wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2023 – 11:32 PM EDT

PDB ID	:	4V53
Title	:	Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin.
Authors	:	Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on	:	2007-06-16
Resolution	:	3.54 Å(reported)

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

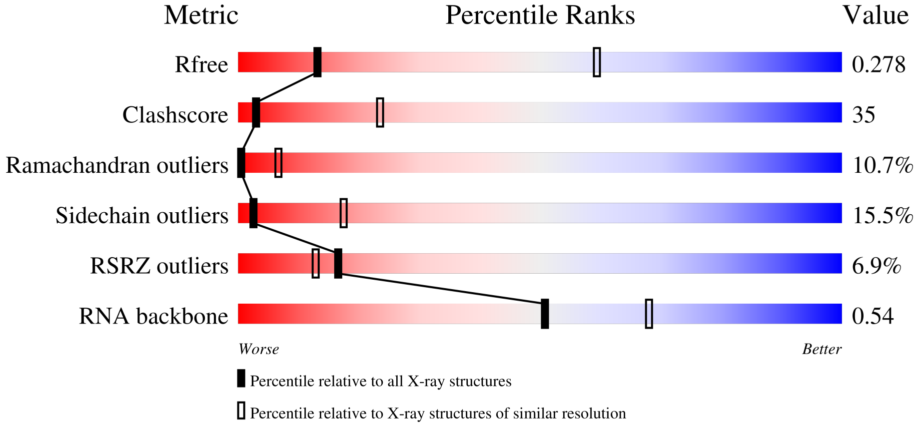
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance ⓘ

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

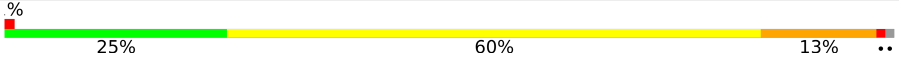
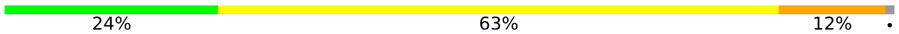
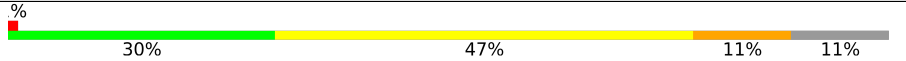
The reported resolution of this entry is 3.54 Å.

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	1028 (3.60-3.48)
Clashscore	141614	1109 (3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)
RNA backbone	3102	1003 (4.02-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	CA	1542	
2	AC	232	

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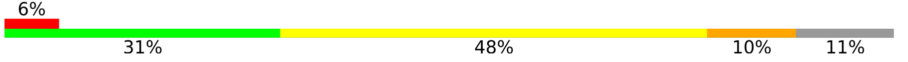
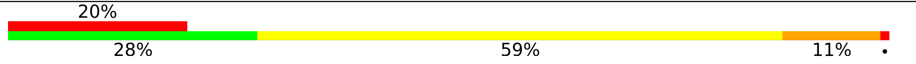
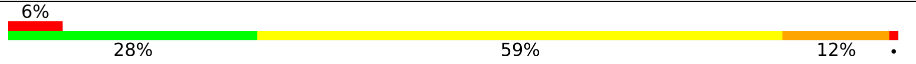
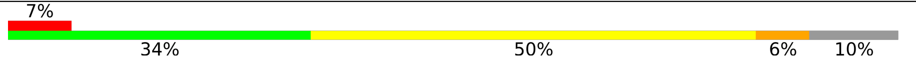
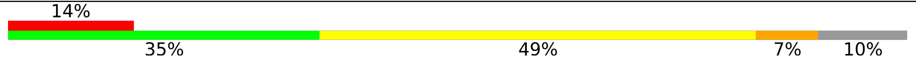
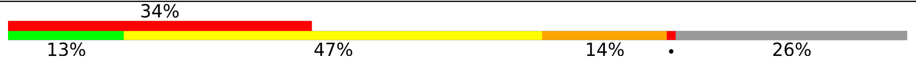
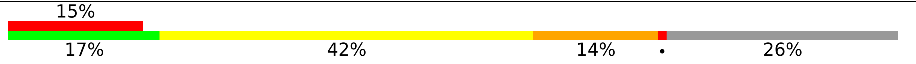
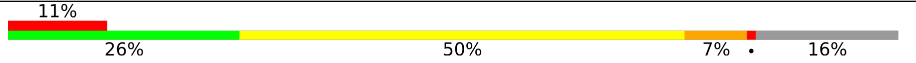
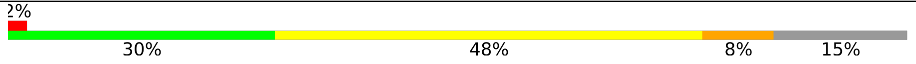
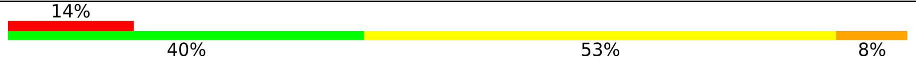
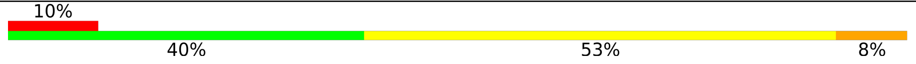
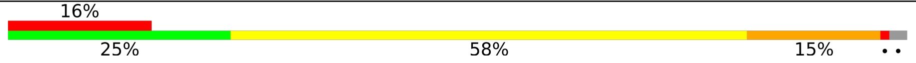
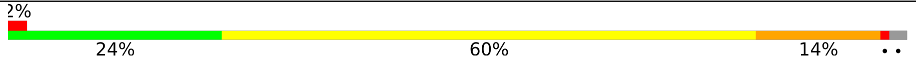
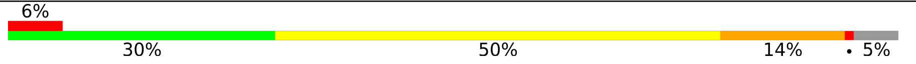
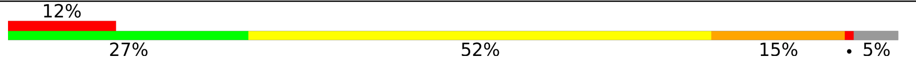
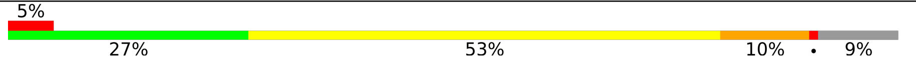
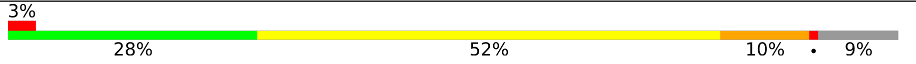
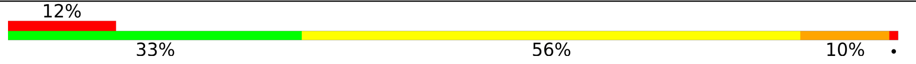
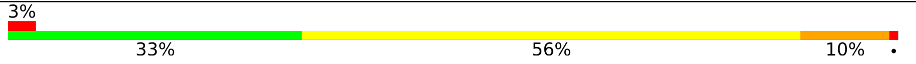
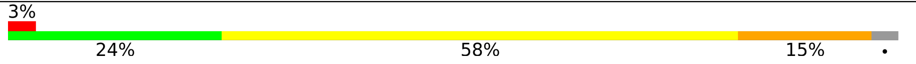
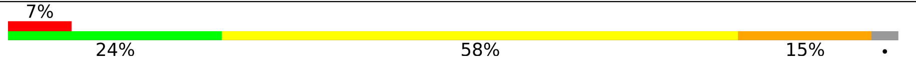
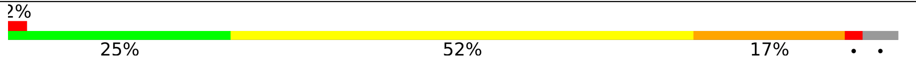
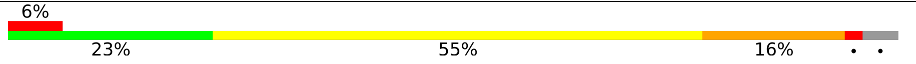
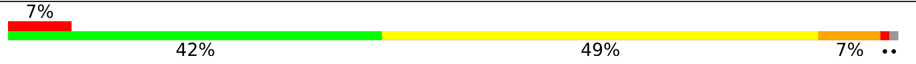
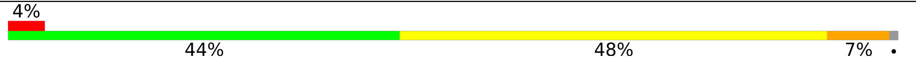
Mol	Chain	Length	Quality of chain
2	CC	232	 6% 31% 48% 10% 11%
3	AD	205	 20% 28% 59% 11% •
3	CD	205	 6% 28% 59% 12% •
4	AE	166	 7% 34% 50% 6% 10%
4	CE	166	 14% 35% 49% 7% 10%
5	AF	135	 34% 13% 47% 14% • 26%
5	CF	135	 15% 17% 42% 14% • 26%
6	AG	178	 11% 26% 50% 7% • 16%
6	CG	178	 2% 30% 48% 8% 15%
7	AH	129	 14% 40% 53% 8%
7	CH	129	 10% 40% 53% 8%
8	AI	129	 16% 25% 58% 15% • •
8	CI	129	 2% 24% 60% 14% • •
9	AJ	103	 6% 30% 50% 14% • 5%
9	CJ	103	 12% 27% 52% 15% • 5%
10	AK	128	 5% 27% 53% 10% • 9%
10	CK	128	 3% 28% 52% 10% • 9%
11	AL	123	 12% 33% 56% 10% •
11	CL	123	 3% 33% 56% 10% •
12	AM	117	 3% 24% 58% 15% •
12	CM	117	 7% 24% 58% 15% •
13	AN	100	 2% 25% 52% 17% • •
13	CN	100	 6% 23% 55% 16% • •
14	AO	89	 7% 42% 49% 7% ••
14	CO	89	 4% 44% 48% 7% •

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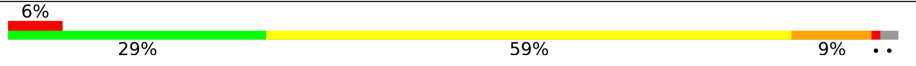
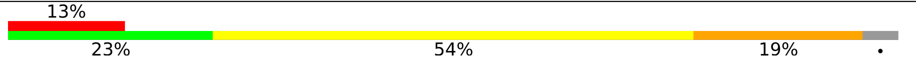
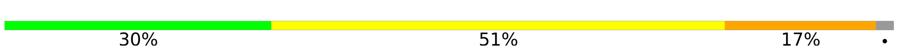
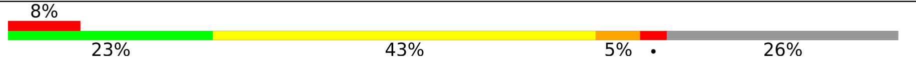
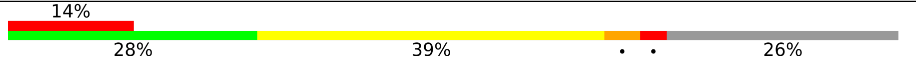
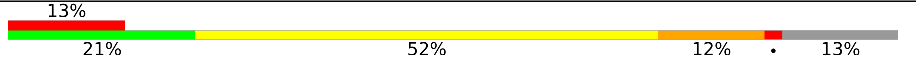
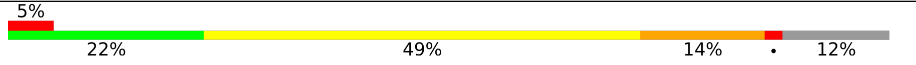
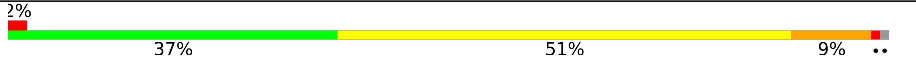
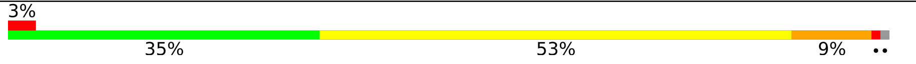
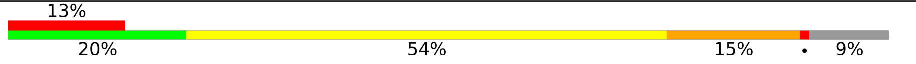
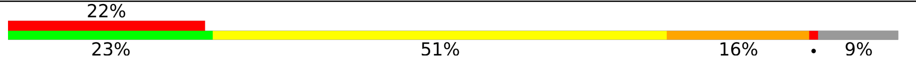
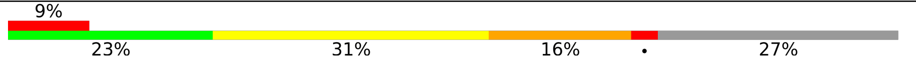
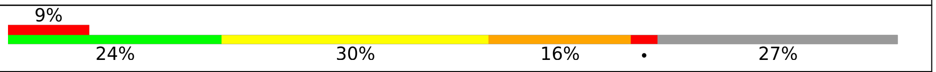
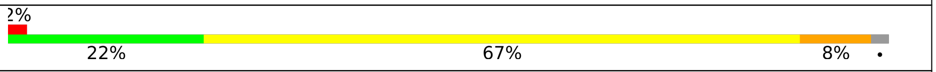
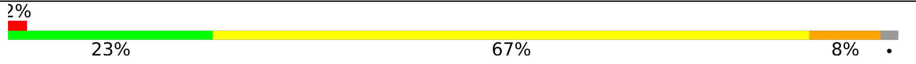
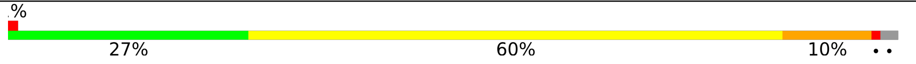
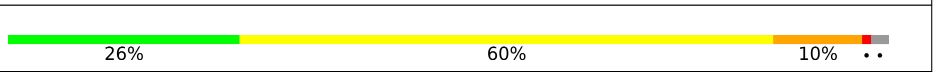
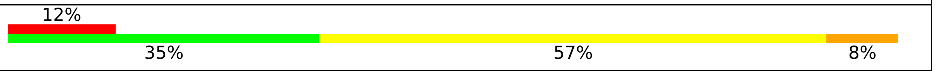
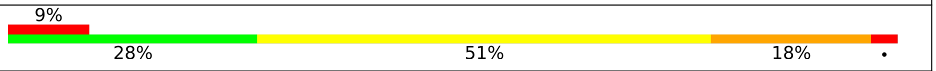
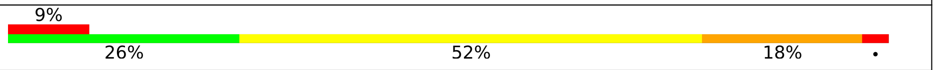
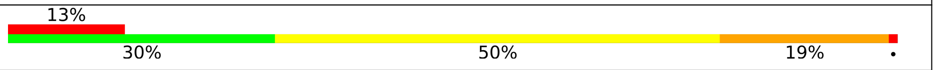
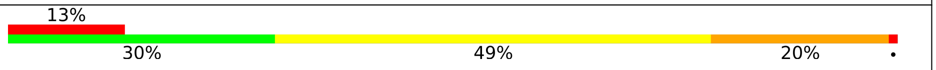
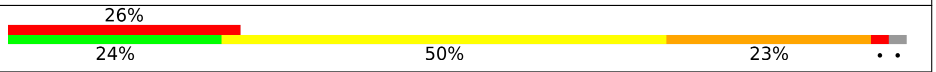
Mol	Chain	Length	Quality of chain
15	AP	82	
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	

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Mol	Chain	Length	Quality of chain
27	DK	123	2% 25% 49% 23% • •
28	BP	114	26% 26% 52% 18% •
28	DP	114	3% 27% 51% 18% •
29	BE	201	16% 28% 57% 15%
29	DE	201	9% 31% 54% 15%
30	BY	58	10% 26% 55% 17% •
30	DY	58	5% 24% 57% 17% •
31	B0	56	11% 30% 54% 14% •
31	D0	56	29% 54% 16% •
32	B4	38	11% 16% 45% 37% •
32	D4	38	18% 42% 37% •
33	B1	54	31% 20% 50% 22% 7%
33	D1	54	17% 19% 54% 20% 7%
34	B3	64	9% 41% 47% 12%
34	D3	64	12% 42% 44% 14%
35	BV	94	7% 28% 55% 17%
35	DV	94	9% 28% 55% 17%
36	B2	46	7% 35% 48% 17%
36	D2	46	4% 35% 50% 15%
37	BL	144	5% 39% 41% 19% ••
37	DL	144	19% 35% 44% 20% ••
38	BM	136	10% 29% 54% 16%
38	DM	136	5% 31% 54% 15%
39	BX	63	22% 17% 63% 19%
39	DX	63	3% 14% 67% 19%

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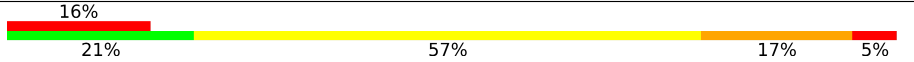
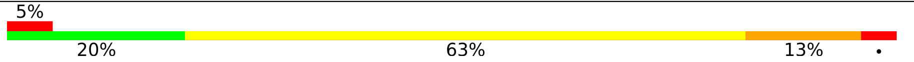
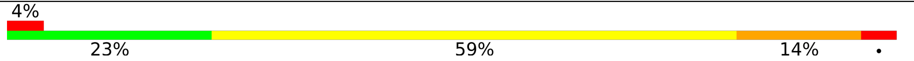
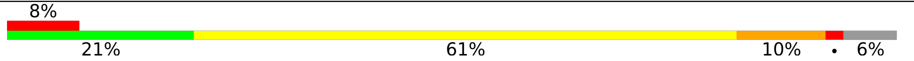
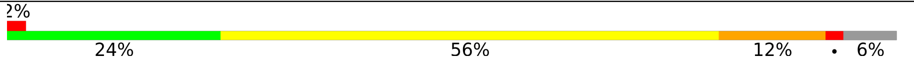
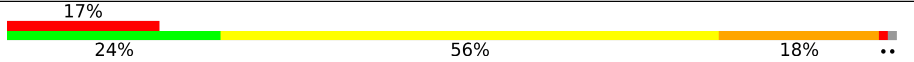
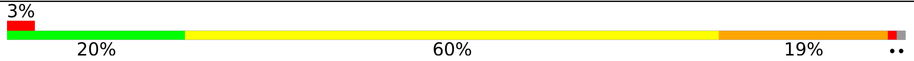
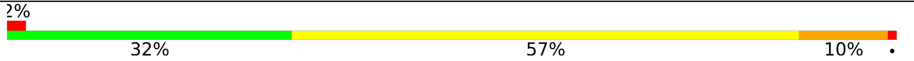
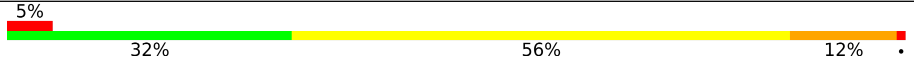
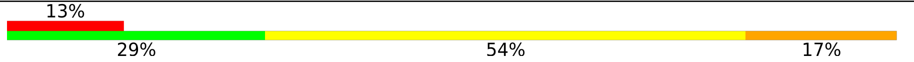
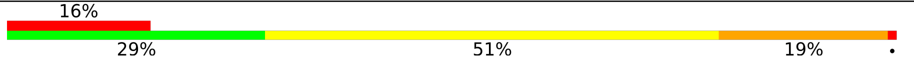
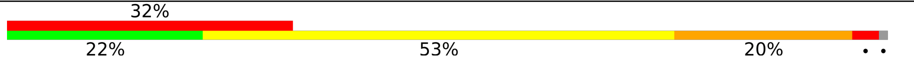
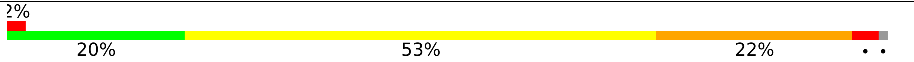
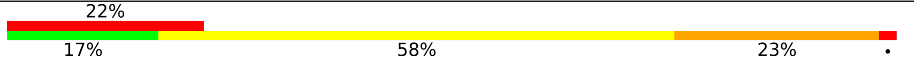
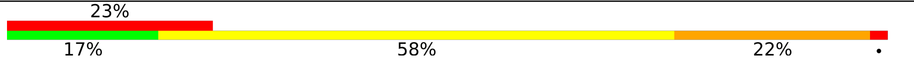
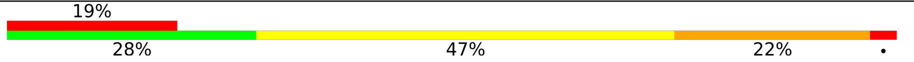
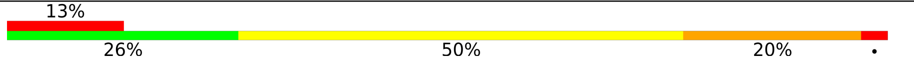
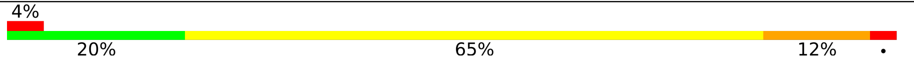
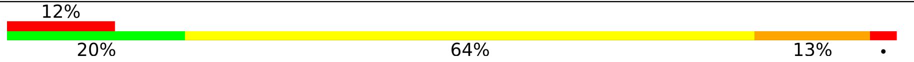
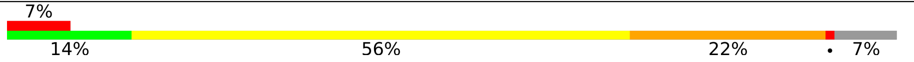
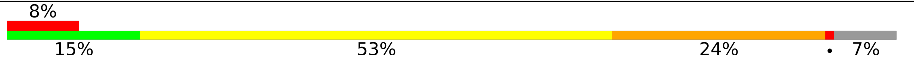
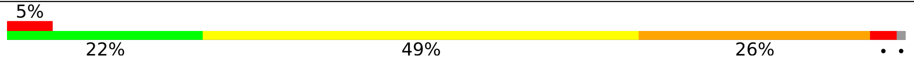
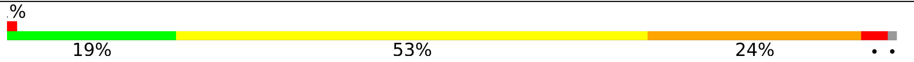
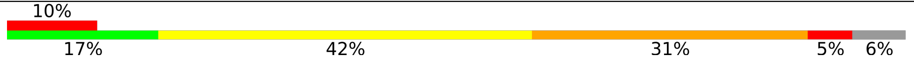
Mol	Chain	Length	Quality of chain
40	BH	149	
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW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

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Mol	Chain	Length	Quality of chain
52	DW	84	

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	MG	AA	2023	-	-	-	X
53	MG	AA	2037	-	-	-	X
53	MG	DB	3059	-	-	-	X

2 Entry composition ⓘ

There are 56 unique types of molecules in this entry. The entry contains 284252 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
			Total	C	N	O	P			
1	AA	1530	32831	14642	6024	10635	1530	0	0	0
1	CA	1530	32831	14642	6024	10635	1530	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 648 411 121 113 3	0	0	0
16	CQ	81	Total C N O S 657 417 122 115 3	0	0	0

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

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

- 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 637 408 120 107 2	0	0	0
18	CS	80	Total C N O S 644 413 121 108 2	0	0	0

- 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 665 411 137 114 3	0	0	0
19	CT	85	Total C N O S 665 411 137 114 3	0	0	0

- 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 1704 1081 305 311 7	0	0	0
20	CB	218	Total C N O S 1704 1081 305 311 7	0	0	0

- 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 425 265 86 73 1	0	0	0
21	CU	51	Total C N O S 425 265 86 73 1	0	0	0

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

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

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

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

- 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 1032 651 179 196 6	0	0	0
24	DI	141	Total C N O S 1032 651 179 196 6	0	0	0

- 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 2082 1288 423 364 7	0	0	0
25	DC	271	Total C N O S 2082 1288 423 364 7	0	0	0

- 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 1565 979 288 294 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 504 323 105 74 2	0	0	0
34	D3	64	Total C N O S 504 323 105 74 2	0	0	0

- 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 753 479 137 134 3	0	0	0
35	DV	94	Total C N O S 753 479 137 134 3	0	0	0

- 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 377 228 90 57 2	0	0	0
36	D2	46	Total C N O S 377 228 90 57 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
42	DN	120	Total C N O S 960 593 196 166 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 C N O 892 552 178 162	0	0	0
43	DO	116	Total C N O 892 552 178 162	0	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
45	BS	110	Total C N O S 857 532 166 156 3	0	0	0
45	DS	110	Total C N O S 857 532 166 156 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 C N O 779 492 146 141	0	0	0
46	DU	102	Total C N O 779 492 146 141	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
47	BF	178	Total C N O S 1420 905 251 258 6	0	0	0
47	DF	178	Total C N O S 1420 905 251 258 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 1323 832 243 246 2	0	0	0
48	DG	176	Total C N O S 1323 832 243 246 2	0	0	0

- 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 816 516 153 145 2	0	0	0
49	DR	103	Total C N O S 816 516 153 145 2	0	0	0

- 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 738 466 139 131 2	0	0	0
50	DT	93	Total C N O S 738 466 139 131 2	0	0	0

- 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 625 388 129 106 2	0	0	0
51	DZ	77	Total C N O S 625 388 129 106 2	0	0	0

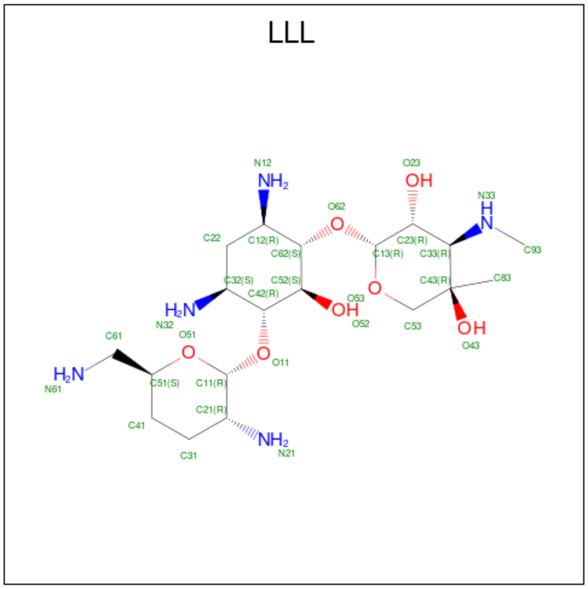
- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 54 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDR OXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: $C_{19}H_{39}N_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
54	AA	1	31	19	5	7	0	0
			Total	C	N	O		
54	AA	1	31	19	5	7	0	0
			Total	C	N	O		
54	AA	1	31	19	5	7	0	0
			Total	C	N	O		
54	BB	1	31	19	5	7	0	0
			Total	C	N	O		
54	CA	1	31	19	5	7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	CA	1	Total C N O 31 19 5 7	0	0
54	CA	1	Total C N O 31 19 5 7	0	0
54	DB	1	Total C N O 31 19 5 7	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	292	Total O 292 292	0	0
56	AE	1	Total O 1 1	0	0
56	AK	1	Total O 1 1	0	0
56	AL	2	Total O 2 2	0	0
56	AN	2	Total O 2 2	0	0
56	AT	2	Total O 2 2	0	0
56	BB	492	Total O 492 492	0	0
56	BC	7	Total O 7 7	0	0
56	BE	3	Total O 3 3	0	0
56	B2	1	Total O 1 1	0	0
56	BL	3	Total O 3 3	0	0
56	BH	1	Total O 1 1	0	0

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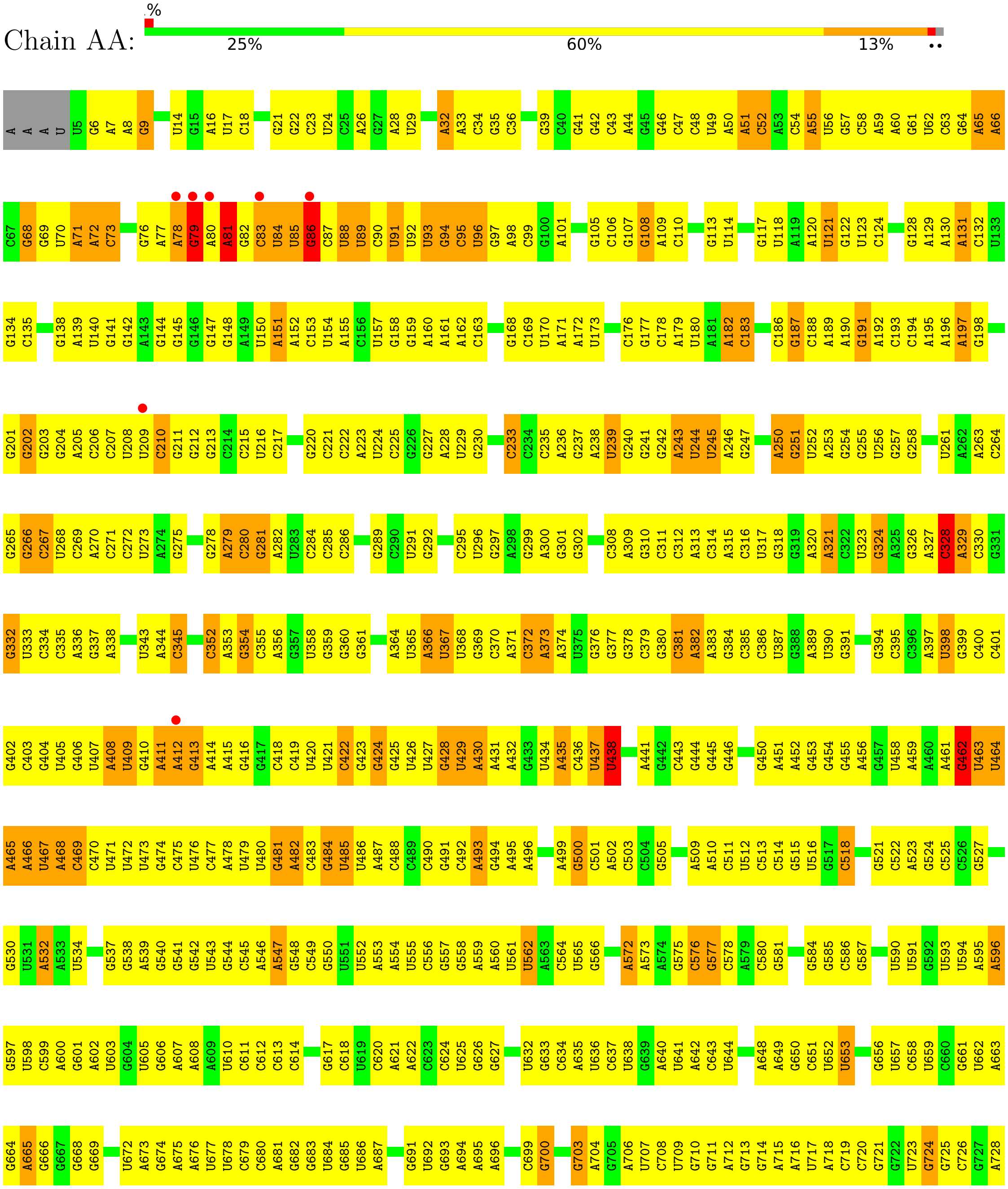
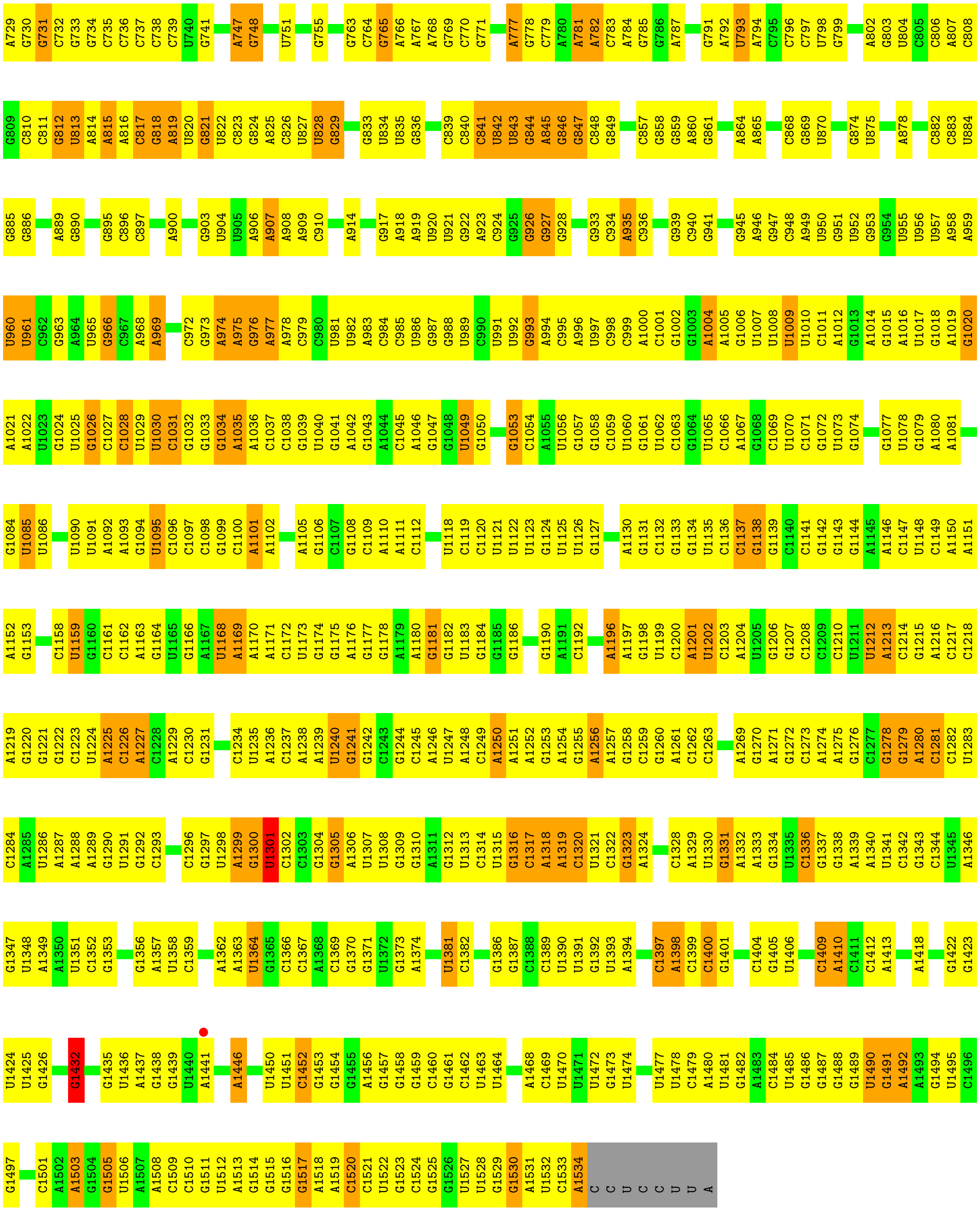
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	CA	297	Total O 297 297	0	0
56	CE	2	Total O 2 2	0	0
56	CK	1	Total O 1 1	0	0
56	CL	2	Total O 2 2	0	0
56	CN	4	Total O 4 4	0	0
56	CT	2	Total O 2 2	0	0
56	DB	502	Total O 502 502	0	0
56	DC	4	Total O 4 4	0	0
56	DE	2	Total O 2 2	0	0
56	DL	4	Total O 4 4	0	0

3 Residue-property plots ⓘ

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

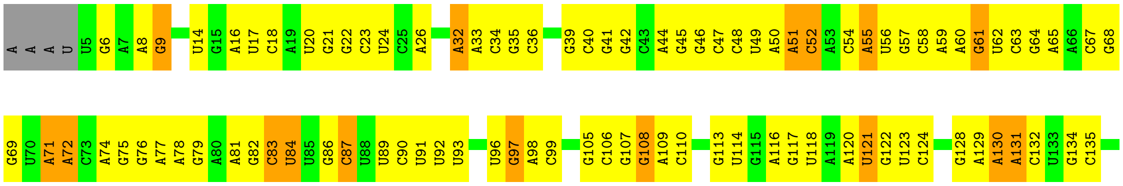
- Molecule 1: 16S rRNA

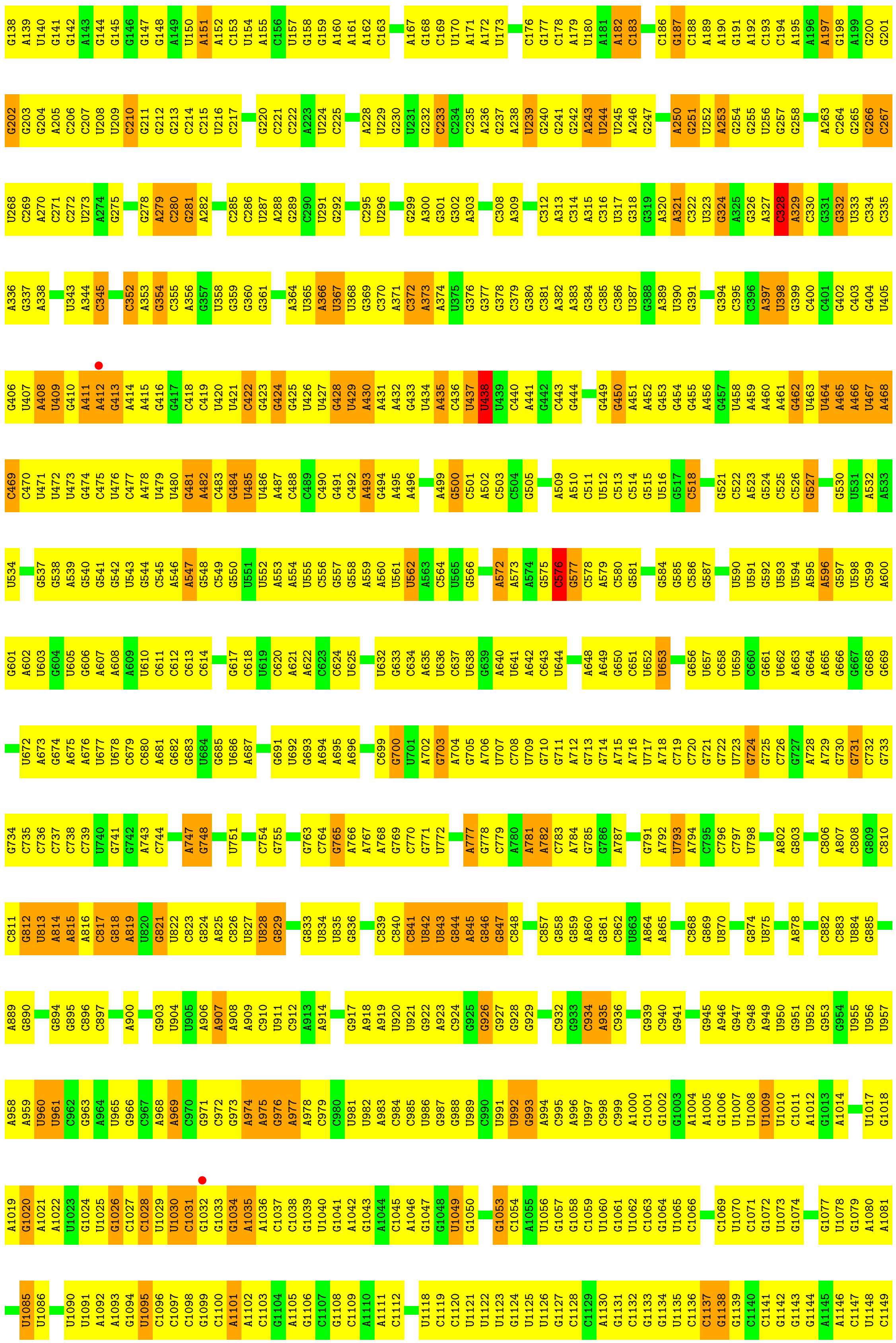




- Molecule 1: 16S rRNA

Chain CA:

