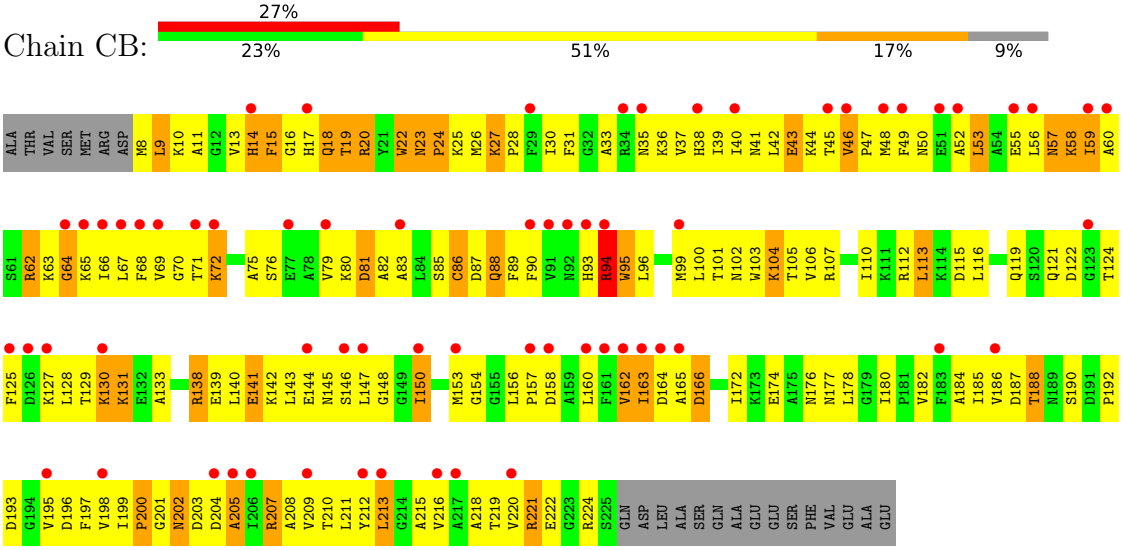
• Molecule 20: 30S ribosomal protein S2

Chain AB:



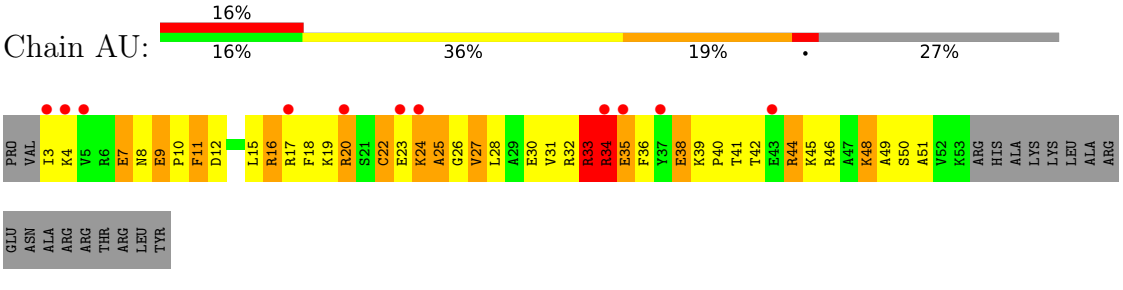
• Molecule 20: 30S ribosomal protein S2

Chain CB:



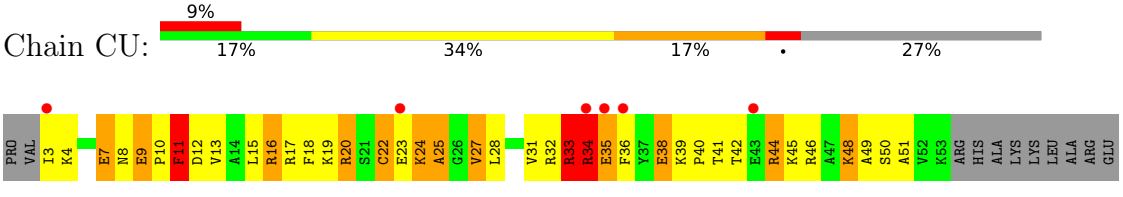
• Molecule 21: 30S ribosomal protein S21

Chain AU:



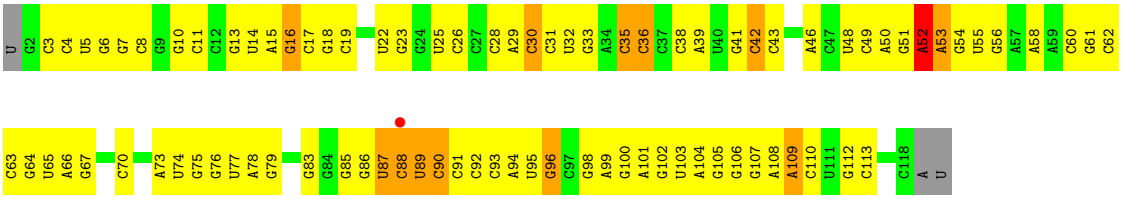
• Molecule 21: 30S ribosomal protein S21

Chain CU:



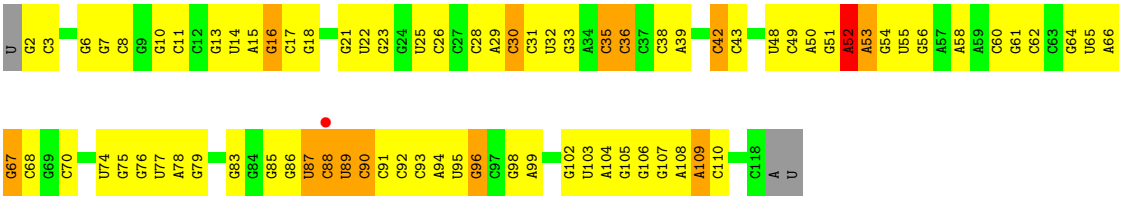
• Molecule 22: 5S rRNA

Chain BA:



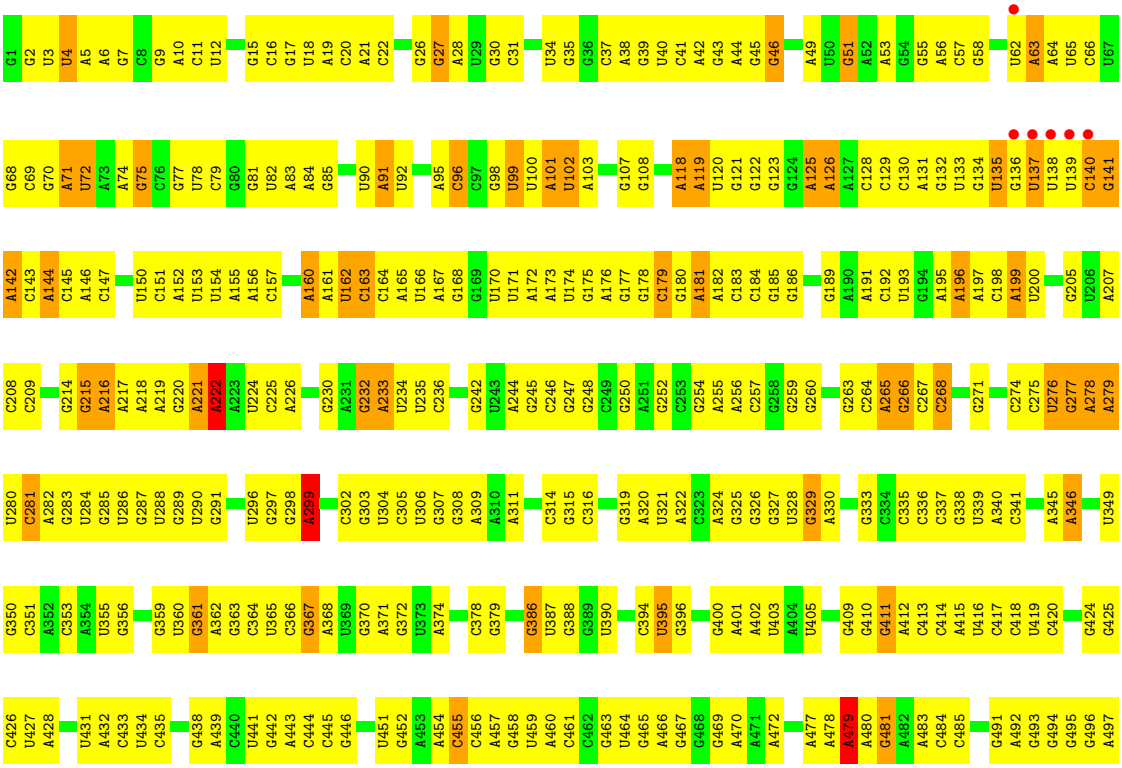
• Molecule 22: 5S rRNA

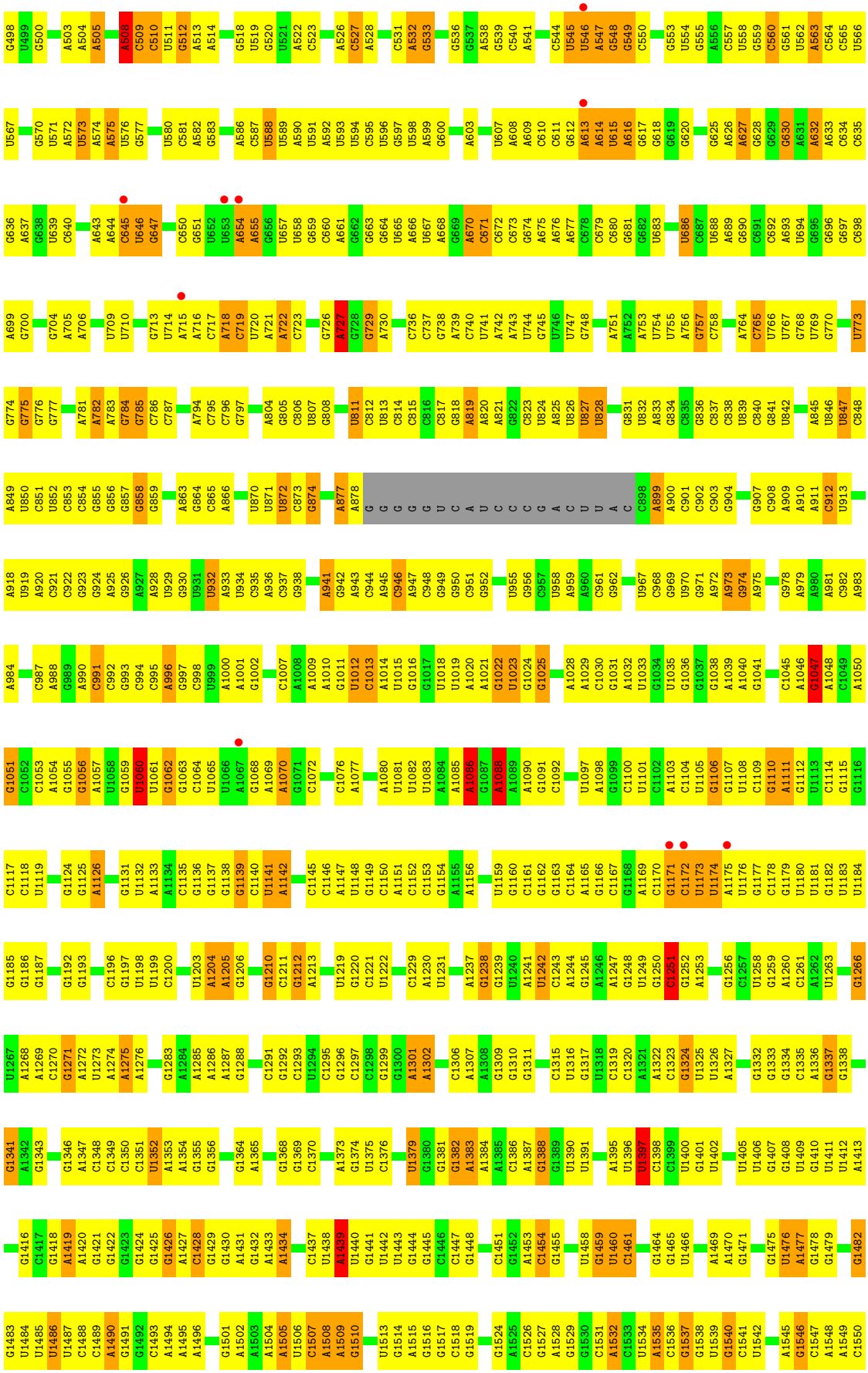
Chain DA:

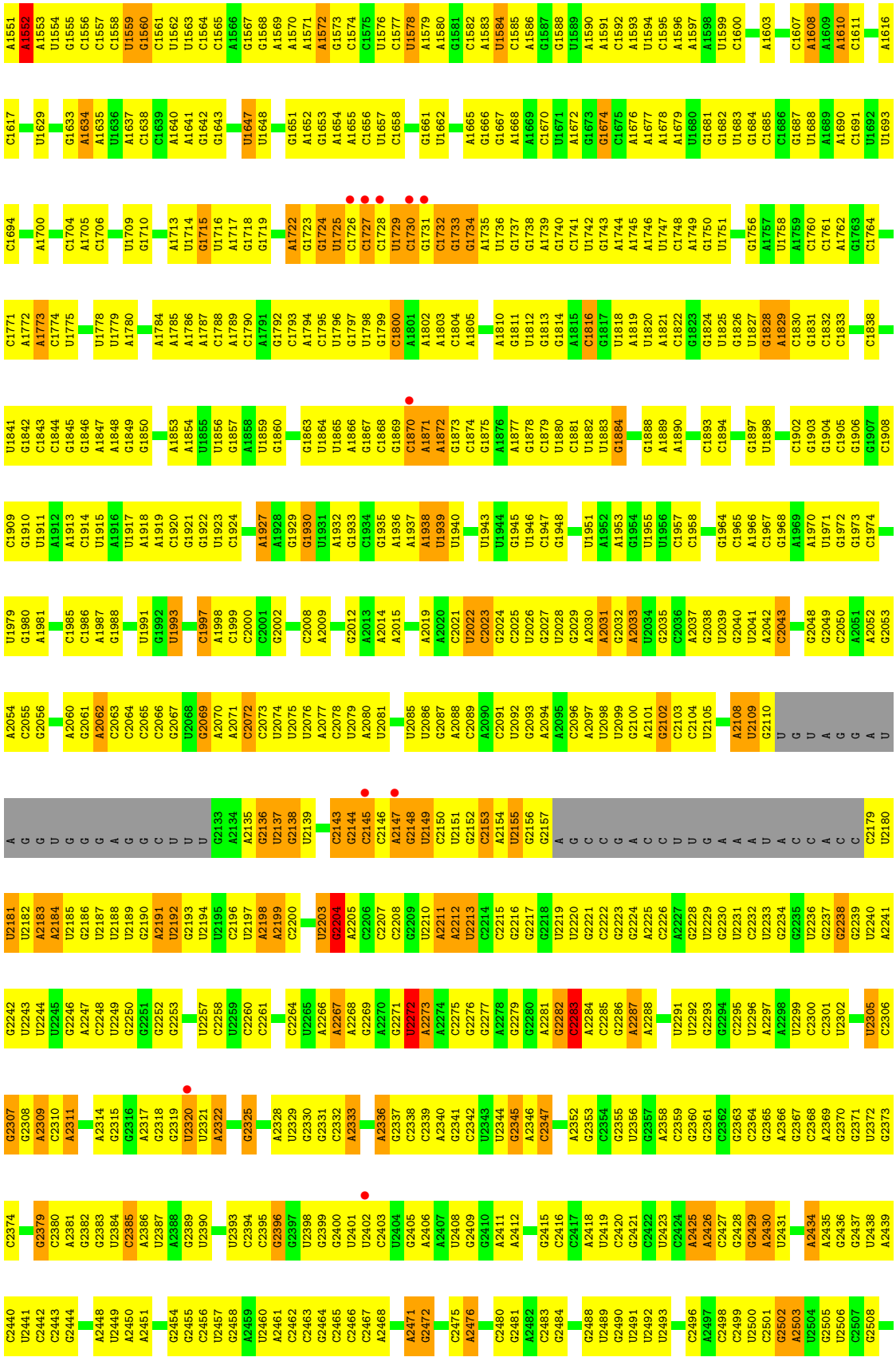


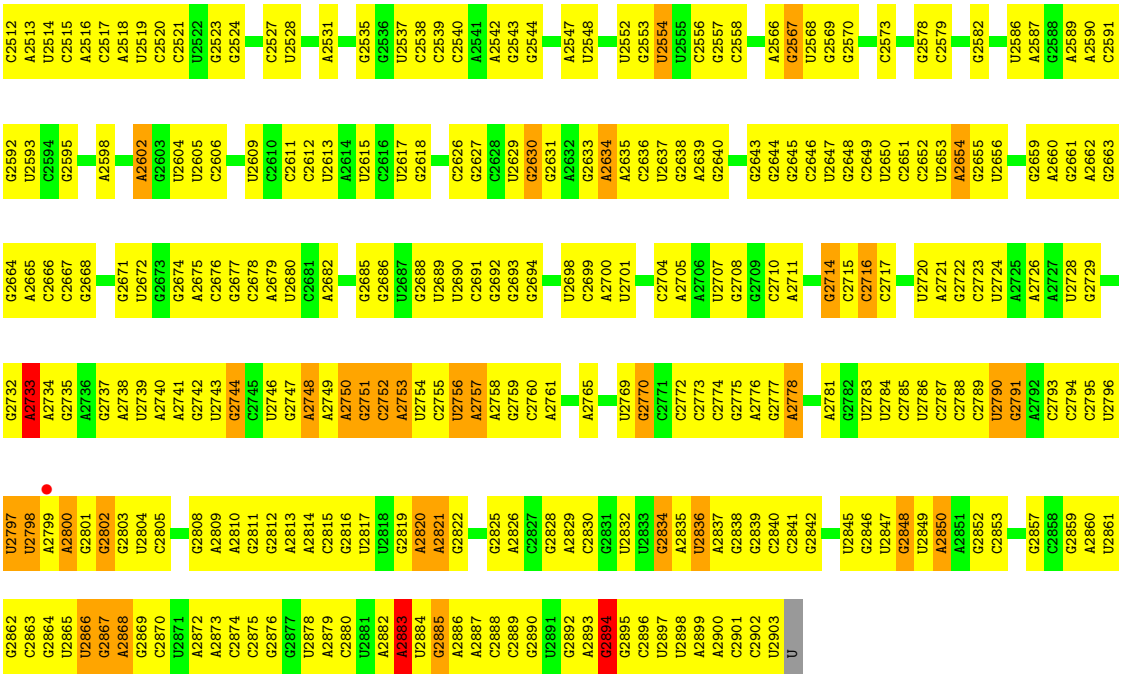
• Molecule 23: 23S rRNA

Chain BB:



