



## 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 Å 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](mailto: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>.

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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

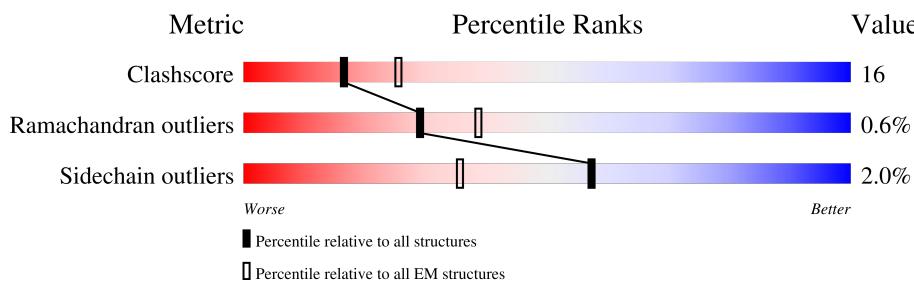
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *ELECTRON MICROSCOPY*

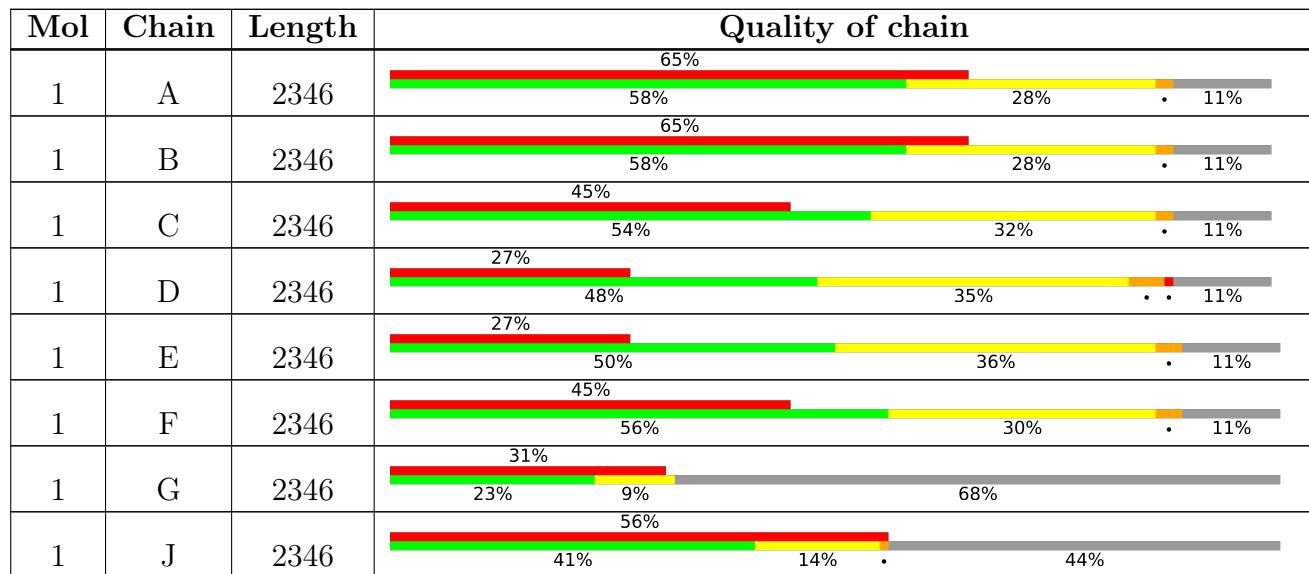
The reported resolution of this entry is 5.90 Å.

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.