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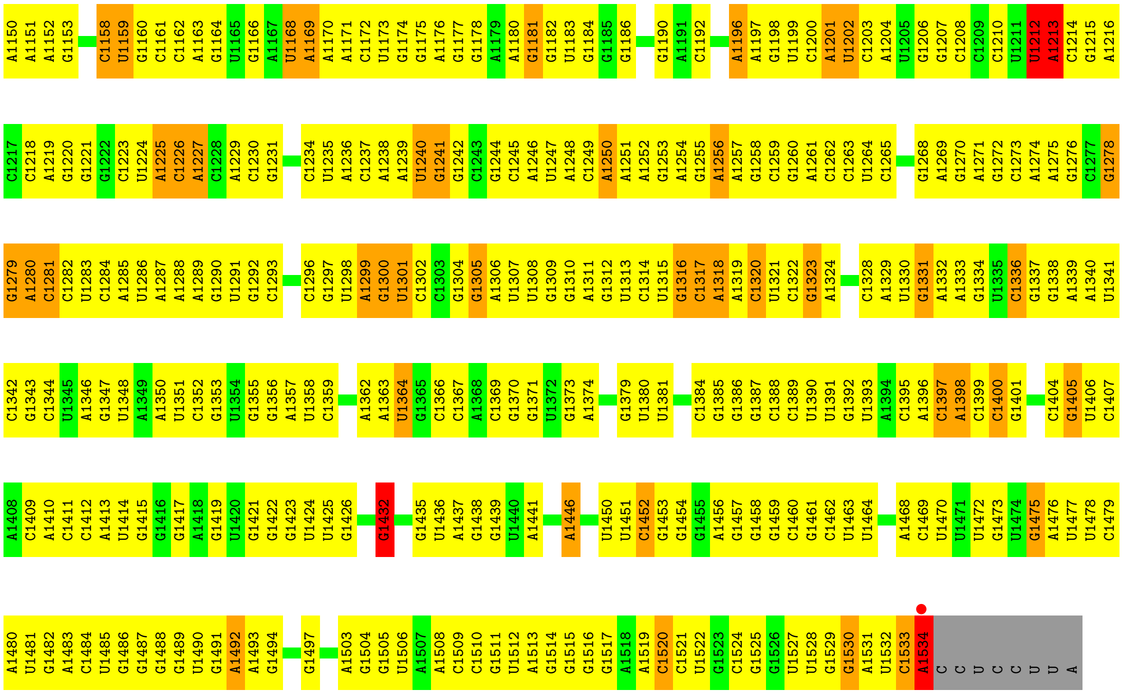
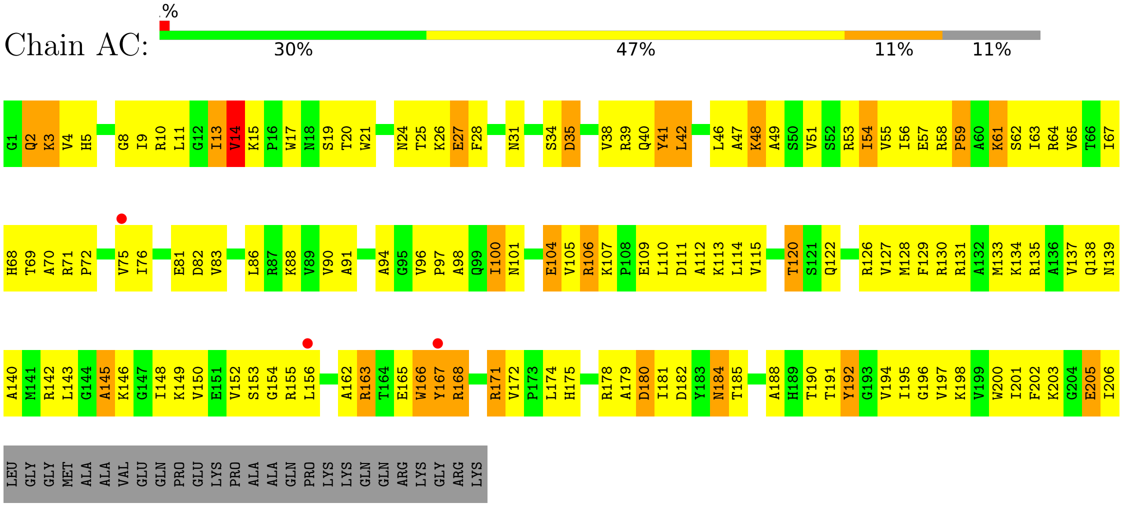
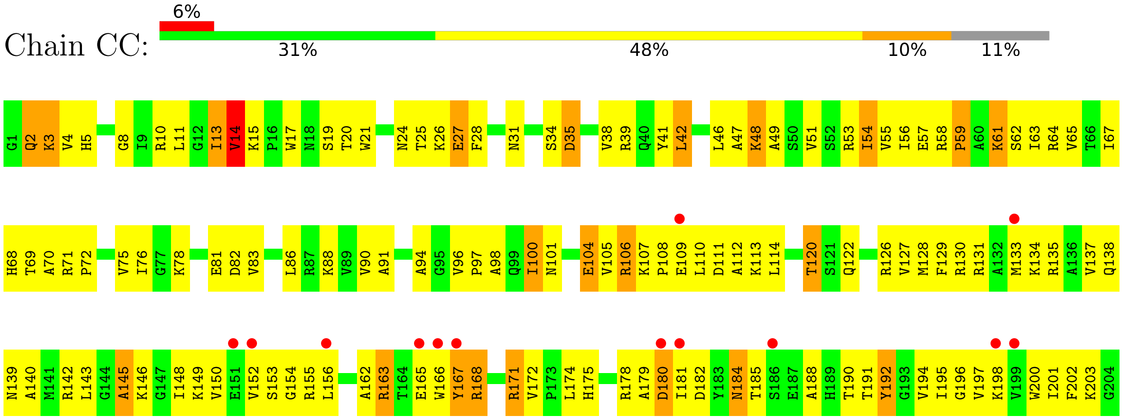
G202 G203 G204 A205 C206 C207 U208 U209 C210 G211 G212 G213 C214 C215 U216 C217 G220 C221 C222 A223 U224 C225 A228 U229 G230 U231 G232 C233 C234 C235 A236 G237 A238 U239 G240 G241 G242 A243 U244 U245 A246 G247 A250 G251 U252 A253 G254 G255 U256 G257 G258 A263 C264 G265 G266 C267
U268 C269 A270 C271 C272 U273 A274 G275 G278 A279 C280 G281 A282 C285 C286 U287 A288 G289 C290 U291 G292 C295 U296 G299 A300 G301 G302 A303 C308 A309 C312 A313 C314 A315 C316 U317 G318 G319 A320 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 G331 G332 U333 C334 C335
A336 G337 A338 U343 A344 C345 C352 A353 G354 C355 A356 G357 U358 G359 G360 G361 A364 U365 A366 U367 C368 G369 C370 A371 C372 A373 A374 U375 G376 G377 G378 C379 G380 C381 A382 A383 G384 C385 C386 U387 G388 A389 U390 G391 G394 C395 C396 A397 U398 G399 C400 C401 G402 C403 G404 U405
G406 U407 A408 U409 G410 A411 A412 G413 A414 A415 G416 G417 C418 C419 U420 U421 C422 G423 G424 G425 U426 U427 G428 U429 A430 A431 A432 G433 U434 A435 C436 U437 U438 U439 C440 A441 G442 C443 G444 G449 G450 A451 A452 G453 G454 G455 A456 G457 U458 A459 A460 A461 G462 U463 U464 A465 A466 U467 A468
C469 C470 U471 U472 U473 G474 C475 U476 C477 A478 U479 U480 G481 A482 C483 G484 U485 U486 A487 C488 C489 C490 G491 C492 A493 G494 A495 A496 A499 G500 C501 A502 C503 C504 G505 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 G521 C522 A523 G524 C525 C526 G527 G530 U531 A532 A533
U534 G537 G538 A539 G540 G541 G542 U543 G544 C545 A546 A547 G548 C549 G550 U551 U552 A553 A554 U555 C556 G557 G558 A559 A560 U561 U562 A563 C564 U565 G566 A572 A573 A574 G575 C576 G577 C578 A579 C580 G581 G584 G585 C586 G587 U590 U591 G592 U593 U594 A595 A596 G597 U598 C599 A600
G601 A602 U603 G604 U605 G606 A607 A608 A609 U610 C611 C612 C613 C614 G617 C618 U619 C620 A621 A622 C623 C624 U625 U632 G633 C634 A635 U636 C637 U638 G639 A640 U641 A642 C643 U644 A648 A649 G650 C651 U652 U653 G656 U657 C658 U659 C660 G661 U662 A663 A664 A665 G666 G667 G668 G669
U672 A673 G674 A675 A676 U677 U678 C679 C680 A681 G682 G683 U684 G685 U686 A687 G691 U692 G693 A694 A695 A696 C699 G700 U701 A702 G703 A704 G705 A706 U707 C708 U709 G710 G711 A712 G713 G714 A715 A716 U717 A718 C719 C720 G721 G722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 G733
G734 C735 C736 C737 C738 C739 U740 G741 G742 A743 C744 A747 G748 U751 C754 G755 G763 C764 G765 A766 A767 A768 G769 C770 G771 U772 A777 G778 C779 A780 A781 A782 C783 A784 G785 G786 A787 G791 A792 U793 A794 C795 C796 C797 U798 A802 G803 C806 A807 C808 G809 C810
C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829 G833 U834 U835 G836 C839 C840 C841 U842 U843 G844 A845 G846 G847 C848 C857 G858 G859 A860 G861 C862 U863 A864 A865 C868 G869 U870 G874 U875 A878 C882 C883 U884 G885
A889 G890 G894 G895 C896 C897 A900 G903 U904 U905 A906 A907 A908 A909 C910 U911 C912 A913 A914 G917 A918 U919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C932 G933 C934 A935 C936 G939 C940 G941 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 U957
A958 A959 U960 U961 C962 G963 A964 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 U986 G987 G988 U989 C990 U991 U992 G993 A994 C995 A996 U997 C998 C999 A1000 C1001 G1002 G1003 A1004 A1005 G1006 U1007 U1008 U1009 U1010 C1011 A1012 G1013 A1014 U1017 G1018
A1019 G1020 A1021 A1022 U1023 G1024 U1025 G1026 C1027 C1028 U1029 U1030 C1031 G1032 G1033 G1034 A1035 A1036 C1037 C1038 G1039 U1040 G1041 A1042 G1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 G1053 C1054 A1055 U1056 G1057 G1058 C1059 U1060 G1061 U1062 C1063 G1064 U1065 C1066 C1069 U1070 C1071 G1072 U1073 G1074 G1077 U1078 G1079 A1080 A1081
U1085 U1086 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 U1118 C1119 C1120 U1121 U1122 U1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 C1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 C1144 A1145 A1146 C1147 U1148 C1149



- Molecule 2: 30S ribosomal protein S3



- Molecule 2: 30S ribosomal protein S3



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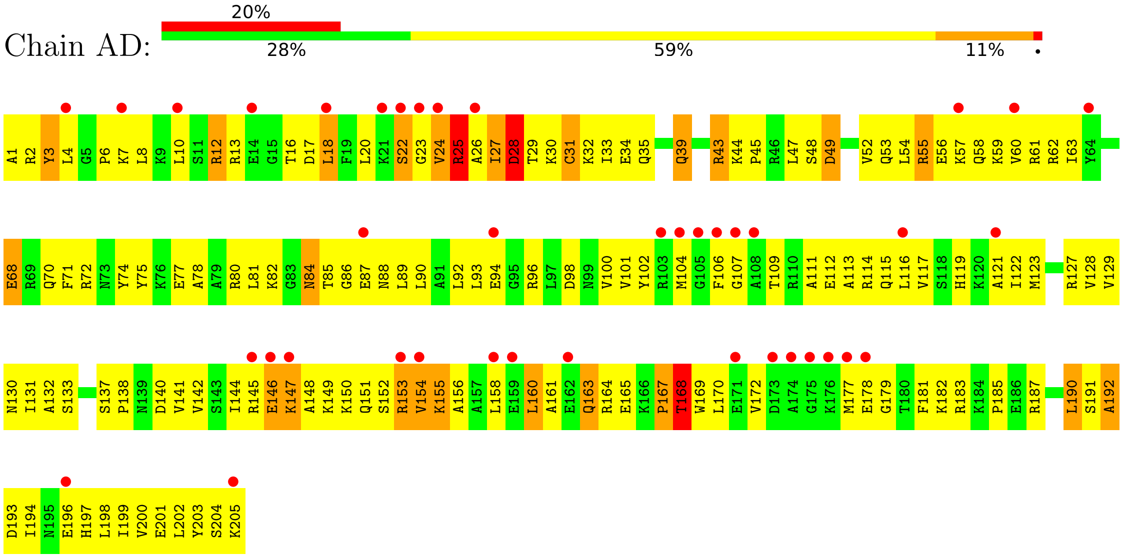
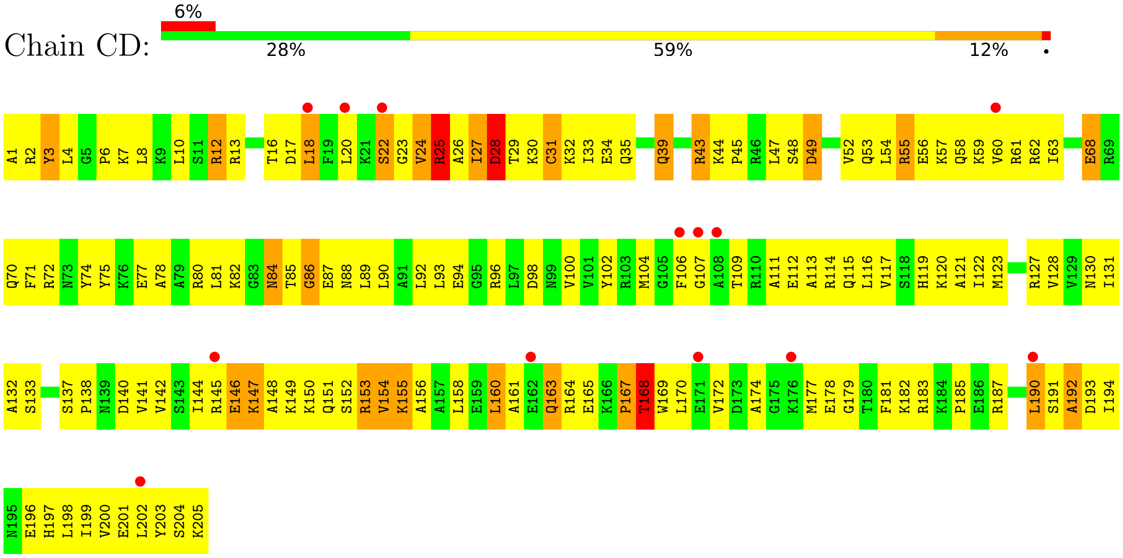


- Molecule 3: 30S ribosomal protein S4



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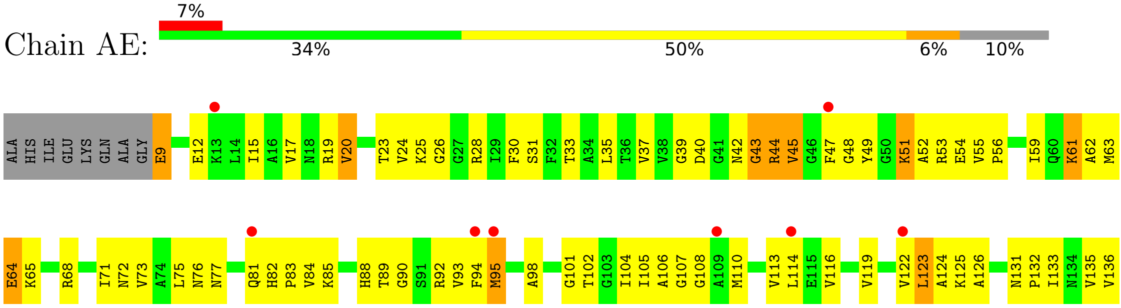
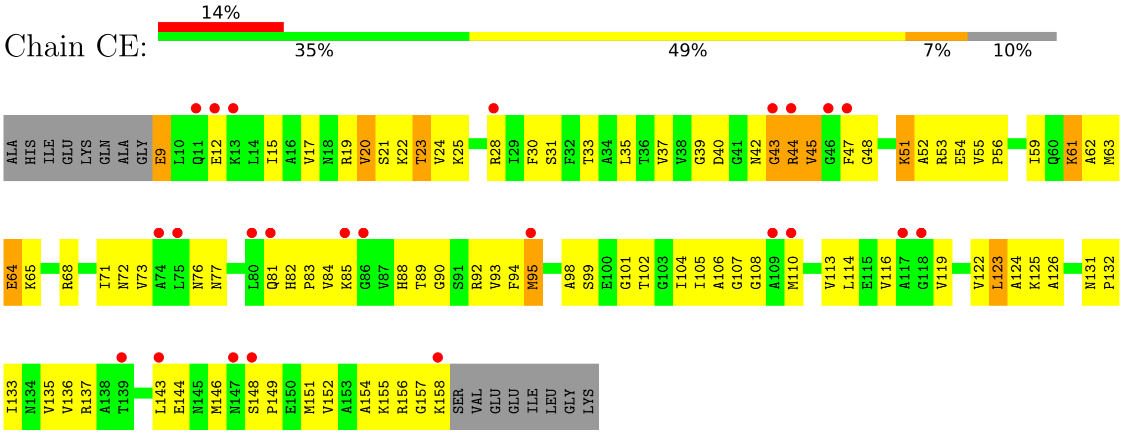
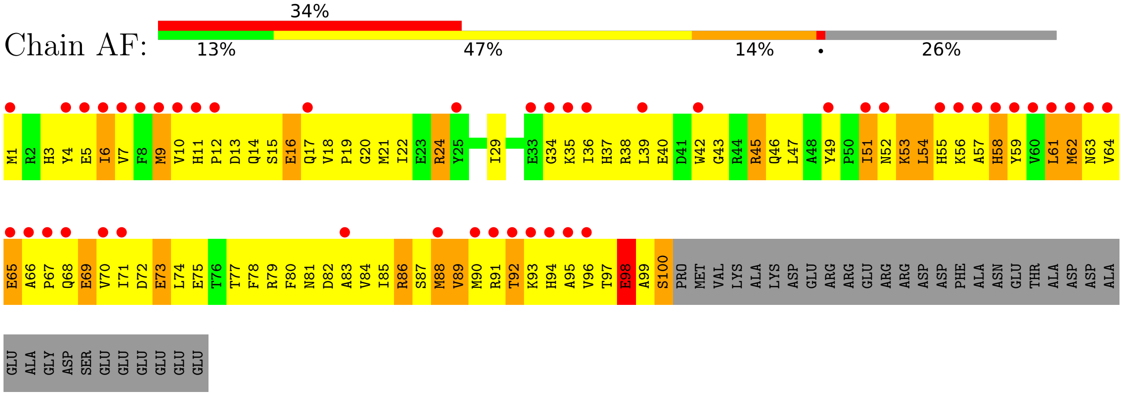


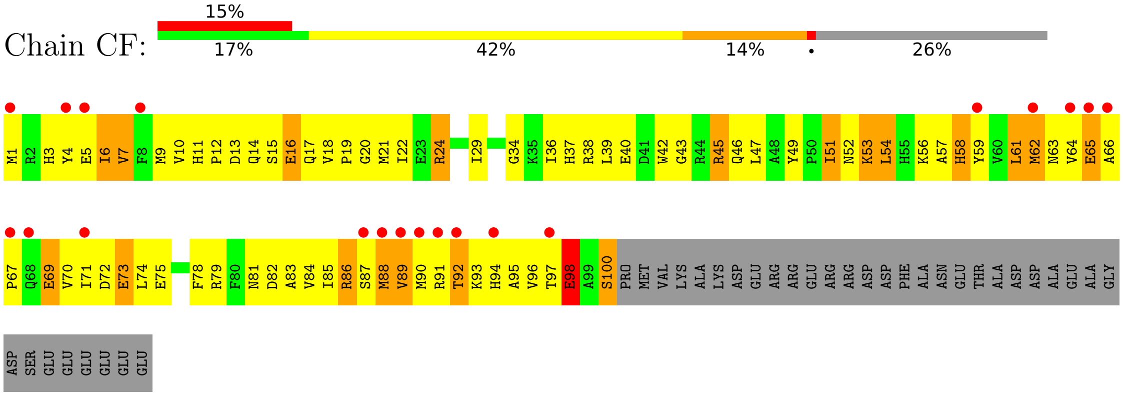
- Molecule 4: 30S ribosomal protein S5



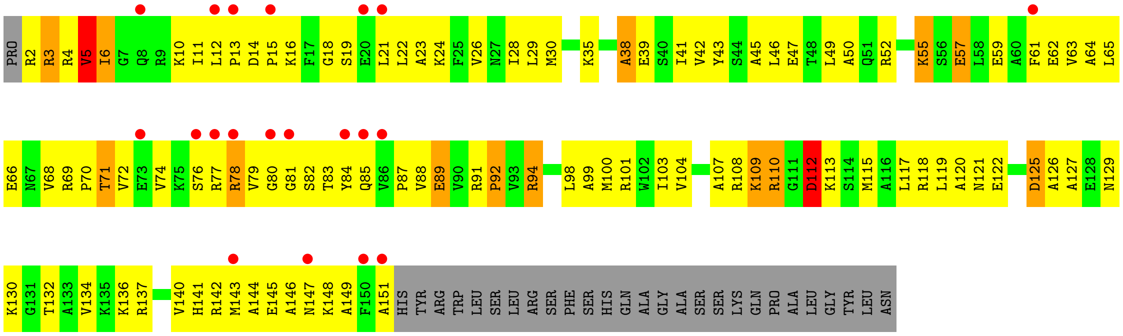
- Molecule 5: 30S ribosomal protein S6



- Molecule 5: 30S ribosomal protein S6

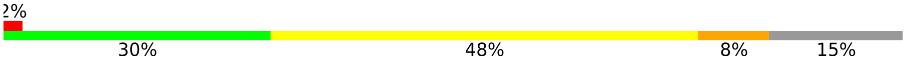


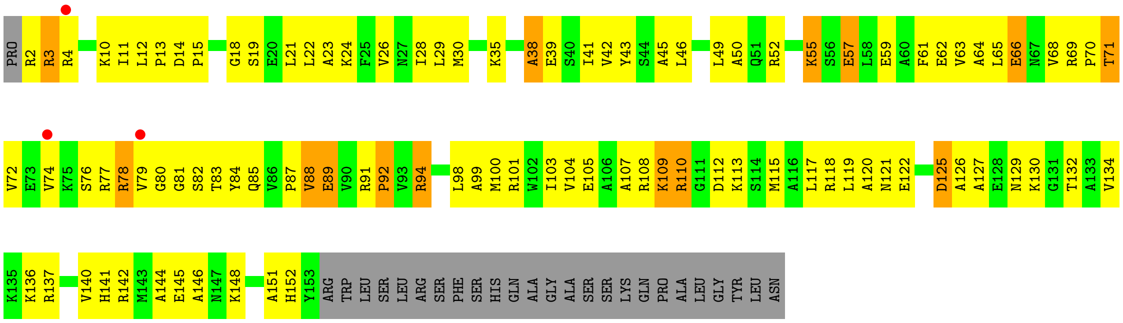
- Molecule 6: 30S ribosomal protein S7



- Molecule 6: 30S ribosomal protein S7

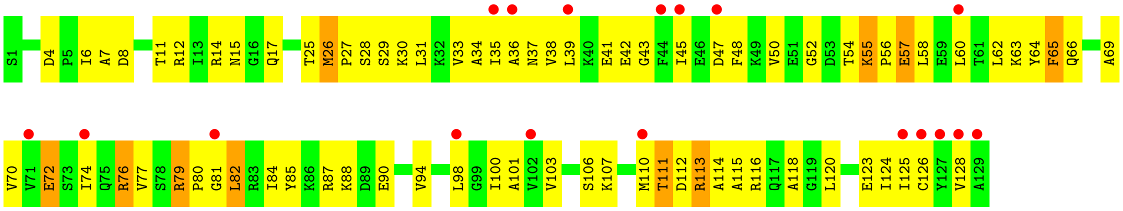
Chain CG:





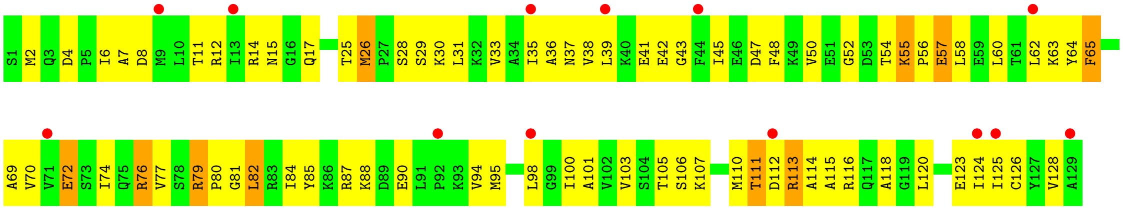
- Molecule 7: 30S ribosomal protein S8

Chain AH:



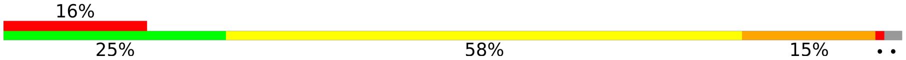
- Molecule 7: 30S ribosomal protein S8

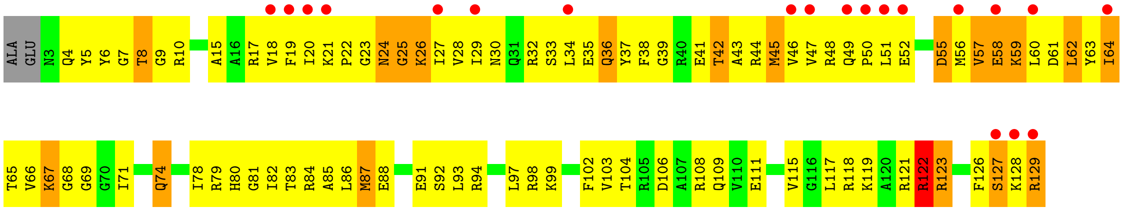
Chain CH:



- Molecule 8: 30S ribosomal protein S9

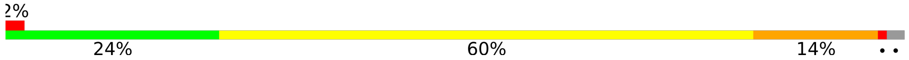
Chain AI:

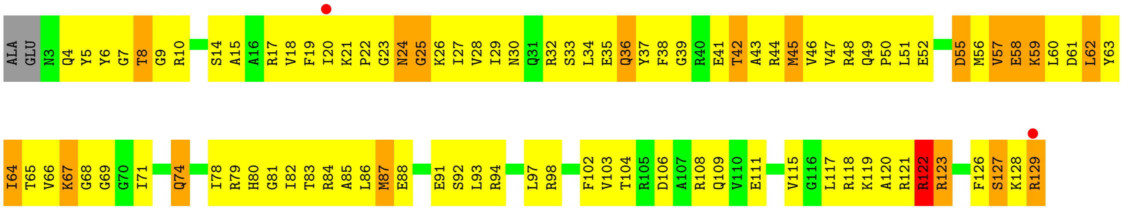




- Molecule 8: 30S ribosomal protein S9

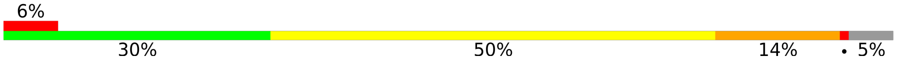
Chain CI:

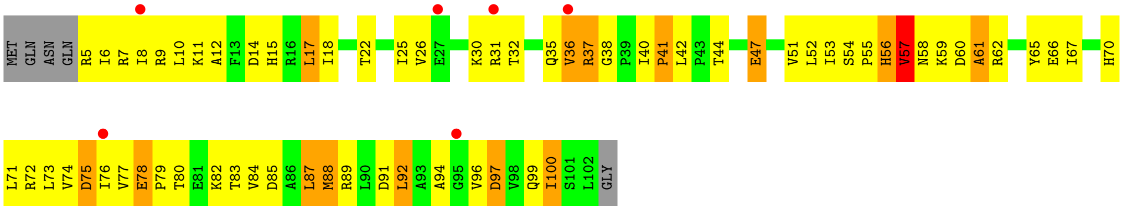




- Molecule 9: 30S ribosomal protein S10

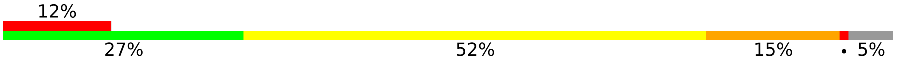
Chain AJ:

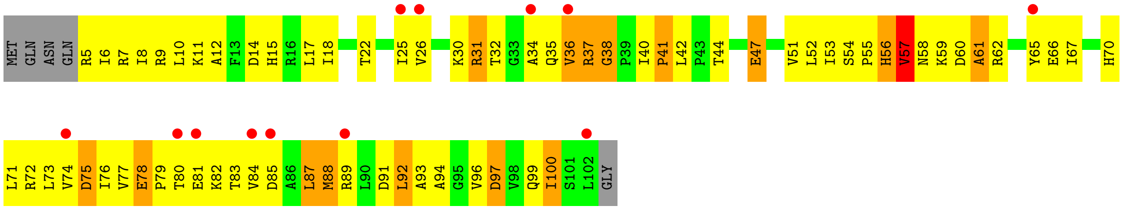




- Molecule 9: 30S ribosomal protein S10

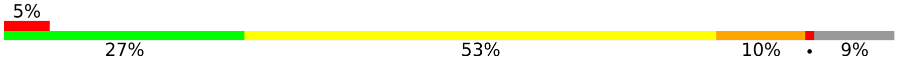
Chain CJ:

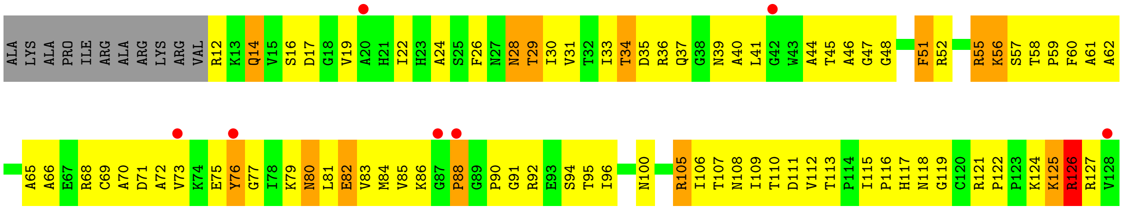




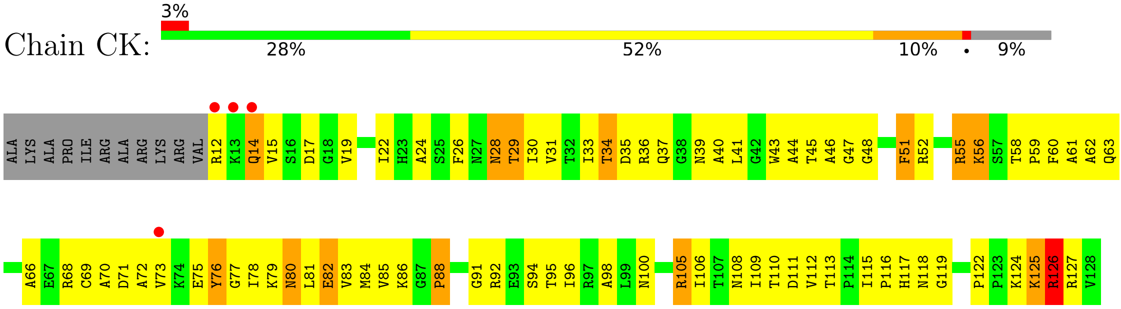
- Molecule 10: 30S ribosomal protein S11

Chain AK:

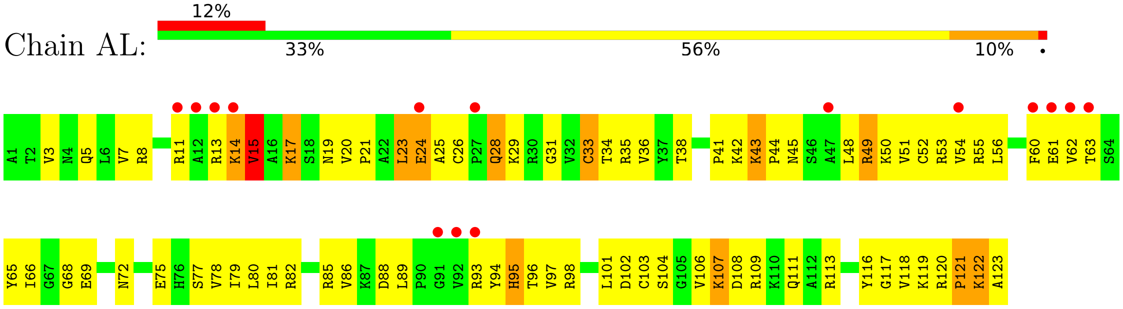




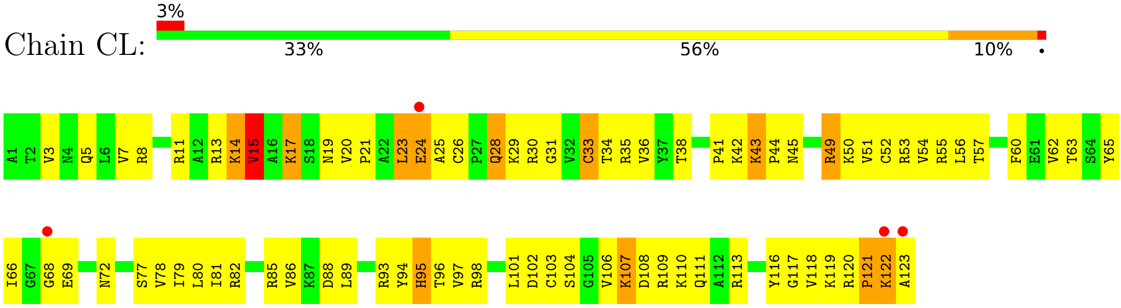
- Molecule 10: 30S ribosomal protein S11



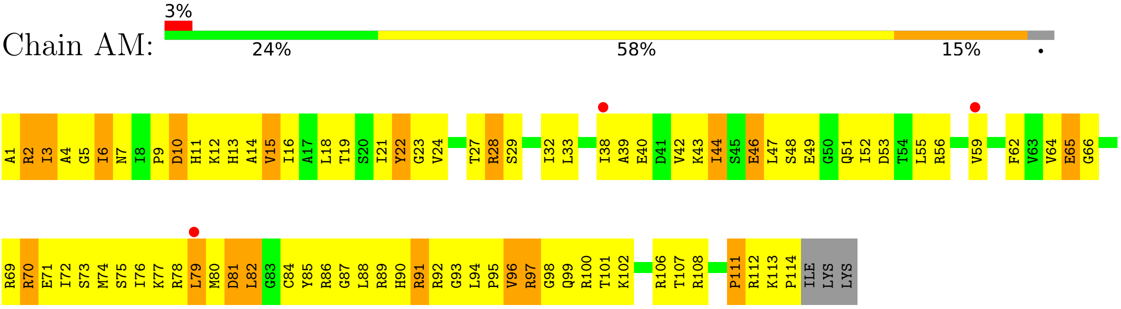
- Molecule 11: 30S ribosomal protein S12



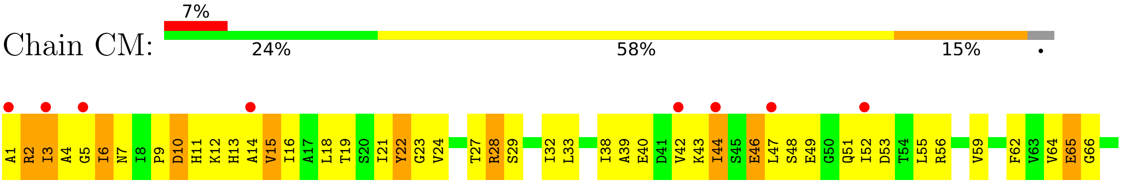
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

