wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 08:28 pm GMT

PDB ID	:	6G2I
EMDB ID	:	EMD-4344
Title	:	Filament of acetyl-CoA carboxylase and BRCT domains of BRCA1 (ACC-BRCT) at 5.9 A resolution
Authors	:	Hunkeler, M.; Hagmann, A.; Stuttfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on	:	2018-03-23
Resolution	:	5.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

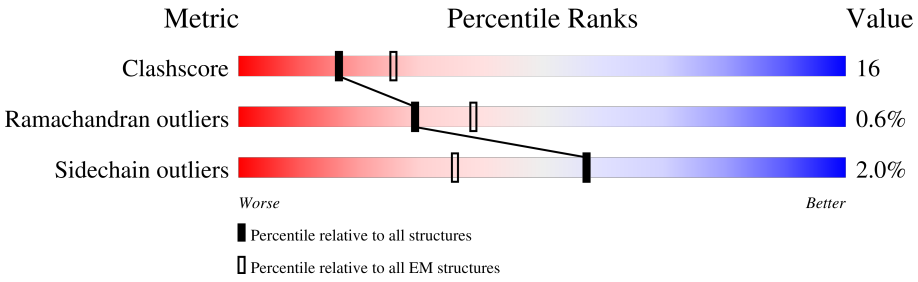
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2346	65% 58% 28% • 11%
1	B	2346	65% 58% 28% • 11%
1	C	2346	45% 54% 32% • 11%
1	D	2346	27% 48% 35% • • 11%
1	E	2346	27% 50% 36% • 11%
1	F	2346	45% 56% 30% • 11%
1	G	2346	31% 23% 9% 68%
1	J	2346	56% 41% 14% • 44%

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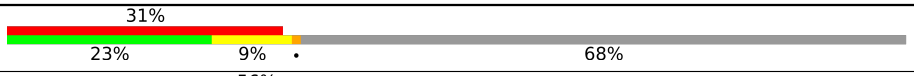
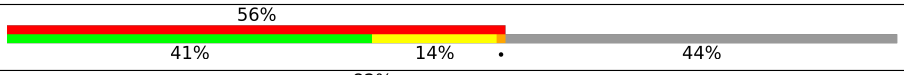
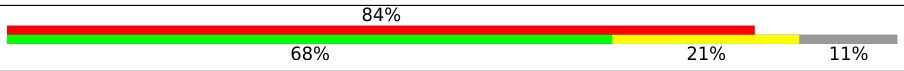
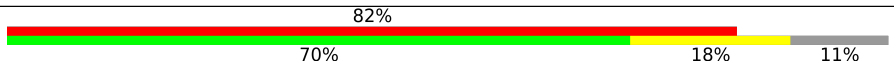
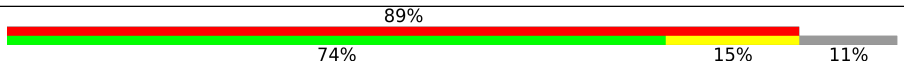
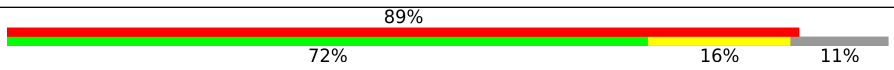
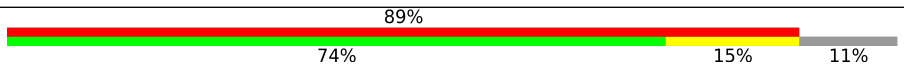
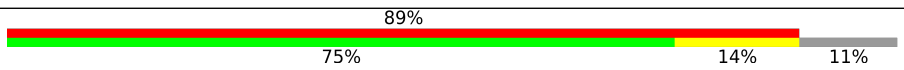
Mol	Chain	Length	Quality of chain
1	Q	2346	
1	R	2346	
2	H	240	
2	K	240	
2	M	240	
2	O	240	
2	S	240	
2	U	240	
2	W	240	
2	Y	240	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 288810 atoms, of which 143374 are hydrogens and 0 are deuteriums.

In the tables below, 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 Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms							AltConf	Trace
1	D	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	E	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	C	2080	Total	C	H	N	O	P	S	0	0
			32757	10493	16275	2855	3033	1	100		
1	F	2080	Total	C	H	N	O	P	S	0	0
			32757	10493	16275	2855	3033	1	100		
1	B	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	A	2080	Total	C	H	N	O	P	S	0	0
			32758	10493	16276	2855	3033	1	100		
1	G	757	Total	C	H	N	O	S		0	0
			12055	3855	5997	1050	1124	29			
1	Q	757	Total	C	H	N	O	S		0	0
			12055	3855	5997	1050	1124	29			
1	J	1323	Total	C	H	N	O	P	S	0	0
			20703	6638	10279	1805	1909	1	71		
1	R	1323	Total	C	H	N	O	P	S	0	0
			20703	6638	10279	1805	1909	1	71		

- Molecule 2 is a protein called Breast cancer type 1 susceptibility protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		
2	K	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		
2	M	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		
2	O	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		
2	S	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	U	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		
2	Y	214	Total	C	H	N	O	S	0	0
			3347	1084	1648	289	312	14		
2	W	214	Total	C	H	N	O	S	0	0
			3340	1083	1644	286	313	14		

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1620	MET	-	initiating methionine	UNP P38398
H	1621	LYS	-	expression tag	UNP P38398
H	1622	HIS	-	expression tag	UNP P38398
H	1623	HIS	-	expression tag	UNP P38398
H	1624	HIS	-	expression tag	UNP P38398
H	1625	HIS	-	expression tag	UNP P38398
H	1626	HIS	-	expression tag	UNP P38398
H	1627	HIS	-	expression tag	UNP P38398
H	1628	PRO	-	expression tag	UNP P38398
H	1629	MET	-	expression tag	UNP P38398
H	1630	THR	-	expression tag	UNP P38398
H	1631	SER	-	expression tag	UNP P38398
H	1632	LEU	-	expression tag	UNP P38398
H	1633	TYR	-	expression tag	UNP P38398
H	1634	LYS	-	expression tag	UNP P38398
H	1635	LYS	-	expression tag	UNP P38398
H	1636	ALA	-	expression tag	UNP P38398
H	1637	GLY	-	expression tag	UNP P38398
H	1638	LEU	-	expression tag	UNP P38398
H	1639	GLU	-	expression tag	UNP P38398
H	1640	ASN	-	expression tag	UNP P38398
H	1641	LEU	-	expression tag	UNP P38398
H	1642	TYR	-	expression tag	UNP P38398
H	1643	PHE	-	expression tag	UNP P38398
H	1644	GLN	-	expression tag	UNP P38398
H	1645	GLY	-	expression tag	UNP P38398
K	1620	MET	-	initiating methionine	UNP P38398
K	1621	LYS	-	expression tag	UNP P38398
K	1622	HIS	-	expression tag	UNP P38398
K	1623	HIS	-	expression tag	UNP P38398
K	1624	HIS	-	expression tag	UNP P38398
K	1625	HIS	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1626	HIS	-	expression tag	UNP P38398
K	1627	HIS	-	expression tag	UNP P38398
K	1628	PRO	-	expression tag	UNP P38398
K	1629	MET	-	expression tag	UNP P38398
K	1630	THR	-	expression tag	UNP P38398
K	1631	SER	-	expression tag	UNP P38398
K	1632	LEU	-	expression tag	UNP P38398
K	1633	TYR	-	expression tag	UNP P38398
K	1634	LYS	-	expression tag	UNP P38398
K	1635	LYS	-	expression tag	UNP P38398
K	1636	ALA	-	expression tag	UNP P38398
K	1637	GLY	-	expression tag	UNP P38398
K	1638	LEU	-	expression tag	UNP P38398
K	1639	GLU	-	expression tag	UNP P38398
K	1640	ASN	-	expression tag	UNP P38398
K	1641	LEU	-	expression tag	UNP P38398
K	1642	TYR	-	expression tag	UNP P38398
K	1643	PHE	-	expression tag	UNP P38398
K	1644	GLN	-	expression tag	UNP P38398
K	1645	GLY	-	expression tag	UNP P38398
M	1620	MET	-	initiating methionine	UNP P38398
M	1621	LYS	-	expression tag	UNP P38398
M	1622	HIS	-	expression tag	UNP P38398
M	1623	HIS	-	expression tag	UNP P38398
M	1624	HIS	-	expression tag	UNP P38398
M	1625	HIS	-	expression tag	UNP P38398
M	1626	HIS	-	expression tag	UNP P38398
M	1627	HIS	-	expression tag	UNP P38398
M	1628	PRO	-	expression tag	UNP P38398
M	1629	MET	-	expression tag	UNP P38398
M	1630	THR	-	expression tag	UNP P38398
M	1631	SER	-	expression tag	UNP P38398
M	1632	LEU	-	expression tag	UNP P38398
M	1633	TYR	-	expression tag	UNP P38398
M	1634	LYS	-	expression tag	UNP P38398
M	1635	LYS	-	expression tag	UNP P38398
M	1636	ALA	-	expression tag	UNP P38398
M	1637	GLY	-	expression tag	UNP P38398
M	1638	LEU	-	expression tag	UNP P38398
M	1639	GLU	-	expression tag	UNP P38398
M	1640	ASN	-	expression tag	UNP P38398
M	1641	LEU	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1642	TYR	-	expression tag	UNP P38398
M	1643	PHE	-	expression tag	UNP P38398
M	1644	GLN	-	expression tag	UNP P38398
M	1645	GLY	-	expression tag	UNP P38398
O	1620	MET	-	initiating methionine	UNP P38398
O	1621	LYS	-	expression tag	UNP P38398
O	1622	HIS	-	expression tag	UNP P38398
O	1623	HIS	-	expression tag	UNP P38398
O	1624	HIS	-	expression tag	UNP P38398
O	1625	HIS	-	expression tag	UNP P38398
O	1626	HIS	-	expression tag	UNP P38398
O	1627	HIS	-	expression tag	UNP P38398
O	1628	PRO	-	expression tag	UNP P38398
O	1629	MET	-	expression tag	UNP P38398
O	1630	THR	-	expression tag	UNP P38398
O	1631	SER	-	expression tag	UNP P38398
O	1632	LEU	-	expression tag	UNP P38398
O	1633	TYR	-	expression tag	UNP P38398
O	1634	LYS	-	expression tag	UNP P38398
O	1635	LYS	-	expression tag	UNP P38398
O	1636	ALA	-	expression tag	UNP P38398
O	1637	GLY	-	expression tag	UNP P38398
O	1638	LEU	-	expression tag	UNP P38398
O	1639	GLU	-	expression tag	UNP P38398
O	1640	ASN	-	expression tag	UNP P38398
O	1641	LEU	-	expression tag	UNP P38398
O	1642	TYR	-	expression tag	UNP P38398
O	1643	PHE	-	expression tag	UNP P38398
O	1644	GLN	-	expression tag	UNP P38398
O	1645	GLY	-	expression tag	UNP P38398
S	1620	MET	-	initiating methionine	UNP P38398
S	1621	LYS	-	expression tag	UNP P38398
S	1622	HIS	-	expression tag	UNP P38398
S	1623	HIS	-	expression tag	UNP P38398
S	1624	HIS	-	expression tag	UNP P38398
S	1625	HIS	-	expression tag	UNP P38398
S	1626	HIS	-	expression tag	UNP P38398
S	1627	HIS	-	expression tag	UNP P38398
S	1628	PRO	-	expression tag	UNP P38398
S	1629	MET	-	expression tag	UNP P38398
S	1630	THR	-	expression tag	UNP P38398
S	1631	SER	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
S	1632	LEU	-	expression tag	UNP P38398
S	1633	TYR	-	expression tag	UNP P38398
S	1634	LYS	-	expression tag	UNP P38398
S	1635	LYS	-	expression tag	UNP P38398
S	1636	ALA	-	expression tag	UNP P38398
S	1637	GLY	-	expression tag	UNP P38398
S	1638	LEU	-	expression tag	UNP P38398
S	1639	GLU	-	expression tag	UNP P38398
S	1640	ASN	-	expression tag	UNP P38398
S	1641	LEU	-	expression tag	UNP P38398
S	1642	TYR	-	expression tag	UNP P38398
S	1643	PHE	-	expression tag	UNP P38398
S	1644	GLN	-	expression tag	UNP P38398
S	1645	GLY	-	expression tag	UNP P38398
U	1620	MET	-	initiating methionine	UNP P38398
U	1621	LYS	-	expression tag	UNP P38398
U	1622	HIS	-	expression tag	UNP P38398
U	1623	HIS	-	expression tag	UNP P38398
U	1624	HIS	-	expression tag	UNP P38398
U	1625	HIS	-	expression tag	UNP P38398
U	1626	HIS	-	expression tag	UNP P38398
U	1627	HIS	-	expression tag	UNP P38398
U	1628	PRO	-	expression tag	UNP P38398
U	1629	MET	-	expression tag	UNP P38398
U	1630	THR	-	expression tag	UNP P38398
U	1631	SER	-	expression tag	UNP P38398
U	1632	LEU	-	expression tag	UNP P38398
U	1633	TYR	-	expression tag	UNP P38398
U	1634	LYS	-	expression tag	UNP P38398
U	1635	LYS	-	expression tag	UNP P38398
U	1636	ALA	-	expression tag	UNP P38398
U	1637	GLY	-	expression tag	UNP P38398
U	1638	LEU	-	expression tag	UNP P38398
U	1639	GLU	-	expression tag	UNP P38398
U	1640	ASN	-	expression tag	UNP P38398
U	1641	LEU	-	expression tag	UNP P38398
U	1642	TYR	-	expression tag	UNP P38398
U	1643	PHE	-	expression tag	UNP P38398
U	1644	GLN	-	expression tag	UNP P38398
U	1645	GLY	-	expression tag	UNP P38398
Y	1620	MET	-	initiating methionine	UNP P38398
Y	1621	LYS	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	1622	HIS	-	expression tag	UNP P38398
Y	1623	HIS	-	expression tag	UNP P38398
Y	1624	HIS	-	expression tag	UNP P38398
Y	1625	HIS	-	expression tag	UNP P38398
Y	1626	HIS	-	expression tag	UNP P38398
Y	1627	HIS	-	expression tag	UNP P38398
Y	1628	PRO	-	expression tag	UNP P38398
Y	1629	MET	-	expression tag	UNP P38398
Y	1630	THR	-	expression tag	UNP P38398
Y	1631	SER	-	expression tag	UNP P38398
Y	1632	LEU	-	expression tag	UNP P38398
Y	1633	TYR	-	expression tag	UNP P38398
Y	1634	LYS	-	expression tag	UNP P38398
Y	1635	LYS	-	expression tag	UNP P38398
Y	1636	ALA	-	expression tag	UNP P38398
Y	1637	GLY	-	expression tag	UNP P38398
Y	1638	LEU	-	expression tag	UNP P38398
Y	1639	GLU	-	expression tag	UNP P38398
Y	1640	ASN	-	expression tag	UNP P38398
Y	1641	LEU	-	expression tag	UNP P38398
Y	1642	TYR	-	expression tag	UNP P38398
Y	1643	PHE	-	expression tag	UNP P38398
Y	1644	GLN	-	expression tag	UNP P38398
Y	1645	GLY	-	expression tag	UNP P38398
W	1620	MET	-	initiating methionine	UNP P38398
W	1621	LYS	-	expression tag	UNP P38398
W	1622	HIS	-	expression tag	UNP P38398
W	1623	HIS	-	expression tag	UNP P38398
W	1624	HIS	-	expression tag	UNP P38398
W	1625	HIS	-	expression tag	UNP P38398
W	1626	HIS	-	expression tag	UNP P38398
W	1627	HIS	-	expression tag	UNP P38398
W	1628	PRO	-	expression tag	UNP P38398
W	1629	MET	-	expression tag	UNP P38398
W	1630	THR	-	expression tag	UNP P38398
W	1631	SER	-	expression tag	UNP P38398
W	1632	LEU	-	expression tag	UNP P38398
W	1633	TYR	-	expression tag	UNP P38398
W	1634	LYS	-	expression tag	UNP P38398
W	1635	LYS	-	expression tag	UNP P38398
W	1636	ALA	-	expression tag	UNP P38398
W	1637	GLY	-	expression tag	UNP P38398

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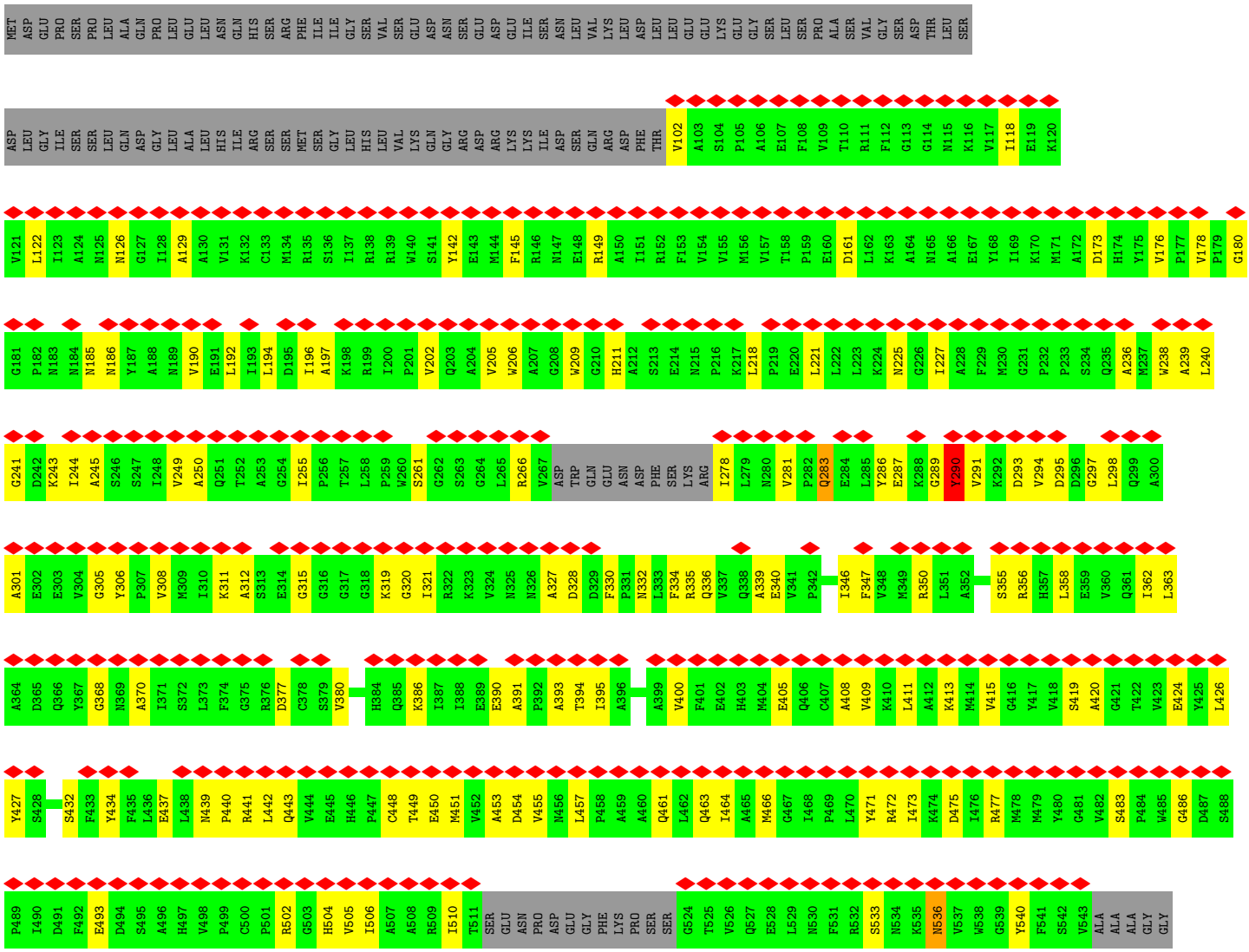
Chain	Residue	Modelled	Actual	Comment	Reference
W	1638	LEU	-	expression tag	UNP P38398
W	1639	GLU	-	expression tag	UNP P38398
W	1640	ASN	-	expression tag	UNP P38398
W	1641	LEU	-	expression tag	UNP P38398
W	1642	TYR	-	expression tag	UNP P38398
W	1643	PHE	-	expression tag	UNP P38398
W	1644	GLN	-	expression tag	UNP P38398
W	1645	GLY	-	expression tag	UNP P38398

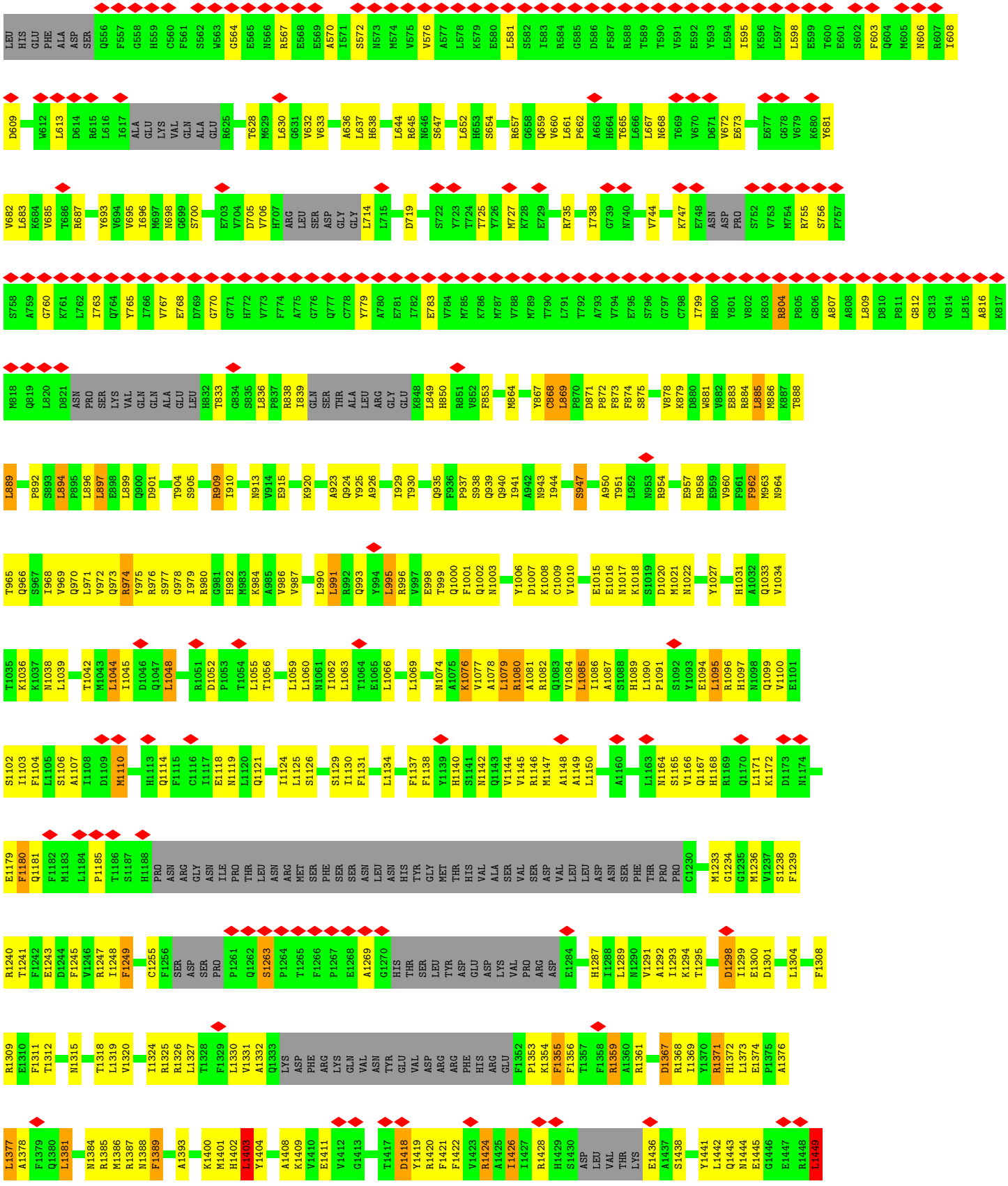
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Acetyl-CoA carboxylase 1

