wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 02:07 AM EDT

PDB ID	:	4YM7
Title	:	RNA polymerase I structure with an alternative dimer hinge
Authors	:	Kostrewa, D.; Kuhn, C.-D.; Engel, C.; Cramer, P.
Deposited on	:	2015-03-06
Resolution	:	5.50 Å(reported)

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

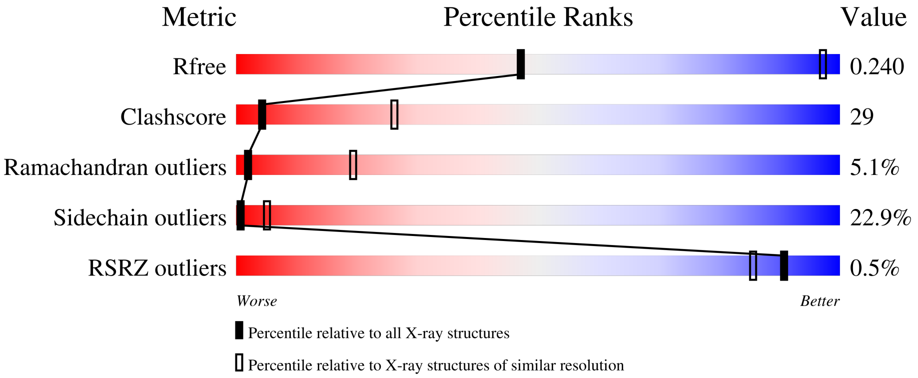
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

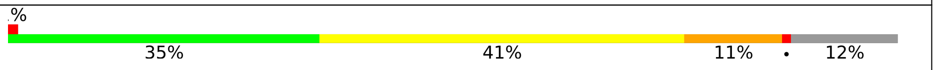
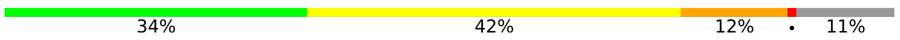
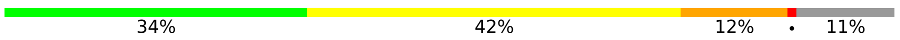
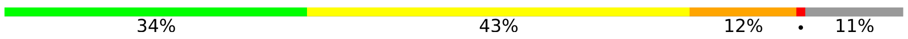
The reported resolution of this entry is 5.50 Å.

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	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)

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	1664	
1	BA	1664	
1	CA	1664	
1	DA	1664	
1	EA	1664	

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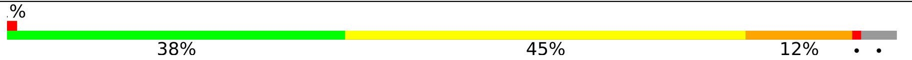
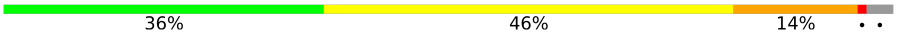
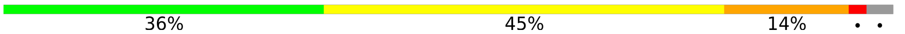
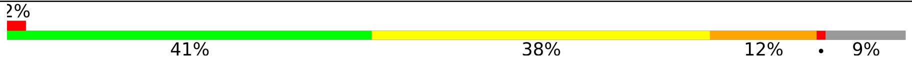
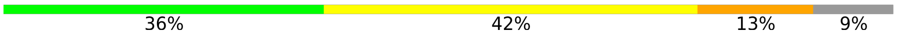
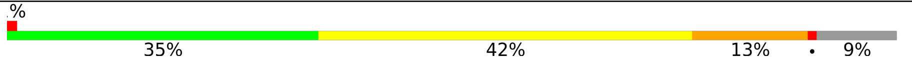
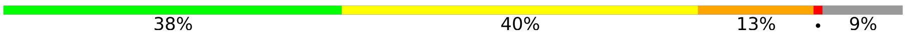
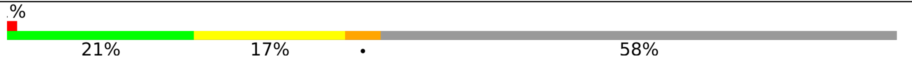
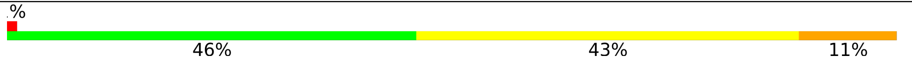
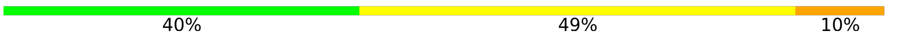
Mol	Chain	Length	Quality of chain
1	FA	1664	
2	AB	1203	
2	BB	1203	
2	CB	1203	
2	DB	1203	
2	EB	1203	
2	FB	1203	
3	AC	335	
3	BC	335	
3	CC	335	
3	DC	335	
3	EC	335	
3	FC	335	
4	AD	137	
4	BD	137	
4	CD	137	
4	DD	137	
4	ED	137	
4	FD	137	
5	AE	215	
5	BE	215	
5	CE	215	
5	DE	215	
5	EE	215	
5	FE	215	

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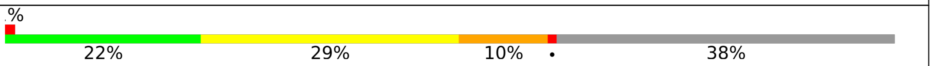
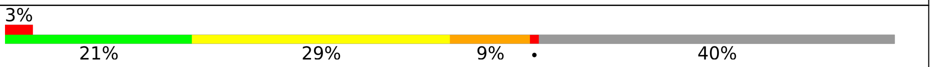
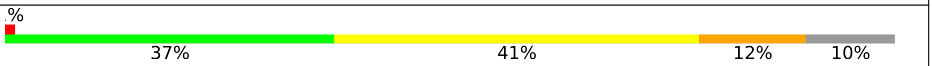
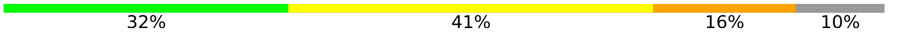
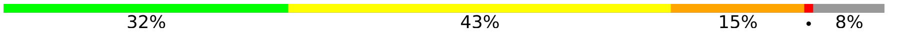
Mol	Chain	Length	Quality of chain
6	AF	155	 29% 28% 6% 37%
6	BF	155	 34% 23% 6% 37%
6	CF	155	 28% 30% 6% 36%
6	DF	155	 31% 27% 6% 36%
6	EF	155	 32% 27% 5% 36%
6	FF	155	 27% 30% 6% 36%
7	AG	326	 % 22% 29% 10% • 38%
7	AO	326	 • 7% 5% 84%
7	BG	326	 3% 21% 29% 9% • 40%
7	BO	326	 • 9% • 84%
7	CG	326	 23% 28% 10% • 38%
7	CO	326	 6% 6% • 85%
7	DG	326	 19% 31% 10% • 38%
7	DO	326	 • 8% 5% 84%
7	EG	326	 21% 30% 9% • 38%
7	EO	326	 • 7% 5% 84%
7	FG	326	 22% 28% 10% • 38%
7	FO	326	 5% 7% • 84%
8	AH	146	 34% 43% 14% 10%
8	BH	146	 % 37% 41% 12% 10%
8	CH	146	 32% 41% 16% 10%
8	DH	146	 32% 43% 15% • 8%
8	EH	146	 33% 43% 15% • 8%
8	FH	146	 32% 45% 16% 8%
9	AI	125	 46% 42% 12% •

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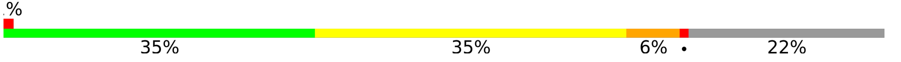
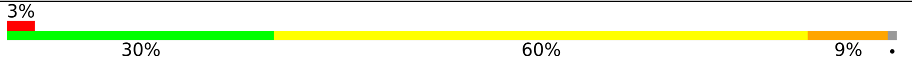
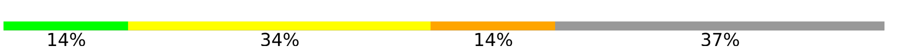
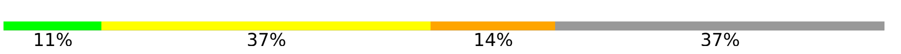
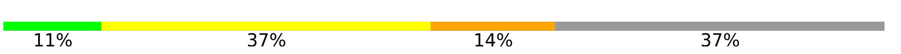
Mol	Chain	Length	Quality of chain
9	BI	125	
9	CI	125	
9	DI	125	
9	EI	125	
9	FI	125	
10	AJ	70	
10	BJ	70	
10	CJ	70	
10	DJ	70	
10	EJ	70	
10	FJ	70	
11	AK	142	
11	BK	142	
11	CK	142	
11	DK	142	
11	EK	142	
11	FK	142	
12	AL	70	
12	BL	70	
12	CL	70	
12	DL	70	
12	EL	70	
12	FL	70	
13	AM	415	
13	BM	415	

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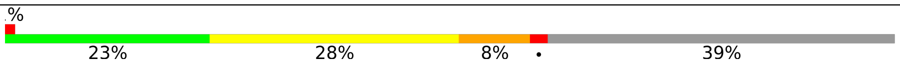
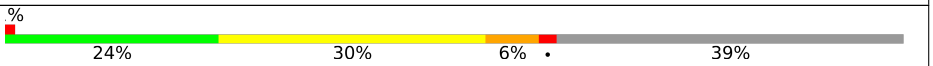
Mol	Chain	Length	Quality of chain
13	CM	415	
13	DM	415	
13	EM	415	
13	FM	415	
14	AN	233	
14	BN	233	
14	CN	233	
14	DN	233	
14	EN	233	
14	FN	233	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 204233 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 protein called DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1484	Total 11703	C 7385	N 2036	O 2220	S 62	0	0	0
1	BA	1462	Total 11540	C 7291	N 2003	O 2184	S 62	0	0	0
1	CA	1483	Total 11695	C 7381	N 2035	O 2217	S 62	0	0	0
1	DA	1483	Total 11697	C 7381	N 2034	O 2220	S 62	0	0	0
1	EA	1484	Total 11706	C 7390	N 2036	O 2218	S 62	0	0	0
1	FA	1484	Total 11709	C 7392	N 2036	O 2219	S 62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	1154	Total 9187	C 5822	N 1606	O 1708	S 51	0	0	0
2	BB	1153	Total 9175	C 5812	N 1603	O 1709	S 51	0	0	0
2	CB	1170	Total 9304	C 5892	N 1629	O 1732	S 51	0	0	0
2	DB	1165	Total 9269	C 5871	N 1622	O 1725	S 51	0	0	0
2	EB	1164	Total 9265	C 5871	N 1619	O 1724	S 51	0	0	0
2	FB	1165	Total 9270	C 5872	N 1622	O 1725	S 51	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	304	2413	1534	414	457	8	0	0	0
3	BC	304	2413	1534	414	457	8	0	0	0
3	CC	304	2413	1534	414	457	8	0	0	0
3	DC	304	2413	1534	414	457	8	0	0	0
3	EC	304	2413	1534	414	457	8	0	0	0
3	FC	304	2413	1534	414	457	8	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	AD	58	459	289	78	92	0	0	0
4	BD	58	459	289	78	92	0	0	0
4	CD	58	459	289	78	92	0	0	0
4	DD	58	459	289	78	92	0	0	0
4	ED	58	459	289	78	92	0	0	0
4	FD	58	459	289	78	92	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	215	1760	1116	310	322	12	0	0	0
5	BE	215	1760	1116	310	322	12	0	0	0
5	CE	215	1760	1116	310	322	12	0	0	0
5	DE	215	1760	1116	310	322	12	0	0	0
5	EE	215	1760	1116	310	322	12	0	0	0
5	FE	215	1760	1116	310	322	12	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	AF	98	Total C N O S 807 512 142 150 3	0	0	0
6	BF	98	Total C N O S 807 512 142 150 3	0	0	0
6	CF	99	Total C N O S 816 517 143 153 3	0	0	0
6	DF	99	Total C N O S 816 517 143 153 3	0	0	0
6	EF	99	Total C N O S 816 517 143 153 3	0	0	0
6	FF	99	Total C N O S 816 517 143 153 3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	AG	202	Total C N O S 1599 1025 276 293 5	0	0	0
7	AO	52	Total C N O 413 253 64 96	0	0	0
7	BG	195	Total C N O S 1539 992 264 278 5	0	0	0
7	BO	51	Total C N O 404 248 63 93	0	0	0
7	CG	202	Total C N O S 1599 1025 276 293 5	0	0	0
7	CO	50	Total C N O 398 245 62 91	0	0	0
7	DG	202	Total C N O S 1599 1025 276 293 5	0	0	0
7	DO	52	Total C N O 413 253 64 96	0	0	0
7	EG	202	Total C N O S 1599 1025 276 293 5	0	0	0
7	EO	52	Total C N O 413 253 64 96	0	0	0
7	FG	202	Total C N O S 1599 1025 276 293 5	0	0	0
7	FO	52	Total C N O 413 253 64 96	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AH	132	Total C N O S 1063 670 180 209 4	0	0	0
8	BH	131	Total C N O S 1052 664 176 208 4	0	0	0
8	CH	131	Total C N O S 1052 664 176 208 4	0	0	0
8	DH	134	Total C N O S 1075 677 182 212 4	0	0	0
8	EH	134	Total C N O S 1075 677 182 212 4	0	0	0
8	FH	134	Total C N O S 1075 677 182 212 4	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AI	124	Total C N O S 943 584 160 190 9	0	0	0
9	BI	97	Total C N O S 716 439 120 148 9	0	0	0
9	CI	124	Total C N O S 943 584 160 190 9	0	0	0
9	DI	124	Total C N O S 943 584 160 190 9	0	0	0
9	EI	117	Total C N O S 898 556 152 181 9	0	0	0
9	FI	124	Total C N O S 943 584 160 190 9	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	AJ	68	Total C N O S 558 356 97 99 6	0	0	0
10	BJ	69	Total C N O S 569 362 101 100 6	0	0	0
10	CJ	68	Total C N O S 558 356 97 99 6	0	0	0
10	DJ	69	Total C N O S 569 362 101 100 6	0	0	0
10	EJ	68	Total C N O S 558 356 97 99 6	0	0	0
10	FJ	68	Total C N O S 558 356 97 99 6	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	AK	101	Total C N O S 793 496 130 162 5	0	0	0
11	BK	100	Total C N O S 786 491 129 161 5	0	0	0
11	CK	101	Total C N O S 793 496 130 162 5	0	0	0
11	DK	101	Total C N O S 793 496 130 162 5	0	0	0
11	EK	100	Total C N O S 786 491 129 161 5	0	0	0
11	FK	100	Total C N O S 786 491 129 161 5	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	AL	44	Total C N O S 352 217 70 61 4	0	0	0
12	BL	44	Total C N O S 352 217 70 61 4	0	0	0
12	CL	44	Total C N O S 352 217 70 61 4	0	0	0
12	DL	44	Total C N O S 352 217 70 61 4	0	0	0
12	EL	44	Total C N O S 352 217 70 61 4	0	0	0
12	FL	44	Total C N O S 352 217 70 61 4	0	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	AM	109	Total C N O 863 548 143 172	0	0	0
13	BM	109	Total C N O 863 548 143 172	0	0	0
13	CM	109	Total C N O 863 548 143 172	0	0	0
13	DM	109	Total C N O 863 548 143 172	0	0	0
13	EM	110	Total C N O 869 551 144 174	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	FM	110	Total C N O 869 551 144 174	0	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	AN	142	Total C N O S 1127 719 183 221 4	0	0	0
14	BN	143	Total C N O S 1130 719 184 223 4	0	0	0
14	CN	143	Total C N O S 1137 728 184 221 4	0	0	0
14	DN	145	Total C N O S 1146 729 186 227 4	0	0	0
14	EN	144	Total C N O S 1140 726 186 224 4	0	0	0
14	FN	145	Total C N O S 1146 729 187 226 4	0	0	0

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	AA	2	Total Zn 2 2	0	0
15	AB	1	Total Zn 1 1	0	0
15	AI	2	Total Zn 2 2	0	0
15	AJ	1	Total Zn 1 1	0	0
15	AL	1	Total Zn 1 1	0	0
15	BA	2	Total Zn 2 2	0	0
15	BB	1	Total Zn 1 1	0	0
15	BI	2	Total Zn 2 2	0	0
15	BJ	1	Total Zn 1 1	0	0
15	BL	1	Total Zn 1 1	0	0

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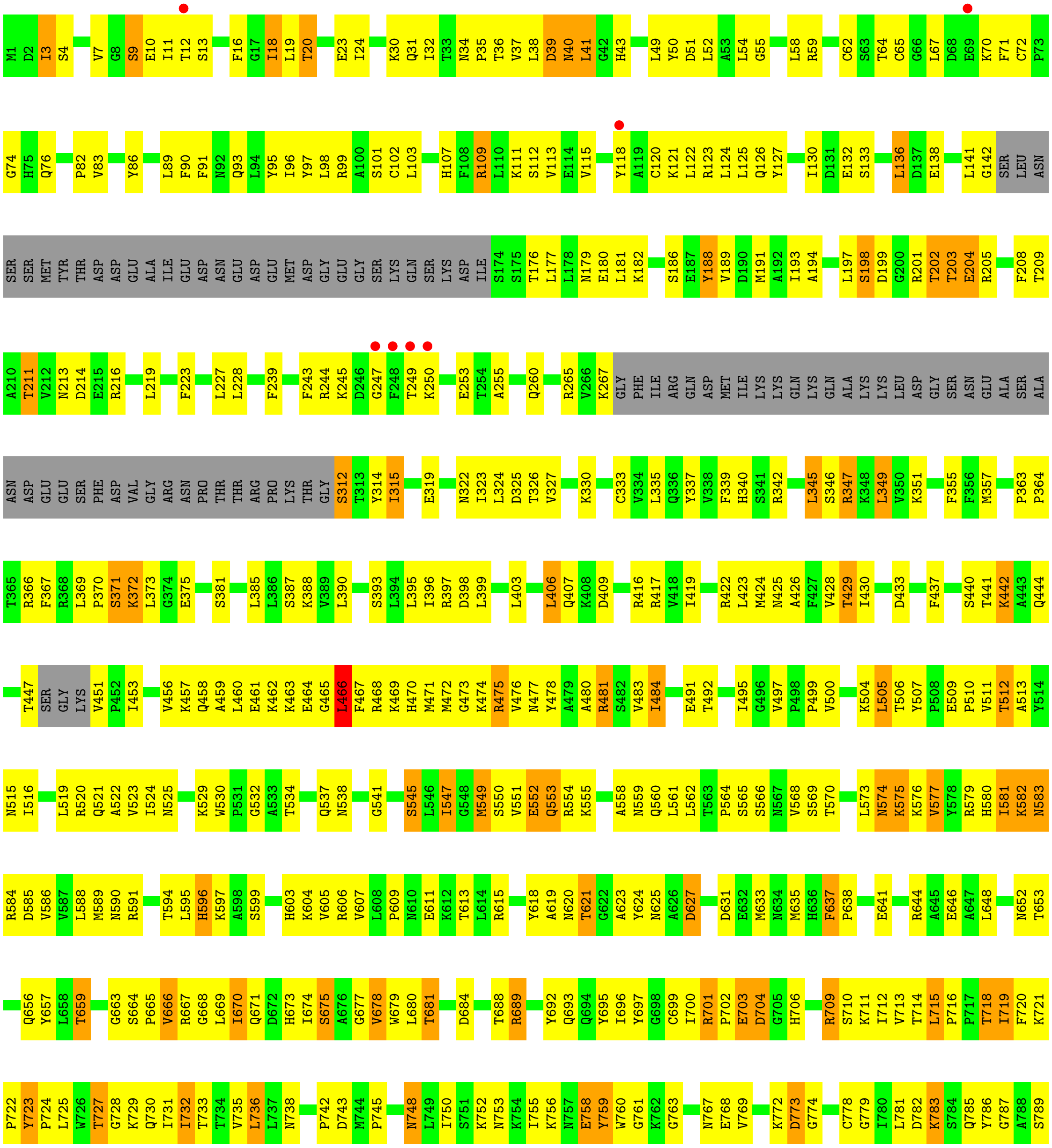
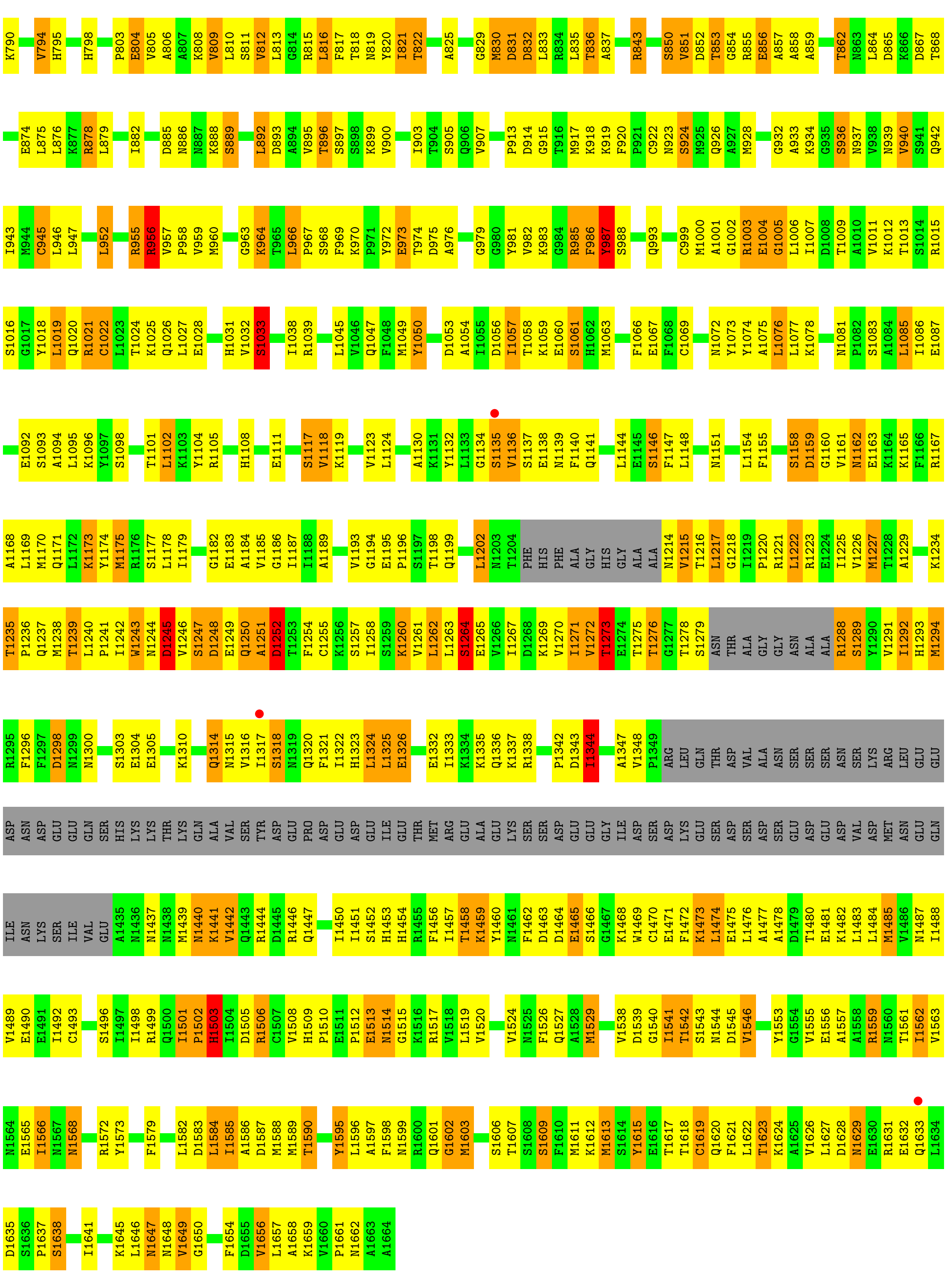
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	CA	2	Total Zn 2 2	0	0
15	CB	1	Total Zn 1 1	0	0
15	CI	2	Total Zn 2 2	0	0
15	CJ	1	Total Zn 1 1	0	0
15	CL	1	Total Zn 1 1	0	0
15	DA	2	Total Zn 2 2	0	0
15	DB	1	Total Zn 1 1	0	0
15	DI	2	Total Zn 2 2	0	0
15	DJ	1	Total Zn 1 1	0	0
15	DL	1	Total Zn 1 1	0	0
15	EA	2	Total Zn 2 2	0	0
15	EB	1	Total Zn 1 1	0	0
15	EI	2	Total Zn 2 2	0	0
15	EJ	1	Total Zn 1 1	0	0
15	EL	1	Total Zn 1 1	0	0
15	FA	2	Total Zn 2 2	0	0
15	FB	1	Total Zn 1 1	0	0
15	FI	2	Total Zn 2 2	0	0
15	FJ	1	Total Zn 1 1	0	0
15	FL	1	Total Zn 1 1	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: DNA-directed RNA polymerase I subunit RPA190





- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

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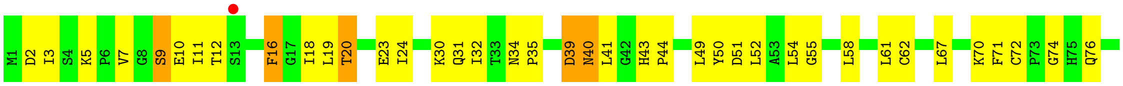

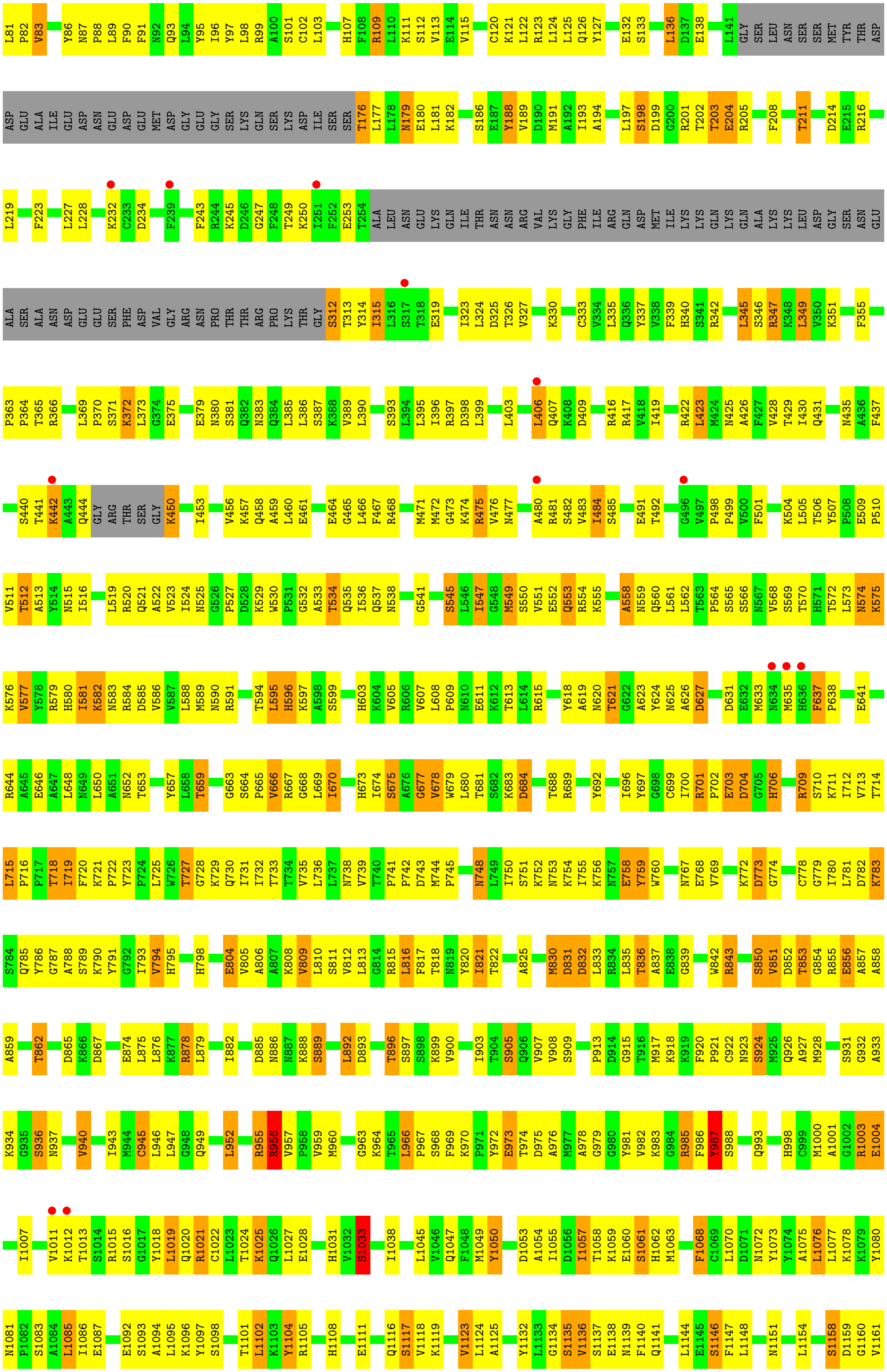
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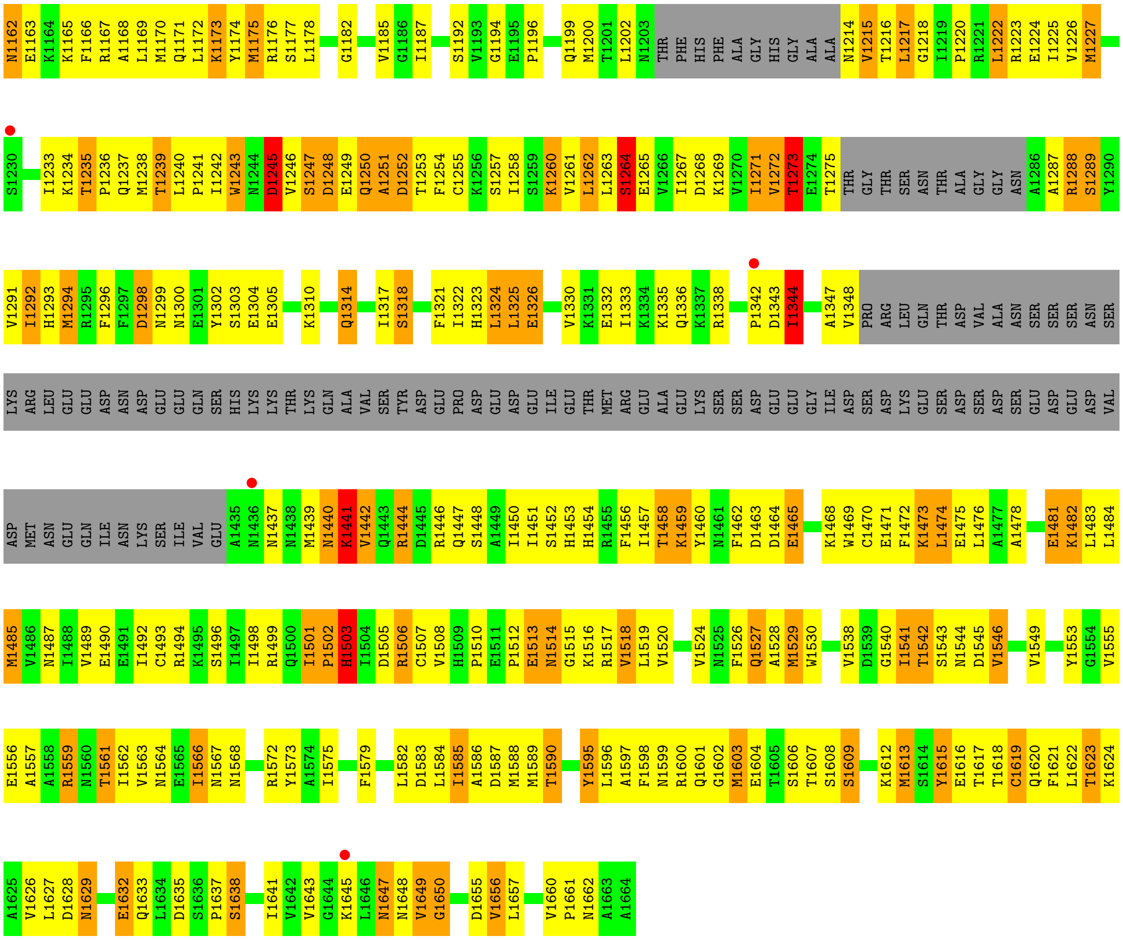

- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

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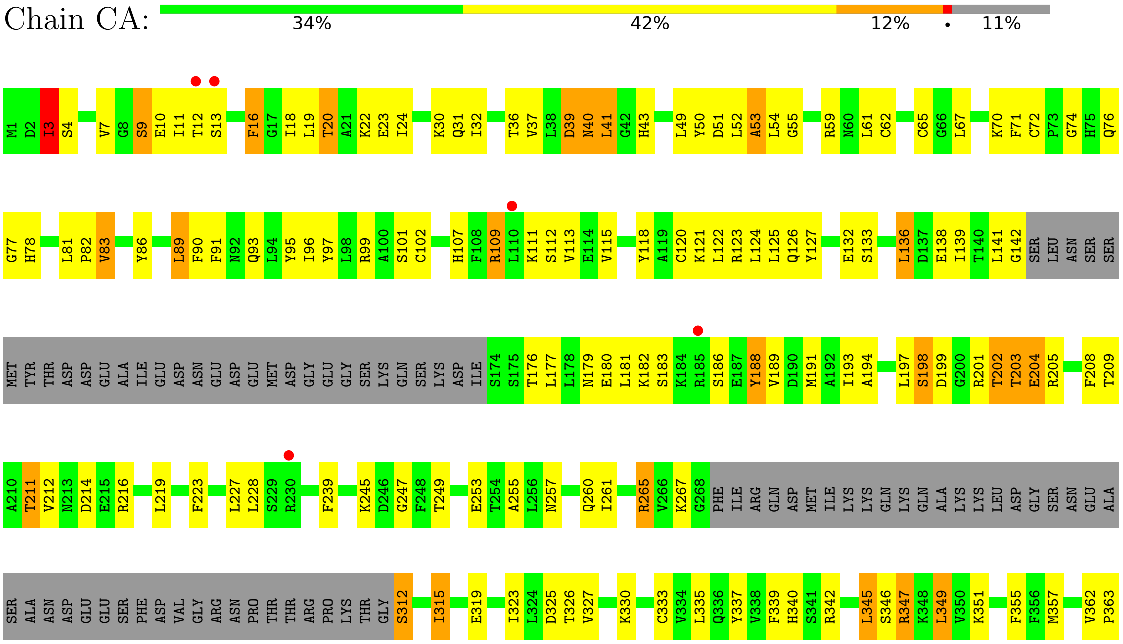

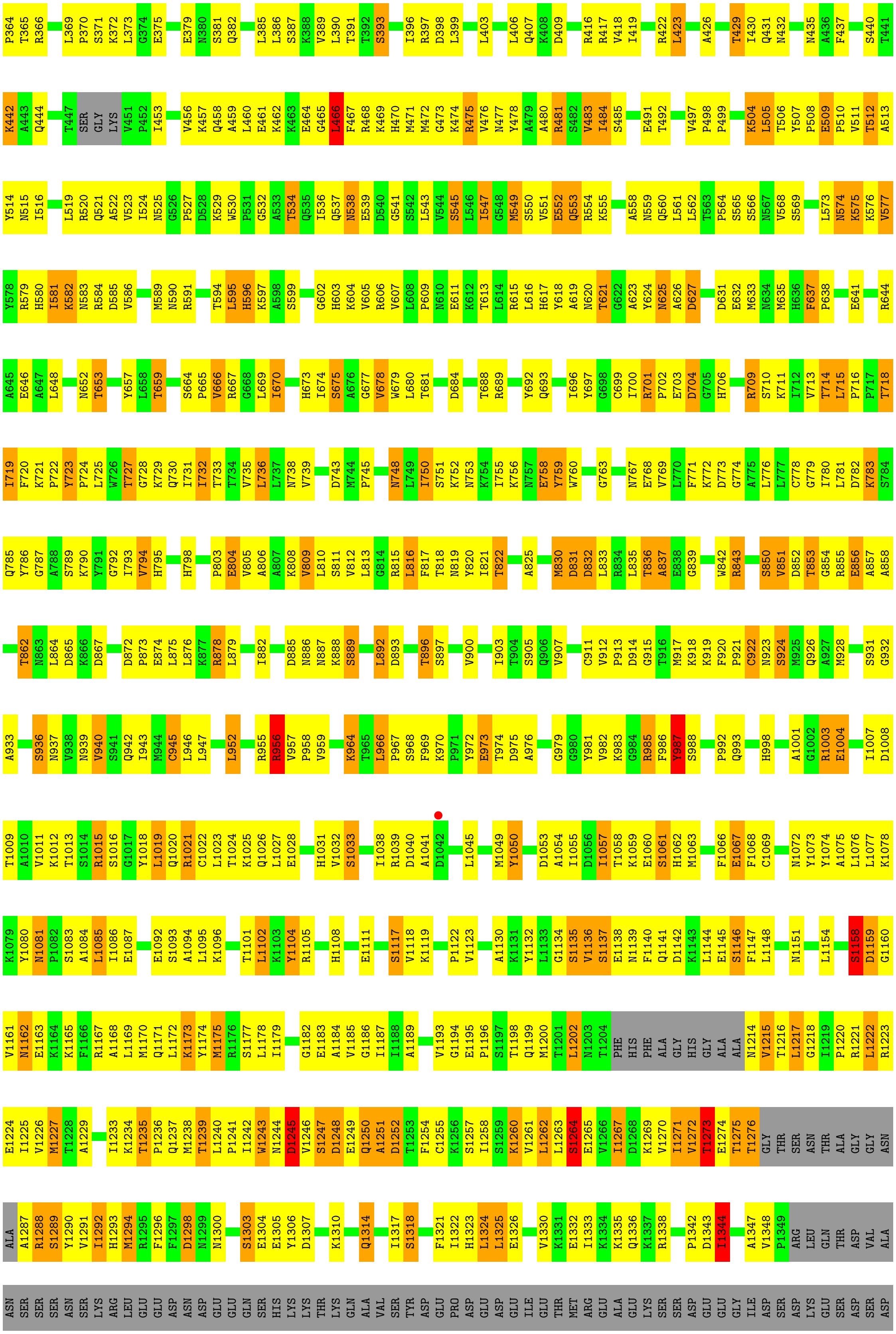
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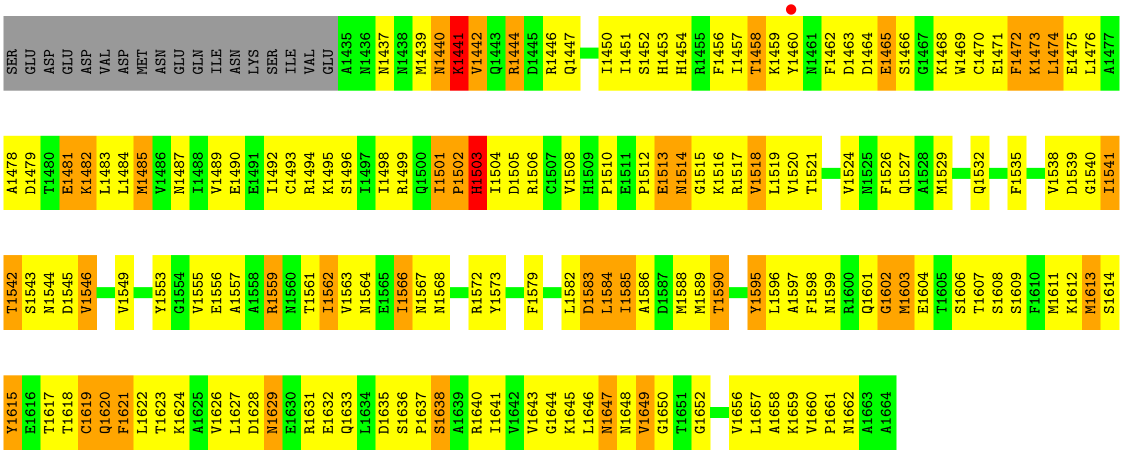

- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

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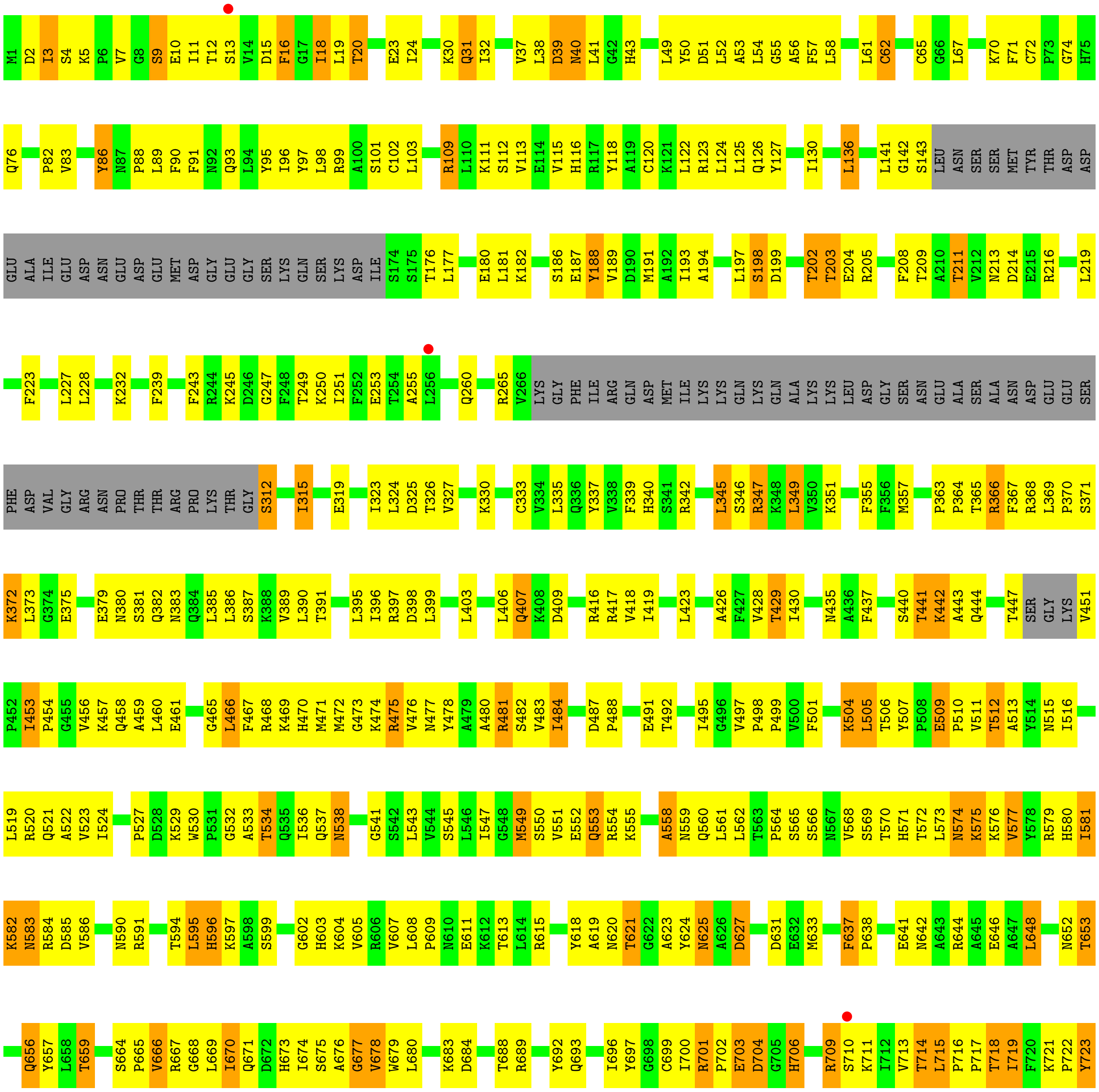

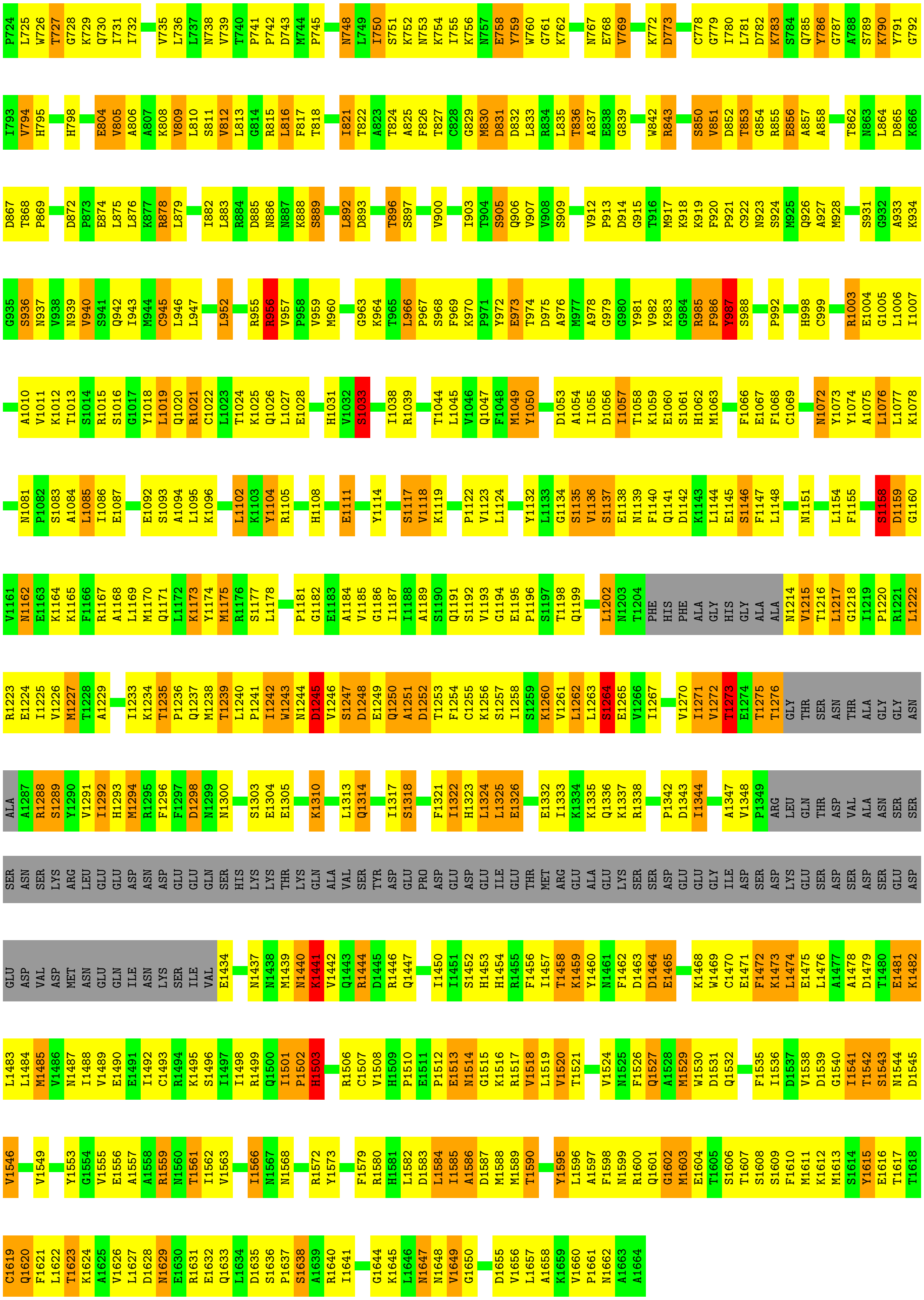

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- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

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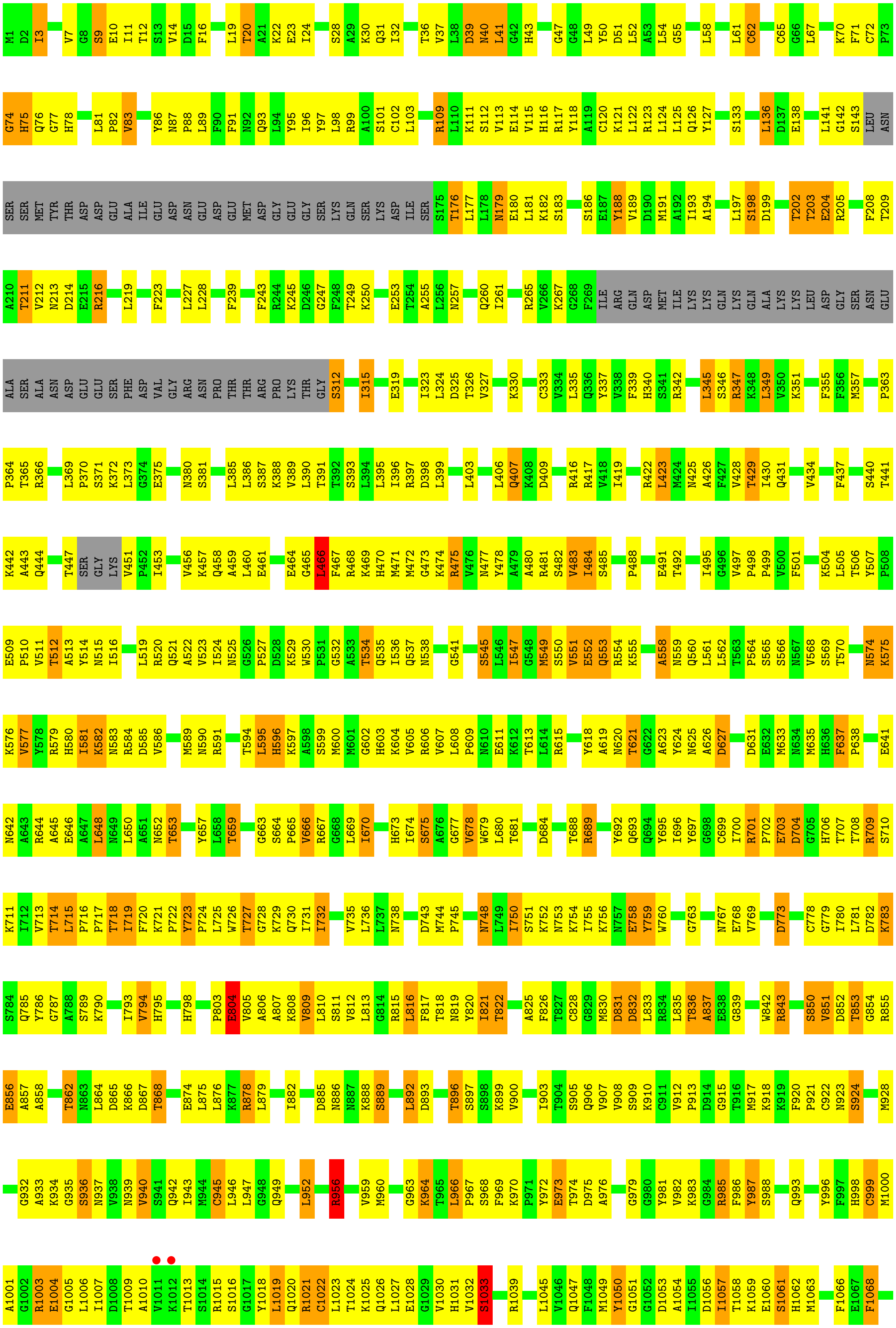
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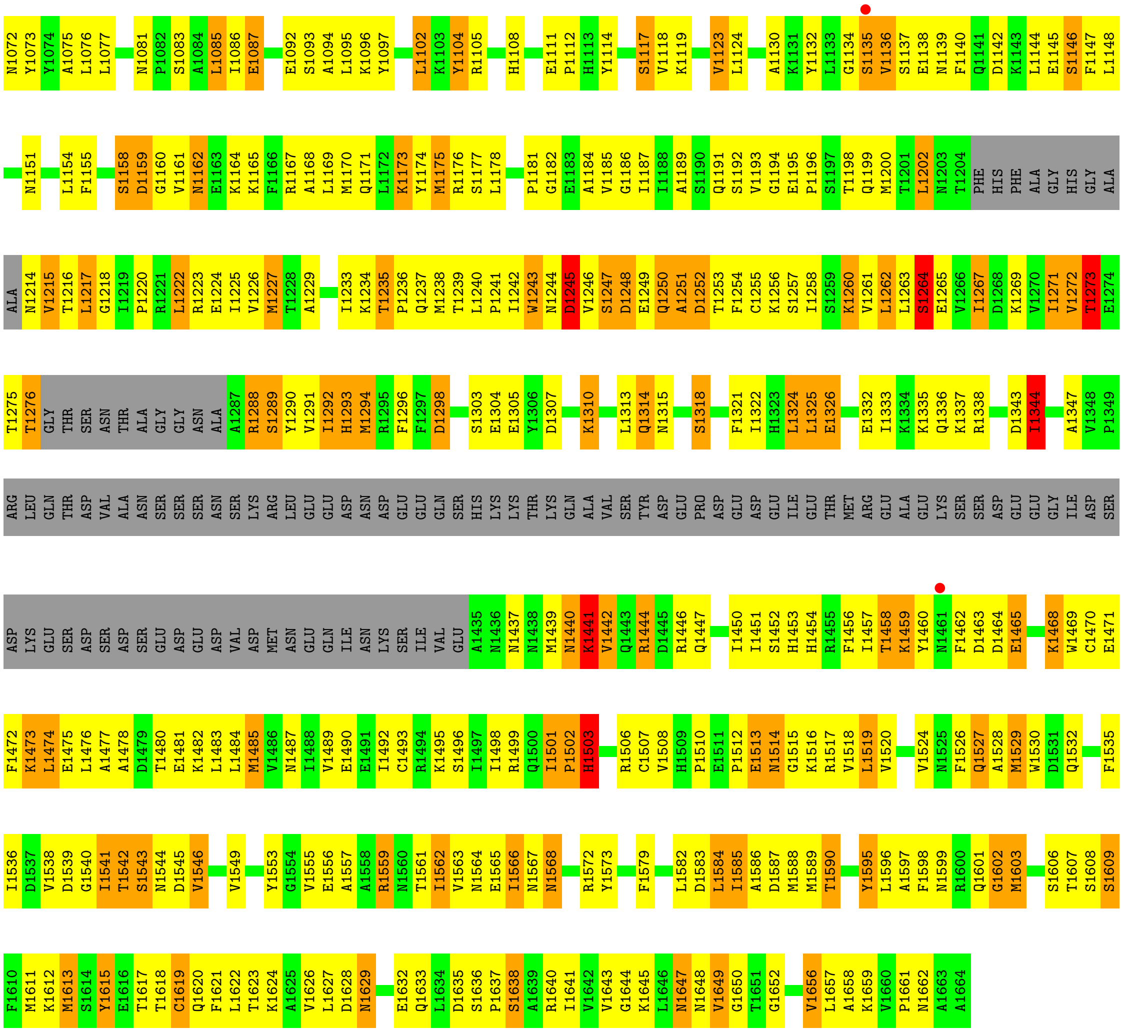

- Molecule 1: DNA-directed RNA polymerase I subunit RPA190

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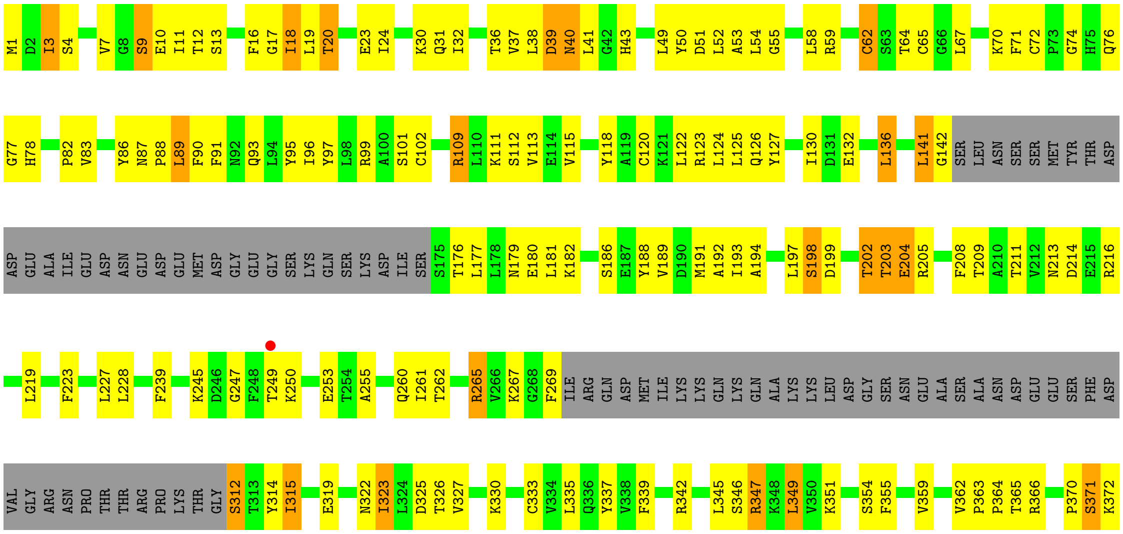

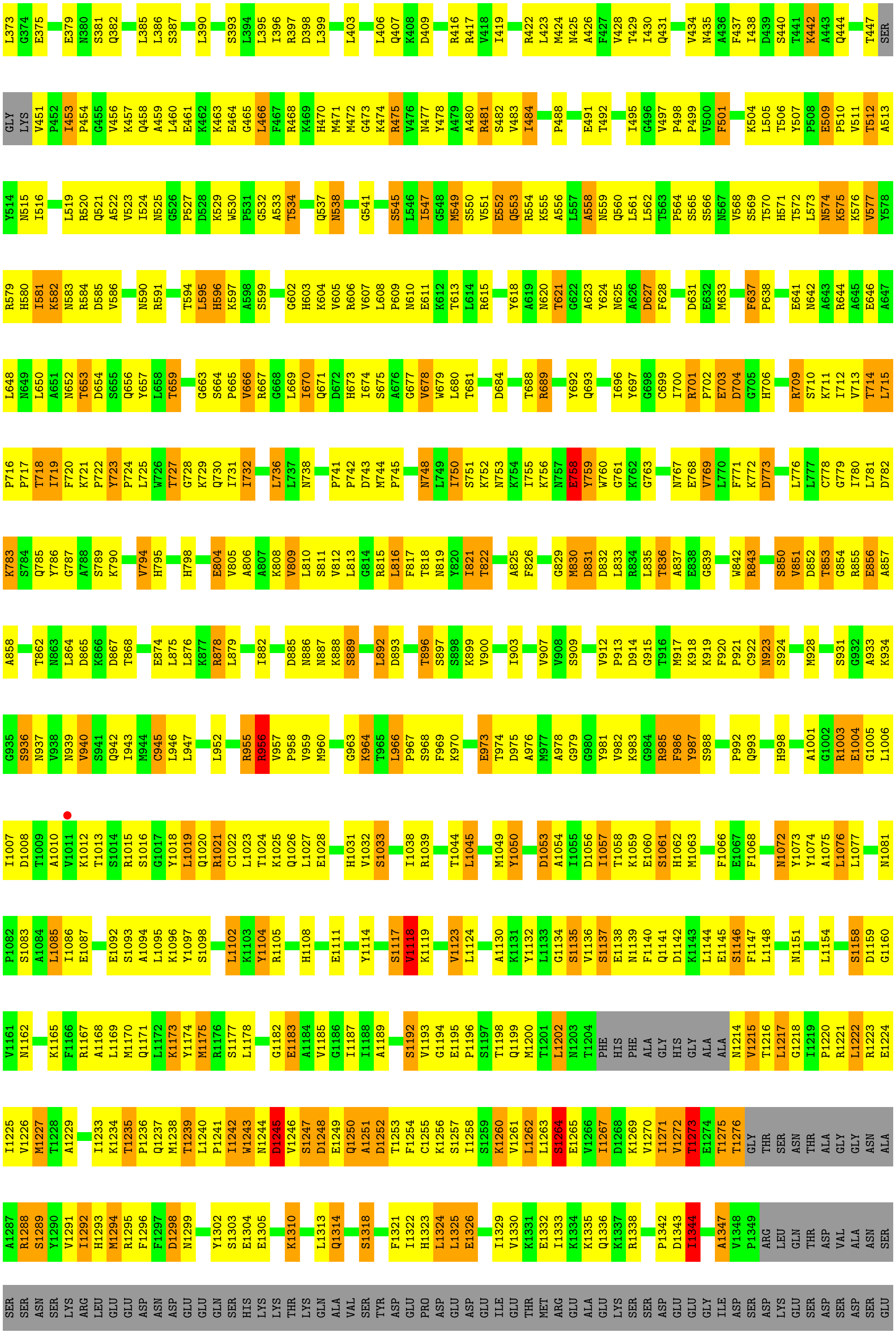
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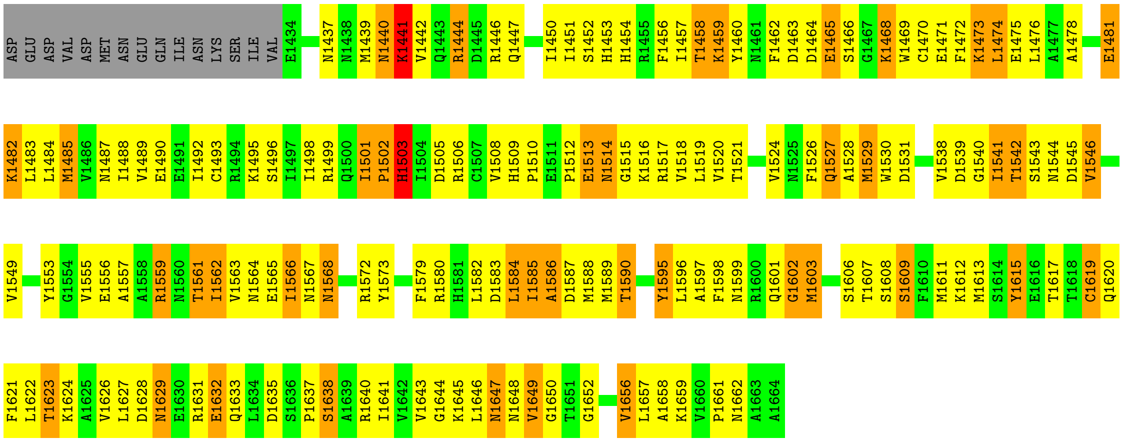
SER SER ASN SER LYS ARG LEU GLU GLU ASP ASN ASP GLU GLN SER HIS LYS LYS THR LYS GLN ALA VAL SER TYR ASP GLU PRO ASP GLU ASP GLU ILE GLU THR MET ARG GLU ALA GLU LYS SER SER ASP GLU GLU GLY ILE ASP SER ASP LYS GLU SER ASP SER ASP SER GLU



- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

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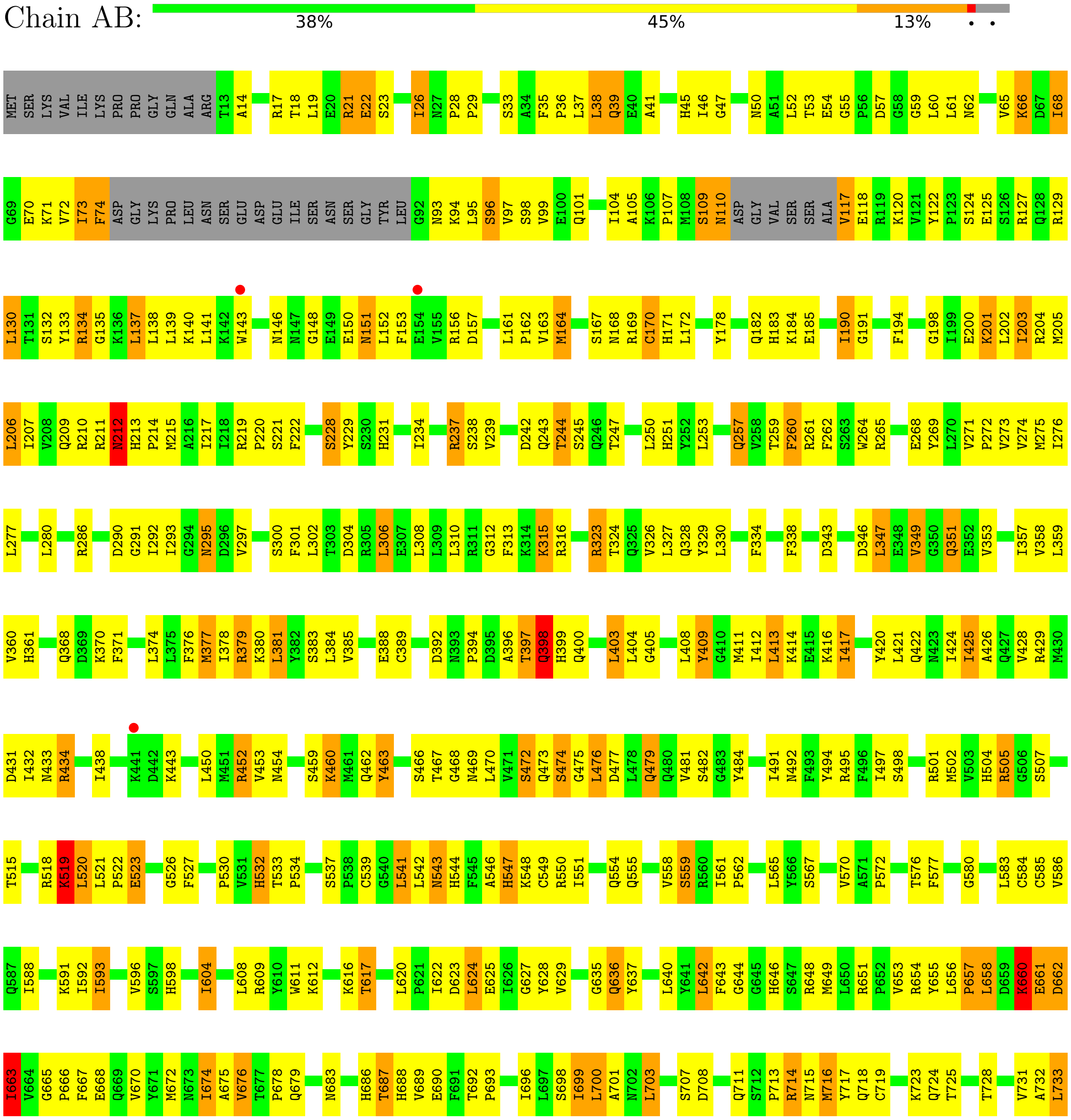

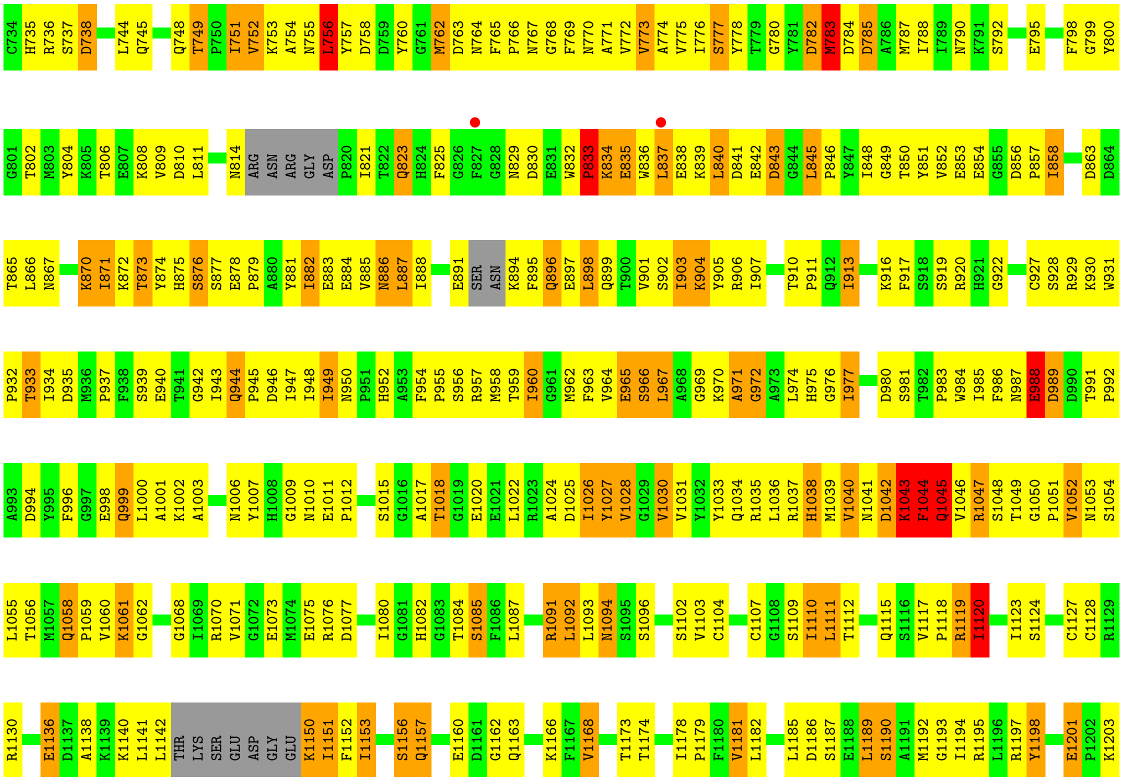

- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

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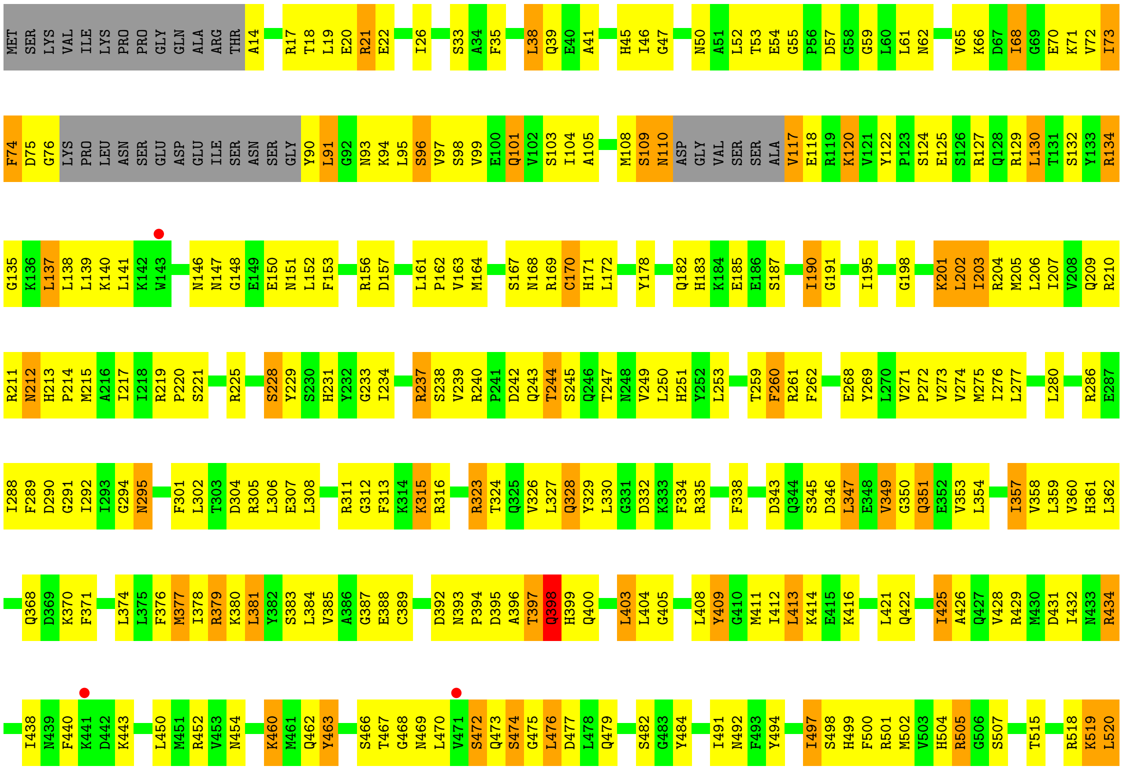
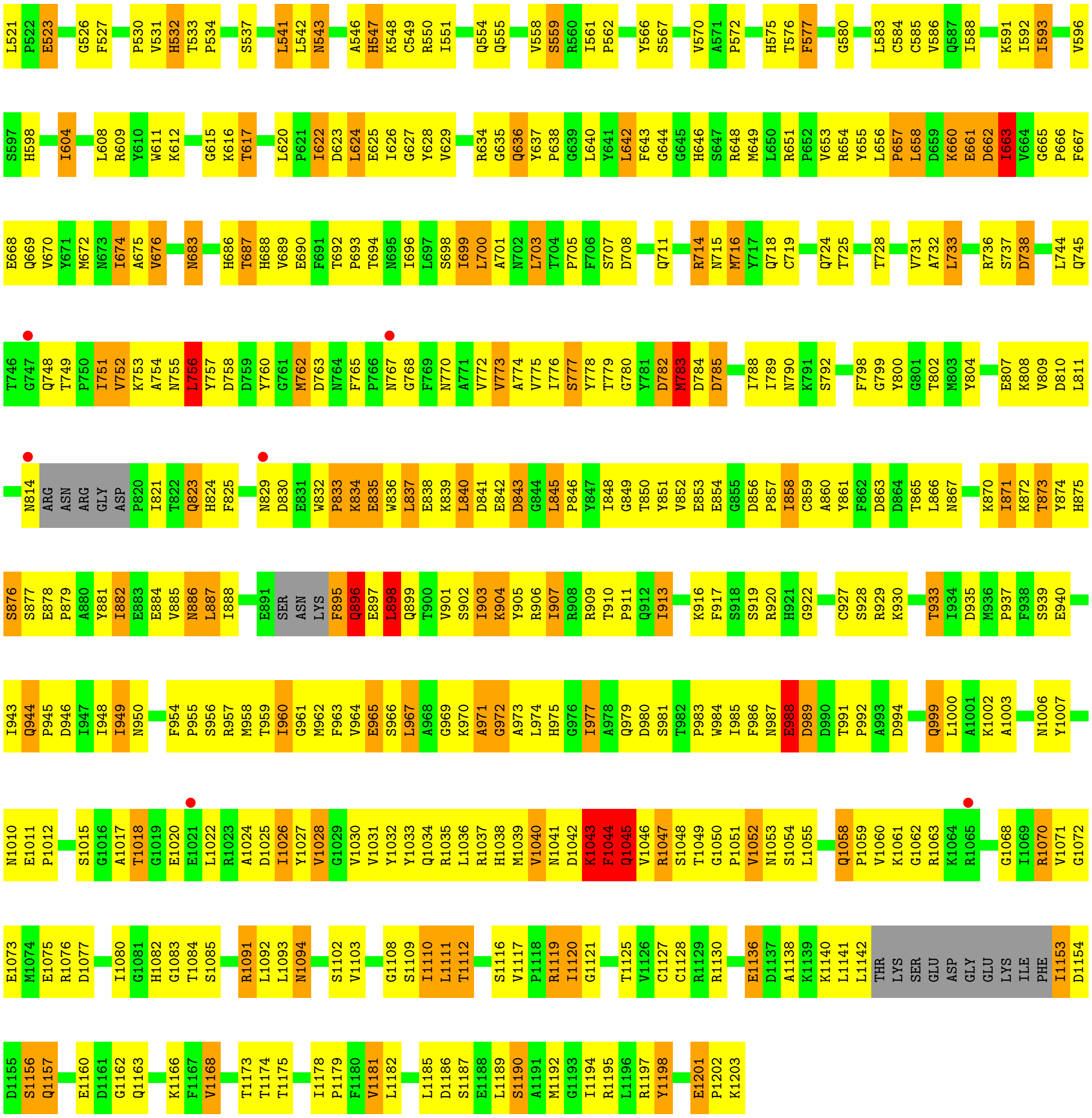
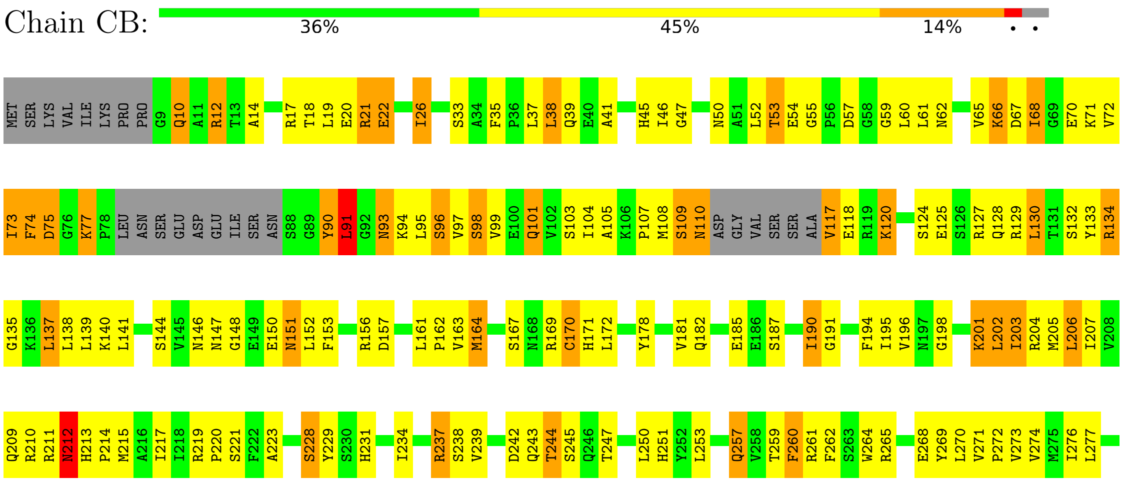
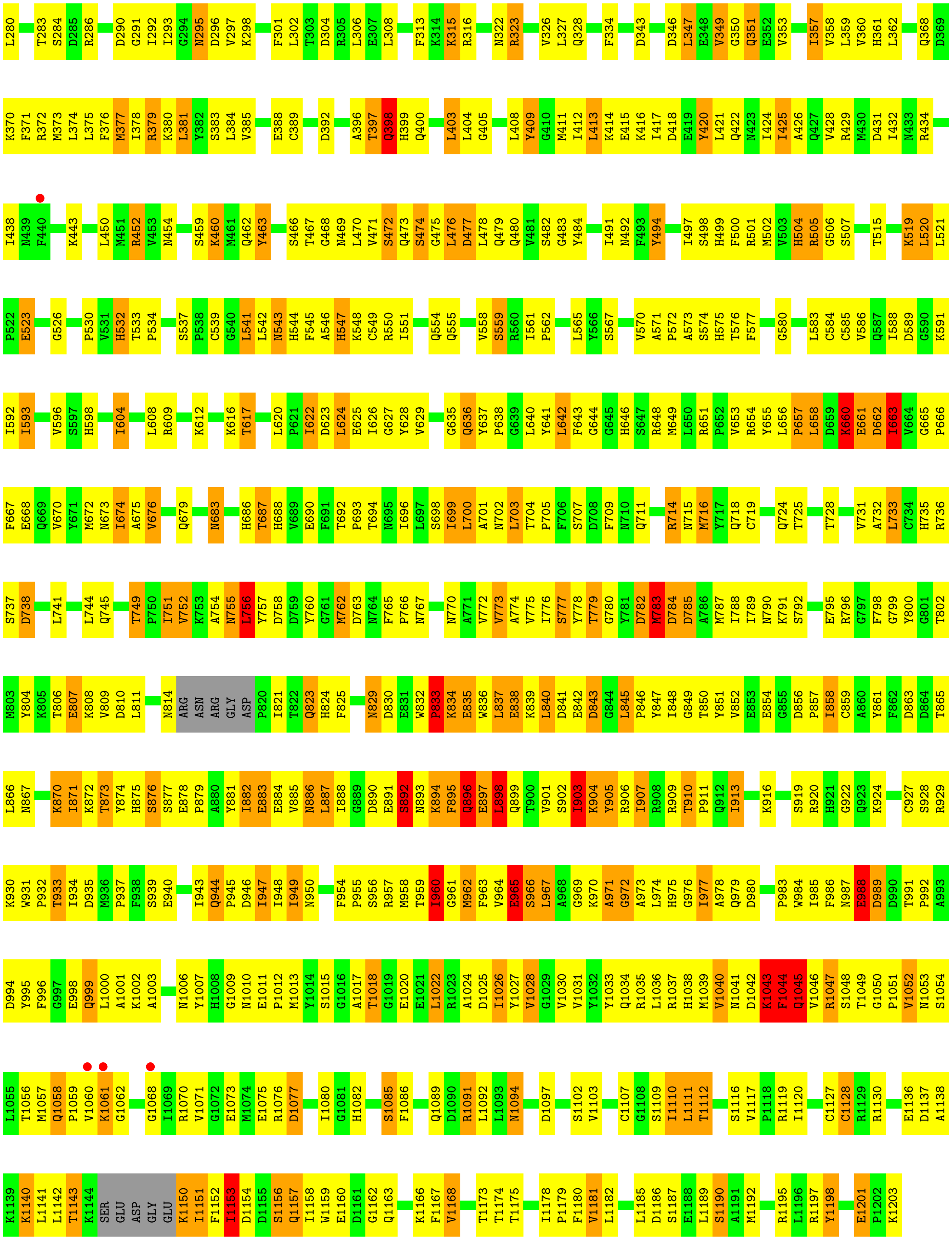




- Molecule 2: DNA-directed RNA polymerase I subunit RPA135





- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

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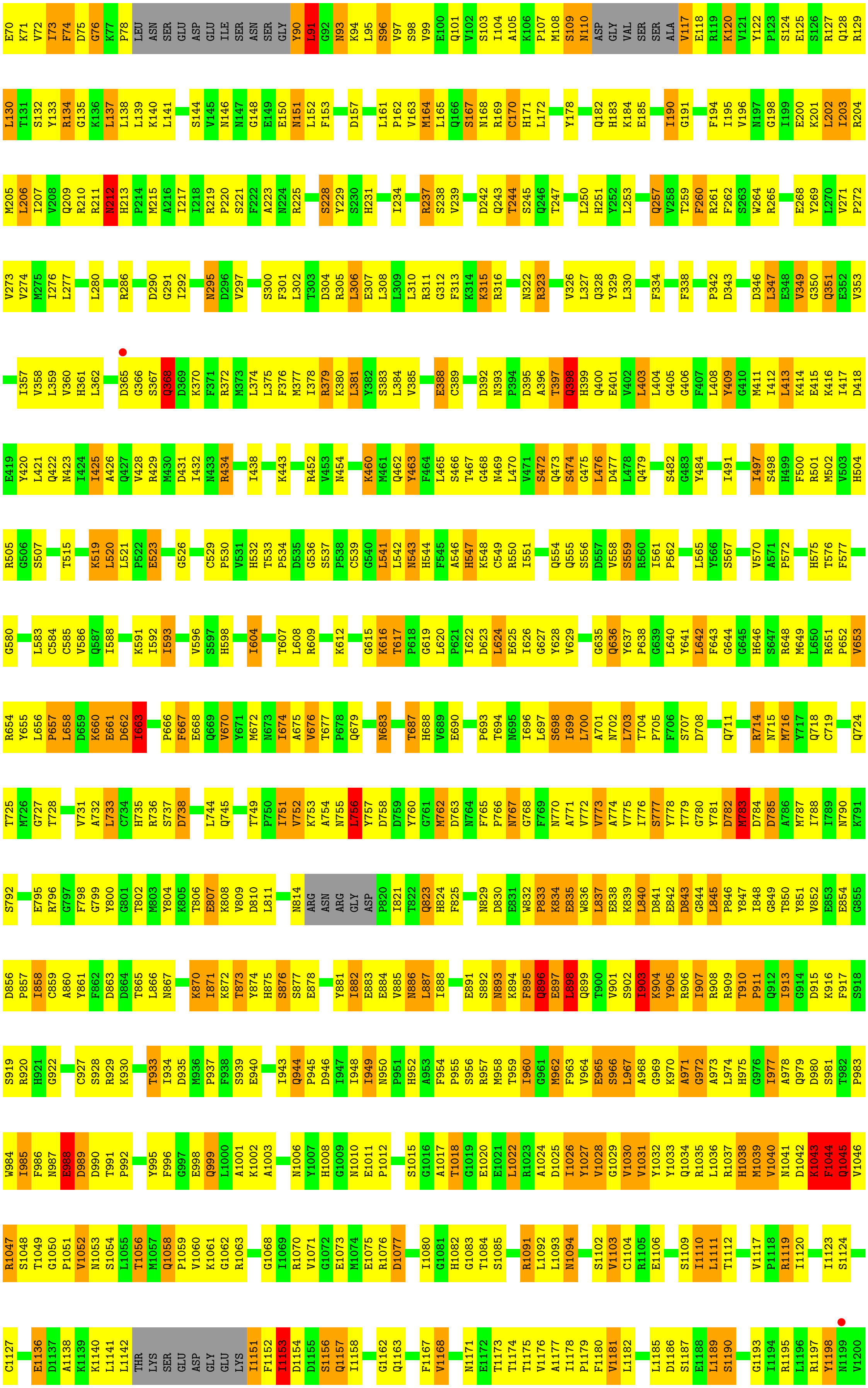
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- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

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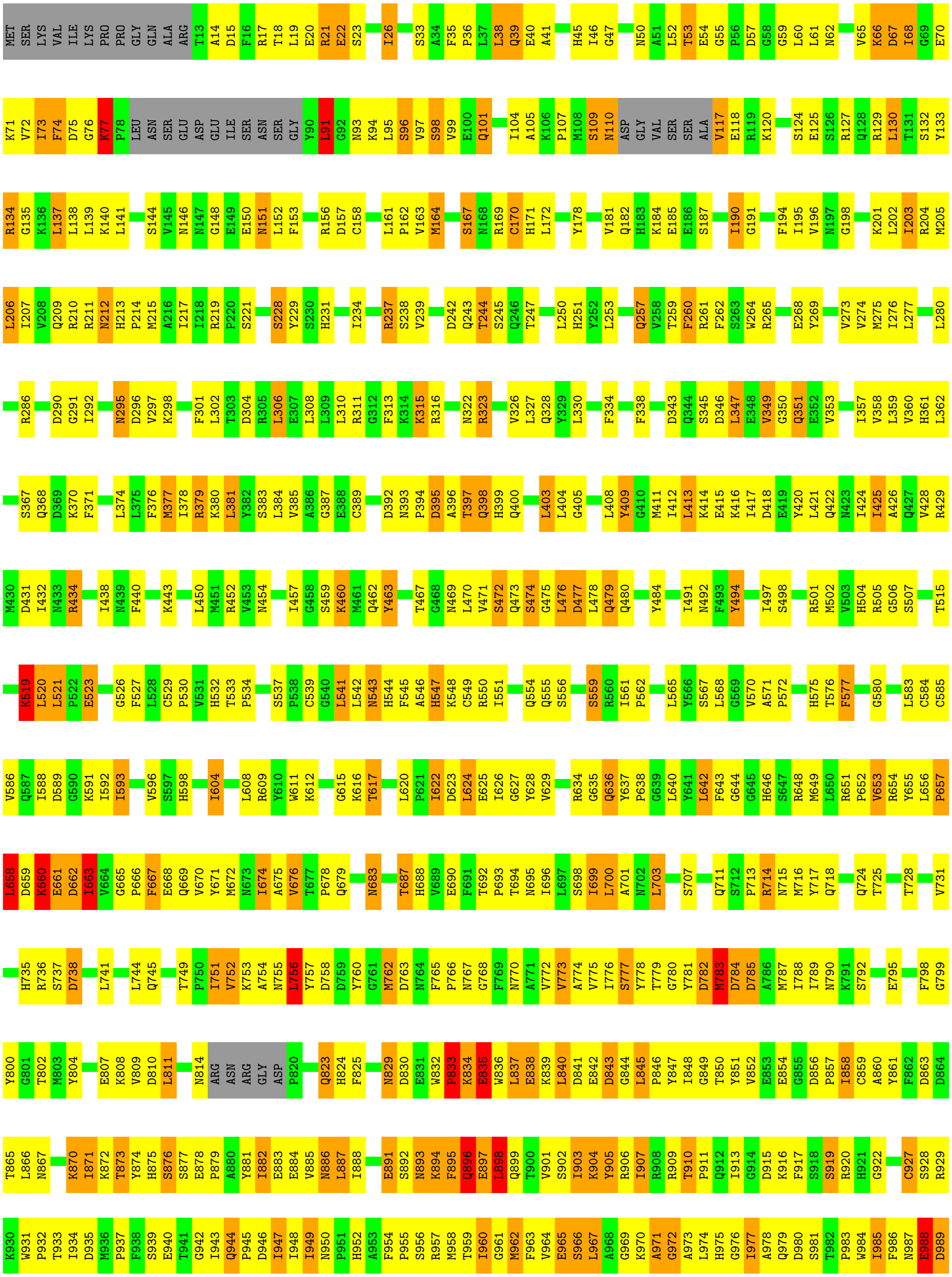

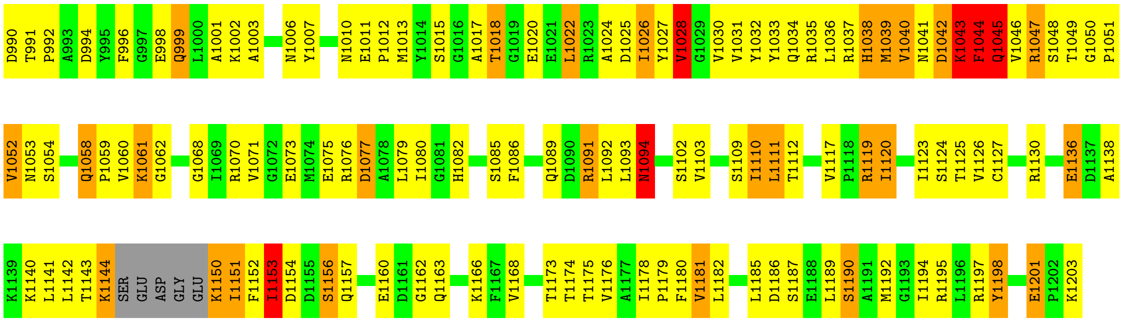

- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

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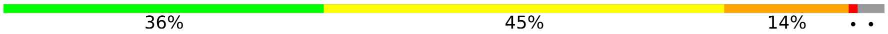

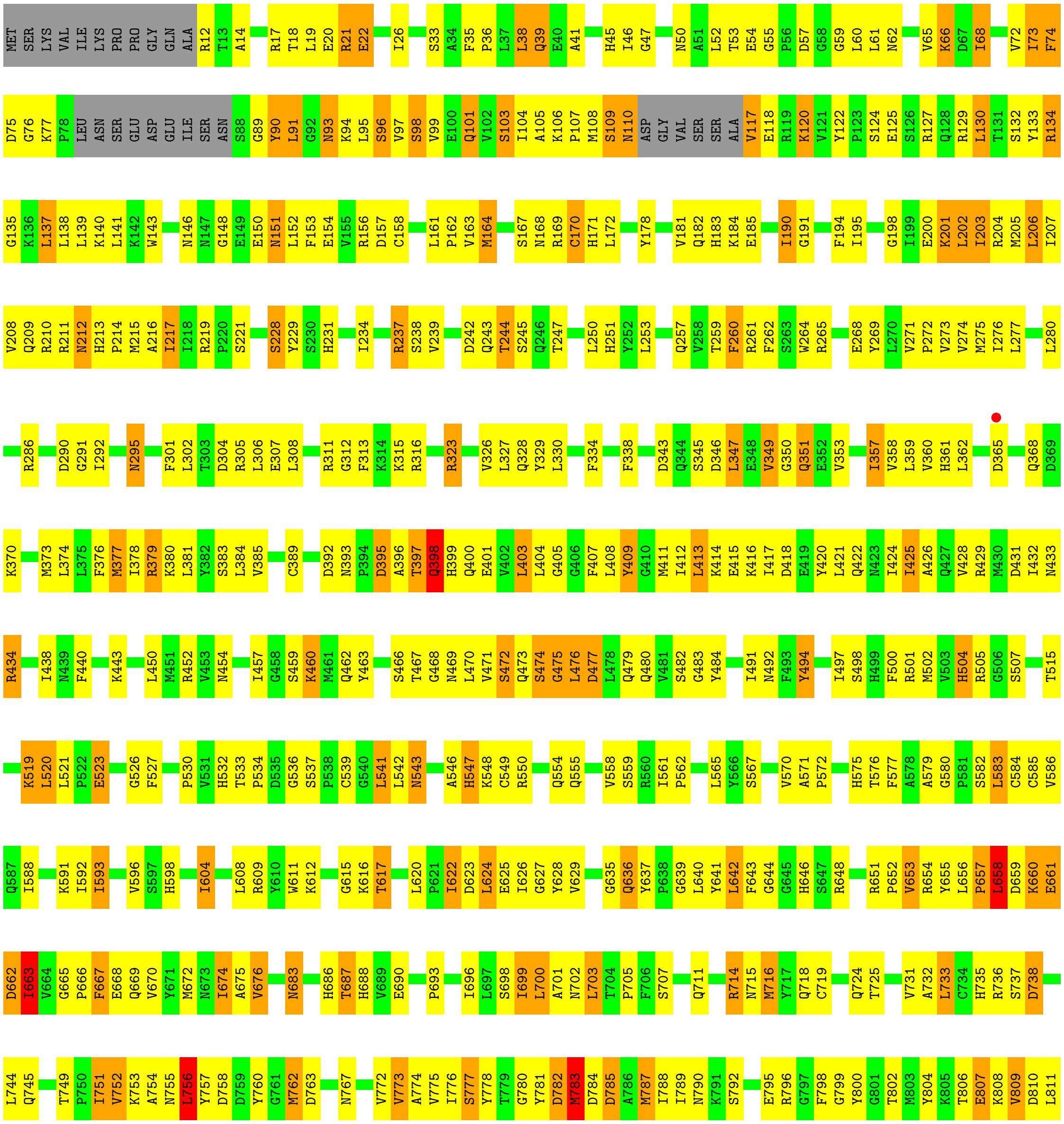

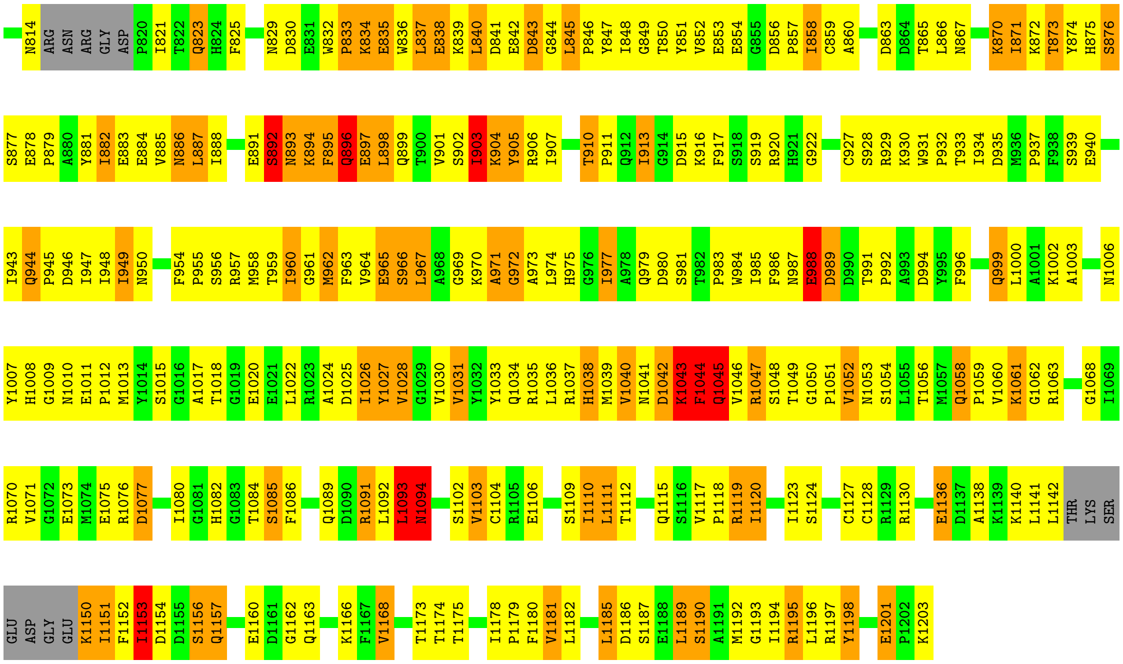

- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

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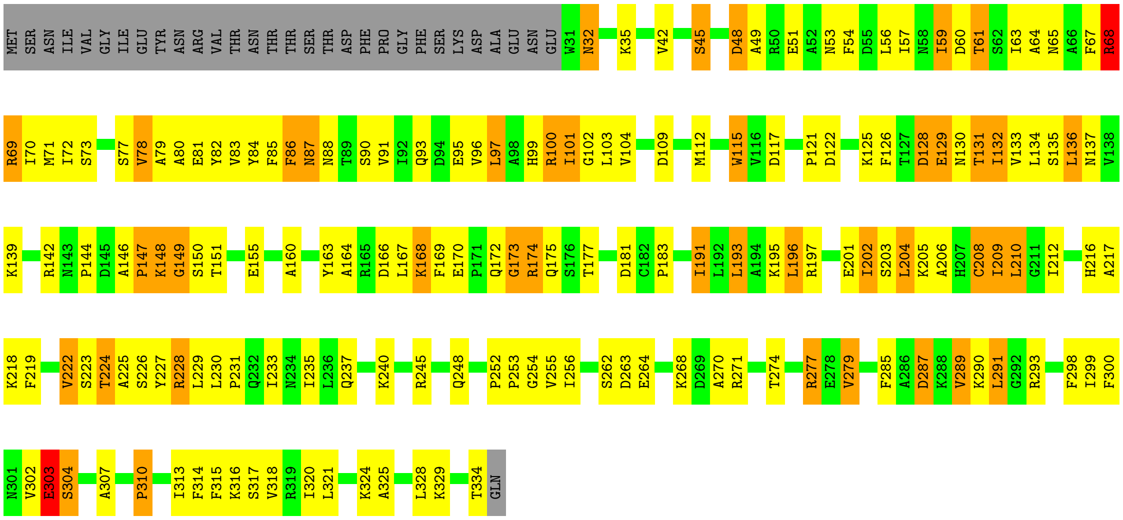

- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

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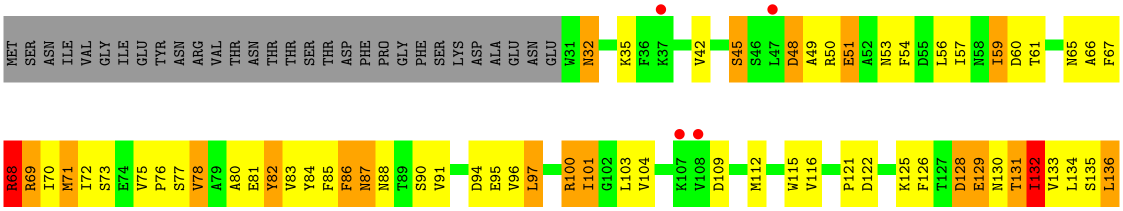

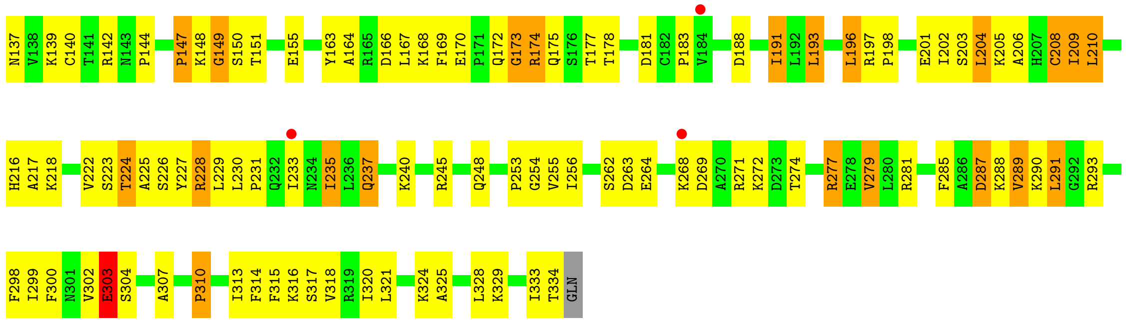

- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

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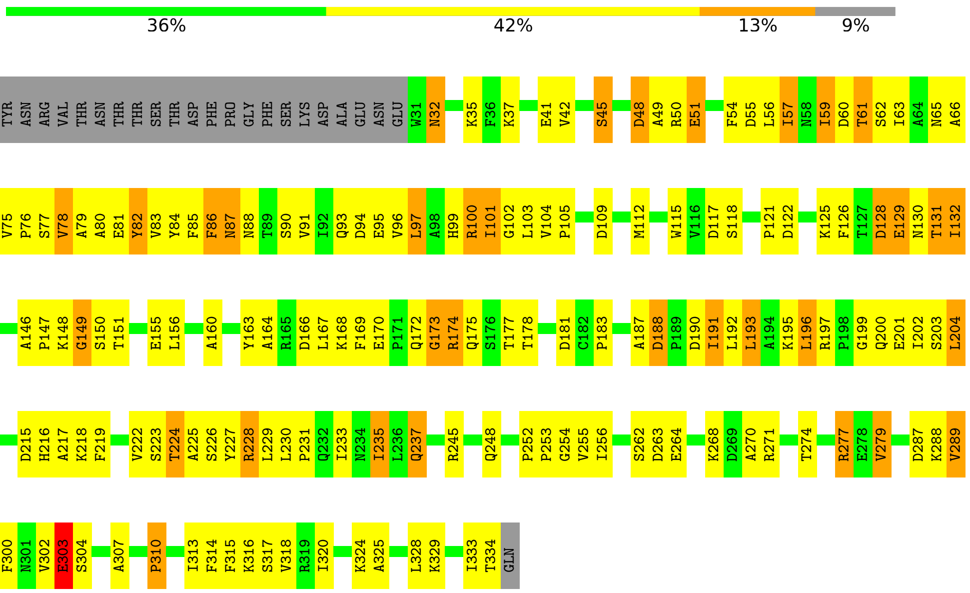

- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

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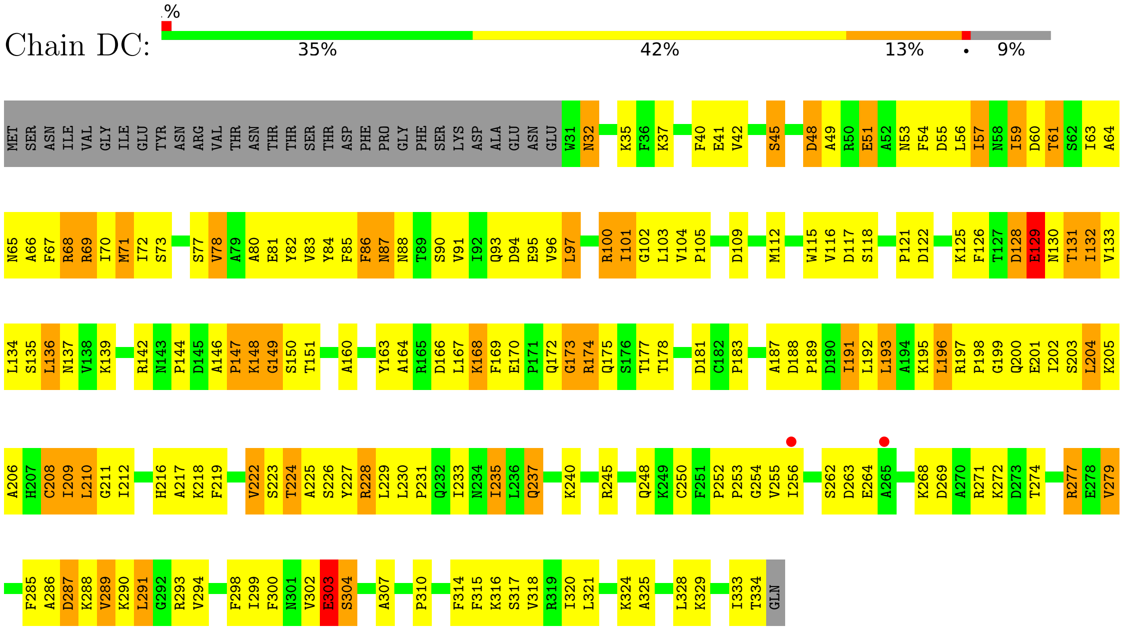
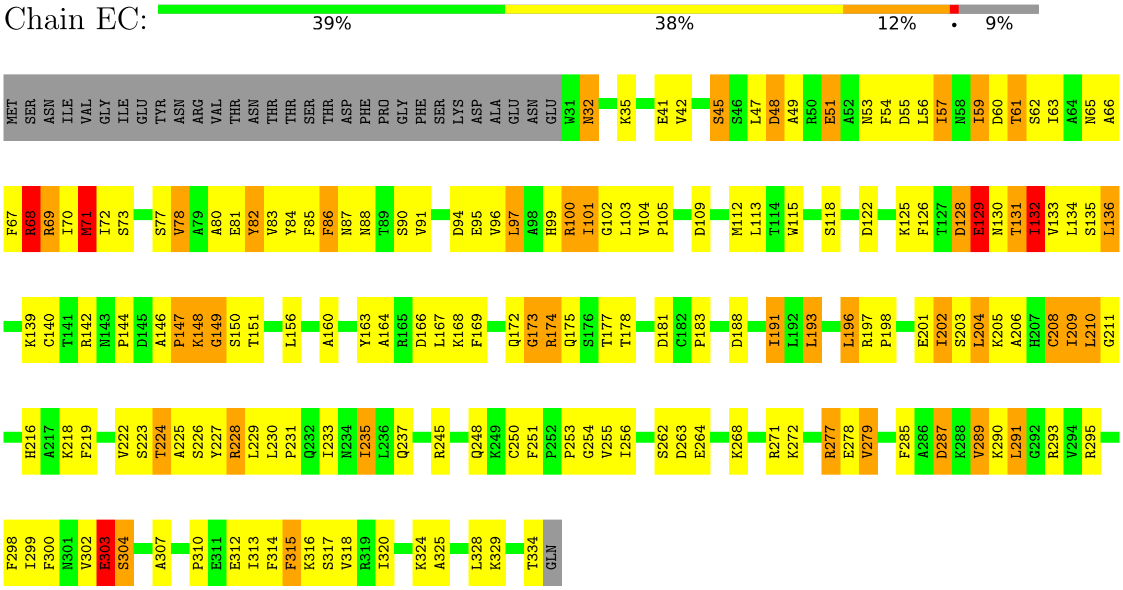
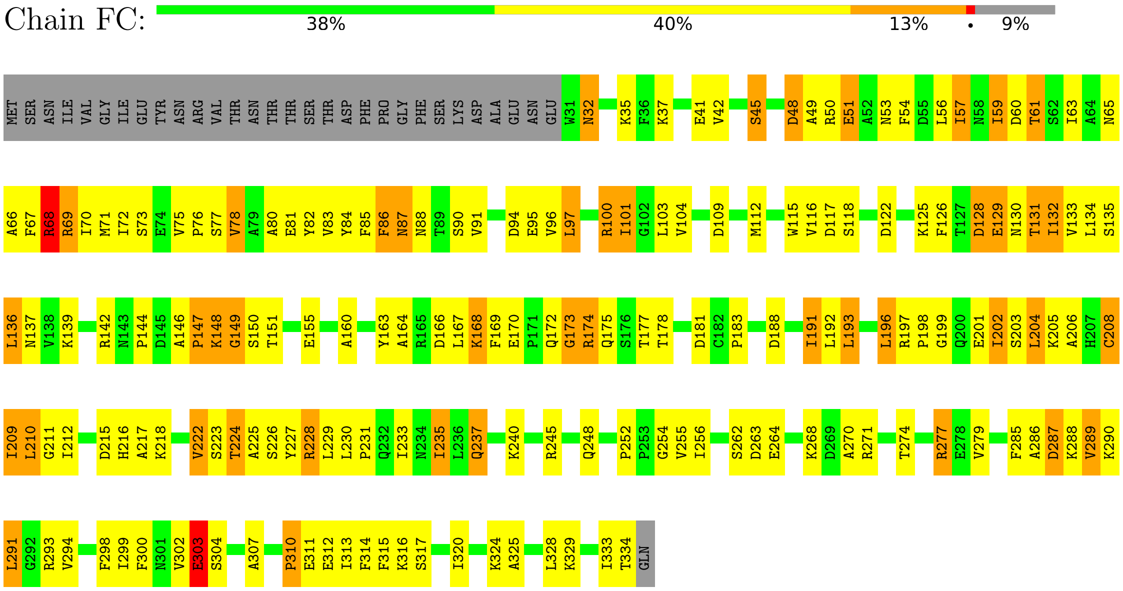


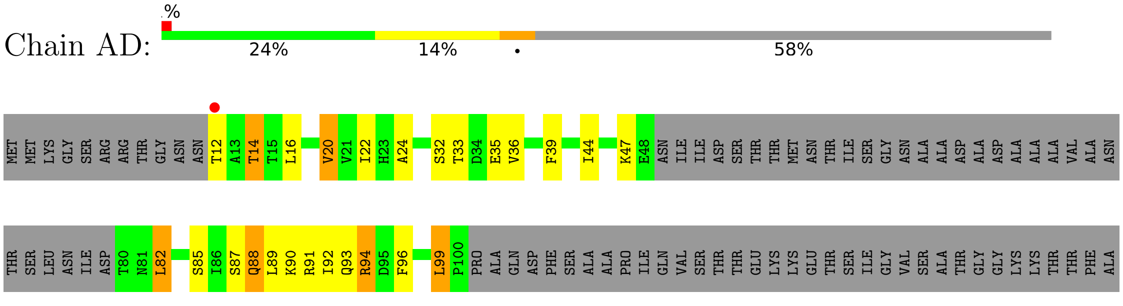
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



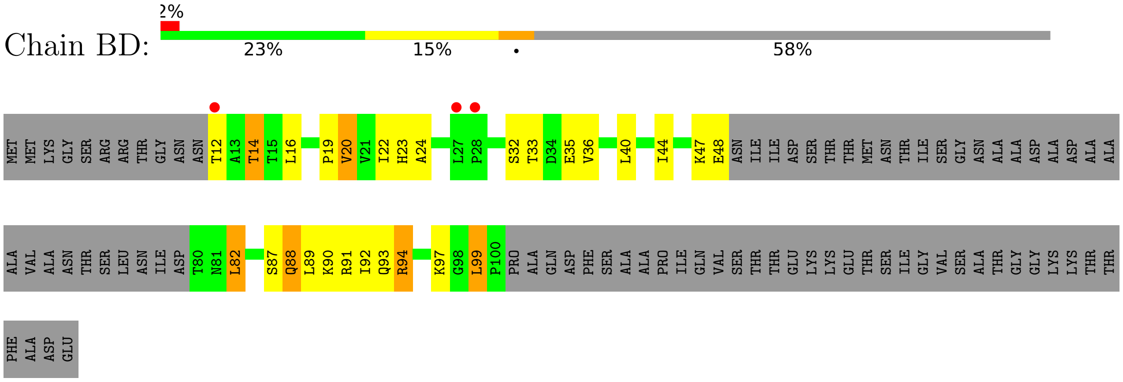
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



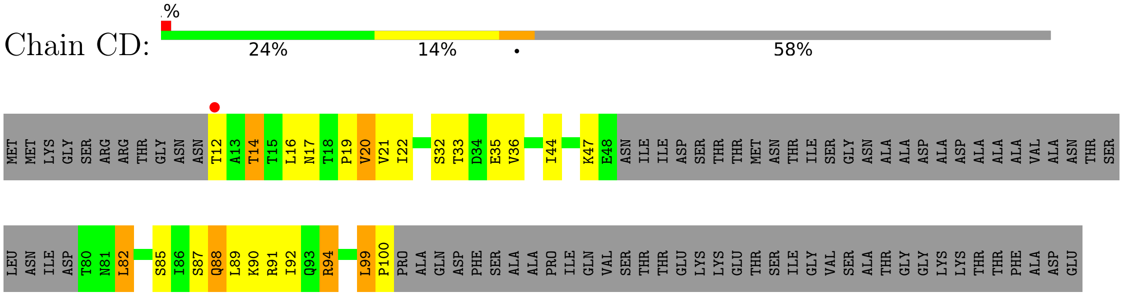
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



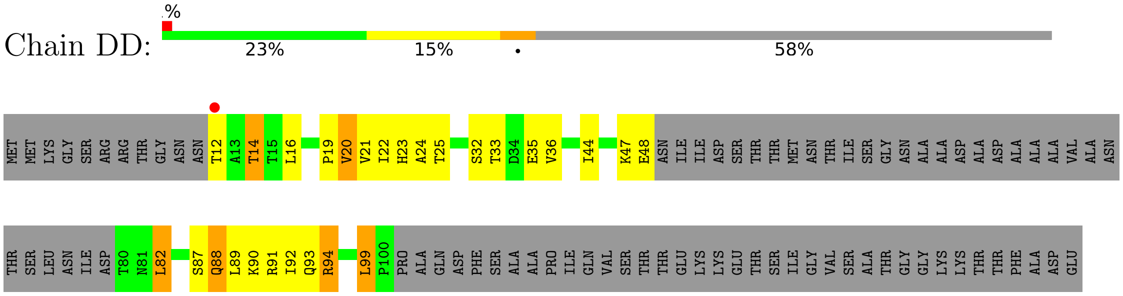
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

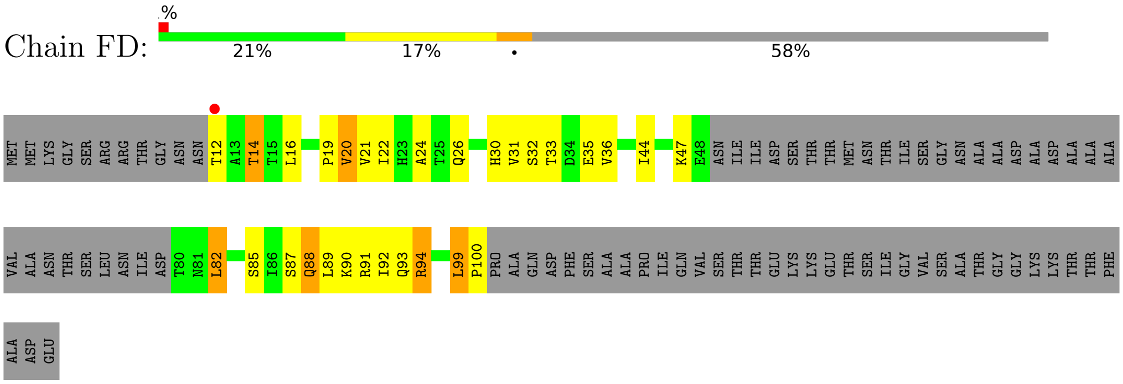


- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

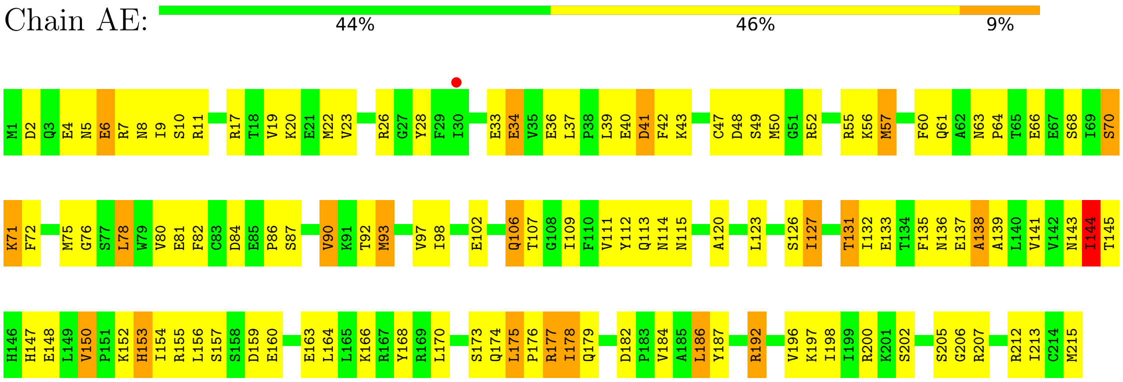


- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

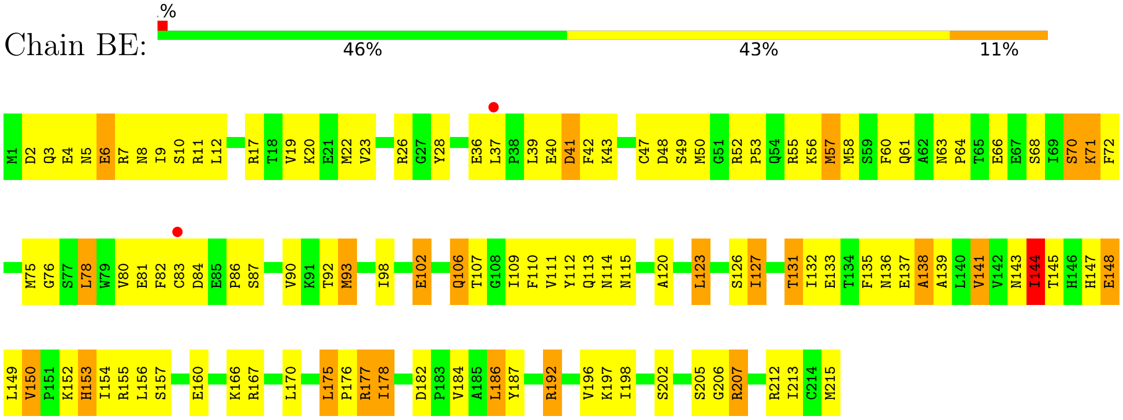
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



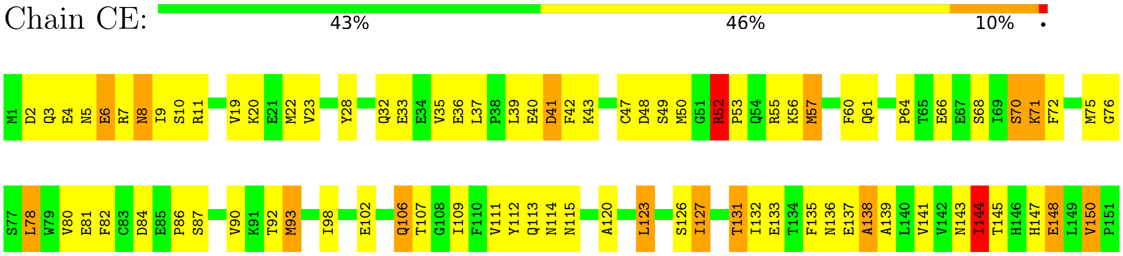
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

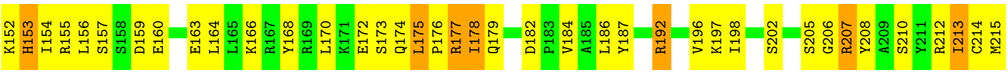


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

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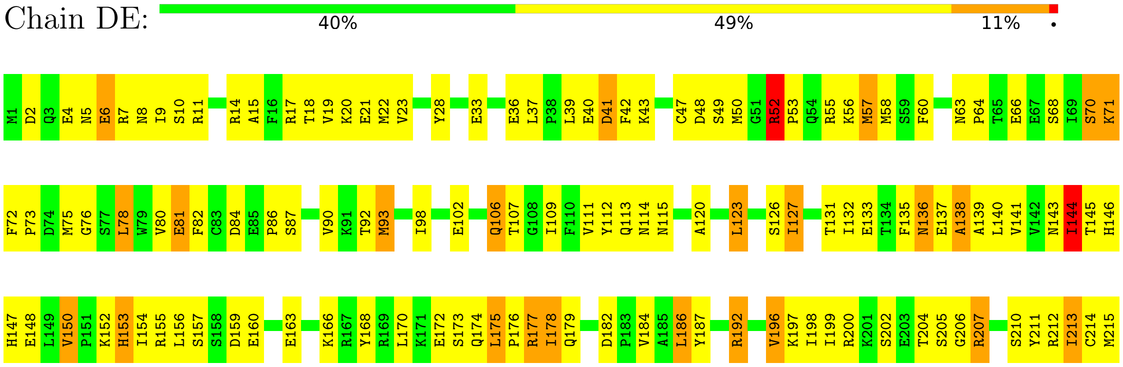

- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

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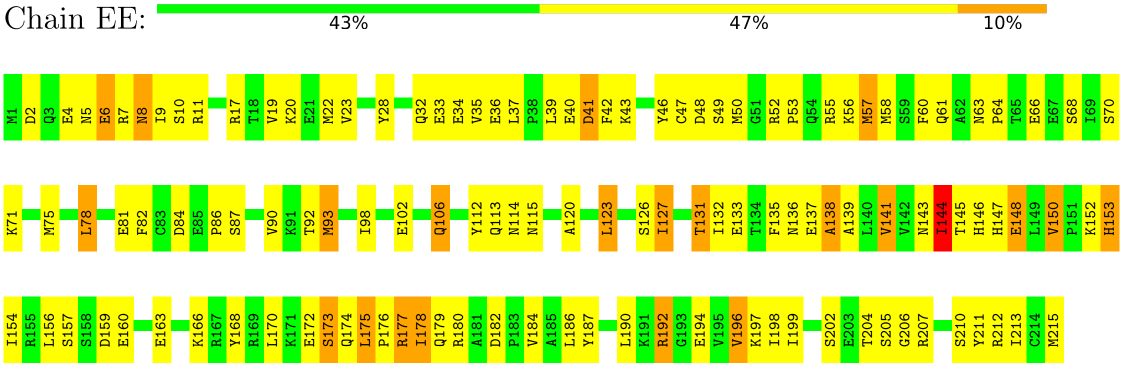

- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

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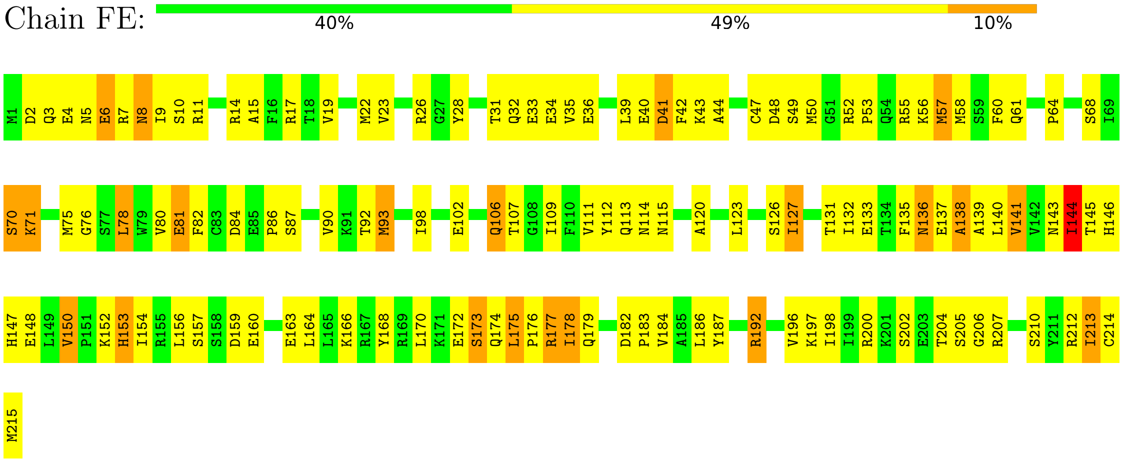

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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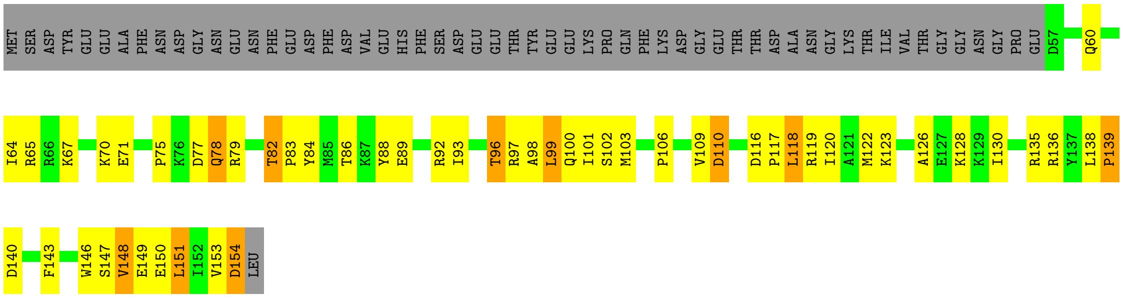

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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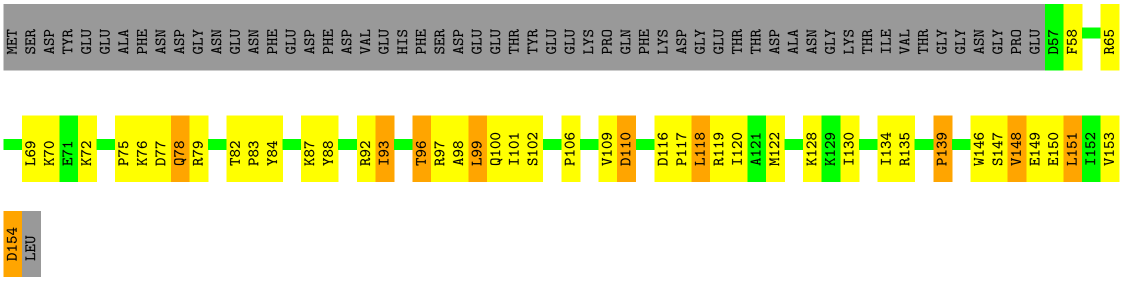

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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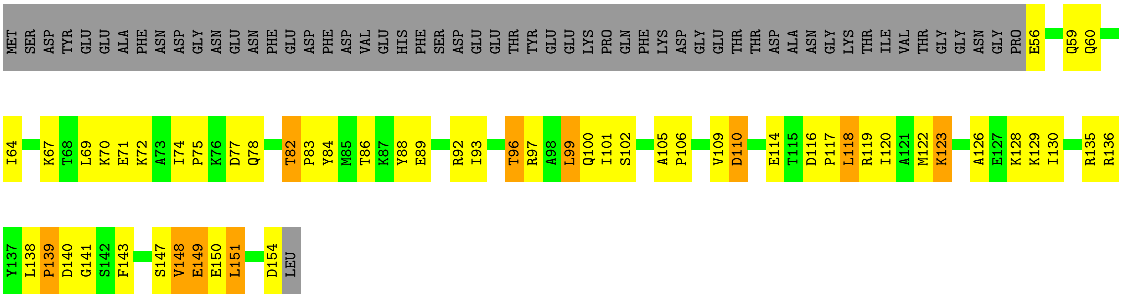

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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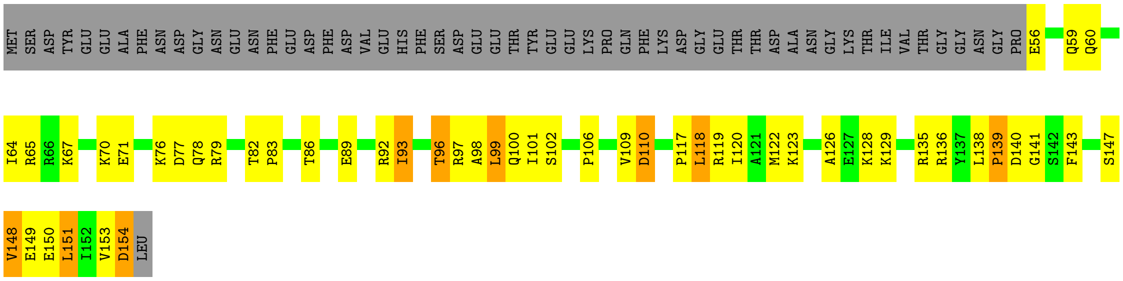