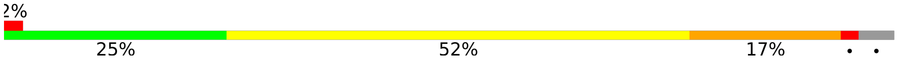


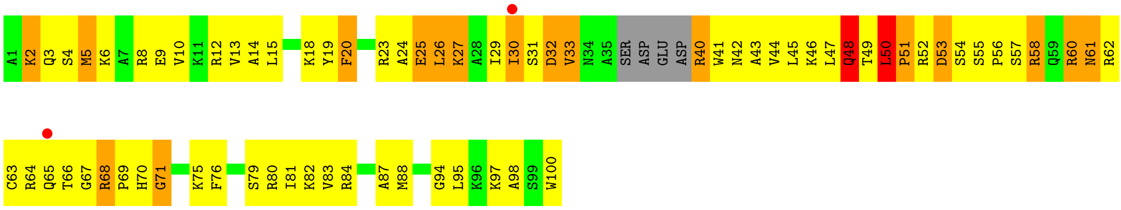
- Molecule 12: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S14

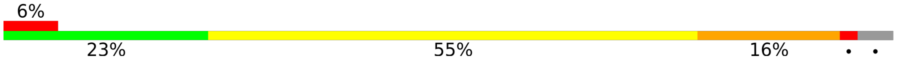
Chain AN:

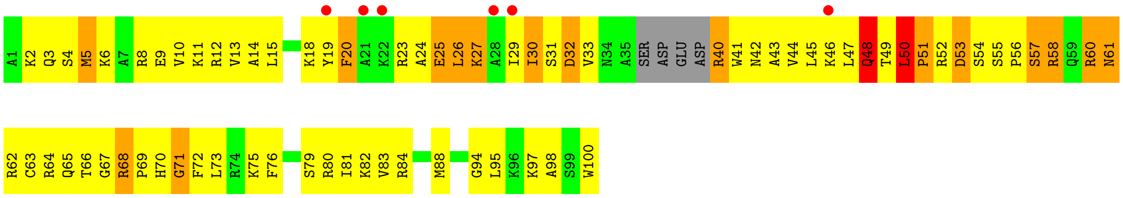




- Molecule 13: 30S ribosomal protein S14

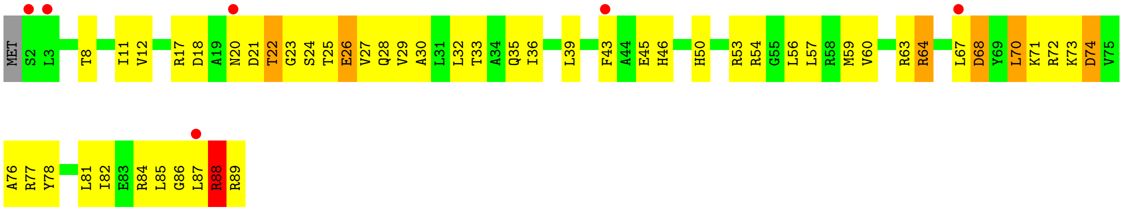
Chain CN:





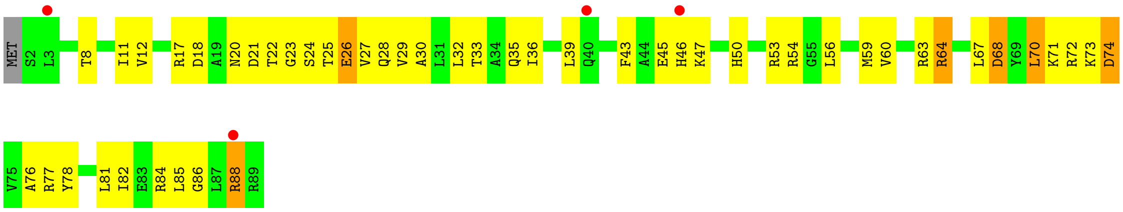
- Molecule 14: 30S ribosomal protein S15

Chain AO:



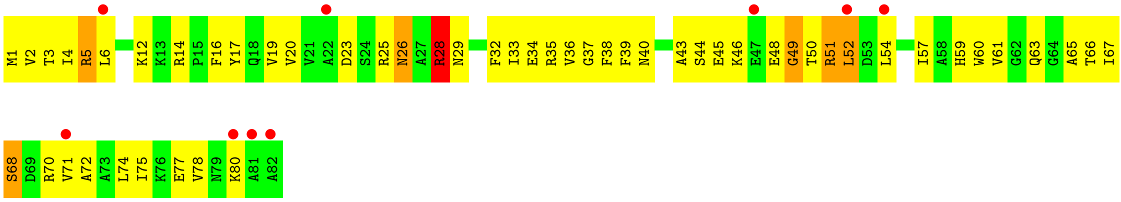
- Molecule 14: 30S ribosomal protein S15

Chain CO:



- Molecule 15: 30S ribosomal protein S16

Chain AP:



- Molecule 15: 30S ribosomal protein S16

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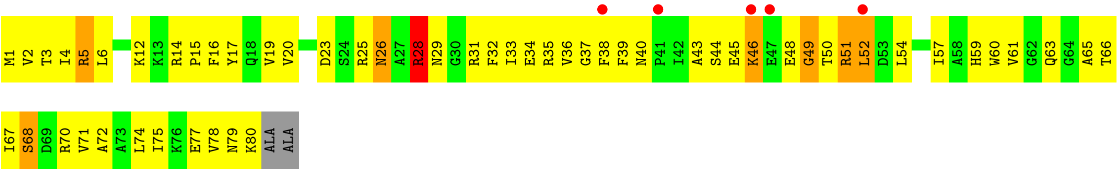
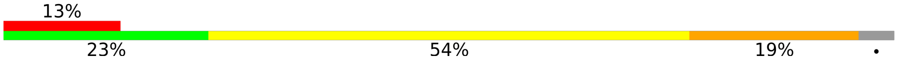
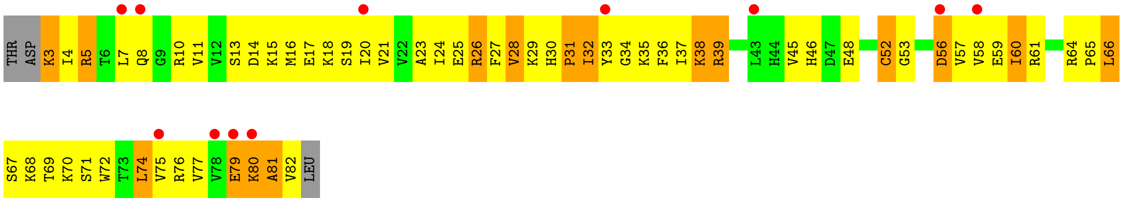


- Molecule 16: 30S ribosomal protein S17

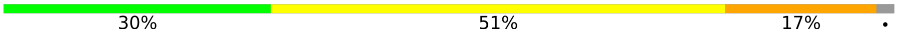
Chain AQ:

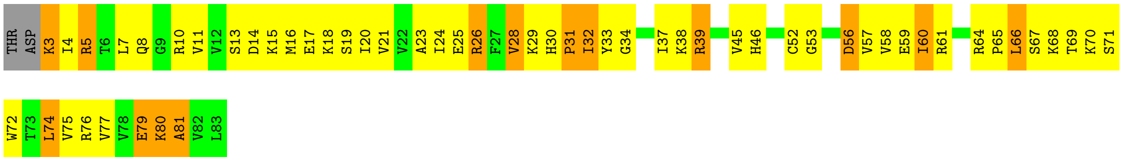




- Molecule 16: 30S ribosomal protein S17

Chain CQ:





- Molecule 17: 30S ribosomal protein S18

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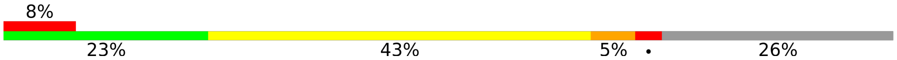

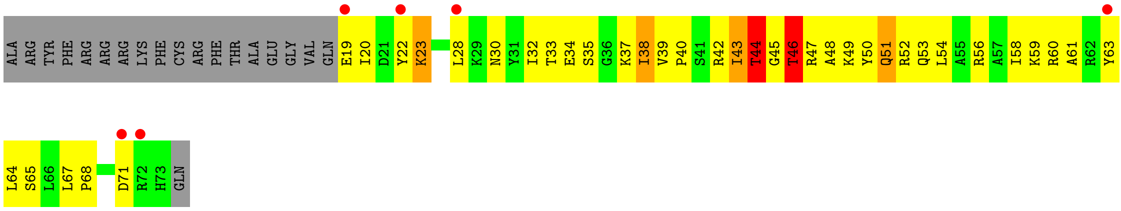

- Molecule 17: 30S ribosomal protein S18

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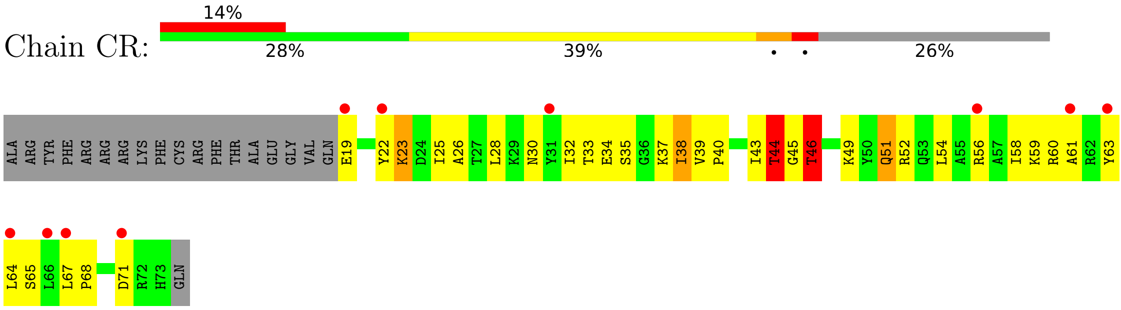
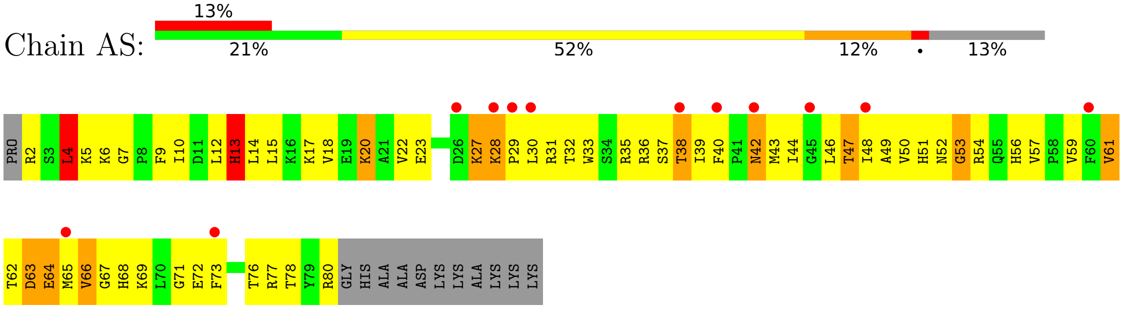


• Molecule 18: 30S ribosomal protein S19

Chain AS:



• Molecule 18: 30S ribosomal protein S19

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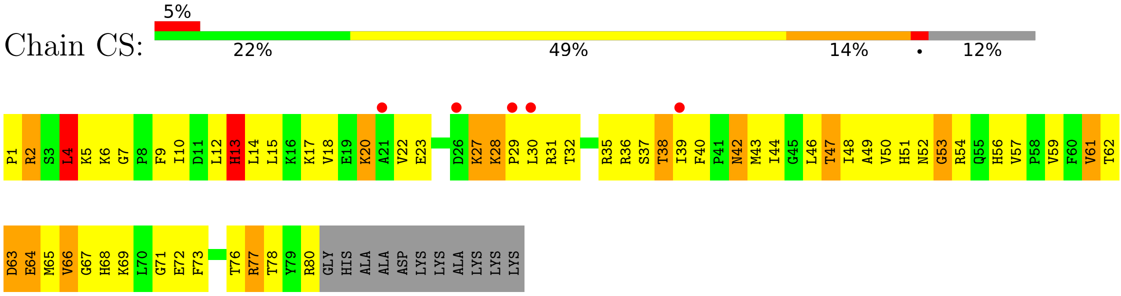
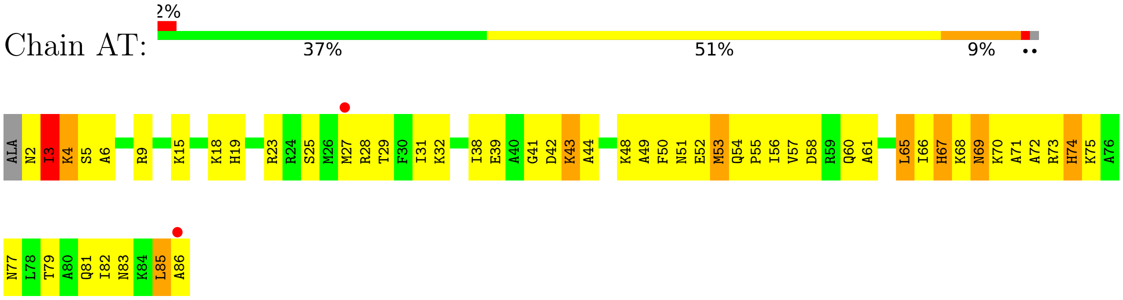


• Molecule 19: 30S ribosomal protein S20

Chain AT:



• Molecule 19: 30S ribosomal protein S20

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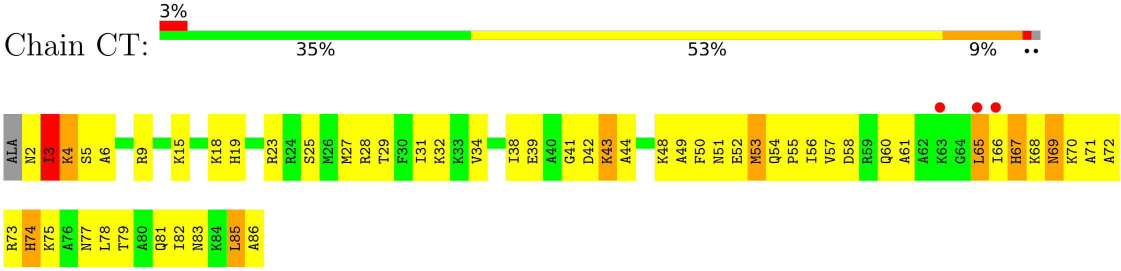

- Molecule 20: 30S ribosomal protein S2

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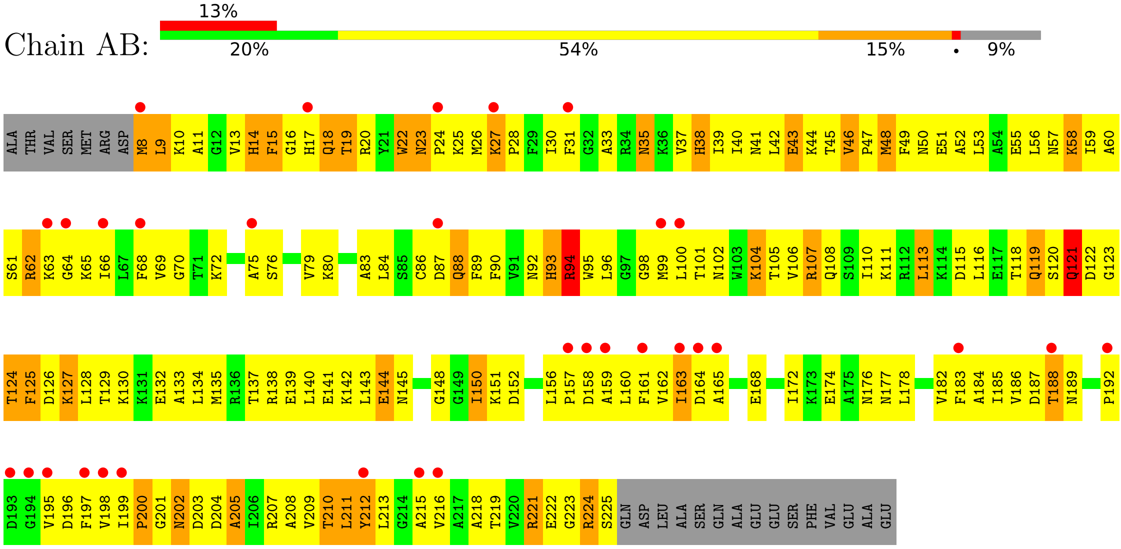

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- Molecule 20: 30S ribosomal protein S2

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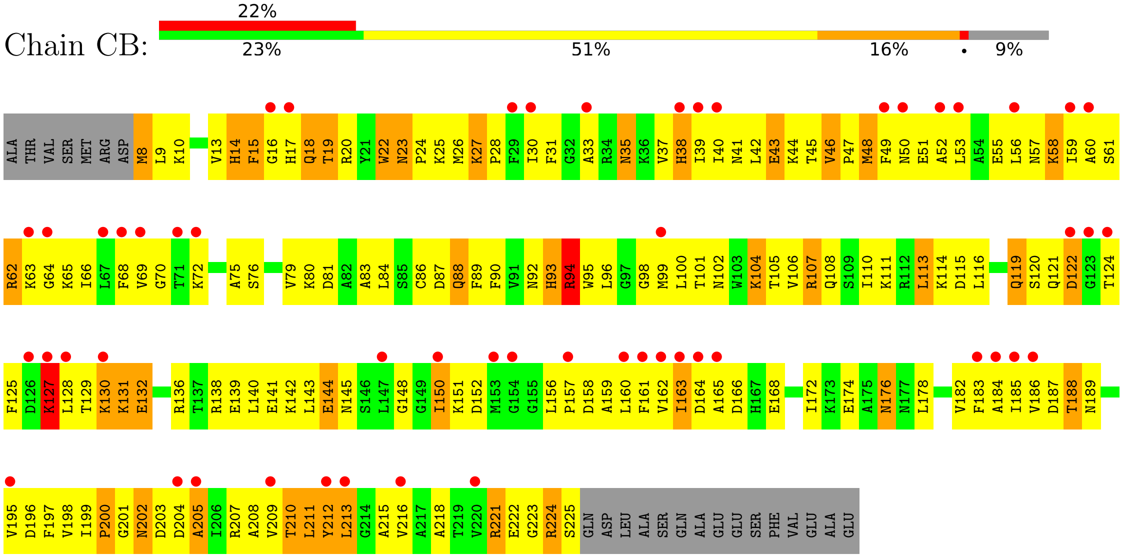

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- Molecule 21: 30S ribosomal protein S21

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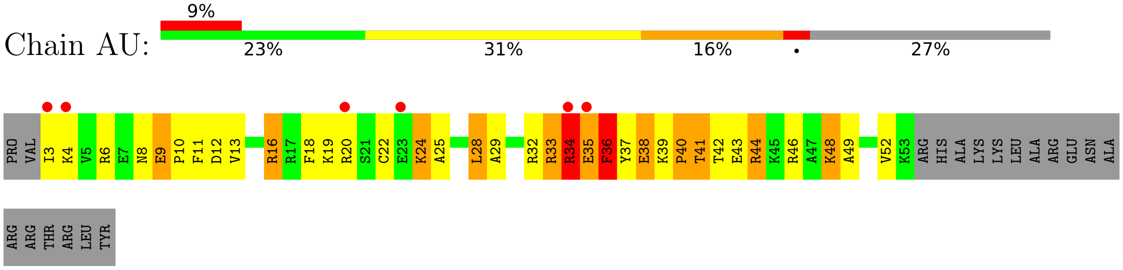

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- Molecule 21: 30S ribosomal protein S21

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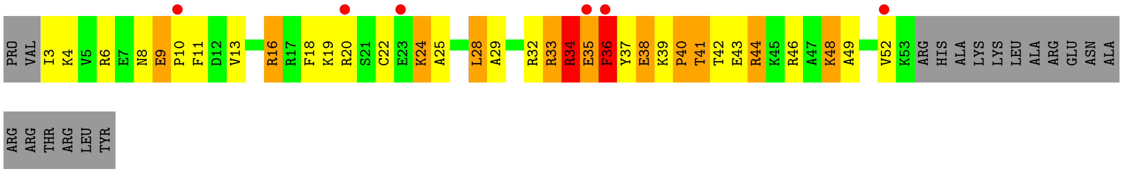

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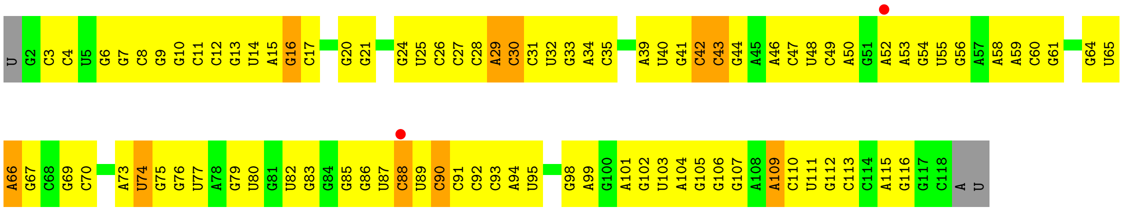

- Molecule 22: 5S rRNA

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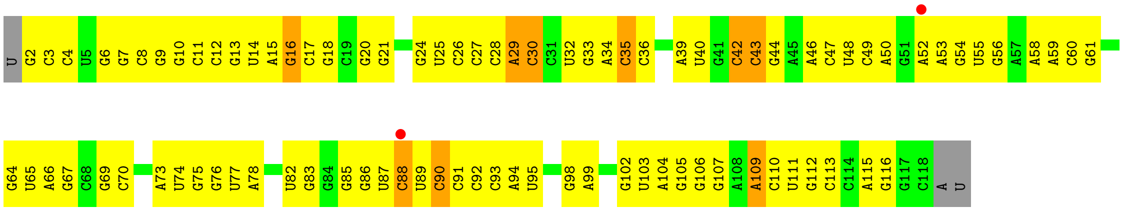

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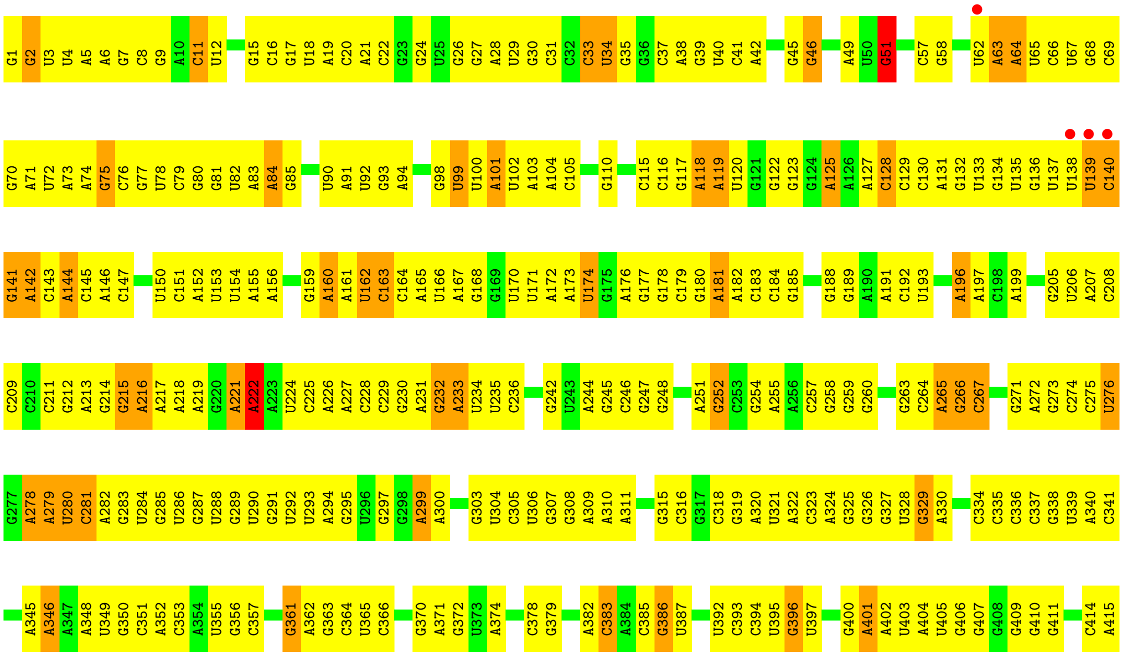

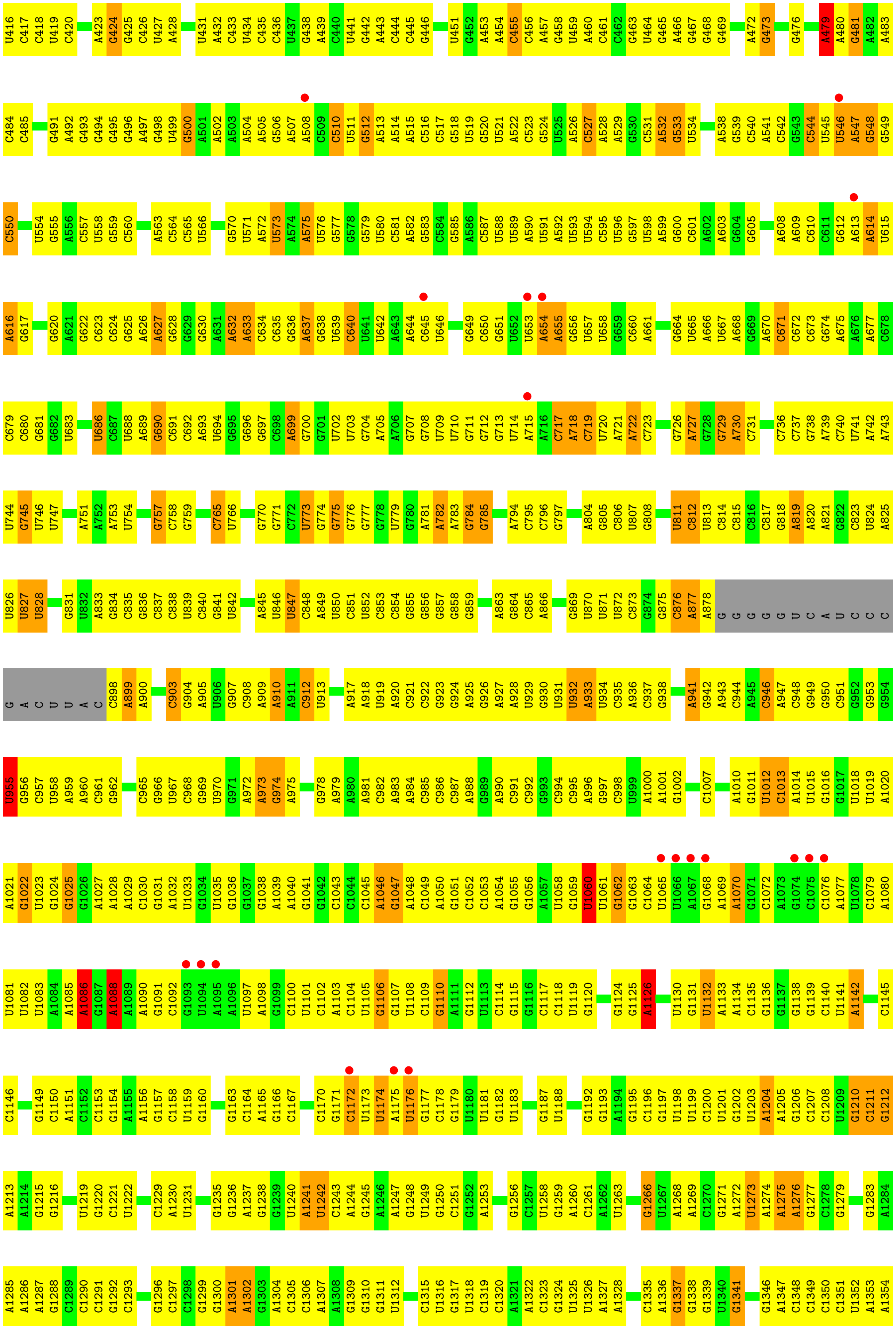
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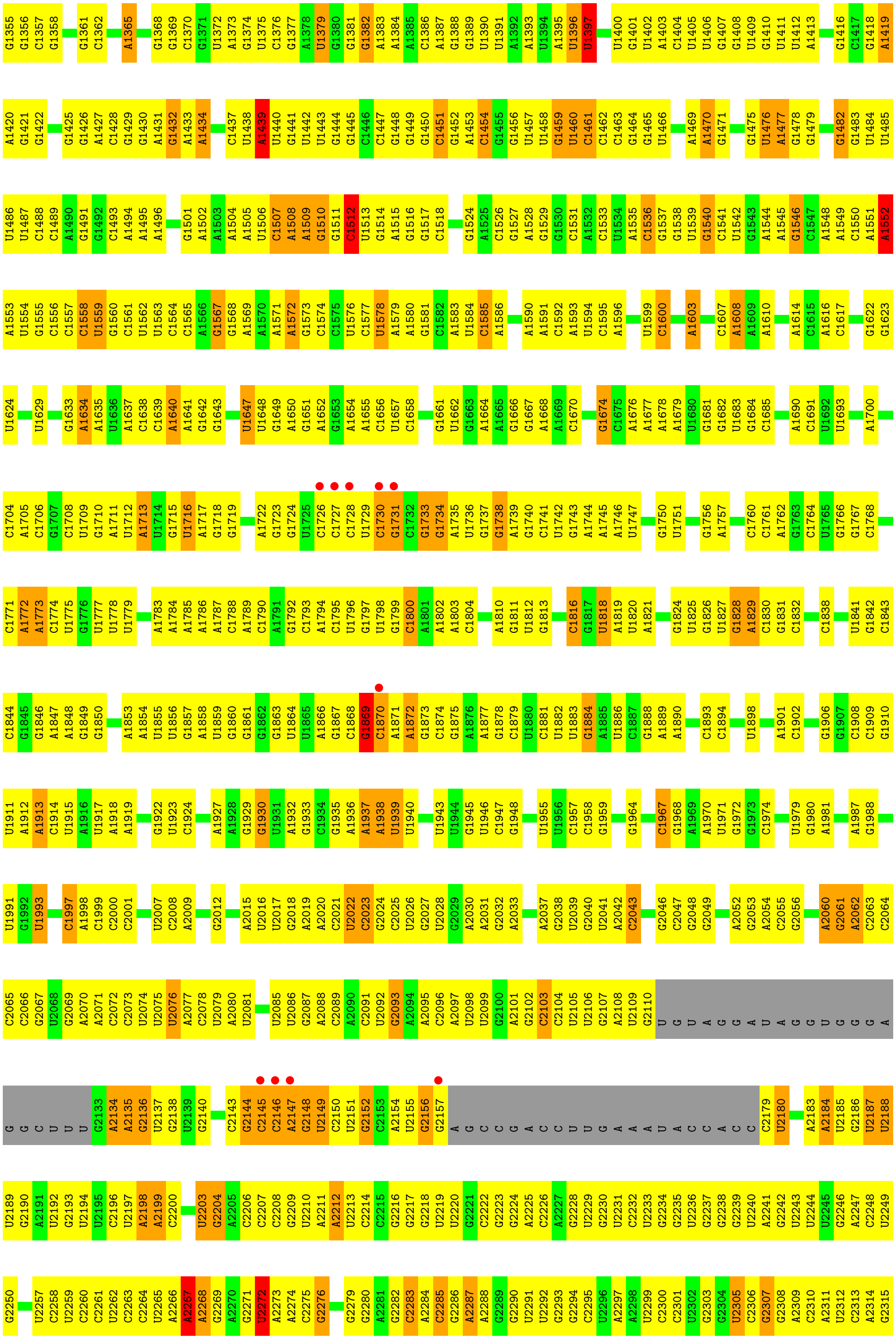
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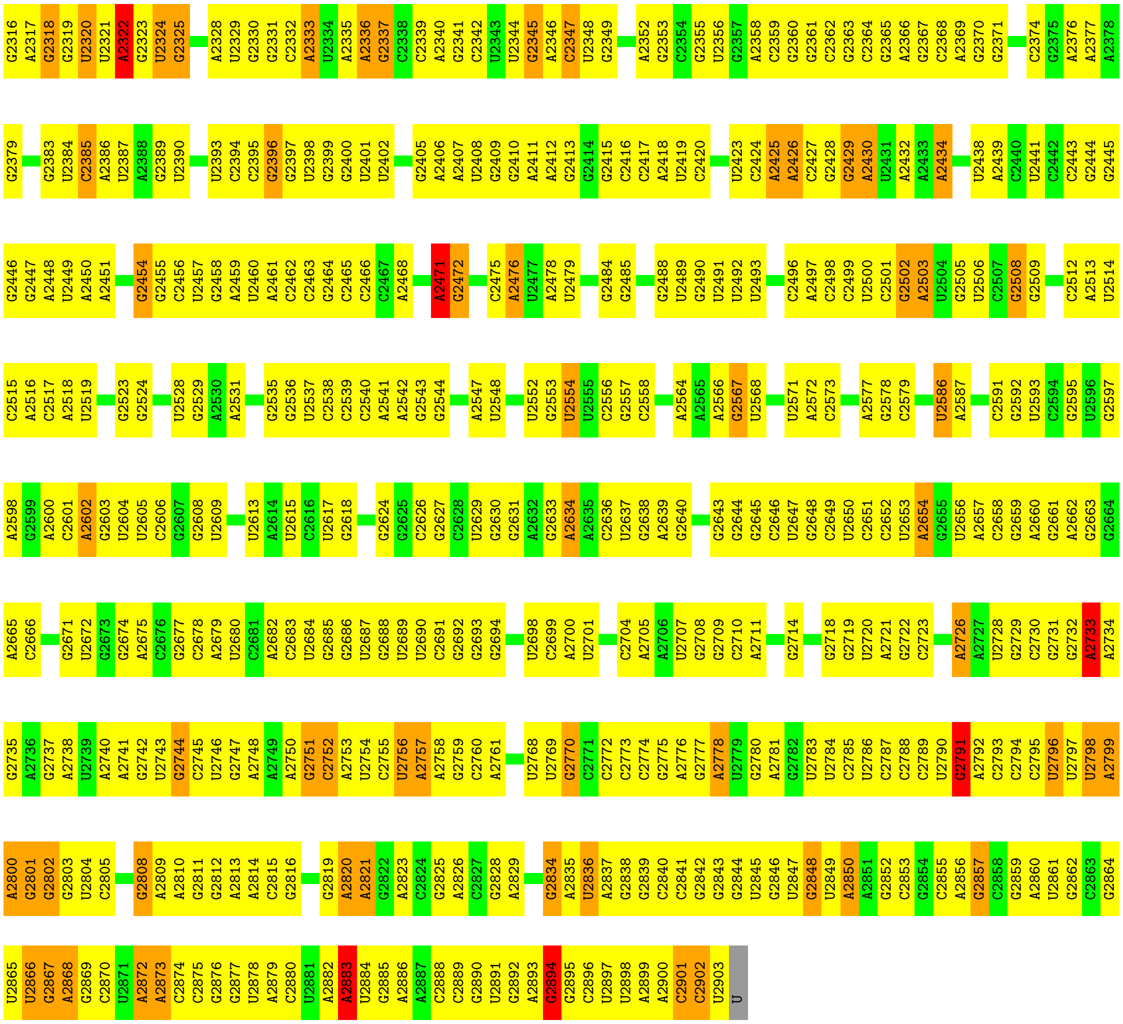

- Molecule 23: 23S rRNA

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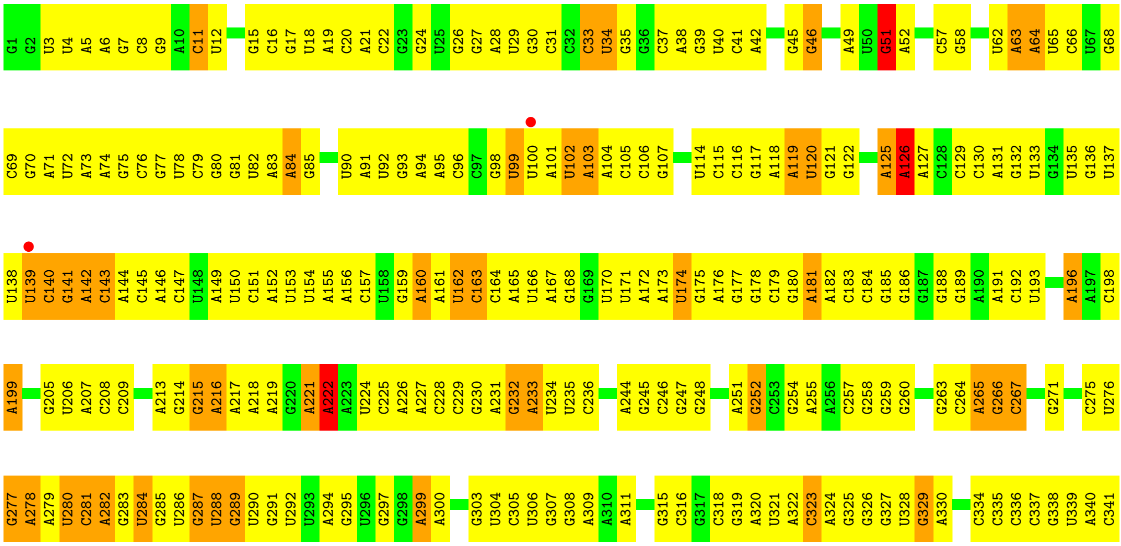