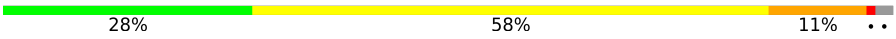


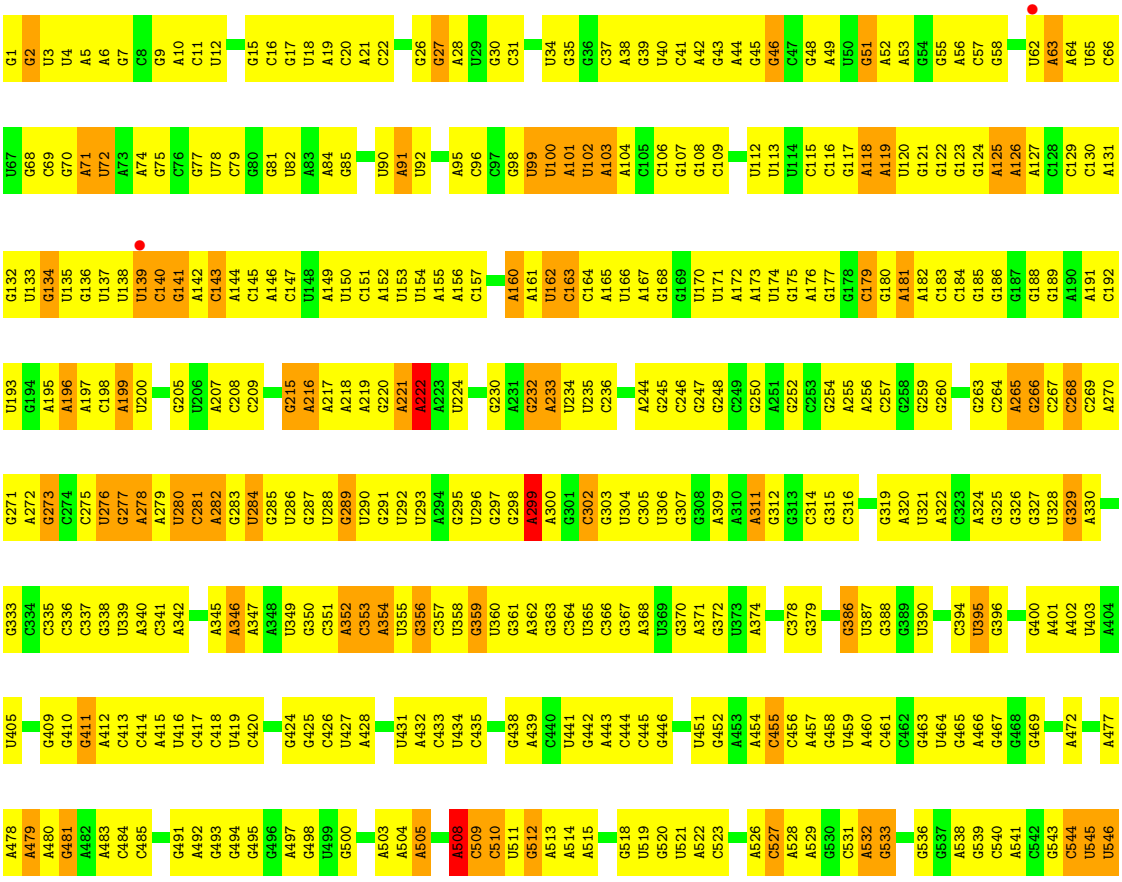


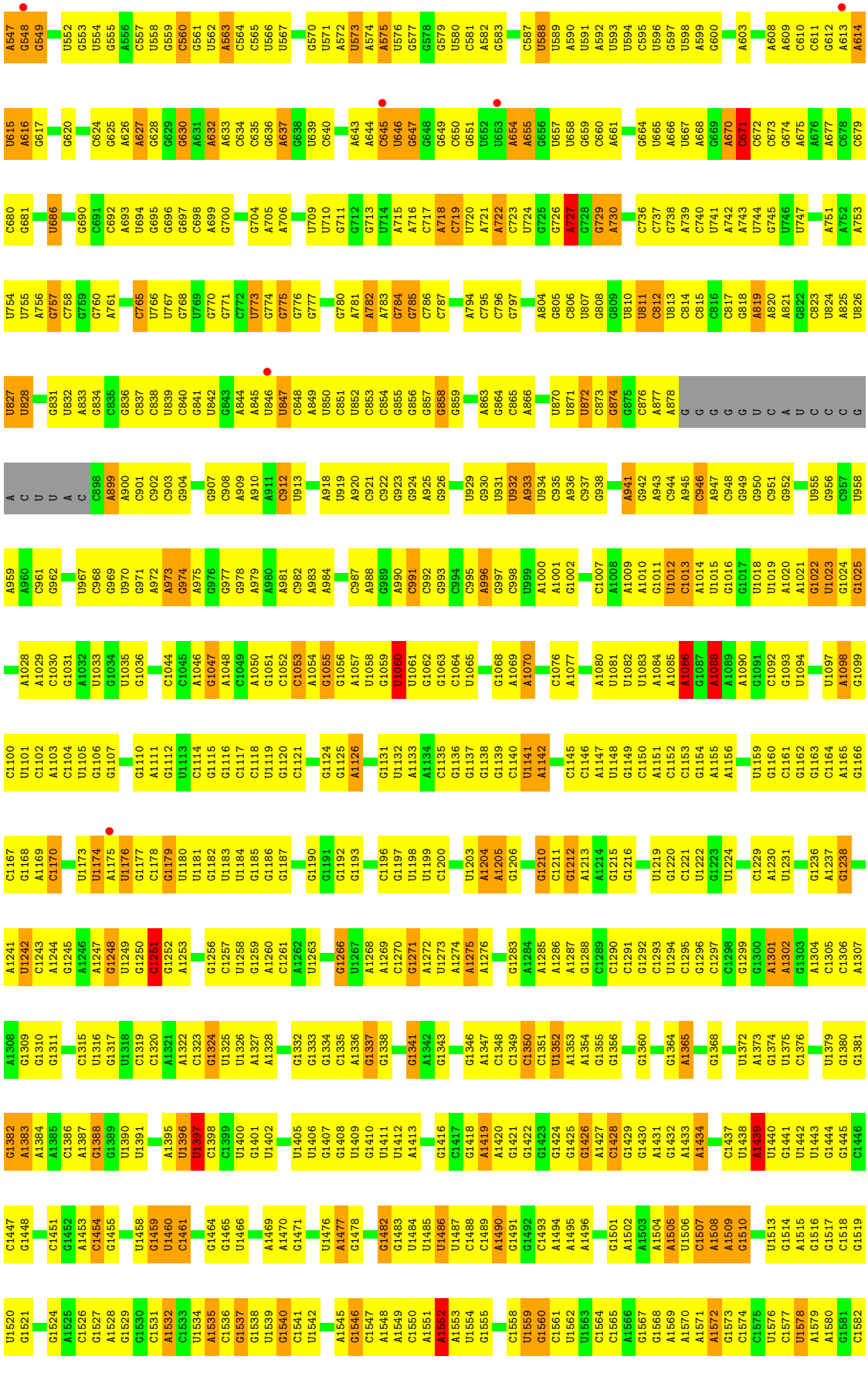


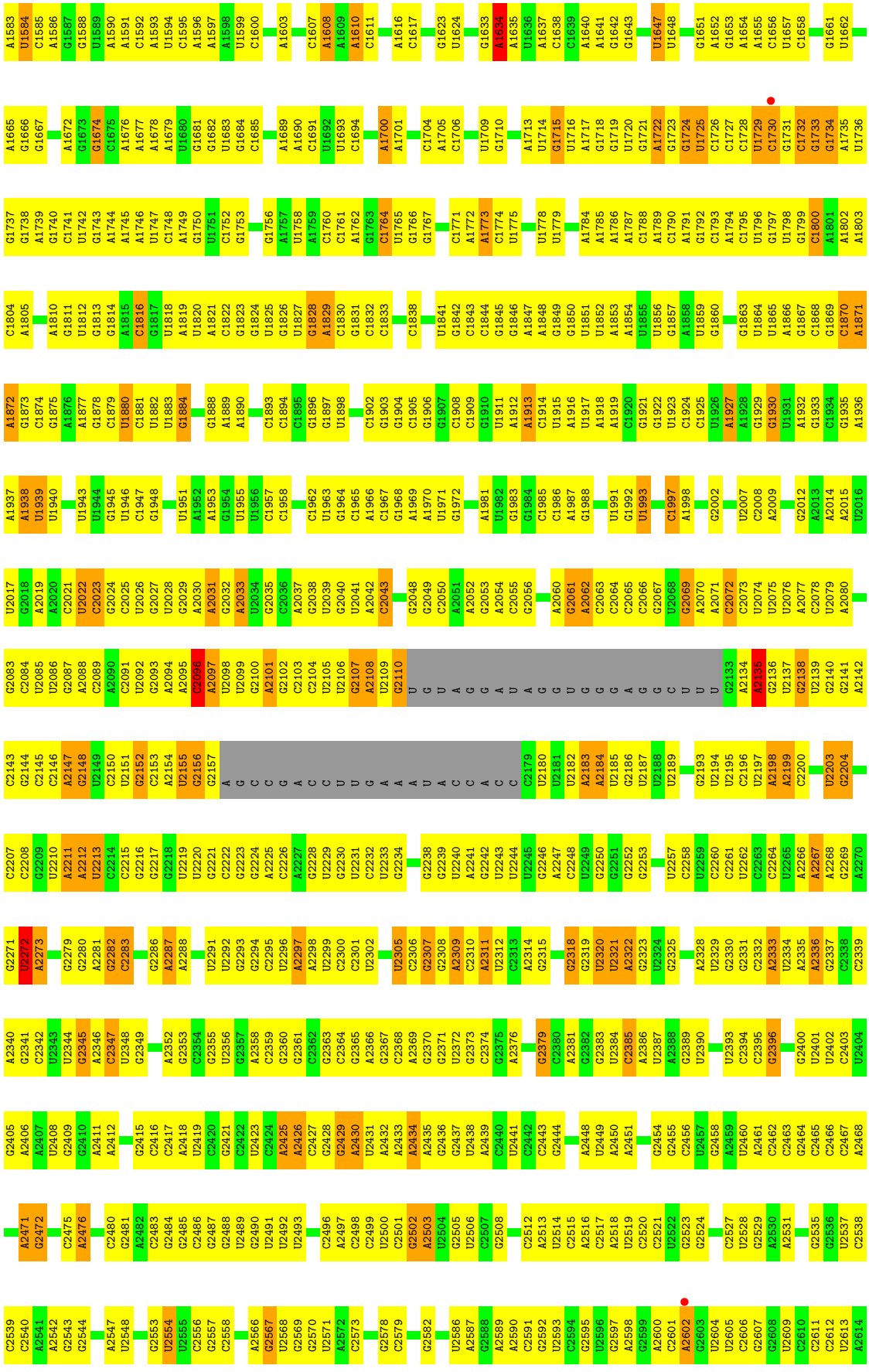
• Molecule 23: 23S rRNA

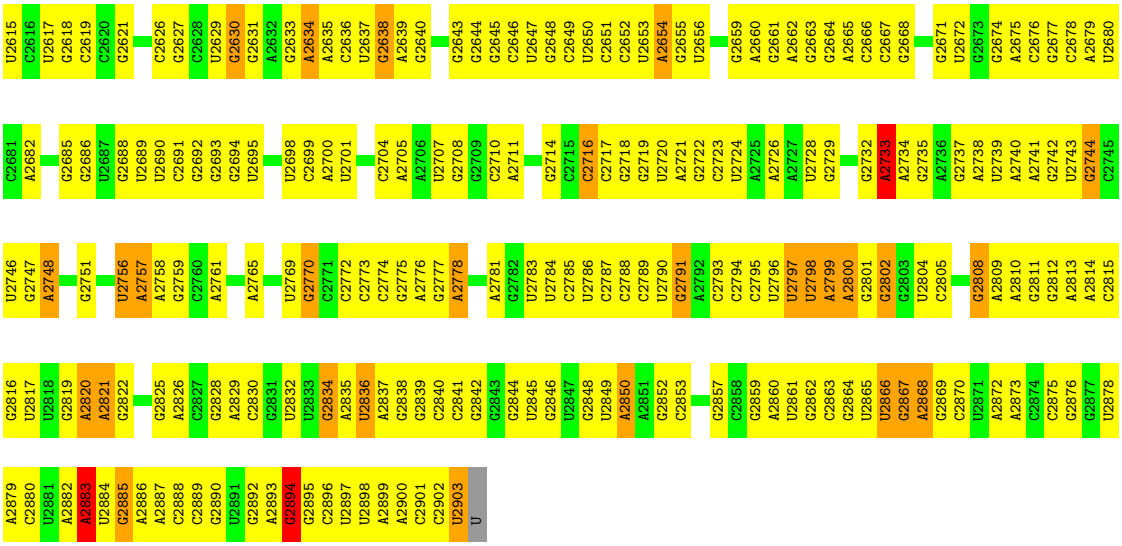
Chain DB:





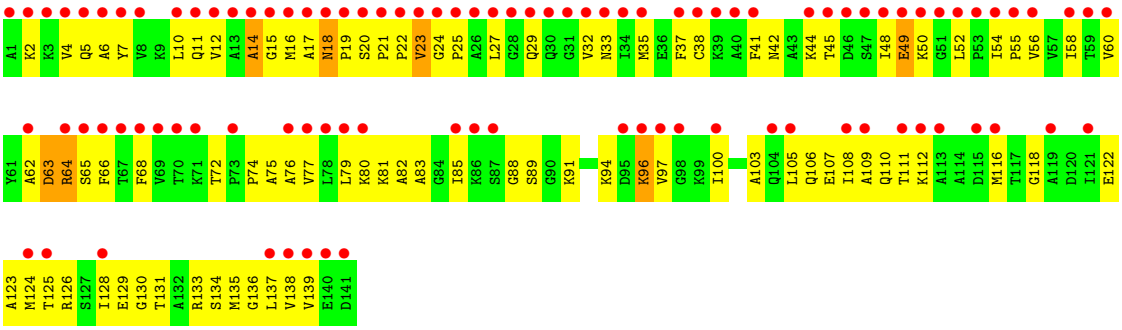






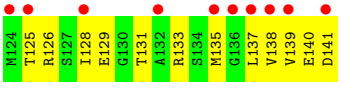
• Molecule 24: 50S ribosomal protein L11

Chain BI:



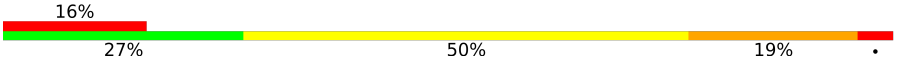
• Molecule 24: 50S ribosomal protein L11

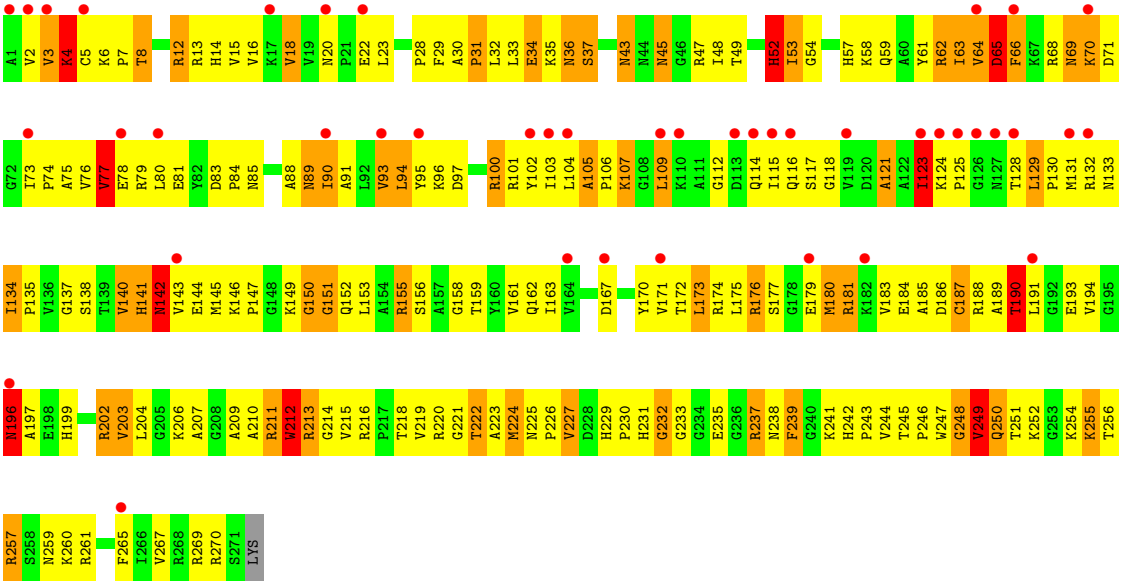
Chain DI:



• Molecule 25: 50S ribosomal protein L2

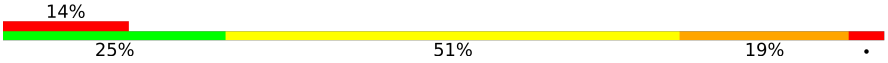
Chain BC:

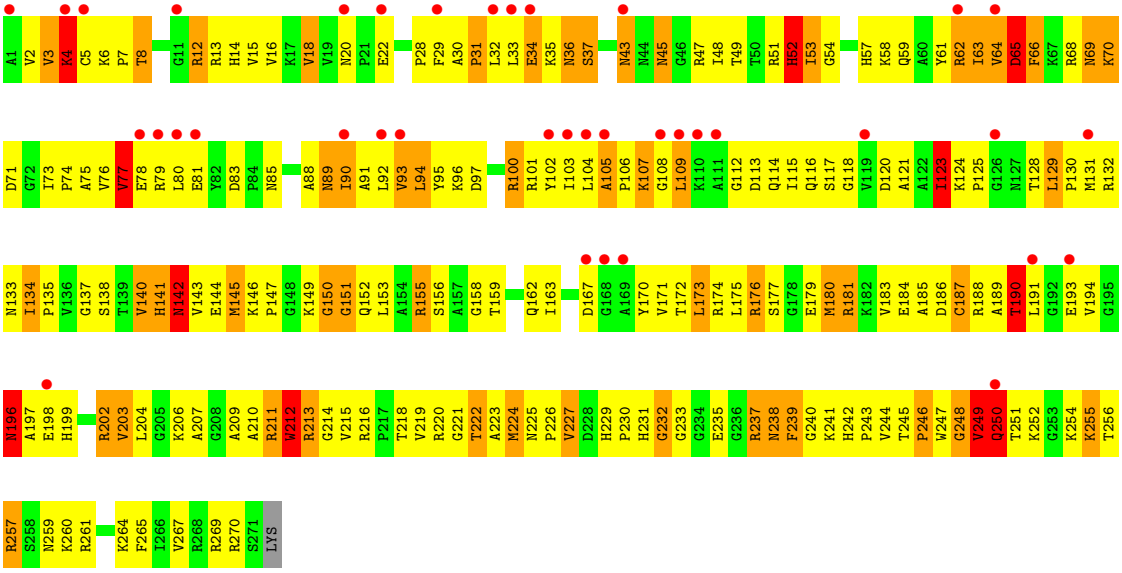




• Molecule 25: 50S ribosomal protein L2

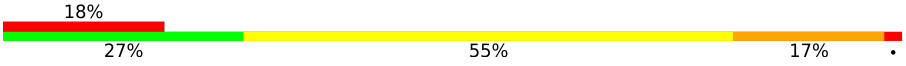
Chain DC:

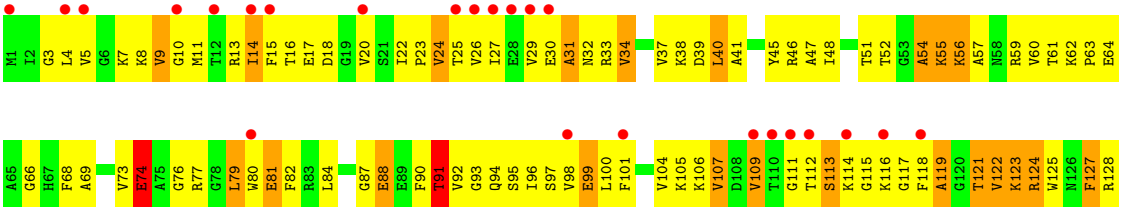


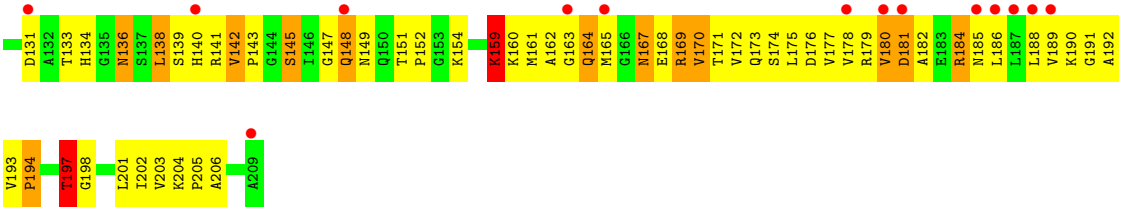


• Molecule 26: 50S ribosomal protein L3

Chain BD:

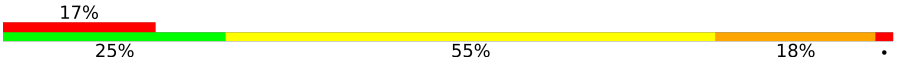


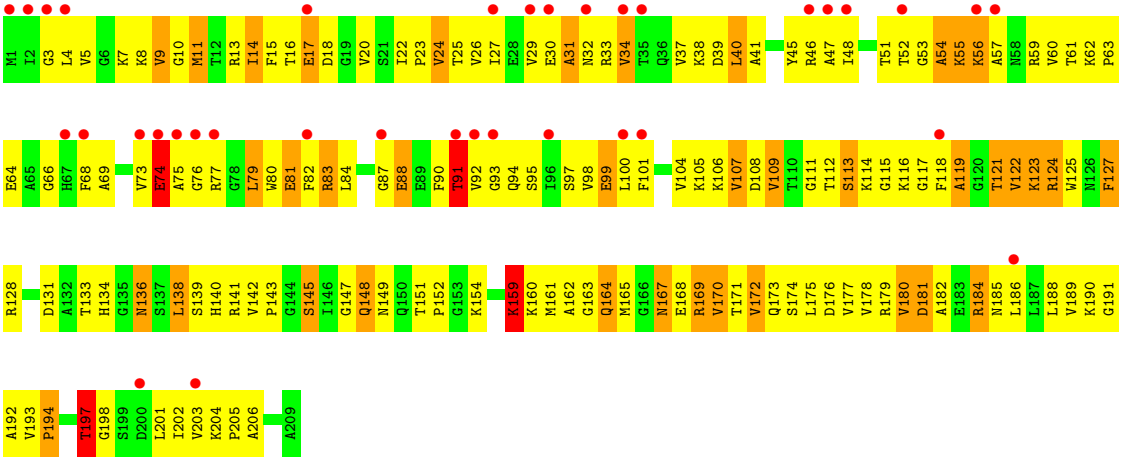




• Molecule 26: 50S ribosomal protein L3

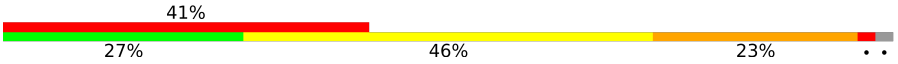
Chain DD:

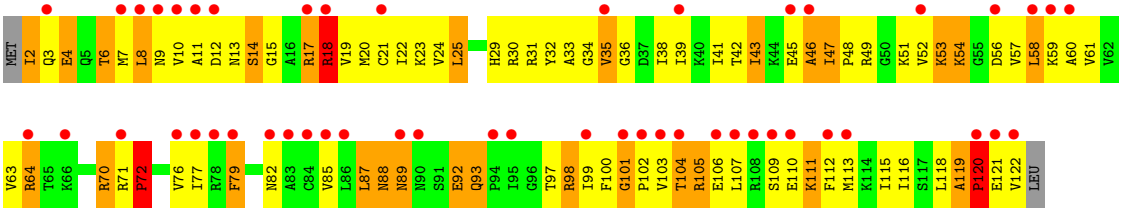




• Molecule 27: 50S ribosomal protein L14

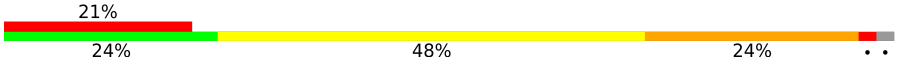
Chain BK:

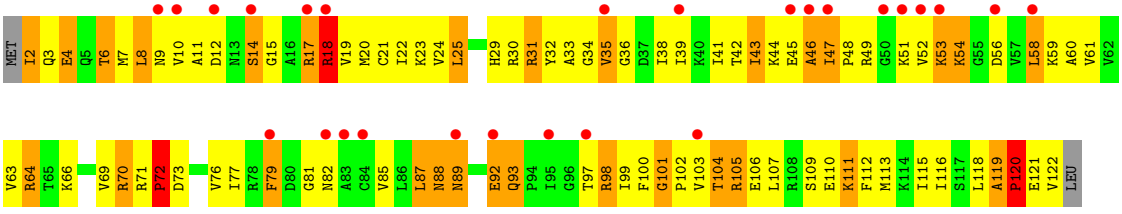




• Molecule 27: 50S ribosomal protein L14

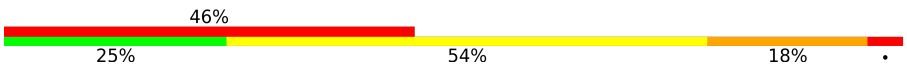
Chain DK:

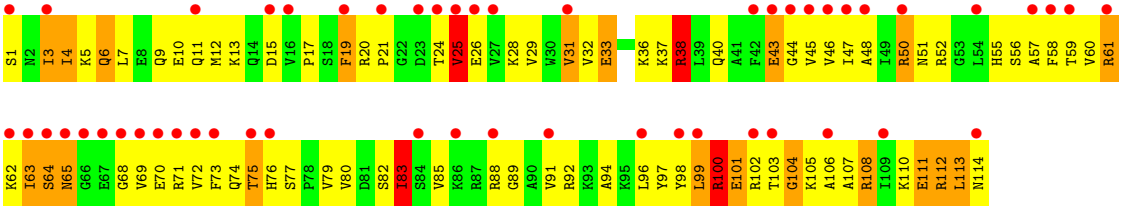




• Molecule 28: 50S ribosomal protein L19

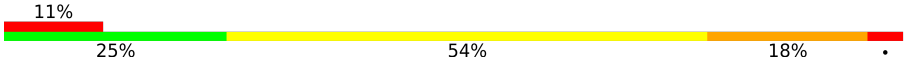
Chain BP:

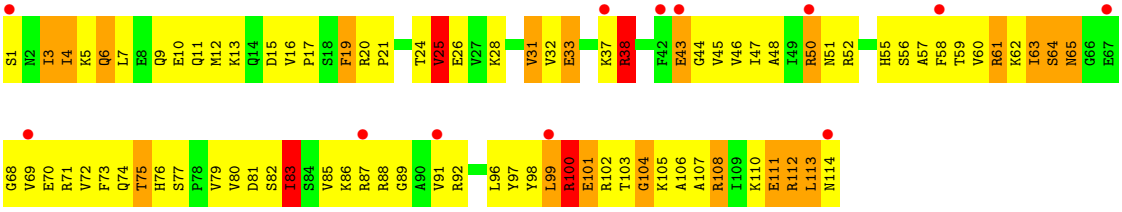




• Molecule 28: 50S ribosomal protein L19

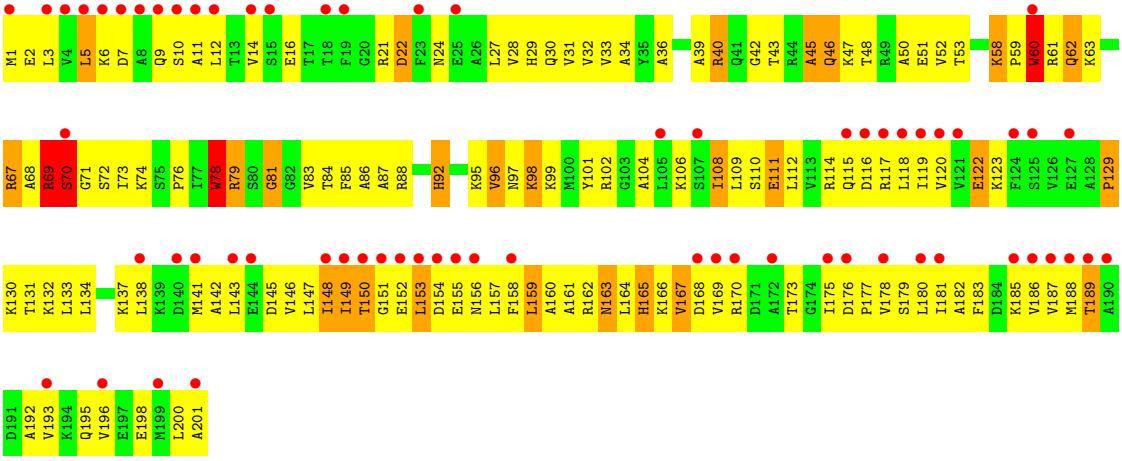
Chain DP:





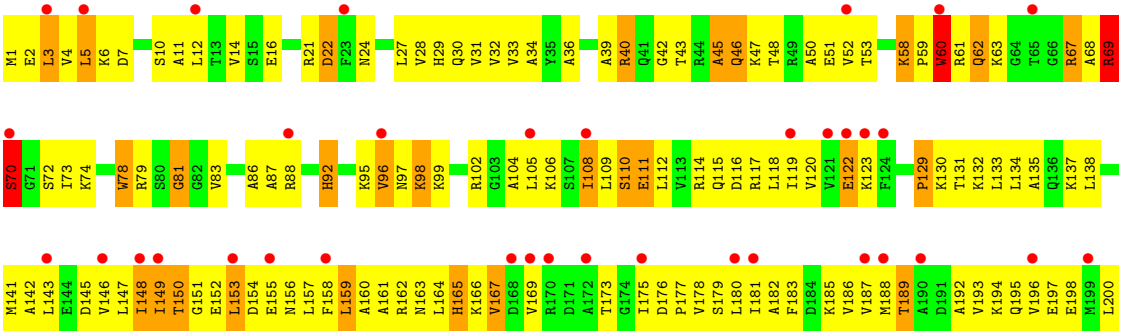
• Molecule 29: 50S ribosomal protein L4

Chain BE:



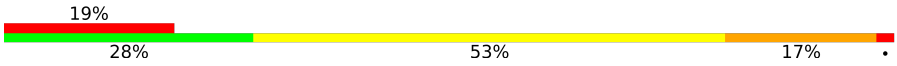
• Molecule 29: 50S ribosomal protein L4

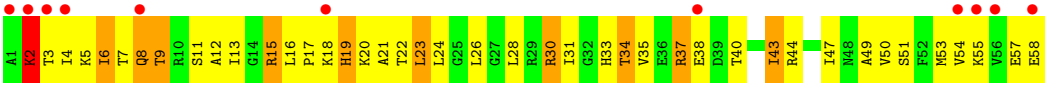
Chain DE:



• Molecule 30: 50S ribosomal protein L30

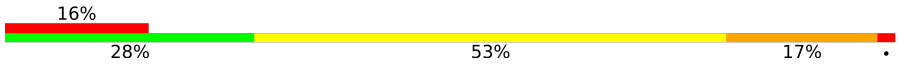
Chain BY:

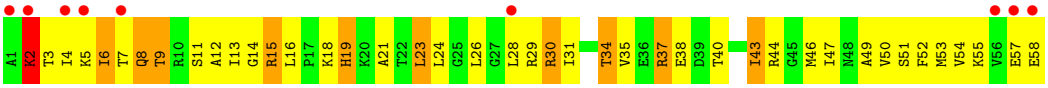




• Molecule 30: 50S ribosomal protein L30

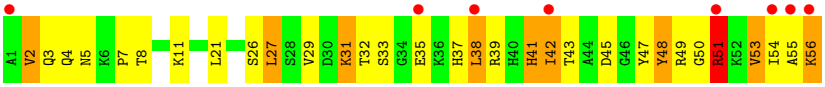
Chain DY:





• Molecule 31: 50S ribosomal protein L32

Chain B0:

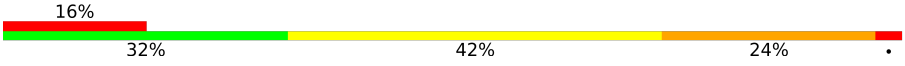


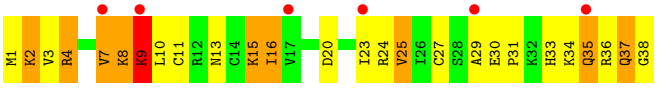
• Molecule 31: 50S ribosomal protein L32

Chain D0:

• Molecule 32: 50S ribosomal protein L36

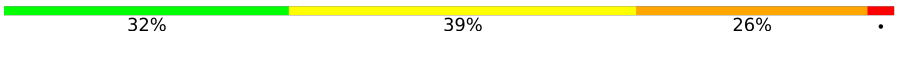
Chain B4:

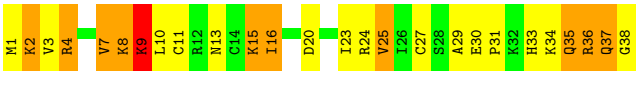




• Molecule 32: 50S ribosomal protein L36

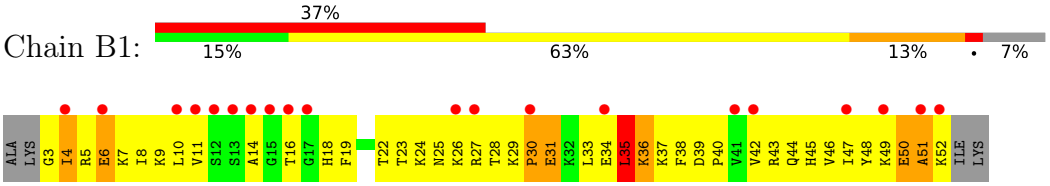
Chain D4:





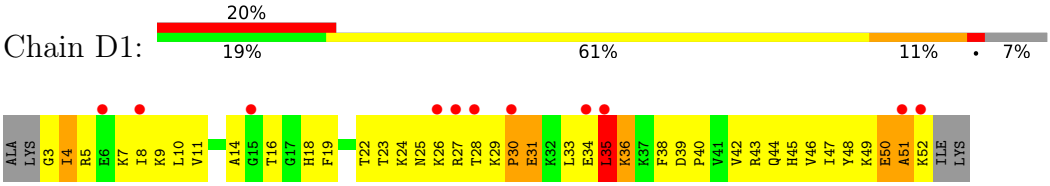
• Molecule 33: 50S ribosomal protein L33

Chain B1:



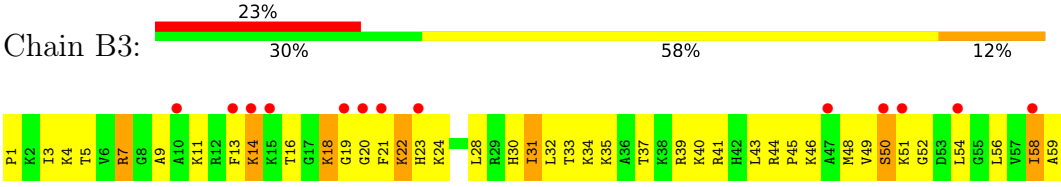
• Molecule 33: 50S ribosomal protein L33

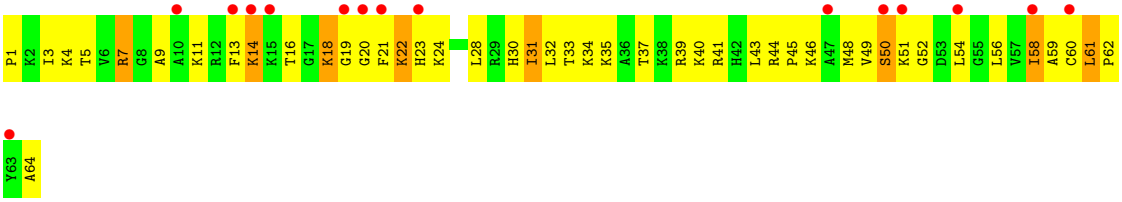
Chain D1:



• Molecule 34: 50S ribosomal protein L35

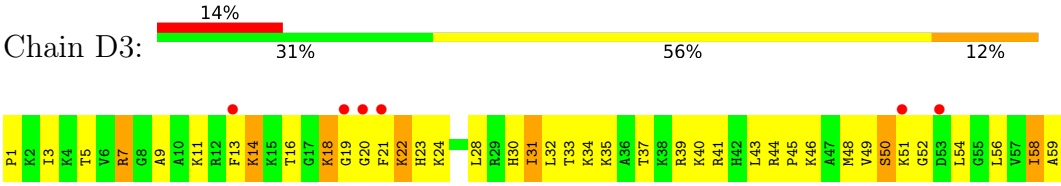
Chain B3:

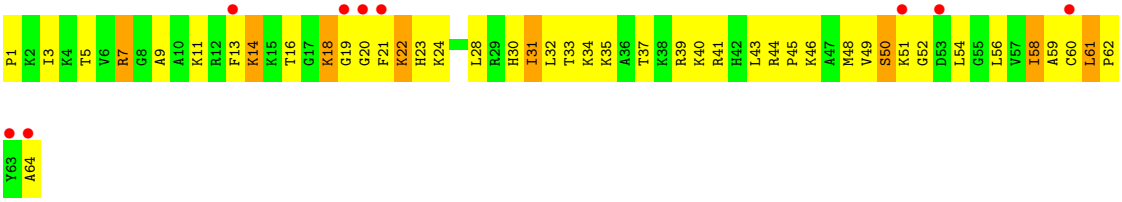




• Molecule 34: 50S ribosomal protein L35

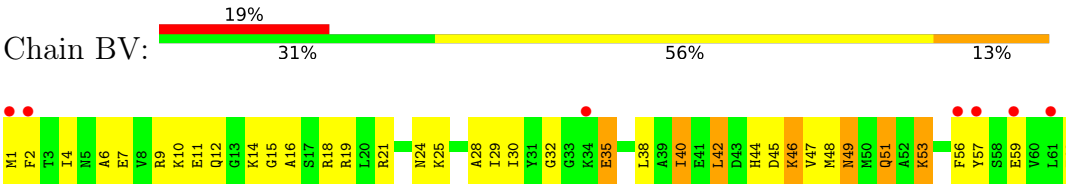
Chain D3:

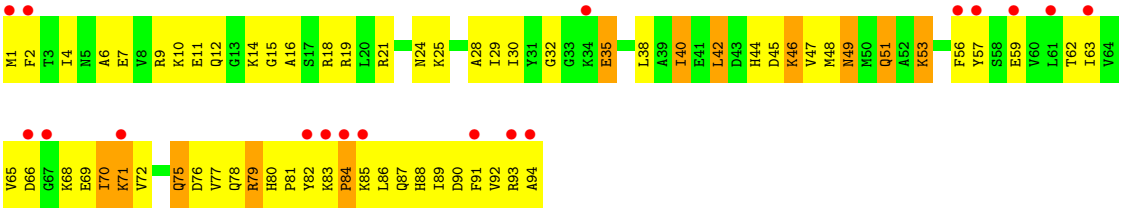




• Molecule 35: 50S ribosomal protein L25

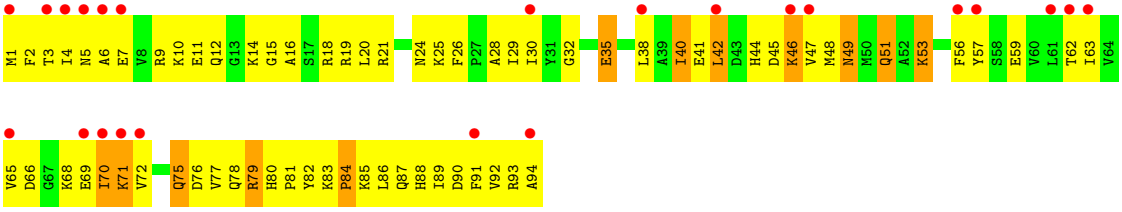
Chain BV:



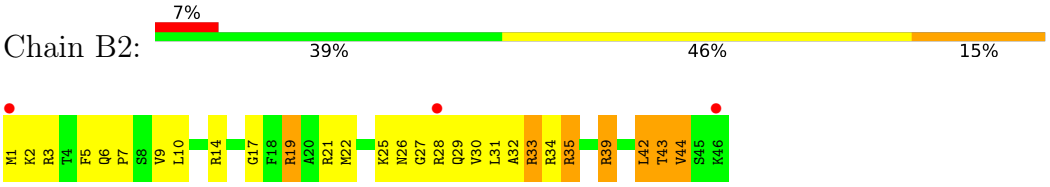


• Molecule 35: 50S ribosomal protein L25

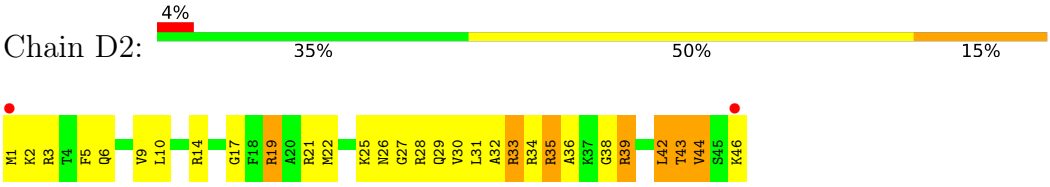
Chain DV:



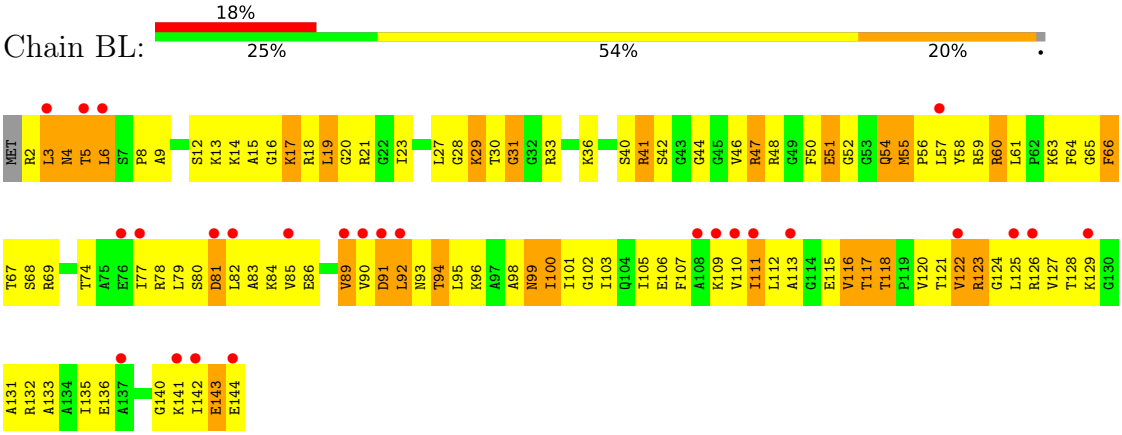
• Molecule 36: 50S ribosomal protein L34



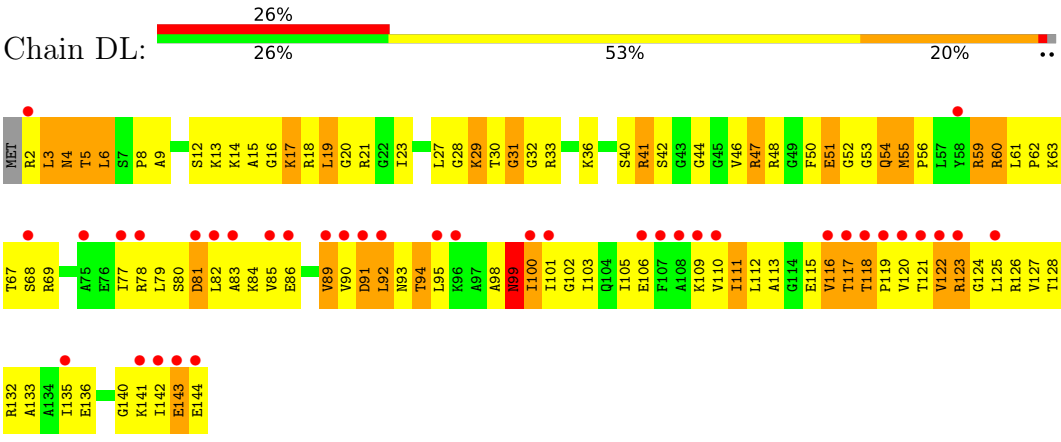
• Molecule 36: 50S ribosomal protein L34



• Molecule 37: 50S ribosomal protein L15

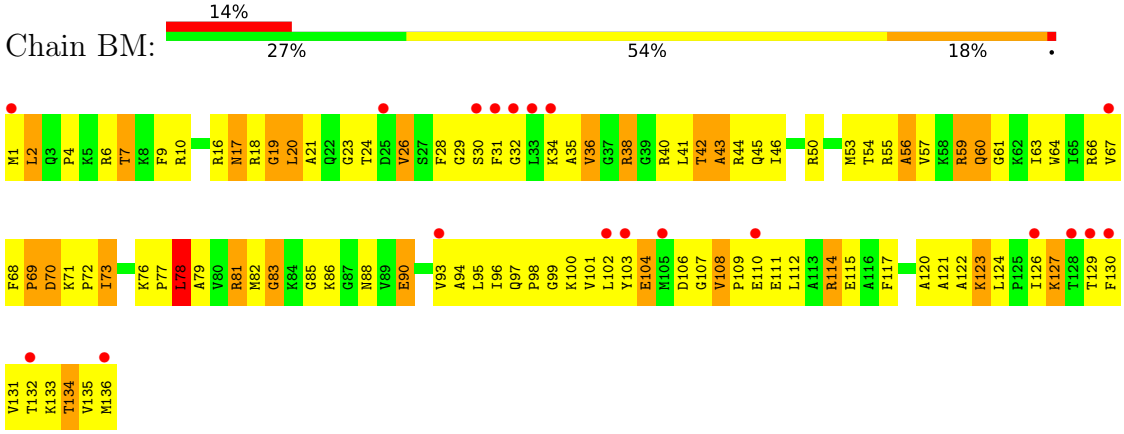


• Molecule 37: 50S ribosomal protein L15



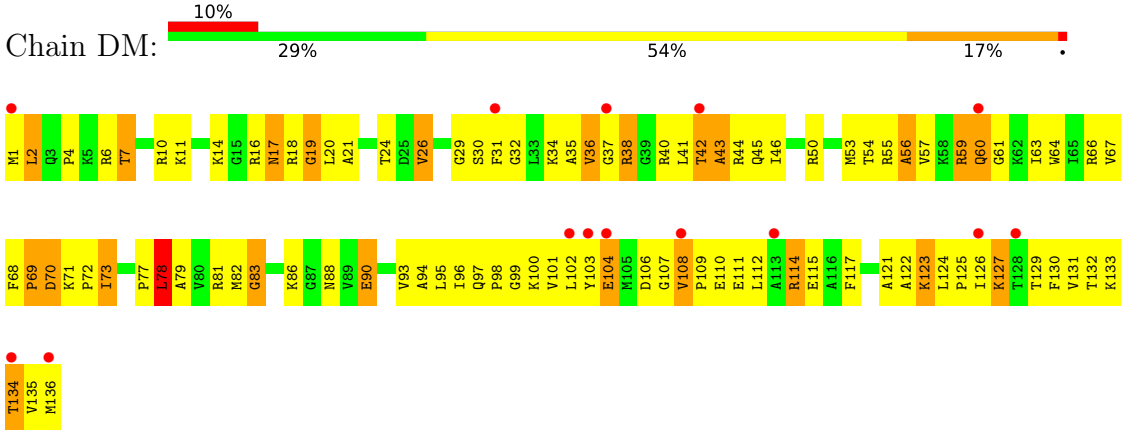
• Molecule 38: 50S ribosomal protein L16

Chain BM:



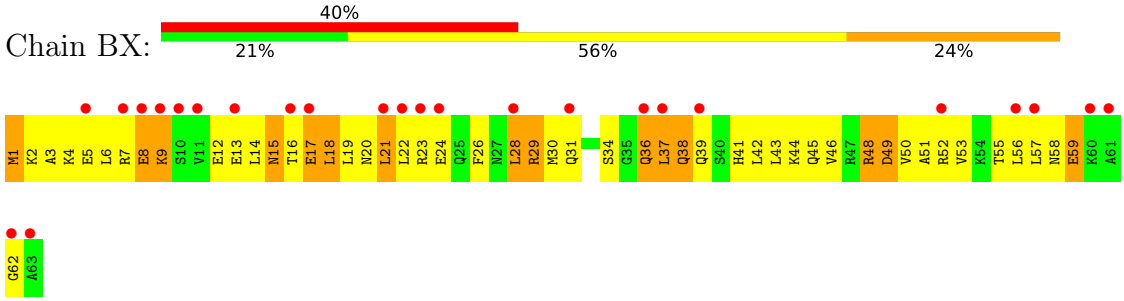
• Molecule 38: 50S ribosomal protein L16

Chain DM:



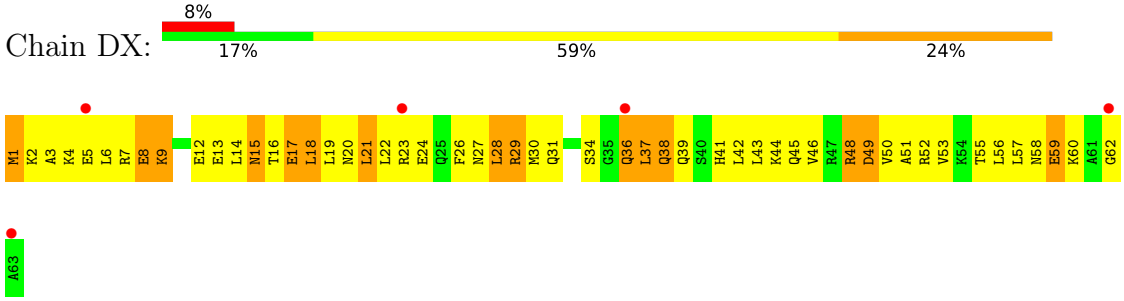
• Molecule 39: 50S ribosomal protein L29

Chain BX:



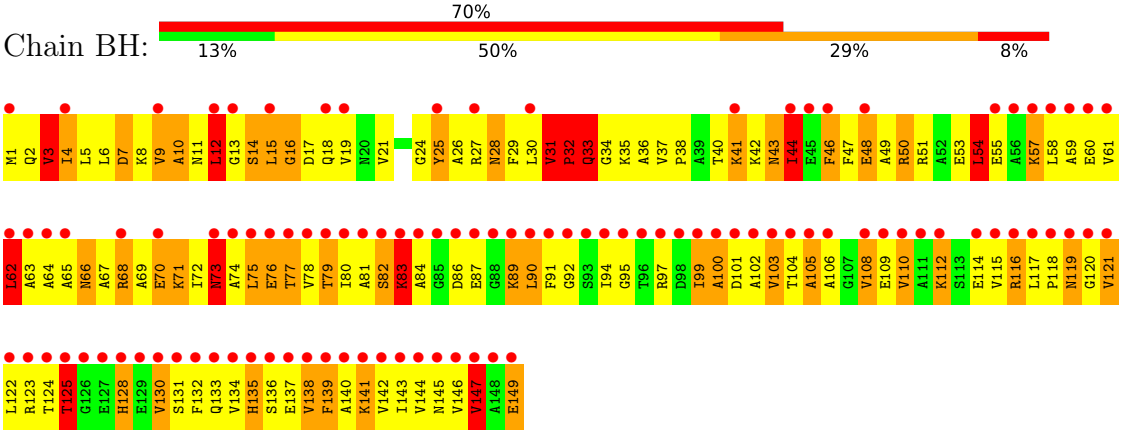
• Molecule 39: 50S ribosomal protein L29