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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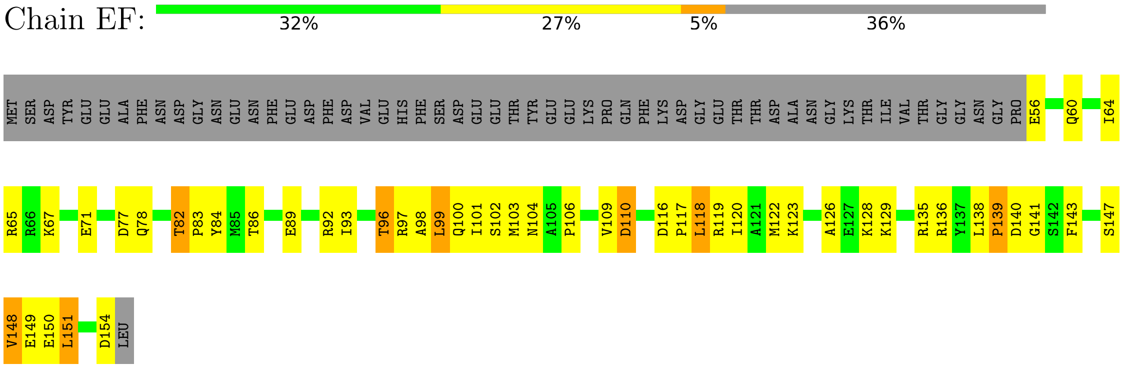

- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

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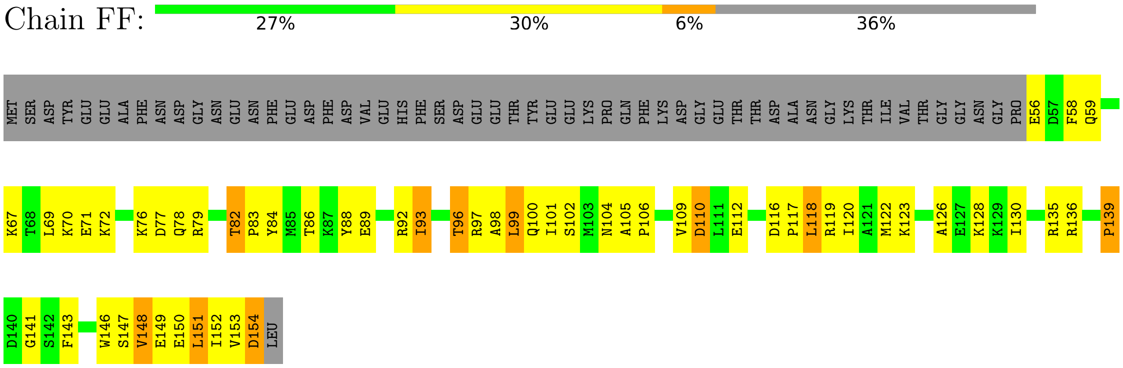

- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

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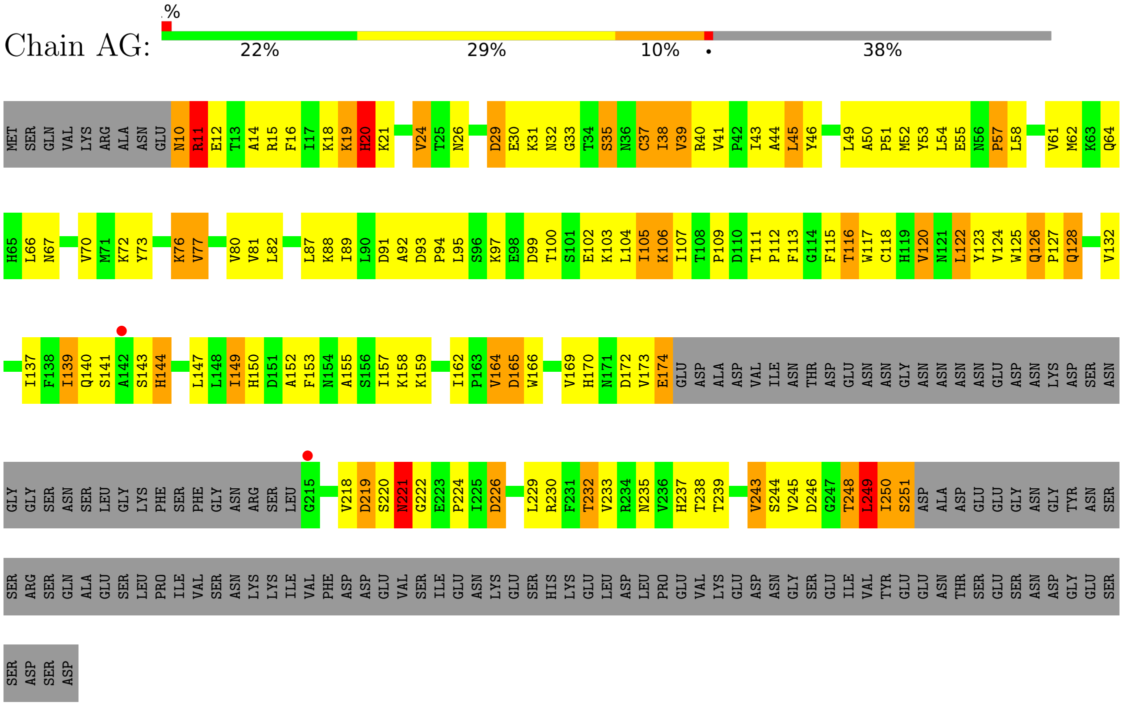

- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

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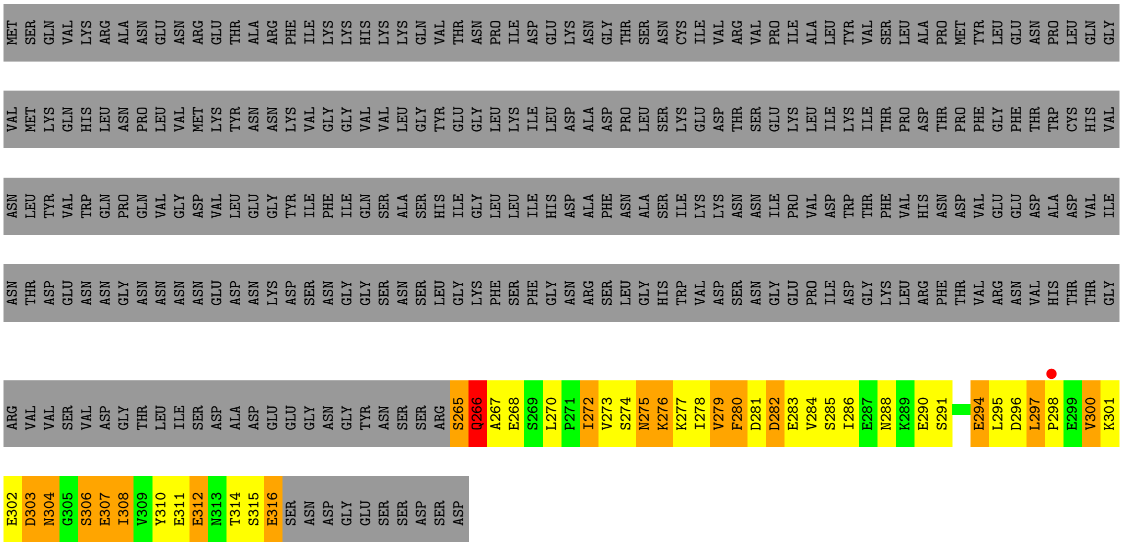

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- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

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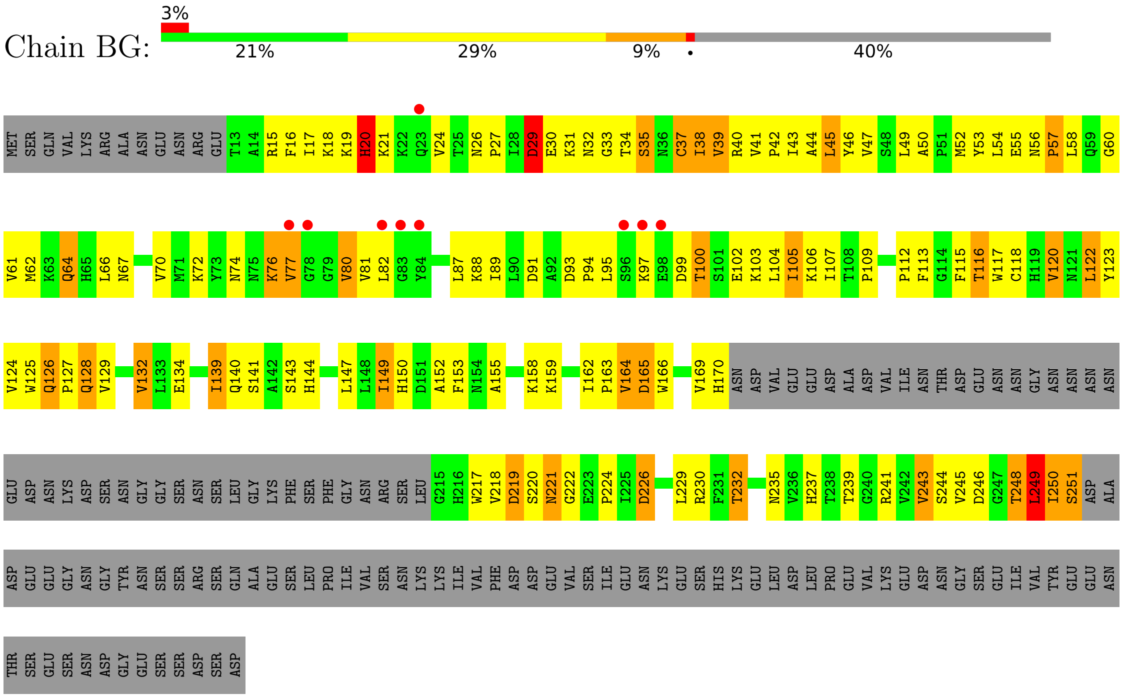

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- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

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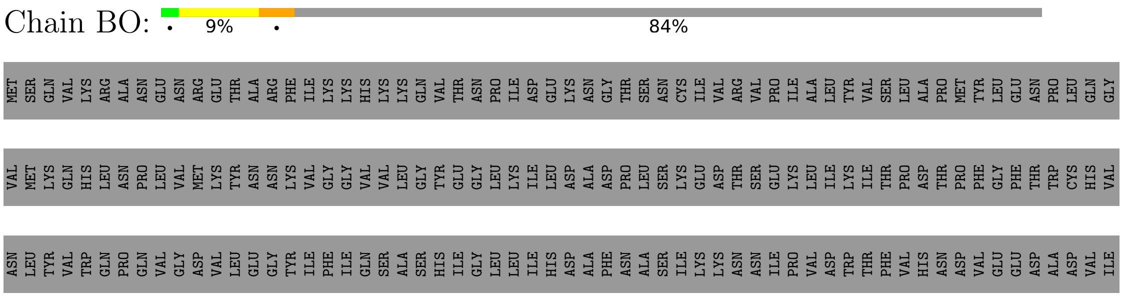

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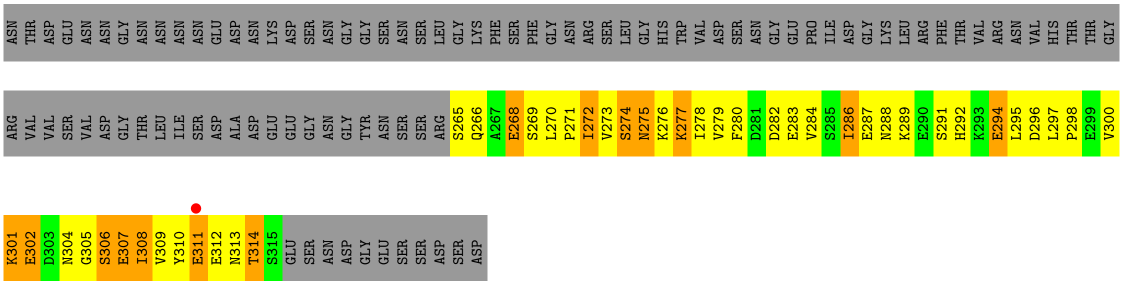

- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

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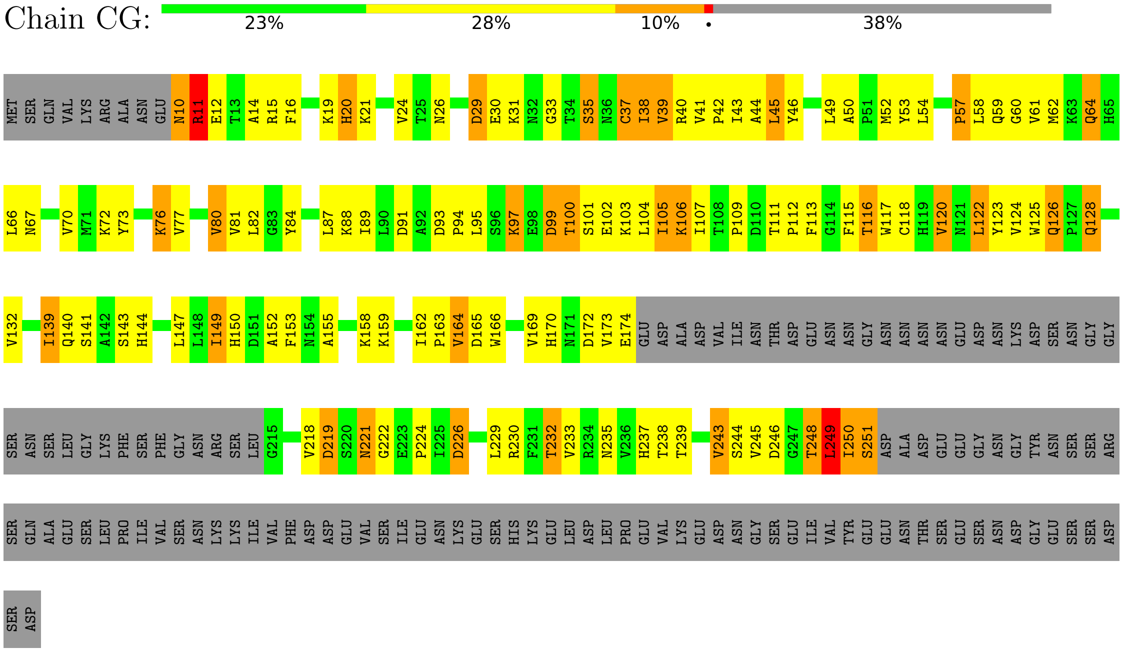

- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

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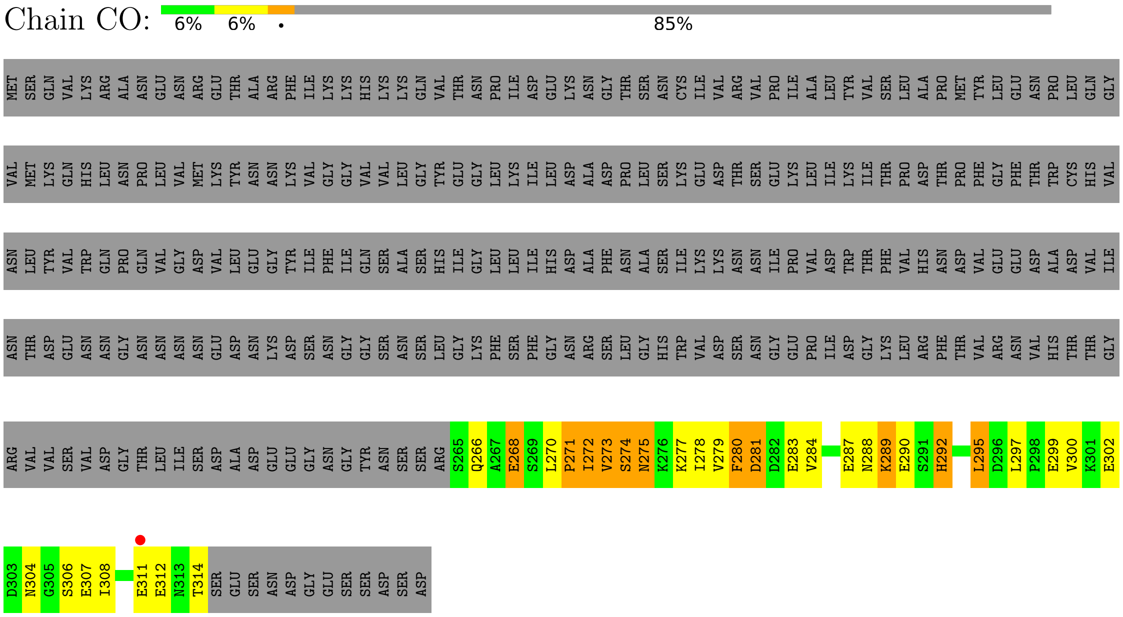
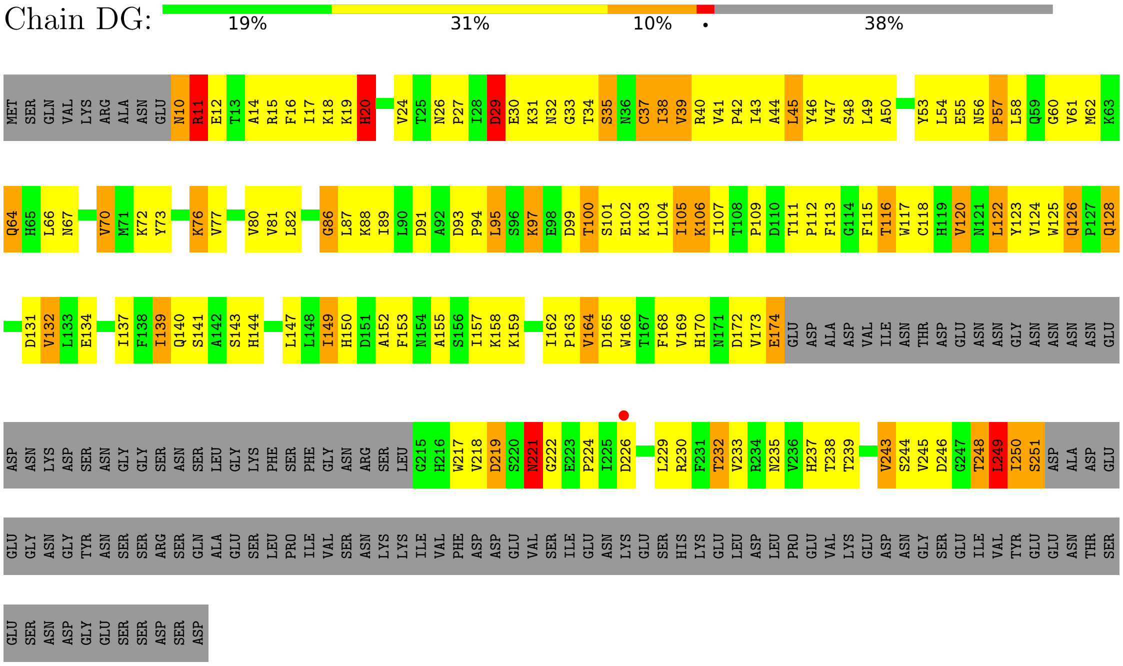
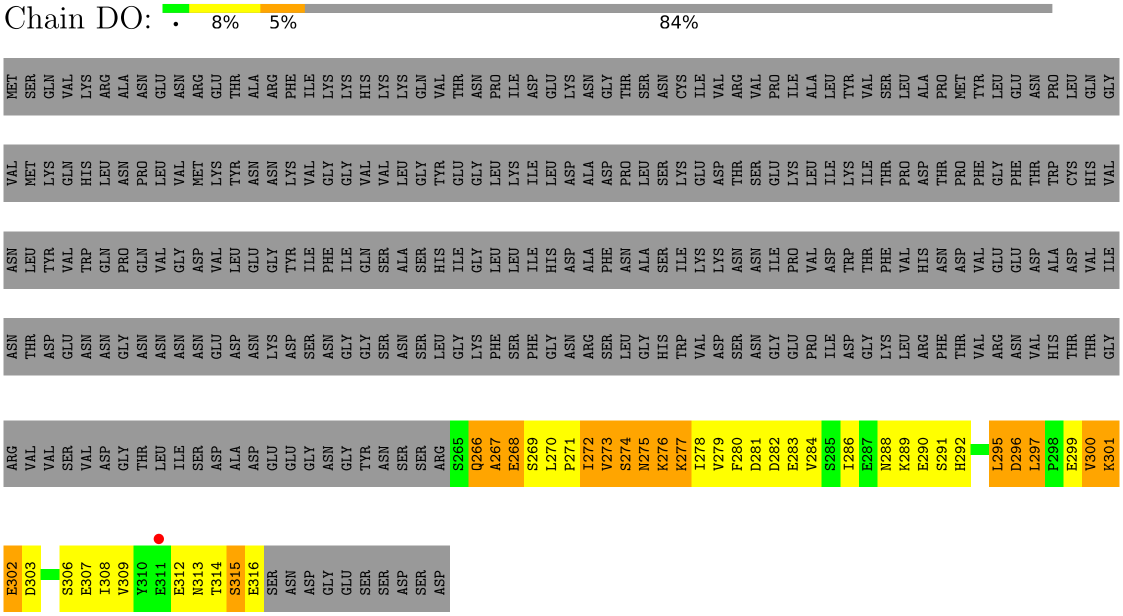


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



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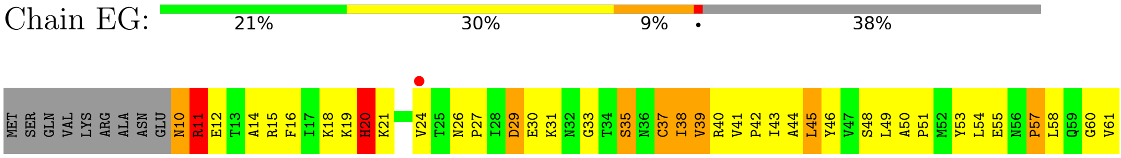

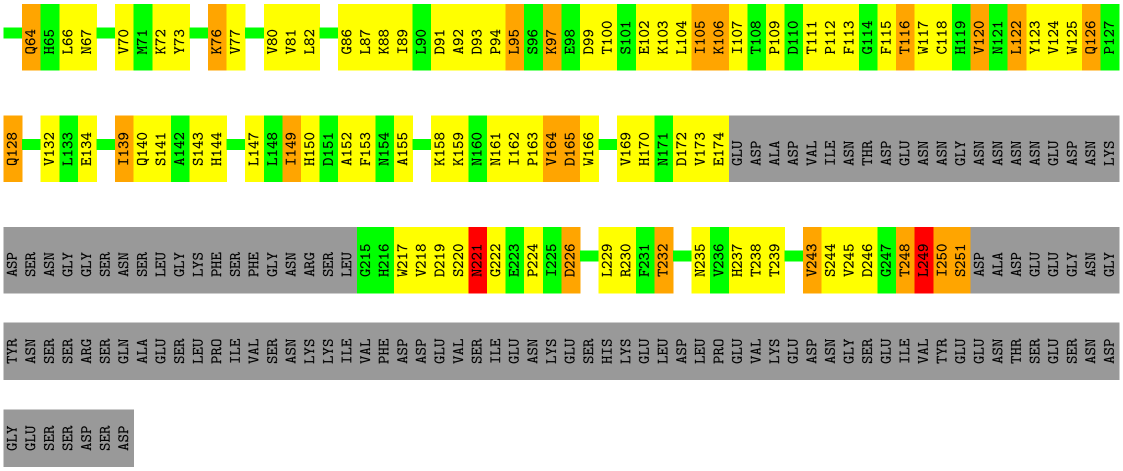

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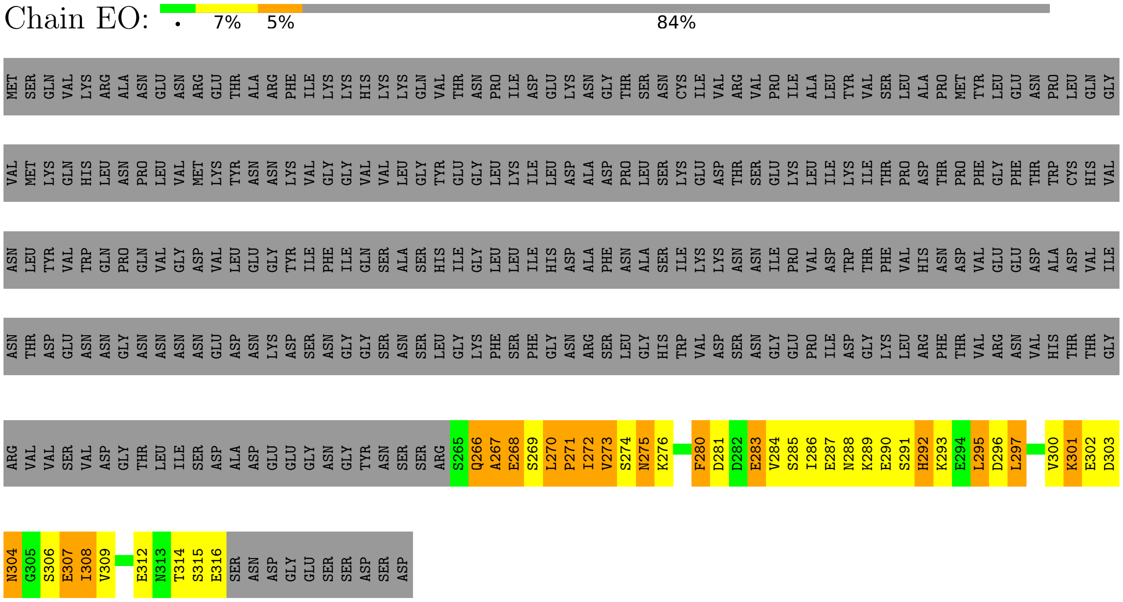
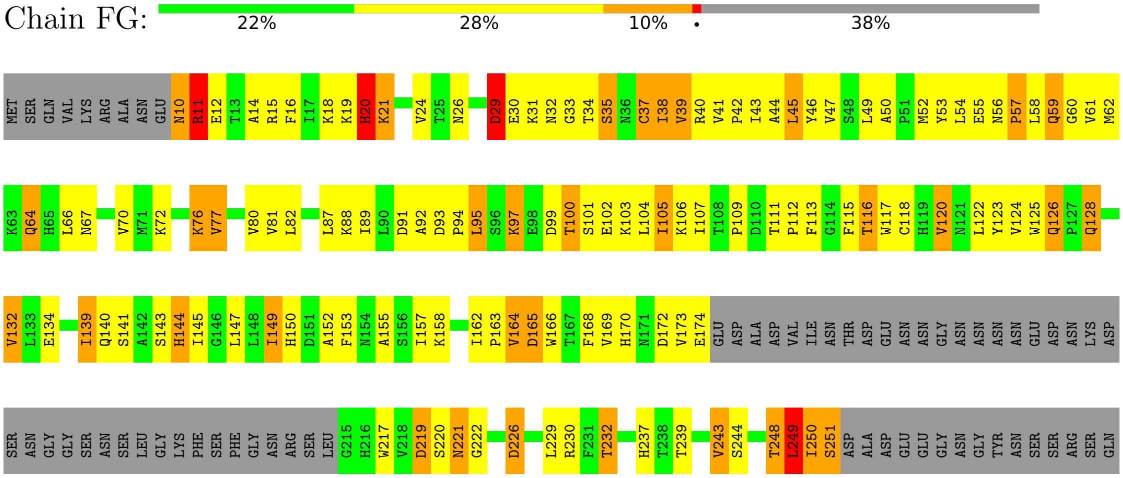
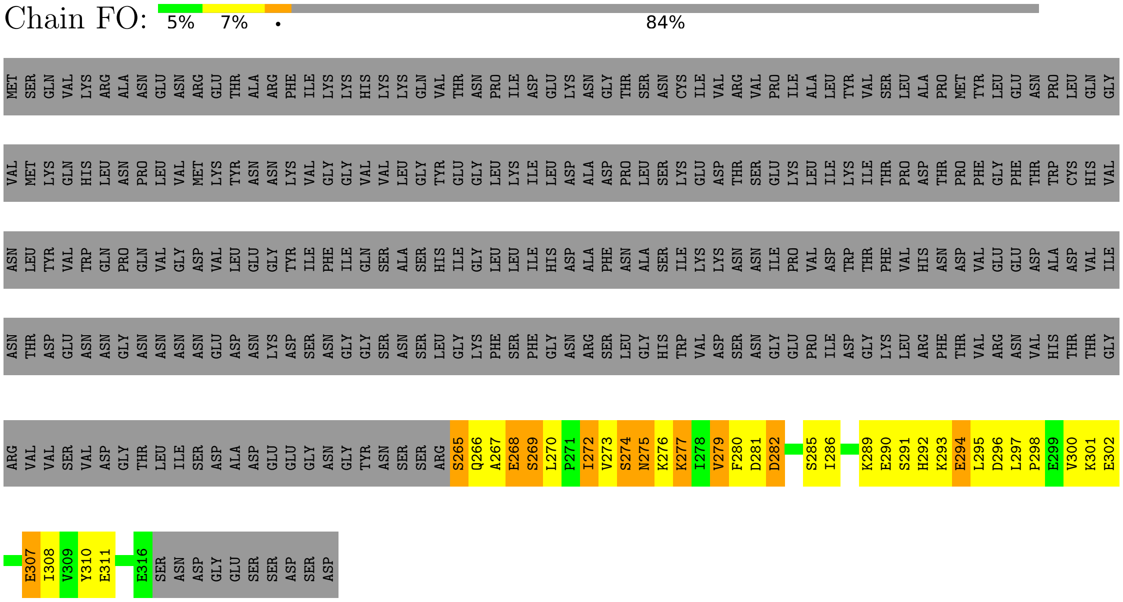


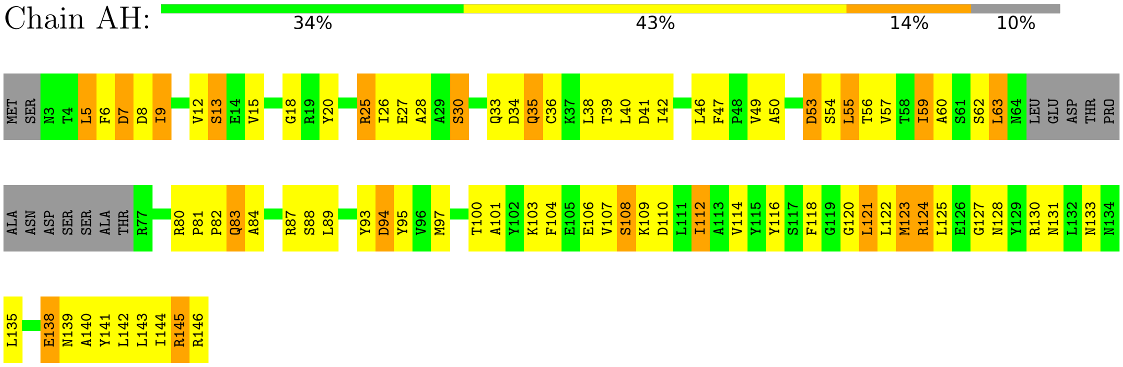
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