Chain D:




LEU HIS GLU PHE ALA ASP SER Q556 F557 G558 H559 C560 F561 S562 W563 G564 E565 N566 R567 E568 E569 A570 I571 S572 N573 M574 V575 V576 A577 L578 K579 E580 L581 S582 I583 R584 G585 D586 F587 R588 T589 T590 V591 E592 Y593 L594 I595 K596 L597 L598 E599 T600 E601 S602 F603 Q604 M605 N606 R607 I608
D609 W612 L613 D614 R615 L616 I617 ALA GLU LYS VAL GLN ALA GLU R625 T628 M629 L630 G631 V632 V633 A636 L637 H638 L644 R645 N646 S647 L652 H653 S654 R657 G658 Q659 V660 L661 P662 A663 H664 T665 L666 L667 N668 T669 V670 D671 V672 E673 E677 G678 V679 K680 Y681
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E1179 F1180 Q1181 F1182 M1183 L1184 P1185 T1186 S1187 H1188 PRO ASN ARG GLY ASN ILE PRO THR LEU ASN ARG MET SER PHE SER SER ASN LEU ASN HIS TYR GLY MET THR HIS VAL ALA SER VAL SER ASP VAL LEU LEU ASP ASN SER PHE THR PRO PRO C1230 M1233 G1234 G1235 M1236 Y1237 S1238 F1239
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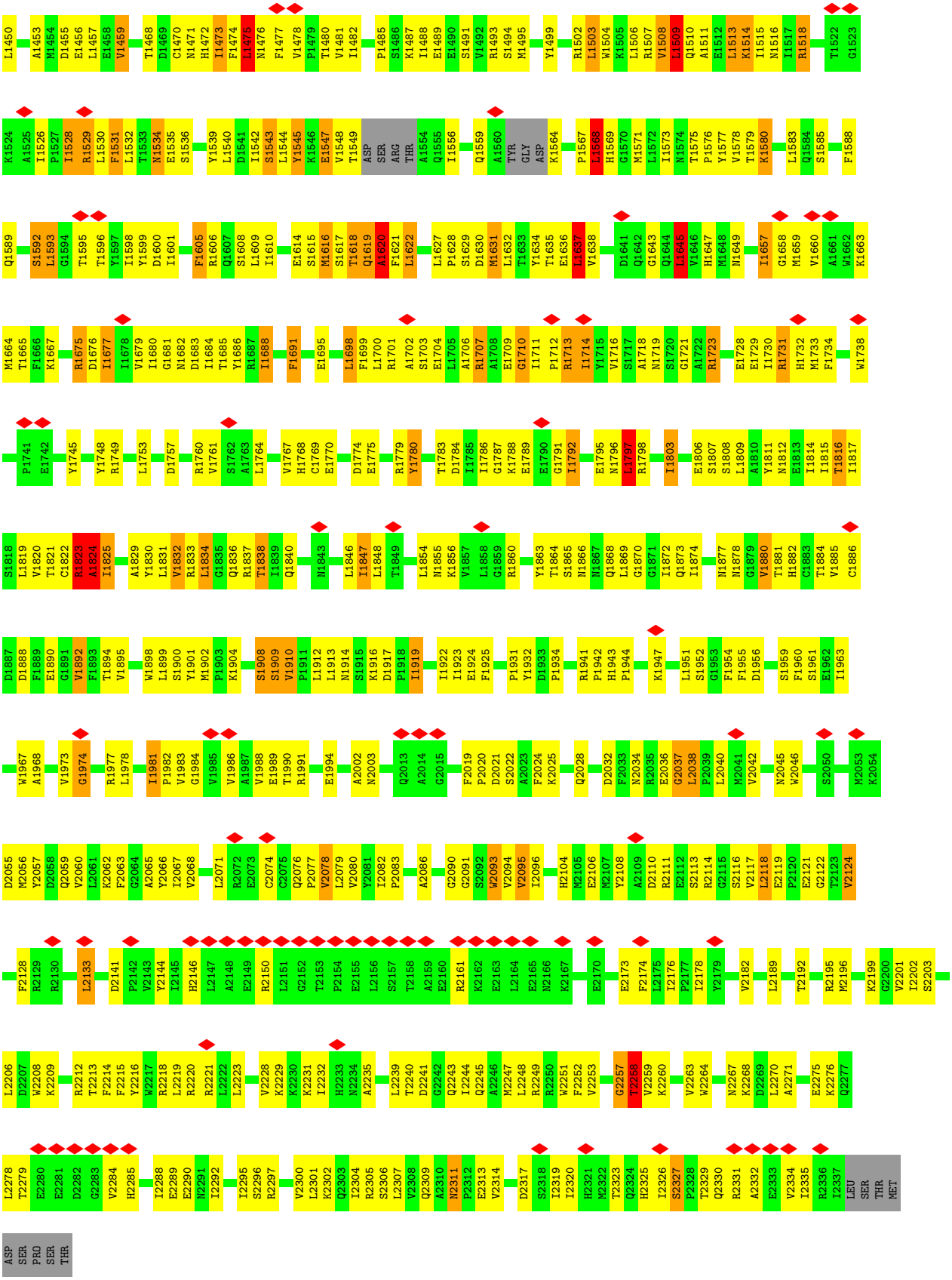
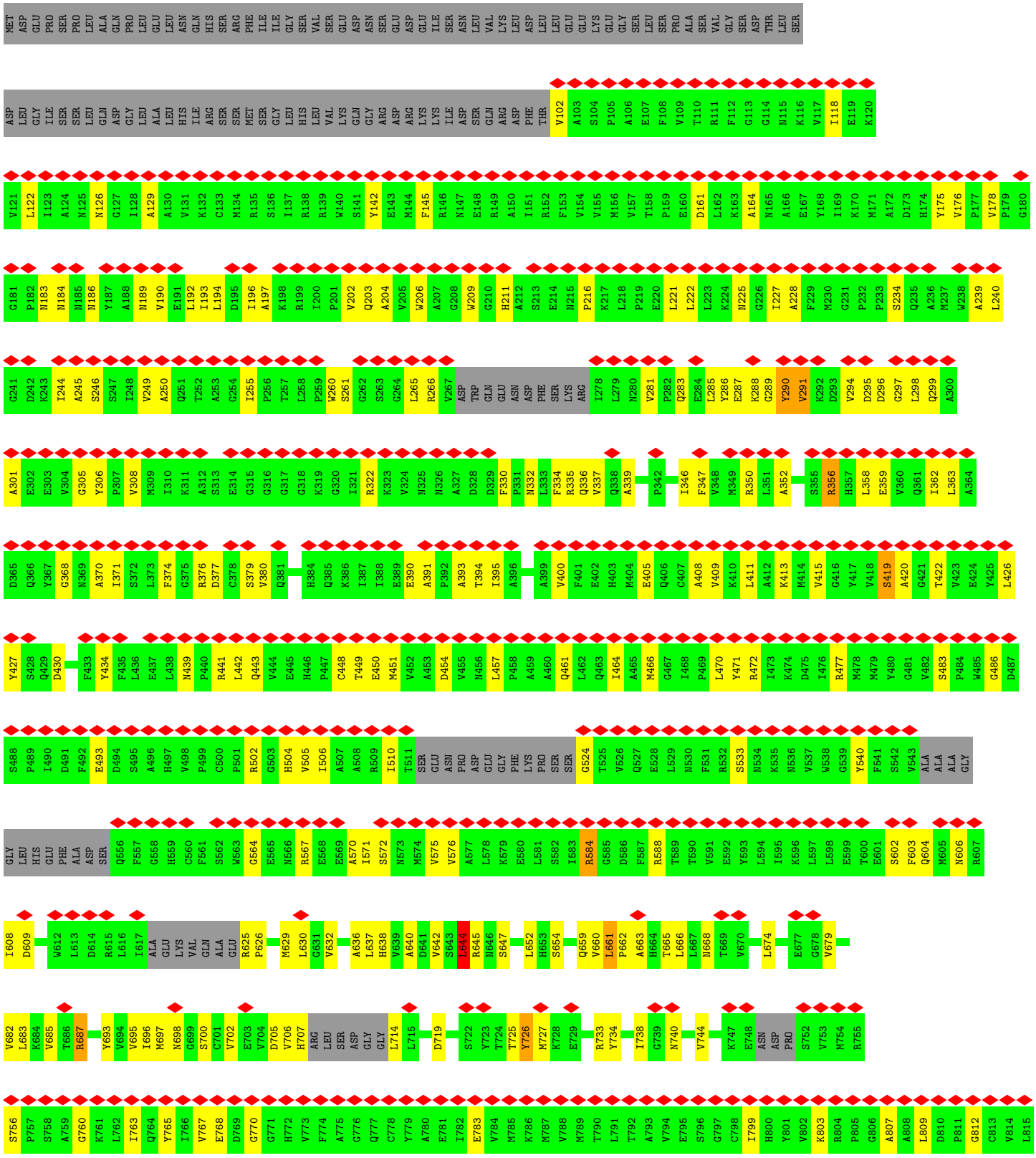


• Molecule 1: Acetyl-CoA carboxylase 1

Chain E:


27%
50%
36%
11%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ASP LEU GLY ILE SER SER LEU GLN ASP GLY LEU ALA LEU HIS ILE ARG SER SER MET SER GLY LEU HIS LEU VAL LYS GLN GLY ARG ASP ARG LYS LYS ILE ASP SER GLN ARG ASP PHE THR V102 A103 S104 P105 A106 E107 F108 V109 T110 R111 F112 G113 G114 N115 K116 V117 I118 E119 K120
V121 L122 I123 A124 N125 N126 G127 I128 A129 A130 V131 K132 C133 M134 R135 S136 I137 R138 R139 W140 S141 Y142 E143 M144 F145 R146 N147 E148 R149 A150 I151 R152 F153 V154 V155 M156 V157 T158 P159 E160 D161 L162 K163 A164 N165 A166 E167 Y168 I169 K170 M171 A172 D173 H174 Y175 V176 P177 V178 P179 G180
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S488 P489 I490 D491 F492 E493 D494 S495 A496 H497 V498 P499 C500 P501 R502 G503 H504 V505 I506 A507 A508 R509 I510 T511 SER GLU ASN PRO ASP GLU GLY PHE LYS PRO SER SER G524 T525 V526 Q527 E528 L529 N530 F531 R532 S533 N534 K535 N536 V537 W538 G539 Y540 F541 S542 V543 ALA ALA ALA GLY
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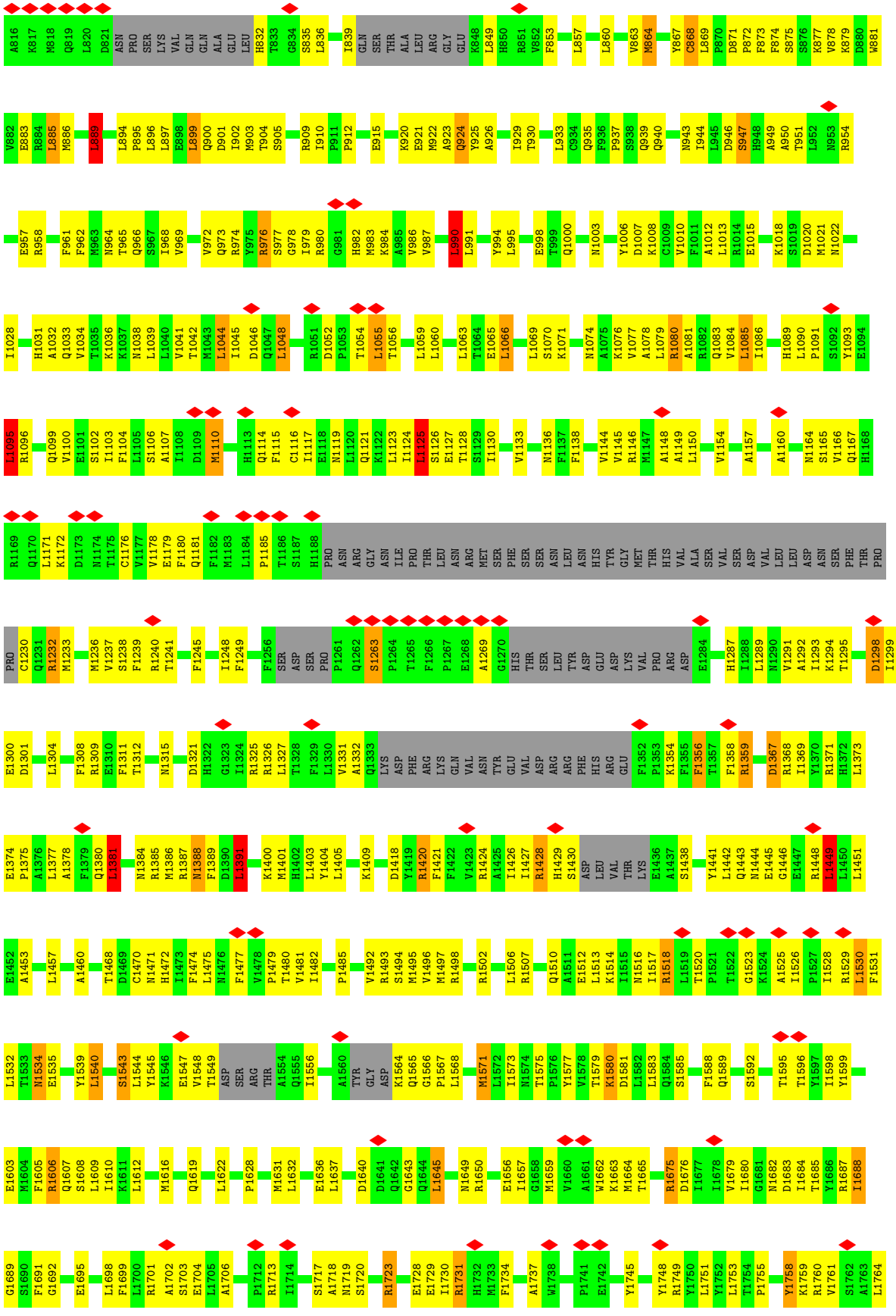
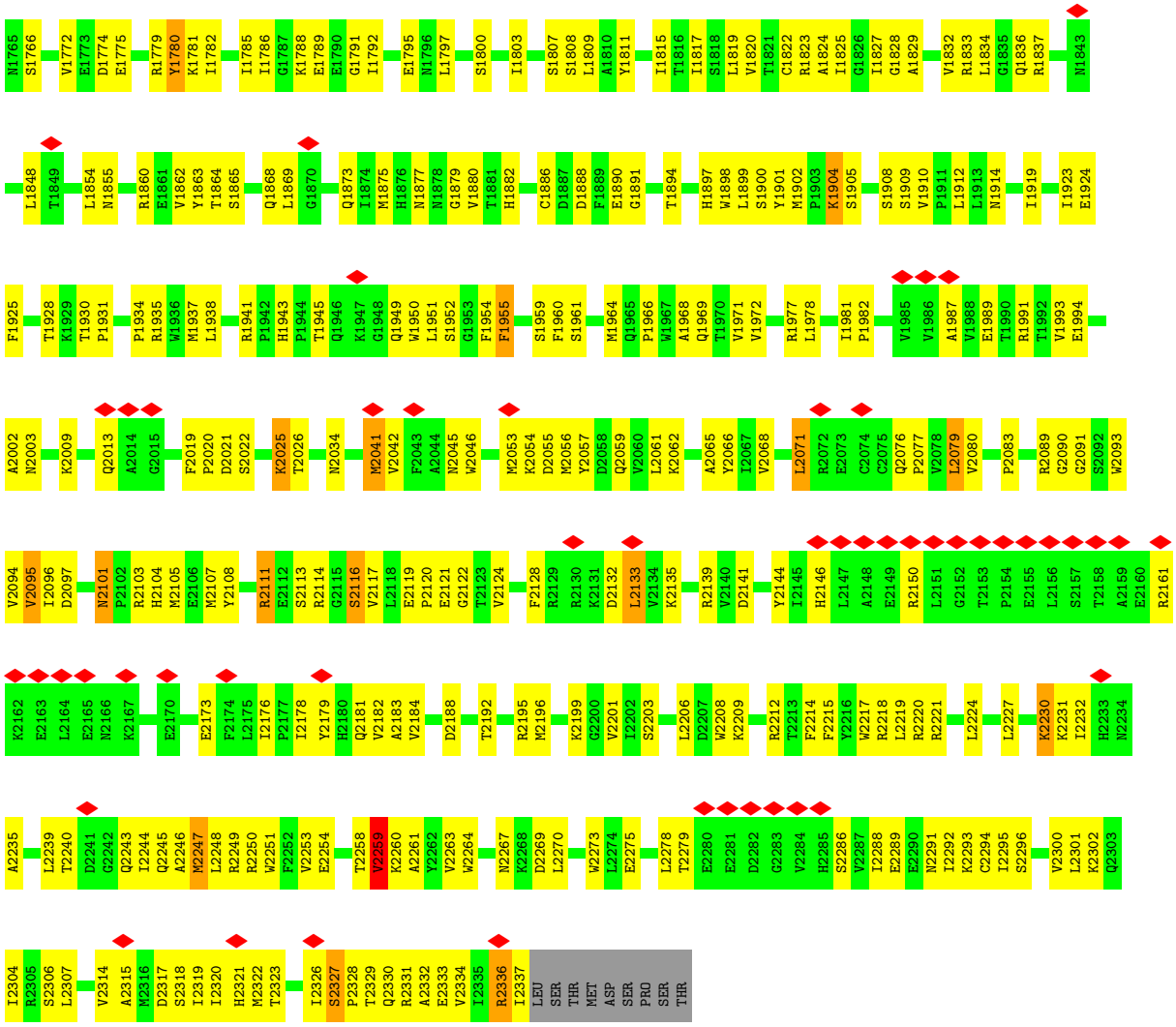
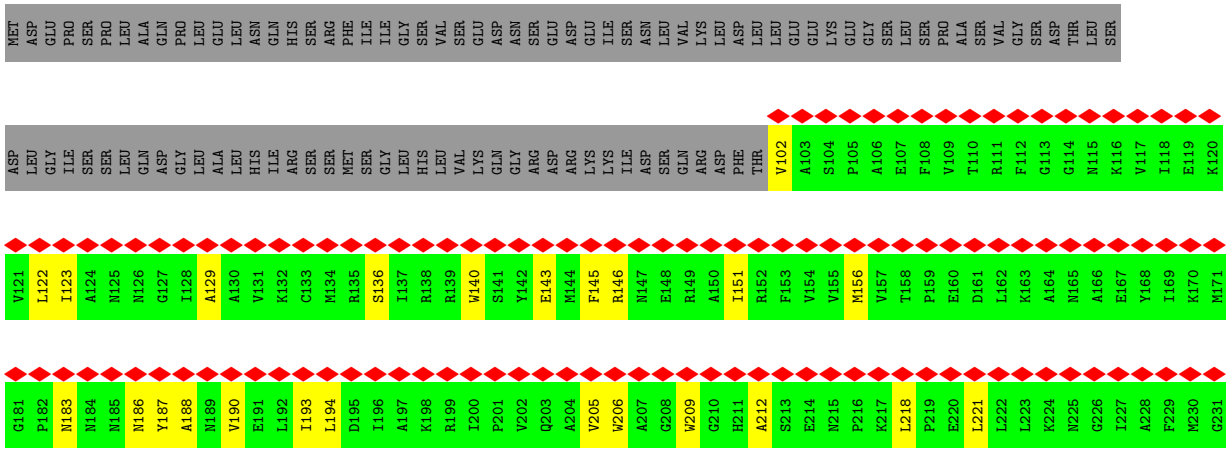
I608 D609 W612 L613 D614 R615 L616 I617 ALA GLU LYS VAL GLN ALA GLU R625 P626 M629 L630 G631 V632 A636 L637 H638 V639 A640 D641 V642 S643 L644 R645 N646 S647 L652 H653 S654 Q659 V660 L661 P662 A663 H664 T665 L666 L667 N668 T669 V670 L674 E677 G678 V679
V682 L683 K684 V685 T686 R687 Y693 V694 V695 I696 M697 N698 G699 S700 C701 V702 E703 V704 D705 V706 H707 ARG LEU SER ASP GLY GLY L714 L715 D719 S722 Y723 T724 T725 Y726 M727 K728 E729 R733 Y734 I738 G739 N740 V744 K747 E748 ASN ASP PRO S752 V753 M754 R755
S756 P757 S758 A759 G760 K761 L762 I763 Q764 Y765 I766 V767 E768 D769 G770 G771 H772 V773 F774 A775 G776 Q777 C778 Y779 A780 E781 I782 E783 V784 M785 K786 M787 V788 M789 T790 L791 T792 A793 V794 E795 S796 G797 C798 I799 H800 Y801 V802 K803 R804 P805 G806 A807 A808 L809 D810 P811 G812 C813 V814 L815