Chain DX:



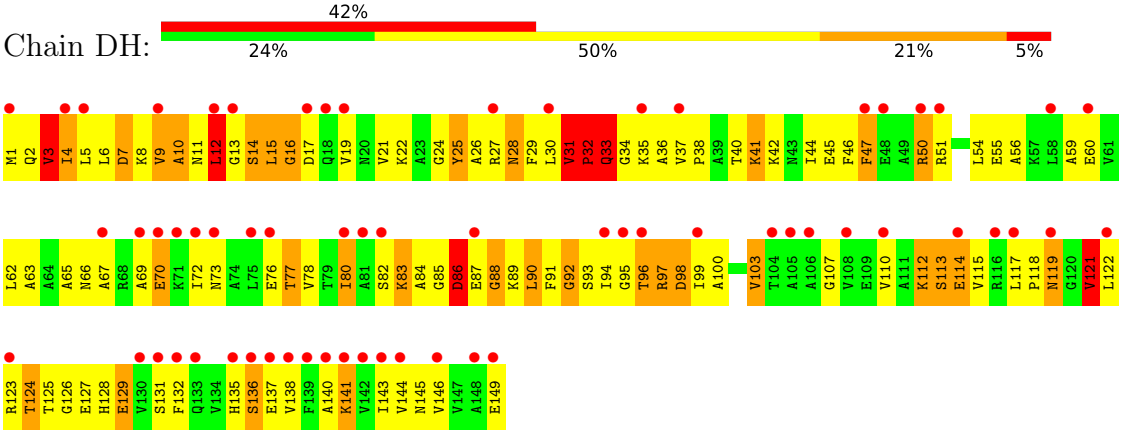
• Molecule 40: 50S ribosomal protein L9

Chain BH:



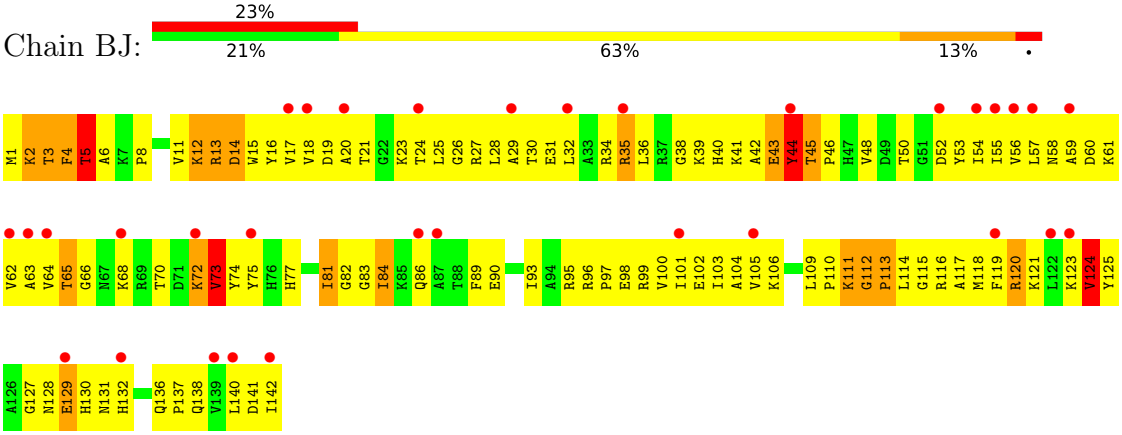
• Molecule 40: 50S ribosomal protein L9

Chain DH:



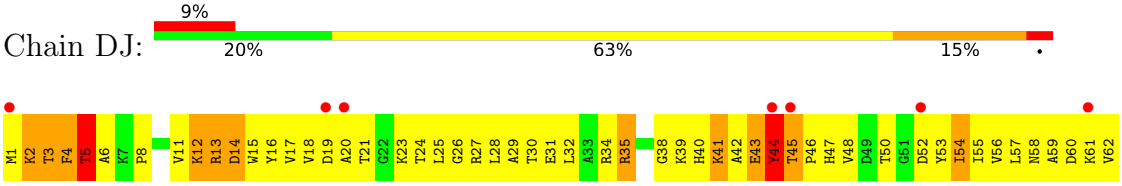
• Molecule 41: 50S ribosomal protein L13

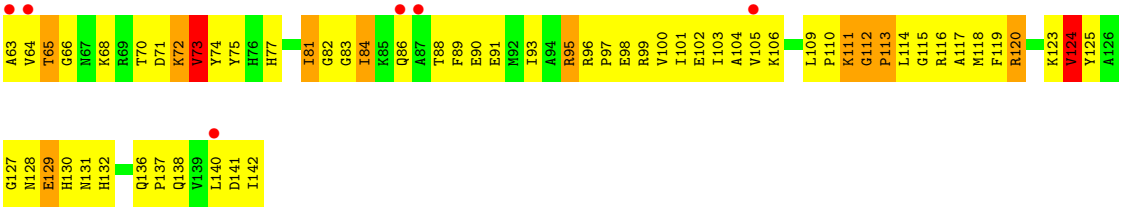
Chain BJ:



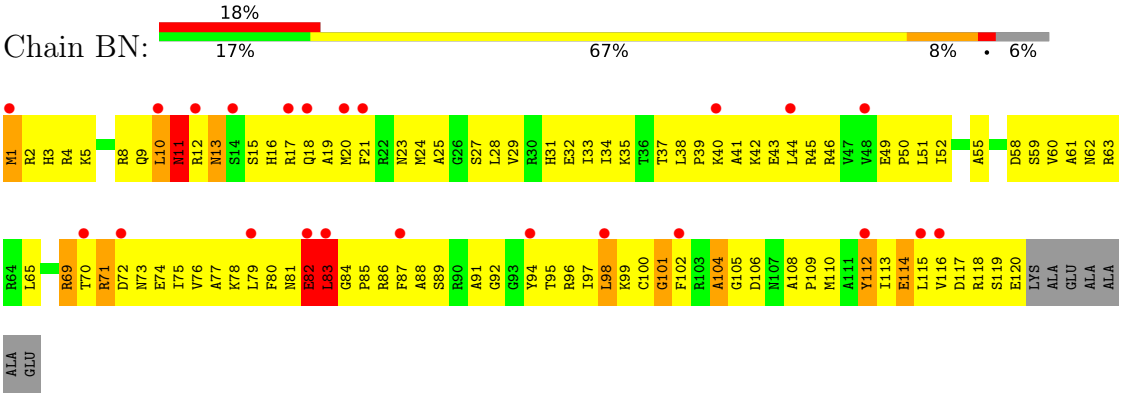
• Molecule 41: 50S ribosomal protein L13

Chain DJ:

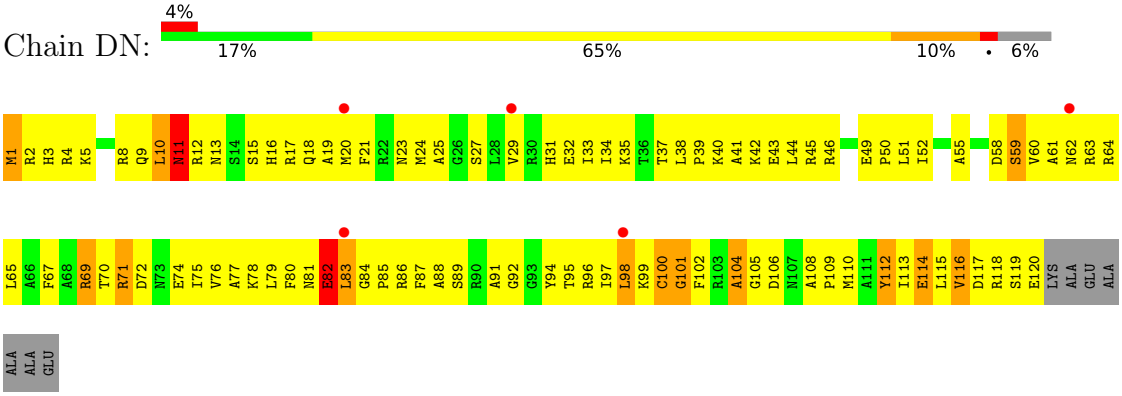




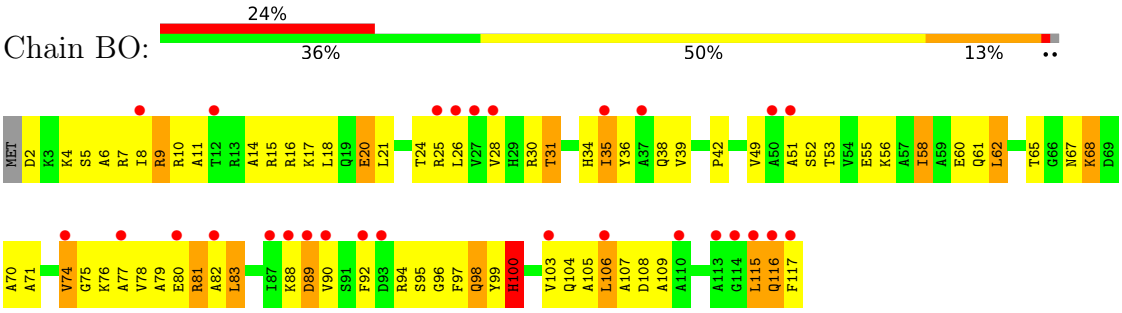
• Molecule 42: 50S ribosomal protein L17



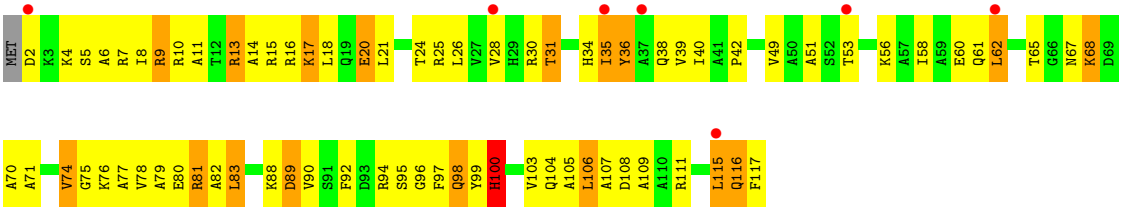
• Molecule 42: 50S ribosomal protein L17

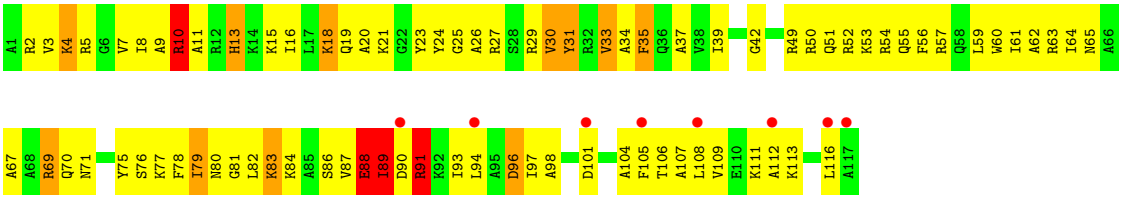


• Molecule 43: 50S ribosomal protein L18



• Molecule 43: 50S ribosomal protein L18



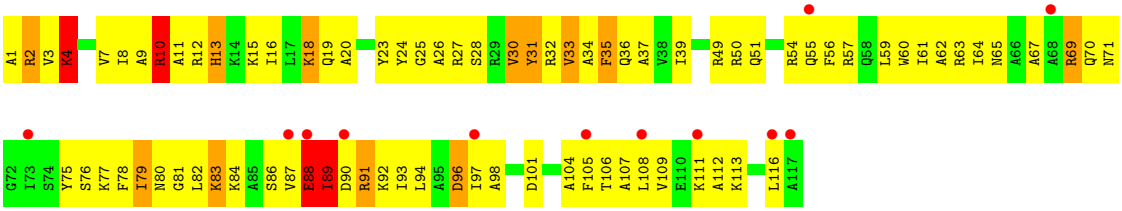


• Molecule 44: 50S ribosomal protein L20

Chain BQ:

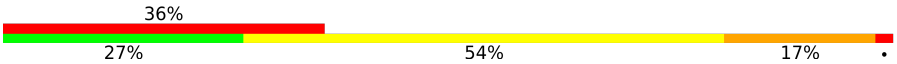
• Molecule 44: 50S ribosomal protein L20

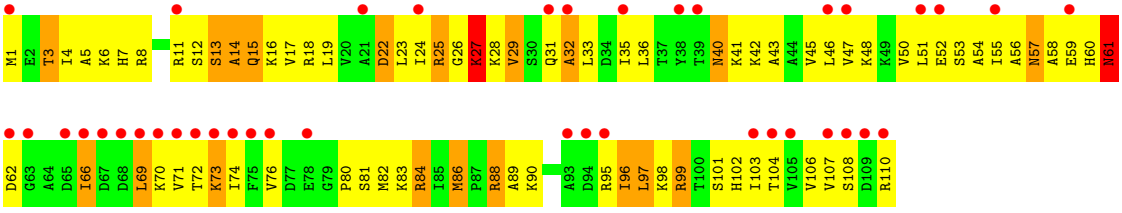
Chain DQ:



• Molecule 45: 50S ribosomal protein L22

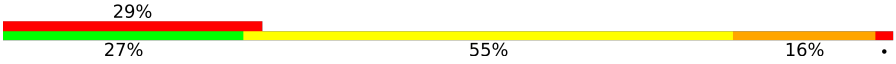
Chain BS:

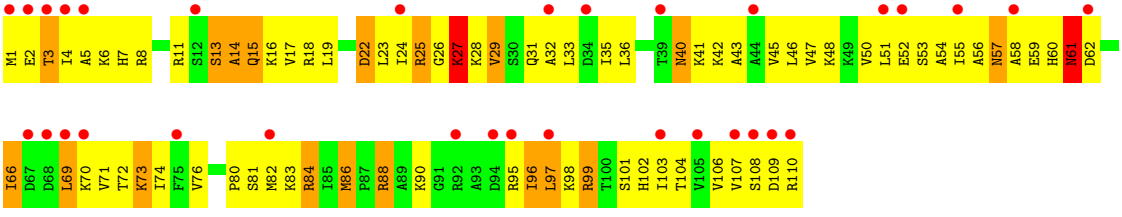




• Molecule 45: 50S ribosomal protein L22

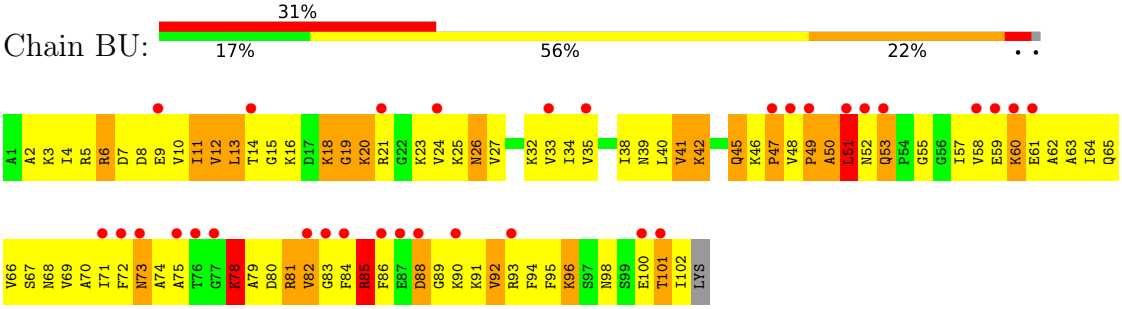
Chain DS:





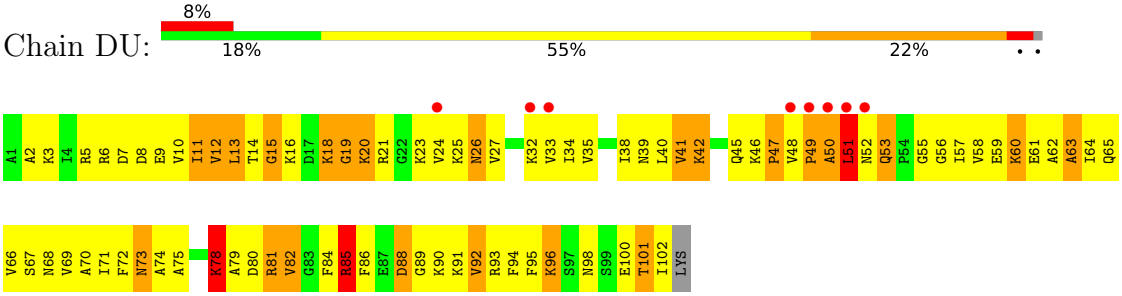
• Molecule 46: 50S ribosomal protein L24

Chain BU:



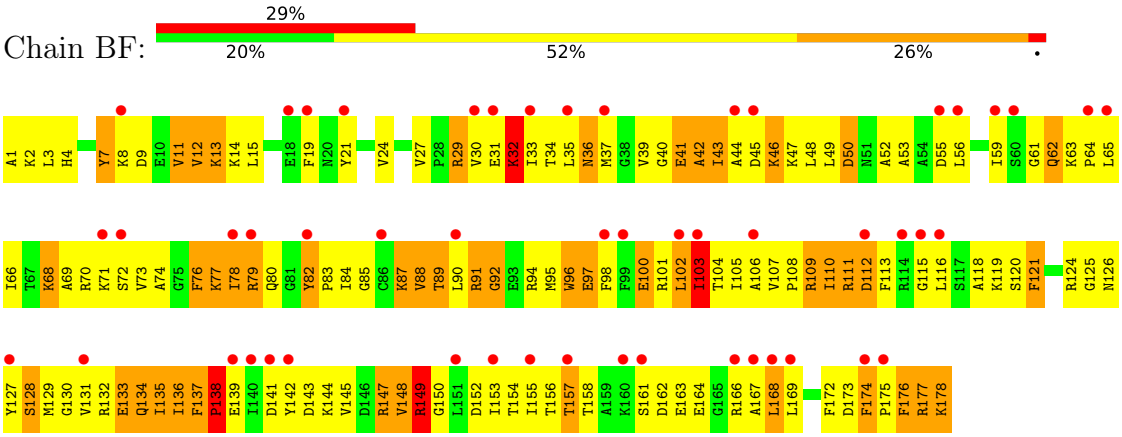
• Molecule 46: 50S ribosomal protein L24

Chain DU:



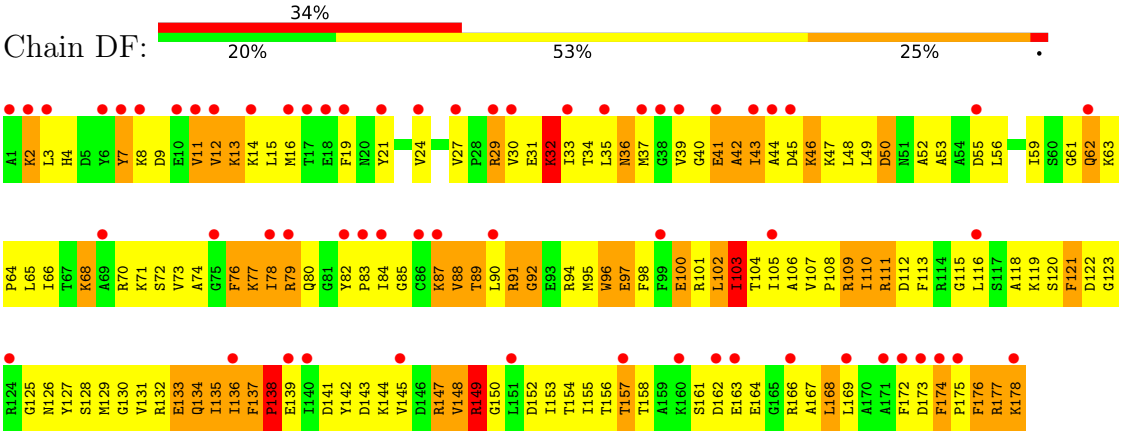
• Molecule 47: 50S ribosomal protein L5

Chain BF:



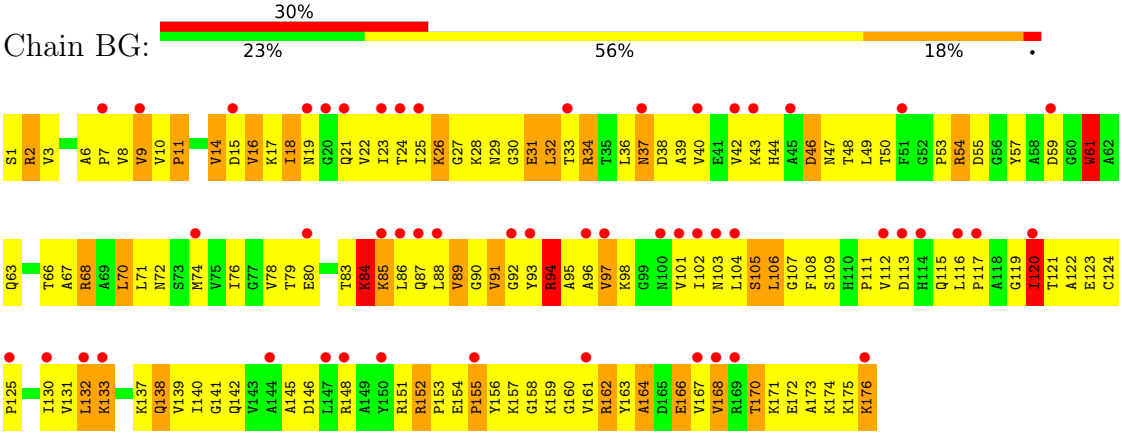
• Molecule 47: 50S ribosomal protein L5

Chain DF:



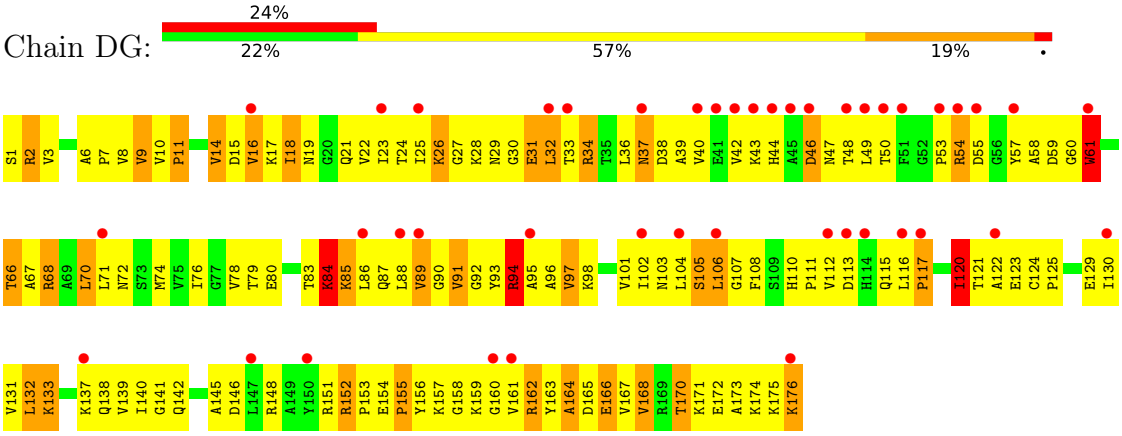
• Molecule 48: 50S ribosomal protein L6

Chain BG:



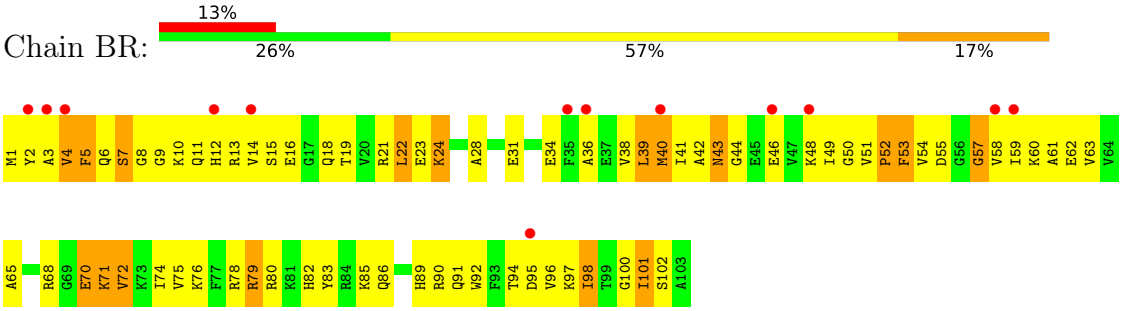
• Molecule 48: 50S ribosomal protein L6

Chain DG:



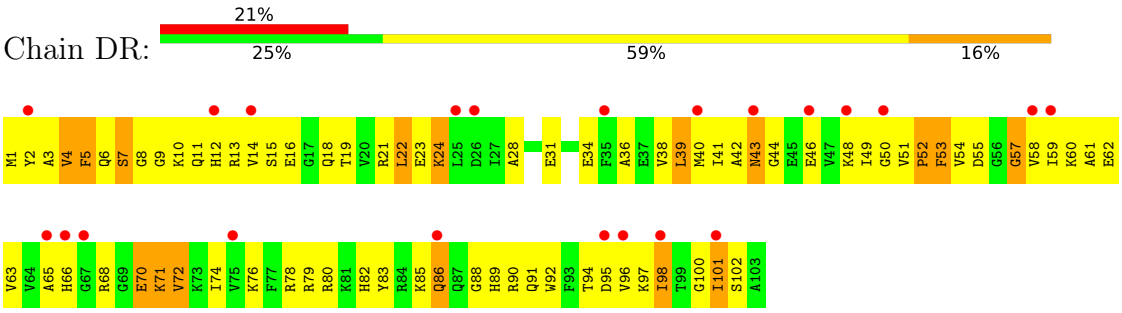
• Molecule 49: 50S ribosomal protein L21

Chain BR:



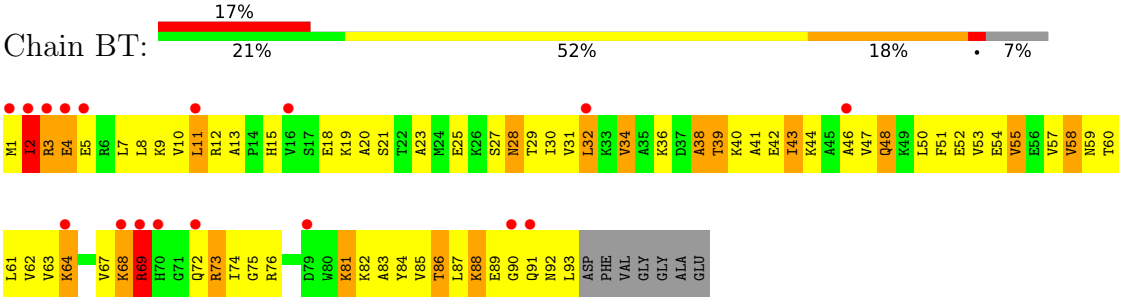
• Molecule 49: 50S ribosomal protein L21

Chain DR:



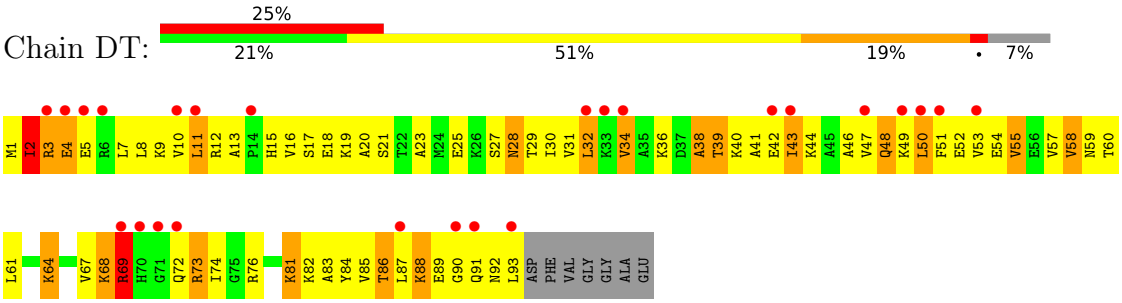
• Molecule 50: 50S ribosomal protein L23

Chain BT:



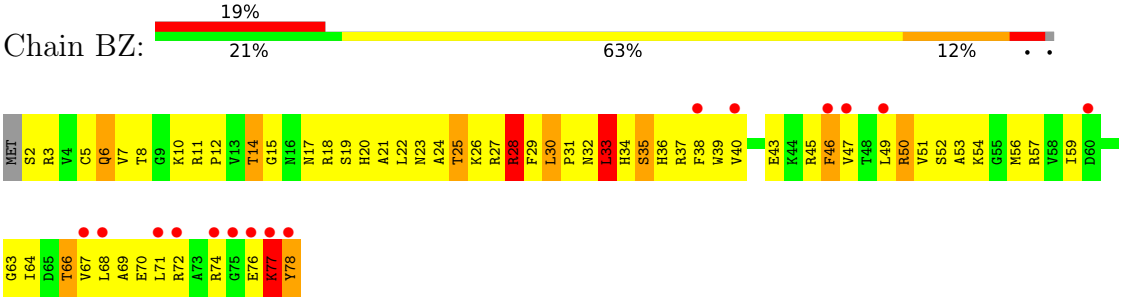
• Molecule 50: 50S ribosomal protein L23

Chain DT:



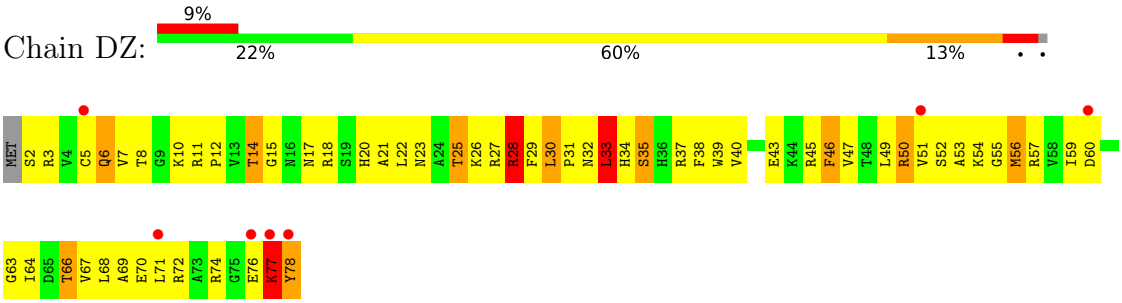
• Molecule 51: 50S ribosomal protein L28

Chain BZ:



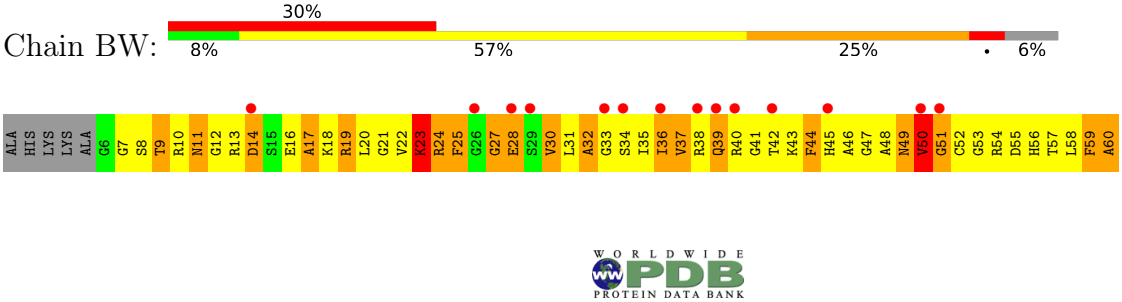
• Molecule 51: 50S ribosomal protein L28

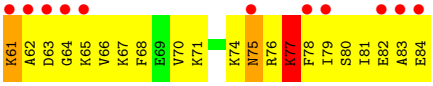
Chain DZ:



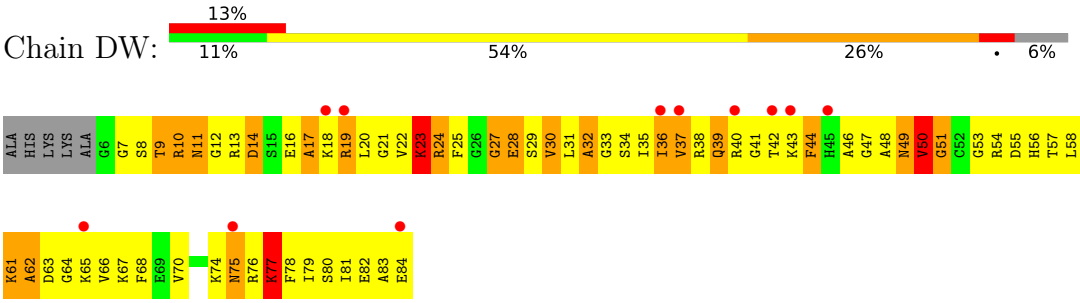
• Molecule 52: 50S ribosomal protein L27

Chain BW:





• Molecule 52: 50S ribosomal protein L27



4 Data and refinement statistics (i)

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 – 3.21 138.41 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.7 (138.41-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.309 0.240 , 0.272	Depositor DCC
R_{free} test set	30053 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	284172	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	0.25	1/36762 (0.0%)	0.75	12/57350 (0.0%)
1	CA	0.26	1/36762 (0.0%)	0.75	16/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.24	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.45	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.47	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.49	0/1300
11	CL	0.22	0/969	0.49	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.48	0/1043
13	CN	0.24	0/785	0.48	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.23	0/666	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.24	0/671	0.40	0/888
19	CT	0.24	0/671	0.40	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.24	0/2803	0.75	1/4371 (0.0%)
22	DA	0.24	0/2803	0.75	1/4371 (0.0%)
23	BB	0.28	8/68314 (0.0%)	0.77	42/106569 (0.0%)
23	DB	0.28	9/68314 (0.0%)	0.77	48/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.49	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.49	0/2134
26	DD	0.24	0/1586	0.49	0/2134
27	BK	0.24	0/939	0.56	0/1258
27	DK	0.24	0/939	0.56	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.51	0/2113
29	DE	0.24	0/1571	0.51	0/2113
30	BY	0.23	0/453	0.50	0/605
30	DY	0.23	0/453	0.50	0/605
31	B0	0.22	0/450	0.56	0/599
31	D0	0.22	0/450	0.56	0/599
32	B4	0.23	0/303	0.48	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.42	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.26	0/380	0.47	0/498
36	D2	0.26	0/380	0.47	0/498
37	BL	0.23	0/1054	0.48	0/1403
37	DL	0.24	0/1054	0.49	0/1403
38	BM	0.25	0/1093	0.49	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.53	0/677
39	DX	0.24	0/510	0.53	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.23	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.52	0/1301
42	DN	0.24	0/973	0.52	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.26	0/960	0.50	0/1278
44	DQ	0.26	0/960	0.50	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.48	0/1051
47	BF	0.26	0/1444	0.52	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.49	0/1107
49	DR	0.25	0/829	0.49	0/1107
50	BT	0.23	0/744	0.57	0/994
50	DT	0.23	0/744	0.57	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.53	0/797
52	DW	0.28	0/603	0.53	0/797
All	All	0.26	19/306360 (0.0%)	0.70	120/457969 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	13
1	CA	0	11
23	BB	0	43
23	DB	0	42
All	All	0	109

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	DB	1086	A	C5-C6	-16.27	1.26	1.41
23	BB	1086	A	C5-C6	-16.18	1.26	1.41
23	BB	1088	A	C6-N1	-10.58	1.28	1.35
23	DB	1088	A	C6-N1	-10.47	1.28	1.35
23	DB	2323	G	O3'-P	9.74	1.72	1.61

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	DB	2204	G	O5'-P-OP1	-29.64	75.14	110.70
23	BB	2204	G	O5'-P-OP2	-28.20	76.86	110.70
23	BB	2791	G	O5'-P-OP1	-27.64	77.53	110.70
23	DB	2791	G	O5'-P-OP2	-26.90	78.42	110.70
23	BB	2791	G	O5'-P-OP2	18.64	133.06	110.70

There are no chirality outliers.

5 of 109 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	78	A	Sidechain
1	AA	86	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1156	0
1	CA	32831	0	16521	1152	0
2	AC	1624	0	1699	127	0
2	CC	1624	0	1699	127	0
3	AD	1643	0	1710	158	0
3	CD	1643	0	1710	151	0
4	AE	1105	0	1148	92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	CE	1105	0	1148	95	0
5	AF	817	0	808	83	0
5	CF	817	0	808	79	0
6	AG	1174	0	1230	89	0
6	CG	1196	0	1246	88	0
7	AH	979	0	1034	83	0
7	CH	979	0	1034	82	0
8	AI	1022	0	1070	128	0
8	CI	1022	0	1070	118	0
9	AJ	786	0	828	85	0
9	CJ	786	0	828	89	0
10	AK	877	0	887	94	0
10	CK	877	0	887	93	0
11	AL	955	0	1019	75	0
11	CL	955	0	1019	73	0
12	AM	883	0	944	116	0
12	CM	876	0	937	115	0
13	AN	774	0	827	101	0
13	CN	774	0	827	105	0
14	AO	714	0	734	57	0
14	CO	714	0	734	52	0
15	AP	649	0	666	54	0
15	CP	638	0	656	51	0
16	AQ	648	0	691	42	0
16	CQ	657	0	702	45	0
17	AR	455	0	478	28	0
17	CR	455	0	478	26	0
18	AS	637	0	665	86	0
18	CS	644	0	675	89	0
19	AT	665	0	714	55	0
19	CT	665	0	714	52	0
20	AB	1704	0	1732	199	0
20	CB	1704	0	1732	199	0
21	AU	425	0	449	61	0
21	CU	425	0	449	59	0
22	BA	2507	0	1270	96	0
22	DA	2507	0	1270	89	0
23	BB	60995	0	30678	2146	0
23	DB	60995	0	30677	2248	0
24	BI	1032	0	1088	111	0
24	DI	1032	0	1088	196	0
25	BC	2082	0	2157	259	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	DC	2082	0	2157	244	0
26	BD	1565	0	1616	204	0
26	DD	1565	0	1616	214	0
27	BK	930	0	1000	117	0
27	DK	930	0	1000	121	0
28	BP	917	0	965	119	0
28	DP	917	0	965	117	0
29	BE	1552	0	1619	185	0
29	DE	1552	0	1619	165	0
30	BY	449	0	491	52	0
30	DY	449	0	491	47	0
31	B0	444	0	461	45	0
31	D0	444	0	461	46	0
32	B4	302	0	340	30	0
32	D4	302	0	341	28	0
33	B1	409	0	440	51	0
33	D1	409	0	440	42	0
34	B3	504	0	574	56	0
34	D3	504	0	574	51	0
35	BV	753	0	780	80	0
35	DV	753	0	780	83	0
36	B2	377	0	418	44	0
36	D2	377	0	418	47	0
37	BL	1045	0	1117	142	0
37	DL	1045	0	1117	152	0
38	BM	1074	0	1157	115	0
38	DM	1074	0	1157	114	0
39	BX	509	0	543	62	0
39	DX	509	0	543	58	0
40	BH	1111	0	1148	196	0
40	DH	1111	0	1148	153	0
41	BJ	1129	0	1162	146	0
41	DJ	1129	0	1162	148	0
42	BN	960	0	1000	116	0
42	DN	960	0	1000	116	0
43	BO	892	0	923	79	0
43	DO	892	0	923	91	0
44	BQ	947	0	1022	142	0
44	DQ	947	0	1022	147	0
45	BS	857	0	922	103	0
45	DS	857	0	922	100	0
46	BU	779	0	834	125	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DU	779	0	834	118	0
47	BF	1420	0	1460	231	0
47	DF	1420	0	1460	237	0
48	BG	1323	0	1374	187	0
48	DG	1323	0	1374	189	0
49	BR	816	0	839	97	0
49	DR	816	0	839	102	0
50	BT	738	0	807	129	0
50	DT	738	0	807	122	0
51	BZ	625	0	652	82	0
51	DZ	625	0	652	83	0
52	BW	596	0	610	136	0
52	DW	596	0	610	143	0
53	AA	42	0	46	2	0
53	BB	42	0	46	0	0
53	CA	42	0	46	0	0
53	DB	42	0	46	1	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	60	0	0	0	0
54	CE	1	0	0	0	0
54	CN	1	0	0	0	0
54	DB	111	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	291	0	0	2	0
56	AL	4	0	0	0	0
56	AN	4	0	0	0	0
56	AT	1	0	0	0	0
56	BB	497	0	0	8	0
56	BC	5	0	0	0	0
56	BE	1	0	0	0	0
56	BL	1	0	0	0	0
56	BN	1	0	0	0	0
56	BR	1	0	0	0	0
56	CA	298	0	0	1	0
56	CE	3	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CP	1	0	0	0	0
56	CT	1	0	0	0	0
56	DB	502	0	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DC	6	0	0	0	0
56	DE	1	0	0	0	0
56	DL	2	0	0	0	0
56	DR	1	0	0	0	0
All	All	284172	0	190846	16001	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 34.

The worst 5 of 16001 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.38	1.21
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.32	1.11
40:DH:31:VAL:HB	40:DH:32:PRO:HD2	1.30	1.11
6:CG:2:ARG:HH11	6:CG:2:ARG:HB3	1.10	1.11
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.29	1.10

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	204/232 (88%)	155 (76%)	35 (17%)	14 (7%)	1 8
2	CC	204/232 (88%)	155 (76%)	36 (18%)	13 (6%)	1 9
3	AD	203/205 (99%)	154 (76%)	34 (17%)	15 (7%)	1 7
3	CD	203/205 (99%)	151 (74%)	37 (18%)	15 (7%)	1 7
4	AE	148/166 (89%)	120 (81%)	25 (17%)	3 (2%)	7 36
4	CE	148/166 (89%)	120 (81%)	24 (16%)	4 (3%)	5 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	AF	98/135 (73%)	67 (68%)	26 (26%)	5 (5%)	2 15
5	CF	98/135 (73%)	65 (66%)	28 (29%)	5 (5%)	2 15
6	AG	148/178 (83%)	124 (84%)	18 (12%)	6 (4%)	3 19
6	CG	150/178 (84%)	127 (85%)	18 (12%)	5 (3%)	4 24
7	AH	127/129 (98%)	98 (77%)	25 (20%)	4 (3%)	4 26
7	CH	127/129 (98%)	97 (76%)	27 (21%)	3 (2%)	6 32
8	AI	125/129 (97%)	95 (76%)	20 (16%)	10 (8%)	1 5
8	CI	125/129 (97%)	97 (78%)	19 (15%)	9 (7%)	1 7
9	AJ	96/103 (93%)	73 (76%)	15 (16%)	8 (8%)	1 5
9	CJ	96/103 (93%)	74 (77%)	13 (14%)	9 (9%)	0 3
10	AK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	2 19
10	CK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	2 19
11	AL	121/123 (98%)	79 (65%)	33 (27%)	9 (7%)	1 7
11	CL	121/123 (98%)	80 (66%)	32 (26%)	9 (7%)	1 7
12	AM	112/117 (96%)	76 (68%)	27 (24%)	9 (8%)	1 5
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	1 7
13	AN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	0 2
13	CN	92/100 (92%)	58 (63%)	23 (25%)	11 (12%)	0 2
14	AO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3 23
14	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	3 23
15	AP	80/82 (98%)	60 (75%)	14 (18%)	6 (8%)	1 6
15	CP	78/82 (95%)	58 (74%)	14 (18%)	6 (8%)	1 6
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	2 15
16	CQ	79/83 (95%)	59 (75%)	16 (20%)	4 (5%)	2 15
17	AR	53/74 (72%)	43 (81%)	8 (15%)	2 (4%)	3 21
17	CR	53/74 (72%)	43 (81%)	9 (17%)	1 (2%)	8 38
18	AS	77/91 (85%)	54 (70%)	17 (22%)	6 (8%)	1 6
18	CS	78/91 (86%)	54 (69%)	17 (22%)	7 (9%)	1 4
19	AT	83/86 (96%)	65 (78%)	12 (14%)	6 (7%)	1 7
19	CT	83/86 (96%)	66 (80%)	11 (13%)	6 (7%)	1 7
20	AB	216/240 (90%)	150 (69%)	44 (20%)	22 (10%)	0 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	CB	216/240 (90%)	147 (68%)	48 (22%)	21 (10%)	0 3
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0 0
21	CU	49/70 (70%)	28 (57%)	10 (20%)	11 (22%)	0 0
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3 22
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3 22
25	BC	269/272 (99%)	174 (65%)	49 (18%)	46 (17%)	0 0
25	DC	269/272 (99%)	174 (65%)	47 (18%)	48 (18%)	0 0
26	BD	207/209 (99%)	112 (54%)	63 (30%)	32 (16%)	0 1
26	DD	207/209 (99%)	114 (55%)	58 (28%)	35 (17%)	0 0
27	BK	119/123 (97%)	75 (63%)	28 (24%)	16 (13%)	0 1
27	DK	119/123 (97%)	75 (63%)	27 (23%)	17 (14%)	0 1
28	BP	112/114 (98%)	62 (55%)	35 (31%)	15 (13%)	0 1
28	DP	112/114 (98%)	63 (56%)	34 (30%)	15 (13%)	0 1
29	BE	199/201 (99%)	131 (66%)	51 (26%)	17 (8%)	1 4
29	DE	199/201 (99%)	130 (65%)	53 (27%)	16 (8%)	1 5
30	BY	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	0 2
30	DY	56/58 (97%)	37 (66%)	13 (23%)	6 (11%)	0 2
31	B0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0 3
31	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	0 3
32	B4	36/38 (95%)	21 (58%)	7 (19%)	8 (22%)	0 0
32	D4	36/38 (95%)	20 (56%)	7 (19%)	9 (25%)	0 0
33	B1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	0 1
33	D1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	0 1
34	B3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1 5
34	D3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1 5
35	BV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	2 19
35	DV	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	2 19
36	B2	44/46 (96%)	29 (66%)	14 (32%)	1 (2%)	6 33
36	D2	44/46 (96%)	28 (64%)	15 (34%)	1 (2%)	6 33
37	BL	141/144 (98%)	88 (62%)	30 (21%)	23 (16%)	0 1
37	DL	141/144 (98%)	88 (62%)	29 (21%)	24 (17%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	BM	134/136 (98%)	86 (64%)	31 (23%)	17 (13%)	0 1
38	DM	134/136 (98%)	86 (64%)	32 (24%)	16 (12%)	0 2
39	BX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1 5
39	DX	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1 5
40	BH	147/149 (99%)	77 (52%)	41 (28%)	29 (20%)	0 0
40	DH	147/149 (99%)	85 (58%)	39 (26%)	23 (16%)	0 1
41	BJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	0 2
41	DJ	140/142 (99%)	89 (64%)	33 (24%)	18 (13%)	0 1
42	BN	118/127 (93%)	72 (61%)	34 (29%)	12 (10%)	0 3
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	0 3
43	BO	114/117 (97%)	84 (74%)	25 (22%)	5 (4%)	2 18
43	DO	114/117 (97%)	83 (73%)	25 (22%)	6 (5%)	2 14
44	BQ	115/117 (98%)	73 (64%)	34 (30%)	8 (7%)	1 7
44	DQ	115/117 (98%)	70 (61%)	38 (33%)	7 (6%)	1 11
45	BS	108/110 (98%)	69 (64%)	28 (26%)	11 (10%)	0 3
45	DS	108/110 (98%)	69 (64%)	29 (27%)	10 (9%)	0 3
46	BU	100/103 (97%)	53 (53%)	25 (25%)	22 (22%)	0 0
46	DU	100/103 (97%)	54 (54%)	23 (23%)	23 (23%)	0 0
47	BF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0 1
47	DF	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0 1
48	BG	174/176 (99%)	100 (58%)	48 (28%)	26 (15%)	0 1
48	DG	174/176 (99%)	101 (58%)	48 (28%)	25 (14%)	0 1
49	BR	101/103 (98%)	65 (64%)	25 (25%)	11 (11%)	0 2
49	DR	101/103 (98%)	64 (63%)	28 (28%)	9 (9%)	1 4
50	BT	91/100 (91%)	50 (55%)	31 (34%)	10 (11%)	0 2
50	DT	91/100 (91%)	51 (56%)	30 (33%)	10 (11%)	0 2
51	BZ	75/78 (96%)	53 (71%)	18 (24%)	4 (5%)	2 14
51	DZ	75/78 (96%)	50 (67%)	21 (28%)	4 (5%)	2 14
52	BW	77/84 (92%)	29 (38%)	27 (35%)	21 (27%)	0 0
52	DW	77/84 (92%)	29 (38%)	26 (34%)	22 (29%)	0 0
All	All	11241/11914 (94%)	7579 (67%)	2528 (22%)	1134 (10%)	0 3