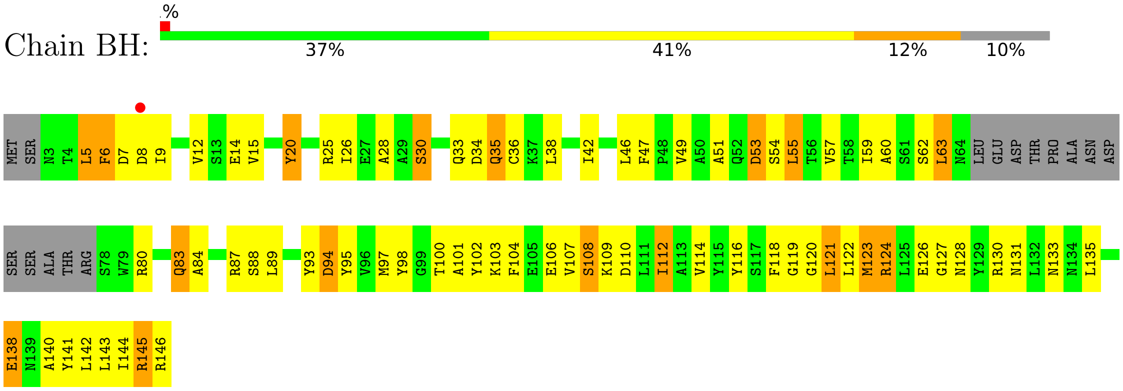
- Molecule 7: DNA-directed RNA polymerase I subunit RPA43



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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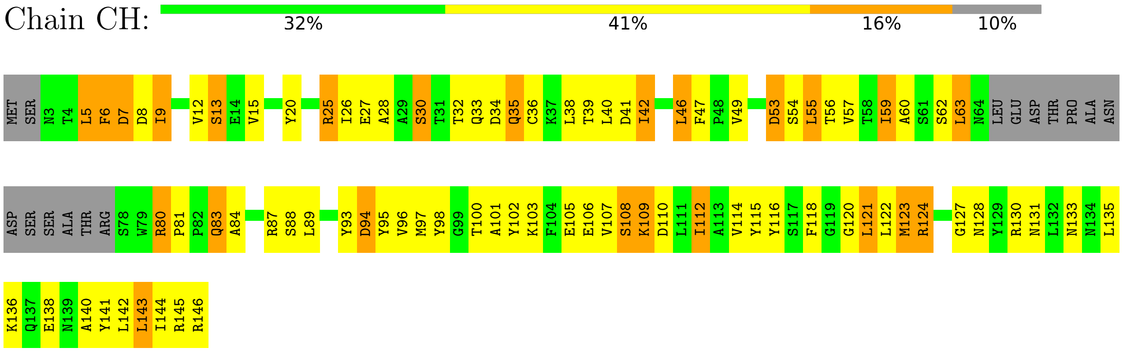

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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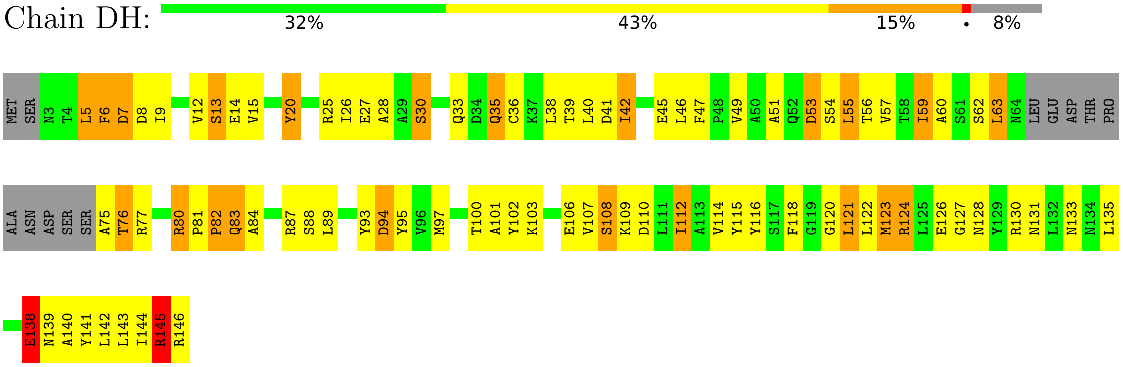

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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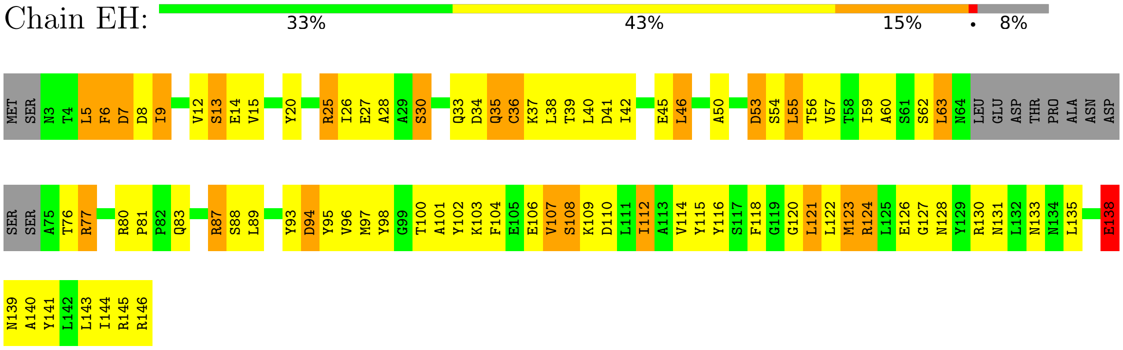

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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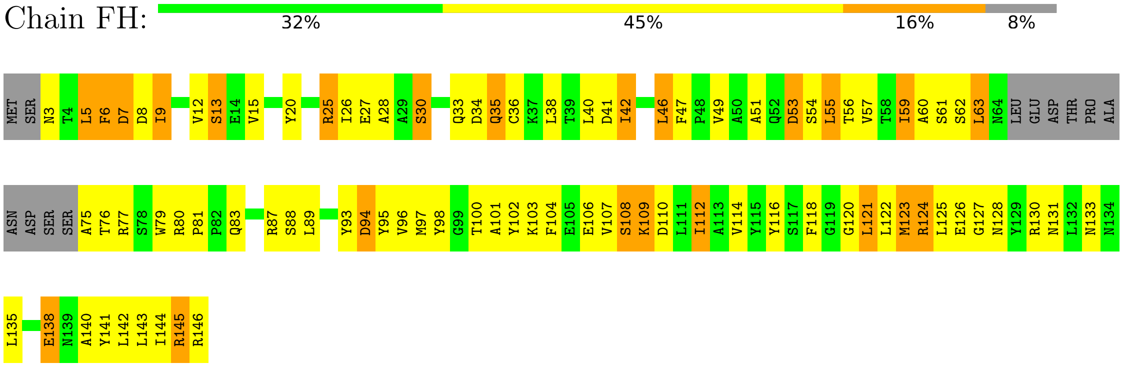
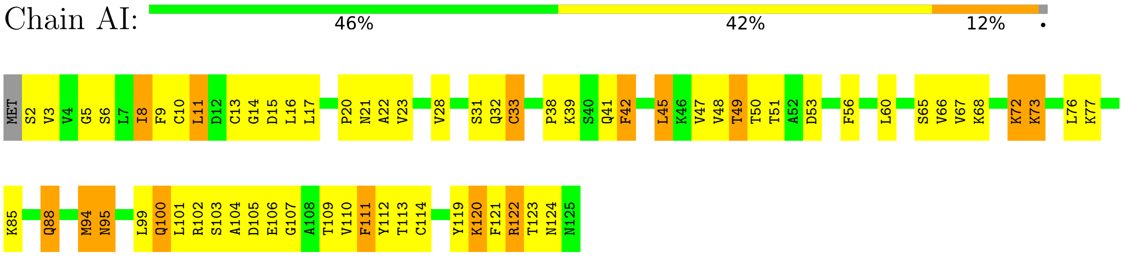


- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain AI:



- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

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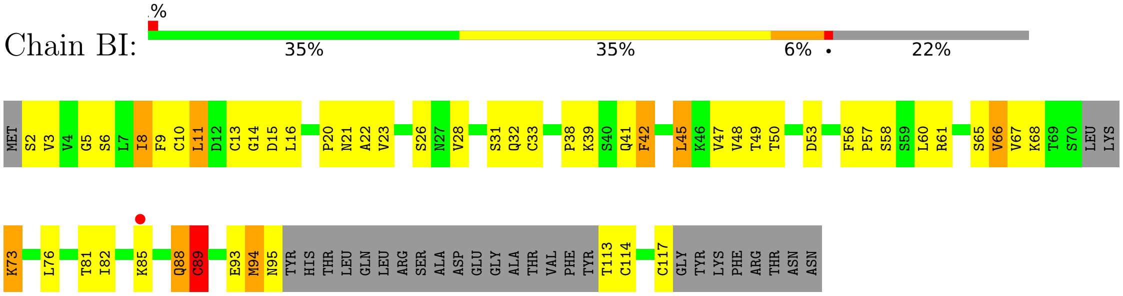
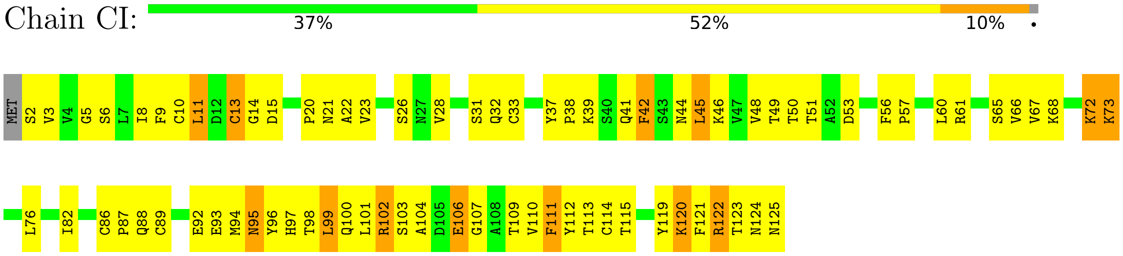


- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain CI:



- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

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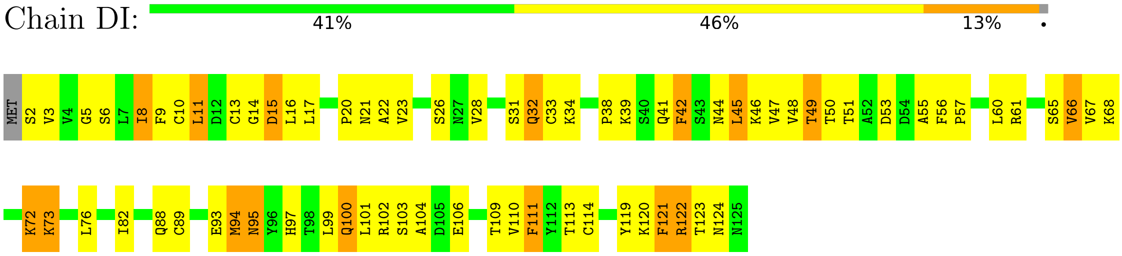
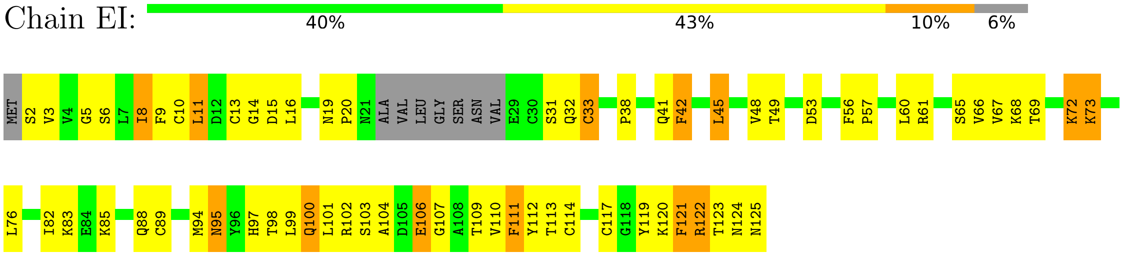


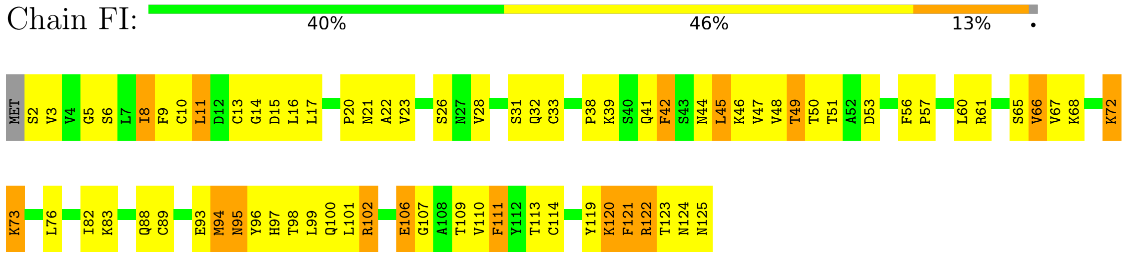
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain EI:



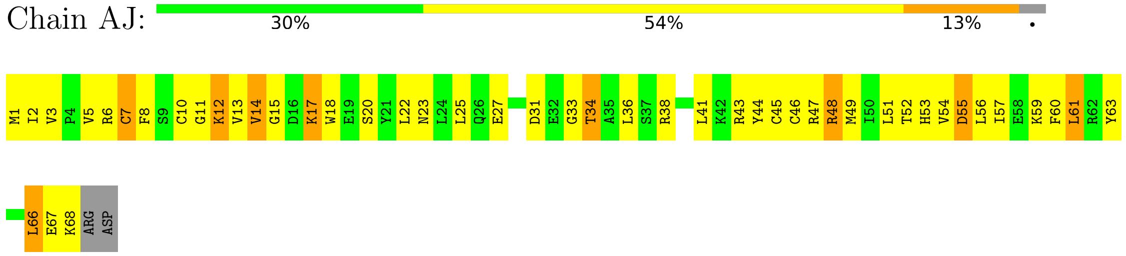
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain FI:



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain AJ:



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

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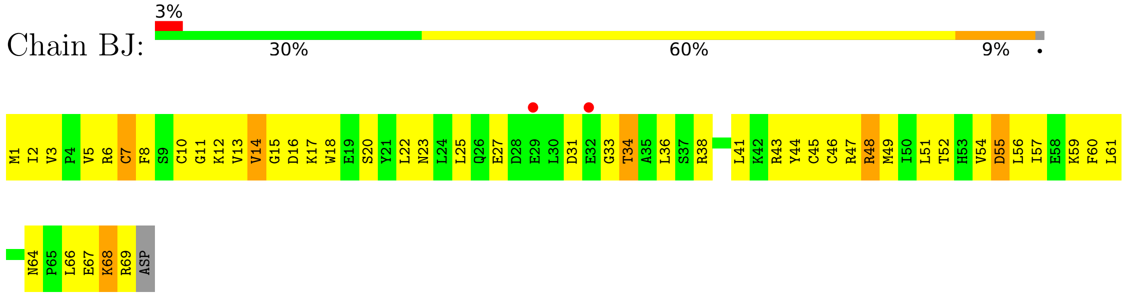

- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

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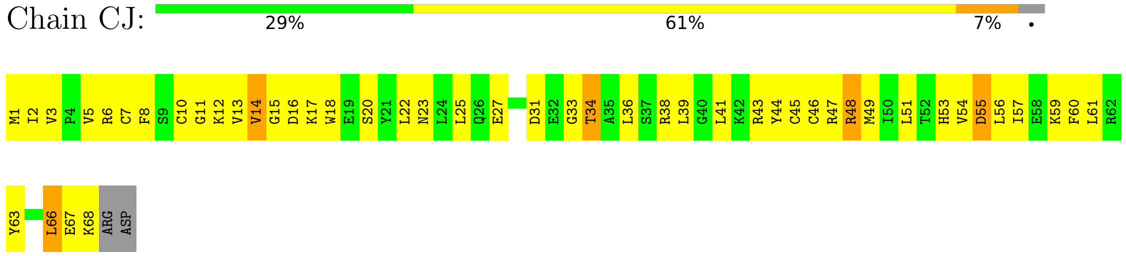

- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

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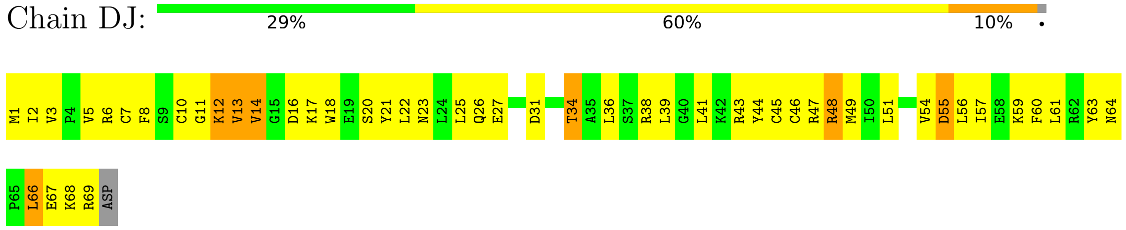
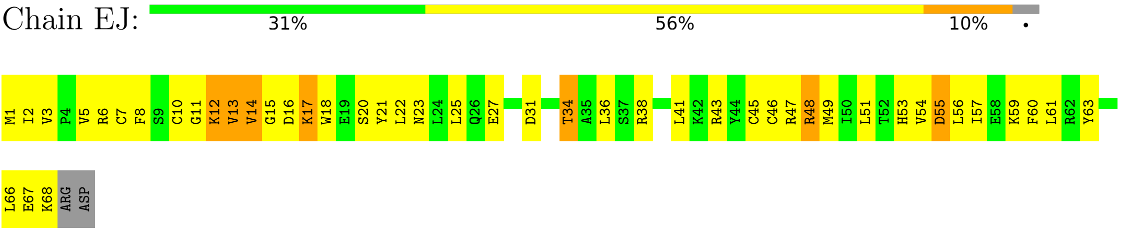


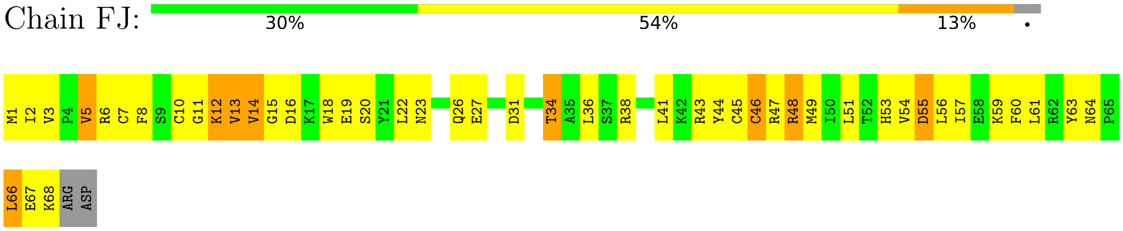
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain EJ:



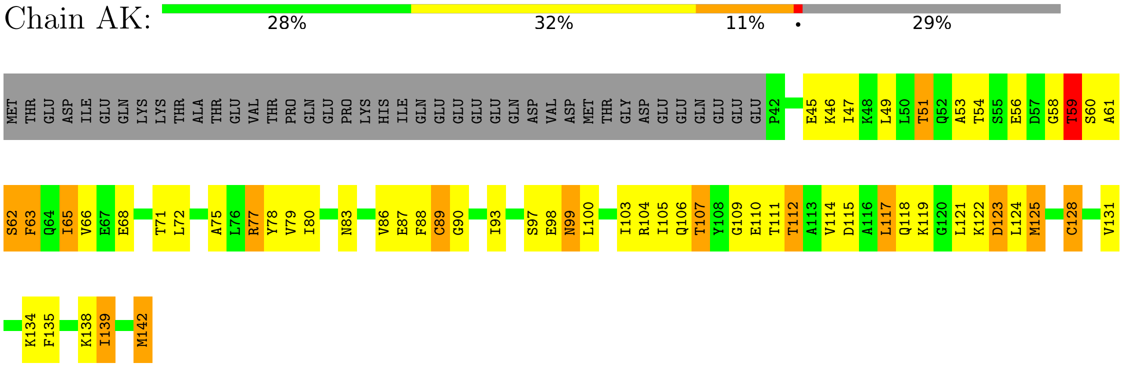
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain FJ:



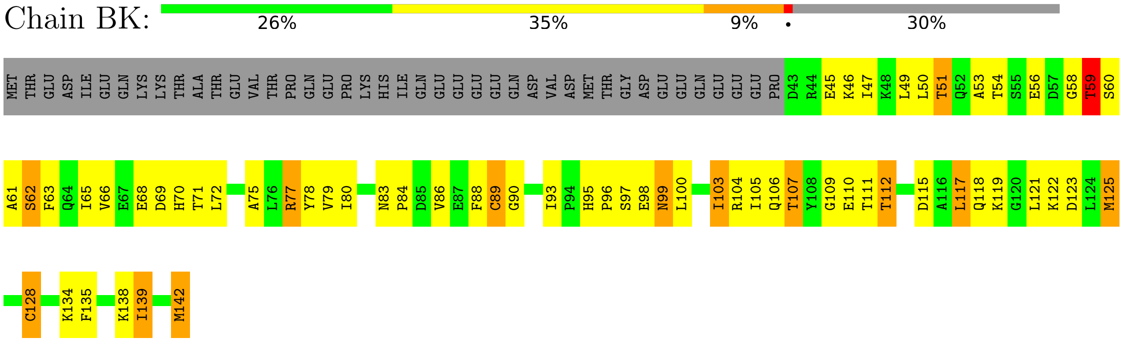
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain AK:



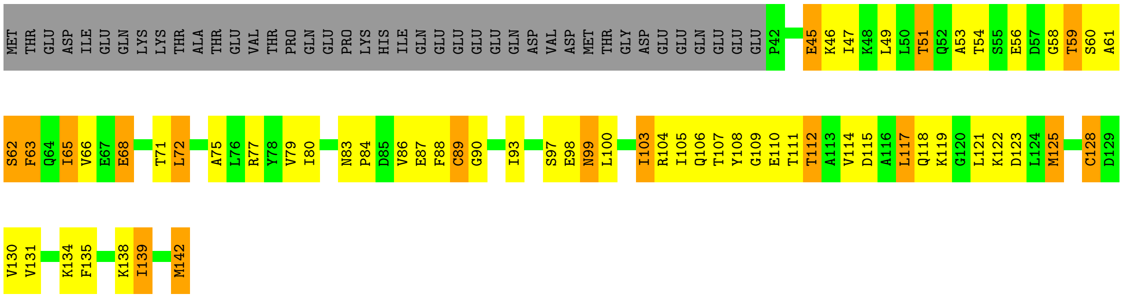
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain BK:



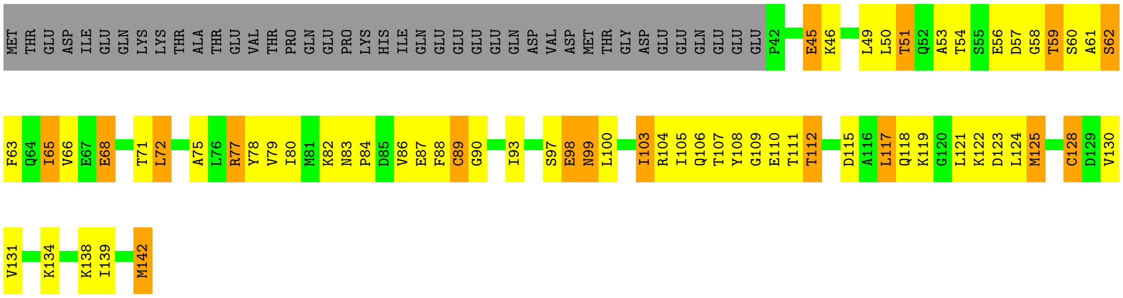
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain CK:



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain DK:



- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

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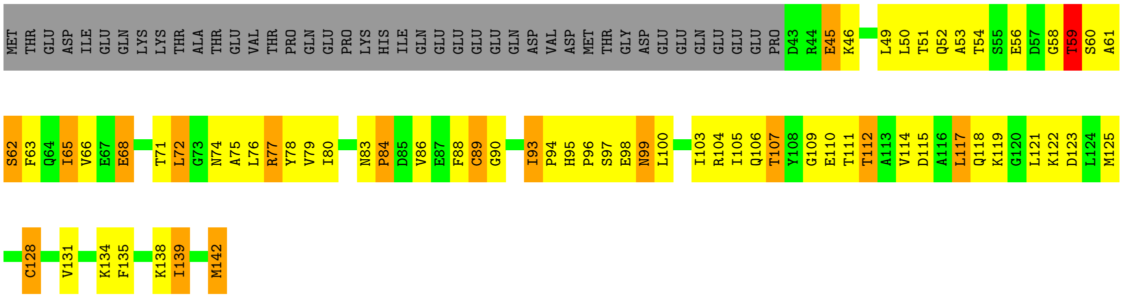

- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

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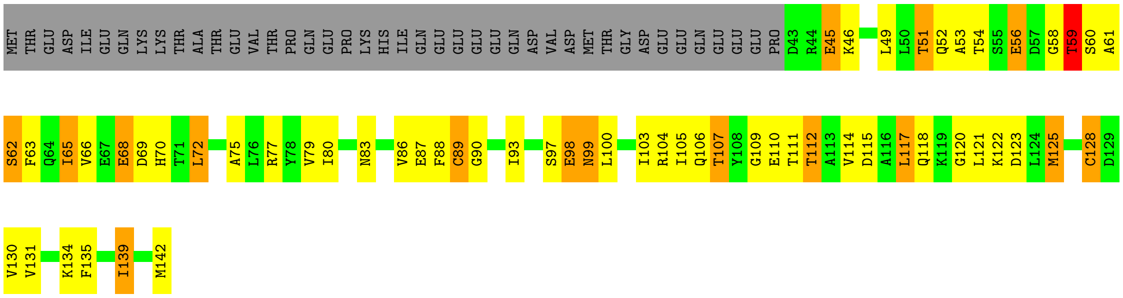
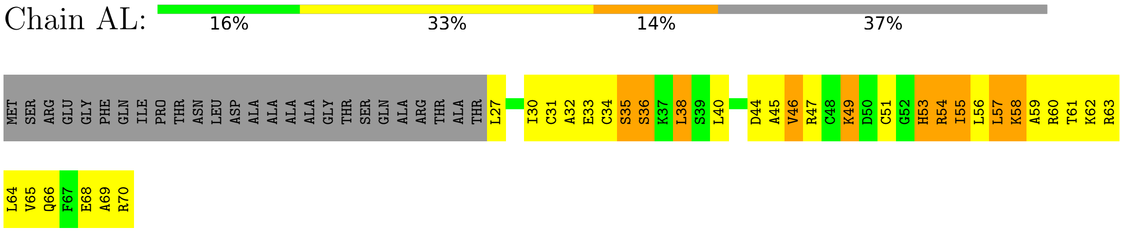


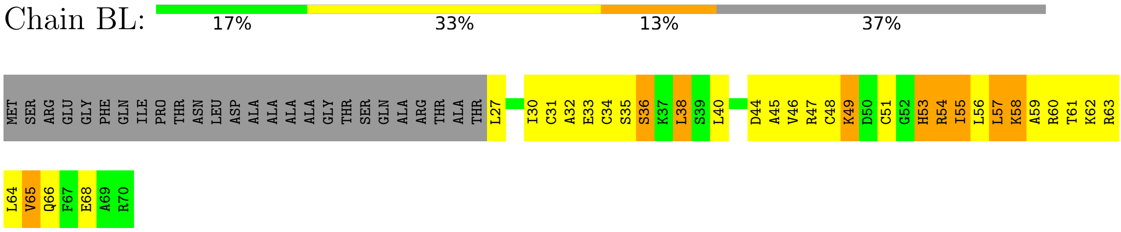
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain AL:



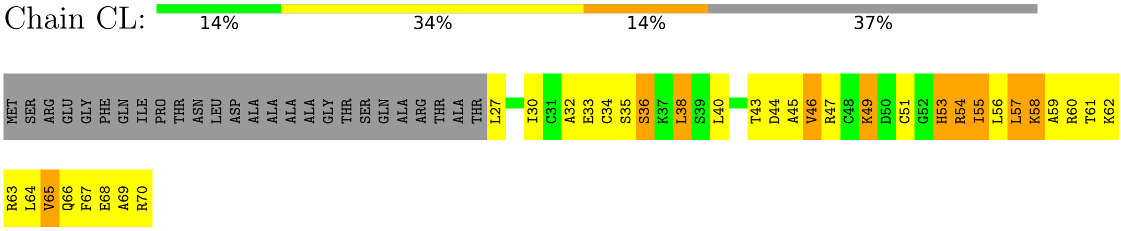
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain BL:



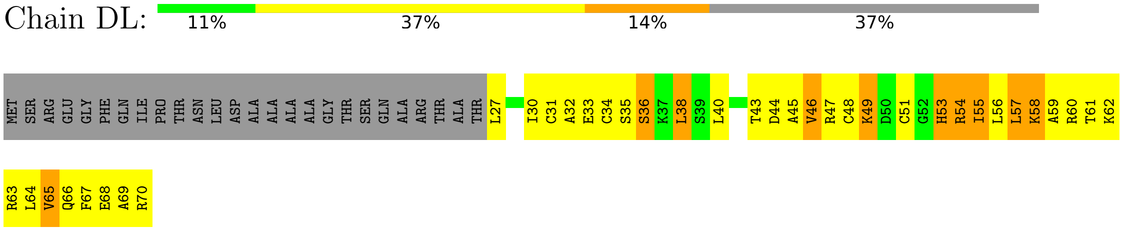
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain CL:



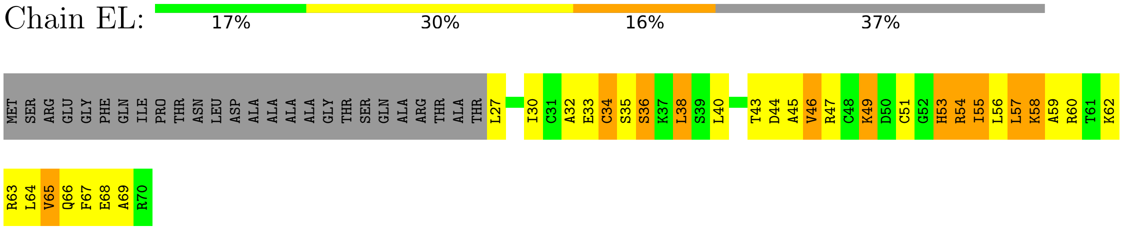
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain DL:



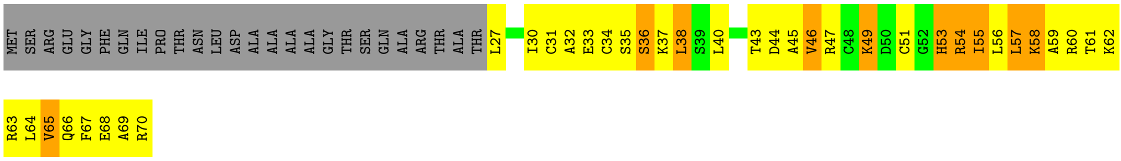
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain EL:



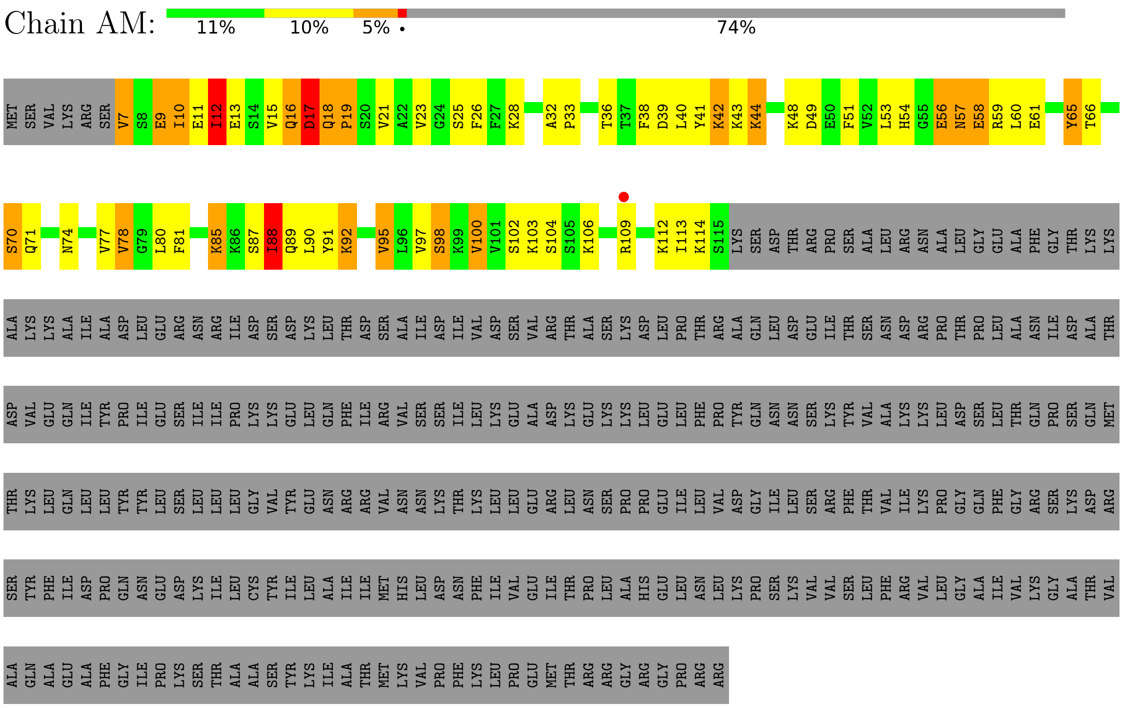
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain FL:



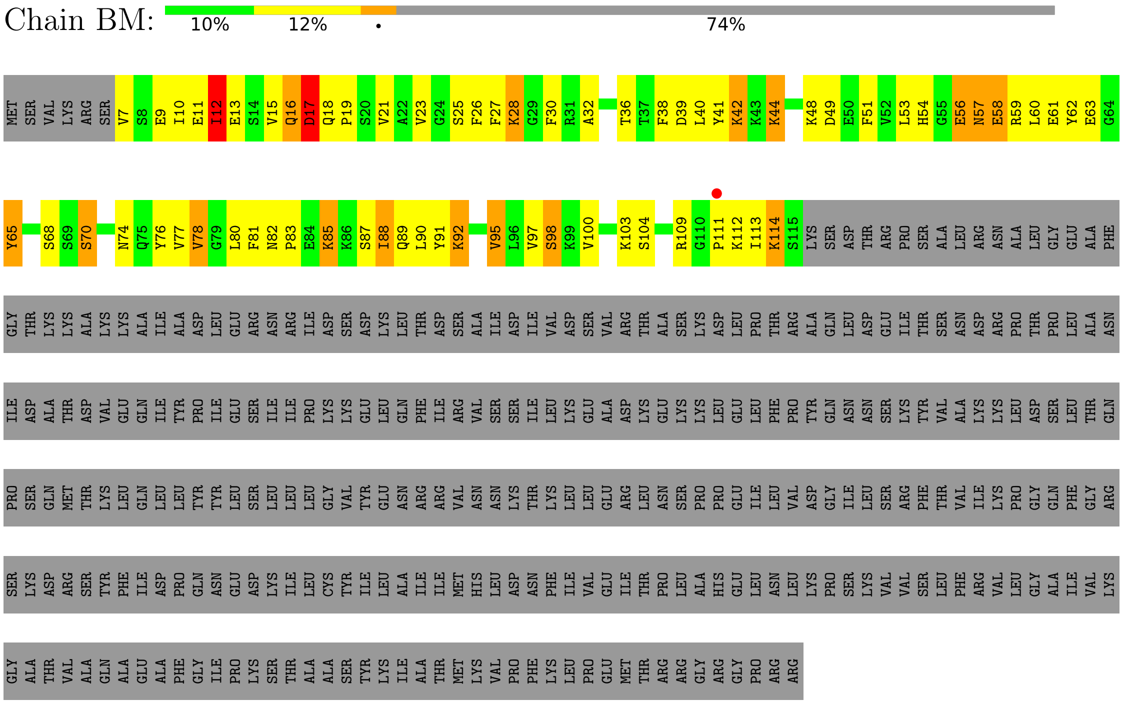
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain AM:



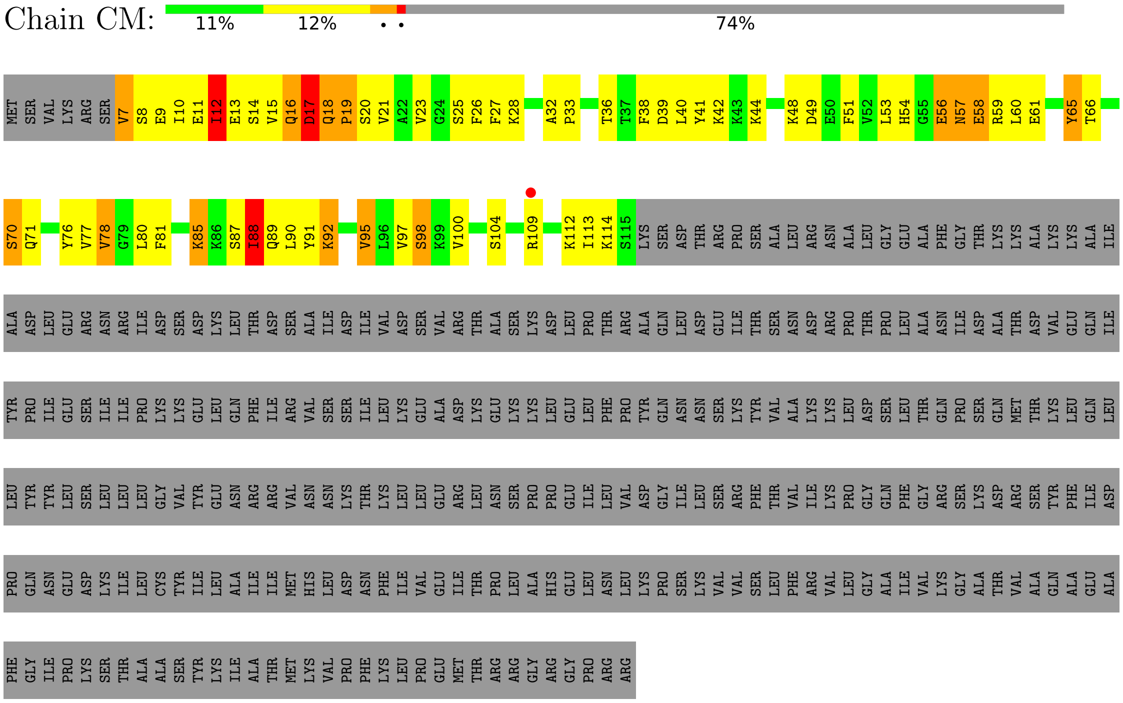
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain BM:



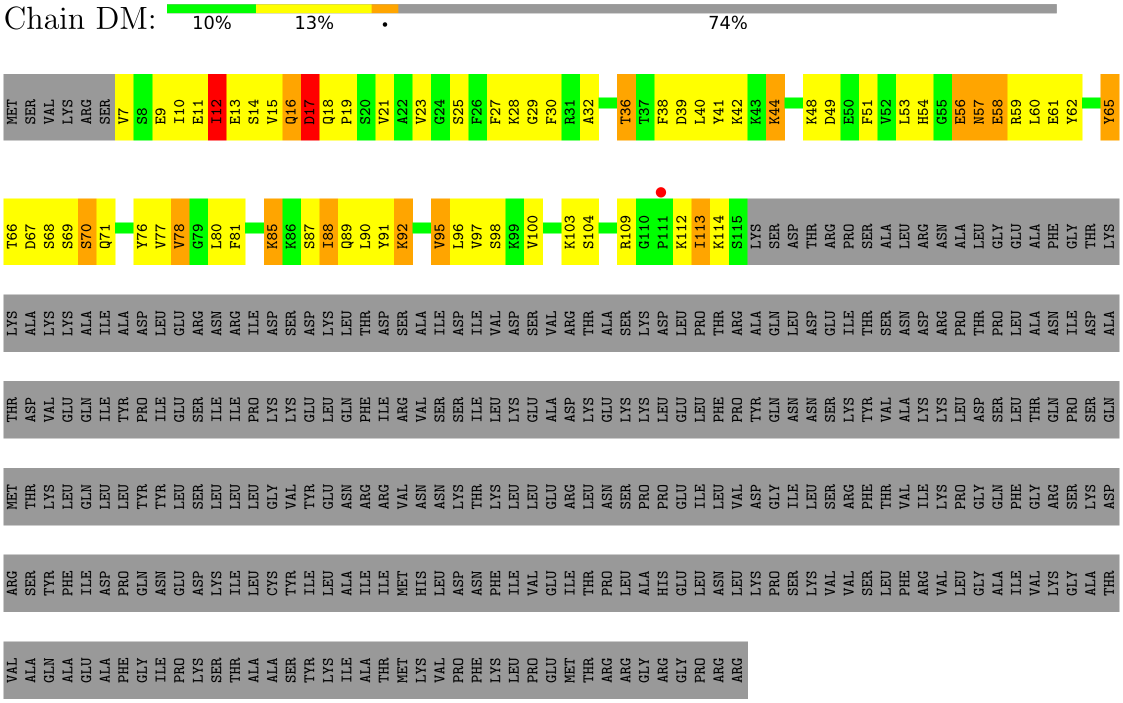
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain CM:



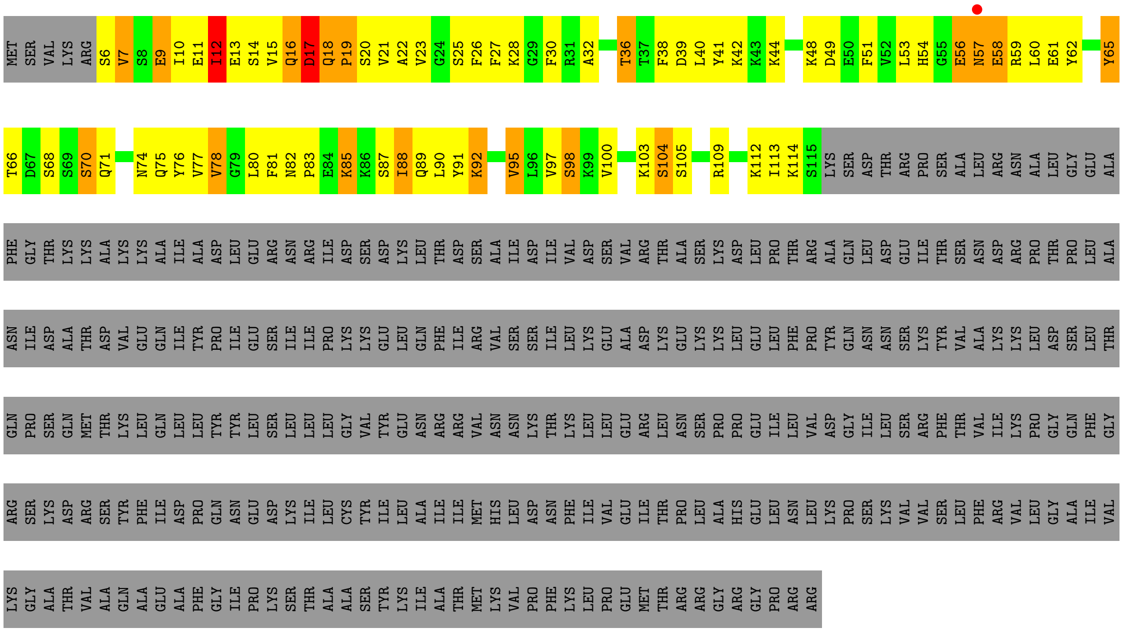
- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain DM:

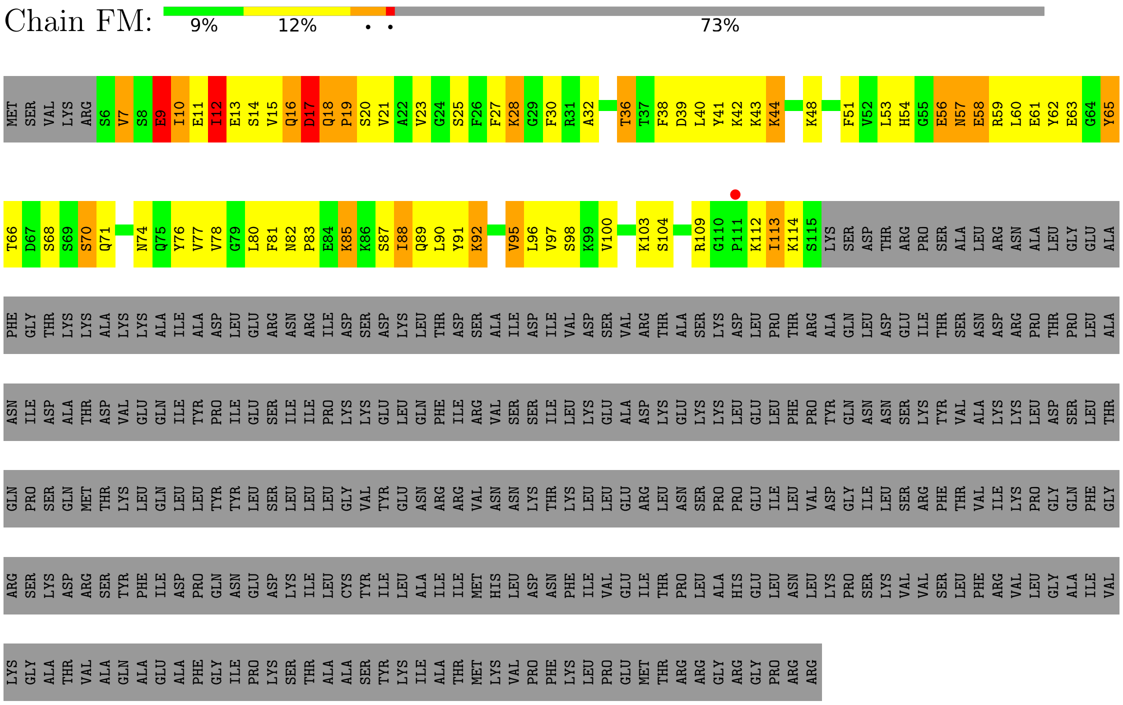


- Molecule 13: DNA-directed RNA polymerase I subunit RPA49

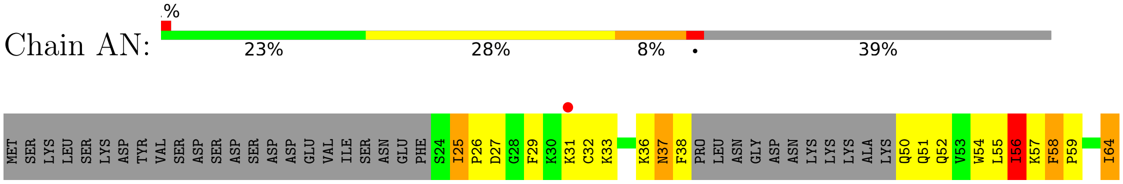
Chain EM:

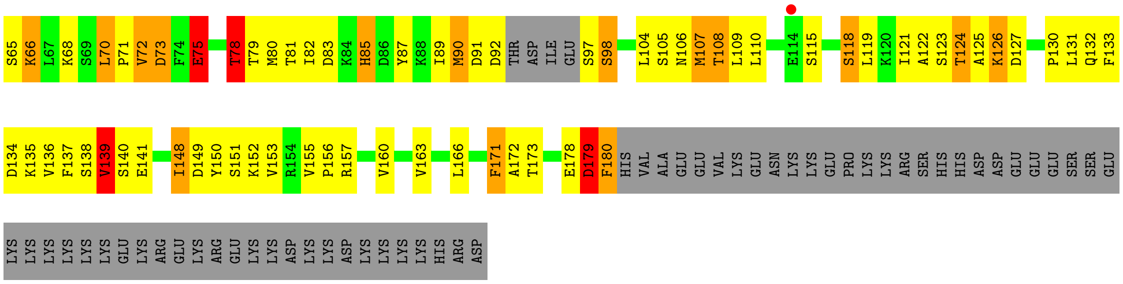


- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



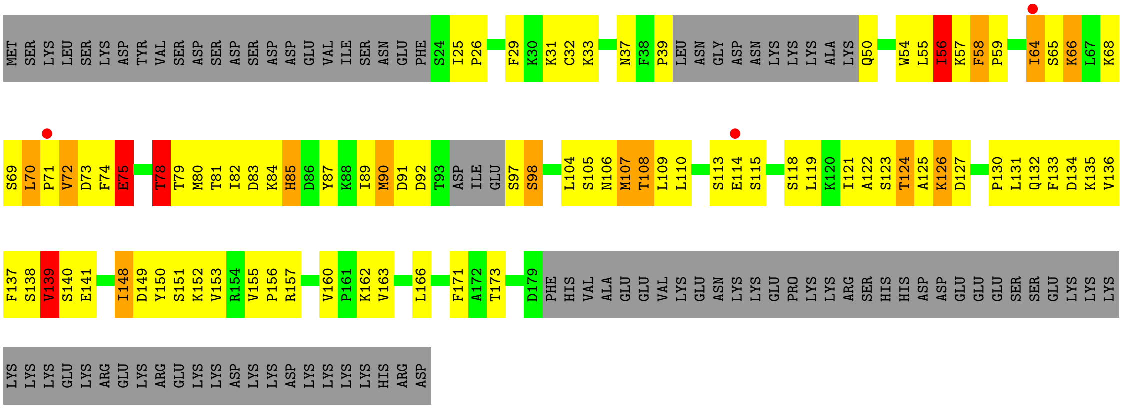
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34





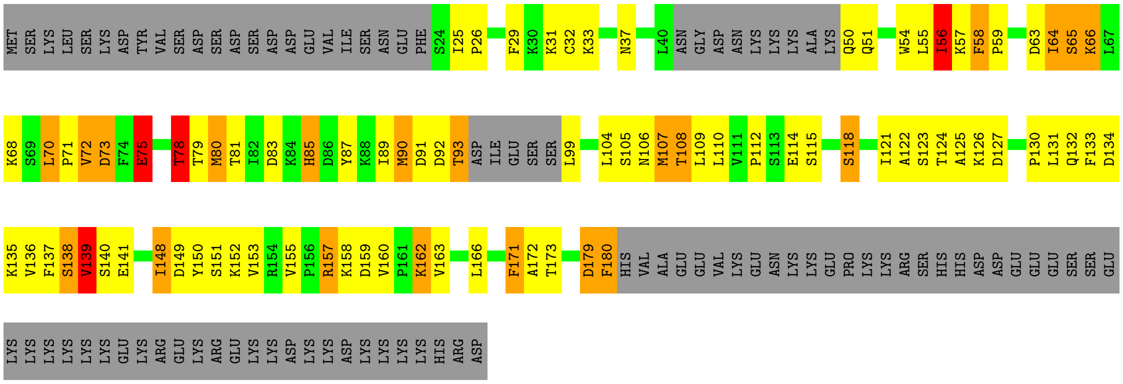
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain BN:



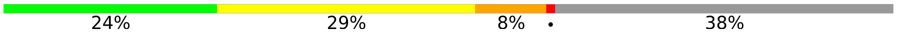
- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

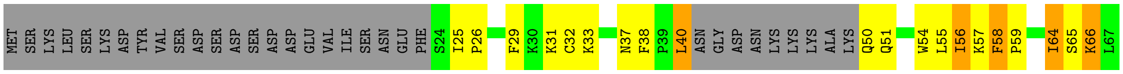
Chain CN:

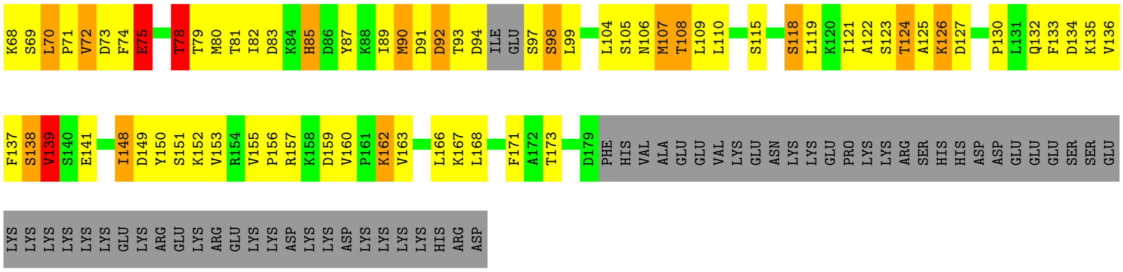


- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain DN:

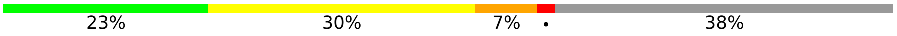


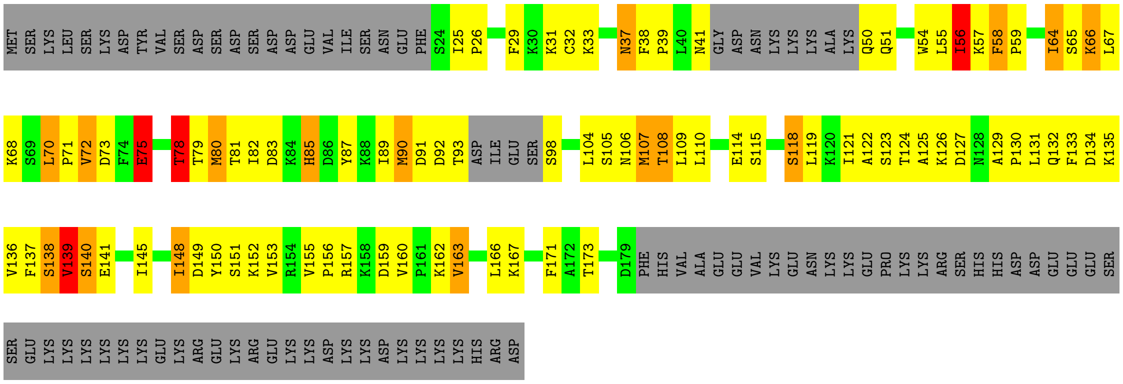




- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

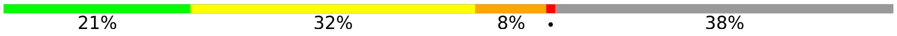
Chain EN:

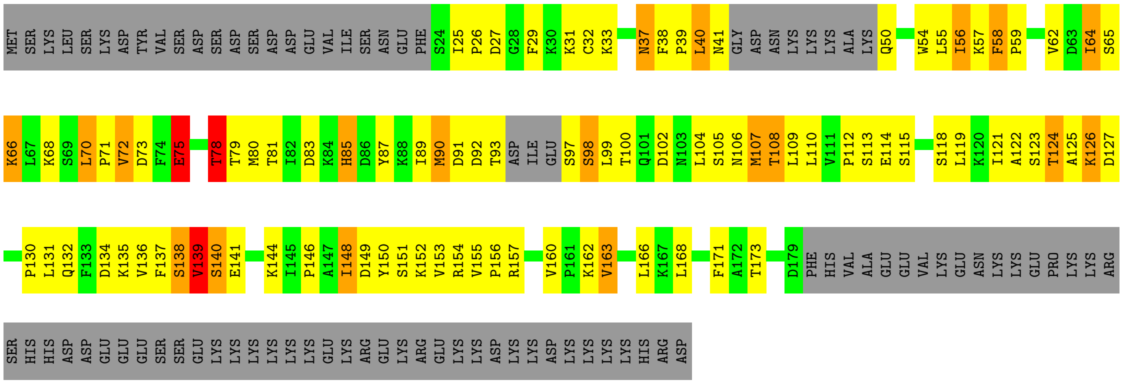




- Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain FN:





4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	619.48Å 306.62Å 251.78Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	49.69 – 5.50 49.69 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.69-5.50) 99.1 (49.69-5.50)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 5.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.235 0.200 , 0.240	Depositor DCC
R_{free} test set	1987 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å^2)	117.0	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 213.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	204233	wwPDB-VP
Average B, all atoms (Å^2)	195.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	AA	0.61	0/11916	0.69	0/16097
1	BA	0.53	0/11752	0.66	0/15875
1	CA	0.66	2/11908 (0.0%)	0.72	0/16086
1	DA	0.67	2/11910 (0.0%)	0.72	0/16090
1	EA	0.68	3/11919 (0.0%)	0.74	2/16099 (0.0%)
1	FA	0.69	2/11923 (0.0%)	0.73	0/16106
2	AB	0.60	0/9389	0.70	0/12685
2	BB	0.57	1/9377 (0.0%)	0.69	0/12671
2	CB	0.70	7/9509 (0.1%)	0.75	1/12847 (0.0%)
2	DB	0.69	4/9474 (0.0%)	0.75	2/12802 (0.0%)
2	EB	0.70	2/9470 (0.0%)	0.75	1/12796 (0.0%)
2	FB	0.70	1/9475 (0.0%)	0.75	1/12802 (0.0%)
3	AC	0.61	0/2465	0.70	0/3342
3	BC	0.53	0/2465	0.66	0/3342
3	CC	0.68	0/2465	0.73	0/3342
3	DC	0.67	0/2465	0.72	0/3342
3	EC	0.73	0/2465	0.76	0/3342
3	FC	0.70	0/2465	0.73	0/3342
4	AD	0.58	0/465	0.69	0/630
4	BD	0.52	0/465	0.68	0/630
4	CD	0.69	0/465	0.76	0/630
4	DD	0.64	0/465	0.75	0/630
4	ED	0.67	0/465	0.74	0/630
4	FD	0.71	0/465	0.78	0/630
5	AE	0.54	0/1796	0.66	0/2416
5	BE	0.49	0/1796	0.64	0/2416
5	CE	0.60	0/1796	0.71	2/2416 (0.1%)
5	DE	0.60	0/1796	0.72	2/2416 (0.1%)
5	EE	0.59	0/1796	0.69	0/2416
5	FE	0.64	0/1796	0.71	0/2416
6	AF	0.56	0/821	0.64	0/1106
6	BF	0.50	0/821	0.59	0/1106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	CF	0.66	0/830	0.68	0/1118
6	DF	0.64	0/830	0.68	0/1118
6	EF	0.66	0/830	0.68	0/1118
6	FF	0.65	0/830	0.68	0/1118
7	AG	0.59	0/1637	0.72	1/2226 (0.0%)
7	AO	0.83	0/417	0.78	0/562
7	BG	0.52	0/1577	0.67	0/2145
7	BO	0.84	0/408	0.78	0/550
7	CG	0.68	0/1637	0.76	1/2226 (0.0%)
7	CO	1.02	3/402 (0.7%)	0.93	0/542
7	DG	0.66	0/1637	0.77	1/2226 (0.0%)
7	DO	0.95	0/417	0.91	0/562
7	EG	0.65	0/1637	0.73	2/2226 (0.1%)
7	EO	0.94	0/417	0.86	0/562
7	FG	0.70	0/1637	0.79	2/2226 (0.1%)
7	FO	0.97	2/417 (0.5%)	0.90	0/562
8	AH	0.70	0/1081	0.72	0/1463
8	BH	0.52	0/1070	0.63	0/1449
8	CH	0.70	0/1070	0.72	0/1449
8	DH	0.71	0/1093	0.71	0/1480
8	EH	0.73	1/1093 (0.1%)	0.75	0/1480
8	FH	0.78	0/1093	0.78	0/1480
9	AI	0.69	0/956	0.73	0/1288
9	BI	0.61	1/721 (0.1%)	0.66	0/969
9	CI	0.72	2/956 (0.2%)	0.75	1/1288 (0.1%)
9	DI	0.71	0/956	0.73	0/1288
9	EI	0.83	1/910 (0.1%)	0.77	0/1223
9	FI	0.81	2/956 (0.2%)	0.75	0/1288
10	AJ	0.60	0/567	0.64	0/761
10	BJ	0.59	0/578	0.65	0/775
10	CJ	0.72	0/567	0.69	0/761
10	DJ	0.64	0/578	0.67	0/775
10	EJ	0.74	0/567	0.71	0/761
10	FJ	0.71	1/567 (0.2%)	0.70	0/761
11	AK	0.64	0/804	0.69	0/1083
11	BK	0.50	0/796	0.63	0/1072
11	CK	0.69	0/804	0.70	0/1083
11	DK	0.64	0/804	0.69	0/1083
11	EK	0.68	0/796	0.71	0/1072
11	FK	0.66	0/796	0.70	0/1072
12	AL	0.71	0/354	0.74	0/468
12	BL	0.64	1/354 (0.3%)	0.71	0/468
12	CL	0.77	0/354	0.79	0/468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	DL	0.71	1/354 (0.3%)	0.77	0/468
12	EL	0.83	1/354 (0.3%)	0.85	0/468
12	FL	0.72	0/354	0.75	0/468
13	AM	0.68	0/879	0.73	0/1180
13	BM	0.66	0/879	0.73	0/1180
13	CM	0.77	0/879	0.76	0/1180
13	DM	0.75	0/879	0.75	0/1180
13	EM	0.78	2/885 (0.2%)	0.78	0/1188
13	FM	0.79	1/885 (0.1%)	0.79	0/1188
14	AN	0.68	0/1148	0.76	1/1546 (0.1%)
14	BN	0.64	0/1151	0.77	1/1552 (0.1%)
14	CN	0.76	0/1159	0.82	1/1563 (0.1%)
14	DN	0.73	0/1167	0.82	0/1574
14	EN	0.78	0/1161	0.82	1/1566 (0.1%)
14	FN	0.76	1/1167 (0.1%)	0.82	0/1574
All	All	0.66	44/208122 (0.0%)	0.72	23/281066 (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	EA	0	1

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	FO	294	GLU	CB-CG	7.84	1.67	1.52
1	EA	65	CYS	CB-SG	-7.74	1.69	1.82
9	EI	33	CYS	CB-SG	-7.71	1.69	1.82
1	EA	75	HIS	CA-CB	-7.70	1.37	1.53
7	FO	294	GLU	CG-CD	6.88	1.62	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	FG	11	ARG	NE-CZ-NH1	9.99	125.30	120.30
7	DG	11	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	EA	75	HIS	CG-ND1-CE1	9.08	120.91	108.20
7	CG	11	ARG	NE-CZ-NH1	8.63	124.62	120.30
7	AG	11	ARG	NE-CZ-NH1	8.54	124.57	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	EA	75	HIS	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	11703	0	11787	744	0
1	BA	11540	0	11624	709	0
1	CA	11695	0	11780	785	0
1	DA	11697	0	11775	791	0
1	EA	11706	0	11788	781	0
1	FA	11709	0	11790	792	0
2	AB	9187	0	9100	594	0
2	BB	9175	0	9074	571	0
2	CB	9304	0	9216	623	0
2	DB	9269	0	9175	644	0
2	EB	9265	0	9179	642	0
2	FB	9270	0	9180	644	0
3	AC	2413	0	2404	153	0
3	BC	2413	0	2404	145	0
3	CC	2413	0	2404	172	0
3	DC	2413	0	2404	170	0
3	EC	2413	0	2404	160	0
3	FC	2413	0	2404	161	0
4	AD	459	0	462	25	0
4	BD	459	0	462	32	0
4	CD	459	0	462	26	0
4	DD	459	0	462	26	0
4	ED	459	0	462	29	0
4	FD	459	0	462	32	0
5	AE	1760	0	1788	79	0
5	BE	1760	0	1788	84	0
5	CE	1760	0	1788	83	0
5	DE	1760	0	1788	98	0
5	EE	1760	0	1788	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	FE	1760	0	1788	101	0
6	AF	807	0	827	43	0
6	BF	807	0	827	43	0
6	CF	816	0	833	40	0
6	DF	816	0	833	37	0
6	EF	816	0	833	42	0
6	FF	816	0	833	39	0
7	AG	1599	0	1602	112	0
7	AO	413	0	389	47	0
7	BG	1539	0	1552	106	0
7	BO	404	0	383	47	0
7	CG	1599	0	1602	101	0
7	CO	398	0	378	42	0
7	DG	1599	0	1602	115	0
7	DO	413	0	389	34	0
7	EG	1599	0	1602	116	0
7	EO	413	0	389	47	0
7	FG	1599	0	1602	112	0
7	FO	413	0	389	38	0
8	AH	1063	0	1034	58	0
8	BH	1052	0	1021	59	0
8	CH	1052	0	1021	70	0
8	DH	1075	0	1046	72	0
8	EH	1075	0	1046	63	0
8	FH	1075	0	1046	63	0
9	AI	943	0	929	62	0
9	BI	716	0	709	37	0
9	CI	943	0	929	63	0
9	DI	943	0	929	64	0
9	EI	898	0	880	54	0
9	FI	943	0	929	65	0
10	AJ	558	0	572	42	0
10	BJ	569	0	585	37	0
10	CJ	558	0	572	43	0
10	DJ	569	0	585	39	0
10	EJ	558	0	572	35	0
10	FJ	558	0	572	39	0
11	AK	793	0	790	41	0
11	BK	786	0	782	42	0
11	CK	793	0	790	46	0
11	DK	793	0	790	50	0
11	EK	786	0	782	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	FK	786	0	782	45	0
12	AL	352	0	374	48	0
12	BL	352	0	374	25	0
12	CL	352	0	374	42	0
12	DL	352	0	374	42	0
12	EL	352	0	374	34	0
12	FL	352	0	374	45	0
13	AM	863	0	864	59	0
13	BM	863	0	864	77	0
13	CM	863	0	864	61	0
13	DM	863	0	864	58	0
13	EM	869	0	869	67	0
13	FM	869	0	869	71	0
14	AN	1127	0	1133	85	0
14	BN	1130	0	1138	79	0
14	CN	1137	0	1148	84	0
14	DN	1146	0	1153	78	0
14	EN	1140	0	1150	77	0
14	FN	1146	0	1155	78	0
15	AA	2	0	0	0	0
15	AB	1	0	0	0	0
15	AI	2	0	0	0	0
15	AJ	1	0	0	0	0
15	AL	1	0	0	0	0
15	BA	2	0	0	0	0
15	BB	1	0	0	0	0
15	BI	2	0	0	0	0
15	BJ	1	0	0	0	0
15	BL	1	0	0	0	0
15	CA	2	0	0	0	0
15	CB	1	0	0	0	0
15	CI	2	0	0	0	0
15	CJ	1	0	0	0	0
15	CL	1	0	0	0	0
15	DA	2	0	0	0	0
15	DB	1	0	0	0	0
15	DI	2	0	0	0	0
15	DJ	1	0	0	0	0
15	DL	1	0	0	0	0
15	EA	2	0	0	0	0
15	EB	1	0	0	0	0
15	EI	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	EJ	1	0	0	0	0
15	EL	1	0	0	0	0
15	FA	2	0	0	0	0
15	FB	1	0	0	0	0
15	FI	2	0	0	0	0
15	FJ	1	0	0	0	0
15	FL	1	0	0	0	0
All	All	204233	0	204265	11918	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 29.