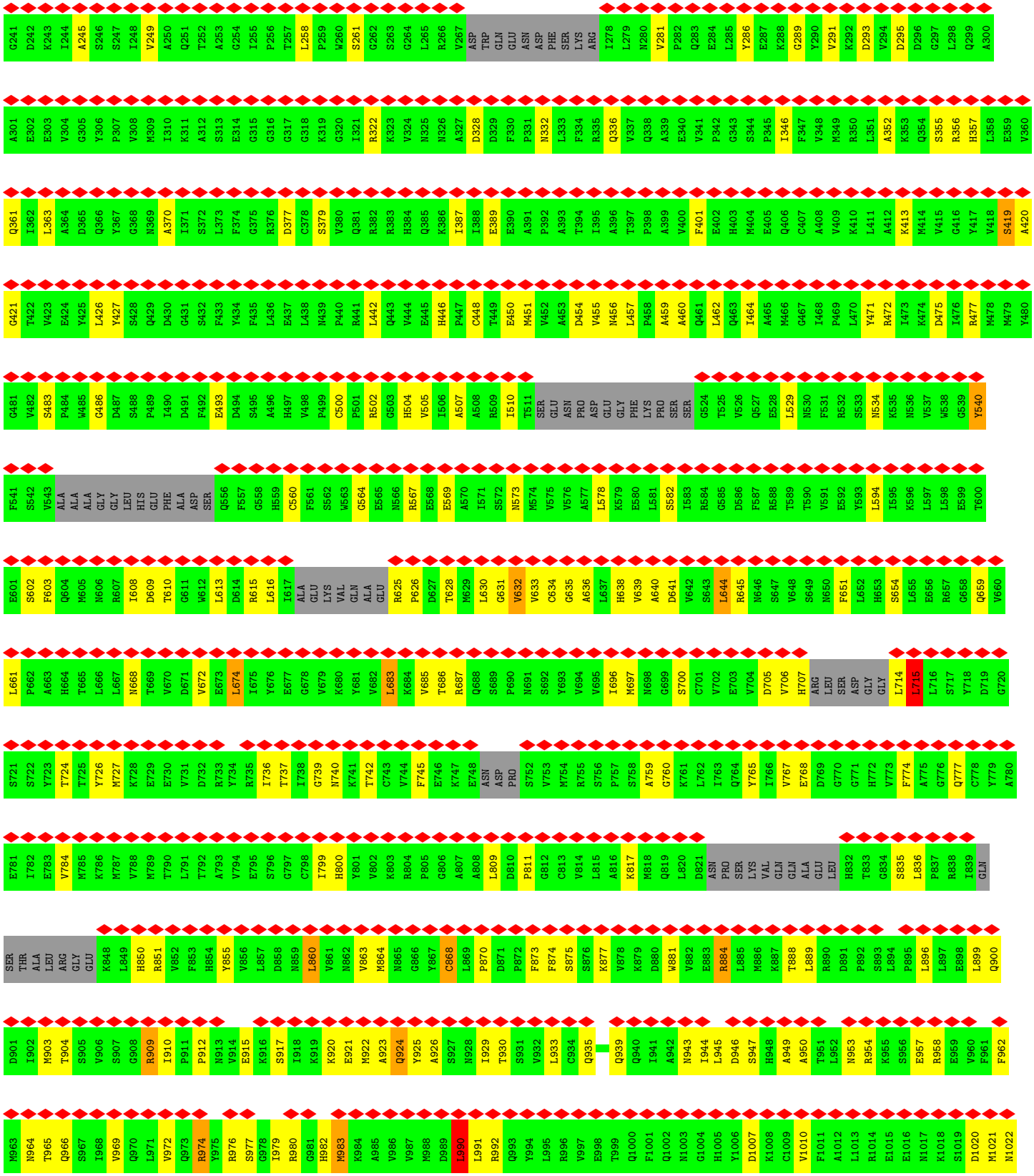




• Molecule 1: Acetyl-CoA carboxylase 1

Chain C:

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A301 E302 E303 V304 G305 Y306 P307 V308 M309 I310 K311 A312 S313 E314 G315 G316 G317 G318 K319 G320 I321 R322 K323 V324 N325 N326 A327 D328 D329 F330 P331 N332 L333 F334 R335 Q336 V337 Q338 A339 E340 V341 P342 G343 S344 P345 I346 F347 V348 M349 R350 L351 A352 K353 Q354 S355 R356 H357 L358 E359 V360
Q361 I362 L363 A364 D365 Q366 Y367 G368 N369 A370 I371 S372 L373 F374 G375 R376 D377 C378 S379 V380 Q381 R382 R383 H384 Q385 K386 I387 I388 E389 E390 A391 P392 A393 T394 I395 A396 T397 P398 A399 V400 F401 E402 H403 M404 E405 Q406 C407 A408 V409 K410 L411 A412 K413 M414 V415 G416 Y417 V418 S419 A420
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G481 V482 S483 P484 W485 G486 D487 S488 P489 I490 D491 F492 E493 D494 S495 A496 H497 V498 P499 C500 P501 R502 G503 H504 V505 I506 A507 A508 R509 I510 T511 SER GLU ASN PRO ASP GLU GLY PHE LYS PRO SER SER G524 T525 V526 Q527 E528 L529 N530 F531 R532 S533 N534 K535 N536 V537 W538 G539 Y540
F541 S542 V543 ALA ALA ALA GLY GLY LEU HIS GLU PHE ALA ASP SER Q556 F557 G558 H559 C560 F561 S562 W563 G564 E565 N566 R567 E568 E569 A570 I571 S572 N573 M574 V575 V576 A577 L578 K579 E580 L581 S582 I583 R584 G585 D586 F587 R588 T589 T590 V591 E592 Y593 L594 I595 K596 L597 L598 E599 T600
E601 S602 F603 Q604 M605 N606 R607 I608 D609 T610 G611 W612 L613 D614 R615 L616 I617 ALA GLU LYS VAL GLN ALA GLU R625 P626 D627 T628 W629 L630 G631 V632 V633 C634 G635 A636 L637 H638 V639 A640 D641 V642 S643 L644 R645 N646 S647 V648 S649 N650 F651 L652 H653 S654 L655 E656 R657 G658 Q659 V660
L661 P662 A663 H664 T665 L666 L667 N668 T669 V670 D671 V672 E673 L674 I675 Y676 E677 G678 V679 K680 Y681 V682 L683 K684 V685 T686 R687 Q688 S689 P690 N691 S692 Y693 V694 V695 I696 M697 N698 G699 S700 C701 V702 E703 V704 D705 V706 H707 ARG LEU SER ASP GLY GLY L714 L715 L716 S717 Y718 D719 G720
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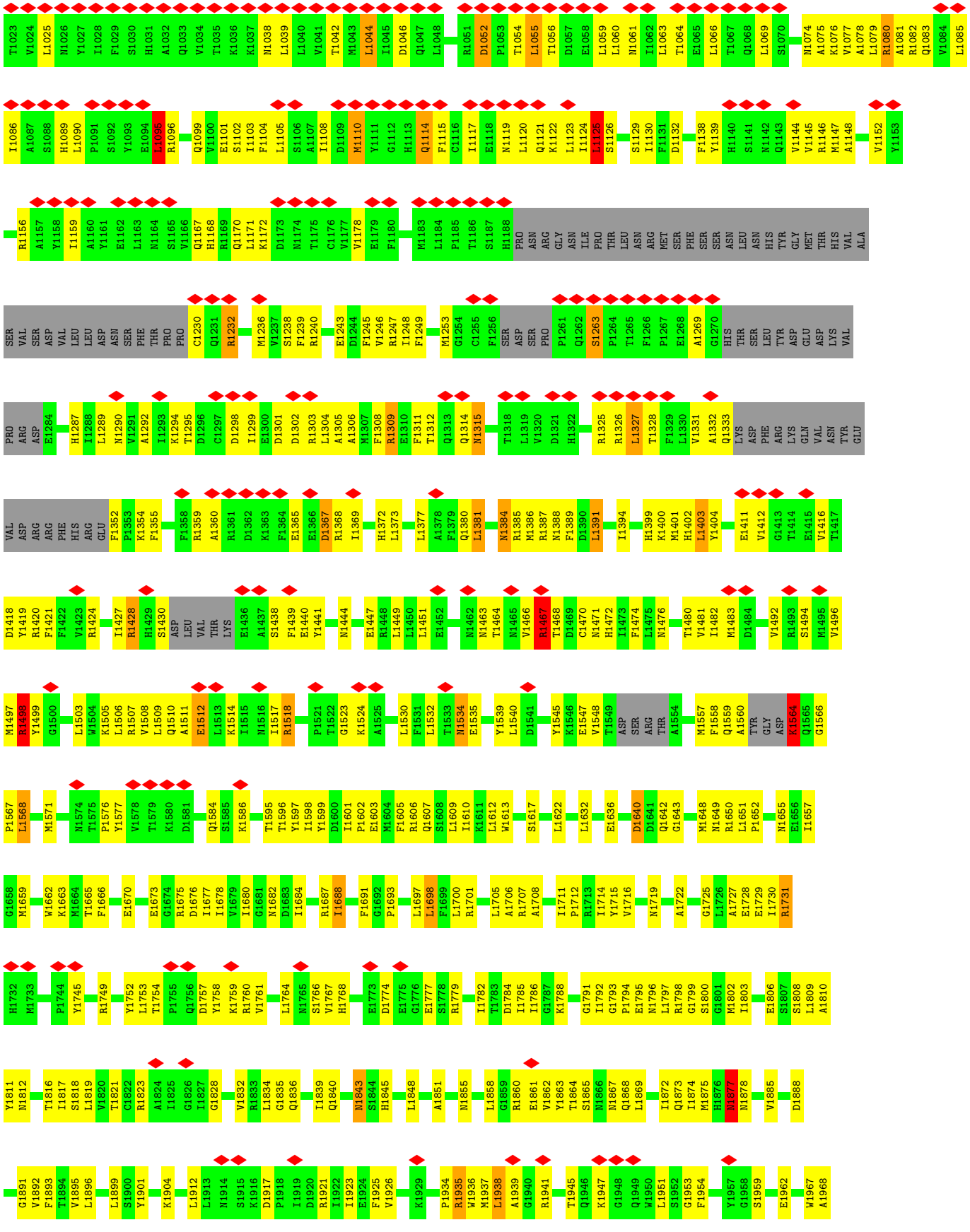
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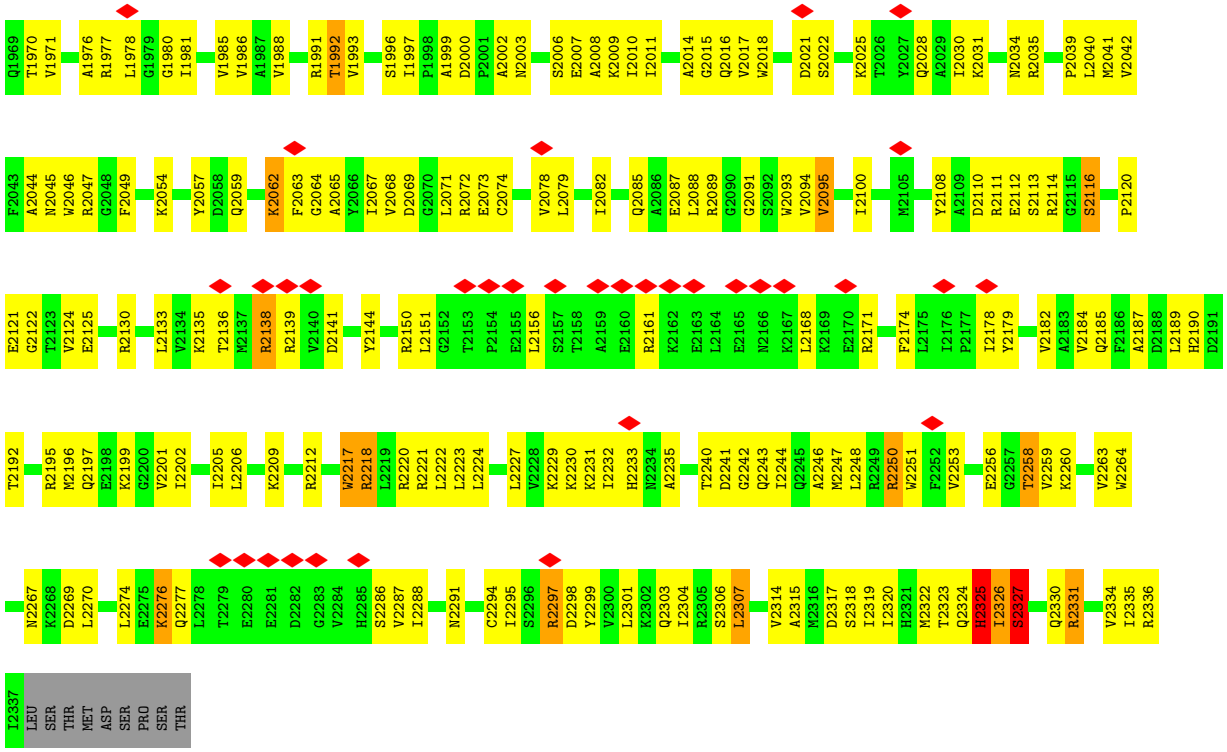
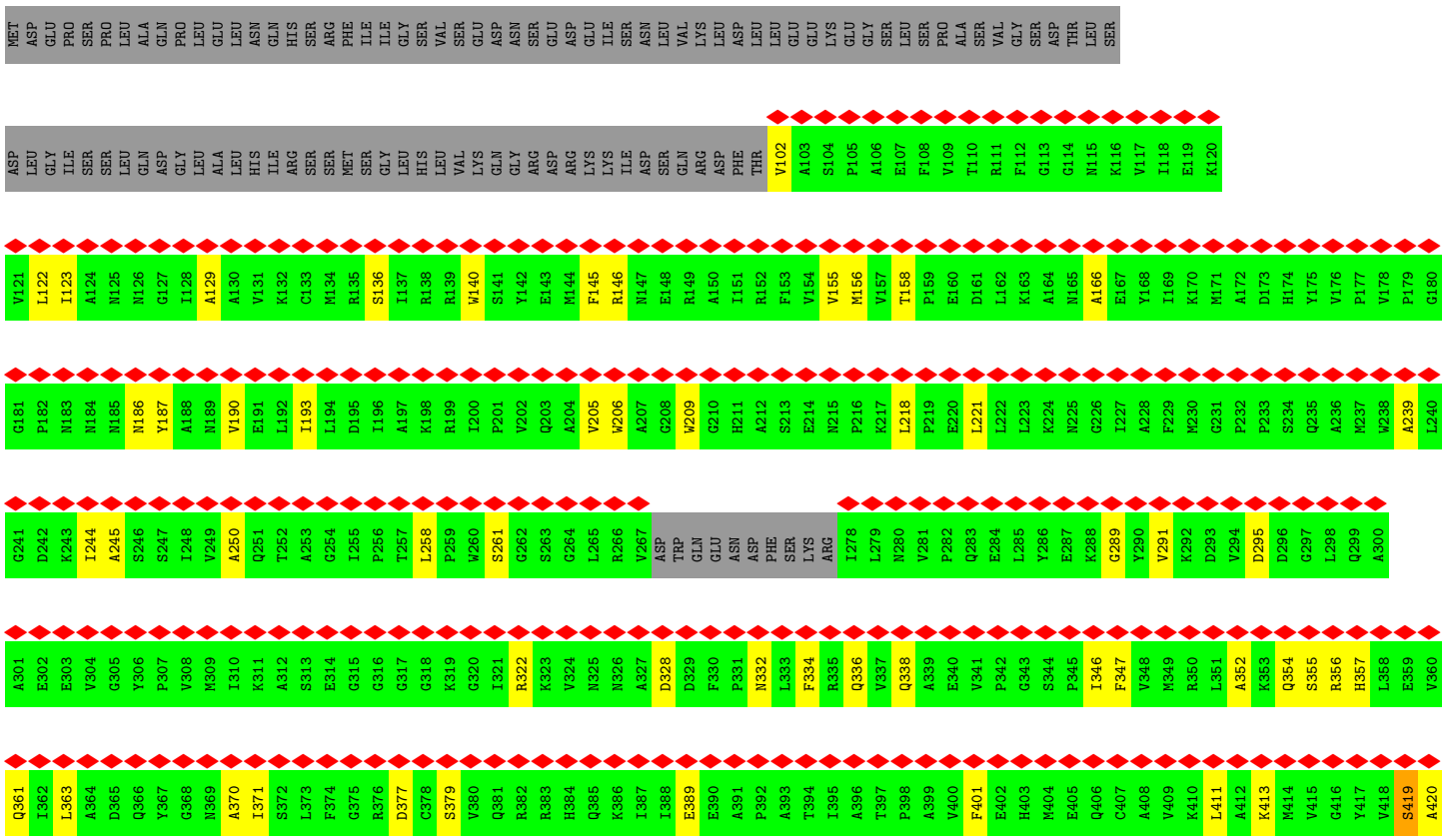
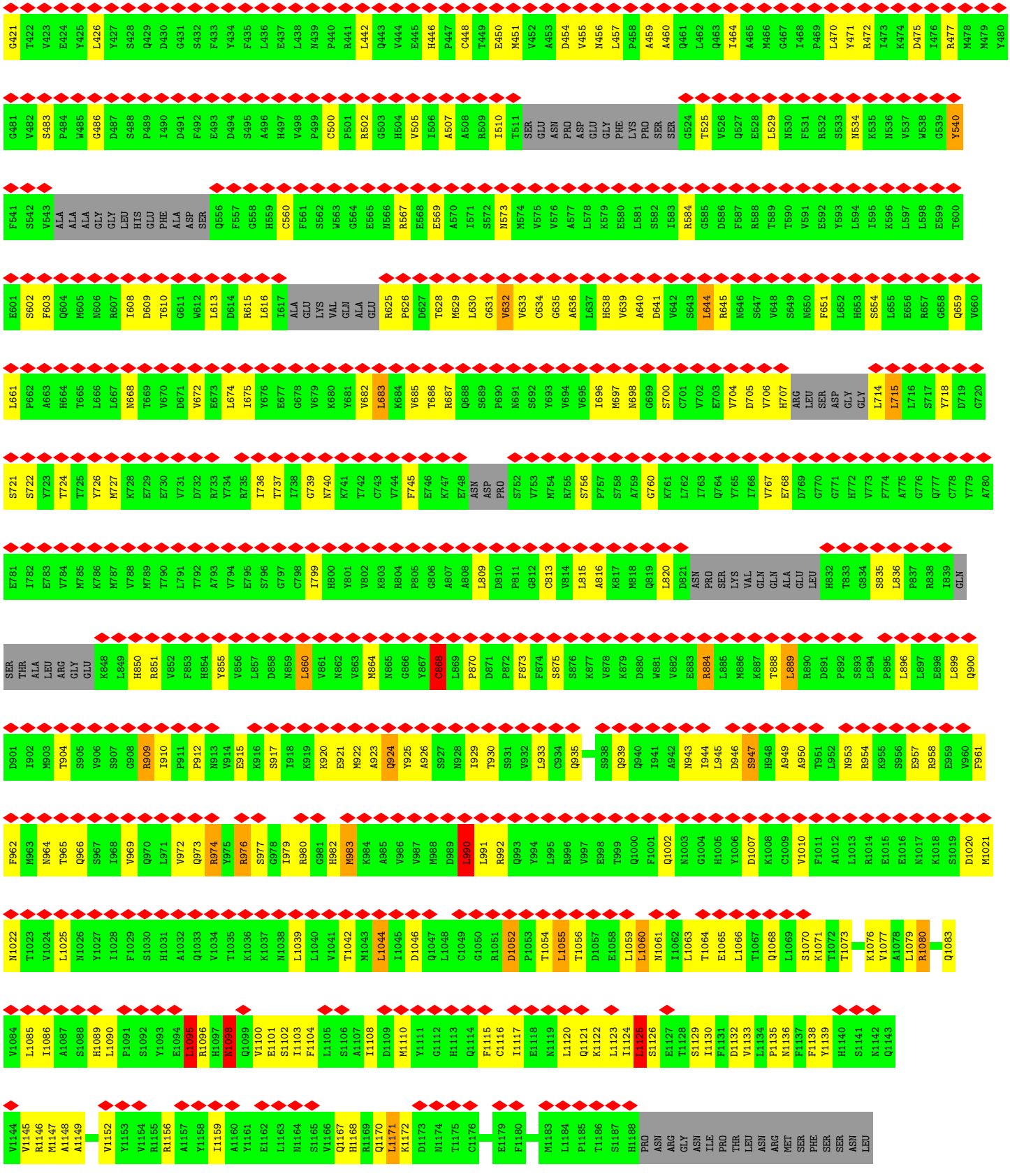


• Molecule 1: Acetyl-CoA carboxylase 1

Chain F:

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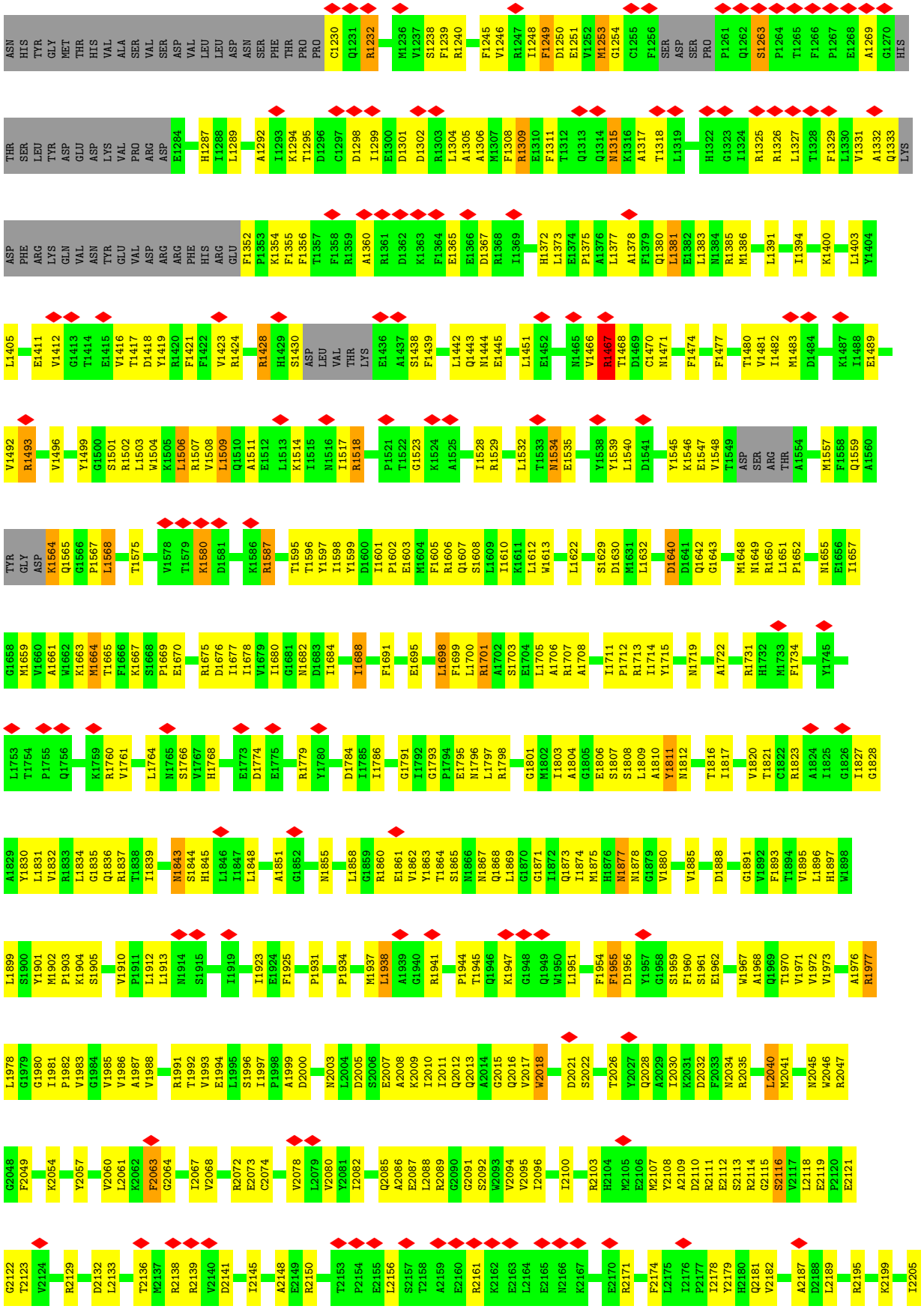
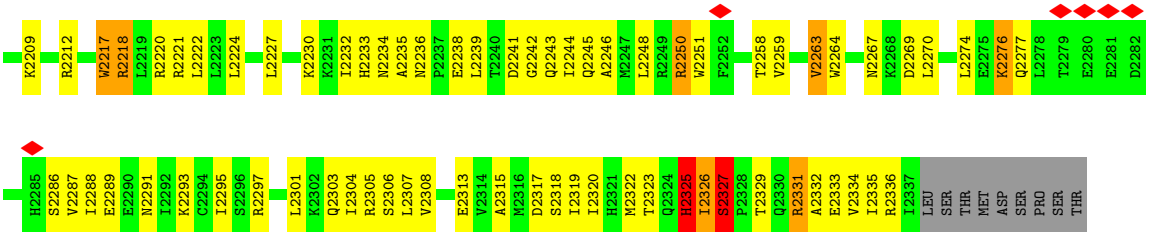
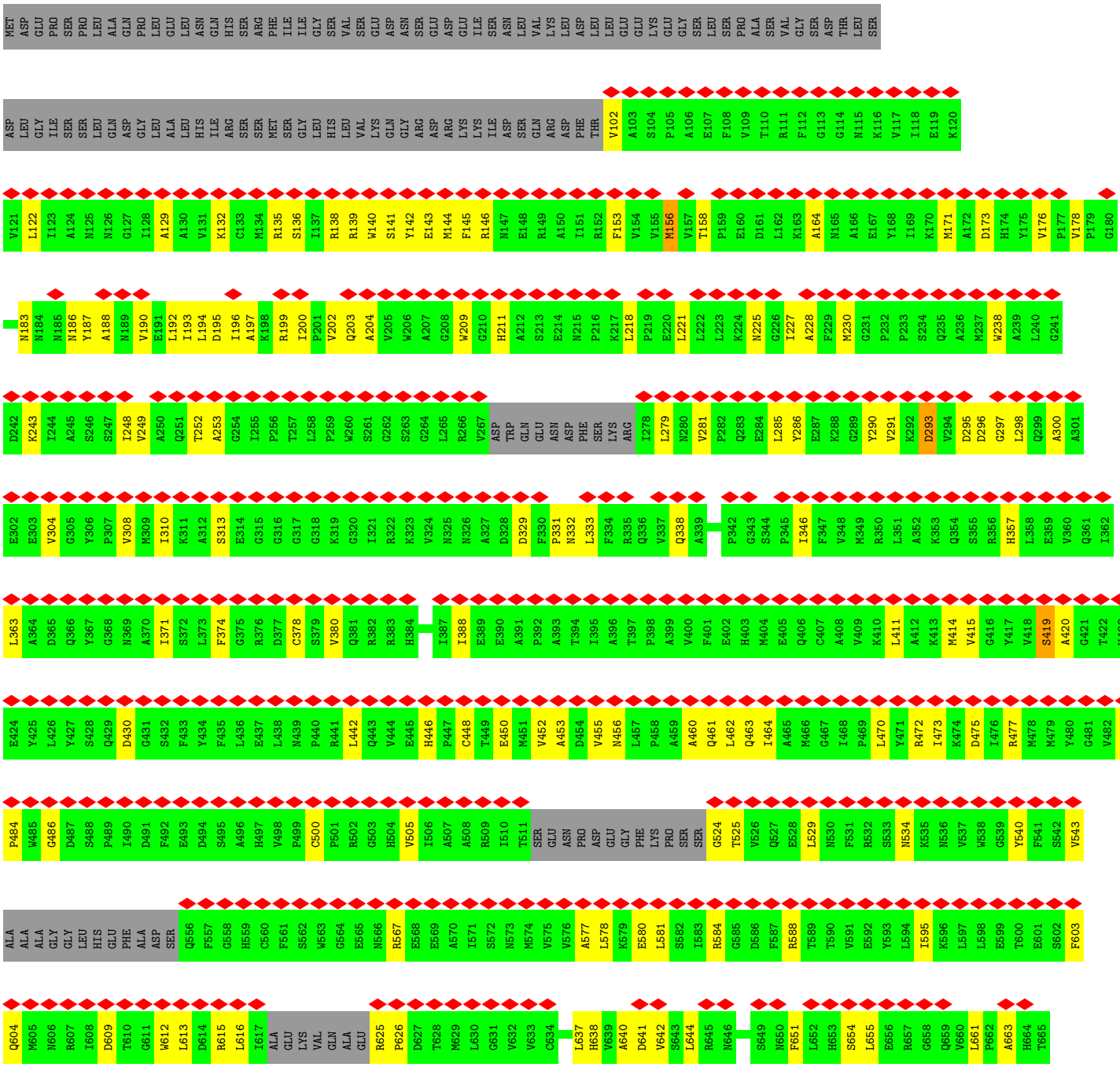
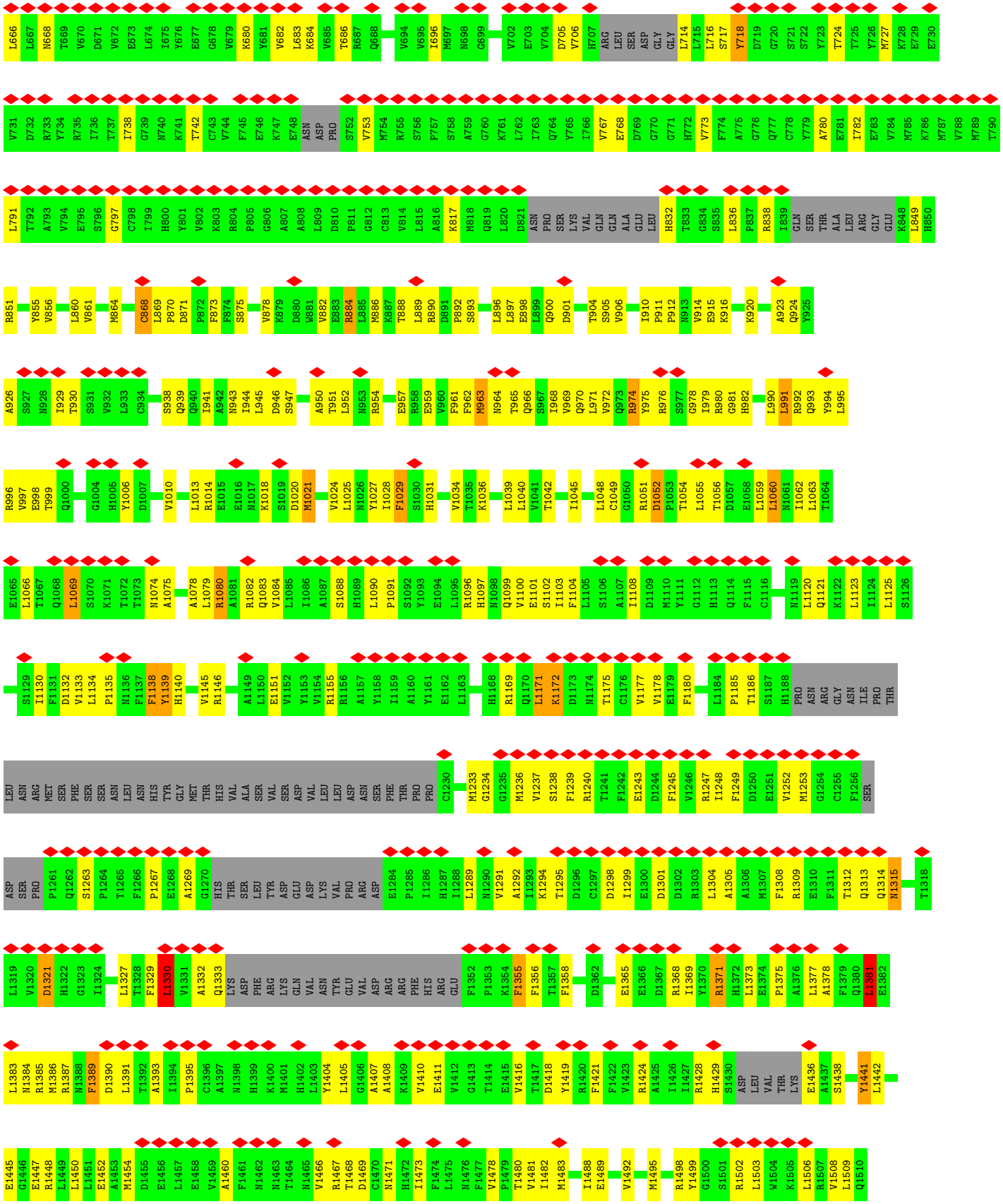




• Molecule 1: Acetyl-CoA carboxylase 1

Chain B:

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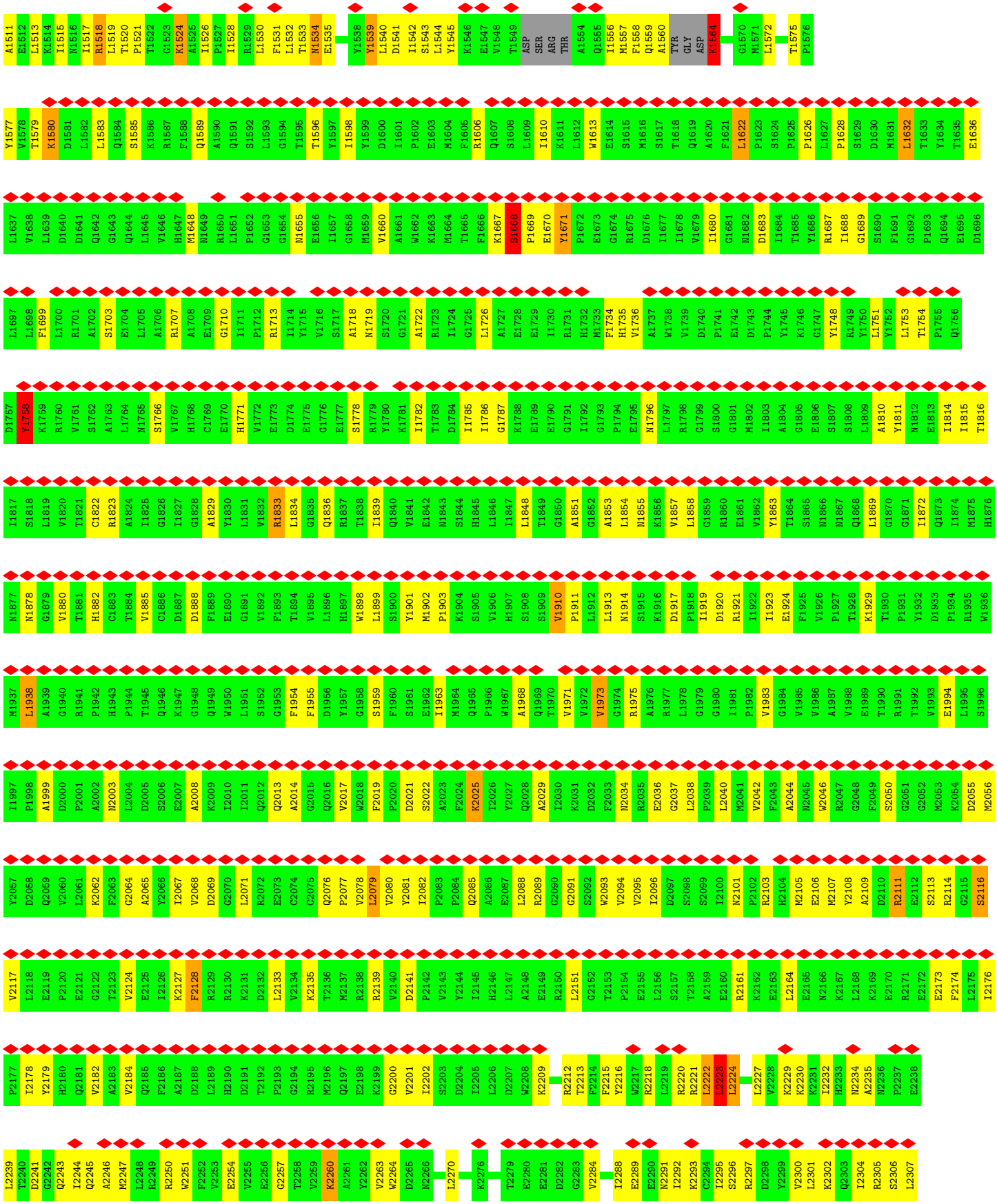
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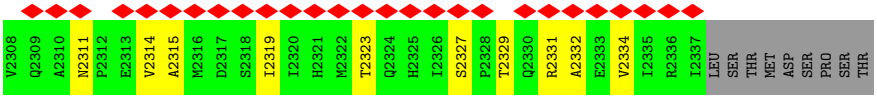
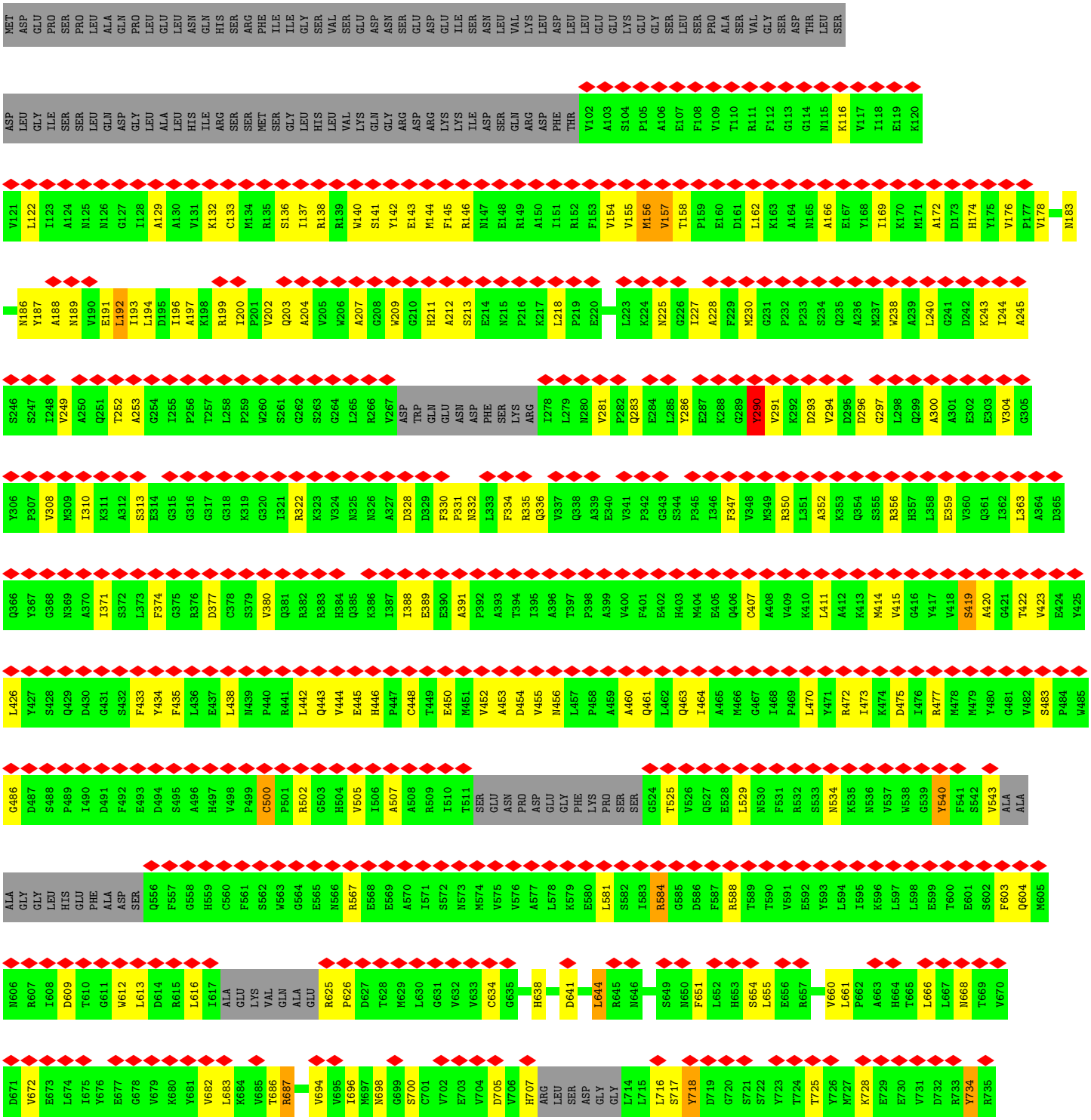
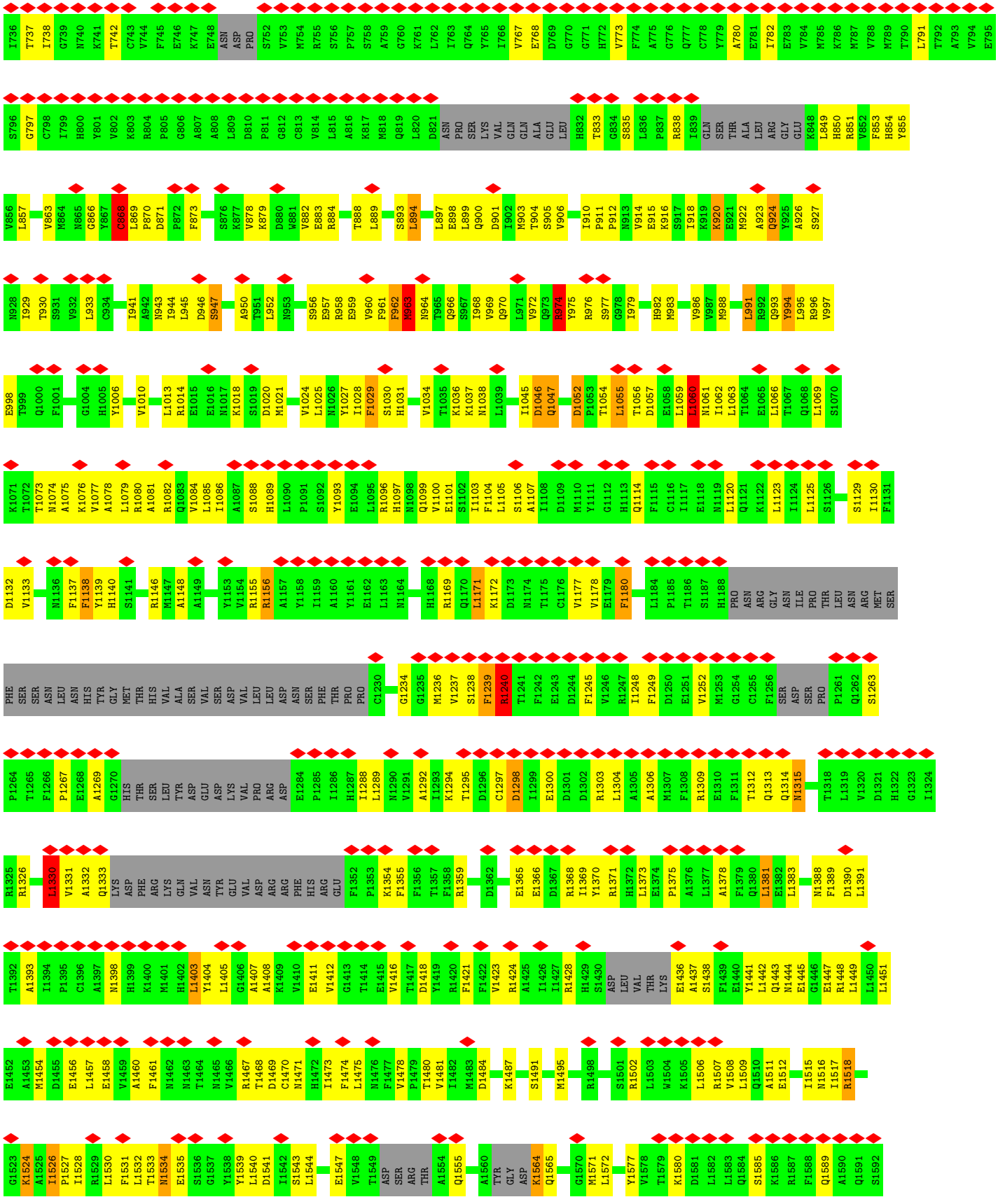


• Molecule 1: Acetyl-CoA carboxylase 1

Chain A:

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PHE SER SER ASN LEU ASN HIS TYR GLY MET THR THR HIS VAL ALA SER VAL SER ASP VAL LEU LEU ASP ASN SER PHE THR PRO PRO C1230 G1234 G1235 M1236 V1237 S1238 F1239 R1240 T1241 F1242 E1243 D1244 F1245 V1246 R1247 I1248 F1249 D1250 E1251 V1252 M1253 G1254 C1255 F1256 SER ASP SER PRO P1261 Q1262 S1263
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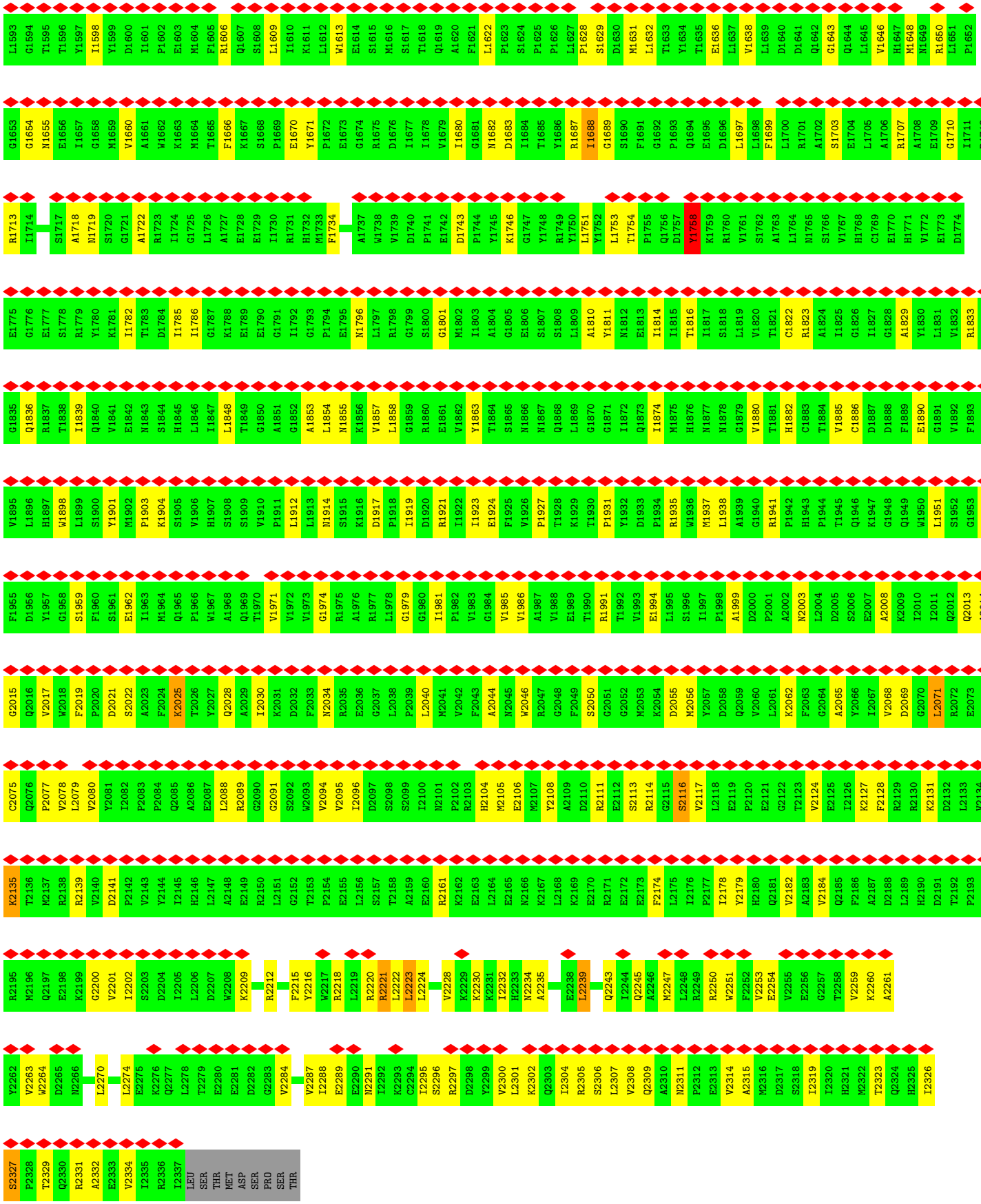
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S2327 P2328 T2329 Q2330 R2331 A2332 E2333 V2334 I2335 R2336 I2337 LEU SER THR MET ASP SER PRO SER THR

• Molecule 1: Acetyl-CoA carboxylase 1

Chain G:

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

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

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

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

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

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

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

TYR GLY ASP LYS GLN GLY PRO LEU HIS GLY MET LEU ILE ASN THR PRO TYR VAL THR LYS D1581 L1582 L1583 Q1584 S1585 K1586 R1587 F1588 Q1589 A1590 Q1591 S1592 L1593 G1594 T1595 T1596 Y1597 I1598 Y1599 D1600 I1601 P1602 E1603 M1604 F1605 R1606 Q1607 S1608 L1609 I1610 K1611 L1612 W1613 E1614 S1615 M1616 S1617 T1618 Q1619 A1620

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G1801 M1802 I1803 A1804 G1805 E1806 S1807 S1808 L1809 A1810 Y1811 N1812 E1813 I1814 I1815 T1816 I1817 S1818 L1819 V1820 T1821 C1822 R1823 A1824 I1825 G1826 I1827 G1828 A1829 Y1830 L1831 V1832 R1833 L1834 G1835 Q1836 R1837 T1838 I1839 Q1840 V1841 E1842 N1843 S1844 H1845 L1846 I1847 L1848 T1849 G1850 A1851 G1852 A1853 L1854 N1855 K1856 V1857 L1858 G1859 R1860

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R1921 I1922 I1923 E1924 F1925 V1926 P1927 T1928 K1929 T1930 P1931 Y1932 D1933 P1934 R1935 W1936 M1937 L1938 A1939 G1940 R1941 P1942 H1943 P1944 T1945 Q1946 K1947 G1948 Q1949 W1950 L1951 S1952 G1953 F1954 F1955 D1956 Y1957 G1958 S1959 F1960 S1961 E1962 I1963 M1964 Q1965 P1966 W1967 A1968 Q1969 T1970 V1971 V1972 V1973 G1974 R1975 A1976 R1977 L1978 G1979 G1980

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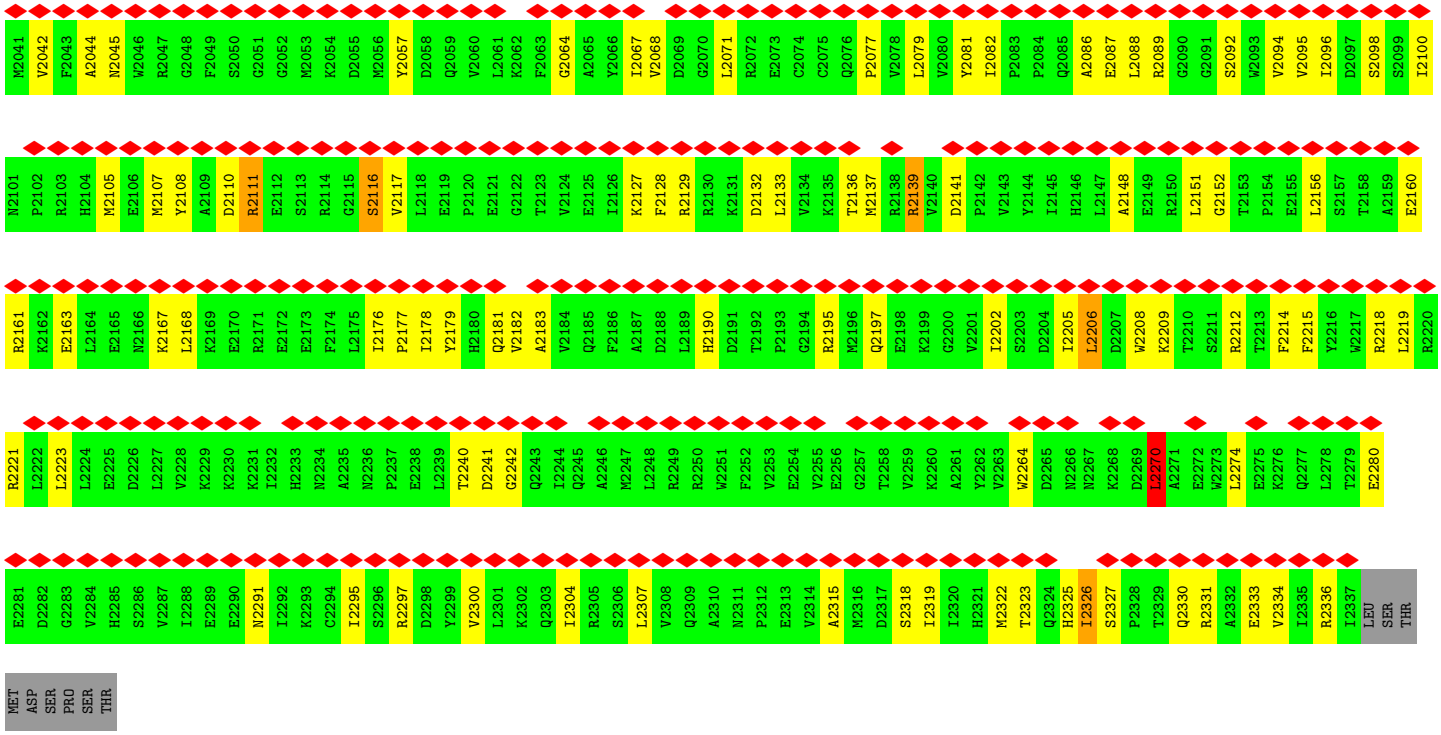
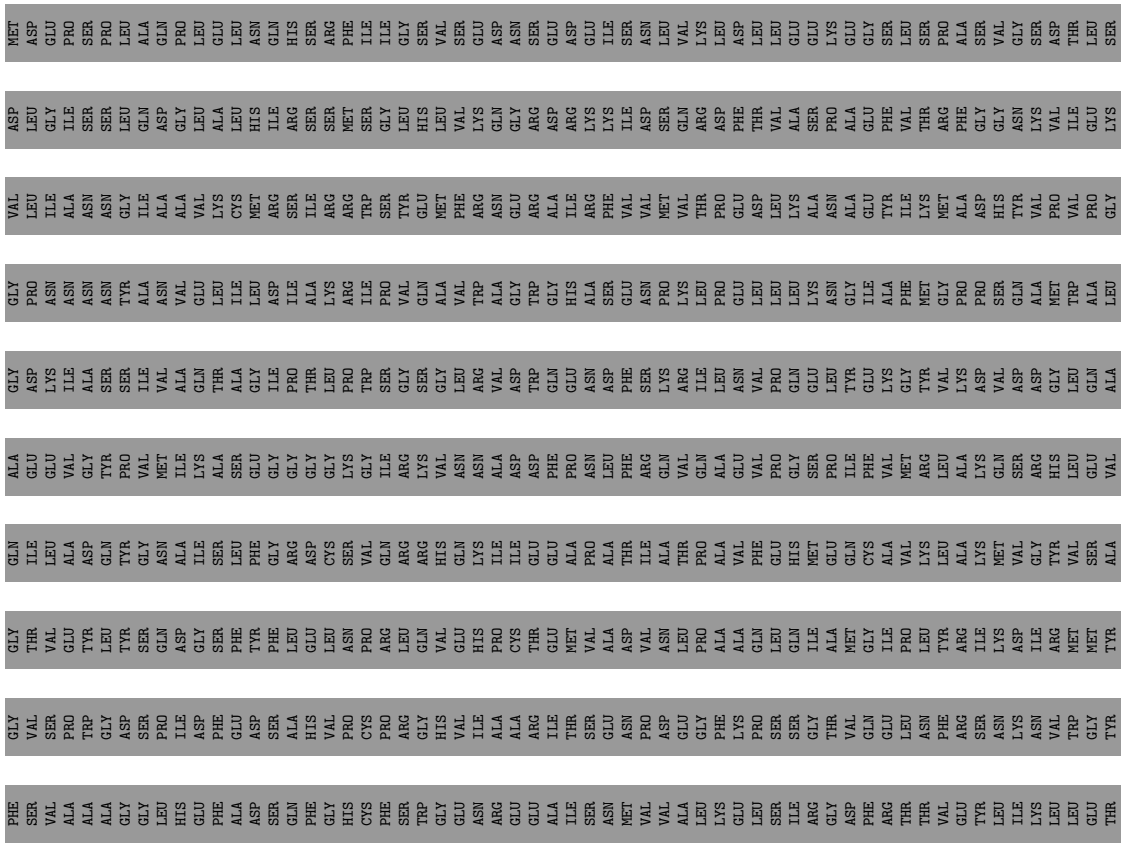


- Molecule 1: Acetyl-CoA carboxylase 1

Chain Q:



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

TYR GLY ASP LYS GLN GLY PRO LEU HIS GLY MET LEU ILE ASN THR PRO TYR VAL THR LYS D1581 L1582 L1583 Q1584 S1585 K1586 R1587 F1588 Q1589 A1590 Q1591 S1592 L1593 G1594 T1595 T1596 Y1597 I1598 Y1599 D1600 I1601 P1602 E1603 M1604 F1605 R1606 Q1607 S1608 L1609 I1610 K1611 L1612 W1613 E1614 S1615 M1616 S1617 T1618 Q1619 A1620

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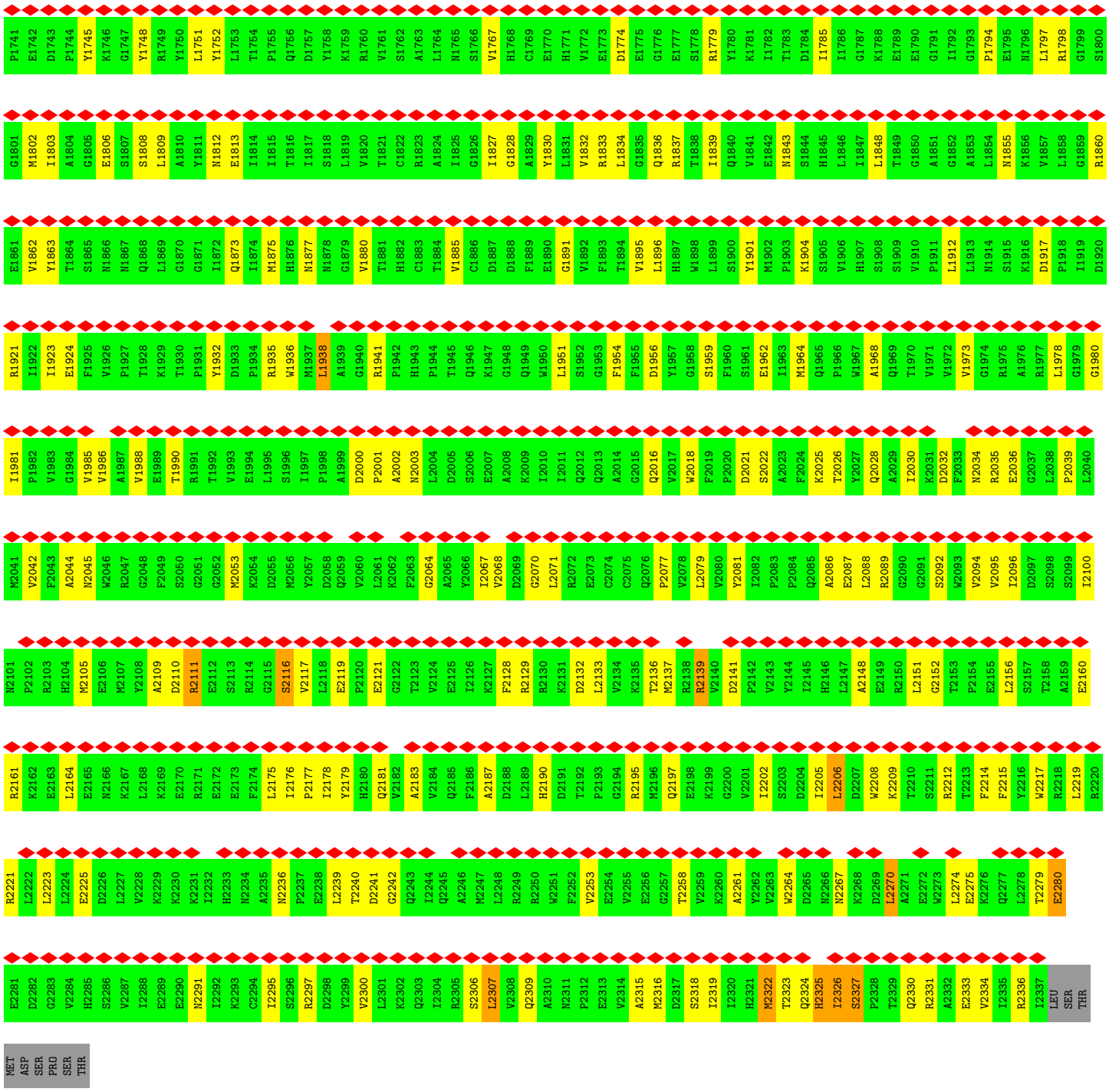
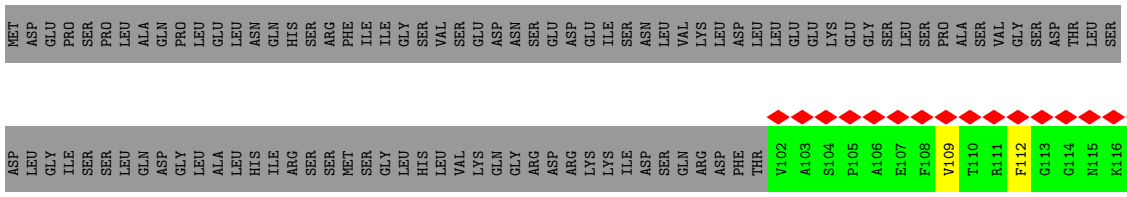
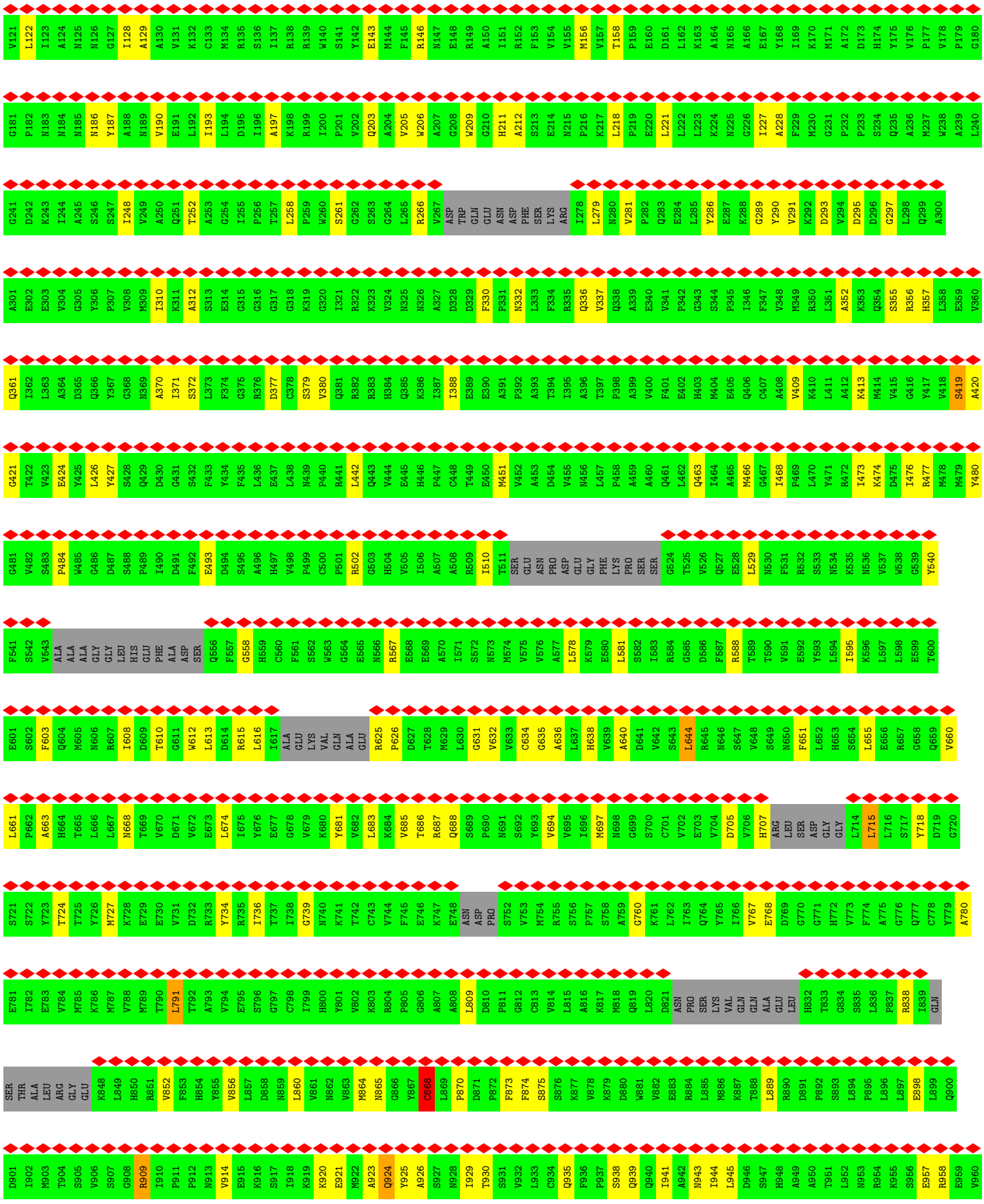