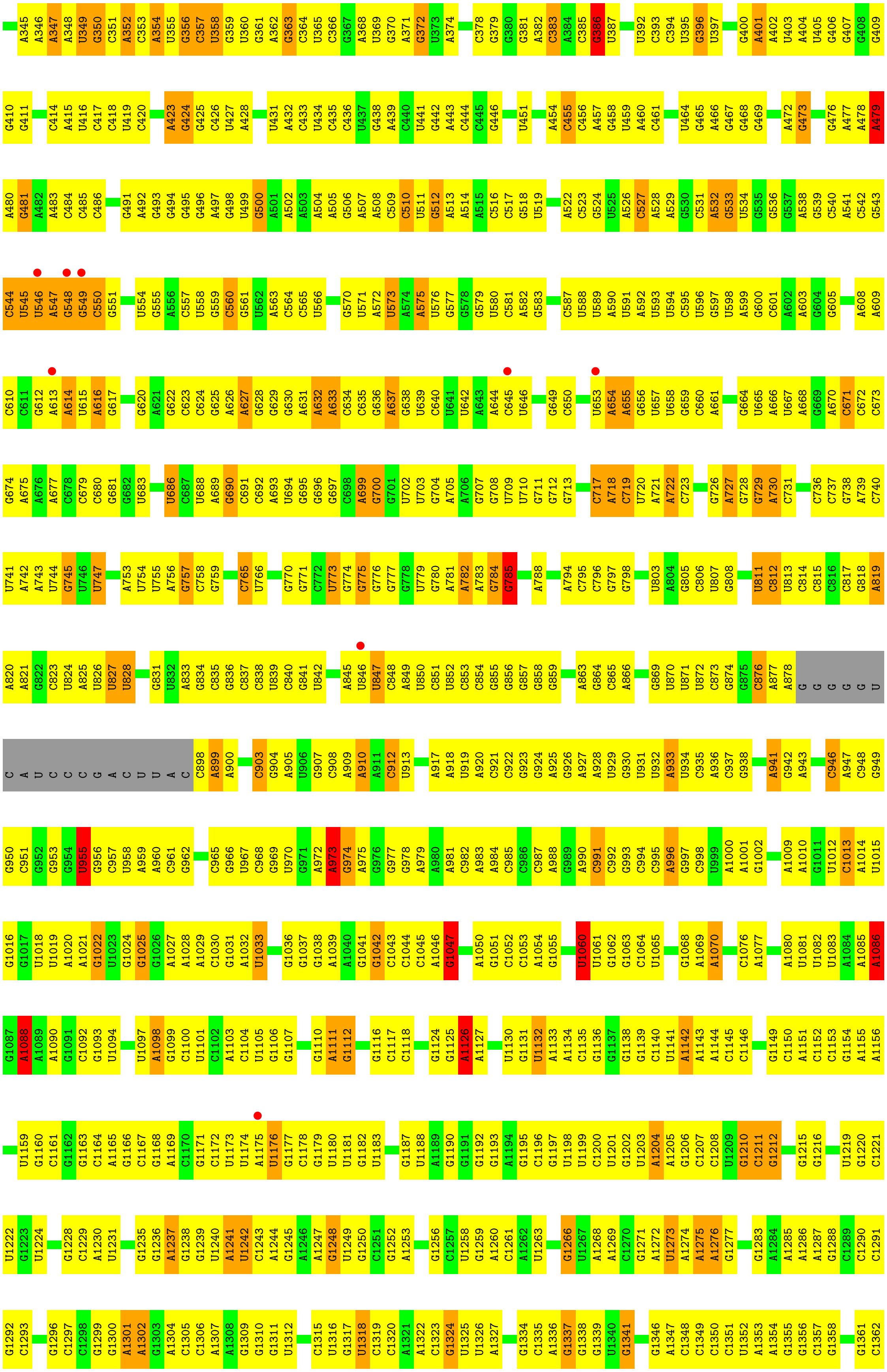
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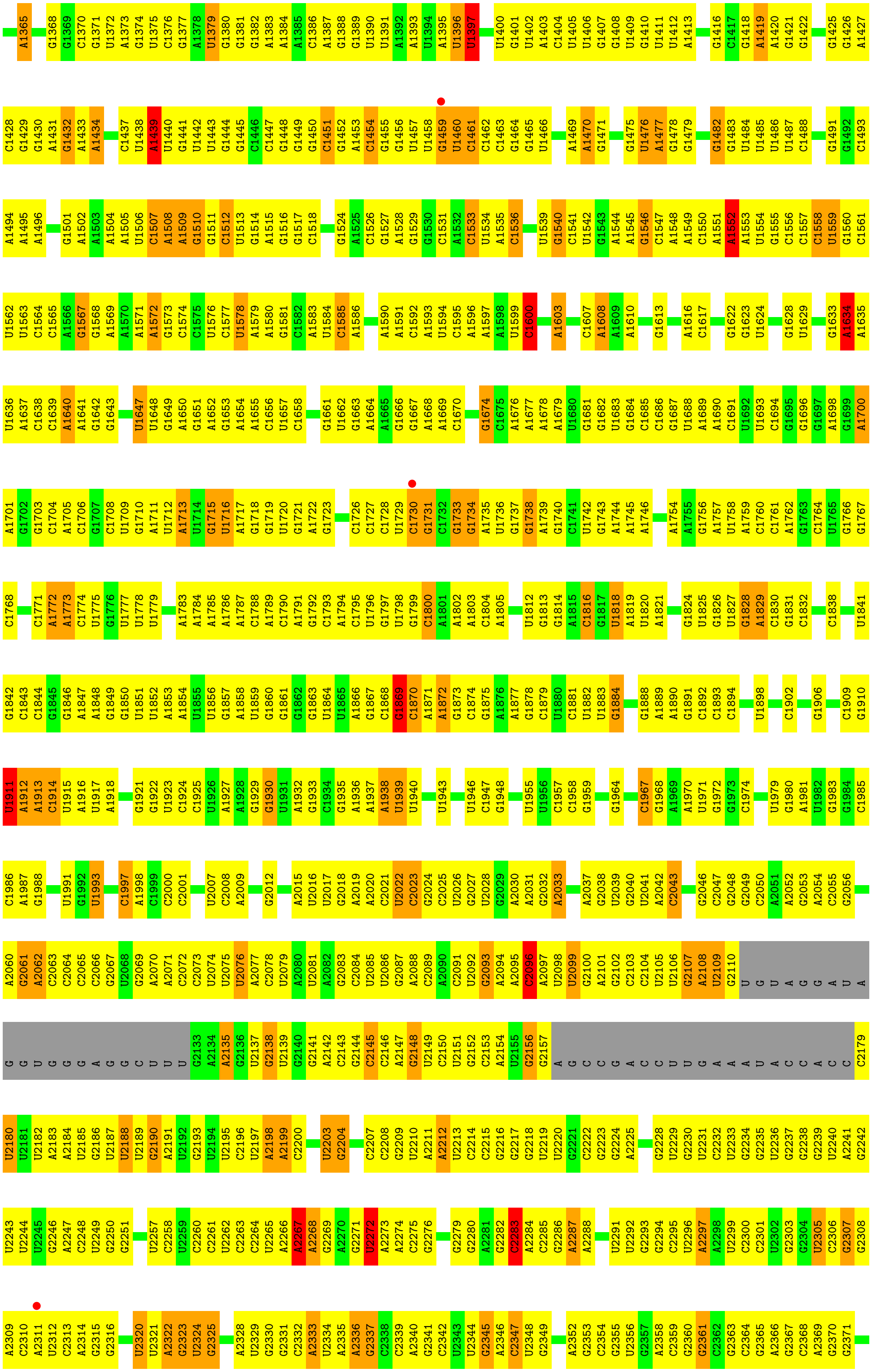
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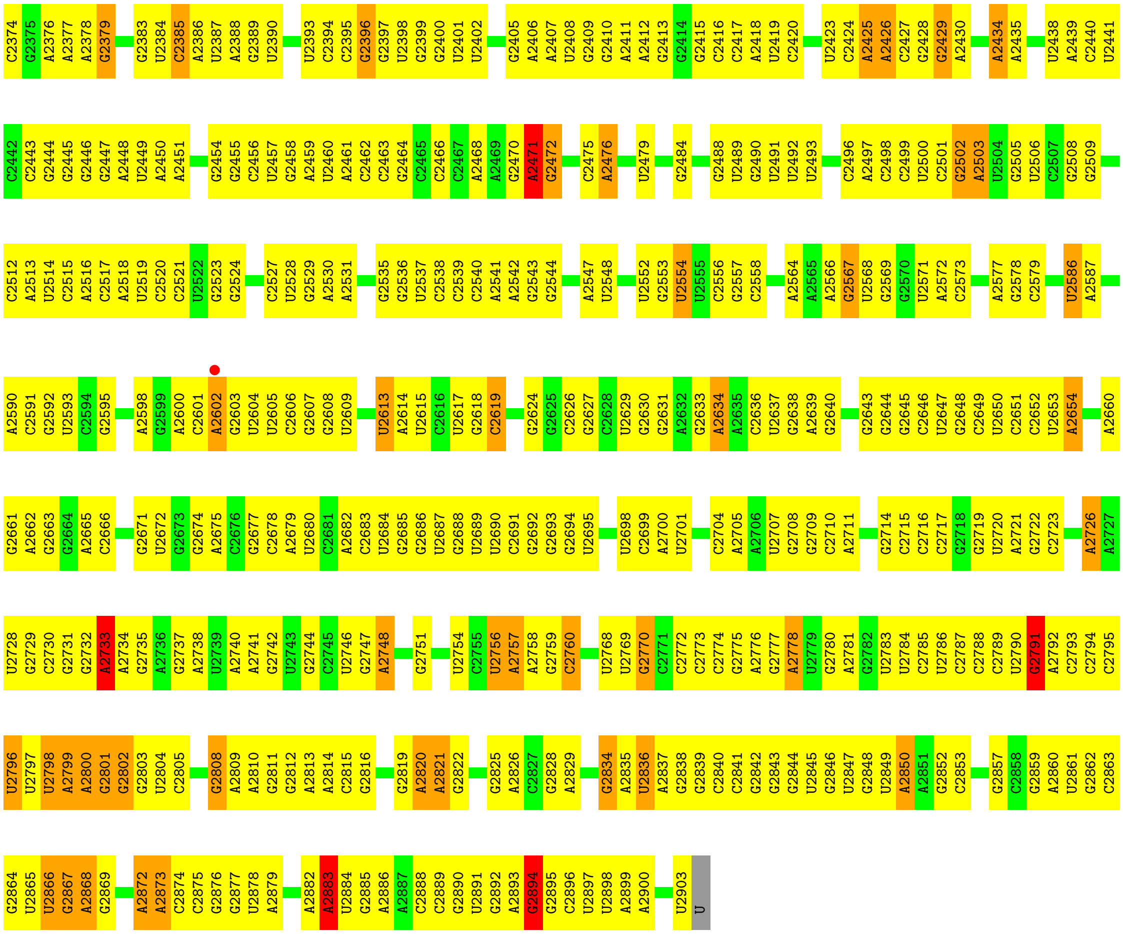

- Molecule 24: 50S ribosomal protein L11

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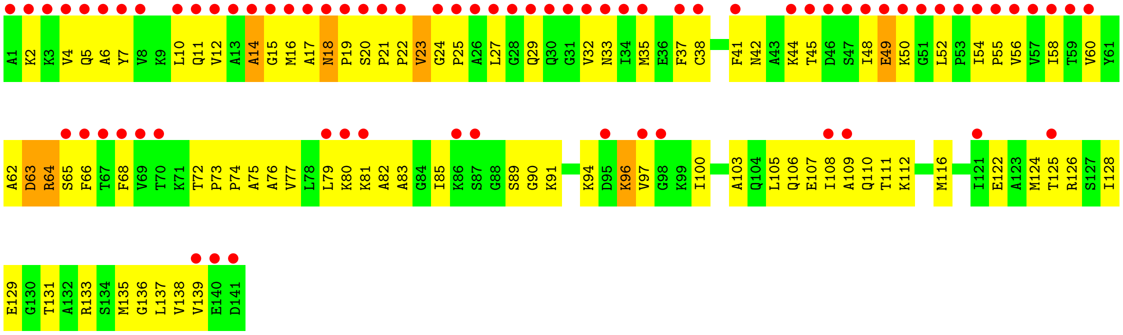

- Molecule 24: 50S ribosomal protein L11

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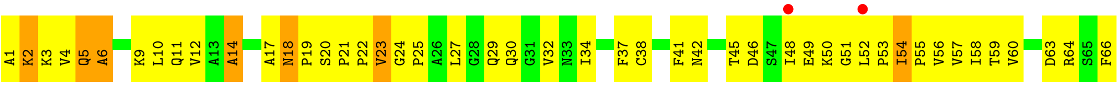
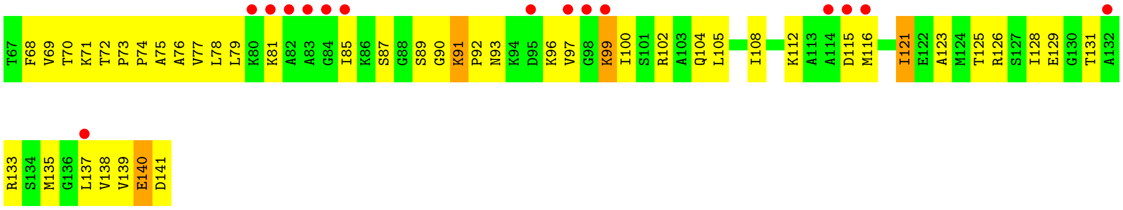
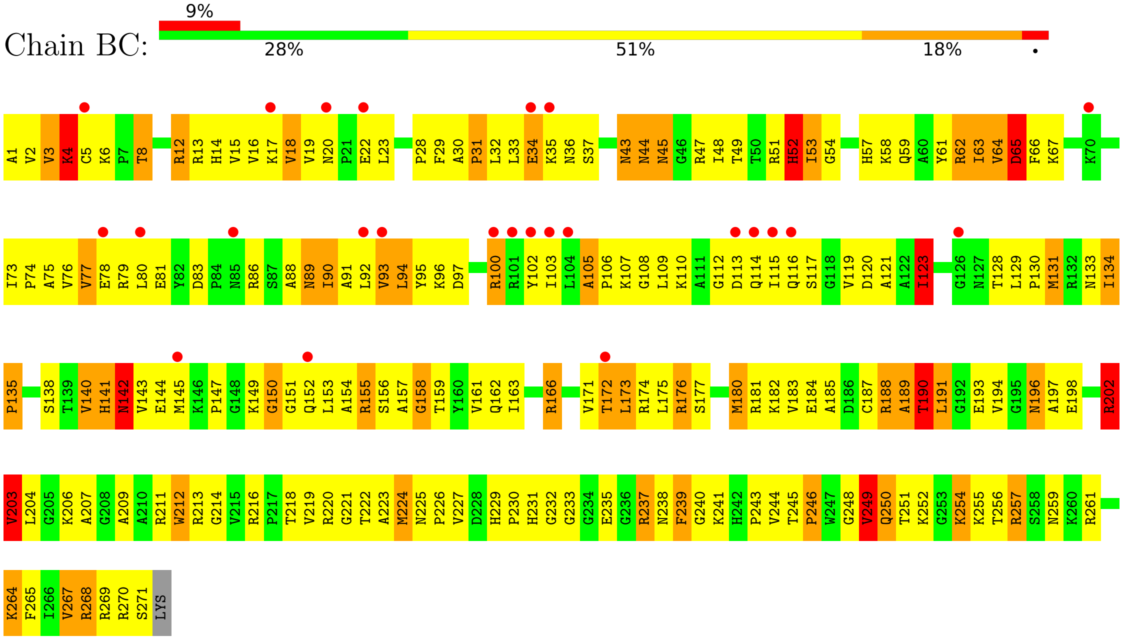
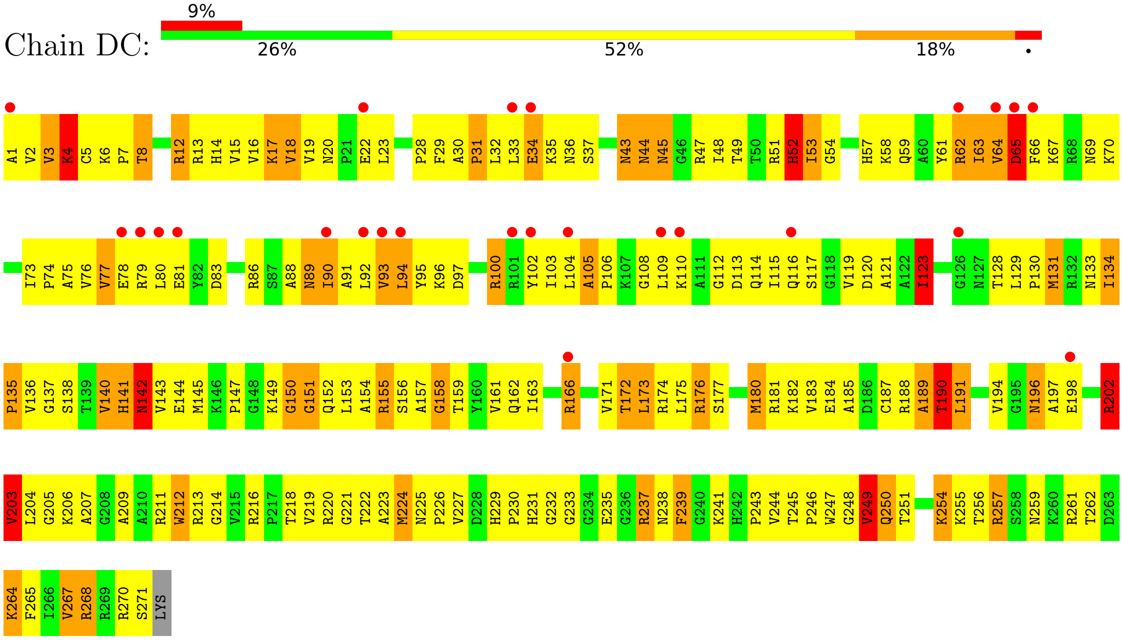




- Molecule 25: 50S ribosomal protein L2



- Molecule 25: 50S ribosomal protein L2



- Molecule 26: 50S ribosomal protein L3

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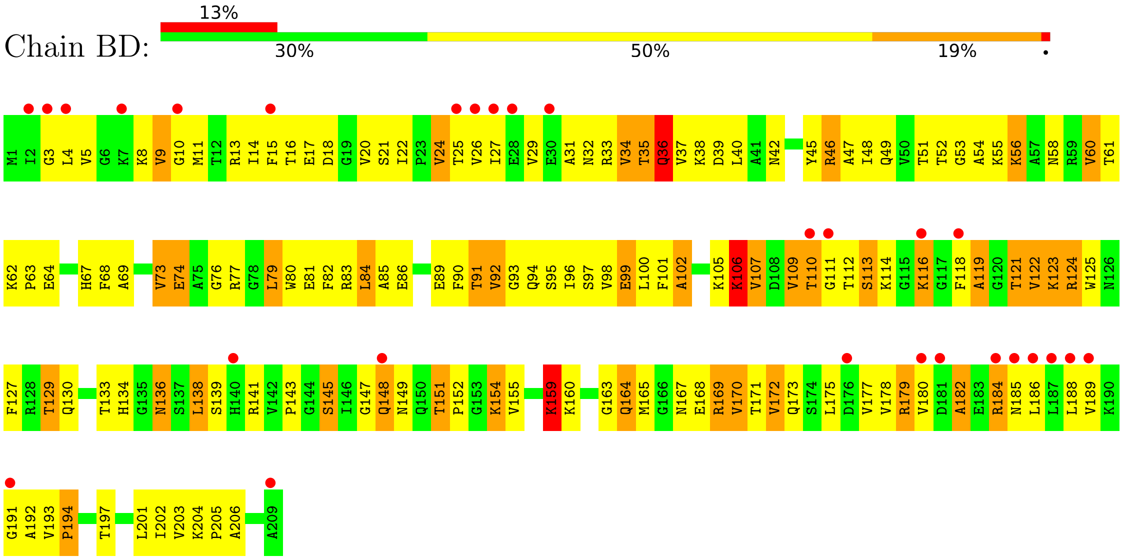
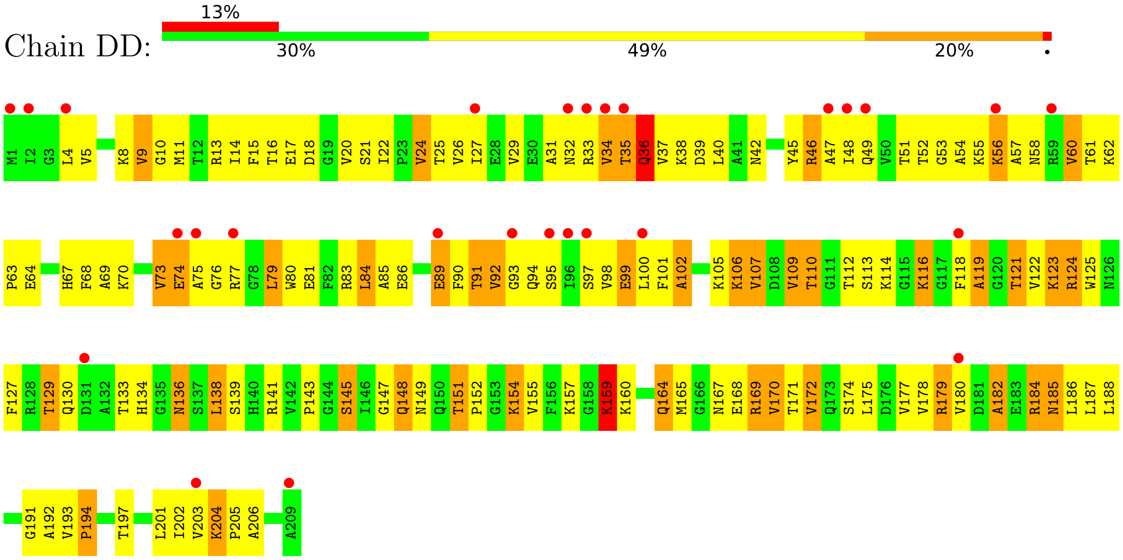


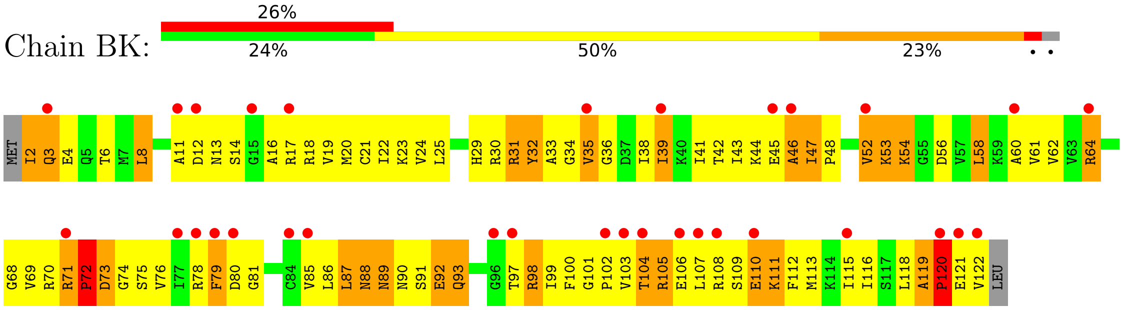
- Molecule 26: 50S ribosomal protein L3

Chain DD:



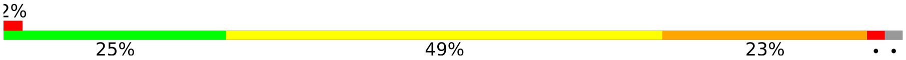
- Molecule 27: 50S ribosomal protein L14

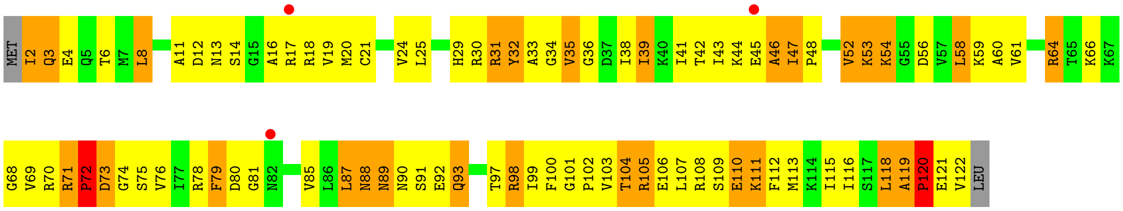
Chain BK:



- Molecule 27: 50S ribosomal protein L14

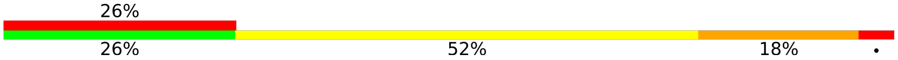
Chain DK:

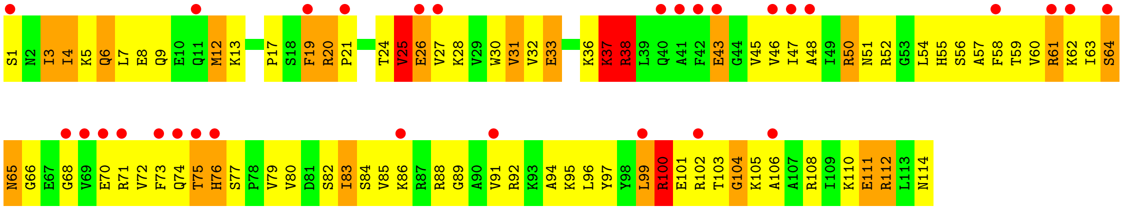




- Molecule 28: 50S ribosomal protein L19

Chain BP:





- Molecule 28: 50S ribosomal protein L19

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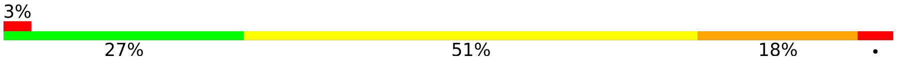
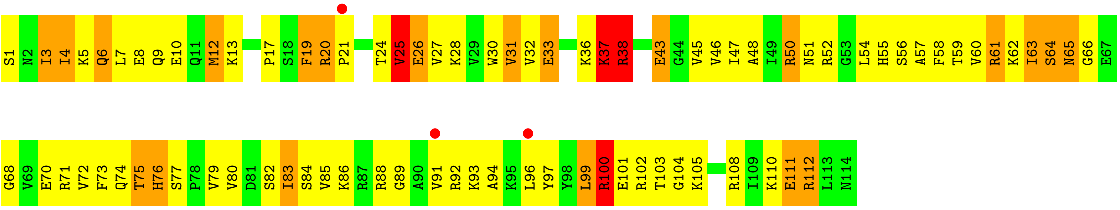
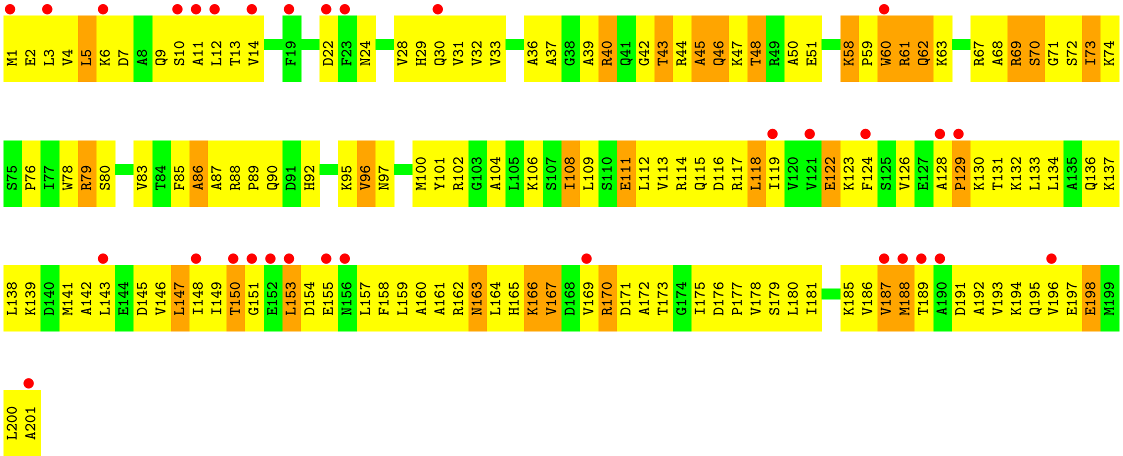




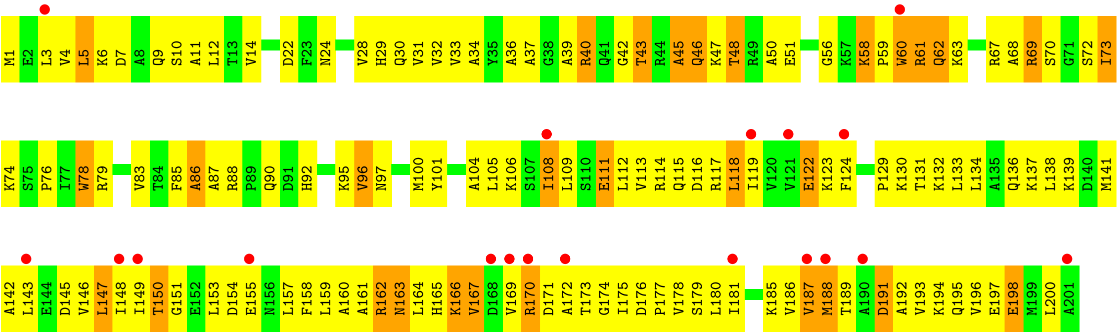
- Molecule 29: 50S ribosomal protein L4

Chain BE:



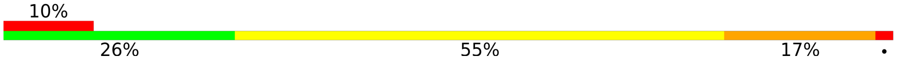
- Molecule 29: 50S ribosomal protein L4

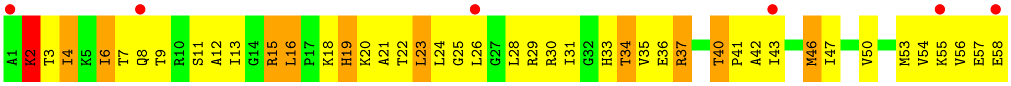
Chain DE:



- Molecule 30: 50S ribosomal protein L30

Chain BY:





- Molecule 30: 50S ribosomal protein L30

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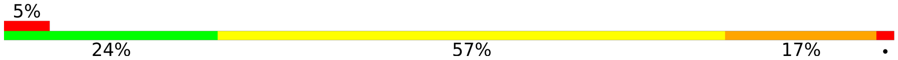
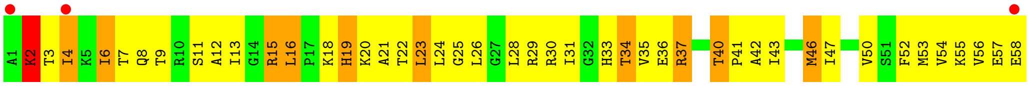


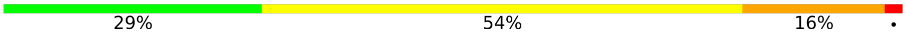


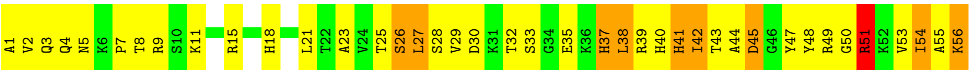
- Molecule 31: 50S ribosomal protein L32

Chain B0:

- Molecule 31: 50S ribosomal protein L32

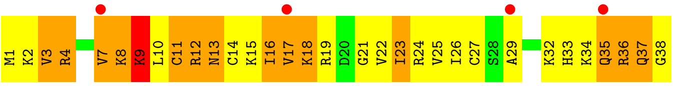
Chain D0:





- Molecule 32: 50S ribosomal protein L36

Chain B4:



- Molecule 32: 50S ribosomal protein L36

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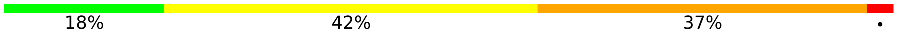
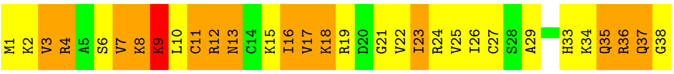
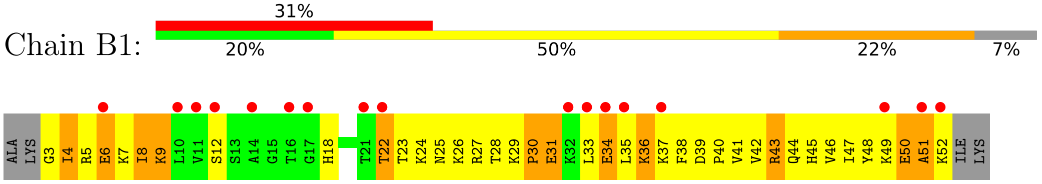
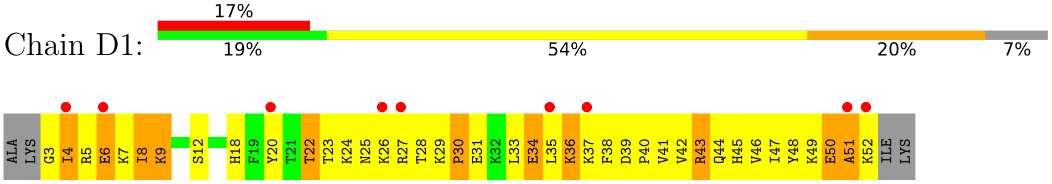




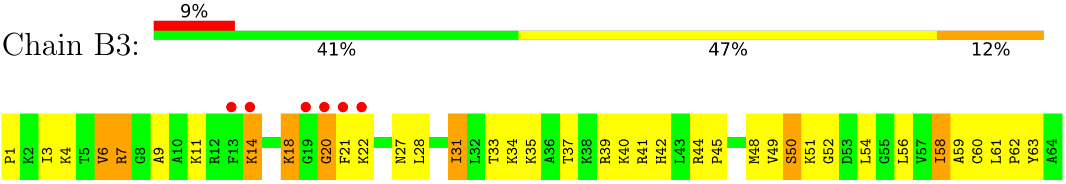
- Molecule 33: 50S ribosomal protein L33



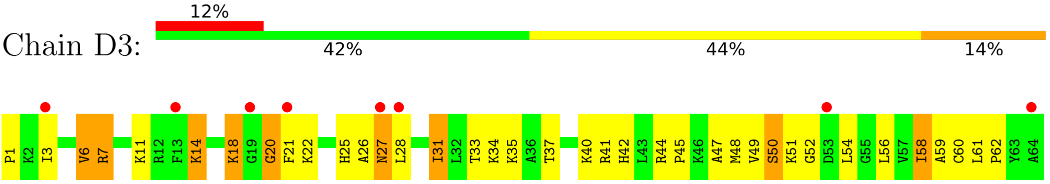
- Molecule 33: 50S ribosomal protein L33



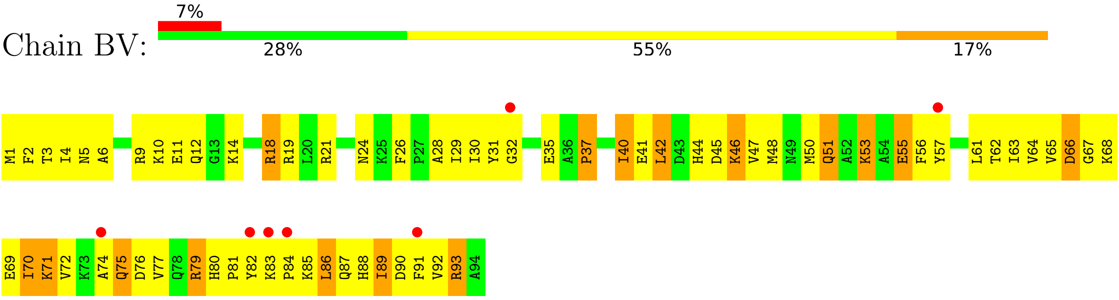
- Molecule 34: 50S ribosomal protein L35



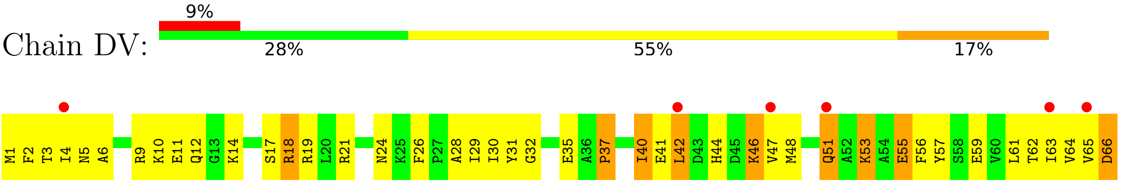
- Molecule 34: 50S ribosomal protein L35

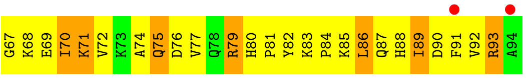


- Molecule 35: 50S ribosomal protein L25

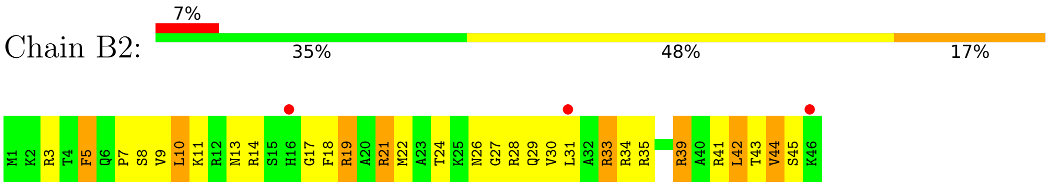


- Molecule 35: 50S ribosomal protein L25

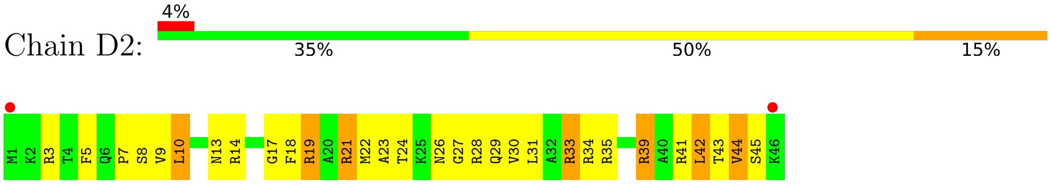




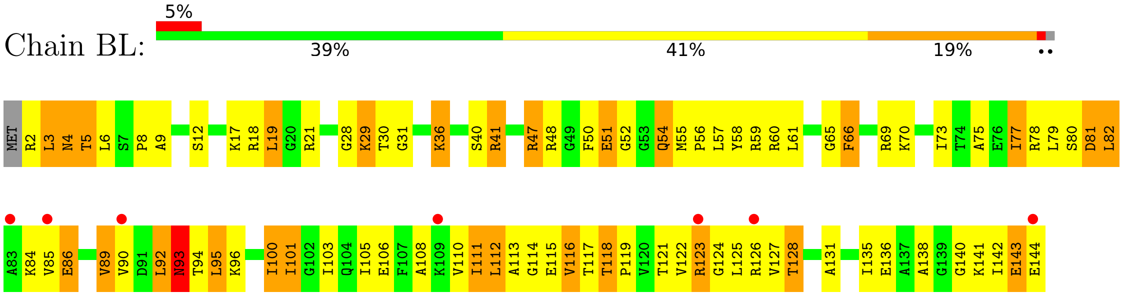
- Molecule 36: 50S ribosomal protein L34