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Mol	Chain	Length	Quality of chain				
1	Q	2346	31%	23%	9%	•	68%
1	R	2346	56%	41%	14%	•	44%
2	H	240	82%	69%			20% 11%
2	K	240	84%	68%			21% 11%
2	M	240	86%	68%			20% 11%
2	O	240	82%	70%			18% 11%
2	S	240	89%	74%			15% 11%
2	U	240	89%	72%			16% 11%
2	W	240	89%	74%			15% 11%
2	Y	240	89%	75%			14% 11%

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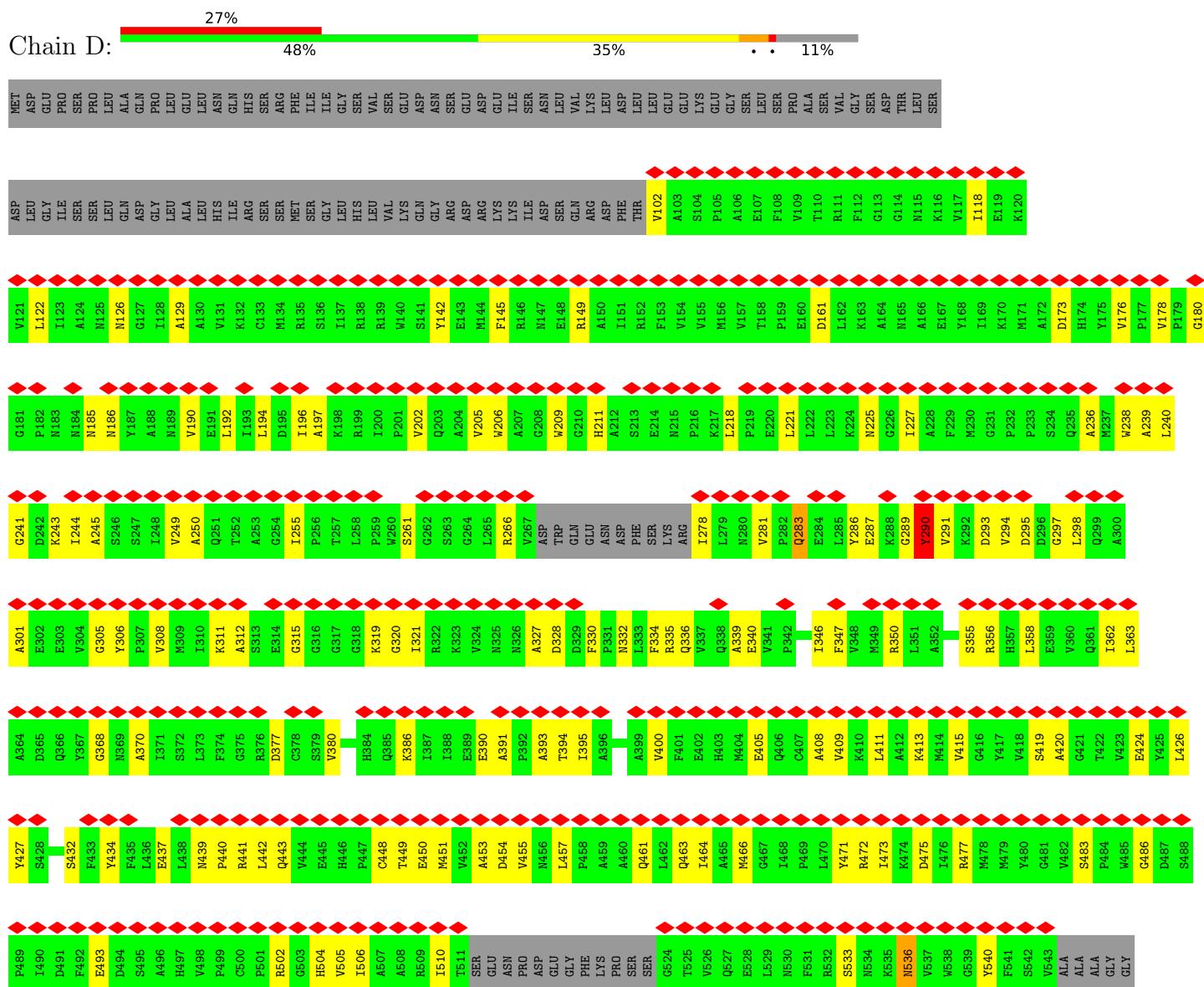