• Molecule 1: Acetyl-CoA carboxylase 1

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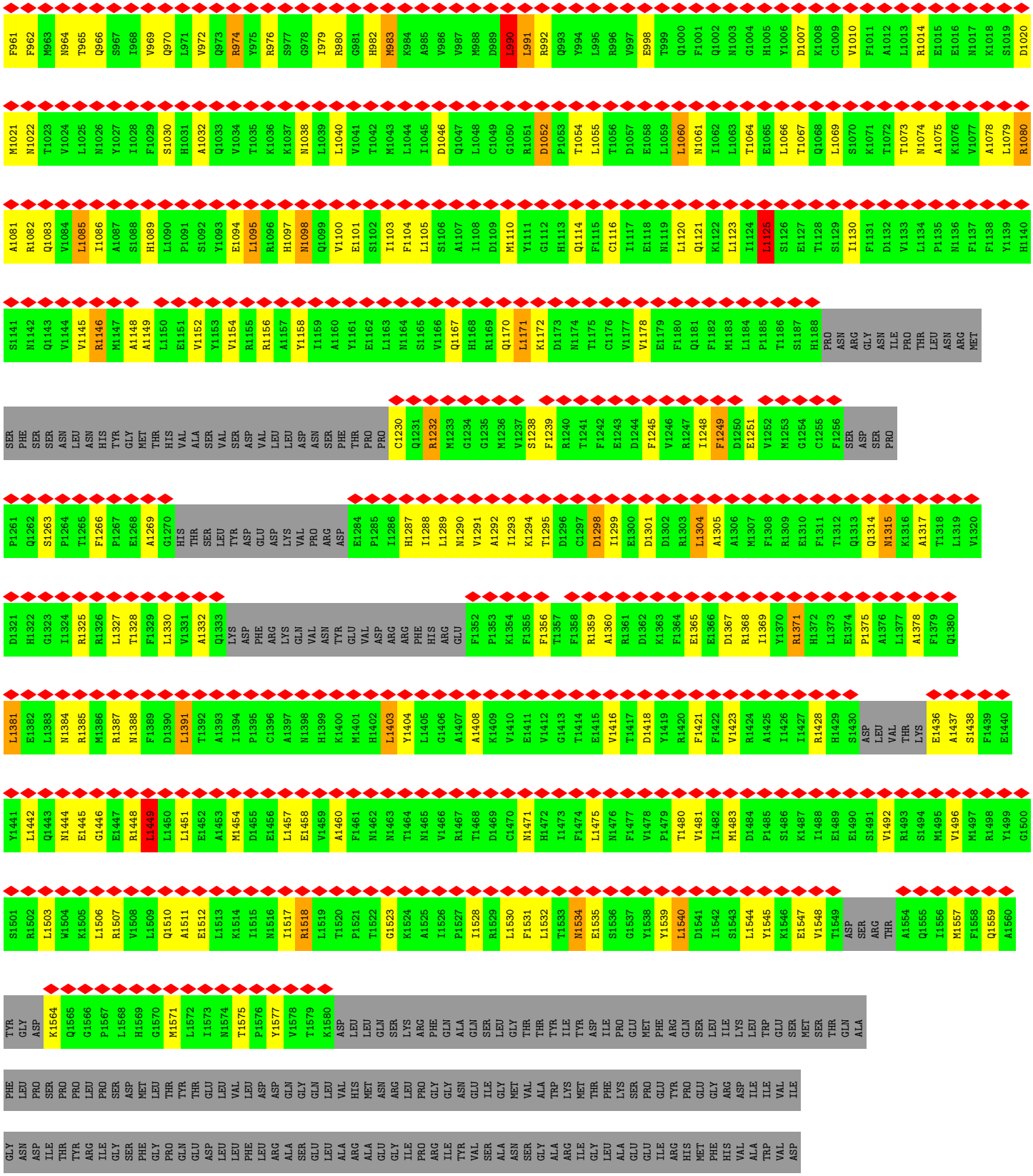
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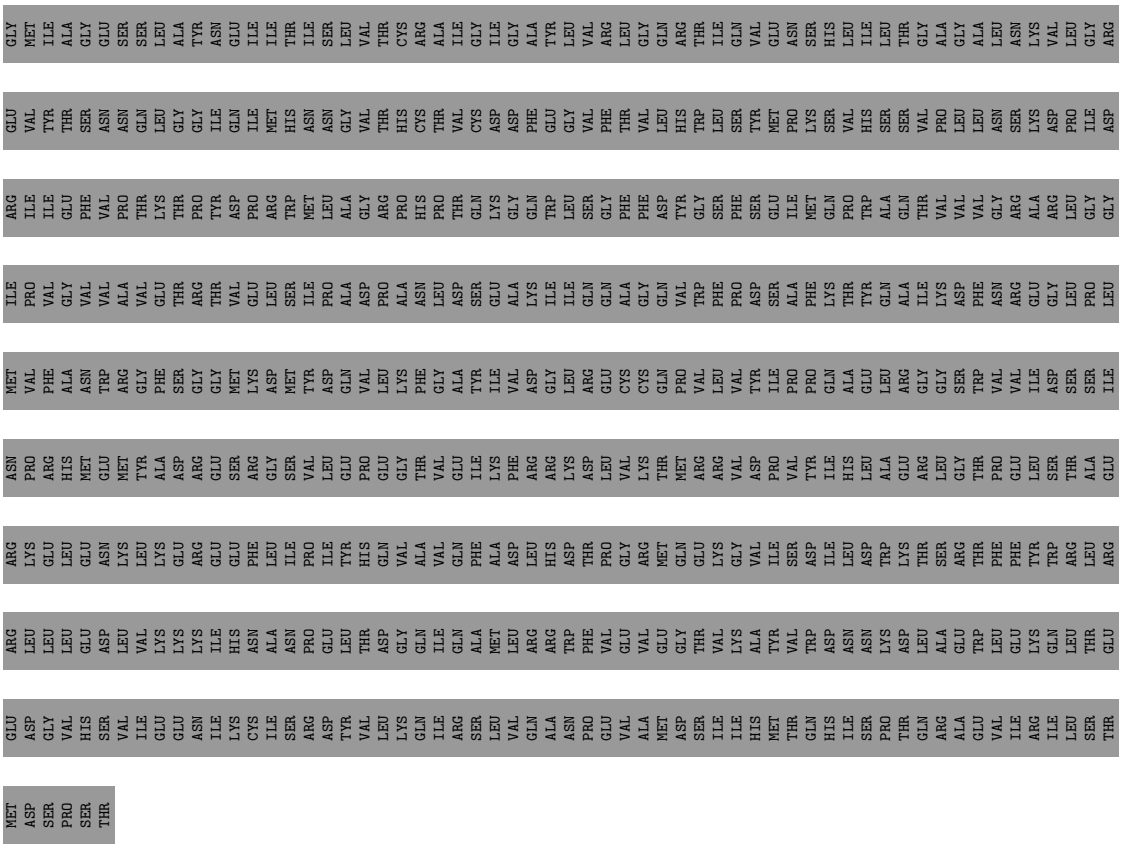
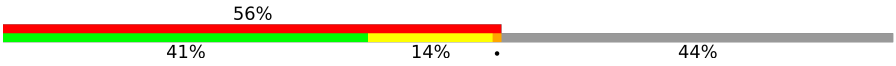
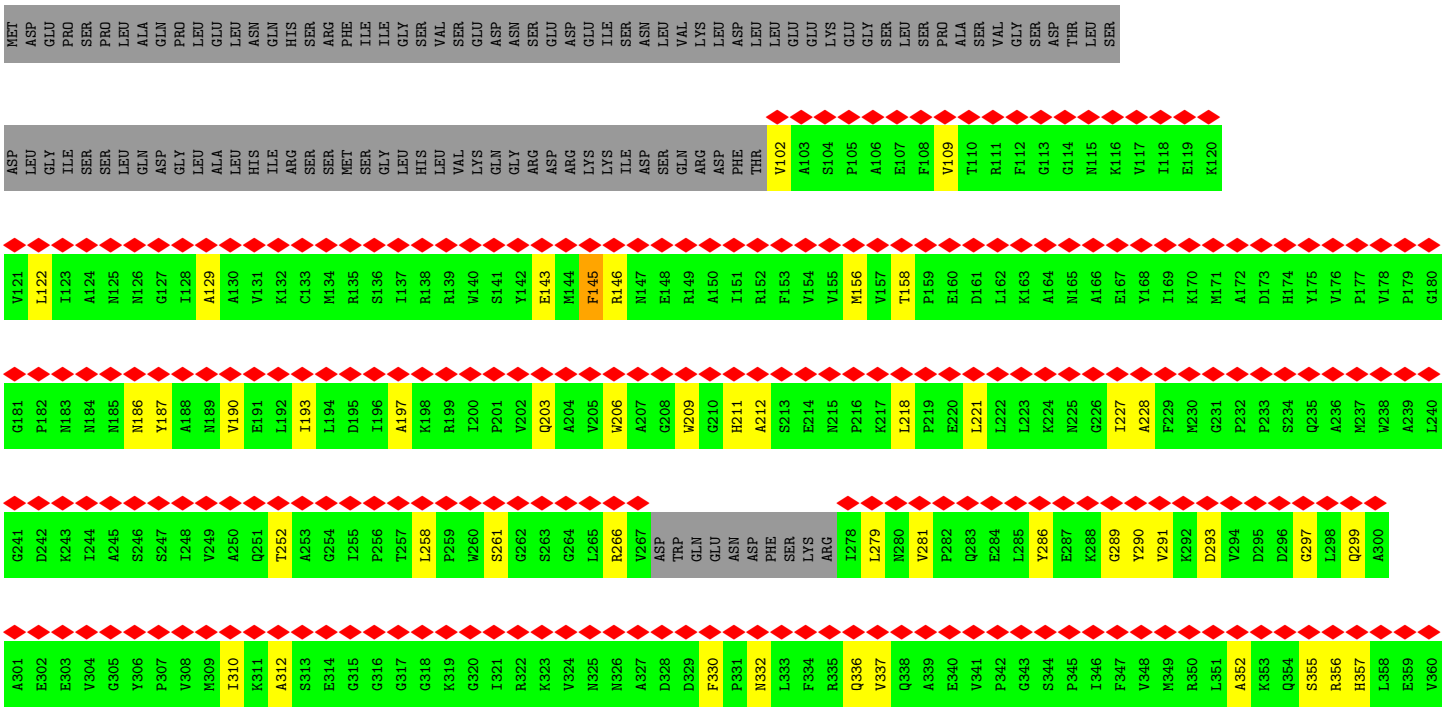
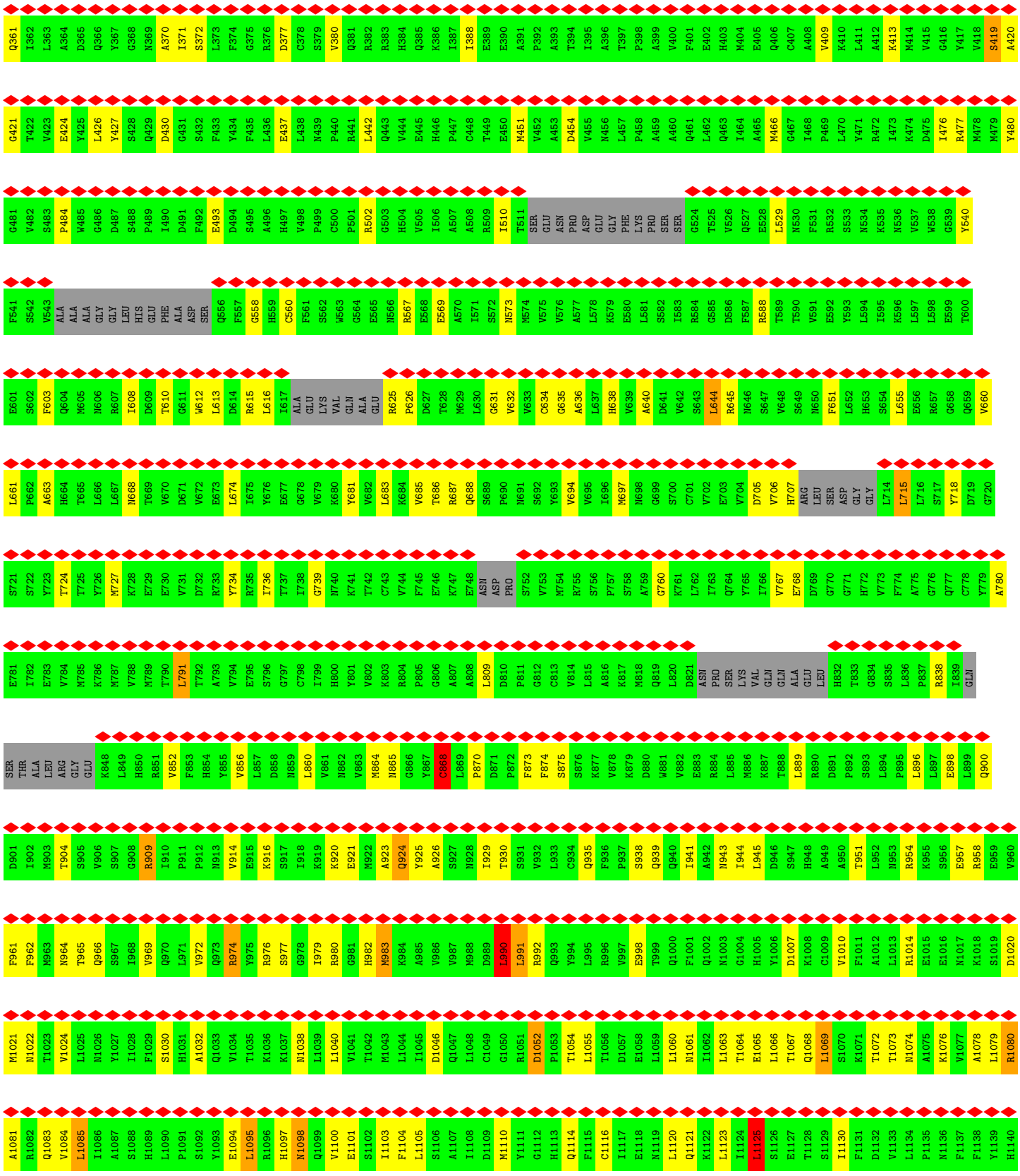


• Molecule 1: Acetyl-CoA carboxylase 1

Chain R:



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Y1441 L1442 Q1443 N1444 E1445 G1446 E1447 R1448 L1449 L1450 L1451 E1452 A1453 M1454 D1455 E1456 L1457 E1458 V1459 A1460 F1461 N1462 N1463 T1464 N1465 V1466 R1467 T1468 D1469 C1470 N1471 H1472 I1473 F1474 L1475 N1476 F1477 V1478 P1479 T1480 V1481 I1482 M1483 D1484 P1485 S1486 K1487 I1488 E1489 E1490 S1491 V1492 R1493 S1494 M1495 V1496 M1497 R1498 Y1499 G1500

S1501 R1502 L1503 W1504 K1505 L1506 R1507 V1508 L1509 Q1510 A1511 E1512 L1513 K1514 I1515 N1516 I1517 R1518 L1519 T1520 P1521 T1522 G1523 K1524 A1525 I1526 P1527 I1528 R1529 L1530 F1531 L1532 T1533 N1534 E1535 S1536 G1537 Y1538 Y1539 L1540 D1541 I1542 S1543 L1544 Y1545 K1546 E1547 V1548 T1549 ASP SER ARG THR A1554 Q1555 I1556 M1557 F1558 Q1559 A1560

TYR GLY ASP K1564 Q1565 G1566 P1567 L1568 H1569 G1570 M1571 L1572 I1573 N1574 T1575 P1576 Y1577 V1578 T1579 K1580 ASP LEU LEU GLN SER LYS ARG PHE GLN ALA GLN SER LEU GLY THR THR TYR ILE TYR ASP ILE PRO GLU MET PHE ARG GLN SER LEU ILE LYS LEU TRP GLU SER MET SER THR GLN ALA

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

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

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

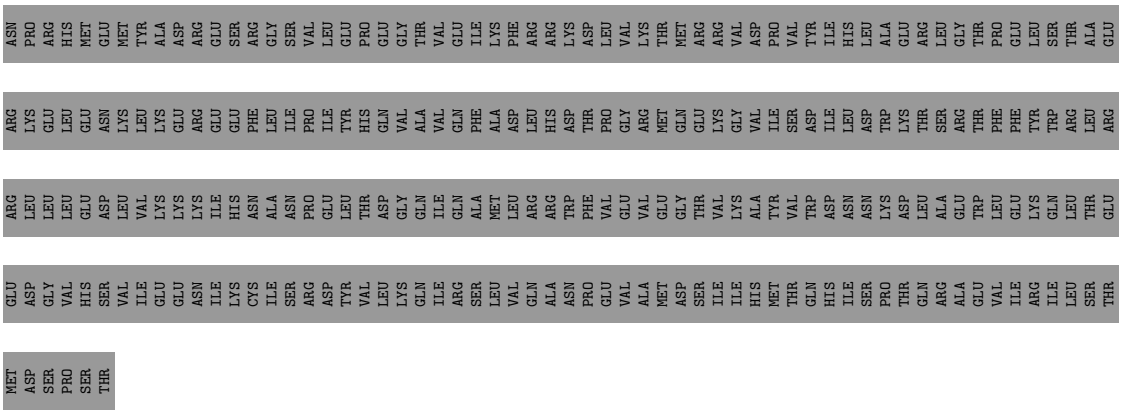
GLY MET ILE ALA GLY GLU SER SER LEU ALA TYR ASN GLU ILE ILE THR ILE SER LEU VAL THR CYS ARG ALA ILE GLY ILE GLY ALA TYR LEU VAL ARG LEU GLY GLN ARG THR ILE GLN VAL GLU ASN SER HIS LEU ILE LEU THR GLY ALA GLY ALA LEU ASN LYS VAL LEU GLY ARG

GLU VAL TYR THR SER ASN ASN GLN LEU GLY GLY ILE GLN ILE MET HIS ASN ASN GLY VAL THR HIS CYS THR VAL CYS ASP ASP PHE GLU GLY VAL PHE THR VAL LEU HIS TRP LEU SER TYR MET PRO LYS SER VAL HIS SER SER VAL PRO LEU LEU ASN SER LYS ASP PRO ILE ASP

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

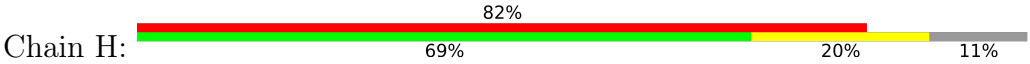
ILE PRO VAL GLY VAL VAL ALA VAL GLU THR ARG THR VAL GLU LEU SER ILE PRO ALA ASP PRO ALA ASN LEU ASP SER GLU ALA LYS ILE ILE GLN GLN ALA GLY GLN VAL TRP PHE PRO ASP SER ALA PHE LYS THR TYR GLN ALA ILE LYS ASP PHE ASN ARG GLU GLY LEU PRO LEU

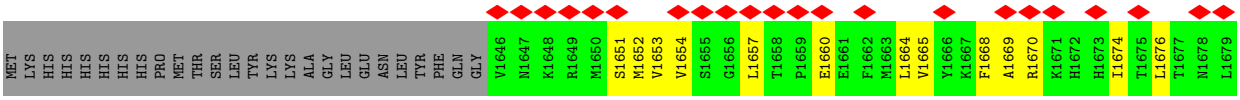
MET VAL PHE ALA ASN TRP ARG GLY PHE SER GLY GLY MET LYS ASP MET TYR ASP GLN VAL LEU LYS PHE GLY ALA TYR ILE VAL ASP GLY LEU ARG GLU CYS CYS GLN PRO VAL LEU VAL TYR ILE PRO PRO GLN ALA GLU LEU ARG GLY GLY SER TRP VAL VAL ILE ASP SER SER ILE

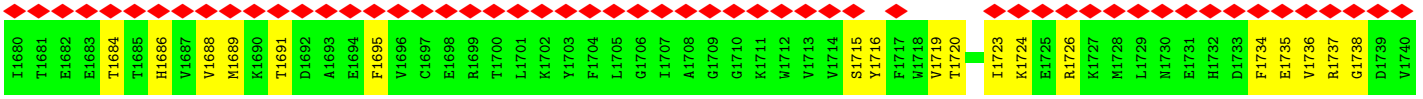


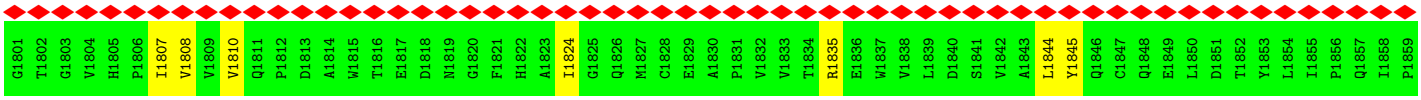
• Molecule 2: Breast cancer type 1 susceptibility protein

Chain H:



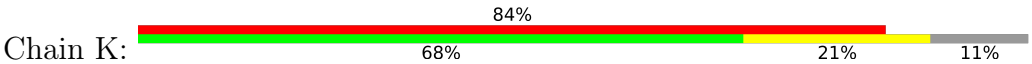


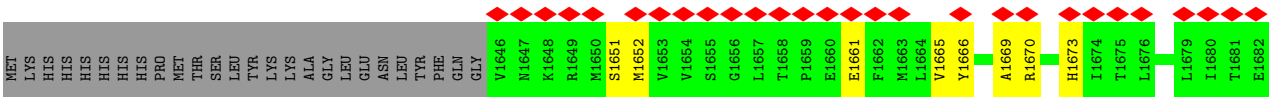


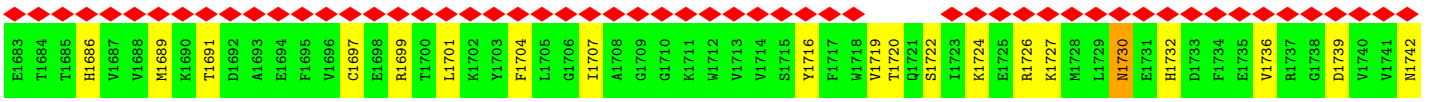


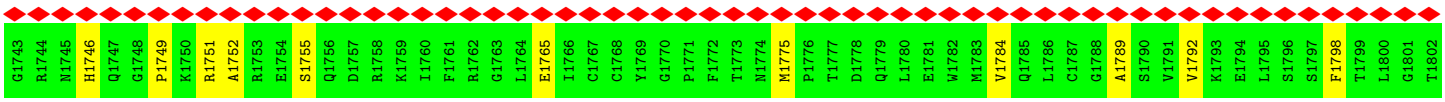
• Molecule 2: Breast cancer type 1 susceptibility protein

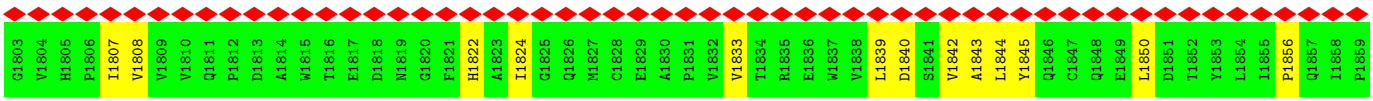
Chain K:





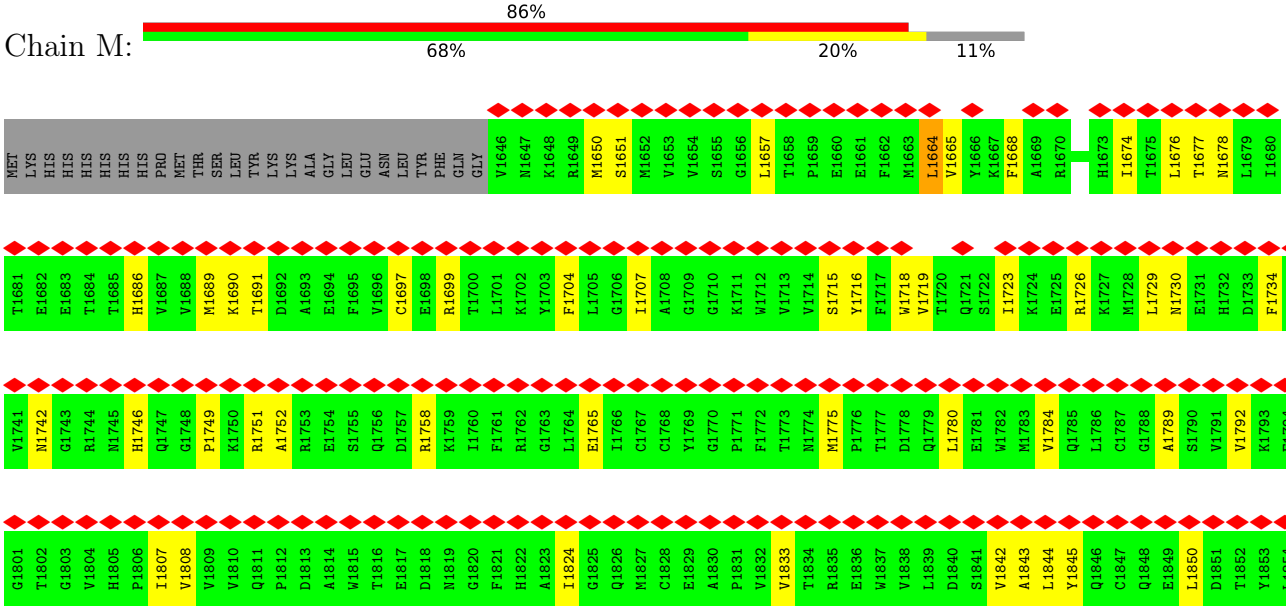






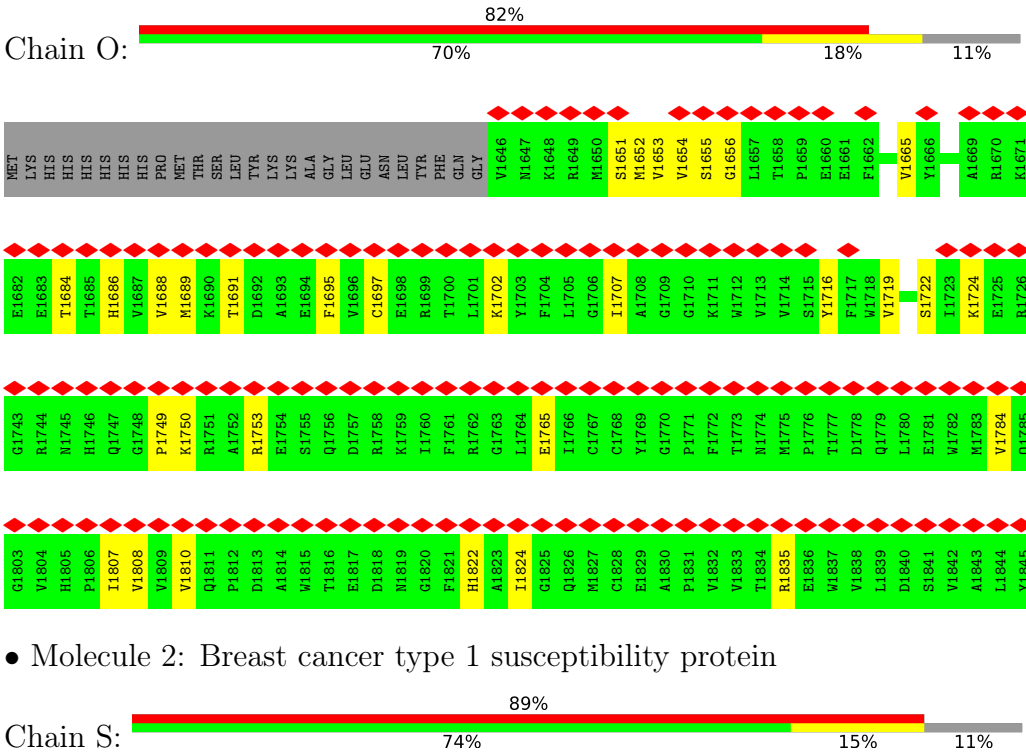
• Molecule 2: Breast cancer type 1 susceptibility protein