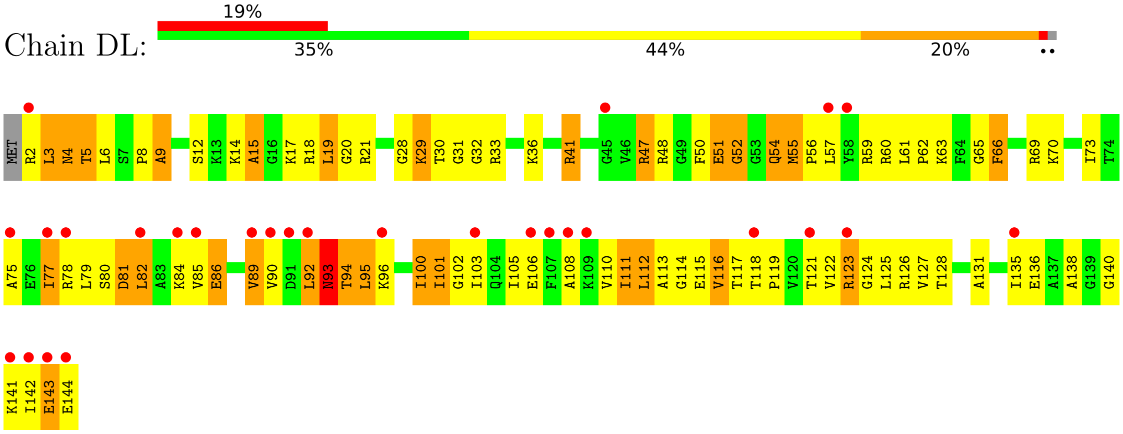
- Molecule 36: 50S ribosomal protein L34



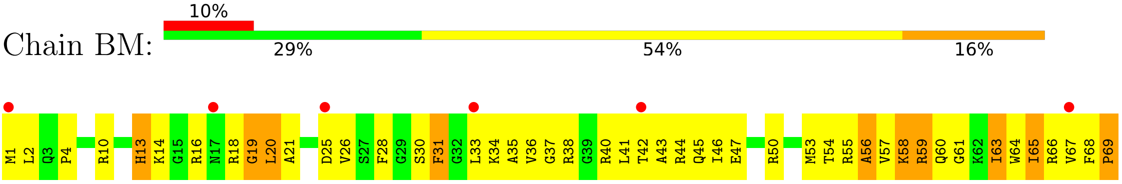
- Molecule 37: 50S ribosomal protein L15

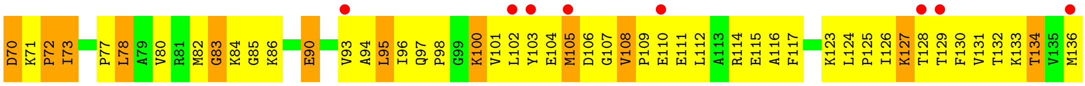


- Molecule 37: 50S ribosomal protein L15

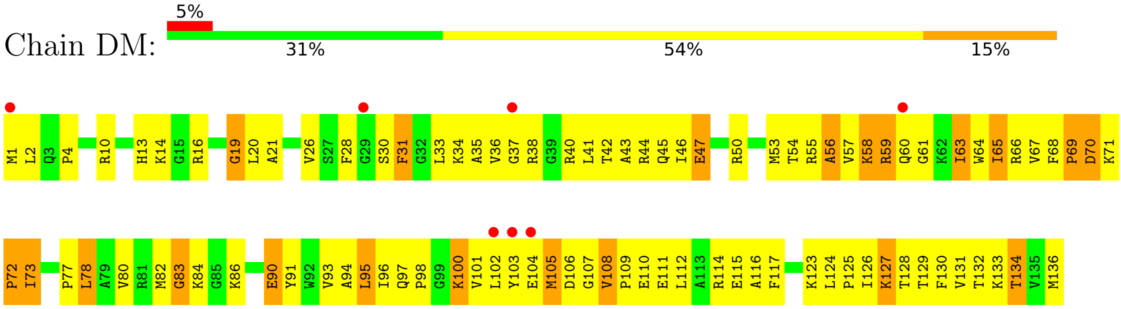


- Molecule 38: 50S ribosomal protein L16

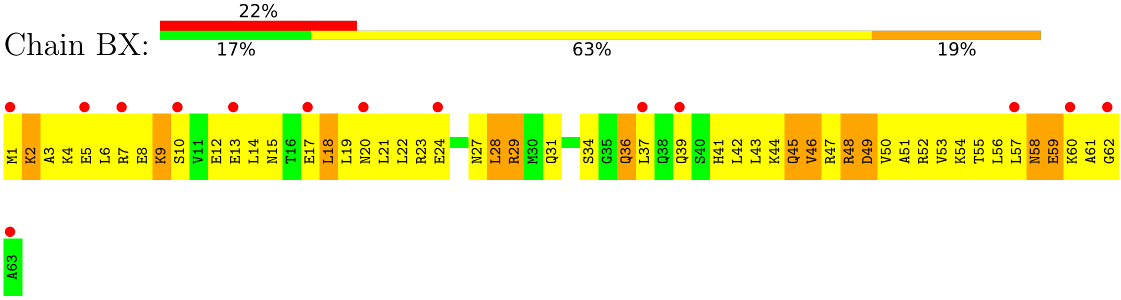




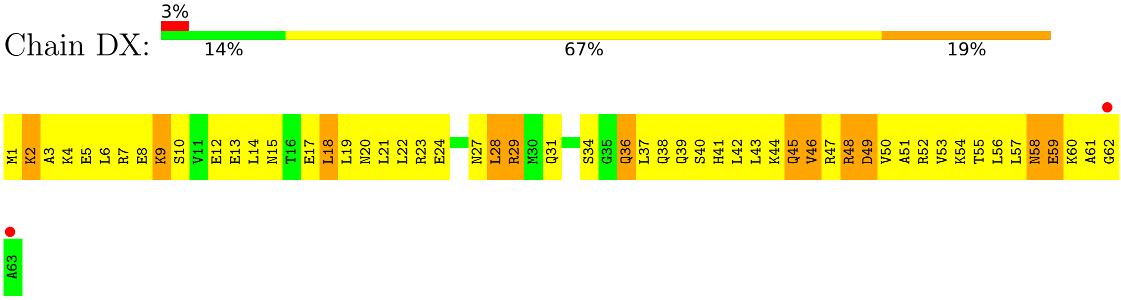
- Molecule 38: 50S ribosomal protein L16



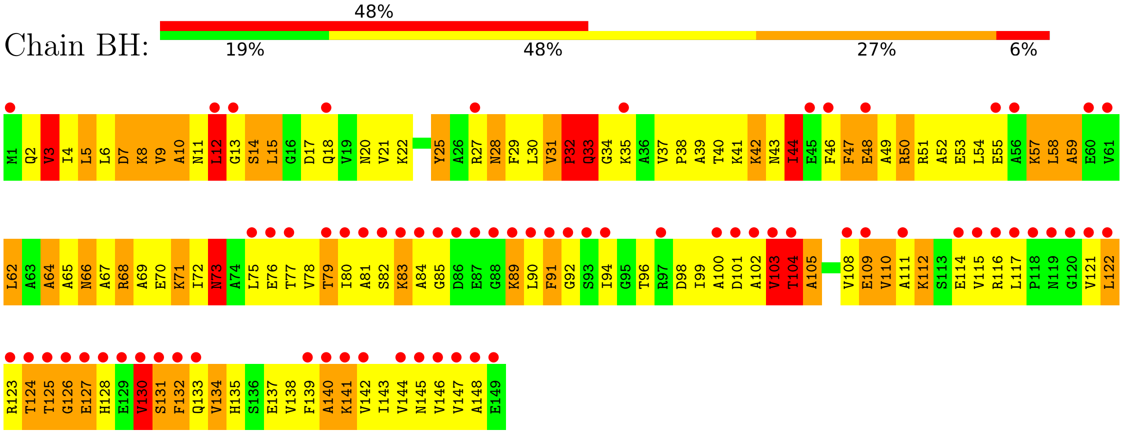
- Molecule 39: 50S ribosomal protein L29



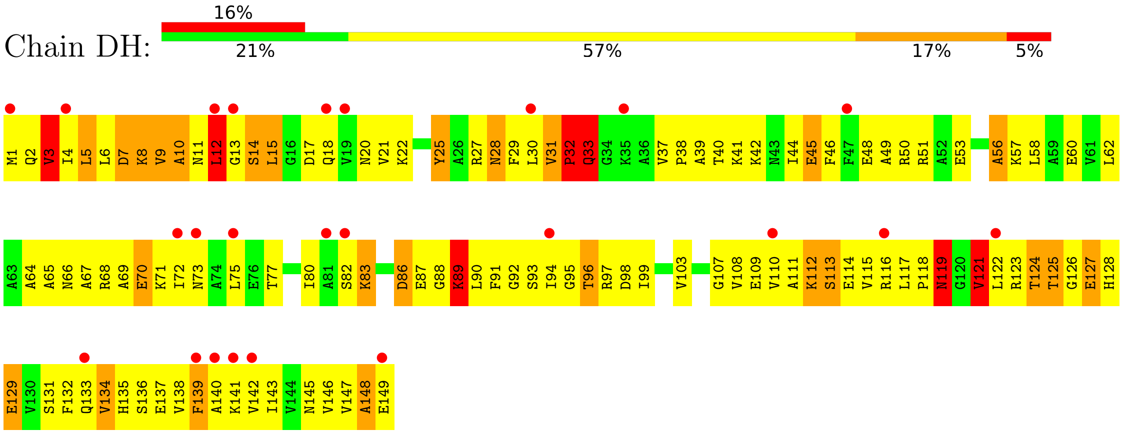
- Molecule 39: 50S ribosomal protein L29



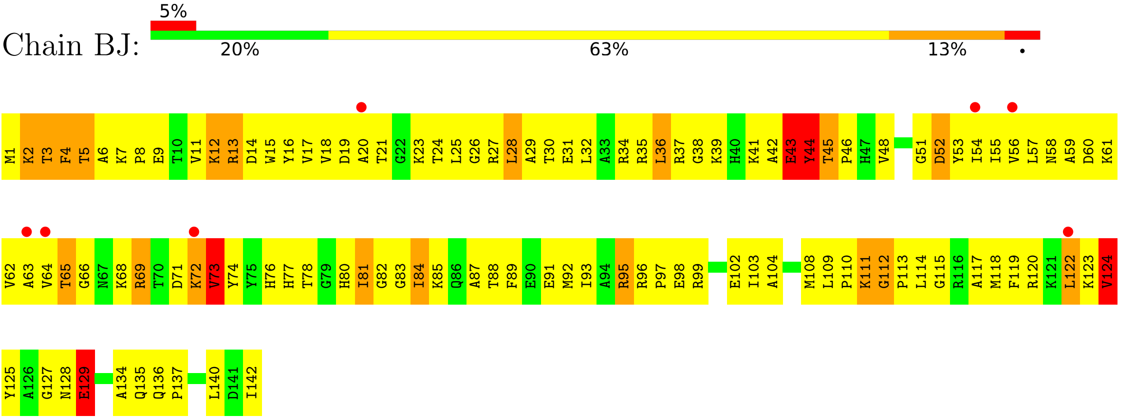
- Molecule 40: 50S ribosomal protein L9



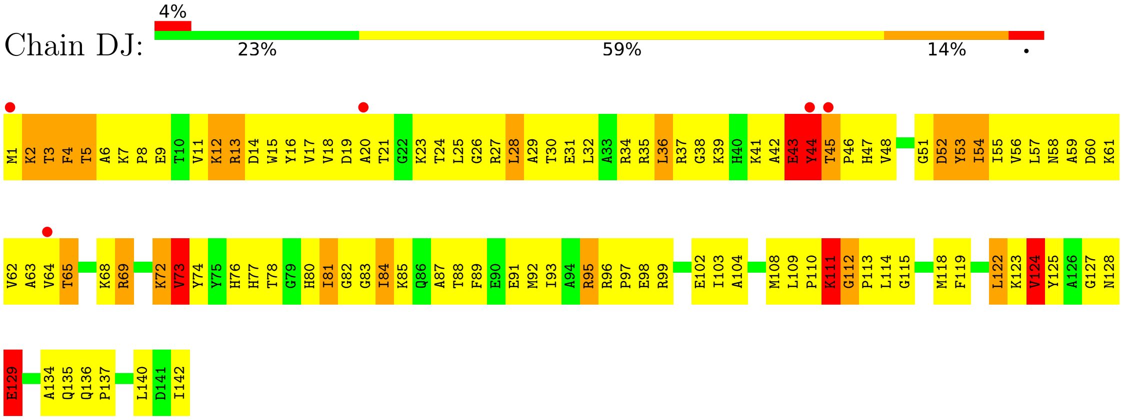
- Molecule 40: 50S ribosomal protein L9



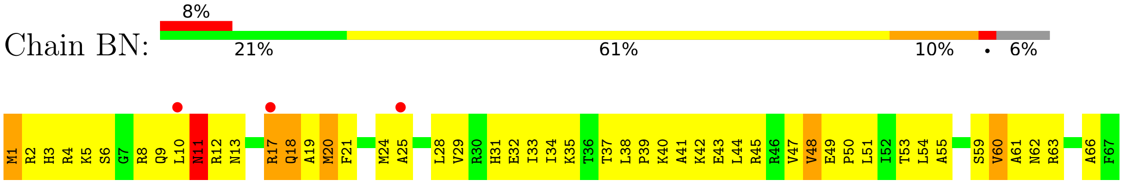
- Molecule 41: 50S ribosomal protein L13

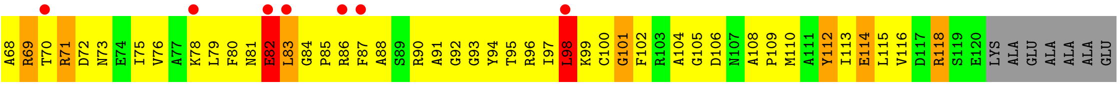


- Molecule 41: 50S ribosomal protein L13



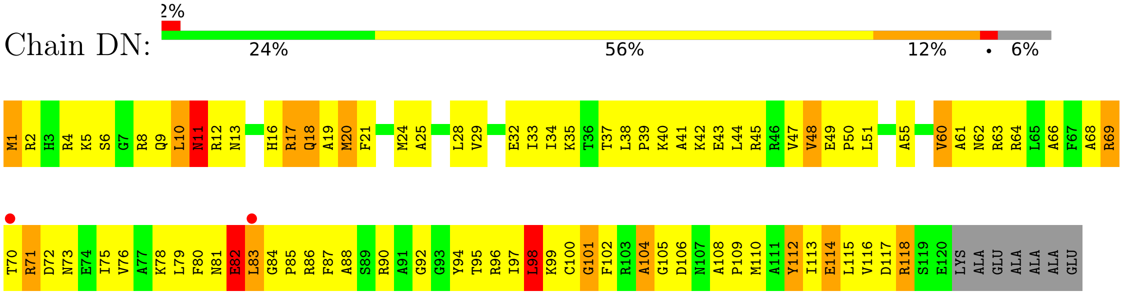
- Molecule 42: 50S ribosomal protein L17





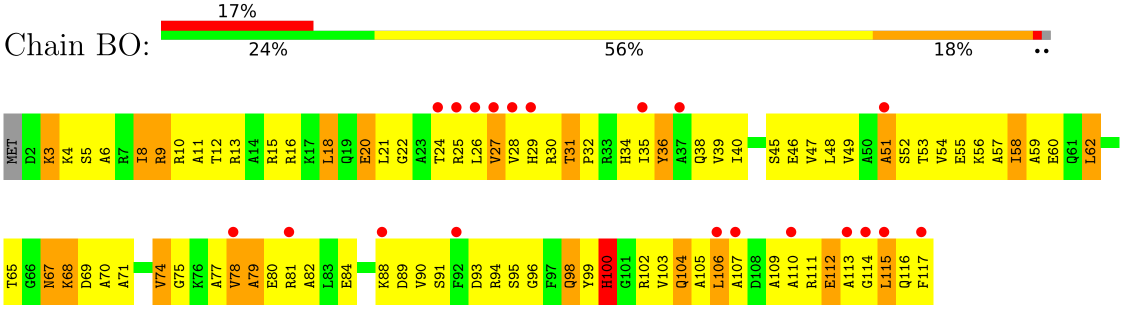
• Molecule 42: 50S ribosomal protein L17

Chain DN:



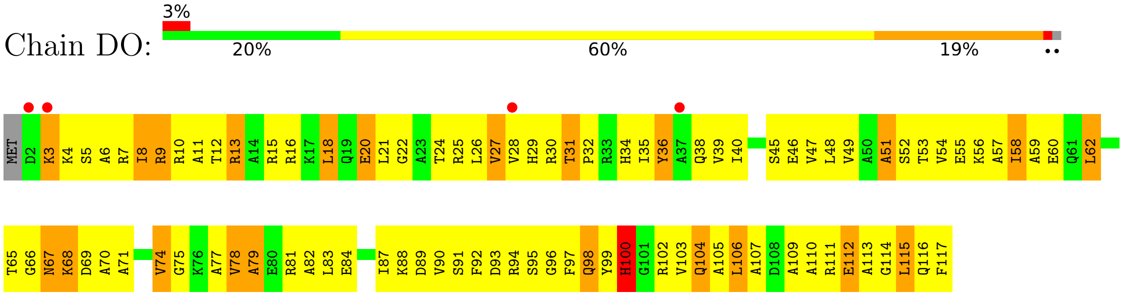
• Molecule 43: 50S ribosomal protein L18

Chain BO:



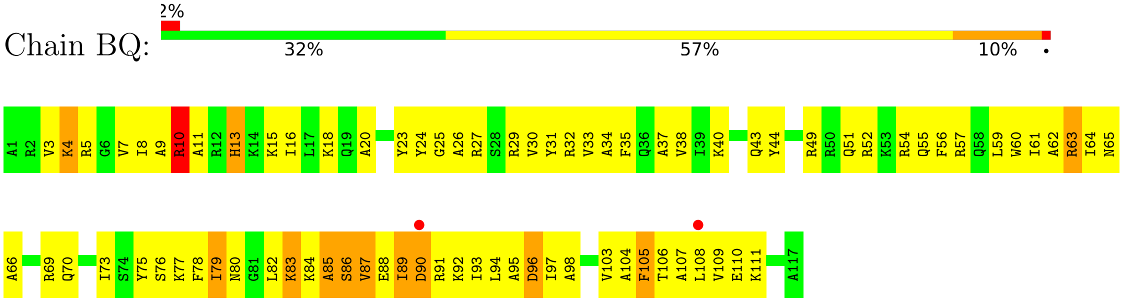
• Molecule 43: 50S ribosomal protein L18

Chain DO:



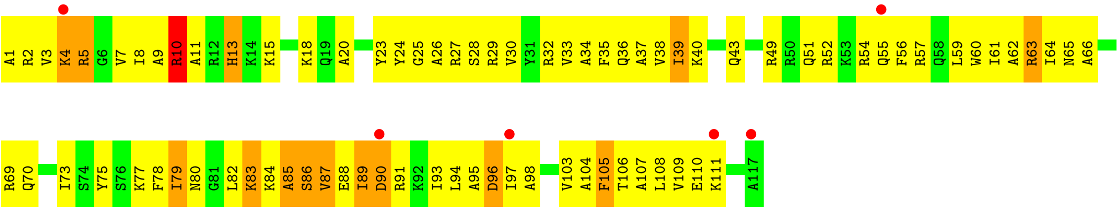
• Molecule 44: 50S ribosomal protein L20

Chain BQ:



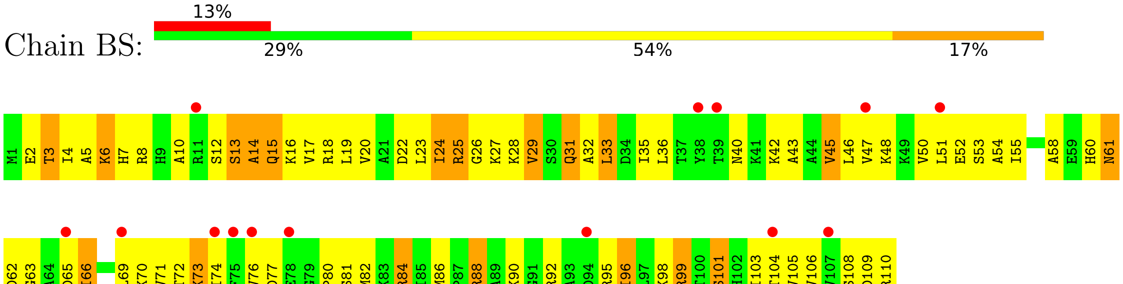
• Molecule 44: 50S ribosomal protein L20

Chain DQ:



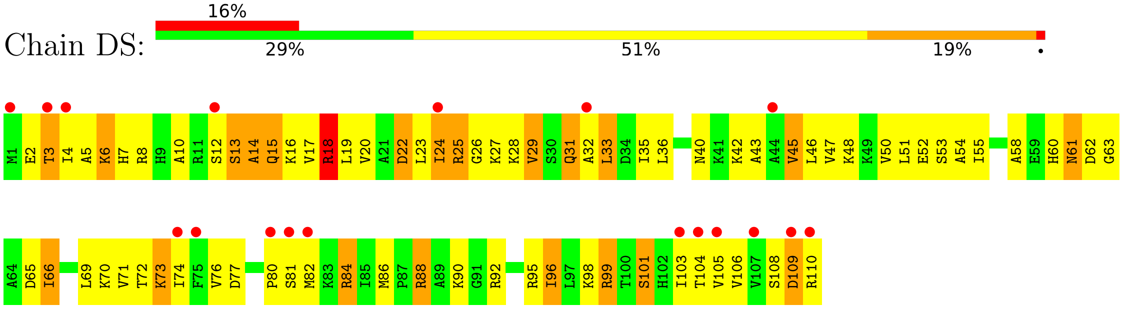
- Molecule 45: 50S ribosomal protein L22

Chain BS:



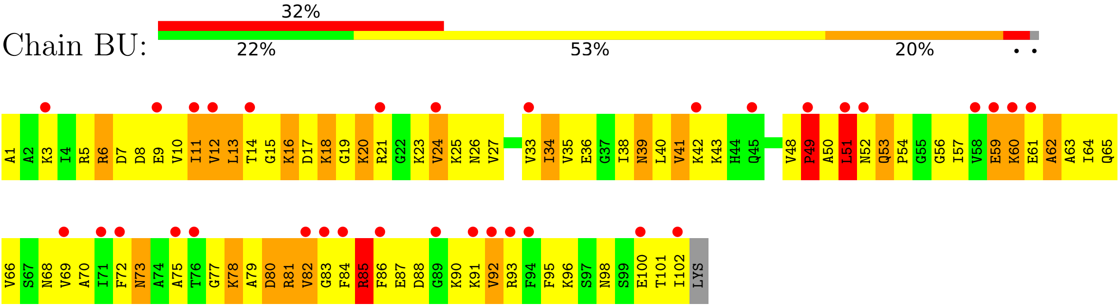
- Molecule 45: 50S ribosomal protein L22

Chain DS:



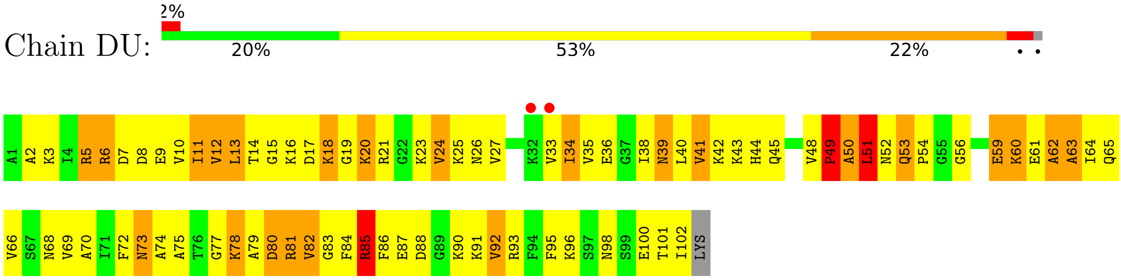
- Molecule 46: 50S ribosomal protein L24

Chain BU:



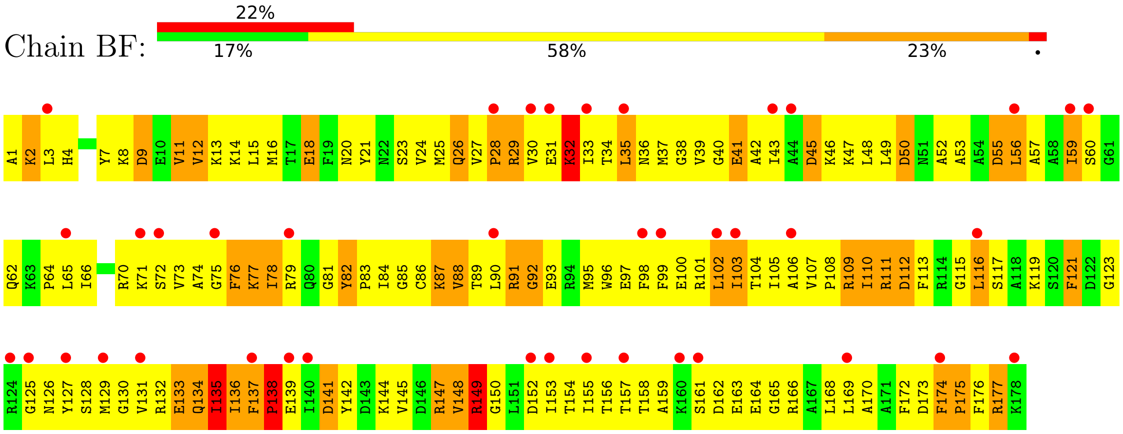
- Molecule 46: 50S ribosomal protein L24

Chain DU:



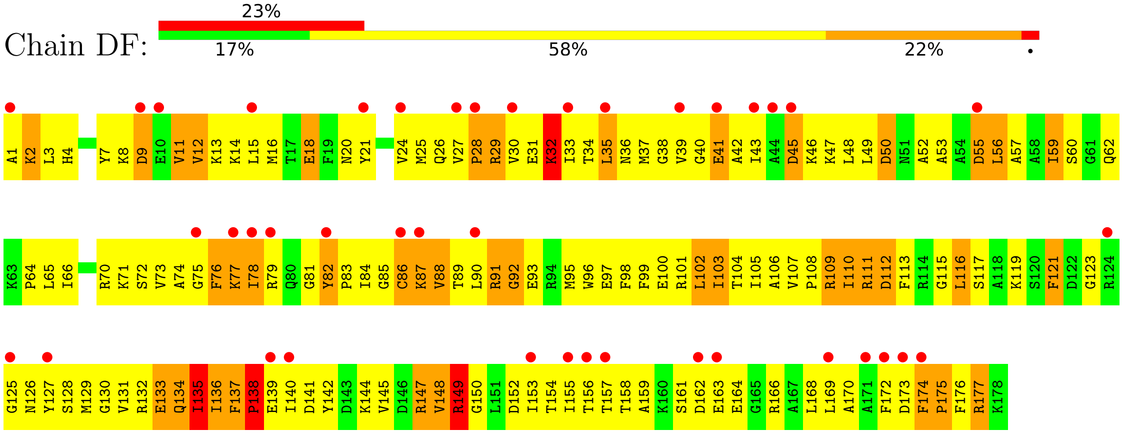
- Molecule 47: 50S ribosomal protein L5

Chain BF:



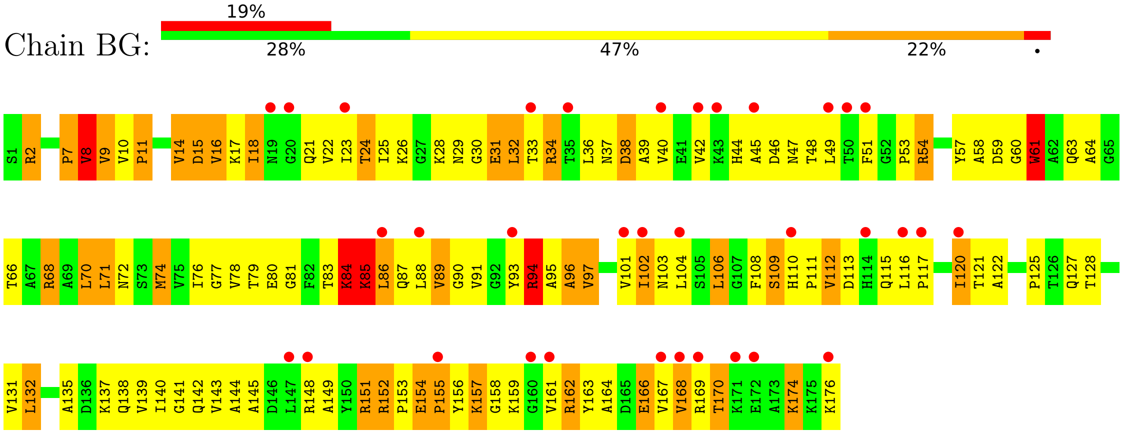
- Molecule 47: 50S ribosomal protein L5

Chain DF:



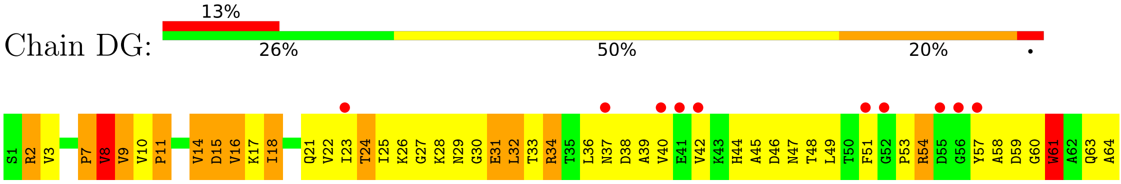
- Molecule 48: 50S ribosomal protein L6

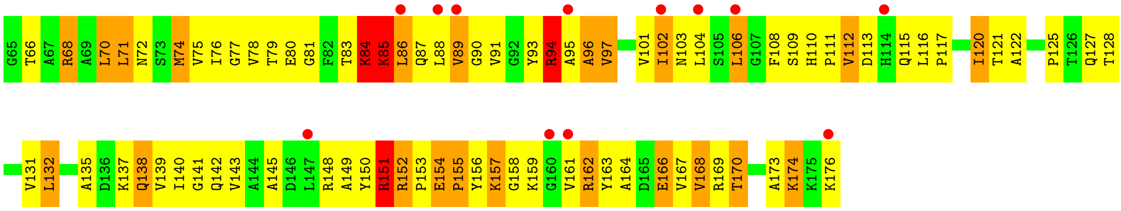
Chain BG:



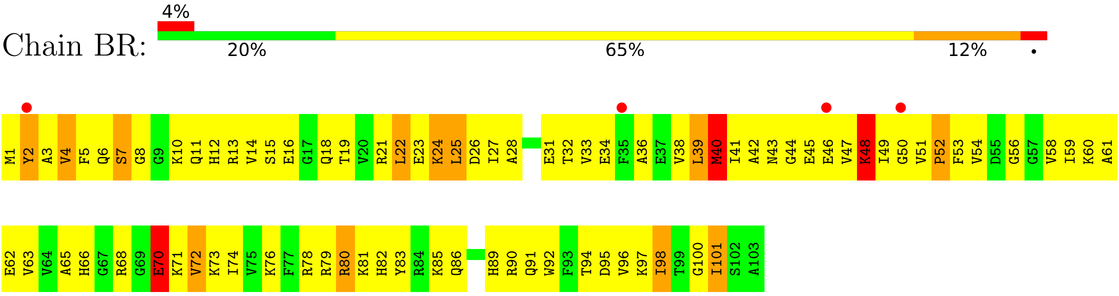
- Molecule 48: 50S ribosomal protein L6

Chain DG:

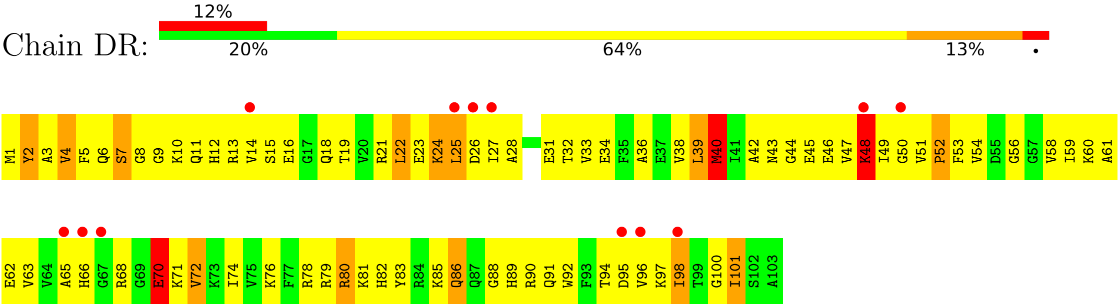




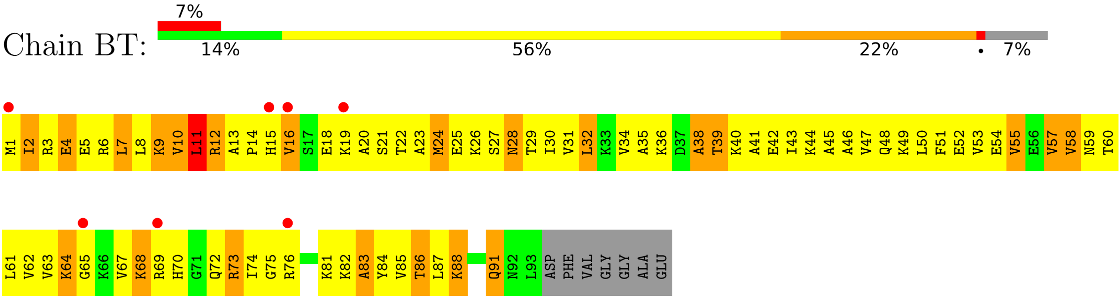
- Molecule 49: 50S ribosomal protein L21



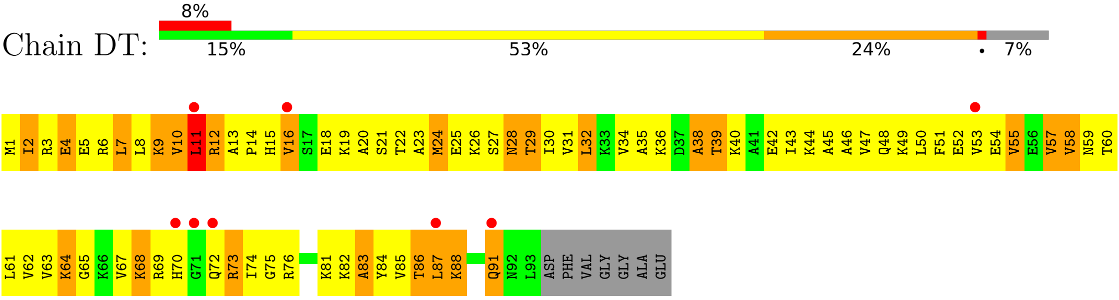
- Molecule 49: 50S ribosomal protein L21



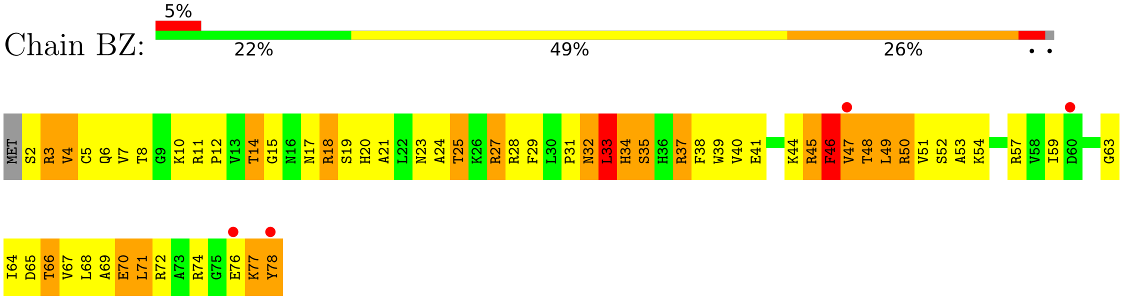
- Molecule 50: 50S ribosomal protein L23



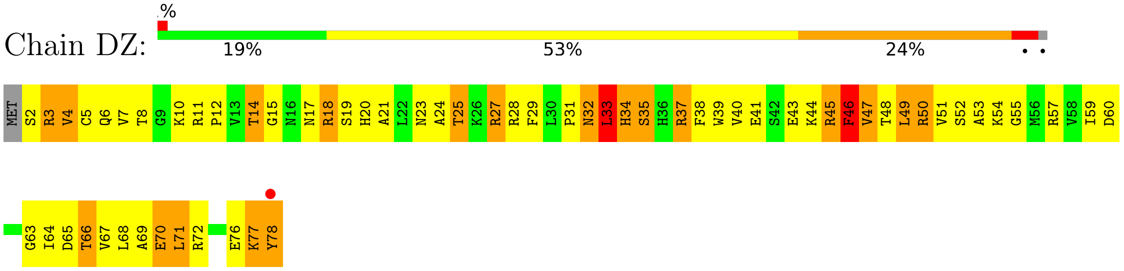
- Molecule 50: 50S ribosomal protein L23



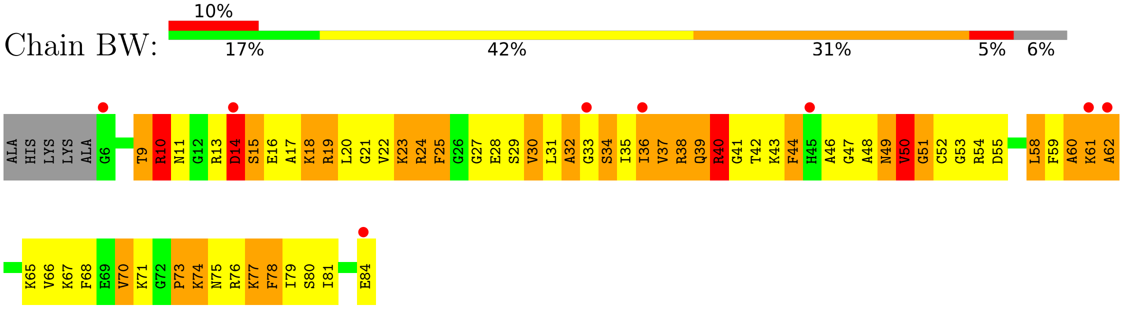
- Molecule 51: 50S ribosomal protein L28