5 of 1134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	153	SER
2	AC	205	GLU
5	AF	92	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AC	170/189 (90%)	137 (81%)	33 (19%)	1 7
2	CC	170/189 (90%)	137 (81%)	33 (19%)	1 7
3	AD	172/172 (100%)	148 (86%)	24 (14%)	3 15
3	CD	172/172 (100%)	148 (86%)	24 (14%)	3 15
4	AE	113/125 (90%)	95 (84%)	18 (16%)	2 11
4	CE	113/125 (90%)	95 (84%)	18 (16%)	2 11
5	AF	87/116 (75%)	71 (82%)	16 (18%)	1 8
5	CF	87/116 (75%)	70 (80%)	17 (20%)	1 7
6	AG	123/146 (84%)	104 (85%)	19 (15%)	2 12
6	CG	125/146 (86%)	103 (82%)	22 (18%)	2 9
7	AH	104/104 (100%)	95 (91%)	9 (9%)	10 36
7	CH	104/104 (100%)	94 (90%)	10 (10%)	8 31
8	AI	105/106 (99%)	88 (84%)	17 (16%)	2 11
8	CI	105/106 (99%)	87 (83%)	18 (17%)	2 9
9	AJ	86/90 (96%)	71 (83%)	15 (17%)	2 9
9	CJ	86/90 (96%)	71 (83%)	15 (17%)	2 9
10	AK	90/98 (92%)	76 (84%)	14 (16%)	2 11
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2 9
11	AL	103/103 (100%)	88 (85%)	15 (15%)	3 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	CL	103/103 (100%)	88 (85%)	15 (15%)	3 14
12	AM	92/95 (97%)	76 (83%)	16 (17%)	2 9
12	CM	91/95 (96%)	75 (82%)	16 (18%)	2 9
13	AN	79/83 (95%)	65 (82%)	14 (18%)	2 9
13	CN	79/83 (95%)	65 (82%)	14 (18%)	2 9
14	AO	76/77 (99%)	70 (92%)	6 (8%)	12 42
14	CO	76/77 (99%)	70 (92%)	6 (8%)	12 42
15	AP	65/65 (100%)	58 (89%)	7 (11%)	6 26
15	CP	65/65 (100%)	59 (91%)	6 (9%)	9 33
16	AQ	74/77 (96%)	65 (88%)	9 (12%)	5 21
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	5 21
17	AR	48/64 (75%)	40 (83%)	8 (17%)	2 10
17	CR	48/64 (75%)	41 (85%)	7 (15%)	3 14
18	AS	70/78 (90%)	56 (80%)	14 (20%)	1 6
18	CS	71/78 (91%)	57 (80%)	14 (20%)	1 6
19	AT	65/65 (100%)	54 (83%)	11 (17%)	2 10
19	CT	65/65 (100%)	54 (83%)	11 (17%)	2 10
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2 9
20	CB	180/198 (91%)	150 (83%)	30 (17%)	2 10
21	AU	44/60 (73%)	30 (68%)	14 (32%)	0 0
21	CU	44/60 (73%)	30 (68%)	14 (32%)	0 0
24	BI	109/109 (100%)	107 (98%)	2 (2%)	59 81
24	DI	109/109 (100%)	104 (95%)	5 (5%)	27 62
25	BC	216/217 (100%)	176 (82%)	40 (18%)	1 8
25	DC	216/217 (100%)	176 (82%)	40 (18%)	1 8
26	BD	164/164 (100%)	142 (87%)	22 (13%)	4 17
26	DD	164/164 (100%)	141 (86%)	23 (14%)	3 15
27	BK	102/104 (98%)	79 (78%)	23 (22%)	1 4
27	DK	102/104 (98%)	79 (78%)	23 (22%)	1 4
28	BP	99/99 (100%)	81 (82%)	18 (18%)	1 8
28	DP	99/99 (100%)	81 (82%)	18 (18%)	1 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	BE	165/165 (100%)	136 (82%)	29 (18%)	2 9
29	DE	165/165 (100%)	137 (83%)	28 (17%)	2 9
30	BY	48/48 (100%)	38 (79%)	10 (21%)	1 5
30	DY	48/48 (100%)	38 (79%)	10 (21%)	1 5
31	B0	47/47 (100%)	36 (77%)	11 (23%)	1 3
31	D0	47/47 (100%)	35 (74%)	12 (26%)	0 2
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2 9
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2 9
33	B1	45/48 (94%)	40 (89%)	5 (11%)	6 25
33	D1	45/48 (94%)	41 (91%)	4 (9%)	9 35
34	B3	51/51 (100%)	47 (92%)	4 (8%)	12 42
34	D3	51/51 (100%)	47 (92%)	4 (8%)	12 42
35	BV	78/78 (100%)	62 (80%)	16 (20%)	1 6
35	DV	78/78 (100%)	62 (80%)	16 (20%)	1 6
36	B2	38/38 (100%)	32 (84%)	6 (16%)	2 11
36	D2	38/38 (100%)	32 (84%)	6 (16%)	2 11
37	BL	102/103 (99%)	89 (87%)	13 (13%)	4 19
37	DL	102/103 (99%)	88 (86%)	14 (14%)	3 16
38	BM	109/109 (100%)	91 (84%)	18 (16%)	2 10
38	DM	109/109 (100%)	91 (84%)	18 (16%)	2 10
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0 1
39	DX	55/55 (100%)	40 (73%)	15 (27%)	0 1
40	BH	114/114 (100%)	64 (56%)	50 (44%)	0 0
40	DH	114/114 (100%)	86 (75%)	28 (25%)	0 2
41	BJ	116/116 (100%)	101 (87%)	15 (13%)	4 19
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	3 16
42	BN	100/103 (97%)	87 (87%)	13 (13%)	4 18
42	DN	100/103 (97%)	87 (87%)	13 (13%)	4 18
43	BO	86/87 (99%)	70 (81%)	16 (19%)	1 8
43	DO	86/87 (99%)	70 (81%)	16 (19%)	1 8
44	BQ	89/89 (100%)	74 (83%)	15 (17%)	2 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
44	DQ	89/89 (100%)	74 (83%)	15 (17%)	2 10
45	BS	93/93 (100%)	79 (85%)	14 (15%)	3 13
45	DS	93/93 (100%)	79 (85%)	14 (15%)	3 13
46	BU	83/84 (99%)	68 (82%)	15 (18%)	1 8
46	DU	83/84 (99%)	68 (82%)	15 (18%)	1 8
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1 3
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1 4
48	BG	137/137 (100%)	113 (82%)	24 (18%)	2 9
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2 9
49	BR	84/84 (100%)	73 (87%)	11 (13%)	4 18
49	DR	84/84 (100%)	73 (87%)	11 (13%)	4 18
50	BT	80/84 (95%)	66 (82%)	14 (18%)	2 9
50	DT	80/84 (95%)	65 (81%)	15 (19%)	1 8
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1 4
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1 4
52	BW	59/62 (95%)	45 (76%)	14 (24%)	1 3
52	DW	59/62 (95%)	45 (76%)	14 (24%)	1 3
All	All	9333/9700 (96%)	7746 (83%)	1587 (17%)	2 9

5 of 1587 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	CI	55	ASP
25	DC	187	CYS
9	CJ	90	LEU
8	CI	45	MET
17	CR	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 343 such sidechains are listed below:

Mol	Chain	Res	Type
18	CS	42	ASN
36	D2	6	GLN
20	CB	23	ASN
26	DD	126	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	DJ	40	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	239 (15%)	16 (1%)
1	CA	1529/1542 (99%)	229 (14%)	17 (1%)
22	BA	116/120 (96%)	17 (14%)	1 (0%)
22	DA	116/120 (96%)	17 (14%)	1 (0%)
23	BB	2837/2904 (97%)	435 (15%)	18 (0%)
23	DB	2837/2904 (97%)	433 (15%)	20 (0%)
All	All	8964/9132 (98%)	1370 (15%)	73 (0%)

5 of 1370 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 73 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	DB	546	U
23	DB	2832	U
23	DB	858	G
23	DB	2213	U
23	BB	1419	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 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	NMY	CA	1601	-	45,45,45	2.02	12 (26%)	63,67,67	1.29	8 (12%)
53	NMY	BB	3001	-	45,45,45	2.05	13 (28%)	63,67,67	1.20	7 (11%)
53	NMY	DB	3001	-	45,45,45	2.10	13 (28%)	63,67,67	1.30	7 (11%)
53	NMY	AA	1601	-	45,45,45	2.03	13 (28%)	63,67,67	1.18	5 (7%)

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	NMY	CA	1601	-	-	5/18/94/94	0/4/4/4
53	NMY	BB	3001	-	-	4/18/94/94	0/4/4/4
53	NMY	DB	3001	-	-	4/18/94/94	0/4/4/4
53	NMY	AA	1601	-	-	4/18/94/94	0/4/4/4

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DB	3001	NMY	C23-C22	5.27	1.59	1.52
53	BB	3001	NMY	C23-C22	5.17	1.59	1.52
53	AA	1601	NMY	C23-C22	5.06	1.58	1.52
53	CA	1601	NMY	C23-C22	4.92	1.58	1.52
53	CA	1601	NMY	O22-C18	4.78	1.54	1.41

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DB	3001	NMY	O11-C13-O16	4.60	116.41	111.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	DB	3001	NMY	O18-C18-C19	4.01	115.12	108.22
53	CA	1601	NMY	O18-C18-C19	3.75	114.67	108.22
53	BB	3001	NMY	O18-C18-C19	3.63	114.46	108.22
53	AA	1601	NMY	O18-C18-C19	3.50	114.24	108.22

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	AA	1601	NMY	O16-C16-C17-O17
53	BB	3001	NMY	C19-C18-O18-C15
53	CA	1601	NMY	C14-C13-O11-C11
53	DB	3001	NMY	C19-C18-O18-C15
53	CA	1601	NMY	O16-C16-C17-O17

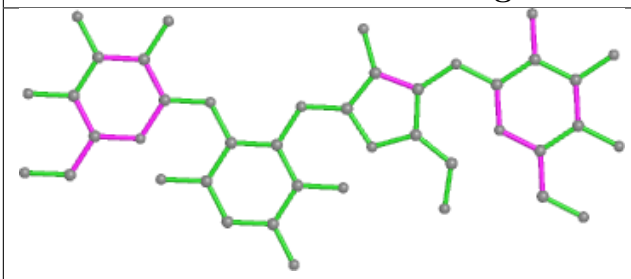
There are no ring outliers.

2 monomers are involved in 3 short contacts:

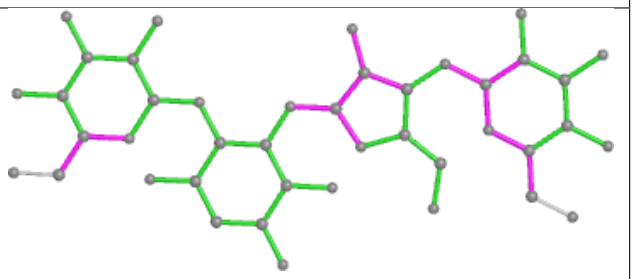
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	DB	3001	NMY	1	0
53	AA	1601	NMY	2	0

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 then 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.