Chain M:



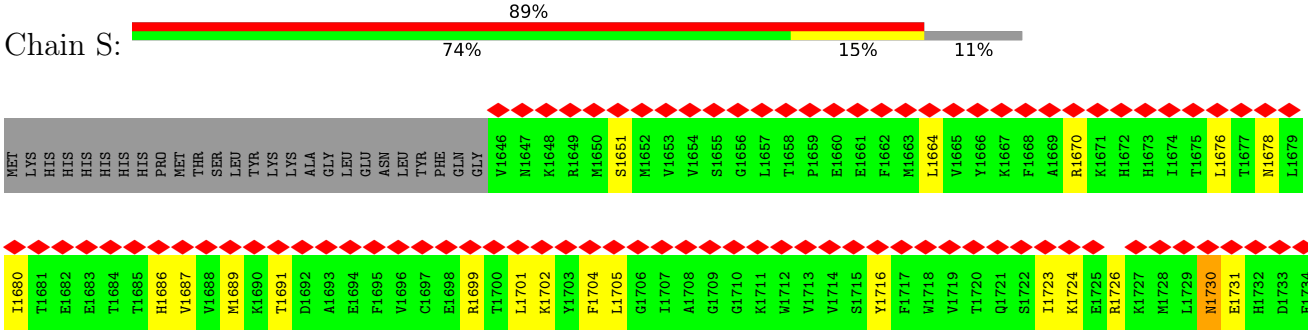
• Molecule 2: Breast cancer type 1 susceptibility protein

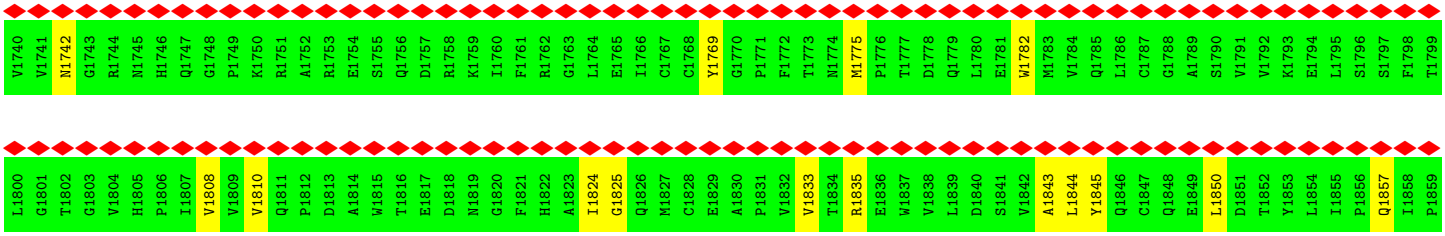
Chain O:



• Molecule 2: Breast cancer type 1 susceptibility protein

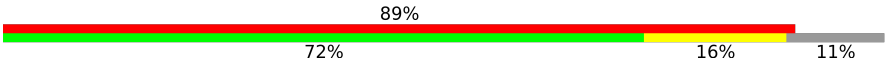
Chain S:

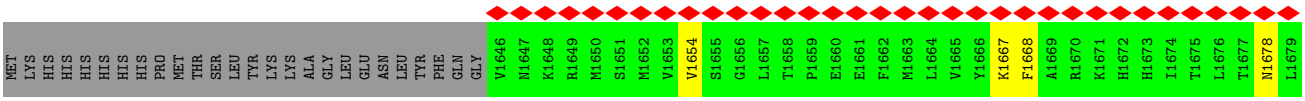




• Molecule 2: Breast cancer type 1 susceptibility protein

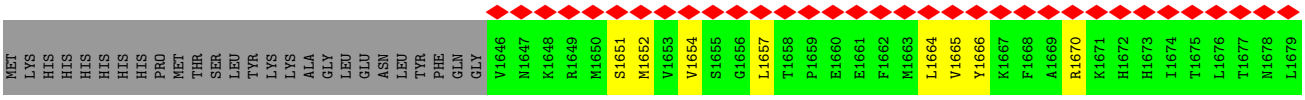
Chain U:





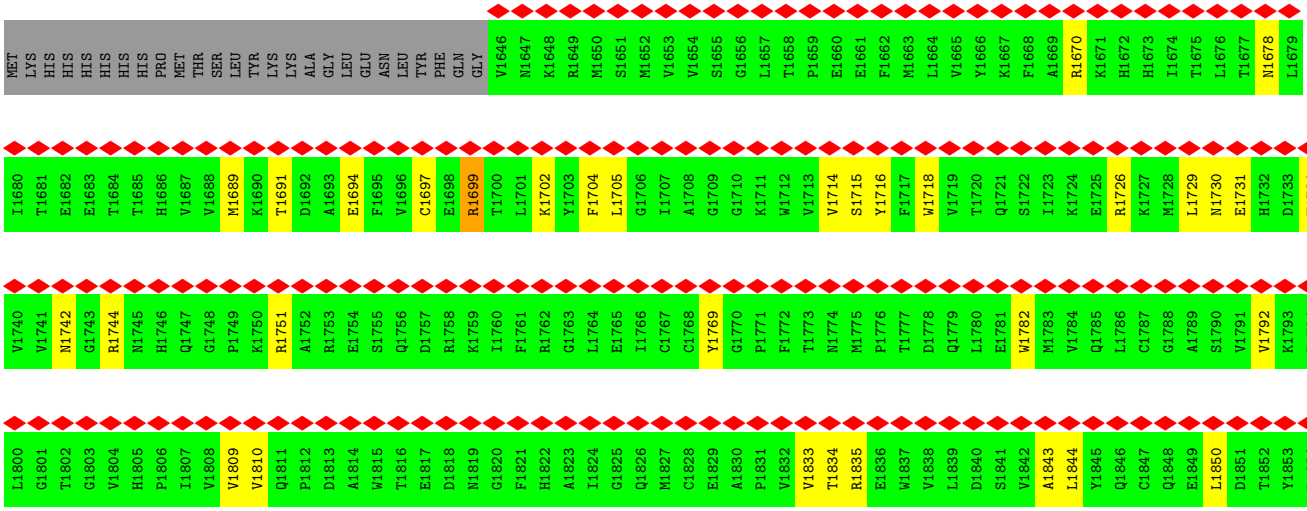
• Molecule 2: Breast cancer type 1 susceptibility protein

Chain Y:



• Molecule 2: Breast cancer type 1 susceptibility protein

Chain W:


MET LYS HIS HIS HIS HIS HIS PRO MET THR SER LEU TYR LYS LYS ALA GLY LEU GLU ASN LEU TYR PHE GLN GLY
V1646 N1647 K1648 R1649 M1650 S1651 M1652 V1653 V1654 S1655 G1656 L1657 T1658 P1659 E1660 E1661 F1662 M1663 L1664 V1665 Y1666 K1667 F1668 A1669 R1670 K1671 H1672 H1673 I1674 T1675 L1676 T1677 N1678 L1679
I1680 T1681 E1682 E1683 T1684 T1685 H1686 V1687 V1688 M1689 K1690 T1691 D1692 A1693 E1694 F1695 V1696 C1697 E1698 R1699 T1700 L1701 K1702 Y1703 F1704 L1705 G1706 I1707 A1708 G1709 G1710 K1711 W1712 V1713 V1714 S1715 Y1716 F1717 W1718 V1719 T1720 Q1721 S1722 I1723 K1724 E1725 R1726 K1727 M1728 L1729 N1730 E1731 H1732 D1733 F1734 E1735 V1736 R1737 G1738 D1739
V1740 V1741 N1742 G1743 R1744 N1745 H1746 Q1747 G1748 P1749 K1750 R1751 A1752 R1753 E1754 S1755 Q1756 D1757 R1758 K1759 I1760 F1761 R1762 G1763 L1764 E1765 I1766 C1767 C1768 Y1769 G1770 P1771 F1772 T1773 N1774 M1775 P1776 T1777 D1778 Q1779 L1780 E1781 W1782 M1783 V1784 Q1785 L1786 C1787 G1788 A1789 S1790 V1791 V1792 K1793 E1794 L1795 S1796 S1797 F1798 T1799
L1800 G1801 T1802 G1803 V1804 H1805 P1806 I1807 V1808 V1809 V1810 Q1811 P1812 D1813 A1814 W1815 T1816 E1817 D1818 N1819 G1820 F1821 H1822 A1823 I1824 G1825 Q1826 M1827 C1828 E1829 A1830 P1831 V1832 V1833 T1834 R1835 E1836 W1837 V1838 L1839 D1840 S1841 V1842 A1843 L1844 Y1845 Q1846 C1847 Q1848 E1849 L1850 D1851 T1852 Y1853 L1854 I1855 P1856 Q1857 I1858 P1859

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	48483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	397.80798, 397.80798, 397.80798	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality

5.1 Standard geometry

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

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	A	0.51	3/16819 (0.0%)	1.02	65/22785 (0.3%)
1	B	0.52	4/16819 (0.0%)	1.06	76/22785 (0.3%)
1	C	0.60	3/16819 (0.0%)	1.05	63/22785 (0.3%)
1	D	0.67	8/16819 (0.0%)	1.20	144/22785 (0.6%)
1	E	0.66	4/16819 (0.0%)	1.11	72/22785 (0.3%)
1	F	0.59	3/16819 (0.0%)	1.04	56/22785 (0.2%)
1	G	0.43	0/6199	0.87	7/8406 (0.1%)
1	J	0.41	0/10619	0.91	26/14376 (0.2%)
1	Q	0.43	0/6199	0.88	10/8406 (0.1%)
1	R	0.41	0/10619	0.92	32/14376 (0.2%)
2	H	0.44	0/1740	0.87	1/2364 (0.0%)
2	K	0.40	0/1737	0.79	0/2360
2	M	0.40	0/1740	0.81	0/2364
2	O	0.43	0/1737	0.84	1/2360 (0.0%)
2	S	0.36	0/1740	0.81	4/2364 (0.2%)
2	U	0.36	0/1737	0.75	0/2360
2	W	0.37	0/1737	0.77	2/2360 (0.1%)
2	Y	0.37	0/1740	0.78	0/2364
All	All	0.54	25/148458 (0.0%)	1.02	559/201170 (0.3%)

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	A	0	13
1	B	0	13
1	C	0	12
1	D	1	18
1	E	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	12
1	J	0	11
1	R	0	11
All	All	1	101

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	2018	TRP	CB-CG	-7.39	1.36	1.50
1	B	1539	TYR	CB-CG	-7.33	1.40	1.51
1	C	2018	TRP	CB-CG	-7.25	1.37	1.50
1	E	1116	CYS	CB-SG	-7.02	1.70	1.82
1	D	1780	TYR	CD2-CE2	-6.97	1.28	1.39

The worst 5 of 559 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1503	LEU	CA-CB-CG	10.94	140.47	115.30
1	E	1449	LEU	CA-CB-CG	10.48	139.40	115.30
1	A	991	LEU	CA-CB-CG	10.27	138.93	115.30
1	E	290	TYR	CB-CG-CD2	10.07	127.04	121.00
1	B	290	TYR	CB-CG-CD2	9.91	126.95	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	1838	THR	CB

5 of 101 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1052	ASP	Peptide
1	D	1087	ALA	Peptide
1	D	1110	MET	Peptide
1	D	924	GLN	Peptide
1	D	957	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16482	16276	16330	551	0
1	B	16482	16276	16330	552	0
1	C	16482	16275	16329	647	0
1	D	16482	16276	16329	769	0
1	E	16482	16276	16330	704	0
1	F	16482	16275	16330	615	0
1	G	6058	5997	6015	151	0
1	J	10424	10279	10314	212	0
1	Q	6058	5997	6015	159	0
1	R	10424	10279	10314	217	0
2	H	1699	1648	1655	30	0
2	K	1696	1644	1651	35	0
2	M	1699	1648	1655	36	0
2	O	1696	1644	1651	30	0
2	S	1699	1648	1655	20	0
2	U	1696	1644	1651	29	0
2	W	1696	1644	1651	23	0
2	Y	1699	1648	1655	20	0
All	All	145436	143374	143860	4549	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 16.

The worst 5 of 4549 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)
1:B:2264:TRP:HA	1:B:2270:LEU:HD21	1.42	1.00
1:A:197:ALA:HB1	1:A:227:ILE:HD13	1.42	0.98
1:B:197:ALA:HB1	1:B:227:ILE:HD13	1.44	0.97
1:F:1123:LEU:HD12	1:F:1152:VAL:HG21	1.48	0.95
1:C:1123:LEU:HD12	1:C:1152:VAL:HG21	1.48	0.93

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 PDB entries followed by that with respect to all EM entries.

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	A	2047/2346 (87%)	1889 (92%)	147 (7%)	11 (0%)	29	69
1	B	2047/2346 (87%)	1888 (92%)	146 (7%)	13 (1%)	25	65
1	C	2047/2346 (87%)	1884 (92%)	150 (7%)	13 (1%)	25	65
1	D	2047/2346 (87%)	1879 (92%)	154 (8%)	14 (1%)	22	62
1	E	2047/2346 (87%)	1895 (93%)	138 (7%)	14 (1%)	22	62
1	F	2047/2346 (87%)	1884 (92%)	150 (7%)	13 (1%)	25	65
1	G	755/2346 (32%)	727 (96%)	25 (3%)	3 (0%)	34	72
1	J	1290/2346 (55%)	1157 (90%)	125 (10%)	8 (1%)	25	65
1	Q	755/2346 (32%)	727 (96%)	24 (3%)	4 (0%)	29	69
1	R	1290/2346 (55%)	1158 (90%)	124 (10%)	8 (1%)	25	65
2	H	212/240 (88%)	207 (98%)	5 (2%)	0	100	100
2	K	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
2	M	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	O	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	S	212/240 (88%)	206 (97%)	6 (3%)	0	100	100
2	U	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	W	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
2	Y	212/240 (88%)	205 (97%)	7 (3%)	0	100	100
All	All	18068/25380 (71%)	16732 (93%)	1235 (7%)	101 (1%)	29	65

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	HIS
1	D	419	SER
1	D	868	CYS
1	D	1688	ILE

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Mol	Chain	Res	Type
1	E	211	HIS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	1784/2056 (87%)	1748 (98%)	36 (2%)	55	74
1	B	1784/2056 (87%)	1755 (98%)	29 (2%)	62	79
1	C	1784/2056 (87%)	1745 (98%)	39 (2%)	52	71
1	D	1784/2056 (87%)	1739 (98%)	45 (2%)	47	68
1	E	1784/2056 (87%)	1734 (97%)	50 (3%)	43	65
1	F	1784/2056 (87%)	1750 (98%)	34 (2%)	57	75
1	G	660/2056 (32%)	655 (99%)	5 (1%)	81	89
1	J	1124/2056 (55%)	1093 (97%)	31 (3%)	43	65
1	Q	660/2056 (32%)	654 (99%)	6 (1%)	78	87
1	R	1124/2056 (55%)	1089 (97%)	35 (3%)	40	62
2	H	186/214 (87%)	185 (100%)	1 (0%)	88	93
2	K	186/214 (87%)	185 (100%)	1 (0%)	88	93
2	M	186/214 (87%)	184 (99%)	2 (1%)	73	84
2	O	186/214 (87%)	185 (100%)	1 (0%)	88	93
2	S	186/214 (87%)	184 (99%)	2 (1%)	73	84
2	U	186/214 (87%)	185 (100%)	1 (0%)	88	93
2	W	186/214 (87%)	185 (100%)	1 (0%)	88	93
2	Y	186/214 (87%)	184 (99%)	2 (1%)	73	84
All	All	15760/22272 (71%)	15439 (98%)	321 (2%)	57	74

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2245	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	916	LYS
1	Q	1667	LYS
1	J	1080	ARG
1	R	1388	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1619	GLN
2	O	1730	ASN
1	B	1181	GLN
2	M	1730	ASN
1	J	1444	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	SEP	A	1263	1	8,9,10	1.54	1 (12%)	8,12,14	1.74	2 (25%)
1	SEP	R	1263	1	8,9,10	1.57	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	B	1263	1	8,9,10	1.53	1 (12%)	8,12,14	0.89	0
1	SEP	C	1263	1	8,9,10	1.55	1 (12%)	8,12,14	1.83	2 (25%)
1	SEP	J	1263	1	8,9,10	1.56	1 (12%)	8,12,14	1.42	2 (25%)
1	SEP	E	1263	1	8,9,10	1.52	1 (12%)	8,12,14	1.32	2 (25%)
1	SEP	F	1263	1	8,9,10	1.54	1 (12%)	8,12,14	0.92	0
1	SEP	D	1263	1	8,9,10	1.51	1 (12%)	8,12,14	1.22	2 (25%)

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
1	SEP	A	1263	1	-	1/5/8/10	-
1	SEP	R	1263	1	-	1/5/8/10	-
1	SEP	B	1263	1	-	1/5/8/10	-
1	SEP	C	1263	1	-	1/5/8/10	-
1	SEP	J	1263	1	-	1/5/8/10	-
1	SEP	E	1263	1	-	1/5/8/10	-
1	SEP	F	1263	1	-	1/5/8/10	-
1	SEP	D	1263	1	-	1/5/8/10	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1263	SEP	P-O1P	3.47	1.61	1.50
1	R	1263	SEP	P-O1P	3.41	1.61	1.50
1	J	1263	SEP	P-O1P	3.40	1.61	1.50
1	B	1263	SEP	P-O1P	3.39	1.61	1.50
1	F	1263	SEP	P-O1P	3.36	1.61	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1263	SEP	OG-CB-CA	3.54	111.59	108.14
1	C	1263	SEP	P-OG-CB	-3.26	109.33	118.30
1	C	1263	SEP	OG-CB-CA	2.92	110.99	108.14
1	J	1263	SEP	OG-CB-CA	2.72	110.79	108.14
1	A	1263	SEP	P-OG-CB	-2.64	111.02	118.30

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	1263	SEP	N-CA-CB-OG
1	E	1263	SEP	N-CA-CB-OG
1	C	1263	SEP	N-CA-CB-OG
1	F	1263	SEP	N-CA-CB-OG
1	B	1263	SEP	N-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1263	SEP	1	0
1	E	1263	SEP	1	0
1	F	1263	SEP	2	0
1	D	1263	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

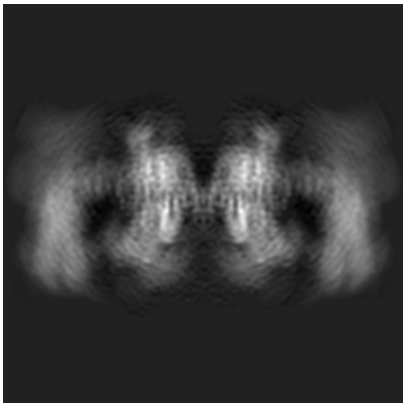
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4344. These allow visual inspection of the internal detail of the map and identification of artifacts.

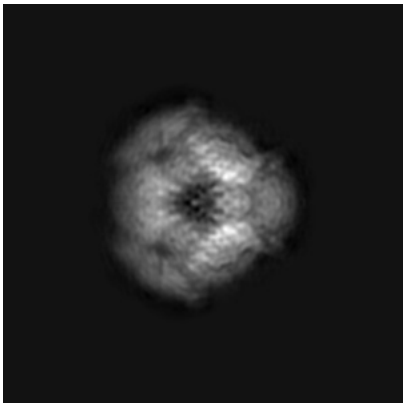
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

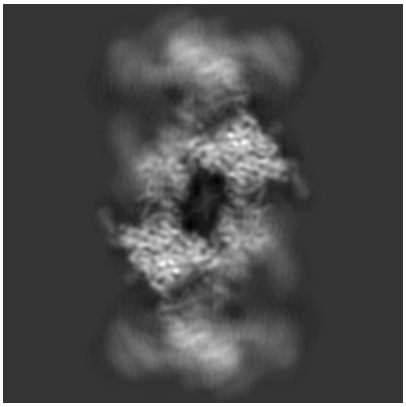
6.1.1 Primary map



X



Y

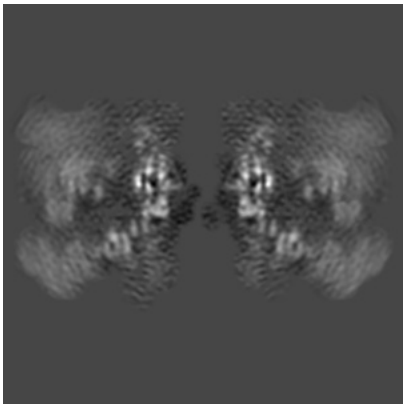


Z

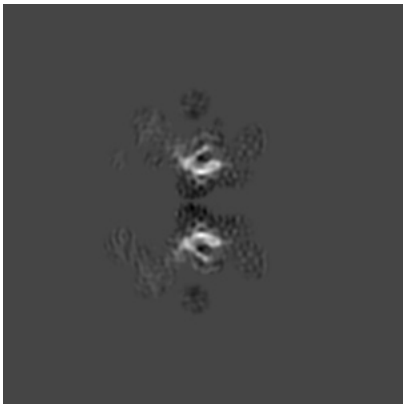
The images above show the map projected in three orthogonal directions.