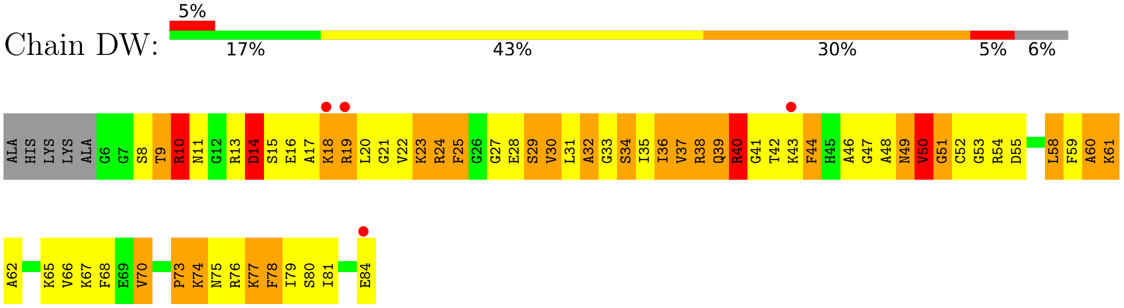
- Molecule 51: 50S ribosomal protein L28



- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.54 138.41 – 3.55	Depositor EDS
% Data completeness (in resolution range)	88.8 (70.00-3.54) 89.9 (138.41-3.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.281 , 0.320 0.246 , 0.278	Depositor DCC
R_{free} test set	30217 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	125.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	284252	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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: LLL, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AA	0.26	2/36762 (0.0%)	0.76	22/57350 (0.0%)
1	CA	0.26	3/36762 (0.0%)	0.76	23/57350 (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	0.23	0/1118	0.45	0/1504
4	CE	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.44	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	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.46	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.47	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	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	0.45	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.22	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	0.24	0/657	0.46	0/881
16	CQ	0.24	0/666	0.46	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.46	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	0.39	0/888
19	CT	0.24	0/671	0.39	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	0.47	0/570
21	CU	0.26	0/430	0.47	0/570
22	BA	0.23	0/2803	0.74	0/4371
22	DA	0.23	0/2803	0.74	0/4371
23	BB	0.29	10/68314 (0.0%)	0.77	47/106569 (0.0%)
23	DB	0.28	9/68314 (0.0%)	0.78	58/106569 (0.1%)
24	BI	0.24	0/1046	0.46	0/1410
24	DI	0.25	0/1046	0.48	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	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.53	0/1258
27	DK	0.24	0/939	0.53	0/1258
28	BP	0.24	0/929	0.50	0/1242
28	DP	0.24	0/929	0.50	0/1242
29	BE	0.24	0/1571	0.50	0/2113
29	DE	0.24	0/1571	0.50	0/2113
30	BY	0.23	0/453	0.48	0/605
30	DY	0.23	0/453	0.48	0/605
31	B0	0.22	0/450	0.53	0/599
31	D0	0.22	0/450	0.53	0/599
32	B4	0.23	0/303	0.46	0/397
32	D4	0.23	0/303	0.46	0/397
33	B1	0.27	0/416	0.48	0/554
33	D1	0.27	0/416	0.48	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.42	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.25	0/380	0.45	0/498
36	D2	0.25	0/380	0.45	0/498
37	BL	0.23	0/1054	0.47	0/1403
37	DL	0.24	0/1054	0.47	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.47	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	0.51	0/1301
42	DN	0.24	0/973	0.51	0/1301
43	BO	0.23	0/902	0.48	0/1209
43	DO	0.23	0/902	0.48	0/1209
44	BQ	0.25	0/960	0.47	0/1278
44	DQ	0.25	0/960	0.47	0/1278
45	BS	0.22	0/864	0.51	0/1156
45	DS	0.22	0/864	0.51	0/1156
46	BU	0.25	0/787	0.46	0/1051
46	DU	0.26	0/787	0.46	0/1051
47	BF	0.26	0/1444	0.50	0/1937
47	DF	0.26	0/1444	0.50	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	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.22	0/744	0.53	0/994
50	DT	0.22	0/744	0.54	0/994
51	BZ	0.25	0/635	0.50	0/848
51	DZ	0.25	0/635	0.50	0/848
52	BW	0.28	0/603	0.48	0/797
52	DW	0.28	0/603	0.48	0/797
All	All	0.26	24/306360 (0.0%)	0.70	150/457969 (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	15
1	CA	1	15
23	BB	0	41
23	DB	0	40
All	All	1	111

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.49	1.26	1.41
23	DB	1086	A	C5-C6	-16.38	1.26	1.41
23	BB	2322	A	O3'-P	14.51	1.78	1.61
23	BB	2318	G	O3'-P	-12.62	1.46	1.61
23	DB	1088	A	C6-N1	-10.61	1.28	1.35

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CA	1213	A	O5'-P-OP1	-32.89	71.23	110.70
23	DB	2204	G	O5'-P-OP1	-29.68	75.08	110.70
1	AA	1213	A	O5'-P-OP2	-28.32	76.72	110.70
23	BB	2204	G	O5'-P-OP2	-28.25	76.80	110.70
23	BB	2791	G	O5'-P-OP1	-28.20	76.86	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	CA	366	A	C3'

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	86	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1241	0
1	CA	32831	0	16521	1247	0
2	AC	1624	0	1699	150	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CC	1624	0	1699	150	0
3	AD	1643	0	1710	174	0
3	CD	1643	0	1710	174	0
4	AE	1105	0	1148	94	0
4	CE	1105	0	1148	93	0
5	AF	817	0	808	99	0
5	CF	817	0	808	93	0
6	AG	1174	0	1230	105	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	82	0
7	CH	979	0	1034	79	0
8	AI	1022	0	1070	133	0
8	CI	1022	0	1070	132	0
9	AJ	786	0	828	81	0
9	CJ	786	0	828	87	0
10	AK	877	0	887	106	0
10	CK	877	0	887	104	0
11	AL	955	0	1019	95	0
11	CL	955	0	1019	95	0
12	AM	883	0	944	107	0
12	CM	876	0	937	111	0
13	AN	774	0	827	108	0
13	CN	774	0	827	110	0
14	AO	714	0	734	47	0
14	CO	714	0	734	41	0
15	AP	649	0	666	65	0
15	CP	638	0	656	66	0
16	AQ	648	0	691	76	0
16	CQ	657	0	702	67	0
17	AR	455	0	478	48	0
17	CR	455	0	478	44	0
18	AS	637	0	665	87	0
18	CS	644	0	675	93	0
19	AT	665	0	714	56	0
19	CT	665	0	714	55	0
20	AB	1704	0	1732	218	0
20	CB	1704	0	1732	205	0
21	AU	425	0	449	75	0
21	CU	425	0	449	69	0
22	BA	2507	0	1270	101	0
22	DA	2507	0	1270	96	0
23	BB	60995	0	30678	2199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	DB	60995	0	30677	2300	0
24	BI	1032	0	1088	106	0
24	DI	1032	0	1088	176	0
25	BC	2082	0	2157	243	0
25	DC	2082	0	2157	245	0
26	BD	1565	0	1616	196	0
26	DD	1565	0	1616	186	0
27	BK	930	0	1000	110	0
27	DK	930	0	1000	108	0
28	BP	917	0	965	111	0
28	DP	917	0	965	109	0
29	BE	1552	0	1619	165	0
29	DE	1552	0	1619	153	0
30	BY	449	0	491	54	0
30	DY	449	0	491	59	0
31	B0	444	0	461	41	0
31	D0	444	0	461	45	0
32	B4	302	0	340	40	0
32	D4	302	0	340	42	0
33	B1	409	0	440	52	0
33	D1	409	0	440	47	0
34	B3	504	0	574	53	0
34	D3	504	0	574	45	0
35	BV	753	0	780	89	0
35	DV	753	0	780	97	0
36	B2	377	0	418	31	0
36	D2	377	0	418	34	0
37	BL	1045	0	1117	132	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	117	0
38	DM	1074	0	1157	119	0
39	BX	509	0	543	71	0
39	DX	509	0	543	72	0
40	BH	1111	0	1148	197	0
40	DH	1111	0	1148	150	0
41	BJ	1129	0	1162	143	0
41	DJ	1129	0	1162	144	0
42	BN	960	0	1000	118	0
42	DN	960	0	1000	118	0
43	BO	892	0	923	88	0
43	DO	892	0	923	103	0
44	BQ	947	0	1022	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DQ	947	0	1022	141	0
45	BS	857	0	922	83	0
45	DS	857	0	922	87	0
46	BU	779	0	834	113	0
46	DU	779	0	834	114	0
47	BF	1420	0	1460	225	0
47	DF	1420	0	1460	228	0
48	BG	1323	0	1374	189	0
48	DG	1323	0	1374	191	0
49	BR	816	0	839	109	0
49	DR	816	0	839	112	0
50	BT	738	0	807	124	0
50	DT	738	0	807	128	0
51	BZ	625	0	652	80	0
51	DZ	625	0	652	77	0
52	BW	596	0	610	128	0
52	DW	596	0	610	131	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CN	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	93	0	117	6	0
54	BB	31	0	39	1	0
54	CA	93	0	117	5	0
54	DB	31	0	39	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	292	0	0	1	0
56	AE	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	2	0	0	0	0
56	AN	2	0	0	0	0
56	AT	2	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	7	0
56	BC	7	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	3	0	0	0	0
56	CA	297	0	0	2	0
56	CE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CT	2	0	0	0	0
56	DB	502	0	0	8	0
56	DC	4	0	0	0	0
56	DE	2	0	0	0	0
56	DL	4	0	0	0	0
All	All	284252	0	190973	16353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

The worst 5 of 16353 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	1.42	1.17
23:DB:855:G:H21	52:DW:23:LYS:HG2	1.12	1.14
26:BD:106:LYS:HB3	26:BD:206:ALA:H	1.13	1.11
26:DD:106:LYS:HB3	26:DD:206:ALA:H	1.13	1.09
37:BL:143:GLU:HG2	37:BL:144:GLU:H	1.18	1.08

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%)	157 (77%)	34 (17%)	13 (6%)	1	16
2	CC	204/232 (88%)	156 (76%)	35 (17%)	13 (6%)	1	16
3	AD	203/205 (99%)	144 (71%)	45 (22%)	14 (7%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CD	203/205 (99%)	143 (70%)	45 (22%)	15 (7%)	1	13
4	AE	148/166 (89%)	114 (77%)	30 (20%)	4 (3%)	5	35
4	CE	148/166 (89%)	115 (78%)	29 (20%)	4 (3%)	5	35
5	AF	98/135 (73%)	71 (72%)	17 (17%)	10 (10%)	0	7
5	CF	98/135 (73%)	70 (71%)	19 (19%)	9 (9%)	1	8
6	AG	148/178 (83%)	117 (79%)	22 (15%)	9 (6%)	1	17
6	CG	150/178 (84%)	121 (81%)	18 (12%)	11 (7%)	1	13
7	AH	127/129 (98%)	99 (78%)	24 (19%)	4 (3%)	4	32
7	CH	127/129 (98%)	99 (78%)	23 (18%)	5 (4%)	3	26
8	AI	125/129 (97%)	88 (70%)	28 (22%)	9 (7%)	1	14
8	CI	125/129 (97%)	86 (69%)	29 (23%)	10 (8%)	1	11
9	AJ	96/103 (93%)	71 (74%)	15 (16%)	10 (10%)	0	7
9	CJ	96/103 (93%)	70 (73%)	15 (16%)	11 (12%)	0	6
10	AK	115/128 (90%)	83 (72%)	26 (23%)	6 (5%)	2	20
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	2	20
11	AL	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	1	16
11	CL	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	1	16
12	AM	112/117 (96%)	76 (68%)	28 (25%)	8 (7%)	1	14
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	1	14
13	AN	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	0	6
13	CN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	0	6
14	AO	86/89 (97%)	63 (73%)	19 (22%)	4 (5%)	2	22
14	CO	86/89 (97%)	64 (74%)	19 (22%)	3 (4%)	3	30
15	AP	80/82 (98%)	57 (71%)	19 (24%)	4 (5%)	2	21
15	CP	78/82 (95%)	55 (70%)	18 (23%)	5 (6%)	1	16
16	AQ	78/83 (94%)	56 (72%)	16 (20%)	6 (8%)	1	11
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	1	12
17	AR	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	1	18
17	CR	53/74 (72%)	40 (76%)	10 (19%)	3 (6%)	1	18
18	AS	77/91 (85%)	60 (78%)	11 (14%)	6 (8%)	1	11
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	1	17
19	CT	83/86 (96%)	64 (77%)	14 (17%)	5 (6%)	1	17
20	AB	216/240 (90%)	149 (69%)	52 (24%)	15 (7%)	1	14
20	CB	216/240 (90%)	149 (69%)	51 (24%)	16 (7%)	1	13
21	AU	49/70 (70%)	28 (57%)	14 (29%)	7 (14%)	0	3
21	CU	49/70 (70%)	27 (55%)	15 (31%)	7 (14%)	0	3
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	3	29
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	3	29
25	BC	269/272 (99%)	168 (62%)	58 (22%)	43 (16%)	0	3
25	DC	269/272 (99%)	167 (62%)	59 (22%)	43 (16%)	0	3
26	BD	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	4
26	DD	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	4
27	BK	119/123 (97%)	79 (66%)	22 (18%)	18 (15%)	0	3
27	DK	119/123 (97%)	78 (66%)	23 (19%)	18 (15%)	0	3
28	BP	112/114 (98%)	61 (54%)	36 (32%)	15 (13%)	0	4
28	DP	112/114 (98%)	60 (54%)	37 (33%)	15 (13%)	0	4
29	BE	199/201 (99%)	126 (63%)	48 (24%)	25 (13%)	0	5
29	DE	199/201 (99%)	127 (64%)	46 (23%)	26 (13%)	0	4
30	BY	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	2	19
30	DY	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	2	19
31	B0	54/56 (96%)	43 (80%)	6 (11%)	5 (9%)	0	8
31	D0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	0	8
32	B4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
32	D4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
33	B1	48/54 (89%)	31 (65%)	12 (25%)	5 (10%)	0	7
33	D1	48/54 (89%)	33 (69%)	10 (21%)	5 (10%)	0	7
34	B3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	10
34	D3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	10
35	BV	92/94 (98%)	67 (73%)	20 (22%)	5 (5%)	2	19
35	DV	92/94 (98%)	67 (73%)	21 (23%)	4 (4%)	2	24
36	B2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	1	15
37	BL	141/144 (98%)	90 (64%)	29 (21%)	22 (16%)	0	3
37	DL	141/144 (98%)	90 (64%)	27 (19%)	24 (17%)	0	2
38	BM	134/136 (98%)	80 (60%)	40 (30%)	14 (10%)	0	7
38	DM	134/136 (98%)	81 (60%)	39 (29%)	14 (10%)	0	7
39	BX	61/63 (97%)	38 (62%)	16 (26%)	7 (12%)	0	6
39	DX	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	0	6
40	BH	147/149 (99%)	83 (56%)	27 (18%)	37 (25%)	0	0
40	DH	147/149 (99%)	89 (60%)	30 (20%)	28 (19%)	0	2
41	BJ	140/142 (99%)	86 (61%)	36 (26%)	18 (13%)	0	4
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	4
42	BN	118/127 (93%)	77 (65%)	30 (25%)	11 (9%)	0	8
42	DN	118/127 (93%)	76 (64%)	30 (25%)	12 (10%)	0	7
43	BO	114/117 (97%)	79 (69%)	24 (21%)	11 (10%)	0	8
43	DO	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	0	8
44	BQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	1	17
44	DQ	115/117 (98%)	77 (67%)	30 (26%)	8 (7%)	1	14
45	BS	108/110 (98%)	67 (62%)	29 (27%)	12 (11%)	0	6
45	DS	108/110 (98%)	66 (61%)	29 (27%)	13 (12%)	0	5
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	2
46	DU	100/103 (97%)	59 (59%)	23 (23%)	18 (18%)	0	2
47	BF	176/178 (99%)	101 (57%)	49 (28%)	26 (15%)	0	3
47	DF	176/178 (99%)	102 (58%)	49 (28%)	25 (14%)	0	3
48	BG	174/176 (99%)	95 (55%)	48 (28%)	31 (18%)	0	2
48	DG	174/176 (99%)	94 (54%)	50 (29%)	30 (17%)	0	2
49	BR	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	4
49	DR	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	4
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	2
50	DT	91/100 (91%)	51 (56%)	23 (25%)	17 (19%)	0	2
51	BZ	75/78 (96%)	51 (68%)	14 (19%)	10 (13%)	0	4
51	DZ	75/78 (96%)	50 (67%)	15 (20%)	10 (13%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BW	77/84 (92%)	32 (42%)	22 (29%)	23 (30%)	0	0
52	DW	77/84 (92%)	30 (39%)	24 (31%)	23 (30%)	0	0
All	All	11241/11914 (94%)	7497 (67%)	2537 (23%)	1207 (11%)	0	7

5 of 1207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	205	GLU
3	AD	24	VAL
3	AD	192	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	145 (85%)	25 (15%)	3	19
2	CC	170/189 (90%)	145 (85%)	25 (15%)	3	19
3	AD	172/172 (100%)	148 (86%)	24 (14%)	3	21
3	CD	172/172 (100%)	148 (86%)	24 (14%)	3	21
4	AE	113/125 (90%)	102 (90%)	11 (10%)	8	35
4	CE	113/125 (90%)	102 (90%)	11 (10%)	8	35
5	AF	87/116 (75%)	70 (80%)	17 (20%)	1	8
5	CF	87/116 (75%)	70 (80%)	17 (20%)	1	8
6	AG	123/146 (84%)	109 (89%)	14 (11%)	5	29
6	CG	125/146 (86%)	114 (91%)	11 (9%)	10	39
7	AH	104/104 (100%)	97 (93%)	7 (7%)	16	49
7	CH	104/104 (100%)	97 (93%)	7 (7%)	16	49
8	AI	105/106 (99%)	89 (85%)	16 (15%)	3	18
8	CI	105/106 (99%)	89 (85%)	16 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	3	21
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	4	24
10	AK	90/98 (92%)	76 (84%)	14 (16%)	2	17
10	CK	90/98 (92%)	77 (86%)	13 (14%)	3	20
11	AL	103/103 (100%)	92 (89%)	11 (11%)	6	32
11	CL	103/103 (100%)	92 (89%)	11 (11%)	6	32
12	AM	92/95 (97%)	79 (86%)	13 (14%)	3	21
12	CM	91/95 (96%)	79 (87%)	12 (13%)	4	23
13	AN	79/83 (95%)	64 (81%)	15 (19%)	1	9
13	CN	79/83 (95%)	64 (81%)	15 (19%)	1	9
14	AO	76/77 (99%)	69 (91%)	7 (9%)	9	38
14	CO	76/77 (99%)	69 (91%)	7 (9%)	9	38
15	AP	65/65 (100%)	59 (91%)	6 (9%)	9	38
15	CP	65/65 (100%)	58 (89%)	7 (11%)	6	31
16	AQ	74/77 (96%)	59 (80%)	15 (20%)	1	7
16	CQ	75/77 (97%)	62 (83%)	13 (17%)	2	12
17	AR	48/64 (75%)	41 (85%)	7 (15%)	3	19
17	CR	48/64 (75%)	41 (85%)	7 (15%)	3	19
18	AS	70/78 (90%)	56 (80%)	14 (20%)	1	8
18	CS	71/78 (91%)	56 (79%)	15 (21%)	1	7
19	AT	65/65 (100%)	58 (89%)	7 (11%)	6	31
19	CT	65/65 (100%)	58 (89%)	7 (11%)	6	31
20	AB	180/198 (91%)	149 (83%)	31 (17%)	2	12
20	CB	180/198 (91%)	147 (82%)	33 (18%)	1	9
21	AU	44/60 (73%)	33 (75%)	11 (25%)	0	4
21	CU	44/60 (73%)	33 (75%)	11 (25%)	0	4
24	BI	109/109 (100%)	107 (98%)	2 (2%)	59	81
24	DI	109/109 (100%)	103 (94%)	6 (6%)	21	56
25	BC	216/217 (100%)	182 (84%)	34 (16%)	2	17
25	DC	216/217 (100%)	183 (85%)	33 (15%)	2	18
26	BD	164/164 (100%)	139 (85%)	25 (15%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	DD	164/164 (100%)	138 (84%)	26 (16%)	2	15
27	BK	102/104 (98%)	77 (76%)	25 (24%)	0	4
27	DK	102/104 (98%)	77 (76%)	25 (24%)	0	4
28	BP	99/99 (100%)	81 (82%)	18 (18%)	1	10
28	DP	99/99 (100%)	81 (82%)	18 (18%)	1	10
29	BE	165/165 (100%)	144 (87%)	21 (13%)	4	24
29	DE	165/165 (100%)	144 (87%)	21 (13%)	4	24
30	BY	48/48 (100%)	37 (77%)	11 (23%)	1	5
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	5
31	B0	47/47 (100%)	38 (81%)	9 (19%)	1	8
31	D0	47/47 (100%)	38 (81%)	9 (19%)	1	8
32	B4	34/34 (100%)	28 (82%)	6 (18%)	2	11
32	D4	34/34 (100%)	28 (82%)	6 (18%)	2	11
33	B1	45/48 (94%)	36 (80%)	9 (20%)	1	8
33	D1	45/48 (94%)	37 (82%)	8 (18%)	2	10
34	B3	51/51 (100%)	46 (90%)	5 (10%)	8	35
34	D3	51/51 (100%)	46 (90%)	5 (10%)	8	35
35	BV	78/78 (100%)	63 (81%)	15 (19%)	1	8
35	DV	78/78 (100%)	63 (81%)	15 (19%)	1	8
36	B2	38/38 (100%)	31 (82%)	7 (18%)	1	9
36	D2	38/38 (100%)	31 (82%)	7 (18%)	1	9
37	BL	102/103 (99%)	91 (89%)	11 (11%)	6	31
37	DL	102/103 (99%)	91 (89%)	11 (11%)	6	31
38	BM	109/109 (100%)	92 (84%)	17 (16%)	2	17
38	DM	109/109 (100%)	93 (85%)	16 (15%)	3	19
39	BX	55/55 (100%)	49 (89%)	6 (11%)	6	31
39	DX	55/55 (100%)	49 (89%)	6 (11%)	6	31
40	BH	114/114 (100%)	86 (75%)	28 (25%)	0	4
40	DH	114/114 (100%)	91 (80%)	23 (20%)	1	7
41	BJ	116/116 (100%)	98 (84%)	18 (16%)	2	17
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BN	100/103 (97%)	85 (85%)	15 (15%)	3	19
42	DN	100/103 (97%)	86 (86%)	14 (14%)	3	21
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	7
43	DO	86/87 (99%)	68 (79%)	18 (21%)	1	7
44	BQ	89/89 (100%)	81 (91%)	8 (9%)	9	38
44	DQ	89/89 (100%)	80 (90%)	9 (10%)	7	34
45	BS	93/93 (100%)	78 (84%)	15 (16%)	2	15
45	DS	93/93 (100%)	76 (82%)	17 (18%)	1	9
46	BU	83/84 (99%)	68 (82%)	15 (18%)	1	10
46	DU	83/84 (99%)	68 (82%)	15 (18%)	1	10
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	6
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	6
48	BG	137/137 (100%)	113 (82%)	24 (18%)	2	11
48	DG	137/137 (100%)	113 (82%)	24 (18%)	2	11
49	BR	84/84 (100%)	71 (84%)	13 (16%)	2	17
49	DR	84/84 (100%)	71 (84%)	13 (16%)	2	17
50	BT	80/84 (95%)	69 (86%)	11 (14%)	3	21
50	DT	80/84 (95%)	68 (85%)	12 (15%)	3	19
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	7
51	DZ	67/68 (98%)	54 (81%)	13 (19%)	1	8
52	BW	59/62 (95%)	44 (75%)	15 (25%)	0	4
52	DW	59/62 (95%)	44 (75%)	15 (25%)	0	4
All	All	9333/9700 (96%)	7889 (84%)	1444 (16%)	2	17

5 of 1444 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	CR	38	ILE
32	D4	3	VAL
20	CB	8	MET
17	CR	35	SER
26	DD	36	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 326 such sidechains are listed below:

Mol	Chain	Res	Type
24	DI	93	ASN
40	DH	28	ASN
25	DC	114	GLN
29	DE	195	GLN
45	DS	15	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	246 (16%)	21 (1%)
1	CA	1529/1542 (99%)	231 (15%)	19 (1%)
22	BA	116/120 (96%)	16 (13%)	0
22	DA	116/120 (96%)	14 (12%)	0
23	BB	2837/2904 (97%)	424 (14%)	20 (0%)
23	DB	2837/2904 (97%)	424 (14%)	21 (0%)
All	All	8964/9132 (98%)	1355 (15%)	81 (0%)

5 of 1355 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 81 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1226	C
23	DB	1911	U
1	CA	1451	U
23	DB	670	A
23	DB	2425	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 353 ligands modelled in this entry, 345 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
54	LLL	AA	2061	-	29,33,33	2.32	10 (34%)	34,49,49	1.28	4 (11%)
54	LLL	DB	3112	-	29,33,33	2.37	12 (41%)	34,49,49	1.19	3 (8%)
54	LLL	AA	2062	-	29,33,33	2.41	15 (51%)	34,49,49	1.27	4 (11%)
54	LLL	CA	2063	-	29,33,33	2.42	13 (44%)	34,49,49	1.24	3 (8%)
54	LLL	BB	3111	-	29,33,33	2.37	12 (41%)	34,49,49	1.22	4 (11%)
54	LLL	CA	2062	-	29,33,33	2.34	12 (41%)	34,49,49	1.20	3 (8%)
54	LLL	AA	2063	-	29,33,33	2.37	12 (41%)	34,49,49	1.34	3 (8%)
54	LLL	CA	2064	-	29,33,33	2.28	11 (37%)	34,49,49	1.20	3 (8%)

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
54	LLL	AA	2061	-	-	1/11/65/65	0/3/3/3
54	LLL	DB	3112	-	-	1/11/65/65	0/3/3/3
54	LLL	AA	2062	-	-	2/11/65/65	0/3/3/3
54	LLL	CA	2063	-	-	4/11/65/65	0/3/3/3
54	LLL	BB	3111	-	-	2/11/65/65	0/3/3/3
54	LLL	CA	2062	-	-	1/11/65/65	0/3/3/3
54	LLL	AA	2063	-	-	2/11/65/65	0/3/3/3
54	LLL	CA	2064	-	-	1/11/65/65	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2063	LLL	O53-C53	6.49	1.52	1.43
54	AA	2062	LLL	O53-C53	6.38	1.52	1.43
54	DB	3112	LLL	O53-C53	6.35	1.52	1.43
54	BB	3111	LLL	O53-C53	6.33	1.52	1.43
54	AA	2061	LLL	O53-C53	6.28	1.52	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	AA	2063	LLL	C53-O53-C13	4.34	118.52	111.53
54	CA	2063	LLL	C53-O53-C13	4.05	118.06	111.53
54	AA	2062	LLL	C53-O53-C13	3.95	117.90	111.53
54	CA	2062	LLL	C53-O53-C13	3.92	117.85	111.53
54	BB	3111	LLL	C53-O53-C13	3.87	117.76	111.53

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	2061	LLL	C23-C33-N33-C93
54	AA	2062	LLL	C23-C33-N33-C93
54	AA	2063	LLL	C23-C33-N33-C93
54	BB	3111	LLL	C23-C33-N33-C93
54	CA	2062	LLL	C23-C33-N33-C93

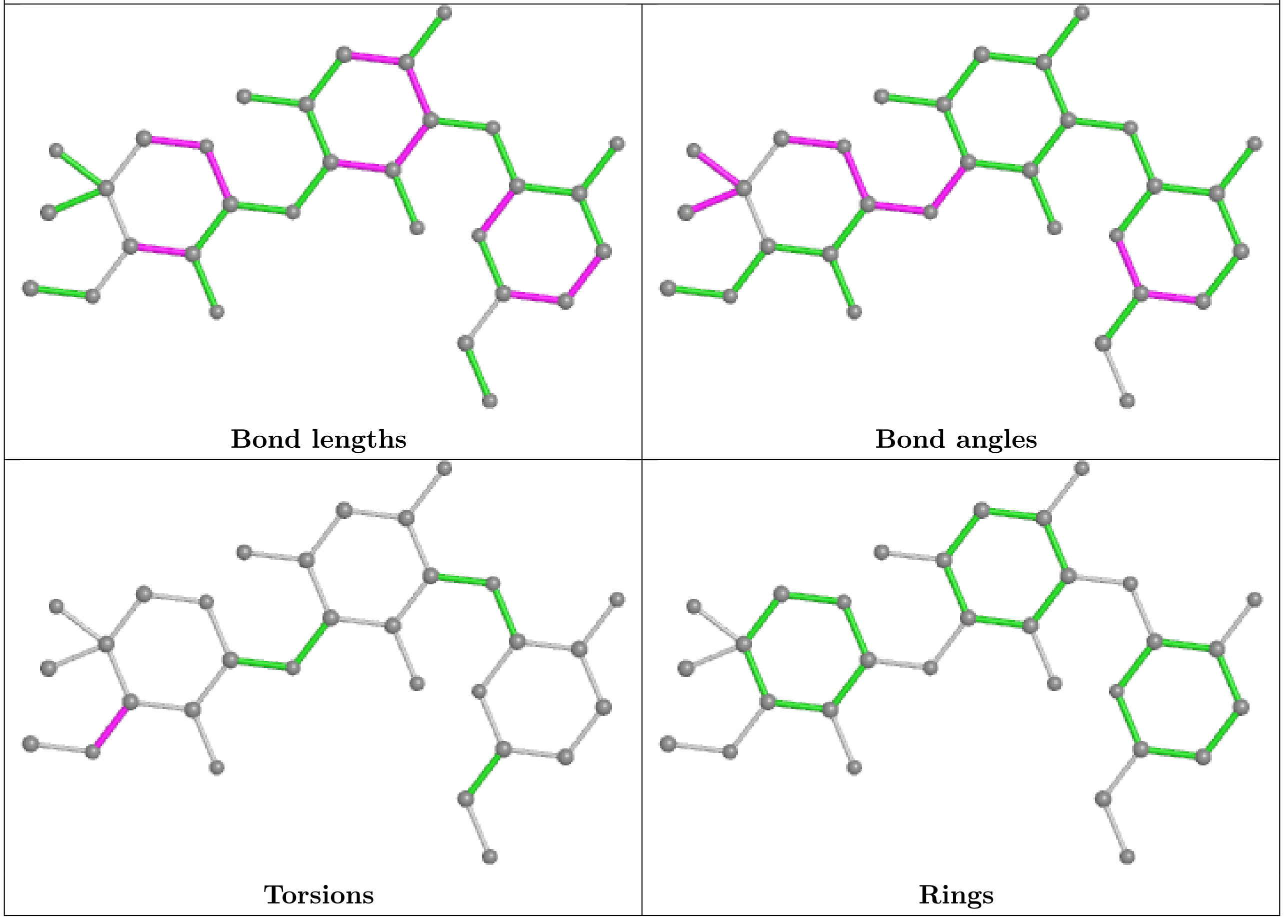
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	AA	2061	LLL	1	0
54	AA	2062	LLL	2	0
54	BB	3111	LLL	1	0
54	CA	2062	LLL	5	0
54	AA	2063	LLL	3	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 LLL AA 2061