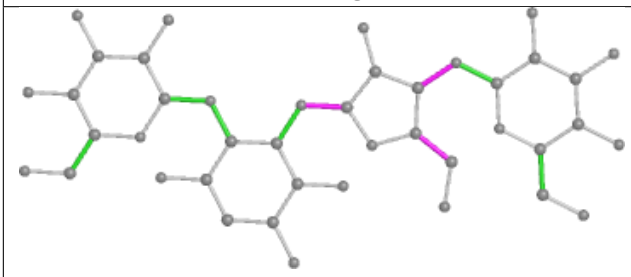
Ligand NMY CA 1601



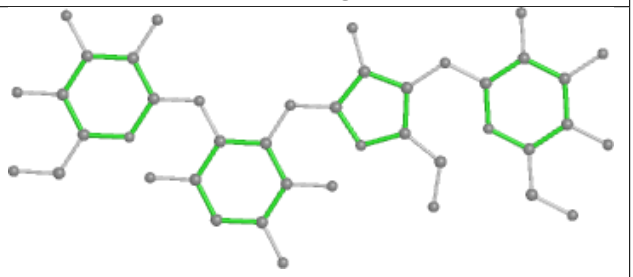
Bond lengths



Bond angles

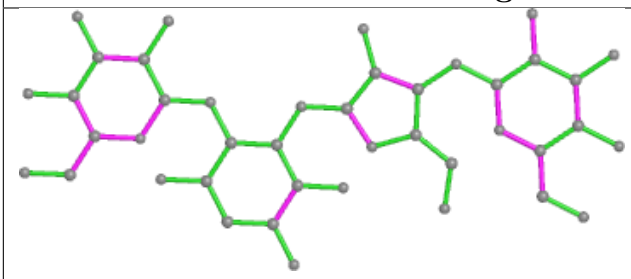


Torsions

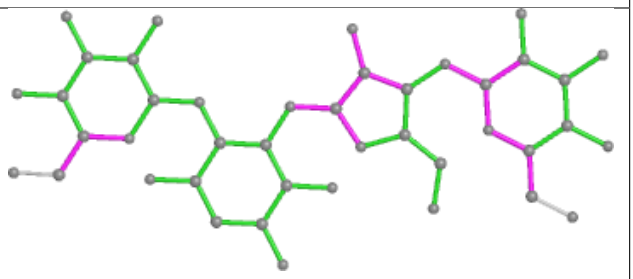


Rings

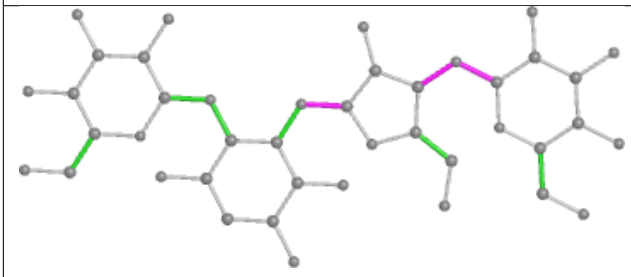
Ligand NMY BB 3001



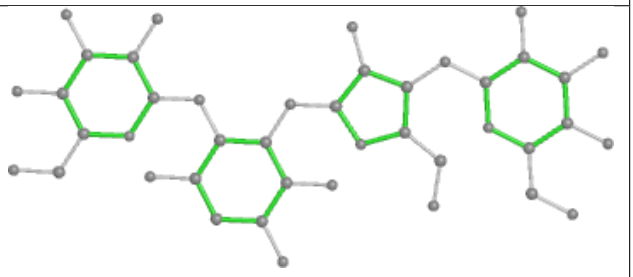
Bond lengths



Bond angles

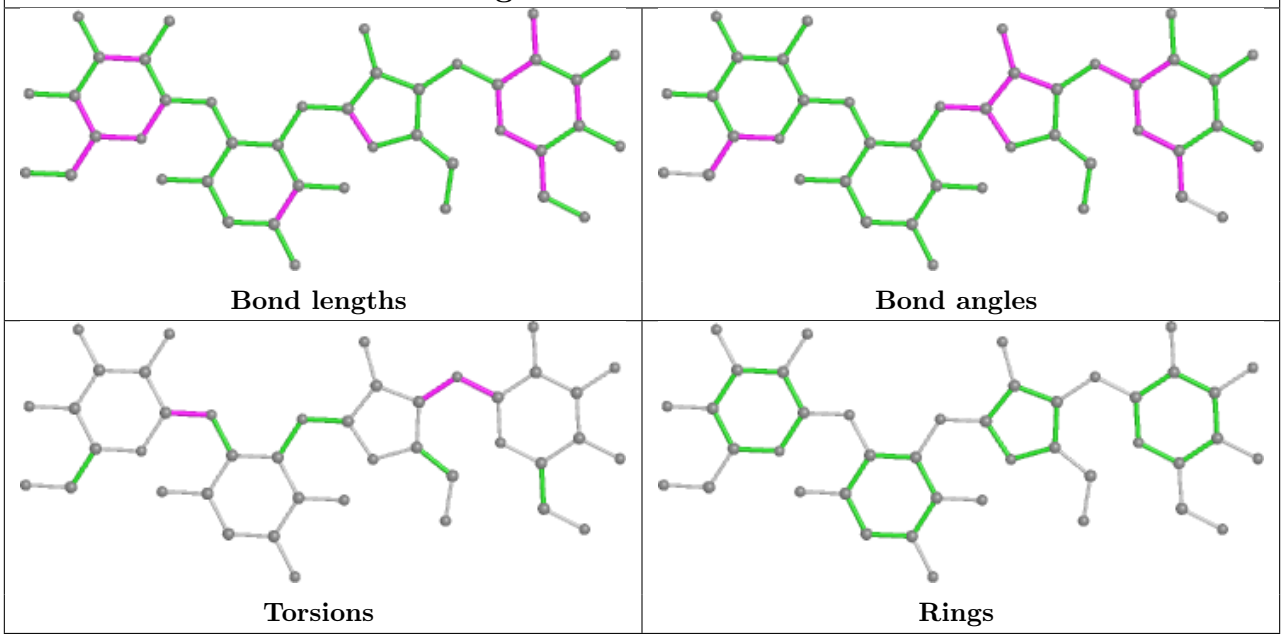


Torsions

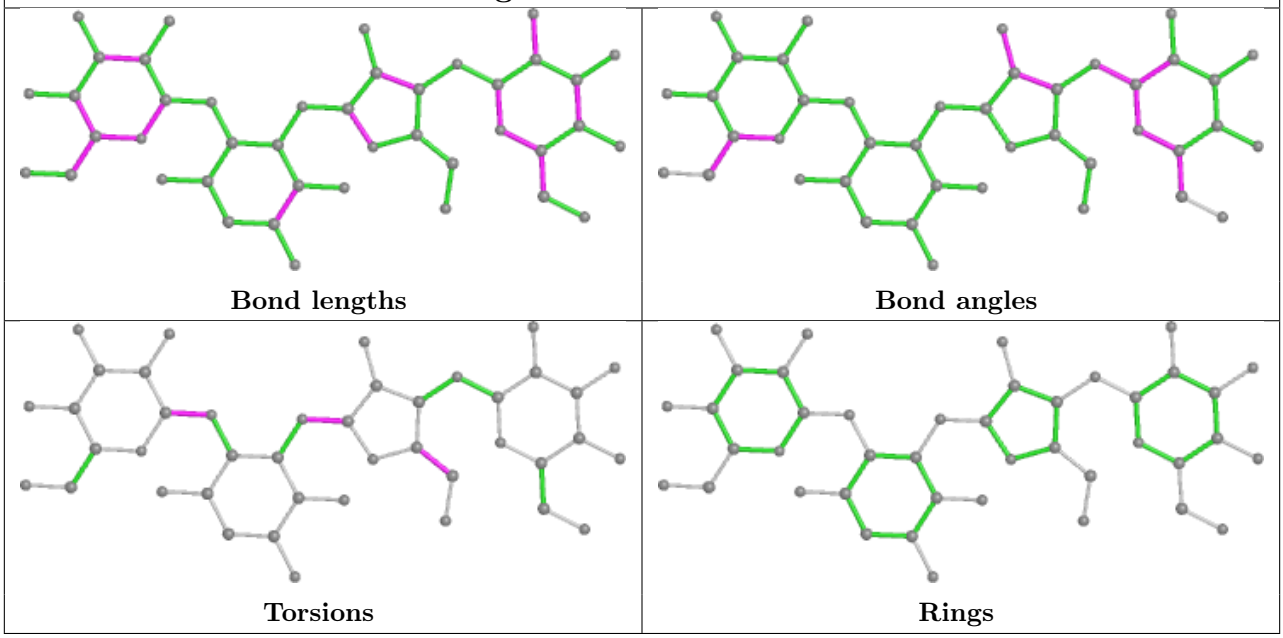


Rings

Ligand NMY DB 3001



Ligand NMY AA 1601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1530/1542 (99%)	-0.62	11 (0%) 87 82	22, 76, 152, 180	0
1	CA	1530/1542 (99%)	-0.63	3 (0%) 95 94	12, 57, 136, 180	0
2	AC	206/232 (88%)	0.76	34 (16%) 1 1	16, 66, 135, 180	0
2	CC	206/232 (88%)	0.73	28 (13%) 3 2	14, 74, 124, 180	0
3	AD	205/205 (100%)	1.28	52 (25%) 0 0	8, 84, 155, 180	0
3	CD	205/205 (100%)	0.85	28 (13%) 3 2	15, 62, 135, 180	0
4	AE	150/166 (90%)	0.71	15 (10%) 7 4	7, 67, 122, 158	0
4	CE	150/166 (90%)	1.10	33 (22%) 0 0	10, 59, 122, 180	0
5	AF	100/135 (74%)	1.48	31 (31%) 0 0	32, 80, 148, 180	0
5	CF	100/135 (74%)	0.97	15 (15%) 2 1	23, 69, 138, 180	0
6	AG	150/178 (84%)	0.70	23 (15%) 2 1	39, 105, 151, 180	0
6	CG	152/178 (85%)	0.22	9 (5%) 22 13	32, 89, 152, 180	0
7	AH	129/129 (100%)	1.30	40 (31%) 0 0	29, 79, 133, 180	0
7	CH	129/129 (100%)	0.61	17 (13%) 3 2	7, 55, 120, 148	0
8	AI	127/129 (98%)	0.80	25 (19%) 1 0	37, 90, 164, 180	0
8	CI	127/129 (98%)	0.59	16 (12%) 3 2	32, 95, 162, 180	0
9	AJ	98/103 (95%)	0.96	19 (19%) 1 0	17, 85, 158, 180	0
9	CJ	98/103 (95%)	1.06	22 (22%) 0 0	22, 89, 150, 180	0
10	AK	117/128 (91%)	0.47	7 (5%) 21 13	17, 63, 128, 162	0
10	CK	117/128 (91%)	0.14	2 (1%) 70 58	10, 51, 116, 164	0
11	AL	123/123 (100%)	0.85	18 (14%) 2 1	19, 74, 135, 180	0
11	CL	123/123 (100%)	0.58	6 (4%) 29 18	6, 50, 127, 180	0
12	AM	114/117 (97%)	0.64	16 (14%) 2 2	52, 119, 180, 180	0
12	CM	113/117 (96%)	0.70	16 (14%) 2 2	53, 105, 167, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AN	96/100 (96%)	0.56	8 (8%) 11 6	24, 79, 118, 152	0
13	CN	96/100 (96%)	0.61	12 (12%) 3 2	26, 82, 119, 139	0
14	AO	88/89 (98%)	1.20	21 (23%) 0 0	39, 76, 123, 180	0
14	CO	88/89 (98%)	0.35	3 (3%) 45 31	15, 55, 123, 154	0
15	AP	82/82 (100%)	1.47	19 (23%) 0 0	30, 86, 150, 180	0
15	CP	80/82 (97%)	0.58	10 (12%) 3 2	8, 56, 135, 180	0
16	AQ	80/83 (96%)	1.20	21 (26%) 0 0	49, 96, 155, 180	0
16	CQ	81/83 (97%)	0.56	8 (9%) 7 5	25, 66, 128, 180	0
17	AR	55/74 (74%)	0.98	8 (14%) 2 1	15, 74, 125, 165	0
17	CR	55/74 (74%)	0.65	7 (12%) 3 2	19, 63, 119, 170	0
18	AS	79/91 (86%)	0.96	19 (24%) 0 0	73, 121, 176, 180	0
18	CS	80/91 (87%)	0.97	16 (20%) 1 0	58, 109, 168, 180	0
19	AT	85/86 (98%)	0.45	9 (10%) 6 4	52, 104, 164, 180	0
19	CT	85/86 (98%)	0.05	4 (4%) 31 20	22, 62, 125, 179	0
20	AB	218/240 (90%)	0.89	45 (20%) 1 0	29, 99, 155, 180	0
20	CB	218/240 (90%)	1.28	65 (29%) 0 0	31, 102, 160, 180	0
21	AU	51/70 (72%)	1.03	11 (21%) 0 0	43, 92, 146, 180	0
21	CU	51/70 (72%)	0.71	6 (11%) 4 3	40, 85, 133, 166	0
22	BA	117/120 (97%)	-0.68	1 (0%) 84 76	49, 83, 138, 174	0
22	DA	117/120 (97%)	-0.58	1 (0%) 84 76	36, 75, 124, 180	0
23	BB	2841/2904 (97%)	-0.38	27 (0%) 82 73	16, 60, 154, 180	0
23	DB	2841/2904 (97%)	-0.41	10 (0%) 92 89	6, 47, 151, 180	0
24	BI	141/141 (100%)	3.62	97 (68%) 0 0	93, 176, 180, 180	0
24	DI	141/141 (100%)	1.95	60 (42%) 0 0	101, 177, 180, 180	0
25	BC	271/272 (99%)	0.91	43 (15%) 1 1	9, 50, 104, 180	0
25	DC	271/272 (99%)	0.84	38 (14%) 2 2	5, 35, 87, 135	0
26	BD	209/209 (100%)	0.91	38 (18%) 1 1	20, 76, 135, 180	0
26	DD	209/209 (100%)	1.00	36 (17%) 1 1	5, 50, 126, 180	0
27	BK	121/123 (98%)	1.90	50 (41%) 0 0	14, 72, 133, 180	0
27	DK	121/123 (98%)	1.25	26 (21%) 0 0	6, 43, 104, 164	0
28	BP	114/114 (100%)	1.94	52 (45%) 0 0	35, 86, 151, 180	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DP	114/114 (100%)	0.68	12 (10%) 6 4	6, 49, 113, 160	0
29	BE	201/201 (100%)	1.42	65 (32%) 0 0	10, 67, 144, 180	0
29	DE	201/201 (100%)	0.99	37 (18%) 1 0	5, 72, 137, 180	0
30	BY	58/58 (100%)	0.83	11 (18%) 1 0	34, 74, 139, 180	0
30	DY	58/58 (100%)	0.60	9 (15%) 2 1	21, 60, 141, 177	0
31	B0	56/56 (100%)	0.84	8 (14%) 2 2	15, 74, 151, 180	0
31	D0	56/56 (100%)	0.49	4 (7%) 16 10	9, 49, 124, 180	0
32	B4	38/38 (100%)	0.78	6 (15%) 2 1	35, 91, 145, 151	0
32	D4	38/38 (100%)	-0.13	0 100 100	18, 68, 129, 150	0
33	B1	50/54 (92%)	2.09	20 (40%) 0 0	52, 90, 134, 174	0
33	D1	50/54 (92%)	1.17	11 (22%) 0 0	14, 76, 127, 175	0
34	B3	64/64 (100%)	1.02	15 (23%) 0 0	26, 59, 87, 158	0
34	D3	64/64 (100%)	0.79	9 (14%) 2 2	9, 49, 112, 156	0
35	BV	94/94 (100%)	0.90	18 (19%) 1 0	29, 97, 155, 178	0
35	DV	94/94 (100%)	1.02	23 (24%) 0 0	21, 89, 153, 167	0
36	B2	46/46 (100%)	0.55	3 (6%) 18 11	14, 50, 83, 144	0
36	D2	46/46 (100%)	0.48	2 (4%) 35 23	5, 38, 76, 180	0
37	BL	143/144 (99%)	0.87	26 (18%) 1 1	25, 70, 133, 180	0
37	DL	143/144 (99%)	1.21	38 (26%) 0 0	9, 59, 117, 147	0
38	BM	136/136 (100%)	1.00	19 (13%) 2 2	21, 68, 136, 180	0
38	DM	136/136 (100%)	0.65	14 (10%) 6 4	13, 54, 118, 167	0
39	BX	63/63 (100%)	1.59	25 (39%) 0 0	21, 81, 149, 175	0
39	DX	63/63 (100%)	0.52	5 (7%) 12 7	38, 97, 156, 180	0
40	BH	149/149 (100%)	4.15	104 (69%) 0 0	31, 134, 180, 180	0
40	DH	149/149 (100%)	1.89	63 (42%) 0 0	32, 110, 160, 180	0
41	BJ	142/142 (100%)	1.05	32 (22%) 0 0	23, 82, 140, 169	0
41	DJ	142/142 (100%)	0.75	13 (9%) 9 5	17, 61, 126, 180	0
42	BN	120/127 (94%)	0.91	23 (19%) 1 0	24, 71, 139, 180	0
42	DN	120/127 (94%)	0.33	5 (4%) 36 24	7, 43, 91, 172	0
43	BO	116/117 (99%)	1.00	28 (24%) 0 0	35, 83, 145, 180	0
43	DO	116/117 (99%)	0.50	7 (6%) 21 13	19, 73, 135, 172	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BQ	117/117 (100%)	0.29	8 (6%) 17 10	10, 66, 129, 167	0
44	DQ	117/117 (100%)	0.76	12 (10%) 6 4	8, 50, 104, 180	0
45	BS	110/110 (100%)	1.58	40 (36%) 0 0	6, 62, 123, 152	0
45	DS	110/110 (100%)	1.55	32 (29%) 0 0	12, 48, 129, 180	0
46	BU	102/103 (99%)	1.58	32 (31%) 0 0	21, 77, 140, 180	0
46	DU	102/103 (99%)	0.29	8 (7%) 13 7	22, 94, 154, 180	0
47	BF	178/178 (100%)	1.32	51 (28%) 0 0	56, 128, 177, 180	0
47	DF	178/178 (100%)	1.81	61 (34%) 0 0	30, 107, 168, 180	0
48	BG	176/176 (100%)	1.36	52 (29%) 0 0	49, 112, 163, 180	0
48	DG	176/176 (100%)	1.18	43 (24%) 0 0	35, 97, 161, 180	0
49	BR	103/103 (100%)	0.59	13 (12%) 3 2	25, 87, 151, 176	0
49	DR	103/103 (100%)	1.09	22 (21%) 0 0	23, 76, 139, 161	0
50	BT	93/100 (93%)	1.06	17 (18%) 1 0	22, 77, 159, 180	0
50	DT	93/100 (93%)	1.07	25 (26%) 0 0	24, 64, 156, 179	0
51	BZ	77/78 (98%)	0.93	15 (19%) 1 0	12, 51, 112, 143	0
51	DZ	77/78 (98%)	0.56	7 (9%) 9 5	9, 48, 94, 128	0
52	BW	79/84 (94%)	1.57	25 (31%) 0 0	18, 85, 141, 159	0
52	DW	79/84 (94%)	0.86	11 (13%) 2 2	20, 71, 134, 180	0
All	All	20417/21046 (97%)	0.37	2386 (11%) 4 3	5, 69, 156, 180	0

The worst 5 of 2386 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	84	ALA	19.9
40	BH	85	GLY	18.2
40	BH	142	VAL	14.1
40	BH	130	VAL	14.0
40	BH	86	ASP	13.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	DB	3067	1/1	0.11	0.13	178,178,178,178	0
54	MG	AA	1660	1/1	0.24	0.35	163,163,163,163	0
54	MG	AA	1603	1/1	0.41	0.15	133,133,133,133	0
54	MG	AA	1615	1/1	0.46	0.08	110,110,110,110	0
54	MG	DB	3061	1/1	0.48	0.08	115,115,115,115	0
54	MG	BB	3101	1/1	0.54	0.12	138,138,138,138	0
54	MG	AA	1626	1/1	0.55	0.19	64,64,64,64	1
54	MG	AA	1638	1/1	0.56	0.36	147,147,147,147	0
53	NMY	BB	3001	42/42	0.59	0.49	100,100,100,100	42
54	MG	BB	3011	1/1	0.65	0.13	66,66,66,66	0
54	MG	BB	3098	1/1	0.67	0.12	80,80,80,80	0
54	MG	CA	1635	1/1	0.68	0.09	96,96,96,96	0
53	NMY	DB	3001	42/42	0.68	0.53	88,88,88,88	42
54	MG	AA	1623	1/1	0.68	0.28	129,129,129,129	0
54	MG	DB	3053	1/1	0.70	0.09	102,102,102,102	0
54	MG	AA	1636	1/1	0.70	0.12	88,88,88,88	0
54	MG	CA	1657	1/1	0.70	0.15	91,91,91,91	0
54	MG	CA	1619	1/1	0.72	0.09	59,59,59,59	0
54	MG	DB	3096	1/1	0.72	0.11	127,127,127,127	0
54	MG	BB	3034	1/1	0.73	0.23	136,136,136,136	0
54	MG	DB	3084	1/1	0.74	0.20	92,92,92,92	0
54	MG	AA	1650	1/1	0.74	0.06	114,114,114,114	0
54	MG	CA	1609	1/1	0.76	0.13	121,121,121,121	0
54	MG	CA	1612	1/1	0.76	0.10	84,84,84,84	0
54	MG	BB	3044	1/1	0.77	0.12	108,108,108,108	0
54	MG	DB	3059	1/1	0.77	1.44	180,180,180,180	0
54	MG	BB	3048	1/1	0.78	0.13	128,128,128,128	0
54	MG	CA	1642	1/1	0.78	0.09	94,94,94,94	0
54	MG	AA	1619	1/1	0.78	0.13	85,85,85,85	0
54	MG	AA	1620	1/1	0.79	0.18	130,130,130,130	0
54	MG	CA	1616	1/1	0.79	0.09	167,167,167,167	0
54	MG	AA	1653	1/1	0.79	0.09	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BB	3043	1/1	0.80	0.08	170,170,170,170	0
54	MG	DB	3060	1/1	0.80	0.24	124,124,124,124	0
54	MG	BB	3079	1/1	0.80	0.12	75,75,75,75	0
54	MG	BB	3058	1/1	0.81	0.17	76,76,76,76	0
54	MG	DB	3031	1/1	0.81	0.24	32,32,32,32	0
54	MG	BB	3095	1/1	0.81	0.15	46,46,46,46	0
54	MG	DB	3097	1/1	0.81	0.21	33,33,33,33	0
54	MG	AA	1609	1/1	0.83	0.20	127,127,127,127	0
54	MG	BB	3039	1/1	0.83	0.07	131,131,131,131	0
54	MG	AA	1640	1/1	0.84	0.24	104,104,104,104	0
54	MG	BB	3029	1/1	0.84	0.22	32,32,32,32	0
54	MG	CA	1615	1/1	0.84	0.07	41,41,41,41	0
54	MG	DB	3051	1/1	0.84	0.08	87,87,87,87	0
54	MG	BB	3020	1/1	0.85	0.09	45,45,45,45	0
54	MG	BB	3082	1/1	0.85	0.33	59,59,59,59	0
54	MG	DB	3035	1/1	0.85	0.20	81,81,81,81	0
54	MG	AA	1647	1/1	0.85	0.13	87,87,87,87	0
54	MG	AA	1627	1/1	0.86	0.10	15,15,15,15	1
54	MG	DB	3017	1/1	0.86	0.08	6,6,6,6	0
54	MG	AA	1657	1/1	0.86	0.09	69,69,69,69	0
54	MG	DB	3034	1/1	0.86	0.08	43,43,43,43	0
54	MG	CA	1621	1/1	0.86	0.31	118,118,118,118	0
54	MG	BB	3052	1/1	0.86	0.09	59,59,59,59	0
54	MG	AA	1621	1/1	0.86	0.07	85,85,85,85	0
54	MG	CE	201	1/1	0.87	0.08	97,97,97,97	0
54	MG	DB	3005	1/1	0.87	0.20	30,30,30,30	0
54	MG	CA	1636	1/1	0.87	0.08	56,56,56,56	0
54	MG	BB	3055	1/1	0.87	0.06	58,58,58,58	0
54	MG	AA	1637	1/1	0.87	0.10	89,89,89,89	0
54	MG	AA	1606	1/1	0.88	0.05	47,47,47,47	0
54	MG	CA	1643	1/1	0.88	0.10	43,43,43,43	0
54	MG	AA	1625	1/1	0.88	0.11	72,72,72,72	0
54	MG	CA	1623	1/1	0.88	0.03	131,131,131,131	0
54	MG	AA	1641	1/1	0.88	0.11	56,56,56,56	0
53	NMY	AA	1601	42/42	0.88	0.29	71,71,71,71	0
54	MG	DB	3104	1/1	0.88	0.09	21,21,21,21	0
54	MG	DB	3058	1/1	0.89	0.05	43,43,43,43	0
54	MG	AA	1661	1/1	0.89	0.11	79,79,79,79	0
54	MG	DB	3016	1/1	0.89	0.11	49,49,49,49	0
54	MG	AA	1624	1/1	0.89	0.32	32,32,32,32	1
54	MG	CA	1638	1/1	0.89	0.17	142,142,142,142	0
54	MG	BB	3019	1/1	0.89	0.10	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	AA	1658	1/1	0.89	0.33	115,115,115,115	0
54	MG	CA	1622	1/1	0.89	0.10	75,75,75,75	0
53	NMY	CA	1601	42/42	0.89	0.25	71,71,71,71	0
54	MG	AA	1628	1/1	0.90	0.14	57,57,57,57	0
54	MG	CA	1620	1/1	0.90	0.17	70,70,70,70	0
54	MG	DB	3029	1/1	0.90	0.07	33,33,33,33	0
54	MG	BB	3081	1/1	0.90	0.21	52,52,52,52	0
54	MG	AA	1617	1/1	0.90	0.07	45,45,45,45	0
54	MG	BB	3018	1/1	0.90	0.07	43,43,43,43	0
54	MG	DB	3038	1/1	0.90	0.15	17,17,17,17	0
54	MG	CA	1634	1/1	0.90	0.12	8,8,8,8	0
54	MG	BB	3032	1/1	0.90	0.10	45,45,45,45	0
54	MG	DB	3110	1/1	0.90	0.08	19,19,19,19	0
54	MG	AA	1651	1/1	0.91	0.06	109,109,109,109	0
54	MG	AA	1616	1/1	0.91	0.10	77,77,77,77	0
54	MG	BB	3091	1/1	0.91	0.09	75,75,75,75	0
54	MG	BB	3094	1/1	0.91	0.22	93,93,93,93	0
54	MG	AA	1654	1/1	0.91	0.13	51,51,51,51	0
54	MG	BB	3096	1/1	0.91	0.12	42,42,42,42	0
54	MG	BB	3014	1/1	0.91	0.05	42,42,42,42	0
54	MG	DB	3023	1/1	0.91	0.10	29,29,29,29	0
54	MG	DB	3072	1/1	0.91	0.08	30,30,30,30	0
54	MG	AA	1635	1/1	0.91	0.13	45,45,45,45	0
54	MG	DB	3030	1/1	0.91	0.13	74,74,74,74	0
54	MG	CA	1607	1/1	0.91	0.12	100,100,100,100	0
54	MG	BB	3078	1/1	0.91	0.06	32,32,32,32	0
54	MG	DB	3107	1/1	0.91	0.10	27,27,27,27	0
54	MG	AA	1613	1/1	0.91	0.07	65,65,65,65	0
54	MG	BB	3040	1/1	0.92	0.10	28,28,28,28	0
54	MG	DB	3062	1/1	0.92	0.04	47,47,47,47	0
54	MG	CA	1627	1/1	0.92	0.08	29,29,29,29	1
54	MG	AA	1648	1/1	0.92	0.48	94,94,94,94	0
54	MG	DB	3078	1/1	0.92	0.13	46,46,46,46	0
54	MG	AA	1642	1/1	0.92	0.07	59,59,59,59	0
54	MG	DB	3086	1/1	0.92	0.11	18,18,18,18	0
54	MG	DB	3091	1/1	0.92	0.07	47,47,47,47	0
54	MG	BB	3089	1/1	0.92	0.07	45,45,45,45	0
54	MG	BB	3111	1/1	0.92	0.14	81,81,81,81	0
54	MG	DB	3024	1/1	0.92	0.05	55,55,55,55	0
54	MG	BB	3061	1/1	0.92	0.14	41,41,41,41	0
54	MG	AA	1630	1/1	0.92	0.07	35,35,35,35	0
54	MG	AA	1632	1/1	0.93	0.14	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	AA	1622	1/1	0.93	0.06	27,27,27,27	0
54	MG	CA	1610	1/1	0.93	0.04	79,79,79,79	0
54	MG	BB	3004	1/1	0.93	0.07	38,38,38,38	0
54	MG	DB	3037	1/1	0.93	0.07	15,15,15,15	0
54	MG	CA	1641	1/1	0.93	0.09	63,63,63,63	0
54	MG	DB	3046	1/1	0.93	0.13	55,55,55,55	0
54	MG	BB	3023	1/1	0.93	0.22	41,41,41,41	0
54	MG	BB	3025	1/1	0.93	0.08	14,14,14,14	0
54	MG	DB	3054	1/1	0.93	0.10	65,65,65,65	0
54	MG	CA	1648	1/1	0.93	0.11	55,55,55,55	0
54	MG	CA	1652	1/1	0.93	0.17	77,77,77,77	0
54	MG	CA	1654	1/1	0.93	0.05	78,78,78,78	0
54	MG	BB	3010	1/1	0.93	0.08	82,82,82,82	0
54	MG	CA	1658	1/1	0.93	0.09	52,52,52,52	0
54	MG	CA	1660	1/1	0.93	0.06	69,69,69,69	0
54	MG	CA	1661	1/1	0.93	0.08	61,61,61,61	0
54	MG	BB	3030	1/1	0.93	0.09	36,36,36,36	0
54	MG	DB	3081	1/1	0.93	0.12	18,18,18,18	0
54	MG	CN	201	1/1	0.93	0.07	48,48,48,48	0
54	MG	AA	1612	1/1	0.93	0.06	37,37,37,37	0
54	MG	DB	3014	1/1	0.93	0.14	48,48,48,48	0
54	MG	DB	3093	1/1	0.93	0.09	67,67,67,67	0
54	MG	AA	1652	1/1	0.93	0.06	73,73,73,73	0
54	MG	BB	3073	1/1	0.93	0.10	67,67,67,67	0
54	MG	DB	3098	1/1	0.93	0.15	36,36,36,36	0
54	MG	CA	1626	1/1	0.93	0.15	8,8,8,8	1
54	MG	BB	3038	1/1	0.93	0.08	50,50,50,50	0
54	MG	CA	1629	1/1	0.93	0.08	46,46,46,46	1
54	MG	BB	3076	1/1	0.94	0.14	60,60,60,60	0
54	MG	BB	3103	1/1	0.94	0.09	37,37,37,37	0
54	MG	BB	3110	1/1	0.94	0.07	30,30,30,30	0
54	MG	CA	1631	1/1	0.94	0.07	34,34,34,34	0
54	MG	BB	3035	1/1	0.94	0.08	32,32,32,32	0
54	MG	DB	3010	1/1	0.94	0.07	5,5,5,5	0
54	MG	DB	3013	1/1	0.94	0.18	21,21,21,21	0
54	MG	BB	3015	1/1	0.94	0.04	27,27,27,27	0
54	MG	DB	3065	1/1	0.94	0.07	16,16,16,16	0
54	MG	BB	3054	1/1	0.94	0.05	46,46,46,46	0
54	MG	CA	1637	1/1	0.94	0.06	79,79,79,79	0
54	MG	DB	3018	1/1	0.94	0.09	8,8,8,8	0
54	MG	BB	3005	1/1	0.94	0.04	39,39,39,39	0
54	MG	AA	1634	1/1	0.94	0.04	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	DB	3027	1/1	0.94	0.07	36,36,36,36	0
54	MG	DB	3087	1/1	0.94	0.19	25,25,25,25	0
54	MG	AA	1607	1/1	0.94	0.04	64,64,64,64	0
54	MG	BB	3092	1/1	0.94	0.10	32,32,32,32	0
54	MG	BB	3063	1/1	0.94	0.14	31,31,31,31	0
54	MG	BB	3065	1/1	0.94	0.08	24,24,24,24	0
54	MG	CA	1653	1/1	0.94	0.10	33,33,33,33	0
54	MG	DB	3100	1/1	0.94	0.15	9,9,9,9	0
54	MG	BB	3066	1/1	0.94	0.06	44,44,44,44	0
54	MG	AA	1643	1/1	0.94	0.06	53,53,53,53	0
54	MG	BB	3100	1/1	0.94	0.19	68,68,68,68	0
54	MG	DB	3032	1/1	0.95	0.11	18,18,18,18	0
54	MG	AA	1649	1/1	0.95	0.11	19,19,19,19	0
54	MG	AA	1629	1/1	0.95	0.05	70,70,70,70	0
54	MG	CA	1644	1/1	0.95	0.08	58,58,58,58	0
54	MG	CA	1647	1/1	0.95	0.06	90,90,90,90	0
54	MG	CA	1611	1/1	0.95	0.06	60,60,60,60	0
54	MG	BB	3083	1/1	0.95	0.12	5,5,5,5	0
54	MG	BB	3041	1/1	0.95	0.15	28,28,28,28	0
54	MG	BB	3090	1/1	0.95	0.07	49,49,49,49	0
54	MG	DB	3055	1/1	0.95	0.09	42,42,42,42	0
54	MG	DB	3056	1/1	0.95	0.07	12,12,12,12	0
54	MG	DB	3057	1/1	0.95	0.07	5,5,5,5	0
54	MG	BB	3059	1/1	0.95	0.07	30,30,30,30	0
54	MG	BB	3060	1/1	0.95	0.08	30,30,30,30	0
54	MG	BB	3093	1/1	0.95	0.04	36,36,36,36	0
54	MG	BB	3013	1/1	0.95	0.12	41,41,41,41	0
54	MG	BB	3021	1/1	0.95	0.06	22,22,22,22	0
54	MG	BB	3045	1/1	0.95	0.09	67,67,67,67	0
54	MG	BB	3047	1/1	0.95	0.09	46,46,46,46	0
54	MG	CA	1628	1/1	0.95	0.04	61,61,61,61	0
54	MG	DB	3011	1/1	0.95	0.07	7,7,7,7	0
54	MG	BB	3099	1/1	0.95	0.16	41,41,41,41	0
54	MG	CA	1630	1/1	0.95	0.08	40,40,40,40	0
54	MG	DB	3015	1/1	0.95	0.07	22,22,22,22	0
54	MG	AA	1618	1/1	0.95	0.08	79,79,79,79	0
54	MG	CA	1632	1/1	0.95	0.15	47,47,47,47	0
54	MG	CA	1633	1/1	0.95	0.16	73,73,73,73	0
54	MG	BB	3074	1/1	0.95	0.10	31,31,31,31	0
54	MG	BB	3102	1/1	0.95	0.10	28,28,28,28	0
54	MG	DB	3025	1/1	0.95	0.09	44,44,44,44	0
54	MG	BB	3050	1/1	0.95	0.08	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	BB	3051	1/1	0.95	0.05	41,41,41,41	0
54	MG	DB	3105	1/1	0.95	0.10	40,40,40,40	0
54	MG	AA	1631	1/1	0.95	0.10	107,107,107,107	0
54	MG	BB	3080	1/1	0.95	0.09	37,37,37,37	0
54	MG	DB	3111	1/1	0.95	0.14	28,28,28,28	0
55	ZN	B4	101	1/1	0.95	0.06	72,72,72,72	0
55	ZN	D4	101	1/1	0.95	0.13	57,57,57,57	0
54	MG	BB	3085	1/1	0.96	0.15	44,44,44,44	0
54	MG	DB	3008	1/1	0.96	0.11	16,16,16,16	0
54	MG	BB	3087	1/1	0.96	0.23	41,41,41,41	0
54	MG	BB	3088	1/1	0.96	0.21	57,57,57,57	0
54	MG	AA	1602	1/1	0.96	0.05	29,29,29,29	0
54	MG	AA	1614	1/1	0.96	0.03	64,64,64,64	0
54	MG	BB	3068	1/1	0.96	0.10	55,55,55,55	0
54	MG	CA	1639	1/1	0.96	0.08	14,14,14,14	0
54	MG	DB	3063	1/1	0.96	0.04	71,71,71,71	0
54	MG	BB	3070	1/1	0.96	0.08	15,15,15,15	0
54	MG	BB	3072	1/1	0.96	0.09	52,52,52,52	0
54	MG	DB	3070	1/1	0.96	0.18	23,23,23,23	0
54	MG	AA	1655	1/1	0.96	0.04	38,38,38,38	0
54	MG	BB	3009	1/1	0.96	0.13	64,64,64,64	0
54	MG	CA	1646	1/1	0.96	0.05	72,72,72,72	0
54	MG	BB	3056	1/1	0.96	0.13	34,34,34,34	0
54	MG	DB	3085	1/1	0.96	0.17	25,25,25,25	0
54	MG	BB	3033	1/1	0.96	0.07	55,55,55,55	0
54	MG	CA	1649	1/1	0.96	0.07	73,73,73,73	0
54	MG	CA	1651	1/1	0.96	0.06	40,40,40,40	0
54	MG	AA	1639	1/1	0.96	0.09	57,57,57,57	0
54	MG	DB	3094	1/1	0.96	0.15	21,21,21,21	0
54	MG	DB	3033	1/1	0.96	0.12	62,62,62,62	0
54	MG	CA	1624	1/1	0.96	0.03	34,34,34,34	0
54	MG	AA	1644	1/1	0.96	0.07	24,24,24,24	0
54	MG	BB	3037	1/1	0.96	0.07	42,42,42,42	0
54	MG	DB	3101	1/1	0.96	0.09	5,5,5,5	0
54	MG	AA	1633	1/1	0.96	0.10	51,51,51,51	0
54	MG	DB	3044	1/1	0.96	0.06	12,12,12,12	0
54	MG	BB	3064	1/1	0.96	0.06	26,26,26,26	0
54	MG	DB	3108	1/1	0.96	0.07	21,21,21,21	0
54	MG	DB	3048	1/1	0.96	0.17	23,23,23,23	0
54	MG	BB	3105	1/1	0.96	0.11	21,21,21,21	0
54	MG	BB	3109	1/1	0.96	0.13	32,32,32,32	0
54	MG	BB	3084	1/1	0.96	0.10	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	AA	1659	1/1	0.97	0.05	112,112,112,112	0
54	MG	DB	3019	1/1	0.97	0.14	48,48,48,48	0
54	MG	BB	3104	1/1	0.97	0.04	8,8,8,8	0
54	MG	BB	3031	1/1	0.97	0.03	47,47,47,47	0
54	MG	BB	3107	1/1	0.97	0.07	54,54,54,54	0
54	MG	DB	3066	1/1	0.97	0.06	29,29,29,29	0
54	MG	DB	3026	1/1	0.97	0.13	15,15,15,15	0
54	MG	DB	3068	1/1	0.97	0.07	19,19,19,19	0
54	MG	DB	3069	1/1	0.97	0.10	6,6,6,6	0
54	MG	AA	1646	1/1	0.97	0.03	94,94,94,94	0
54	MG	BB	3075	1/1	0.97	0.10	13,13,13,13	0
54	MG	DB	3074	1/1	0.97	0.05	28,28,28,28	0
54	MG	AA	1656	1/1	0.97	0.13	60,60,60,60	0
54	MG	DB	3079	1/1	0.97	0.09	43,43,43,43	0
54	MG	CA	1656	1/1	0.97	0.07	27,27,27,27	0
54	MG	CA	1602	1/1	0.97	0.05	6,6,6,6	0
54	MG	CA	1603	1/1	0.97	0.12	30,30,30,30	0
54	MG	CA	1659	1/1	0.97	0.07	62,62,62,62	0
54	MG	BB	3077	1/1	0.97	0.08	37,37,37,37	0
54	MG	DB	3088	1/1	0.97	0.10	48,48,48,48	0
54	MG	DB	3090	1/1	0.97	0.17	34,34,34,34	0
54	MG	BB	3012	1/1	0.97	0.17	25,25,25,25	0
54	MG	BB	3062	1/1	0.97	0.04	29,29,29,29	0
54	MG	DB	3041	1/1	0.97	0.14	15,15,15,15	0
54	MG	DB	3095	1/1	0.97	0.05	39,39,39,39	0
54	MG	DB	3043	1/1	0.97	0.09	15,15,15,15	0
54	MG	BB	3022	1/1	0.97	0.10	22,22,22,22	0
54	MG	BB	3036	1/1	0.97	0.07	36,36,36,36	0
54	MG	DB	3007	1/1	0.97	0.07	12,12,12,12	0
54	MG	CA	1613	1/1	0.97	0.09	77,77,77,77	0
54	MG	DB	3052	1/1	0.97	0.20	32,32,32,32	0
54	MG	BB	3097	1/1	0.97	0.05	32,32,32,32	0
54	MG	BB	3002	1/1	0.97	0.05	24,24,24,24	0
54	MG	AA	1610	1/1	0.97	0.10	10,10,10,10	0
54	MG	DB	3109	1/1	0.97	0.05	10,10,10,10	0
54	MG	BB	3026	1/1	0.97	0.10	54,54,54,54	0
54	MG	AA	1605	1/1	0.97	0.15	48,48,48,48	0
54	MG	CA	1645	1/1	0.97	0.16	45,45,45,45	0
54	MG	BB	3086	1/1	0.97	0.14	66,66,66,66	0
54	MG	DB	3004	1/1	0.98	0.09	14,14,14,14	0
54	MG	BB	3053	1/1	0.98	0.08	25,25,25,25	0
54	MG	DB	3006	1/1	0.98	0.07	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	AA	1611	1/1	0.98	0.04	28,28,28,28	0
54	MG	DB	3036	1/1	0.98	0.05	40,40,40,40	0
54	MG	DB	3071	1/1	0.98	0.09	61,61,61,61	0
54	MG	BB	3108	1/1	0.98	0.11	25,25,25,25	0
54	MG	DB	3073	1/1	0.98	0.07	33,33,33,33	0
54	MG	DB	3009	1/1	0.98	0.08	19,19,19,19	0
54	MG	DB	3076	1/1	0.98	0.06	26,26,26,26	0
54	MG	DB	3039	1/1	0.98	0.13	19,19,19,19	0
54	MG	DB	3040	1/1	0.98	0.07	58,58,58,58	0
54	MG	DB	3080	1/1	0.98	0.16	39,39,39,39	0
54	MG	CA	1614	1/1	0.98	0.06	58,58,58,58	0
54	MG	DB	3083	1/1	0.98	0.08	24,24,24,24	0
54	MG	DB	3042	1/1	0.98	0.06	7,7,7,7	0
54	MG	BB	3017	1/1	0.98	0.10	28,28,28,28	0
54	MG	BB	3046	1/1	0.98	0.08	46,46,46,46	0
54	MG	DB	3045	1/1	0.98	0.03	22,22,22,22	0
54	MG	CA	1618	1/1	0.98	0.04	8,8,8,8	0
54	MG	DB	3089	1/1	0.98	0.14	10,10,10,10	0
54	MG	DB	3047	1/1	0.98	0.04	24,24,24,24	0
54	MG	BB	3007	1/1	0.98	0.09	5,5,5,5	0
54	MG	DB	3092	1/1	0.98	0.17	46,46,46,46	0
54	MG	DB	3049	1/1	0.98	0.10	46,46,46,46	0
54	MG	DB	3050	1/1	0.98	0.14	32,32,32,32	0
54	MG	BB	3069	1/1	0.98	0.11	32,32,32,32	0
54	MG	CA	1655	1/1	0.98	0.07	69,69,69,69	0
54	MG	AA	1608	1/1	0.98	0.06	54,54,54,54	0
54	MG	CA	1605	1/1	0.98	0.04	16,16,16,16	0
54	MG	DB	3099	1/1	0.98	0.15	29,29,29,29	0
54	MG	DB	3022	1/1	0.98	0.09	5,5,5,5	0
54	MG	AA	1645	1/1	0.98	0.10	60,60,60,60	0
54	MG	DB	3102	1/1	0.98	0.14	14,14,14,14	0
54	MG	DB	3103	1/1	0.98	0.10	16,16,16,16	0
54	MG	CA	1640	1/1	0.98	0.12	57,57,57,57	0
54	MG	CA	1608	1/1	0.98	0.06	40,40,40,40	0
54	MG	DB	3106	1/1	0.98	0.12	39,39,39,39	0
54	MG	CA	1625	1/1	0.98	0.06	34,34,34,34	0
54	MG	BB	3027	1/1	0.98	0.08	34,34,34,34	0
54	MG	DB	3028	1/1	0.98	0.10	8,8,8,8	0
54	MG	BB	3028	1/1	0.98	0.08	32,32,32,32	0
54	MG	DB	3002	1/1	0.98	0.10	5,5,5,5	0
54	MG	DB	3112	1/1	0.98	0.15	37,37,37,37	0
54	MG	DB	3064	1/1	0.98	0.10	33,33,33,33	0