6.2 Central slices

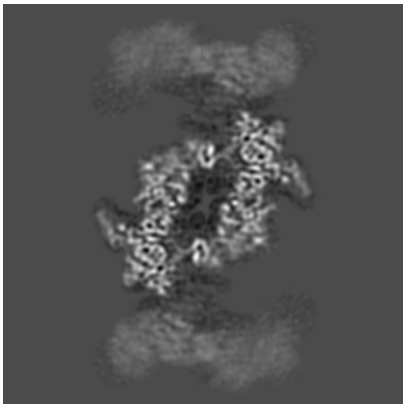
6.2.1 Primary map



X Index: 188



Y Index: 188

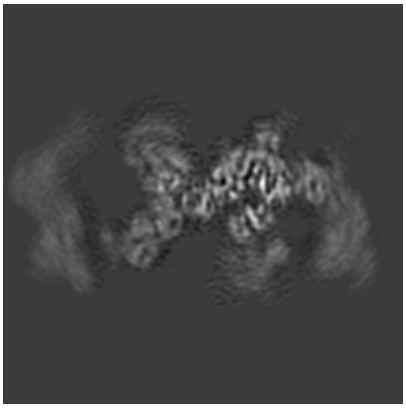


Z Index: 188

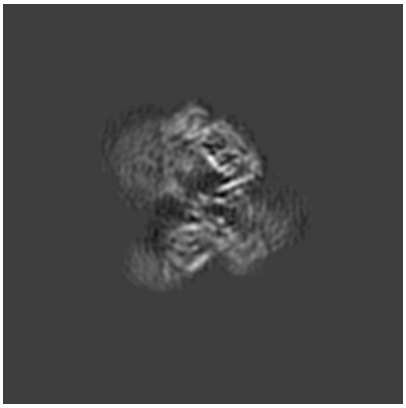
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

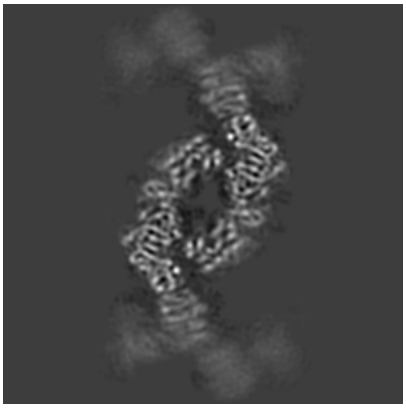
6.3.1 Primary map



X Index: 219



Y Index: 223



Z Index: 201

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

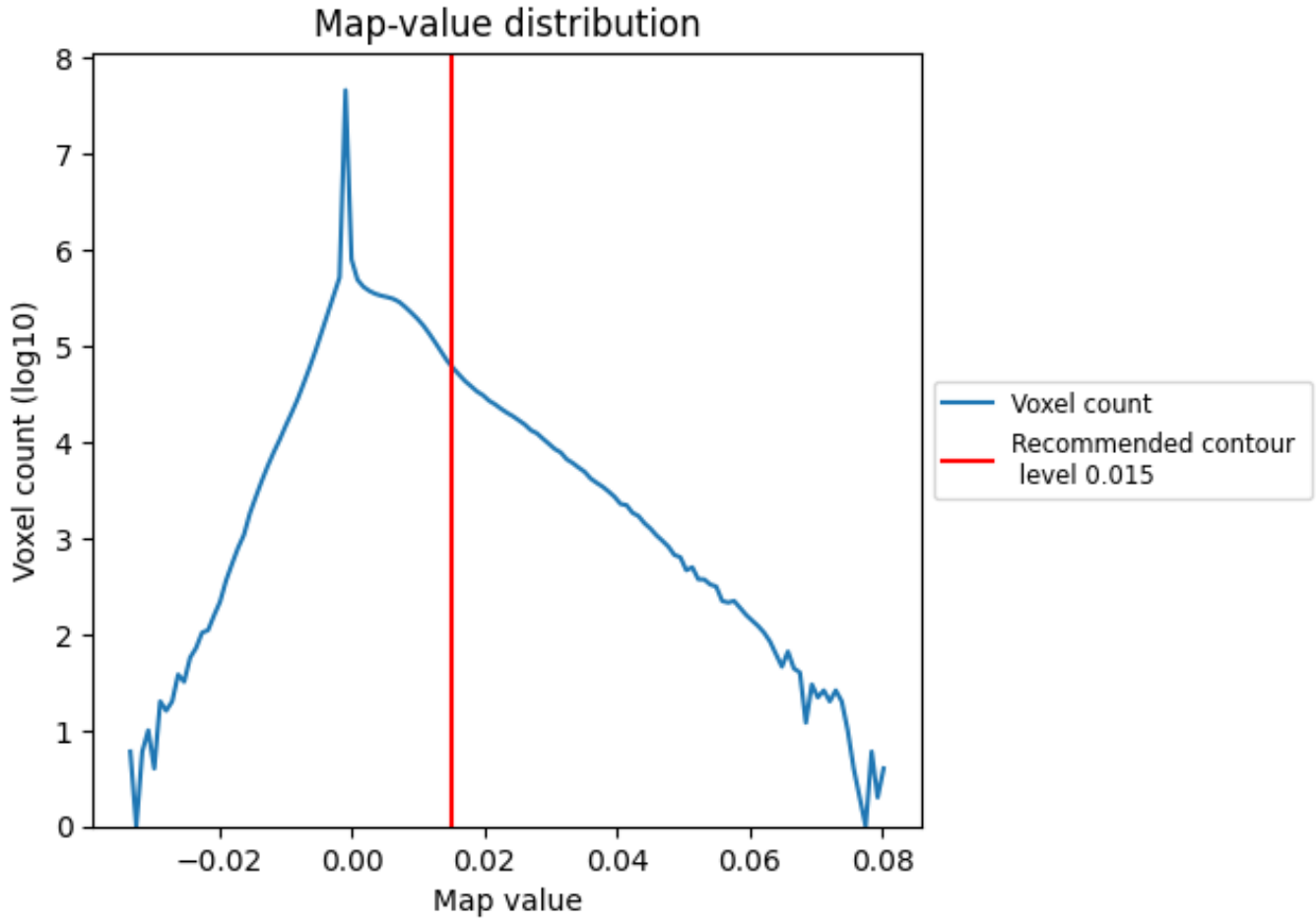
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

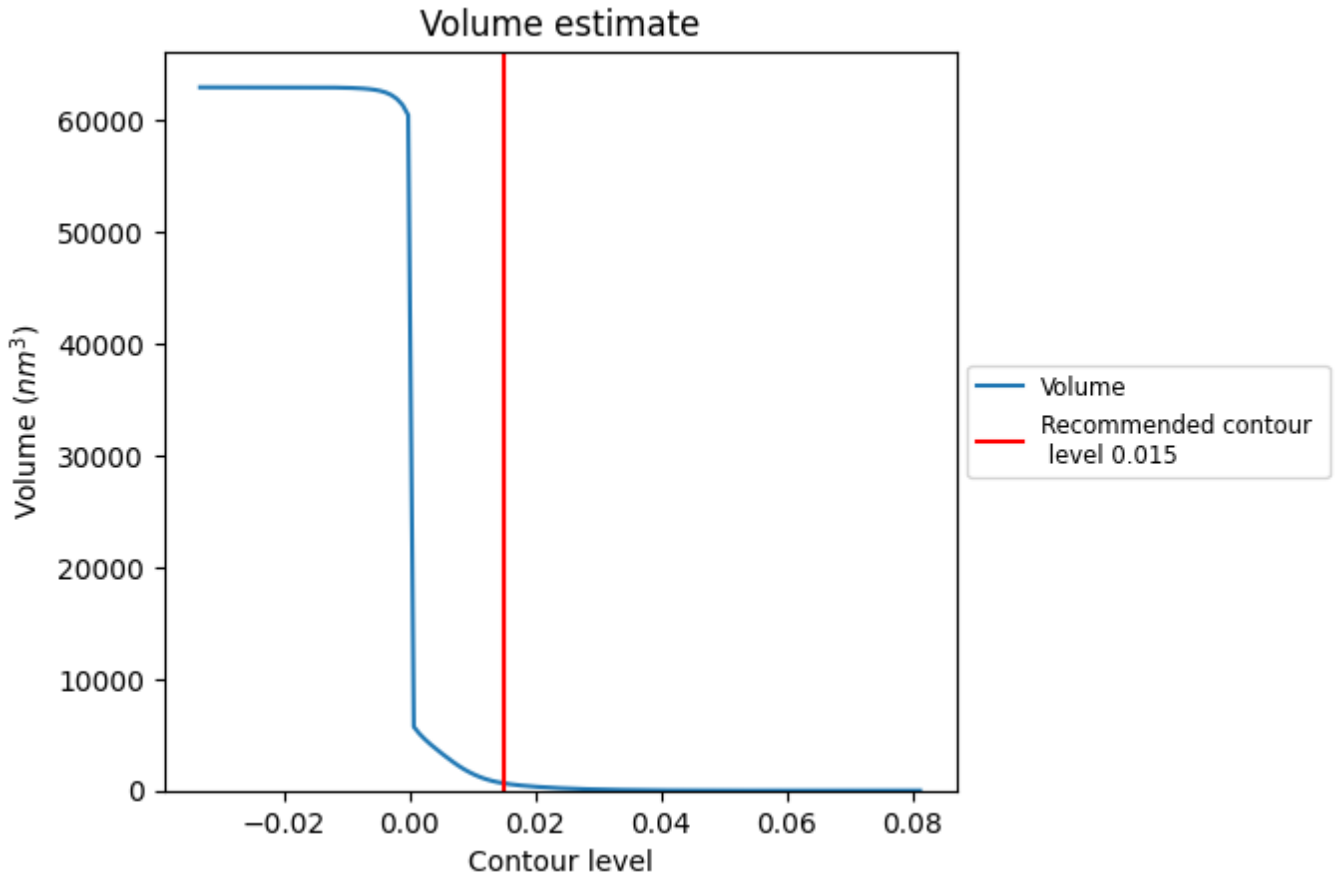
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

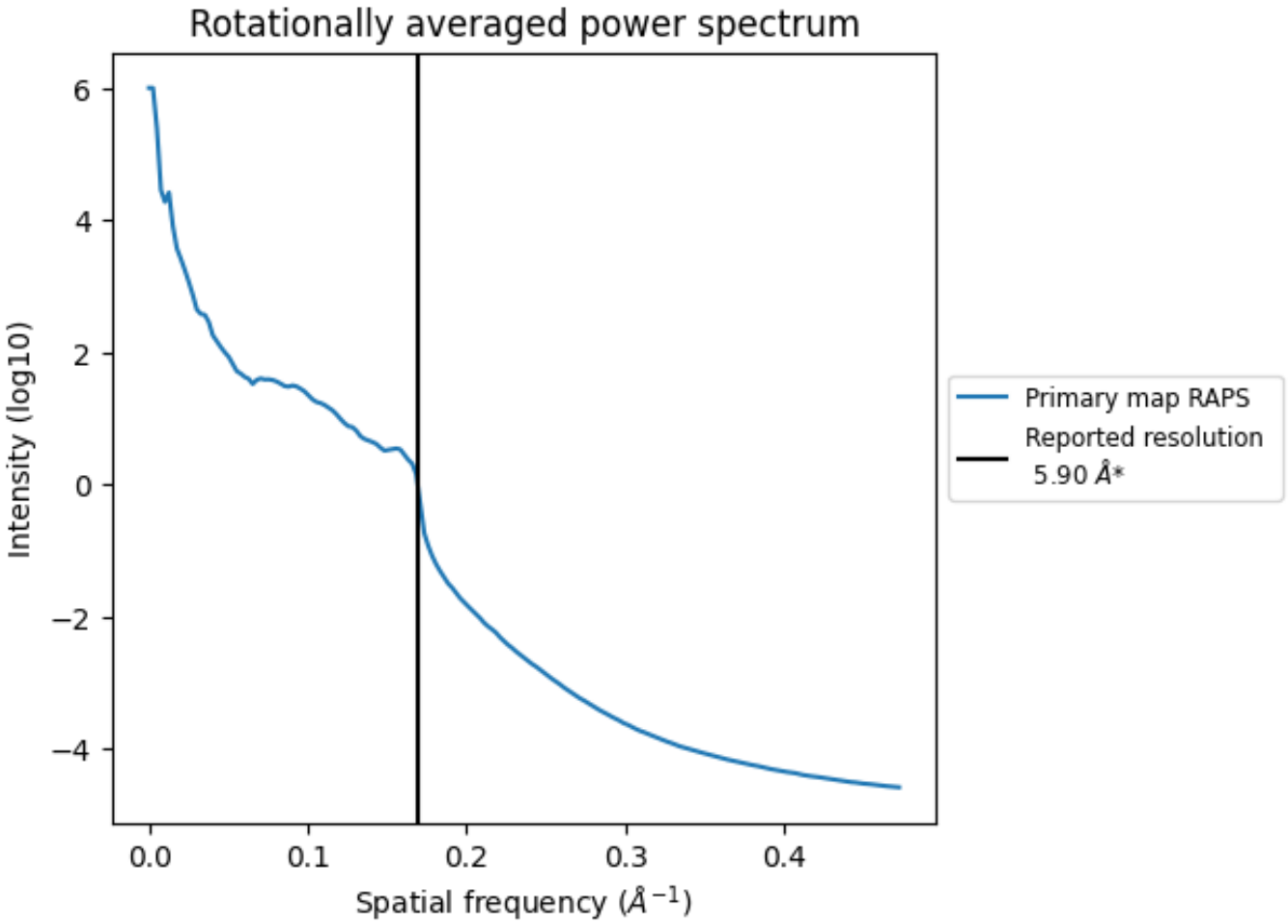
7.2 Volume estimate (i)



The volume at the recommended contour level is 649 nm^3; this corresponds to an approximate mass of 587 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.169 Å^{-1}

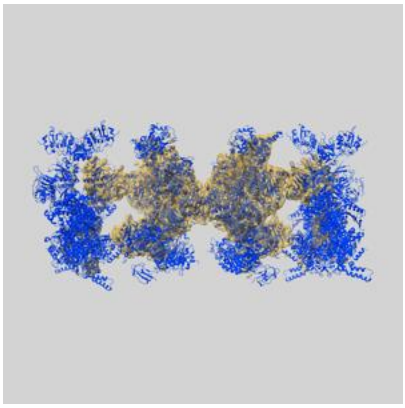
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

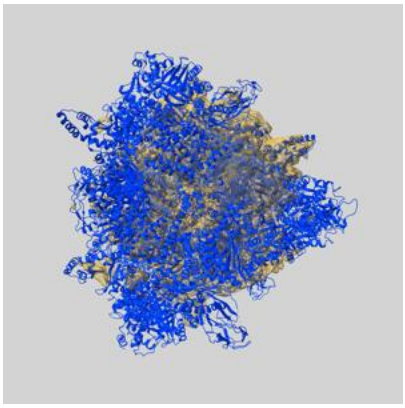
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4344 and PDB model 6G2I. Per-residue inclusion information can be found in section 3 on page 11.

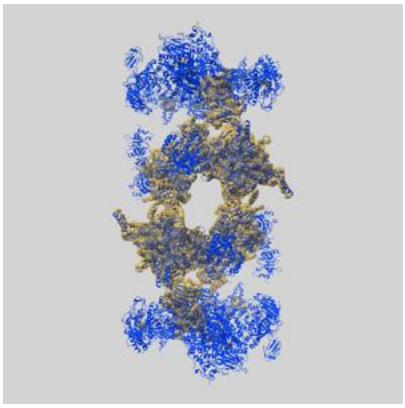
9.1 Map-model overlay



X



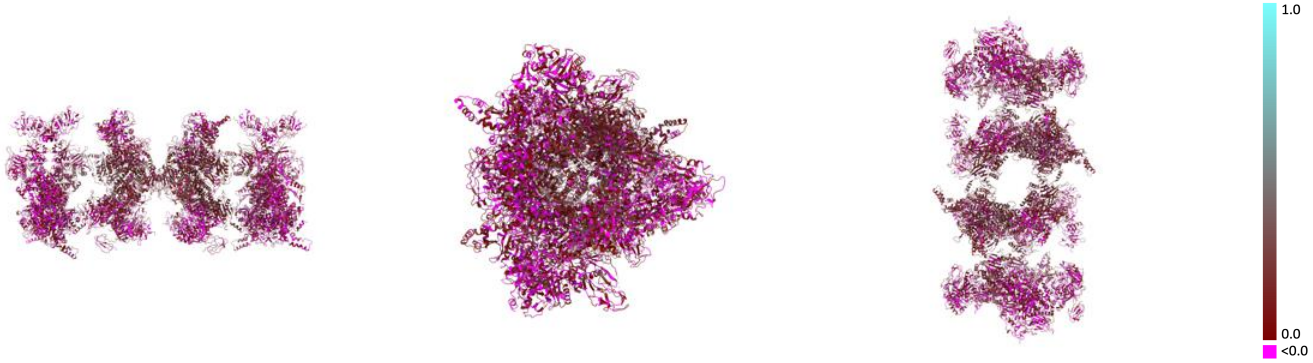
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

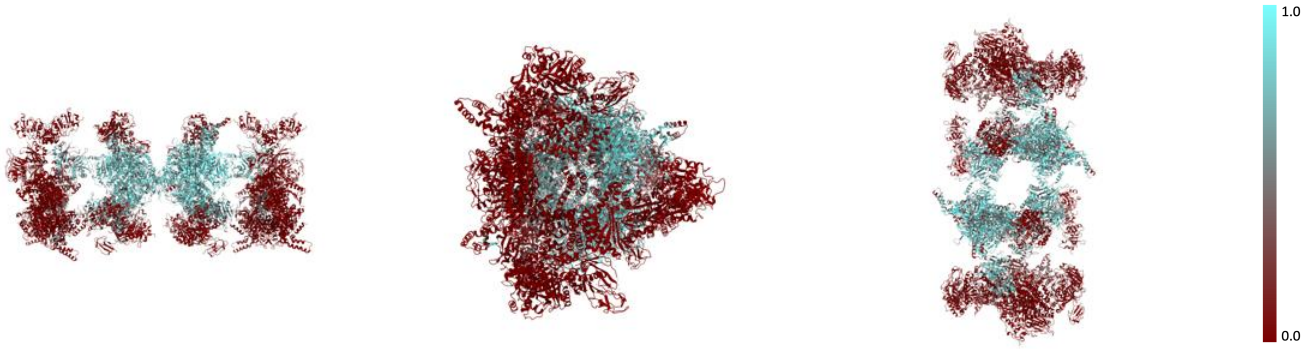
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

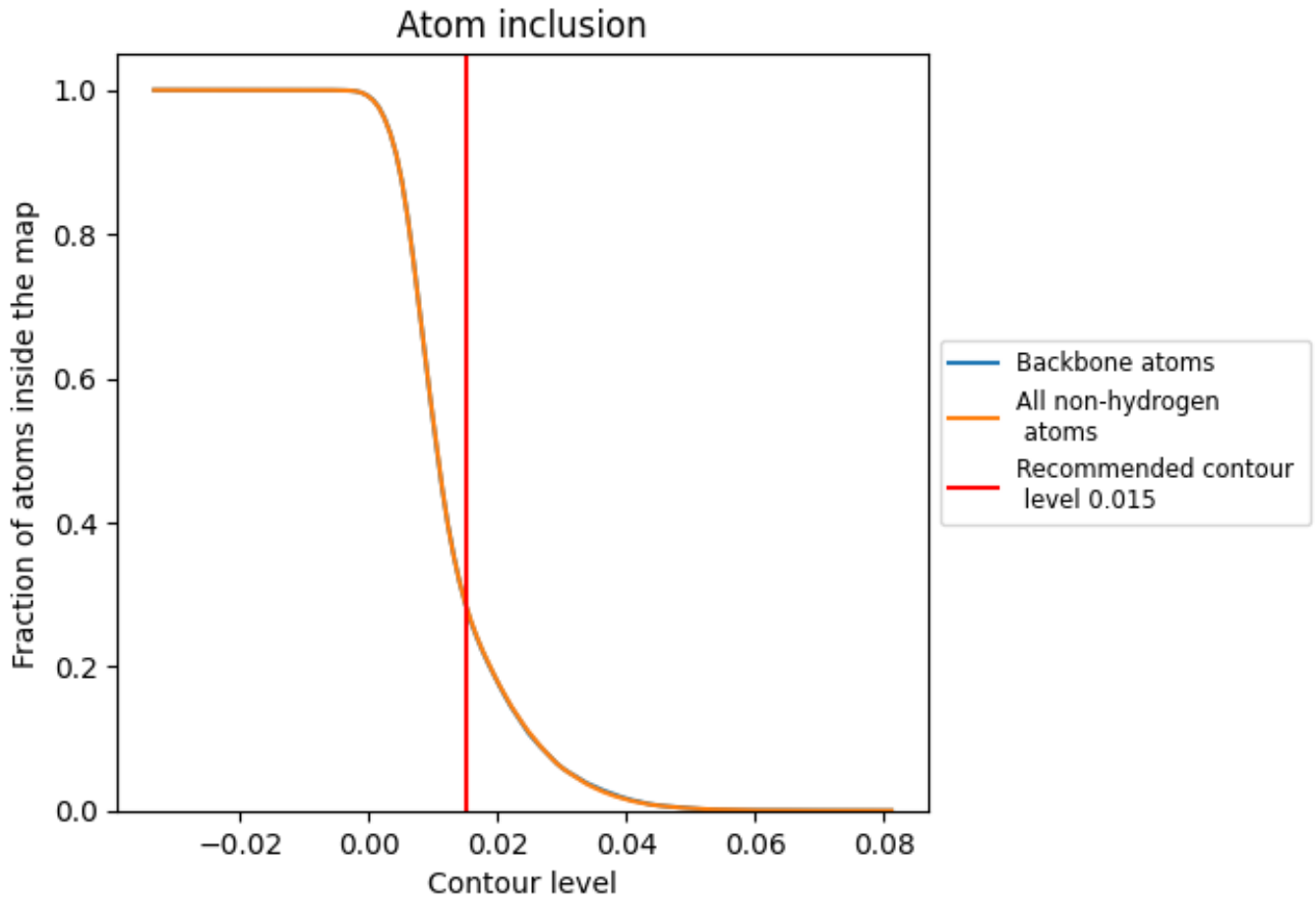
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 29% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2876	0.1080
A	0.2282	0.0990
B	0.2298	0.1000
C	0.4242	0.1330
D	0.5945	0.1610
E	0.5903	0.1610
F	0.4229	0.1330
G	0.0360	0.0800
H	0.0707	0.0540
J	0.0063	0.0540
K	0.0522	0.0450
M	0.0468	0.0510
O	0.0732	0.0580
Q	0.0353	0.0770
R	0.0063	0.0540
S	0.0018	0.0510
U	0.0024	0.0510
W	0.0000	0.0370
Y	0.0012	0.0380