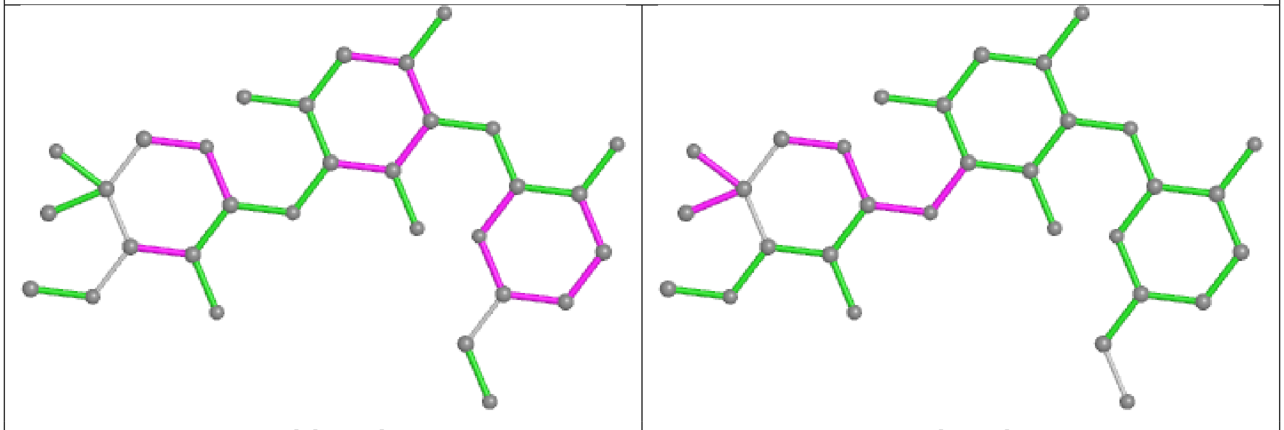
Bond lengths

Bond angles

Torsions

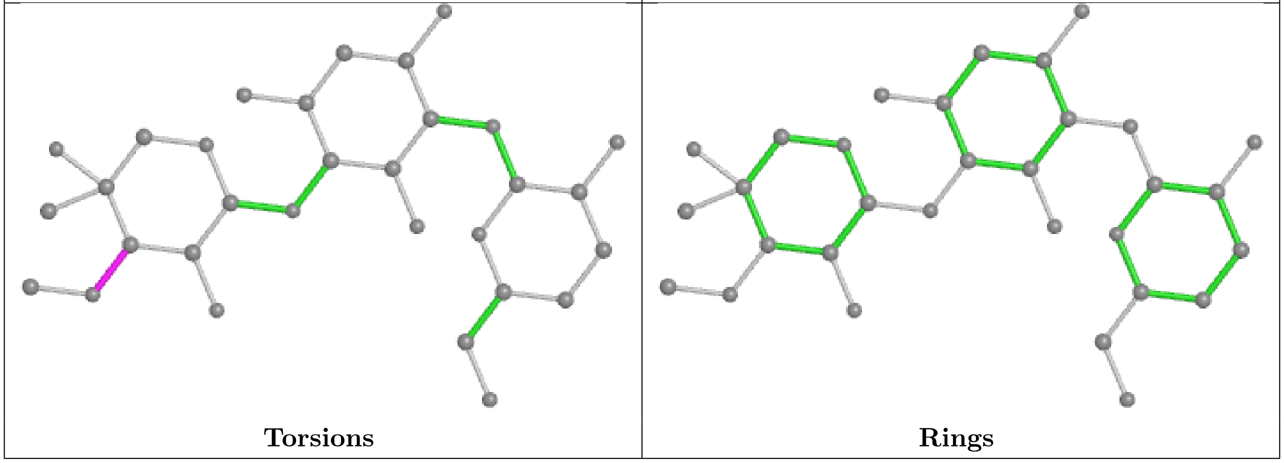
Rings

Ligand LLL DB 3112



Bond lengths

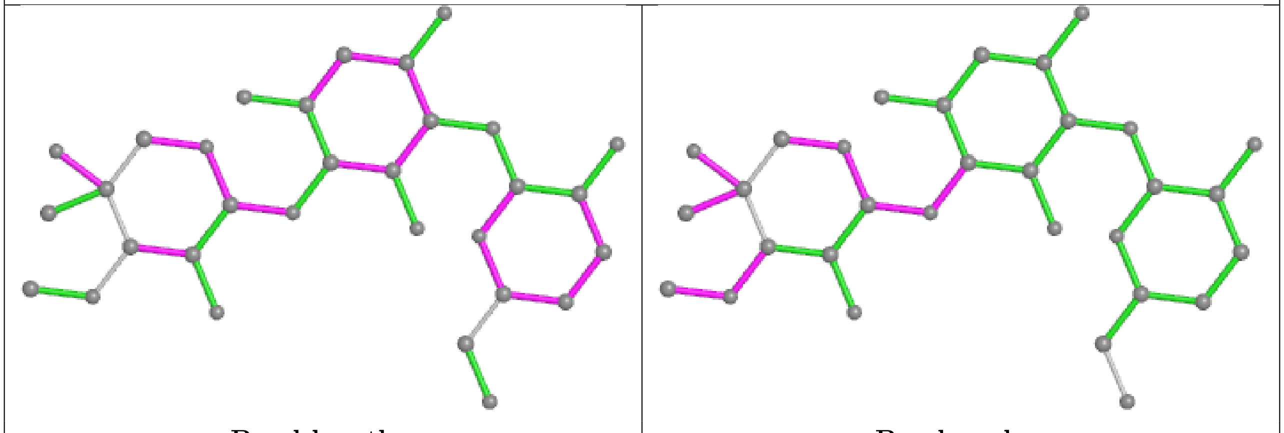
Bond angles



Torsions

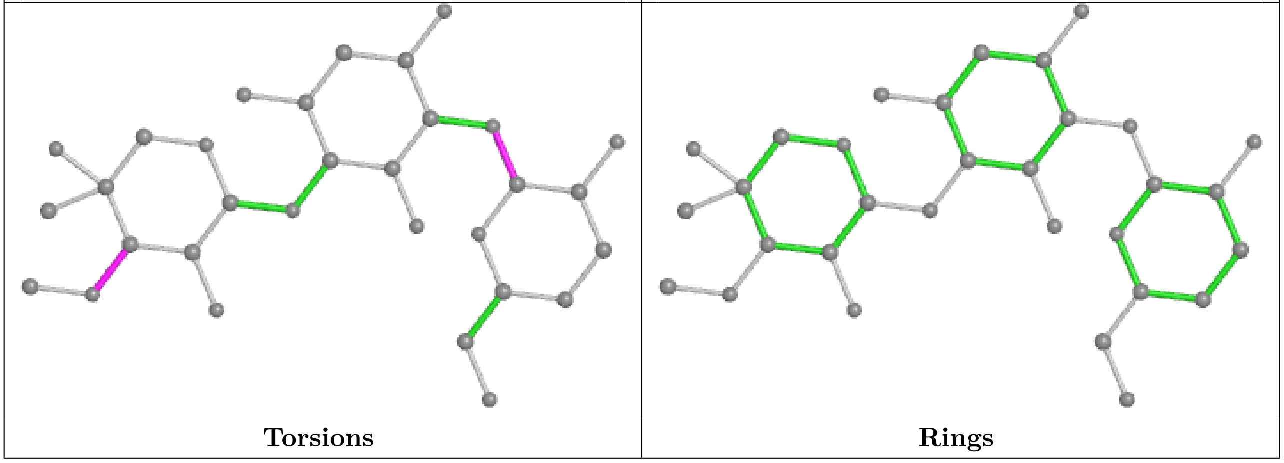
Rings

Ligand LLL AA 2062



Bond lengths

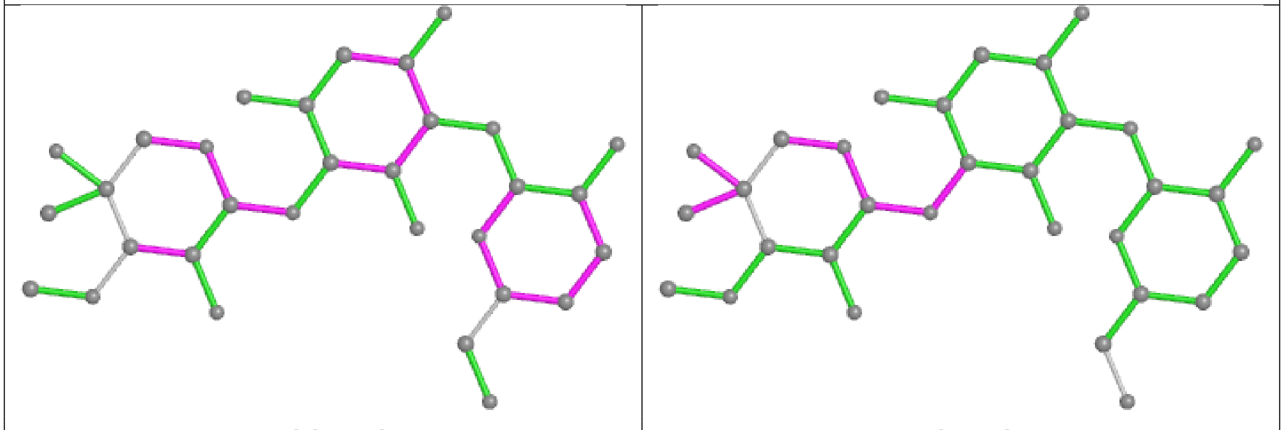
Bond angles



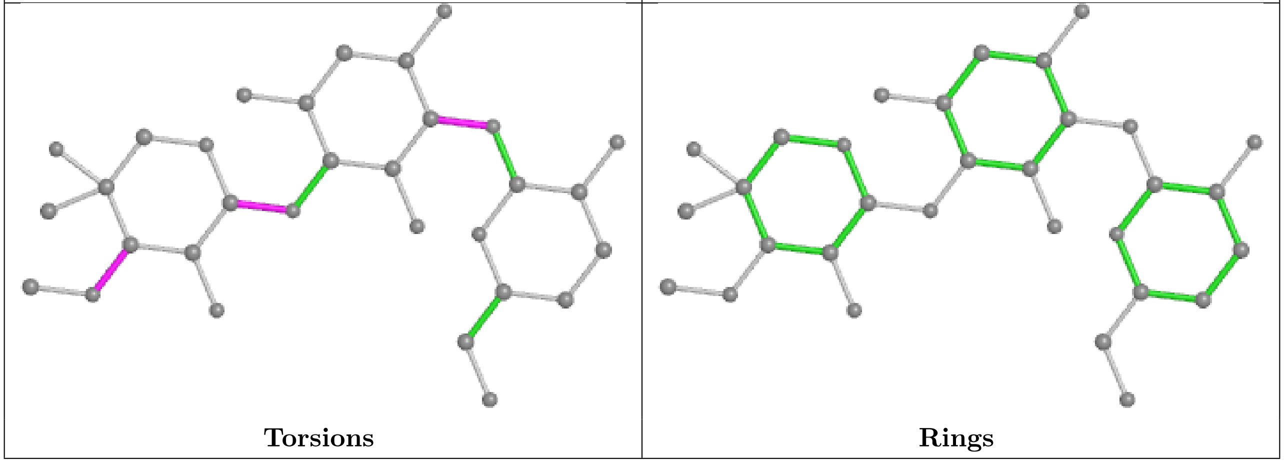
Torsions

Rings

Ligand LLL CA 2063

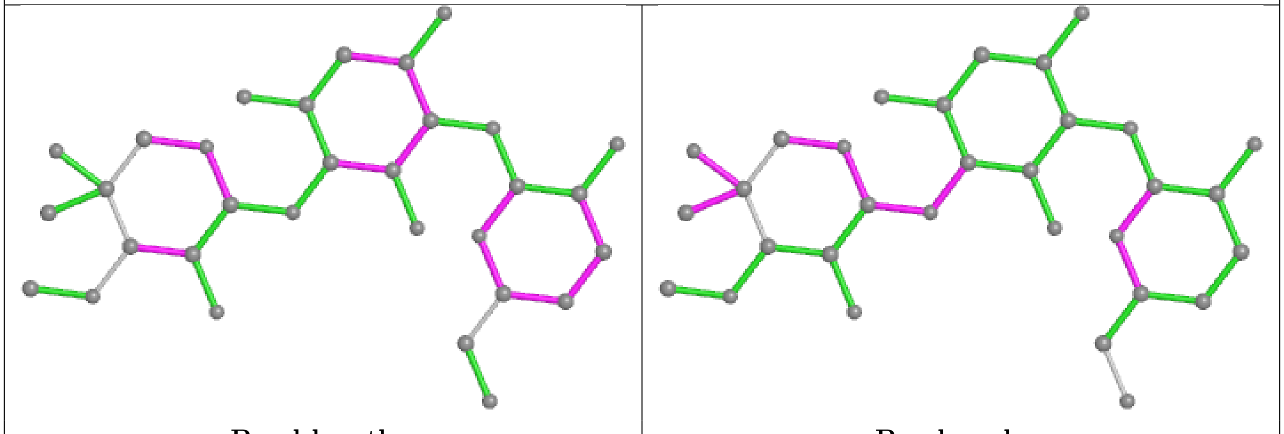


Bond lengths **Bond angles**

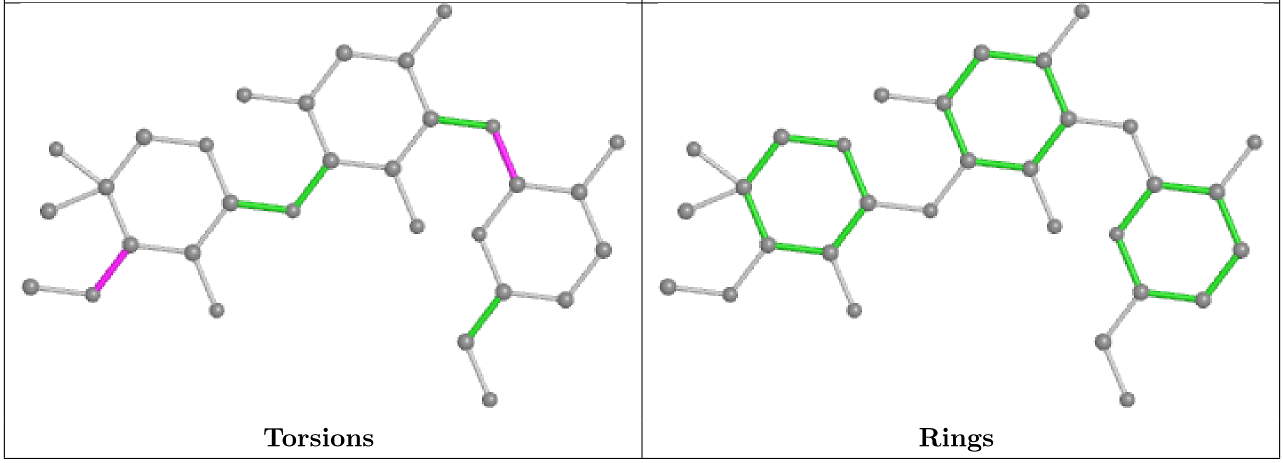


Torsions **Rings**

Ligand LLL BB 3111

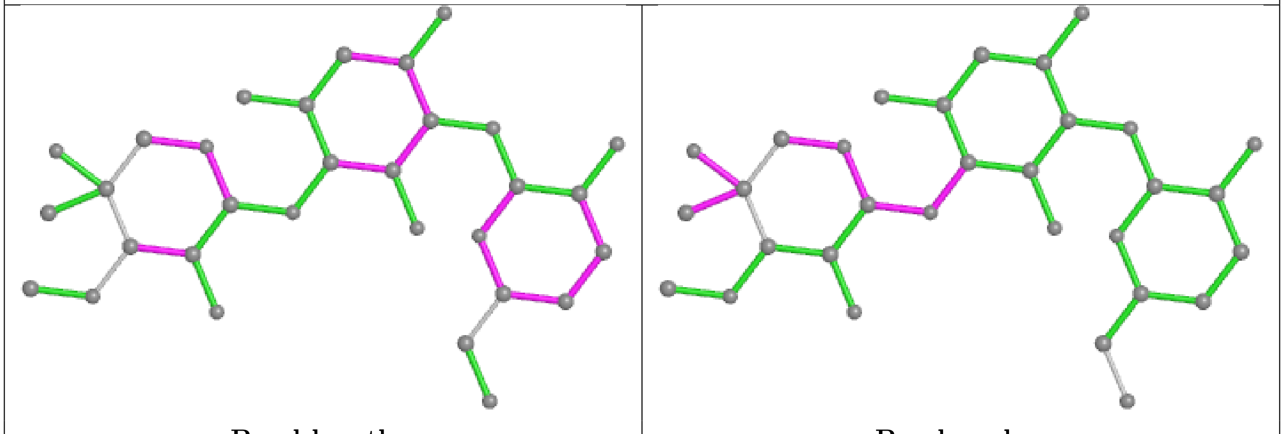


Bond lengths **Bond angles**



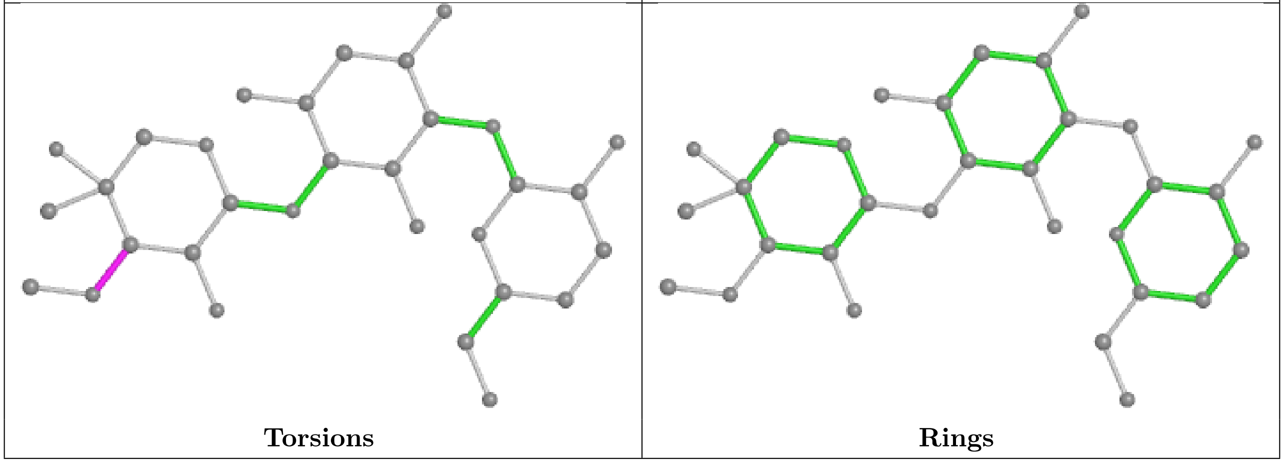
Torsions **Rings**

Ligand LLL CA 2062



Bond lengths

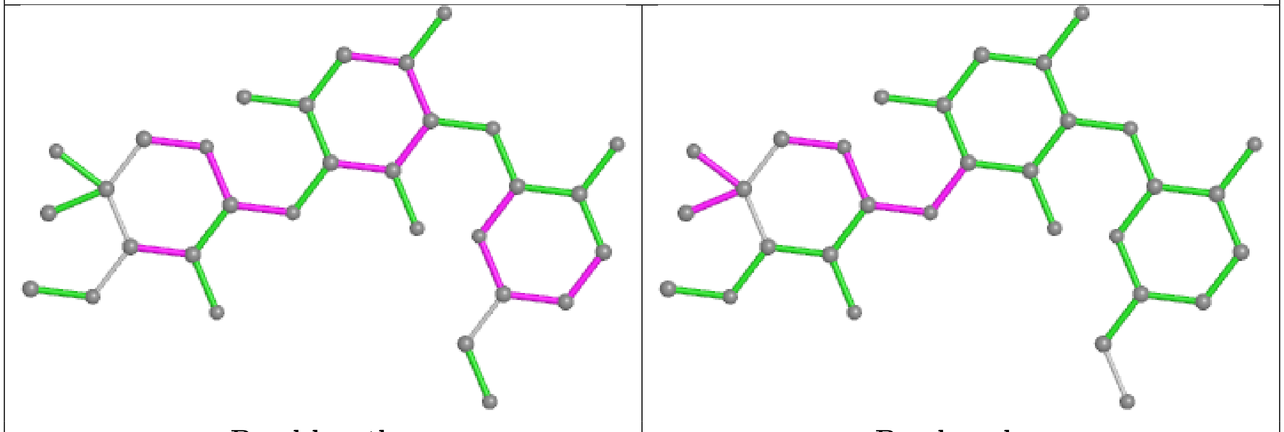
Bond angles



Torsions

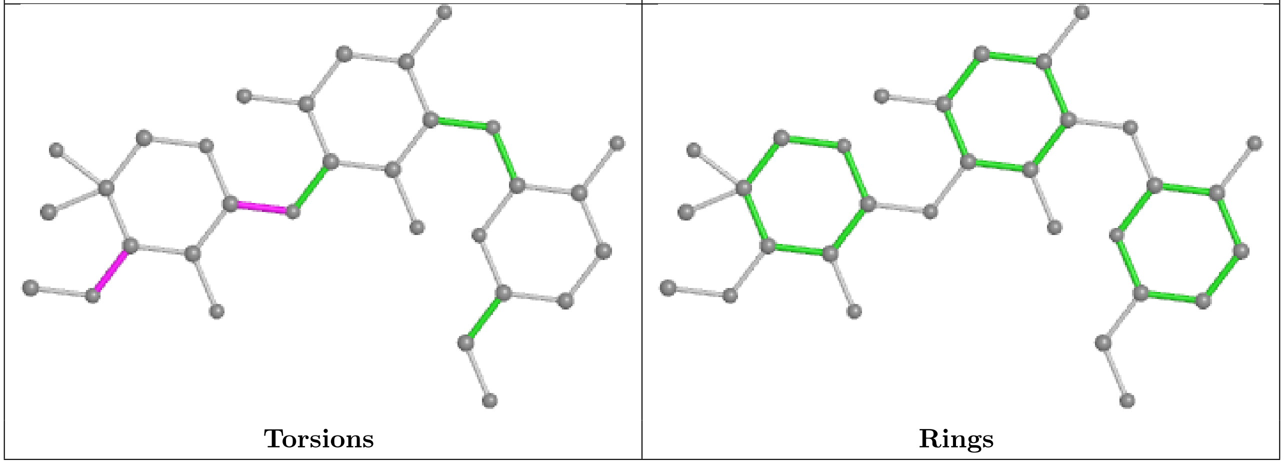
Rings

Ligand LLL AA 2063



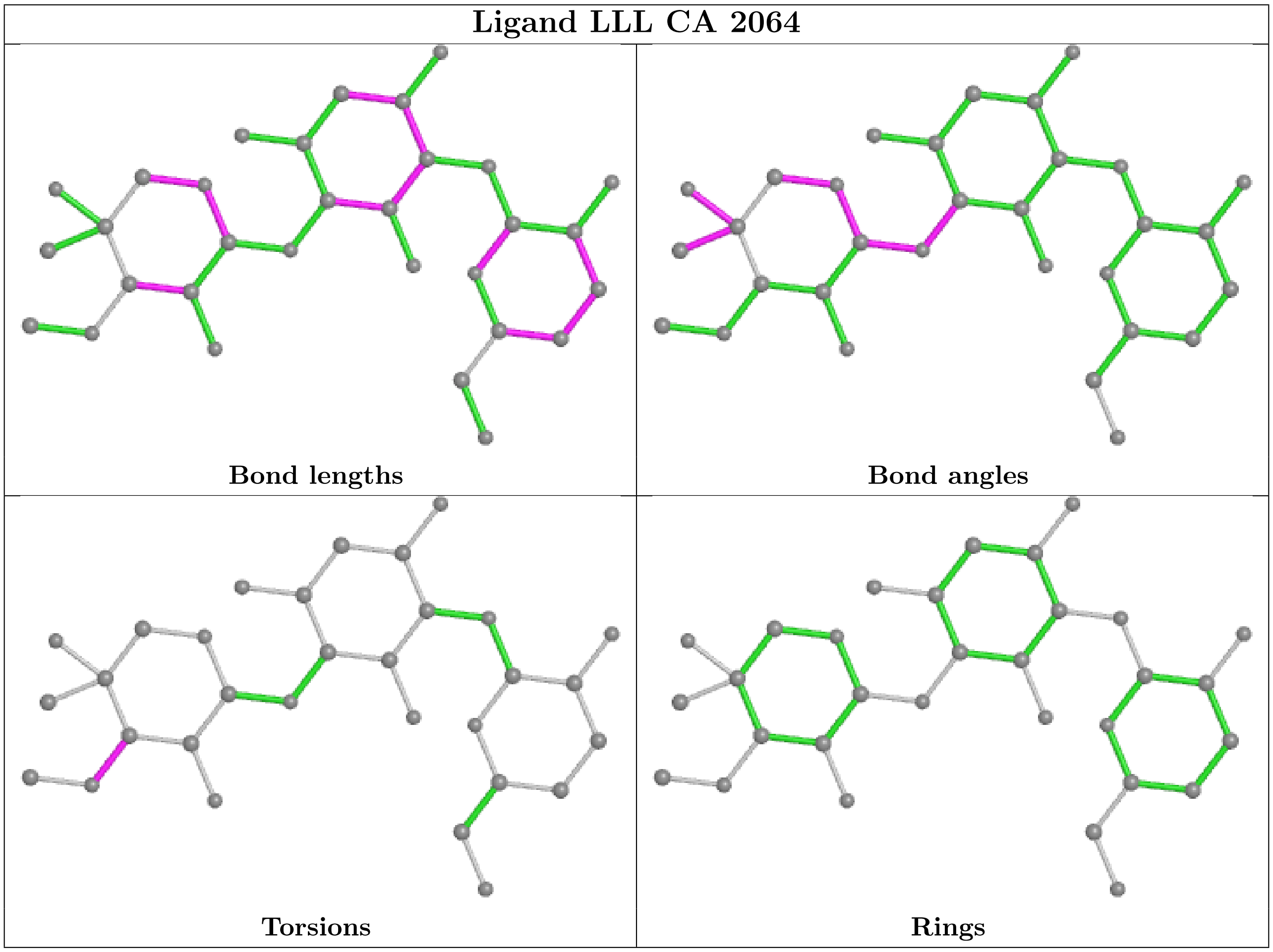
Bond lengths

Bond angles



Torsions

Rings


Ligand LLL CA 2064

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	BB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BB	2322:A	O3’	2323:G	P	1.78

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	1530/1542 (99%)	-0.59	8 (0%) 91 84	22, 85, 131, 156	0
1	CA	1530/1542 (99%)	-0.60	3 (0%) 95 91	5, 60, 120, 167	0
2	AC	206/232 (88%)	0.03	3 (1%) 73 61	14, 72, 111, 136	0
2	CC	206/232 (88%)	0.14	13 (6%) 20 14	5, 74, 103, 160	0
3	AD	205/205 (100%)	0.97	40 (19%) 1 1	21, 87, 115, 135	0
3	CD	205/205 (100%)	0.31	13 (6%) 20 14	8, 65, 107, 121	0
4	AE	150/166 (90%)	0.35	11 (7%) 15 11	6, 74, 105, 134	0
4	CE	150/166 (90%)	0.86	24 (16%) 1 2	5, 59, 96, 125	0
5	AF	100/135 (74%)	1.71	46 (46%) 0 0	22, 72, 114, 148	0
5	CF	100/135 (74%)	1.13	20 (20%) 1 0	12, 72, 109, 123	0
6	AG	150/178 (84%)	0.28	20 (13%) 3 3	47, 89, 116, 152	0
6	CG	152/178 (85%)	-0.13	3 (1%) 65 52	29, 80, 115, 134	0
7	AH	129/129 (100%)	0.50	18 (13%) 2 3	31, 80, 112, 136	0
7	CH	129/129 (100%)	0.42	13 (10%) 7 6	5, 56, 91, 112	0
8	AI	127/129 (98%)	0.49	20 (15%) 2 2	31, 83, 118, 143	0
8	CI	127/129 (98%)	0.01	2 (1%) 72 59	35, 84, 118, 157	0
9	AJ	98/103 (95%)	0.43	6 (6%) 21 15	22, 87, 121, 135	0
9	CJ	98/103 (95%)	0.40	12 (12%) 4 4	33, 84, 110, 125	0
10	AK	117/128 (91%)	0.47	7 (5%) 21 15	5, 67, 102, 117	0
10	CK	117/128 (91%)	-0.06	4 (3%) 45 33	5, 56, 101, 119	0
11	AL	123/123 (100%)	0.52	15 (12%) 4 4	22, 75, 110, 146	0
11	CL	123/123 (100%)	0.31	4 (3%) 46 34	5, 47, 103, 123	0
12	AM	114/117 (97%)	0.15	3 (2%) 56 42	58, 96, 124, 147	0
12	CM	113/117 (96%)	0.22	8 (7%) 16 12	48, 89, 116, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AN	96/100 (96%)	0.05	2 (2%)	63	50	27, 85, 121, 154	0
13	CN	96/100 (96%)	0.08	6 (6%)	20	14	40, 87, 114, 142	0
14	AO	88/89 (98%)	0.52	6 (6%)	17	13	38, 80, 109, 133	0
14	CO	88/89 (98%)	0.32	4 (4%)	33	24	5, 56, 107, 128	0
15	AP	82/82 (100%)	0.75	9 (10%)	5	5	48, 88, 121, 135	0
15	CP	80/82 (97%)	0.18	5 (6%)	20	14	11, 59, 109, 147	0
16	AQ	80/83 (96%)	0.72	11 (13%)	2	3	31, 87, 117, 124	0
16	CQ	81/83 (97%)	0.07	0	100	100	9, 58, 99, 121	0
17	AR	55/74 (74%)	0.79	6 (10%)	5	5	19, 76, 118, 138	0
17	CR	55/74 (74%)	0.91	10 (18%)	1	1	19, 68, 119, 131	0
18	AS	79/91 (86%)	0.82	12 (15%)	2	2	68, 100, 124, 136	0
18	CS	80/91 (87%)	0.14	5 (6%)	20	14	48, 94, 127, 153	0
19	AT	85/86 (98%)	0.20	2 (2%)	59	45	39, 92, 123, 144	0
19	CT	85/86 (98%)	0.04	3 (3%)	44	32	19, 61, 106, 125	0
20	AB	218/240 (90%)	0.79	32 (14%)	2	2	20, 87, 113, 132	0
20	CB	218/240 (90%)	1.16	53 (24%)	0	0	29, 89, 118, 144	0
21	AU	51/70 (72%)	0.74	6 (11%)	4	4	36, 89, 126, 134	0
21	CU	51/70 (72%)	0.32	6 (11%)	4	4	46, 78, 116, 132	0
22	BA	117/120 (97%)	-0.65	2 (1%)	70	57	47, 78, 117, 140	0
22	DA	117/120 (97%)	-0.55	2 (1%)	70	57	30, 80, 115, 155	0
23	BB	2841/2904 (97%)	-0.30	34 (1%)	79	67	9, 58, 127, 165	0
23	DB	2841/2904 (97%)	-0.31	14 (0%)	91	84	5, 45, 124, 163	0
24	BI	141/141 (100%)	2.36	74 (52%)	0	0	59, 117, 149, 158	0
24	DI	141/141 (100%)	0.89	17 (12%)	4	4	70, 117, 148, 160	0
25	BC	271/272 (99%)	0.73	25 (9%)	9	7	5, 47, 88, 105	0
25	DC	271/272 (99%)	0.70	25 (9%)	9	7	5, 32, 80, 112	0
26	BD	209/209 (100%)	0.65	28 (13%)	3	3	12, 71, 107, 141	0
26	DD	209/209 (100%)	0.57	27 (12%)	3	3	5, 49, 98, 135	0
27	BK	121/123 (98%)	1.37	32 (26%)	0	0	16, 67, 106, 134	0
27	DK	121/123 (98%)	0.54	3 (2%)	57	43	5, 37, 90, 130	0
28	BP	114/114 (100%)	1.20	30 (26%)	0	0	25, 81, 113, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	DP	114/114 (100%)	0.33	3 (2%)	56	42	7, 49, 94, 112	0
29	BE	201/201 (100%)	0.78	32 (15%)	1	2	5, 65, 104, 147	0
29	DE	201/201 (100%)	0.42	19 (9%)	8	6	5, 62, 107, 138	0
30	BY	58/58 (100%)	0.59	6 (10%)	6	6	26, 69, 107, 137	0
30	DY	58/58 (100%)	0.12	3 (5%)	27	20	6, 64, 110, 117	0
31	B0	56/56 (100%)	0.57	6 (10%)	6	5	5, 71, 113, 136	0
31	D0	56/56 (100%)	0.06	0	100	100	10, 43, 99, 104	0
32	B4	38/38 (100%)	0.71	4 (10%)	6	6	33, 76, 108, 125	0
32	D4	38/38 (100%)	-0.26	0	100	100	15, 65, 94, 105	0
33	B1	50/54 (92%)	1.84	17 (34%)	0	0	50, 75, 102, 115	0
33	D1	50/54 (92%)	1.26	9 (18%)	1	1	27, 74, 105, 118	0
34	B3	64/64 (100%)	0.55	6 (9%)	8	6	9, 55, 82, 106	0
34	D3	64/64 (100%)	0.57	8 (12%)	3	4	5, 39, 84, 101	0
35	BV	94/94 (100%)	0.20	7 (7%)	14	11	31, 86, 115, 129	0
35	DV	94/94 (100%)	0.43	8 (8%)	10	9	8, 79, 108, 125	0
36	B2	46/46 (100%)	0.39	3 (6%)	18	13	8, 40, 81, 113	0
36	D2	46/46 (100%)	0.12	2 (4%)	35	25	5, 28, 68, 113	0
37	BL	143/144 (99%)	0.38	7 (4%)	29	21	9, 63, 99, 134	0
37	DL	143/144 (99%)	0.81	28 (19%)	1	1	5, 55, 95, 123	0
38	BM	136/136 (100%)	0.75	14 (10%)	6	6	5, 65, 100, 131	0
38	DM	136/136 (100%)	0.39	7 (5%)	28	20	5, 55, 94, 134	0
39	BX	63/63 (100%)	1.04	14 (22%)	0	0	18, 76, 110, 123	0
39	DX	63/63 (100%)	0.09	2 (3%)	47	35	36, 82, 107, 142	0
40	BH	149/149 (100%)	2.55	71 (47%)	0	0	25, 98, 122, 146	0
40	DH	149/149 (100%)	1.00	24 (16%)	1	1	18, 88, 112, 141	0
41	BJ	142/142 (100%)	0.29	7 (4%)	29	21	16, 70, 106, 118	0
41	DJ	142/142 (100%)	0.28	5 (3%)	44	32	5, 60, 101, 131	0
42	BN	120/127 (94%)	0.47	10 (8%)	11	9	14, 65, 101, 145	0
42	DN	120/127 (94%)	0.09	2 (1%)	70	57	5, 42, 75, 118	0
43	BO	116/117 (99%)	0.73	20 (17%)	1	1	40, 78, 104, 128	0
43	DO	116/117 (99%)	-0.04	4 (3%)	45	33	5, 73, 106, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BQ	117/117 (100%)	-0.24	2 (1%) 70 57	5, 60, 95, 109	0
44	DQ	117/117 (100%)	0.44	6 (5%) 28 20	5, 50, 92, 120	0
45	BS	110/110 (100%)	0.81	14 (12%) 3 4	6, 56, 98, 118	0
45	DS	110/110 (100%)	1.14	18 (16%) 1 1	5, 48, 95, 128	0
46	BU	102/103 (99%)	1.45	33 (32%) 0 0	9, 71, 105, 123	0
46	DU	102/103 (99%)	0.25	2 (1%) 65 52	34, 80, 112, 130	0
47	BF	178/178 (100%)	1.11	40 (22%) 0 0	40, 95, 125, 140	0
47	DF	178/178 (100%)	1.25	41 (23%) 0 0	38, 85, 125, 138	0
48	BG	176/176 (100%)	0.92	34 (19%) 1 1	37, 88, 114, 146	0
48	DG	176/176 (100%)	0.55	22 (12%) 3 4	17, 82, 110, 133	0
49	BR	103/103 (100%)	0.05	4 (3%) 39 28	13, 78, 112, 120	0
49	DR	103/103 (100%)	0.52	12 (11%) 4 4	15, 72, 111, 128	0
50	BT	93/100 (93%)	0.43	7 (7%) 14 11	14, 70, 112, 124	0
50	DT	93/100 (93%)	0.47	8 (8%) 10 8	8, 66, 108, 120	0
51	BZ	77/78 (98%)	0.56	4 (5%) 27 20	5, 54, 93, 115	0
51	DZ	77/78 (98%)	0.08	1 (1%) 77 65	5, 43, 87, 114	0
52	BW	79/84 (94%)	0.65	8 (10%) 7 6	8, 75, 111, 136	0
52	DW	79/84 (94%)	0.07	4 (5%) 28 20	12, 65, 103, 122	0
All	All	20417/21046 (97%)	0.15	1415 (6%) 16 13	5, 68, 120, 167	0

The worst 5 of 1415 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
40	BH	86	ASP	9.9
40	BH	93	SER	9.3
40	BH	45	GLU	9.2
40	BH	85	GLY	9.1
40	BH	142	VAL	8.9