Continued on next page...

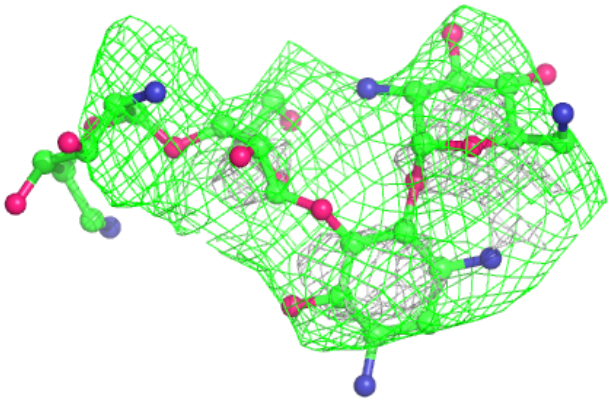
Continued from previous page...

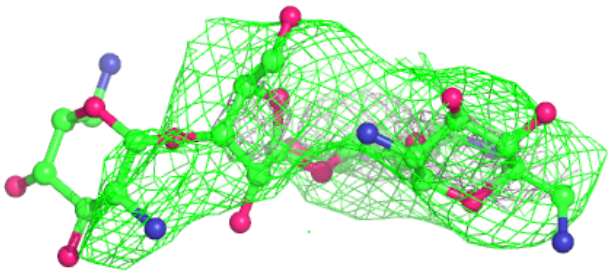
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	DB	3003	1/1	0.98	0.08	9,9,9,9	0
54	MG	CA	1650	1/1	0.99	0.09	12,12,12,12	0
54	MG	DB	3020	1/1	0.99	0.04	5,5,5,5	0
54	MG	DB	3075	1/1	0.99	0.12	7,7,7,7	0
54	MG	DB	3021	1/1	0.99	0.15	9,9,9,9	0
54	MG	DB	3077	1/1	0.99	0.12	47,47,47,47	0
54	MG	BB	3057	1/1	0.99	0.05	20,20,20,20	0
54	MG	BB	3106	1/1	0.99	0.14	33,33,33,33	0
54	MG	AA	1604	1/1	0.99	0.15	36,36,36,36	0
54	MG	BB	3067	1/1	0.99	0.07	34,34,34,34	0
54	MG	DB	3082	1/1	0.99	0.07	6,6,6,6	0
54	MG	BB	3003	1/1	0.99	0.07	24,24,24,24	0
54	MG	BB	3024	1/1	0.99	0.13	7,7,7,7	0
54	MG	BB	3016	1/1	0.99	0.07	18,18,18,18	0
54	MG	BB	3071	1/1	0.99	0.12	29,29,29,29	0
54	MG	DB	3012	1/1	0.99	0.20	37,37,37,37	0
54	MG	BB	3006	1/1	0.99	0.14	5,5,5,5	0
54	MG	CA	1617	1/1	0.99	0.07	9,9,9,9	0
54	MG	CA	1604	1/1	0.99	0.08	52,52,52,52	0
54	MG	BB	3042	1/1	0.99	0.08	8,8,8,8	0
54	MG	CA	1606	1/1	0.99	0.09	19,19,19,19	0
54	MG	BB	3049	1/1	0.99	0.03	14,14,14,14	0
54	MG	BB	3008	1/1	1.00	0.09	64,64,64,64	0

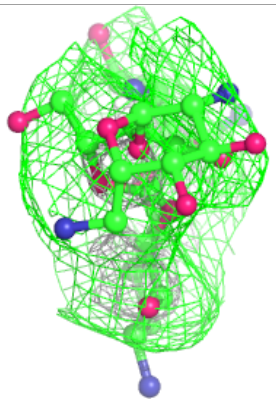
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NMY BB 3001:

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

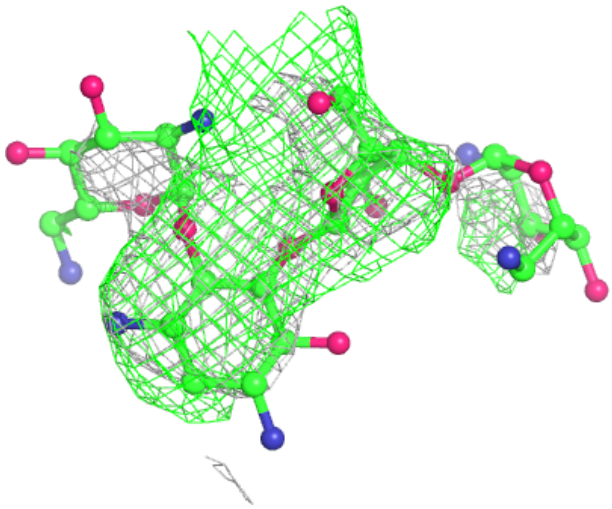


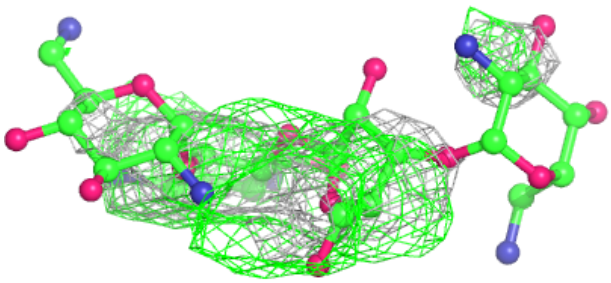


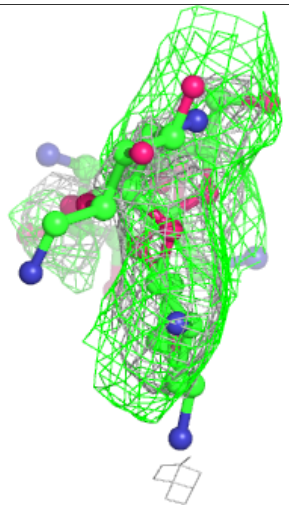


Electron density around NMY DB 3001:

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

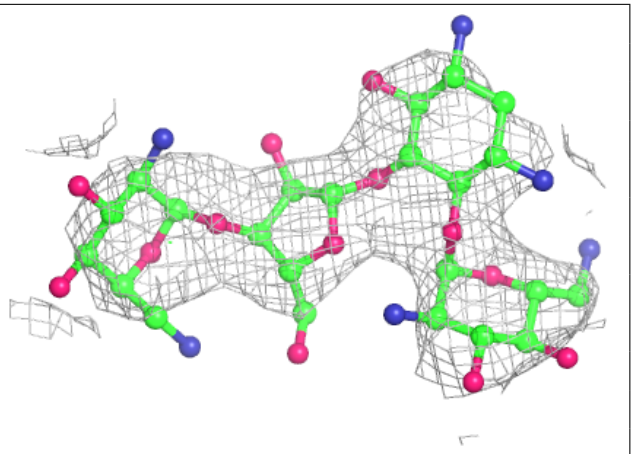


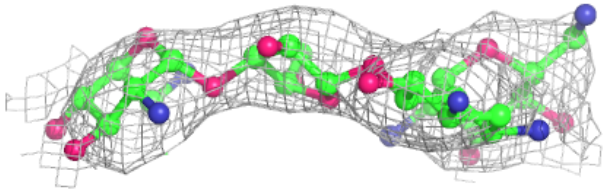


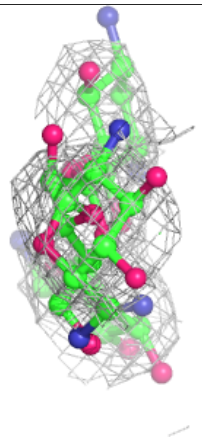


Electron density around NMY AA 1601:

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

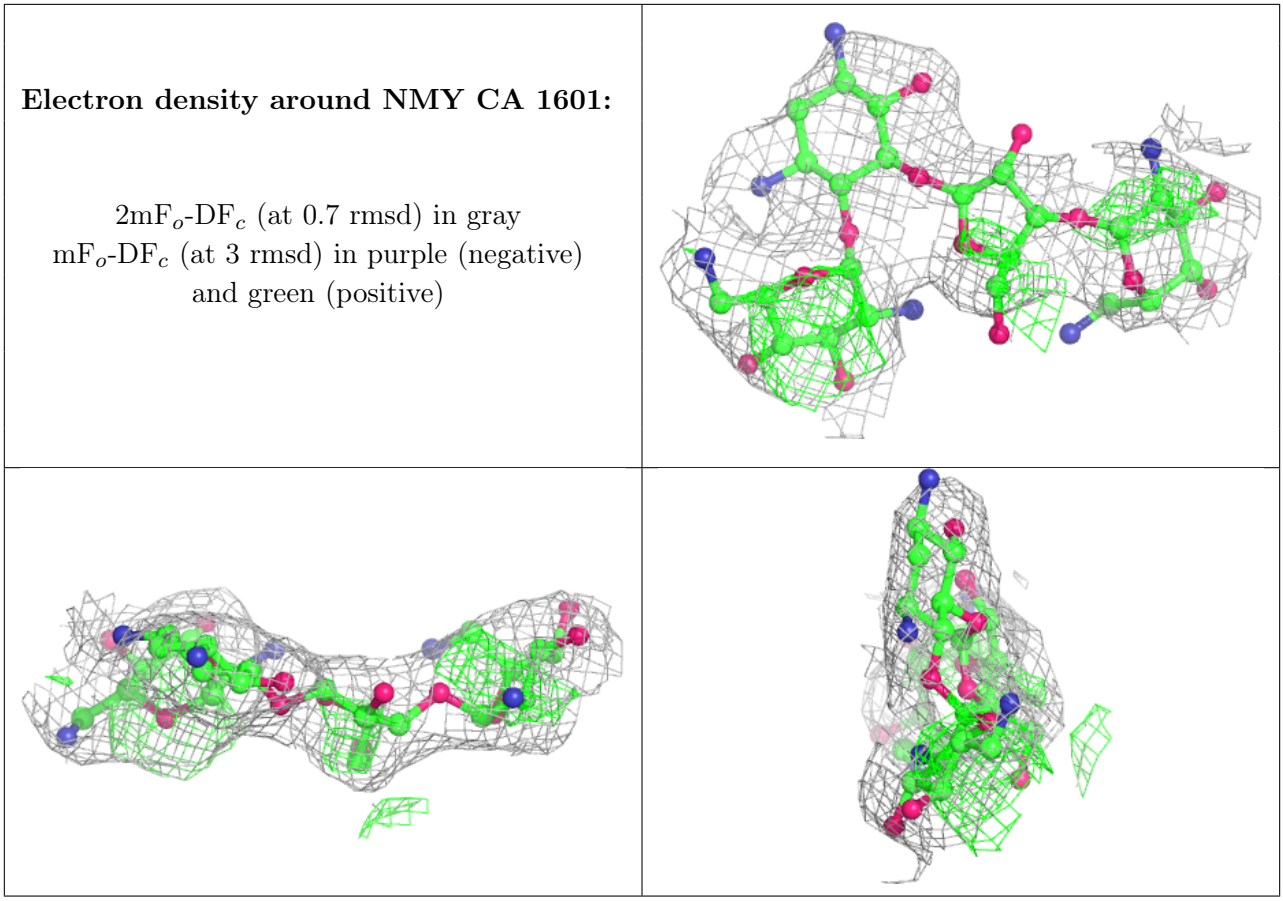






Electron density around NMY CA 1601:

$2mF_o$-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.