The worst 5 of 11918 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)
7:FG:11:ARG:HG2	7:FG:11:ARG:HH11	1.10	1.15
7:DG:11:ARG:HH11	7:DG:11:ARG:HG3	1.13	1.11
7:AG:11:ARG:HH11	7:AG:11:ARG:HG3	1.14	1.10
7:EG:11:ARG:HH11	7:EG:11:ARG:HG2	1.13	1.10
7:CG:11:ARG:HG3	7:CG:11:ARG:HH11	1.11	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	1470/1664 (88%)	1124 (76%)	276 (19%)	70 (5%)	2	21
1	BA	1448/1664 (87%)	1124 (78%)	259 (18%)	65 (4%)	2	22
1	CA	1469/1664 (88%)	1131 (77%)	268 (18%)	70 (5%)	2	21
1	DA	1469/1664 (88%)	1138 (78%)	263 (18%)	68 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EA	1468/1664 (88%)	1127 (77%)	272 (18%)	69 (5%)	2	21
1	FA	1470/1664 (88%)	1127 (77%)	274 (19%)	69 (5%)	2	21
2	AB	1142/1203 (95%)	926 (81%)	158 (14%)	58 (5%)	2	19
2	BB	1141/1203 (95%)	923 (81%)	164 (14%)	54 (5%)	2	21
2	CB	1160/1203 (96%)	921 (79%)	171 (15%)	68 (6%)	1	17
2	DB	1155/1203 (96%)	923 (80%)	172 (15%)	60 (5%)	2	19
2	EB	1154/1203 (96%)	928 (80%)	165 (14%)	61 (5%)	2	19
2	FB	1155/1203 (96%)	925 (80%)	165 (14%)	65 (6%)	2	18
3	AC	302/335 (90%)	231 (76%)	53 (18%)	18 (6%)	1	16
3	BC	302/335 (90%)	232 (77%)	53 (18%)	17 (6%)	2	18
3	CC	302/335 (90%)	234 (78%)	52 (17%)	16 (5%)	2	19
3	DC	302/335 (90%)	233 (77%)	51 (17%)	18 (6%)	1	16
3	EC	302/335 (90%)	233 (77%)	52 (17%)	17 (6%)	2	18
3	FC	302/335 (90%)	233 (77%)	51 (17%)	18 (6%)	1	16
4	AD	54/137 (39%)	49 (91%)	5 (9%)	0	100	100
4	BD	54/137 (39%)	50 (93%)	4 (7%)	0	100	100
4	CD	54/137 (39%)	49 (91%)	5 (9%)	0	100	100
4	DD	54/137 (39%)	50 (93%)	4 (7%)	0	100	100
4	ED	54/137 (39%)	50 (93%)	3 (6%)	1 (2%)	8	38
4	FD	54/137 (39%)	49 (91%)	4 (7%)	1 (2%)	8	38
5	AE	213/215 (99%)	176 (83%)	31 (15%)	6 (3%)	5	30
5	BE	213/215 (99%)	174 (82%)	32 (15%)	7 (3%)	4	26
5	CE	213/215 (99%)	174 (82%)	33 (16%)	6 (3%)	5	30
5	DE	213/215 (99%)	176 (83%)	31 (15%)	6 (3%)	5	30
5	EE	213/215 (99%)	175 (82%)	32 (15%)	6 (3%)	5	30
5	FE	213/215 (99%)	174 (82%)	33 (16%)	6 (3%)	5	30
6	AF	96/155 (62%)	85 (88%)	10 (10%)	1 (1%)	15	53
6	BF	96/155 (62%)	87 (91%)	8 (8%)	1 (1%)	15	53
6	CF	97/155 (63%)	87 (90%)	9 (9%)	1 (1%)	15	53
6	DF	97/155 (63%)	85 (88%)	11 (11%)	1 (1%)	15	53
6	EF	97/155 (63%)	88 (91%)	8 (8%)	1 (1%)	15	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	FF	97/155 (63%)	88 (91%)	7 (7%)	2 (2%)	7	36
7	AG	198/326 (61%)	143 (72%)	40 (20%)	15 (8%)	1	13
7	AO	50/326 (15%)	31 (62%)	11 (22%)	8 (16%)	0	3
7	BG	191/326 (59%)	139 (73%)	37 (19%)	15 (8%)	1	12
7	BO	49/326 (15%)	33 (67%)	11 (22%)	5 (10%)	0	8
7	CG	198/326 (61%)	145 (73%)	38 (19%)	15 (8%)	1	13
7	CO	48/326 (15%)	32 (67%)	10 (21%)	6 (12%)	0	5
7	DG	198/326 (61%)	142 (72%)	38 (19%)	18 (9%)	1	11
7	DO	50/326 (15%)	31 (62%)	12 (24%)	7 (14%)	0	4
7	EG	198/326 (61%)	144 (73%)	40 (20%)	14 (7%)	1	14
7	EO	50/326 (15%)	30 (60%)	13 (26%)	7 (14%)	0	4
7	FG	198/326 (61%)	141 (71%)	40 (20%)	17 (9%)	1	11
7	FO	50/326 (15%)	34 (68%)	13 (26%)	3 (6%)	1	16
8	AH	128/146 (88%)	106 (83%)	19 (15%)	3 (2%)	6	34
8	BH	127/146 (87%)	105 (83%)	17 (13%)	5 (4%)	3	23
8	CH	127/146 (87%)	106 (84%)	18 (14%)	3 (2%)	6	33
8	DH	130/146 (89%)	104 (80%)	20 (15%)	6 (5%)	2	21
8	EH	130/146 (89%)	106 (82%)	17 (13%)	7 (5%)	2	19
8	FH	130/146 (89%)	106 (82%)	19 (15%)	5 (4%)	3	24
9	AI	122/125 (98%)	91 (75%)	28 (23%)	3 (2%)	5	32
9	BI	91/125 (73%)	70 (77%)	19 (21%)	2 (2%)	6	35
9	CI	122/125 (98%)	93 (76%)	25 (20%)	4 (3%)	4	26
9	DI	122/125 (98%)	93 (76%)	26 (21%)	3 (2%)	5	32
9	EI	113/125 (90%)	85 (75%)	25 (22%)	3 (3%)	5	31
9	FI	122/125 (98%)	92 (75%)	25 (20%)	5 (4%)	3	22
10	AJ	66/70 (94%)	45 (68%)	16 (24%)	5 (8%)	1	13
10	BJ	67/70 (96%)	45 (67%)	18 (27%)	4 (6%)	1	16
10	CJ	66/70 (94%)	47 (71%)	15 (23%)	4 (6%)	1	16
10	DJ	67/70 (96%)	47 (70%)	16 (24%)	4 (6%)	1	16
10	EJ	66/70 (94%)	47 (71%)	15 (23%)	4 (6%)	1	16
10	FJ	66/70 (94%)	47 (71%)	16 (24%)	3 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	99/142 (70%)	79 (80%)	17 (17%)	3 (3%)	4	28
11	BK	98/142 (69%)	80 (82%)	15 (15%)	3 (3%)	4	27
11	CK	99/142 (70%)	85 (86%)	11 (11%)	3 (3%)	4	28
11	DK	99/142 (70%)	81 (82%)	14 (14%)	4 (4%)	3	23
11	EK	98/142 (69%)	80 (82%)	14 (14%)	4 (4%)	3	22
11	FK	98/142 (69%)	82 (84%)	13 (13%)	3 (3%)	4	27
12	AL	42/70 (60%)	34 (81%)	5 (12%)	3 (7%)	1	14
12	BL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	14
12	CL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	14
12	DL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	14
12	EL	42/70 (60%)	33 (79%)	6 (14%)	3 (7%)	1	14
12	FL	42/70 (60%)	34 (81%)	5 (12%)	3 (7%)	1	14
13	AM	107/415 (26%)	81 (76%)	17 (16%)	9 (8%)	1	11
13	BM	107/415 (26%)	81 (76%)	17 (16%)	9 (8%)	1	11
13	CM	107/415 (26%)	79 (74%)	19 (18%)	9 (8%)	1	11
13	DM	107/415 (26%)	82 (77%)	15 (14%)	10 (9%)	0	10
13	EM	108/415 (26%)	80 (74%)	18 (17%)	10 (9%)	0	10
13	FM	108/415 (26%)	80 (74%)	18 (17%)	10 (9%)	0	10
14	AN	136/233 (58%)	106 (78%)	17 (12%)	13 (10%)	0	9
14	BN	137/233 (59%)	110 (80%)	16 (12%)	11 (8%)	1	12
14	CN	137/233 (59%)	109 (80%)	17 (12%)	11 (8%)	1	12
14	DN	139/233 (60%)	112 (81%)	16 (12%)	11 (8%)	1	12
14	EN	138/233 (59%)	111 (80%)	15 (11%)	12 (9%)	1	11
14	FN	139/233 (60%)	112 (81%)	15 (11%)	12 (9%)	1	11
All	All	25348/33372 (76%)	19889 (78%)	4164 (16%)	1295 (5%)	2	19

5 of 1295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	39	ASP
1	AA	547	ILE
1	AA	551	VAL
1	AA	710	SER
1	AA	851	VAL

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	
1	AA	1310/1465 (89%)	1024 (78%)	286 (22%)	1	6
1	BA	1290/1465 (88%)	1012 (78%)	278 (22%)	1	6
1	CA	1308/1465 (89%)	1020 (78%)	288 (22%)	1	6
1	DA	1309/1465 (89%)	1019 (78%)	290 (22%)	1	6
1	EA	1309/1465 (89%)	1025 (78%)	284 (22%)	1	6
1	FA	1309/1465 (89%)	1019 (78%)	290 (22%)	1	6
2	AB	1012/1053 (96%)	780 (77%)	232 (23%)	1	5
2	BB	1010/1053 (96%)	783 (78%)	227 (22%)	1	6
2	CB	1024/1053 (97%)	778 (76%)	246 (24%)	0	4
2	DB	1020/1053 (97%)	784 (77%)	236 (23%)	1	5
2	EB	1021/1053 (97%)	782 (77%)	239 (23%)	1	5
2	FB	1021/1053 (97%)	780 (76%)	241 (24%)	1	5
3	AC	268/296 (90%)	217 (81%)	51 (19%)	1	9
3	BC	268/296 (90%)	217 (81%)	51 (19%)	1	9
3	CC	268/296 (90%)	216 (81%)	52 (19%)	1	9
3	DC	268/296 (90%)	217 (81%)	51 (19%)	1	9
3	EC	268/296 (90%)	216 (81%)	52 (19%)	1	9
3	FC	268/296 (90%)	218 (81%)	50 (19%)	1	9
4	AD	55/116 (47%)	47 (86%)	8 (14%)	3	16
4	BD	55/116 (47%)	46 (84%)	9 (16%)	2	13
4	CD	55/116 (47%)	47 (86%)	8 (14%)	3	16
4	DD	55/116 (47%)	46 (84%)	9 (16%)	2	13
4	ED	55/116 (47%)	47 (86%)	8 (14%)	3	16
4	FD	55/116 (47%)	47 (86%)	8 (14%)	3	16
5	AE	197/197 (100%)	158 (80%)	39 (20%)	1	8
5	BE	197/197 (100%)	159 (81%)	38 (19%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CE	197/197 (100%)	157 (80%)	40 (20%)	1	7
5	DE	197/197 (100%)	157 (80%)	40 (20%)	1	7
5	EE	197/197 (100%)	157 (80%)	40 (20%)	1	7
5	FE	197/197 (100%)	156 (79%)	41 (21%)	1	7
6	AF	88/137 (64%)	75 (85%)	13 (15%)	3	16
6	BF	88/137 (64%)	75 (85%)	13 (15%)	3	16
6	CF	89/137 (65%)	73 (82%)	16 (18%)	1	10
6	DF	89/137 (65%)	74 (83%)	15 (17%)	2	12
6	EF	89/137 (65%)	75 (84%)	14 (16%)	2	14
6	FF	89/137 (65%)	73 (82%)	16 (18%)	1	10
7	AG	180/291 (62%)	131 (73%)	49 (27%)	0	3
7	AO	50/291 (17%)	29 (58%)	21 (42%)	0	0
7	BG	173/291 (60%)	128 (74%)	45 (26%)	0	3
7	BO	49/291 (17%)	33 (67%)	16 (33%)	0	2
7	CG	180/291 (62%)	131 (73%)	49 (27%)	0	3
7	CO	48/291 (16%)	35 (73%)	13 (27%)	0	3
7	DG	180/291 (62%)	132 (73%)	48 (27%)	0	3
7	DO	50/291 (17%)	32 (64%)	18 (36%)	0	1
7	EG	180/291 (62%)	133 (74%)	47 (26%)	0	3
7	EO	50/291 (17%)	33 (66%)	17 (34%)	0	1
7	FG	180/291 (62%)	130 (72%)	50 (28%)	0	3
7	FO	50/291 (17%)	36 (72%)	14 (28%)	0	3
8	AH	116/128 (91%)	86 (74%)	30 (26%)	0	4
8	BH	115/128 (90%)	87 (76%)	28 (24%)	0	4
8	CH	115/128 (90%)	84 (73%)	31 (27%)	0	3
8	DH	117/128 (91%)	86 (74%)	31 (26%)	0	3
8	EH	117/128 (91%)	84 (72%)	33 (28%)	0	3
8	FH	117/128 (91%)	85 (73%)	32 (27%)	0	3
9	AI	109/110 (99%)	84 (77%)	25 (23%)	1	5
9	BI	86/110 (78%)	67 (78%)	19 (22%)	1	6
9	CI	109/110 (99%)	83 (76%)	26 (24%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	DI	109/110 (99%)	81 (74%)	28 (26%)	0	4
9	EI	104/110 (94%)	79 (76%)	25 (24%)	0	4
9	FI	109/110 (99%)	80 (73%)	29 (27%)	0	3
10	AJ	63/65 (97%)	47 (75%)	16 (25%)	0	4
10	BJ	64/65 (98%)	49 (77%)	15 (23%)	1	5
10	CJ	63/65 (97%)	49 (78%)	14 (22%)	1	6
10	DJ	64/65 (98%)	49 (77%)	15 (23%)	1	5
10	EJ	63/65 (97%)	50 (79%)	13 (21%)	1	7
10	FJ	63/65 (97%)	49 (78%)	14 (22%)	1	6
11	AK	91/130 (70%)	66 (72%)	25 (28%)	0	3
11	BK	90/130 (69%)	66 (73%)	24 (27%)	0	3
11	CK	91/130 (70%)	67 (74%)	24 (26%)	0	3
11	DK	91/130 (70%)	66 (72%)	25 (28%)	0	3
11	EK	90/130 (69%)	66 (73%)	24 (27%)	0	3
11	FK	90/130 (69%)	65 (72%)	25 (28%)	0	3
12	AL	39/57 (68%)	27 (69%)	12 (31%)	0	2
12	BL	39/57 (68%)	27 (69%)	12 (31%)	0	2
12	CL	39/57 (68%)	27 (69%)	12 (31%)	0	2
12	DL	39/57 (68%)	27 (69%)	12 (31%)	0	2
12	EL	39/57 (68%)	27 (69%)	12 (31%)	0	2
12	FL	39/57 (68%)	27 (69%)	12 (31%)	0	2
13	AM	99/371 (27%)	73 (74%)	26 (26%)	0	3
13	BM	99/371 (27%)	74 (75%)	25 (25%)	0	4
13	CM	99/371 (27%)	74 (75%)	25 (25%)	0	4
13	DM	99/371 (27%)	74 (75%)	25 (25%)	0	4
13	EM	100/371 (27%)	73 (73%)	27 (27%)	0	3
13	FM	100/371 (27%)	75 (75%)	25 (25%)	0	4
14	AN	132/220 (60%)	96 (73%)	36 (27%)	0	3
14	BN	133/220 (60%)	98 (74%)	35 (26%)	0	3
14	CN	133/220 (60%)	95 (71%)	38 (29%)	0	2
14	DN	135/220 (61%)	97 (72%)	38 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	EN	134/220 (61%)	97 (72%)	37 (28%)	0 3
14	FN	135/220 (61%)	99 (73%)	36 (27%)	0 3
All	All	22843/29562 (77%)	17621 (77%)	5222 (23%)	1 5

5 of 5222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EA	1444	ARG
1	FA	1465	GLU
2	EB	403	LEU
1	EA	1439	MET
8	EH	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 426 such sidechains are listed below:

Mol	Chain	Res	Type
2	DB	427	GLN
1	EA	470	HIS
2	FB	1171	ASN
2	DB	893	ASN
7	DG	67	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 42 ligands modelled in this entry, 42 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	EA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	EA	1261:VAL	C	1262:LEU	N	2.28

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
1	AA	1484/1664 (89%)	-0.15	10 (0%)	87	82	174, 197, 249, 308	0
1	BA	1462/1664 (87%)	0.05	18 (1%)	79	70	242, 262, 287, 314	0
1	CA	1483/1664 (89%)	-0.24	7 (0%)	91	85	143, 164, 201, 253	0
1	DA	1483/1664 (89%)	-0.25	3 (0%)	95	93	147, 170, 215, 278	0
1	EA	1484/1664 (89%)	-0.24	4 (0%)	94	90	149, 171, 207, 250	0
1	FA	1484/1664 (89%)	-0.28	2 (0%)	95	94	142, 160, 203, 262	0
2	AB	1154/1203 (95%)	-0.17	5 (0%)	92	87	179, 212, 250, 276	0
2	BB	1153/1203 (95%)	-0.09	9 (0%)	86	79	233, 245, 265, 279	0
2	CB	1170/1203 (97%)	-0.28	4 (0%)	94	90	144, 169, 196, 227	0
2	DB	1165/1203 (96%)	-0.22	2 (0%)	95	93	148, 169, 191, 222	0
2	EB	1164/1203 (96%)	-0.33	0	100	100	148, 162, 188, 225	0
2	FB	1165/1203 (96%)	-0.26	1 (0%)	95	94	142, 164, 191, 212	0
3	AC	304/335 (90%)	-0.07	0	100	100	190, 209, 237, 253	0
3	BC	304/335 (90%)	0.20	7 (2%)	60	52	248, 278, 311, 332	0
3	CC	304/335 (90%)	-0.19	0	100	100	162, 175, 191, 207	0
3	DC	304/335 (90%)	-0.14	2 (0%)	87	82	167, 182, 197, 206	0
3	EC	304/335 (90%)	-0.24	0	100	100	158, 173, 190, 203	0
3	FC	304/335 (90%)	-0.21	0	100	100	154, 170, 187, 198	0
4	AD	58/137 (42%)	-0.03	1 (1%)	70	61	207, 243, 266, 270	0
4	BD	58/137 (42%)	0.44	3 (5%)	27	26	262, 281, 301, 303	0
4	CD	58/137 (42%)	-0.24	1 (1%)	70	61	171, 184, 195, 200	0
4	DD	58/137 (42%)	-0.18	1 (1%)	70	61	177, 190, 204, 207	0
4	ED	58/137 (42%)	-0.28	1 (1%)	70	61	185, 202, 214, 215	0
4	FD	58/137 (42%)	-0.26	1 (1%)	70	61	162, 186, 211, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
5	AE	215/215 (100%)	-0.42	1 (0%)	91	85	186, 214, 234, 243	0
5	BE	215/215 (100%)	0.05	2 (0%)	84	77	255, 281, 296, 307	0
5	CE	215/215 (100%)	-0.52	0	100	100	152, 178, 194, 206	0
5	DE	215/215 (100%)	-0.37	0	100	100	156, 187, 209, 222	0
5	EE	215/215 (100%)	-0.38	0	100	100	158, 189, 211, 228	0
5	FE	215/215 (100%)	-0.43	0	100	100	149, 179, 199, 212	0
6	AF	98/155 (63%)	-0.37	0	100	100	181, 190, 240, 243	0
6	BF	98/155 (63%)	-0.09	0	100	100	251, 265, 299, 302	0
6	CF	99/155 (63%)	-0.36	0	100	100	148, 157, 185, 188	0
6	DF	99/155 (63%)	-0.36	0	100	100	152, 162, 201, 207	0
6	EF	99/155 (63%)	-0.44	0	100	100	154, 168, 211, 214	0
6	FF	99/155 (63%)	-0.34	0	100	100	144, 152, 209, 213	0
7	AG	202/326 (61%)	-0.02	2 (0%)	82	75	199, 249, 286, 305	0
7	AO	52/326 (15%)	0.16	1 (1%)	66	58	209, 235, 287, 294	0
7	BG	195/326 (59%)	0.42	9 (4%)	32	29	259, 290, 311, 319	0
7	BO	51/326 (15%)	0.00	1 (1%)	65	57	244, 259, 301, 312	0
7	CG	202/326 (61%)	-0.30	0	100	100	171, 186, 215, 221	0
7	CO	50/326 (15%)	-0.05	1 (2%)	65	57	159, 187, 235, 247	0
7	DG	202/326 (61%)	-0.00	1 (0%)	91	85	165, 205, 241, 251	0
7	DO	52/326 (15%)	0.03	1 (1%)	66	58	167, 197, 258, 276	0
7	EG	202/326 (61%)	-0.07	1 (0%)	91	85	181, 209, 227, 234	0
7	EO	52/326 (15%)	-0.24	0	100	100	168, 190, 233, 246	0
7	FG	202/326 (61%)	-0.01	0	100	100	158, 197, 226, 232	0
7	FO	52/326 (15%)	-0.25	0	100	100	163, 191, 241, 257	0
8	AH	132/146 (90%)	-0.28	0	100	100	180, 190, 197, 206	0
8	BH	131/146 (89%)	0.46	1 (0%)	86	79	282, 313, 328, 335	0
8	CH	131/146 (89%)	-0.16	0	100	100	162, 175, 183, 187	0
8	DH	134/146 (91%)	-0.25	0	100	100	167, 182, 196, 231	0
8	EH	134/146 (91%)	-0.21	0	100	100	164, 185, 201, 209	0
8	FH	134/146 (91%)	-0.18	0	100	100	151, 162, 173, 203	0
9	AI	124/125 (99%)	0.08	0	100	100	189, 209, 254, 260	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
9	BI	97/125 (77%)	0.22	1 (1%)	82	75	254, 264, 300, 307	0
9	CI	124/125 (99%)	-0.09	0	100	100	162, 179, 201, 206	0
9	DI	124/125 (99%)	-0.04	0	100	100	166, 187, 207, 214	0
9	EI	117/125 (93%)	-0.16	0	100	100	160, 177, 203, 235	0
9	FI	124/125 (99%)	-0.19	0	100	100	159, 181, 203, 211	0
10	AJ	68/70 (97%)	-0.24	0	100	100	194, 209, 227, 240	0
10	BJ	69/70 (98%)	0.01	2 (2%)	51	43	245, 263, 275, 279	0
10	CJ	68/70 (97%)	-0.31	0	100	100	162, 172, 183, 195	0
10	DJ	69/70 (98%)	-0.33	0	100	100	164, 174, 184, 191	0
10	EJ	68/70 (97%)	-0.42	0	100	100	155, 165, 177, 180	0
10	FJ	68/70 (97%)	-0.38	0	100	100	155, 165, 179, 186	0
11	AK	101/142 (71%)	-0.10	0	100	100	186, 193, 213, 220	0
11	BK	100/142 (70%)	0.03	0	100	100	259, 288, 305, 311	0
11	CK	101/142 (71%)	-0.23	0	100	100	157, 168, 182, 190	0
11	DK	101/142 (71%)	-0.36	0	100	100	161, 175, 190, 197	0
11	EK	100/142 (70%)	-0.38	0	100	100	154, 168, 182, 190	0
11	FK	100/142 (70%)	-0.41	0	100	100	150, 159, 174, 180	0
12	AL	44/70 (62%)	-0.04	0	100	100	201, 238, 253, 256	0
12	BL	44/70 (62%)	-0.08	0	100	100	241, 248, 255, 256	0
12	CL	44/70 (62%)	-0.28	0	100	100	163, 184, 192, 193	0
12	DL	44/70 (62%)	-0.17	0	100	100	167, 184, 191, 195	0
12	EL	44/70 (62%)	-0.40	0	100	100	158, 176, 188, 191	0
12	FL	44/70 (62%)	-0.28	0	100	100	159, 183, 193, 196	0
13	AM	109/415 (26%)	0.15	1 (0%)	84	77	228, 248, 259, 263	0
13	BM	109/415 (26%)	0.26	1 (0%)	84	77	247, 257, 278, 284	0
13	CM	109/415 (26%)	-0.12	1 (0%)	84	77	181, 196, 202, 205	0
13	DM	109/415 (26%)	0.09	1 (0%)	84	77	181, 197, 211, 218	0
13	EM	110/415 (26%)	-0.07	1 (0%)	84	77	173, 189, 198, 203	0
13	FM	110/415 (26%)	0.01	1 (0%)	84	77	177, 191, 198, 200	0
14	AN	142/233 (60%)	0.15	2 (1%)	75	66	194, 234, 266, 270	0
14	BN	143/233 (61%)	0.29	3 (2%)	63	55	254, 266, 283, 297	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
14	CN	143/233 (61%)	-0.24	0	100	100	166, 187, 208, 219	0
14	DN	145/233 (62%)	-0.22	0	100	100	167, 197, 213, 220	0
14	EN	144/233 (61%)	-0.35	0	100	100	160, 184, 203, 214	0
14	FN	145/233 (62%)	-0.27	0	100	100	157, 184, 204, 214	0
All	All	25720/33372 (77%)	-0.18	117 (0%)	91	85	142, 184, 273, 335	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	BD	12	THR	6.7
3	BC	184	VAL	3.6
1	BA	634	ASN	3.6
2	BB	441	LYS	3.5
3	BC	108	VAL	3.5

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	ZN	DI	3002	1/1	0.85	0.10	195,195,195,195	0
15	ZN	BJ	3001	1/1	0.88	0.15	267,267,267,267	0
15	ZN	BI	3002	1/1	0.90	0.31	311,311,311,311	0
15	ZN	BA	3002	1/1	0.91	0.16	283,283,283,283	0
15	ZN	AI	3001	1/1	0.92	0.05	247,247,247,247	0
15	ZN	AJ	3001	1/1	0.93	0.25	197,197,197,197	0
15	ZN	FA	3002	1/1	0.93	0.12	202,202,202,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
15	ZN	EA	3002	1/1	0.94	0.10	215,215,215,215	0
15	ZN	BA	3001	1/1	0.94	0.11	248,248,248,248	0
15	ZN	AI	3002	1/1	0.95	0.10	213,213,213,213	0
15	ZN	AA	3001	1/1	0.96	0.07	222,222,222,222	0
15	ZN	CA	3001	1/1	0.96	0.09	168,168,168,168	0
15	ZN	EI	3002	1/1	0.96	0.06	198,198,198,198	0
15	ZN	CA	3002	1/1	0.96	0.11	205,205,205,205	0
15	ZN	CI	3002	1/1	0.97	0.11	195,195,195,195	0
15	ZN	DA	3002	1/1	0.97	0.08	211,211,211,211	0
15	ZN	DB	3001	1/1	0.97	0.18	172,172,172,172	0
15	ZN	BL	3001	1/1	0.97	0.07	245,245,245,245	0
15	ZN	AB	3001	1/1	0.97	0.13	214,214,214,214	0
15	ZN	EB	3001	1/1	0.97	0.16	169,169,169,169	0
15	ZN	EI	3001	1/1	0.97	0.08	187,187,187,187	0
15	ZN	AA	3002	1/1	0.97	0.10	262,262,262,262	0
15	ZN	EL	3001	1/1	0.97	0.09	176,176,176,176	0
15	ZN	CI	3001	1/1	0.97	0.07	194,194,194,194	0
15	ZN	FB	3001	1/1	0.97	0.19	163,163,163,163	0
15	ZN	FI	3001	1/1	0.97	0.09	189,189,189,189	0
15	ZN	FL	3001	1/1	0.97	0.10	184,184,184,184	0
15	ZN	BB	3001	1/1	0.98	0.17	252,252,252,252	0
15	ZN	BI	3001	1/1	0.98	0.09	257,257,257,257	0
15	ZN	AL	3001	1/1	0.98	0.05	241,241,241,241	0
15	ZN	FA	3001	1/1	0.98	0.12	178,178,178,178	0
15	ZN	DJ	3001	1/1	0.98	0.22	167,167,167,167	0
15	ZN	EA	3001	1/1	0.98	0.16	171,171,171,171	0
15	ZN	CL	3001	1/1	0.98	0.07	185,185,185,185	0
15	ZN	FI	3002	1/1	0.98	0.07	190,190,190,190	0
15	ZN	DA	3001	1/1	0.98	0.11	177,177,177,177	0
15	ZN	EJ	3001	1/1	0.99	0.20	159,159,159,159	0
15	ZN	DL	3001	1/1	0.99	0.07	184,184,184,184	0
15	ZN	CB	3001	1/1	0.99	0.13	167,167,167,167	0
15	ZN	FJ	3001	1/1	0.99	0.15	157,157,157,157	0
15	ZN	CJ	3001	1/1	0.99	0.25	164,164,164,164	0
15	ZN	DI	3001	1/1	1.00	0.10	195,195,195,195	0

6.5 Other polymers

There are no such residues in this entry.