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
53	MG	AA	2035	1/1	0.41	0.08	71,71,71,71	0
53	MG	DB	3059	1/1	0.43	0.47	100,100,100,100	0
53	MG	AA	2039	1/1	0.46	0.35	92,92,92,92	0
53	MG	BB	3100	1/1	0.49	0.20	105,105,105,105	0
53	MG	BB	3057	1/1	0.50	0.31	72,72,72,72	0
53	MG	AA	2056	1/1	0.55	0.23	103,103,103,103	0
53	MG	AA	2005	1/1	0.61	0.10	72,72,72,72	0
53	MG	AA	2023	1/1	0.63	0.51	44,44,44,44	1
53	MG	AA	2025	1/1	0.66	0.26	50,50,50,50	1
53	MG	BB	3042	1/1	0.67	0.08	96,96,96,96	0
53	MG	AA	2022	1/1	0.69	0.32	100,100,100,100	0
53	MG	DB	3095	1/1	0.70	0.13	96,96,96,96	0
53	MG	AA	2057	1/1	0.71	0.24	80,80,80,80	0
53	MG	CA	2026	1/1	0.74	0.38	40,40,40,40	1
53	MG	CA	2027	1/1	0.74	0.16	55,55,55,55	1
53	MG	AA	2059	1/1	0.74	0.32	102,102,102,102	0
53	MG	AA	2030	1/1	0.74	0.07	88,88,88,88	0
53	MG	BB	3043	1/1	0.76	0.20	86,86,86,86	0
53	MG	AA	2037	1/1	0.78	0.55	87,87,87,87	0
53	MG	CA	2018	1/1	0.78	0.15	60,60,60,60	0
53	MG	BB	3081	1/1	0.78	0.23	40,40,40,40	0
54	LLL	AA	2062	31/31	0.78	0.37	73,73,73,73	31
53	MG	AA	2014	1/1	0.79	0.07	72,72,72,72	0
53	MG	CA	2036	1/1	0.79	0.06	74,74,74,74	0
53	MG	DB	3013	1/1	0.79	0.18	37,37,37,37	0
53	MG	AA	2049	1/1	0.80	0.07	93,93,93,93	0
53	MG	DB	3060	1/1	0.80	0.11	79,79,79,79	0
53	MG	AA	2012	1/1	0.80	0.07	70,70,70,70	0
53	MG	DB	3030	1/1	0.80	0.28	26,26,26,26	0
54	LLL	AA	2063	31/31	0.80	0.39	62,62,62,62	31
53	MG	AA	2055	1/1	0.81	0.06	57,57,57,57	0
53	MG	AA	2019	1/1	0.82	0.16	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
53	MG	CA	2043	1/1	0.83	0.07	31,31,31,31	0
53	MG	CA	2035	1/1	0.83	0.08	85,85,85,85	0
53	MG	BB	3010	1/1	0.84	0.11	73,73,73,73	0
53	MG	BB	3097	1/1	0.84	0.12	56,56,56,56	0
53	MG	CA	2022	1/1	0.84	0.05	105,105,105,105	0
53	MG	DB	3057	1/1	0.85	0.08	53,53,53,53	0
53	MG	BB	3023	1/1	0.85	0.13	11,11,11,11	0
53	MG	BB	3078	1/1	0.85	0.30	67,67,67,67	0
54	LLL	BB	3111	31/31	0.85	0.33	67,67,67,67	31
53	MG	AA	2015	1/1	0.86	0.20	78,78,78,78	0
53	MG	BB	3095	1/1	0.86	0.14	59,59,59,59	0
53	MG	BB	3038	1/1	0.86	0.12	77,77,77,77	0
53	MG	BB	3077	1/1	0.86	0.10	44,44,44,44	0
53	MG	AA	2047	1/1	0.86	0.46	73,73,73,73	0
53	MG	DB	3092	1/1	0.87	0.14	76,76,76,76	0
53	MG	CA	2052	1/1	0.87	0.10	66,66,66,66	0
53	MG	DB	3111	1/1	0.87	0.20	43,43,43,43	0
53	MG	DB	3058	1/1	0.87	0.79	96,96,96,96	0
53	MG	CA	2008	1/1	0.87	0.07	86,86,86,86	0
53	MG	AA	2017	1/1	0.87	0.07	76,76,76,76	0
54	LLL	DB	3112	31/31	0.87	0.36	54,54,54,54	0
53	MG	AA	2042	1/1	0.88	0.08	28,28,28,28	0
53	MG	BB	3033	1/1	0.88	0.55	90,90,90,90	0
53	MG	AA	2036	1/1	0.88	0.06	62,62,62,62	0
53	MG	AA	2032	1/1	0.88	0.12	67,67,67,67	0
53	MG	BB	3093	1/1	0.88	0.30	80,80,80,80	0
54	LLL	CA	2063	31/31	0.88	0.24	70,70,70,70	0
54	LLL	CA	2064	31/31	0.88	0.28	41,41,41,41	31
53	MG	AA	2024	1/1	0.88	0.13	73,73,73,73	0
53	MG	BB	3024	1/1	0.89	0.05	21,21,21,21	0
53	MG	BB	3027	1/1	0.89	0.10	24,24,24,24	0
53	MG	AA	2034	1/1	0.89	0.06	42,42,42,42	0
53	MG	BB	3094	1/1	0.89	0.12	69,69,69,69	0
53	MG	AA	2002	1/1	0.89	0.32	100,100,100,100	0
53	MG	AA	2046	1/1	0.89	0.11	95,95,95,95	0
53	MG	AA	2031	1/1	0.89	0.13	49,49,49,49	0
53	MG	AA	2013	1/1	0.89	0.04	70,70,70,70	0
53	MG	DB	3023	1/1	0.89	0.06	13,13,13,13	0
53	MG	CA	2014	1/1	0.89	0.05	72,72,72,72	0
53	MG	DB	3034	1/1	0.89	0.20	74,74,74,74	0
53	MG	AA	2053	1/1	0.89	0.16	58,58,58,58	0
53	MG	DB	3032	1/1	0.90	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
53	MG	CA	2015	1/1	0.90	0.06	108,108,108,108	0
53	MG	BB	3079	1/1	0.90	0.14	52,52,52,52	0
53	MG	BB	3004	1/1	0.90	0.05	43,43,43,43	0
53	MG	AA	2011	1/1	0.90	0.08	41,41,41,41	0
53	MG	AA	2050	1/1	0.90	0.05	103,103,103,103	0
53	MG	BB	3052	1/1	0.90	0.09	26,26,26,26	0
53	MG	AA	2051	1/1	0.90	0.22	66,66,66,66	0
53	MG	DB	3097	1/1	0.90	0.19	42,42,42,42	0
53	MG	CA	2042	1/1	0.90	0.09	66,66,66,66	0
53	MG	BB	3099	1/1	0.90	0.10	56,56,56,56	0
53	MG	BB	3061	1/1	0.90	0.06	45,45,45,45	0
53	MG	DB	3009	1/1	0.90	0.08	5,5,5,5	0
53	MG	AA	2058	1/1	0.90	0.07	94,94,94,94	0
53	MG	CA	2009	1/1	0.90	0.05	84,84,84,84	0
53	MG	AA	2007	1/1	0.90	0.09	70,70,70,70	0
55	ZN	B4	101	1/1	0.90	0.08	82,82,82,82	0
53	MG	DB	3045	1/1	0.91	0.08	66,66,66,66	0
53	MG	DB	3107	1/1	0.91	0.08	15,15,15,15	0
53	MG	DB	3052	1/1	0.91	0.17	62,62,62,62	0
53	MG	DB	3015	1/1	0.91	0.10	50,50,50,50	0
53	MG	DB	3022	1/1	0.91	0.07	23,23,23,23	0
53	MG	CA	2037	1/1	0.91	0.08	69,69,69,69	0
53	MG	CA	2057	1/1	0.91	0.05	61,61,61,61	0
53	MG	DB	3066	1/1	0.91	0.31	100,100,100,100	0
53	MG	BB	3030	1/1	0.91	0.05	53,53,53,53	0
53	MG	BB	3107	1/1	0.91	0.12	41,41,41,41	0
53	MG	CA	2011	1/1	0.92	0.08	82,82,82,82	0
53	MG	DB	3004	1/1	0.92	0.20	21,21,21,21	0
53	MG	DB	3099	1/1	0.92	0.18	5,5,5,5	0
53	MG	BB	3088	1/1	0.92	0.08	26,26,26,26	0
53	MG	DB	3055	1/1	0.92	0.18	11,11,11,11	0
53	MG	BB	3022	1/1	0.92	0.19	44,44,44,44	0
53	MG	AA	2026	1/1	0.92	0.13	51,51,51,51	1
53	MG	CA	2020	1/1	0.92	0.52	85,85,85,85	0
53	MG	BB	3036	1/1	0.92	0.14	57,57,57,57	0
53	MG	BB	3063	1/1	0.92	0.18	51,51,51,51	0
53	MG	DB	3087	1/1	0.92	0.23	63,63,63,63	0
53	MG	CA	2056	1/1	0.92	0.09	32,32,32,32	0
53	MG	BB	3102	1/1	0.93	0.10	16,16,16,16	0
53	MG	BB	3051	1/1	0.93	0.12	43,43,43,43	0
53	MG	CA	2038	1/1	0.93	0.17	77,77,77,77	0
53	MG	BB	3110	1/1	0.93	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	BB	3080	1/1	0.93	0.21	56,56,56,56	0
53	MG	CA	2047	1/1	0.93	0.11	74,74,74,74	0
53	MG	BB	3013	1/1	0.93	0.12	41,41,41,41	0
53	MG	DB	3061	1/1	0.93	0.14	58,58,58,58	0
53	MG	CA	2053	1/1	0.93	0.09	51,51,51,51	0
53	MG	DB	3072	1/1	0.93	0.07	25,25,25,25	0
53	MG	DB	3074	1/1	0.93	0.11	5,5,5,5	0
53	MG	BB	3082	1/1	0.93	0.16	5,5,5,5	0
53	MG	BB	3085	1/1	0.93	0.19	59,59,59,59	0
53	MG	CA	2060	1/1	0.93	0.05	55,55,55,55	0
53	MG	BB	3054	1/1	0.93	0.06	39,39,39,39	0
53	MG	BB	3034	1/1	0.93	0.10	52,52,52,52	0
53	MG	BB	3026	1/1	0.93	0.10	24,24,24,24	0
53	MG	DB	3110	1/1	0.93	0.18	29,29,29,29	0
53	MG	BB	3062	1/1	0.93	0.18	29,29,29,29	0
53	MG	CA	2023	1/1	0.93	0.06	54,54,54,54	0
53	MG	AA	2018	1/1	0.93	0.10	76,76,76,76	0
53	MG	AA	2060	1/1	0.93	0.11	46,46,46,46	0
53	MG	CA	2029	1/1	0.93	0.17	57,57,57,57	1
53	MG	DB	3033	1/1	0.93	0.11	18,18,18,18	0
53	MG	BB	3032	1/1	0.93	0.14	36,36,36,36	0
53	MG	DB	3042	1/1	0.93	0.13	22,22,22,22	0
53	MG	AA	2008	1/1	0.94	0.13	81,81,81,81	0
53	MG	BB	3005	1/1	0.94	0.15	5,5,5,5	0
53	MG	DB	3029	1/1	0.94	0.06	66,66,66,66	0
53	MG	BB	3008	1/1	0.94	0.07	80,80,80,80	0
53	MG	DB	3084	1/1	0.94	0.18	25,25,25,25	0
53	MG	AA	2021	1/1	0.94	0.10	23,23,23,23	0
53	MG	DB	3090	1/1	0.94	0.18	57,57,57,57	0
53	MG	BB	3065	1/1	0.94	0.11	44,44,44,44	0
53	MG	BB	3035	1/1	0.94	0.08	35,35,35,35	0
53	MG	DB	3035	1/1	0.94	0.08	54,54,54,54	0
53	MG	DB	3036	1/1	0.94	0.09	26,26,26,26	0
53	MG	DB	3037	1/1	0.94	0.21	5,5,5,5	0
53	MG	DB	3039	1/1	0.94	0.06	36,36,36,36	0
53	MG	CA	2059	1/1	0.94	0.17	51,51,51,51	0
54	LLL	AA	2061	31/31	0.94	0.29	20,20,20,20	0
53	MG	BB	3053	1/1	0.94	0.06	59,59,59,59	0
53	MG	AA	2054	1/1	0.94	0.06	66,66,66,66	0
53	MG	DB	3006	1/1	0.94	0.10	5,5,5,5	0
53	MG	BB	3098	1/1	0.94	0.18	43,43,43,43	0
53	MG	DB	3010	1/1	0.94	0.10	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	BB	3055	1/1	0.94	0.17	40,40,40,40	0
53	MG	CA	2019	1/1	0.94	0.11	63,63,63,63	0
53	MG	CA	2028	1/1	0.95	0.05	77,77,77,77	0
53	MG	BB	3037	1/1	0.95	0.10	29,29,29,29	0
53	MG	CA	2030	1/1	0.95	0.08	31,31,31,31	0
53	MG	BB	3096	1/1	0.95	0.12	44,44,44,44	0
53	MG	AA	2048	1/1	0.95	0.11	48,48,48,48	0
53	MG	BB	3064	1/1	0.95	0.07	37,37,37,37	0
53	MG	AA	2041	1/1	0.95	0.10	57,57,57,57	0
53	MG	DB	3043	1/1	0.95	0.12	5,5,5,5	0
53	MG	BB	3066	1/1	0.95	0.10	37,37,37,37	0
53	MG	DB	3050	1/1	0.95	0.07	73,73,73,73	0
53	MG	BB	3101	1/1	0.95	0.09	11,11,11,11	0
53	MG	DB	3053	1/1	0.95	0.06	66,66,66,66	0
53	MG	BB	3068	1/1	0.95	0.07	37,37,37,37	0
53	MG	CA	2048	1/1	0.95	0.23	65,65,65,65	0
53	MG	CA	2049	1/1	0.95	0.16	63,63,63,63	0
53	MG	BB	3104	1/1	0.95	0.15	18,18,18,18	0
53	MG	BB	3072	1/1	0.95	0.14	57,57,57,57	0
53	MG	CA	2054	1/1	0.95	0.08	91,91,91,91	0
53	MG	BB	3074	1/1	0.95	0.09	9,9,9,9	0
53	MG	AA	2027	1/1	0.95	0.18	56,56,56,56	0
53	MG	CA	2058	1/1	0.95	0.21	63,63,63,63	0
53	MG	BB	3047	1/1	0.95	0.08	77,77,77,77	0
53	MG	BB	3049	1/1	0.95	0.10	20,20,20,20	0
53	MG	CN	201	1/1	0.95	0.07	50,50,50,50	0
53	MG	DB	3003	1/1	0.95	0.12	17,17,17,17	0
53	MG	BB	3029	1/1	0.95	0.07	5,5,5,5	0
53	MG	AA	2045	1/1	0.95	0.10	48,48,48,48	0
53	MG	AA	2003	1/1	0.95	0.13	29,29,29,29	0
53	MG	DB	3105	1/1	0.95	0.11	30,30,30,30	0
53	MG	BB	3019	1/1	0.95	0.08	49,49,49,49	0
53	MG	DB	3108	1/1	0.95	0.08	5,5,5,5	0
53	MG	BB	3021	1/1	0.95	0.12	22,22,22,22	0
53	MG	CA	2021	1/1	0.95	0.11	70,70,70,70	0
53	MG	DB	3018	1/1	0.95	0.14	48,48,48,48	0
53	MG	BB	3089	1/1	0.95	0.17	63,63,63,63	0
53	MG	BB	3091	1/1	0.95	0.15	34,34,34,34	0
53	MG	DB	3027	1/1	0.95	0.13	12,12,12,12	0
54	LLL	CA	2062	31/31	0.95	0.21	9,9,9,9	0
53	MG	DB	3028	1/1	0.95	0.09	37,37,37,37	0
53	MG	CA	2025	1/1	0.95	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	AA	2020	1/1	0.95	0.04	91,91,91,91	0
53	MG	BB	3003	1/1	0.95	0.09	17,17,17,17	0
55	ZN	D4	101	1/1	0.95	0.08	45,45,45,45	0
53	MG	DB	3024	1/1	0.96	0.17	53,53,53,53	0
53	MG	DB	3062	1/1	0.96	0.08	43,43,43,43	0
53	MG	DB	3064	1/1	0.96	0.04	11,11,11,11	0
53	MG	DB	3026	1/1	0.96	0.10	33,33,33,33	0
53	MG	DB	3068	1/1	0.96	0.13	5,5,5,5	0
53	MG	DB	3071	1/1	0.96	0.10	34,34,34,34	0
53	MG	BB	3073	1/1	0.96	0.21	33,33,33,33	0
53	MG	CA	2007	1/1	0.96	0.11	47,47,47,47	0
53	MG	DB	3080	1/1	0.96	0.09	5,5,5,5	0
53	MG	DB	3083	1/1	0.96	0.17	56,56,56,56	0
53	MG	BB	3050	1/1	0.96	0.08	18,18,18,18	0
53	MG	DB	3085	1/1	0.96	0.13	5,5,5,5	0
53	MG	BB	3020	1/1	0.96	0.11	13,13,13,13	0
53	MG	CA	2034	1/1	0.96	0.13	15,15,15,15	0
53	MG	AA	2001	1/1	0.96	0.08	27,27,27,27	0
53	MG	CA	2061	1/1	0.96	0.06	25,25,25,25	0
53	MG	BB	3044	1/1	0.96	0.14	55,55,55,55	0
53	MG	BB	3046	1/1	0.96	0.13	50,50,50,50	0
53	MG	DB	3101	1/1	0.96	0.26	26,26,26,26	0
53	MG	DB	3102	1/1	0.96	0.15	16,16,16,16	0
53	MG	AA	2016	1/1	0.96	0.10	36,36,36,36	0
53	MG	DB	3005	1/1	0.96	0.17	6,6,6,6	0
53	MG	CA	2041	1/1	0.96	0.09	69,69,69,69	0
53	MG	BB	3067	1/1	0.96	0.07	40,40,40,40	0
53	MG	BB	3009	1/1	0.96	0.07	70,70,70,70	0
53	MG	DB	3048	1/1	0.96	0.07	36,36,36,36	0
53	MG	BB	3087	1/1	0.96	0.24	73,73,73,73	0
53	MG	DB	3051	1/1	0.96	0.18	57,57,57,57	0
53	MG	BB	3071	1/1	0.96	0.09	63,63,63,63	0
53	MG	DB	3016	1/1	0.96	0.07	17,17,17,17	0
53	MG	BB	3058	1/1	0.96	0.10	32,32,32,32	0
53	MG	DB	3020	1/1	0.96	0.20	5,5,5,5	0
53	MG	DB	3021	1/1	0.96	0.16	5,5,5,5	0
53	MG	BB	3090	1/1	0.96	0.09	60,60,60,60	0
53	MG	BB	3108	1/1	0.96	0.10	12,12,12,12	0
53	MG	DB	3070	1/1	0.97	0.09	43,43,43,43	0
53	MG	DB	3031	1/1	0.97	0.18	8,8,8,8	0
53	MG	BB	3014	1/1	0.97	0.06	39,39,39,39	0
53	MG	BB	3069	1/1	0.97	0.07	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	DB	3077	1/1	0.97	0.15	50,50,50,50	0
53	MG	DB	3078	1/1	0.97	0.09	48,48,48,48	0
53	MG	BB	3070	1/1	0.97	0.15	24,24,24,24	0
53	MG	DB	3082	1/1	0.97	0.07	42,42,42,42	0
53	MG	CA	2031	1/1	0.97	0.10	37,37,37,37	0
53	MG	BB	3039	1/1	0.97	0.14	35,35,35,35	0
53	MG	BB	3040	1/1	0.97	0.20	40,40,40,40	0
53	MG	DB	3086	1/1	0.97	0.19	24,24,24,24	0
53	MG	DB	3038	1/1	0.97	0.14	17,17,17,17	0
53	MG	DB	3089	1/1	0.97	0.29	52,52,52,52	0
53	MG	CA	2010	1/1	0.97	0.07	59,59,59,59	0
53	MG	BB	3056	1/1	0.97	0.07	22,22,22,22	0
53	MG	BB	3017	1/1	0.97	0.06	16,16,16,16	0
53	MG	BB	3075	1/1	0.97	0.19	33,33,33,33	0
53	MG	CA	2016	1/1	0.97	0.12	10,10,10,10	0
53	MG	CA	2017	1/1	0.97	0.04	5,5,5,5	0
53	MG	DB	3017	1/1	0.97	0.15	5,5,5,5	0
53	MG	DB	3104	1/1	0.97	0.17	55,55,55,55	0
53	MG	CA	2044	1/1	0.97	0.07	67,67,67,67	0
53	MG	DB	3019	1/1	0.97	0.05	6,6,6,6	0
53	MG	DB	3054	1/1	0.97	0.08	13,13,13,13	0
53	MG	AA	2038	1/1	0.97	0.08	45,45,45,45	0
53	MG	DB	3056	1/1	0.97	0.11	5,5,5,5	0
53	MG	BB	3031	1/1	0.97	0.06	32,32,32,32	0
53	MG	BB	3006	1/1	0.97	0.09	19,19,19,19	0
53	MG	AA	2052	1/1	0.97	0.10	69,69,69,69	0
53	MG	BB	3001	1/1	0.97	0.07	8,8,8,8	0
53	MG	AA	2006	1/1	0.97	0.05	57,57,57,57	0
53	MG	CA	2024	1/1	0.97	0.07	23,23,23,23	0
53	MG	DB	3063	1/1	0.97	0.09	21,21,21,21	0
53	MG	BB	3011	1/1	0.97	0.23	21,21,21,21	0
53	MG	BB	3105	1/1	0.97	0.12	34,34,34,34	0
53	MG	AA	2044	1/1	0.97	0.05	48,48,48,48	0
53	MG	BB	3076	1/1	0.98	0.09	23,23,23,23	0
53	MG	AA	2033	1/1	0.98	0.04	69,69,69,69	0
53	MG	AA	2029	1/1	0.98	0.14	50,50,50,50	0
53	MG	DB	3065	1/1	0.98	0.16	16,16,16,16	0
53	MG	CA	2046	1/1	0.98	0.07	70,70,70,70	0
53	MG	AA	2040	1/1	0.98	0.15	65,65,65,65	0
53	MG	DB	3069	1/1	0.98	0.19	21,21,21,21	0
53	MG	BB	3002	1/1	0.98	0.07	5,5,5,5	0
53	MG	DB	3025	1/1	0.98	0.13	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	BB	3012	1/1	0.98	0.07	31,31,31,31	0
53	MG	DB	3073	1/1	0.98	0.10	33,33,33,33	0
53	MG	CA	2050	1/1	0.98	0.16	5,5,5,5	0
53	MG	CA	2051	1/1	0.98	0.07	38,38,38,38	0
53	MG	AA	2010	1/1	0.98	0.06	45,45,45,45	0
53	MG	DB	3079	1/1	0.98	0.14	43,43,43,43	0
53	MG	BB	3083	1/1	0.98	0.18	33,33,33,33	0
53	MG	DB	3081	1/1	0.98	0.12	5,5,5,5	0
53	MG	BB	3103	1/1	0.98	0.11	5,5,5,5	0
53	MG	CA	2055	1/1	0.98	0.09	31,31,31,31	0
53	MG	BB	3084	1/1	0.98	0.30	67,67,67,67	0
53	MG	AA	2004	1/1	0.98	0.15	35,35,35,35	0
53	MG	BB	3106	1/1	0.98	0.08	31,31,31,31	0
53	MG	BB	3016	1/1	0.98	0.18	43,43,43,43	0
53	MG	BB	3041	1/1	0.98	0.12	18,18,18,18	0
53	MG	BB	3109	1/1	0.98	0.12	37,37,37,37	0
53	MG	DB	3091	1/1	0.98	0.26	45,45,45,45	0
53	MG	AA	2043	1/1	0.98	0.09	44,44,44,44	0
53	MG	DB	3093	1/1	0.98	0.19	7,7,7,7	0
53	MG	DB	3094	1/1	0.98	0.04	14,14,14,14	0
53	MG	DB	3040	1/1	0.98	0.13	5,5,5,5	0
53	MG	DB	3096	1/1	0.98	0.17	5,5,5,5	0
53	MG	DB	3041	1/1	0.98	0.14	41,41,41,41	0
53	MG	CA	2001	1/1	0.98	0.05	5,5,5,5	0
53	MG	DB	3100	1/1	0.98	0.09	5,5,5,5	0
53	MG	CA	2006	1/1	0.98	0.15	73,73,73,73	0
53	MG	DB	3044	1/1	0.98	0.06	18,18,18,18	0
53	MG	CA	2032	1/1	0.98	0.15	22,22,22,22	0
53	MG	DB	3046	1/1	0.98	0.10	5,5,5,5	0
53	MG	DB	3106	1/1	0.98	0.17	37,37,37,37	0
53	MG	BB	3018	1/1	0.98	0.23	54,54,54,54	0
53	MG	DB	3049	1/1	0.98	0.08	5,5,5,5	0
53	MG	DB	3007	1/1	0.98	0.16	18,18,18,18	0
53	MG	DB	3008	1/1	0.98	0.12	8,8,8,8	0
53	MG	AA	2028	1/1	0.98	0.08	53,53,53,53	0
53	MG	BB	3092	1/1	0.98	0.09	40,40,40,40	0
53	MG	DB	3011	1/1	0.98	0.21	35,35,35,35	0
53	MG	DB	3012	1/1	0.98	0.17	14,14,14,14	0
53	MG	BB	3059	1/1	0.98	0.09	39,39,39,39	0
53	MG	DB	3014	1/1	0.98	0.08	13,13,13,13	0
53	MG	BB	3045	1/1	0.98	0.07	19,19,19,19	0
53	MG	CA	2039	1/1	0.98	0.14	19,19,19,19	0

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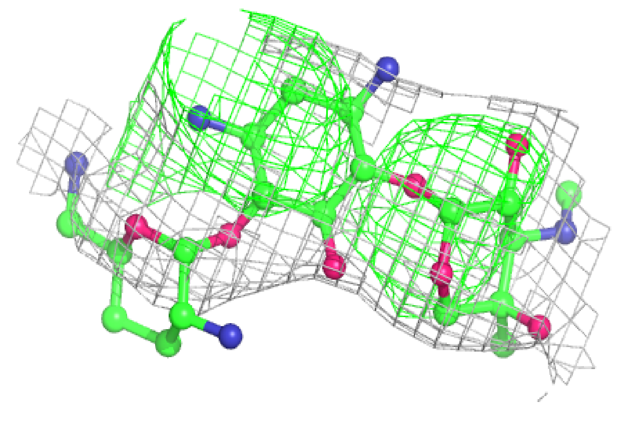
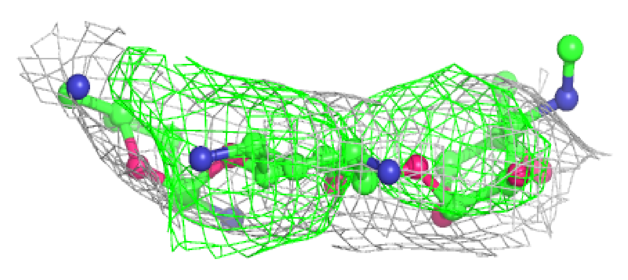
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
53	MG	CA	2040	1/1	0.98	0.08	12,12,12,12	0
53	MG	CA	2013	1/1	0.98	0.13	48,48,48,48	0
53	MG	DB	3098	1/1	0.99	0.22	23,23,23,23	0
53	MG	CA	2003	1/1	0.99	0.08	44,44,44,44	0
53	MG	CA	2004	1/1	0.99	0.05	13,13,13,13	0
53	MG	CA	2005	1/1	0.99	0.10	10,10,10,10	0
53	MG	BB	3060	1/1	0.99	0.19	59,59,59,59	0
53	MG	DB	3103	1/1	0.99	0.08	7,7,7,7	0
53	MG	BB	3025	1/1	0.99	0.09	51,51,51,51	0
53	MG	CA	2045	1/1	0.99	0.16	77,77,77,77	0
53	MG	BB	3086	1/1	0.99	0.19	5,5,5,5	0
53	MG	DB	3047	1/1	0.99	0.20	5,5,5,5	0
53	MG	CA	2033	1/1	0.99	0.17	57,57,57,57	0
53	MG	DB	3109	1/1	0.99	0.10	28,28,28,28	0
53	MG	AA	2009	1/1	0.99	0.14	27,27,27,27	0
53	MG	DB	3067	1/1	0.99	0.11	5,5,5,5	0
53	MG	DB	3088	1/1	0.99	0.27	18,18,18,18	0
53	MG	DB	3001	1/1	0.99	0.12	5,5,5,5	0
53	MG	DB	3002	1/1	0.99	0.13	12,12,12,12	0
53	MG	BB	3007	1/1	0.99	0.06	60,60,60,60	0
53	MG	BB	3048	1/1	0.99	0.04	22,22,22,22	0
53	MG	CA	2012	1/1	0.99	0.08	49,49,49,49	0
53	MG	BB	3028	1/1	0.99	0.15	16,16,16,16	0
53	MG	CA	2002	1/1	0.99	0.12	27,27,27,27	0
53	MG	DB	3075	1/1	0.99	0.08	41,41,41,41	0
53	MG	DB	3076	1/1	0.99	0.12	43,43,43,43	0
53	MG	BB	3015	1/1	1.00	0.06	5,5,5,5	0

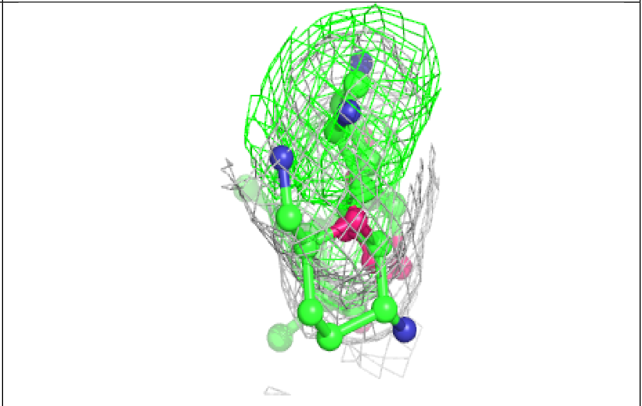
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LLL AA 2062:

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

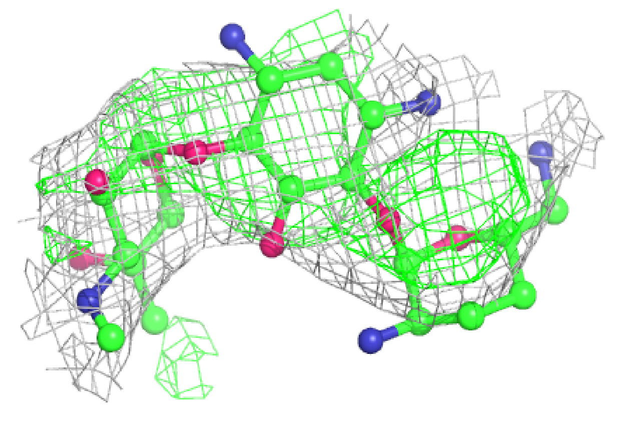


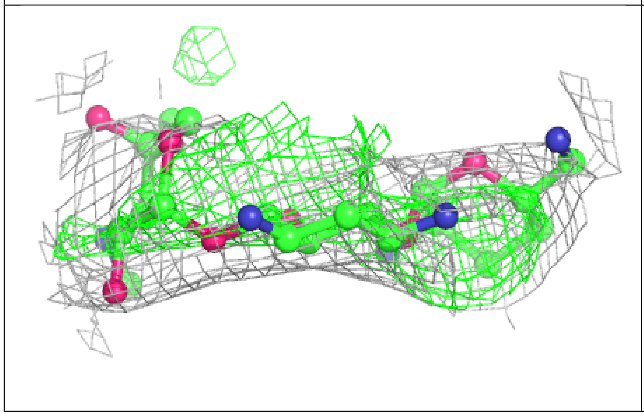


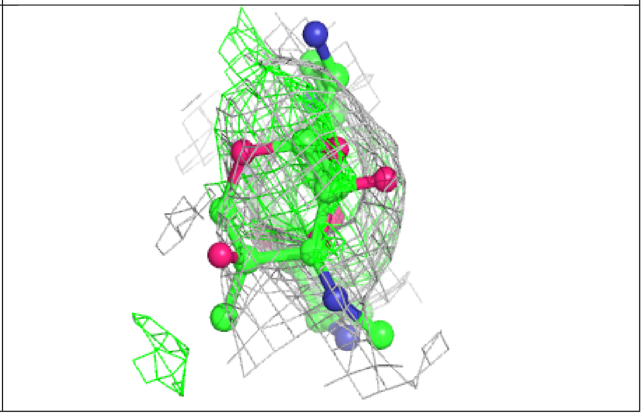


Electron density around LLL AA 2063:

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

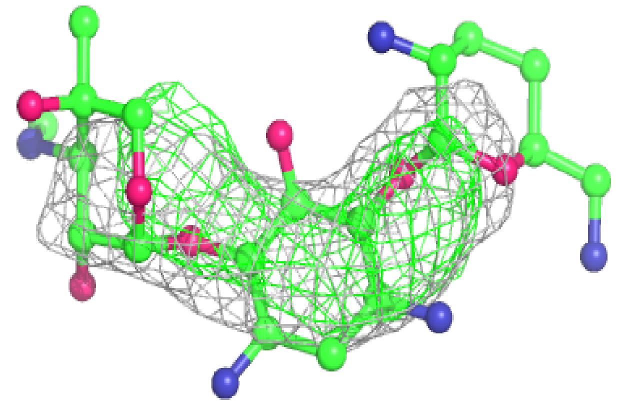


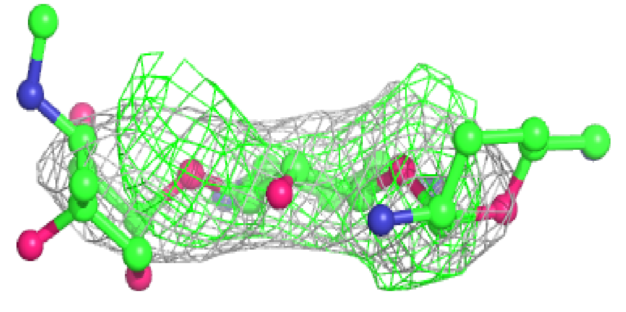


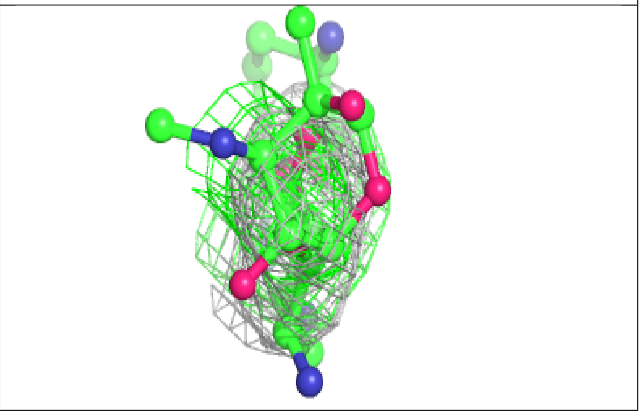


Electron density around LLL BB 3111:

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

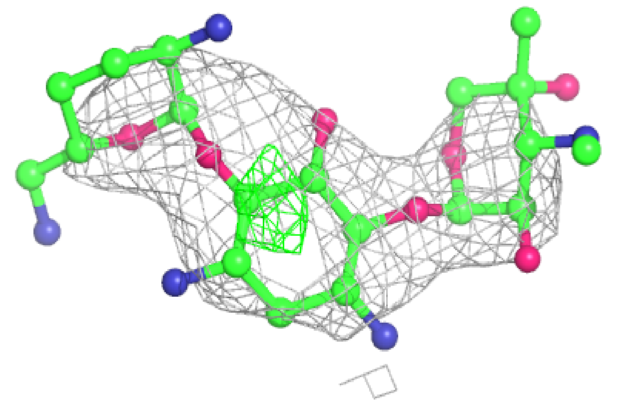


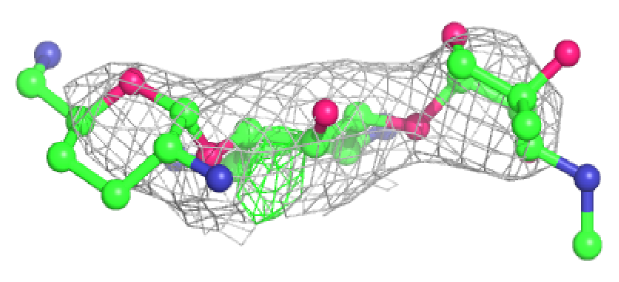


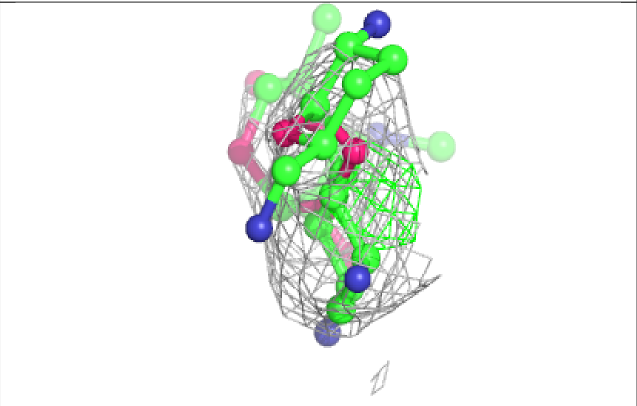


Electron density around LLL DB 3112:

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

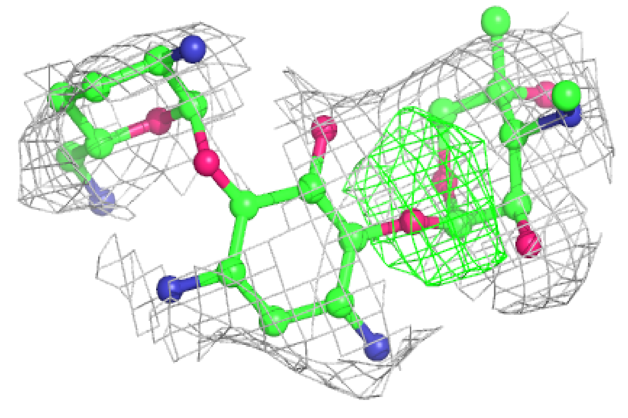


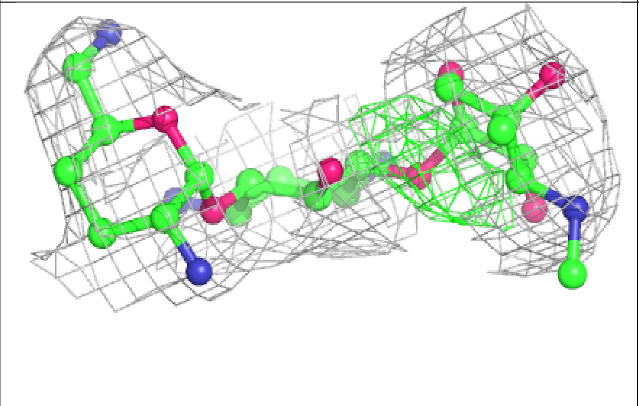


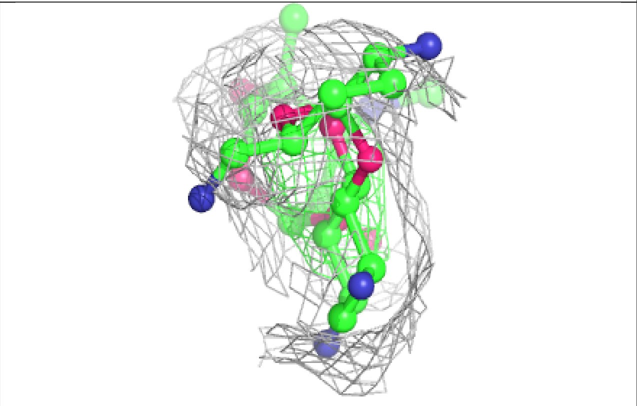


Electron density around LLL CA 2063:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

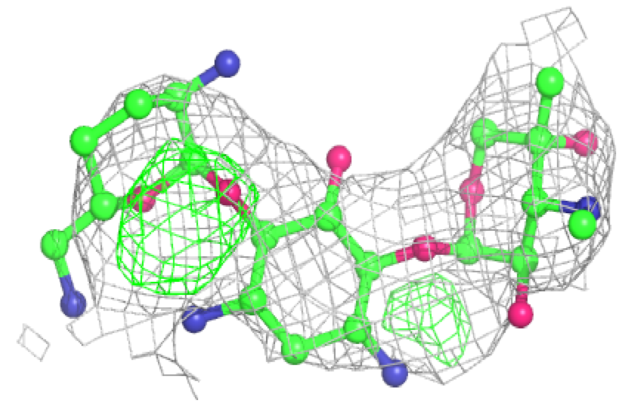


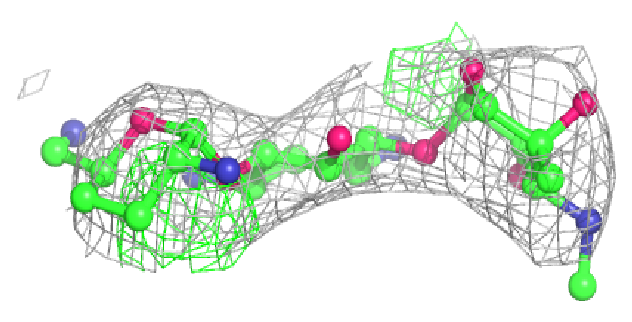


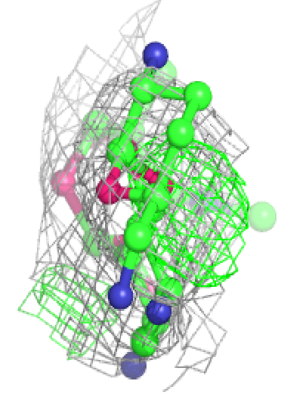


Electron density around LLL CA 2064:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

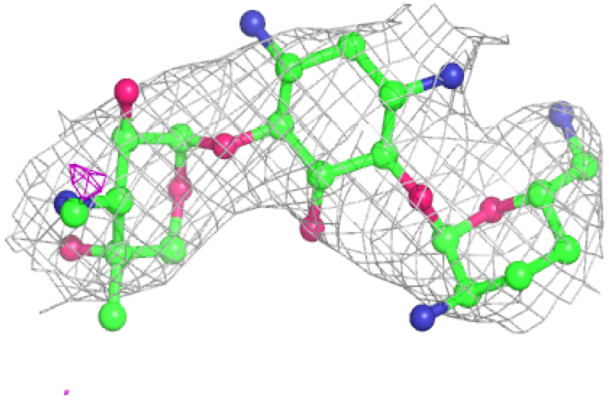


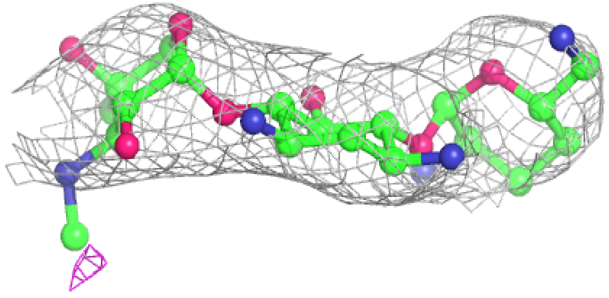


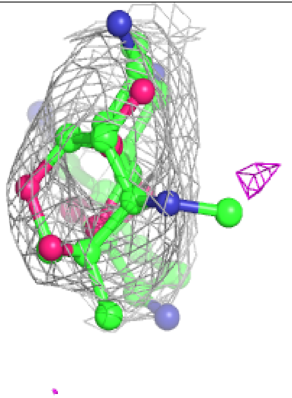


Electron density around LLL AA 2061:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

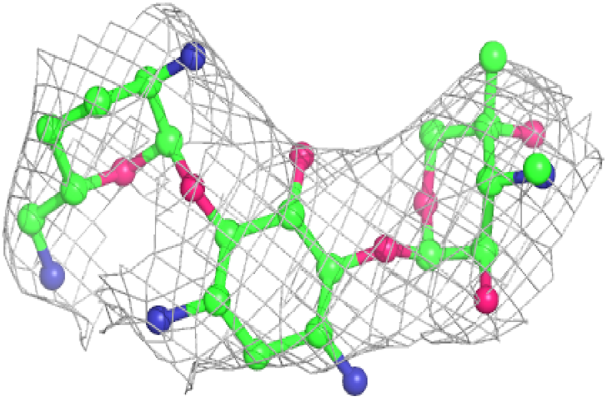


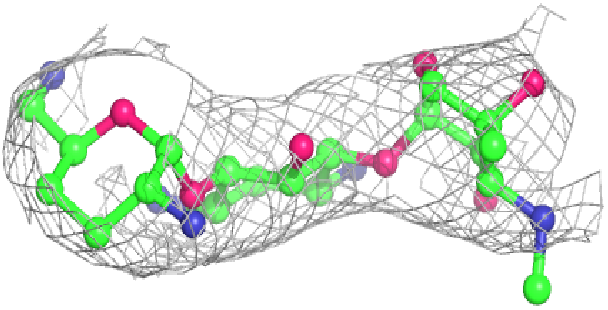


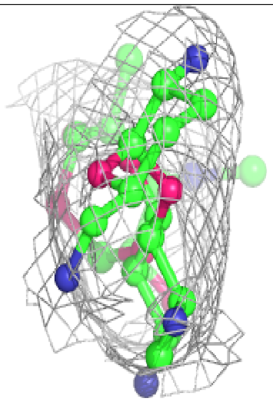


Electron density around LLL CA 2062:

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 ⓘ

There are no such residues in this entry.