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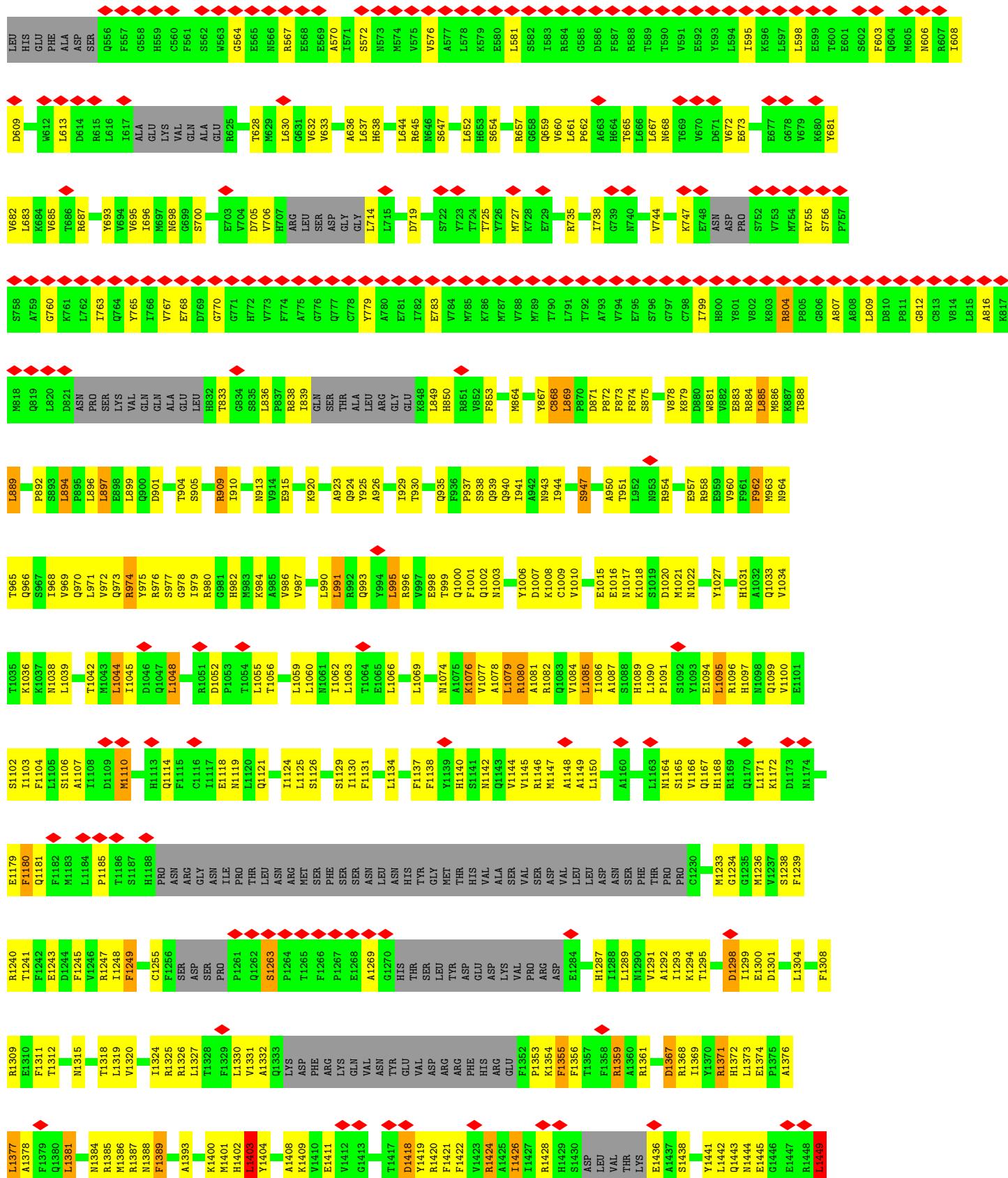
Chain	Residue	Modelled	Actual	Comment	Reference
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W	1639	GLU	-	expression tag	UNP P38398
W	1640	ASN	-	expression tag	UNP P38398
W	1641	LEU	-	expression tag	UNP P38398
W	1642	TYR	-	expression tag	UNP P38398
W	1643	PHE	-	expression tag	UNP P38398
W	1644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

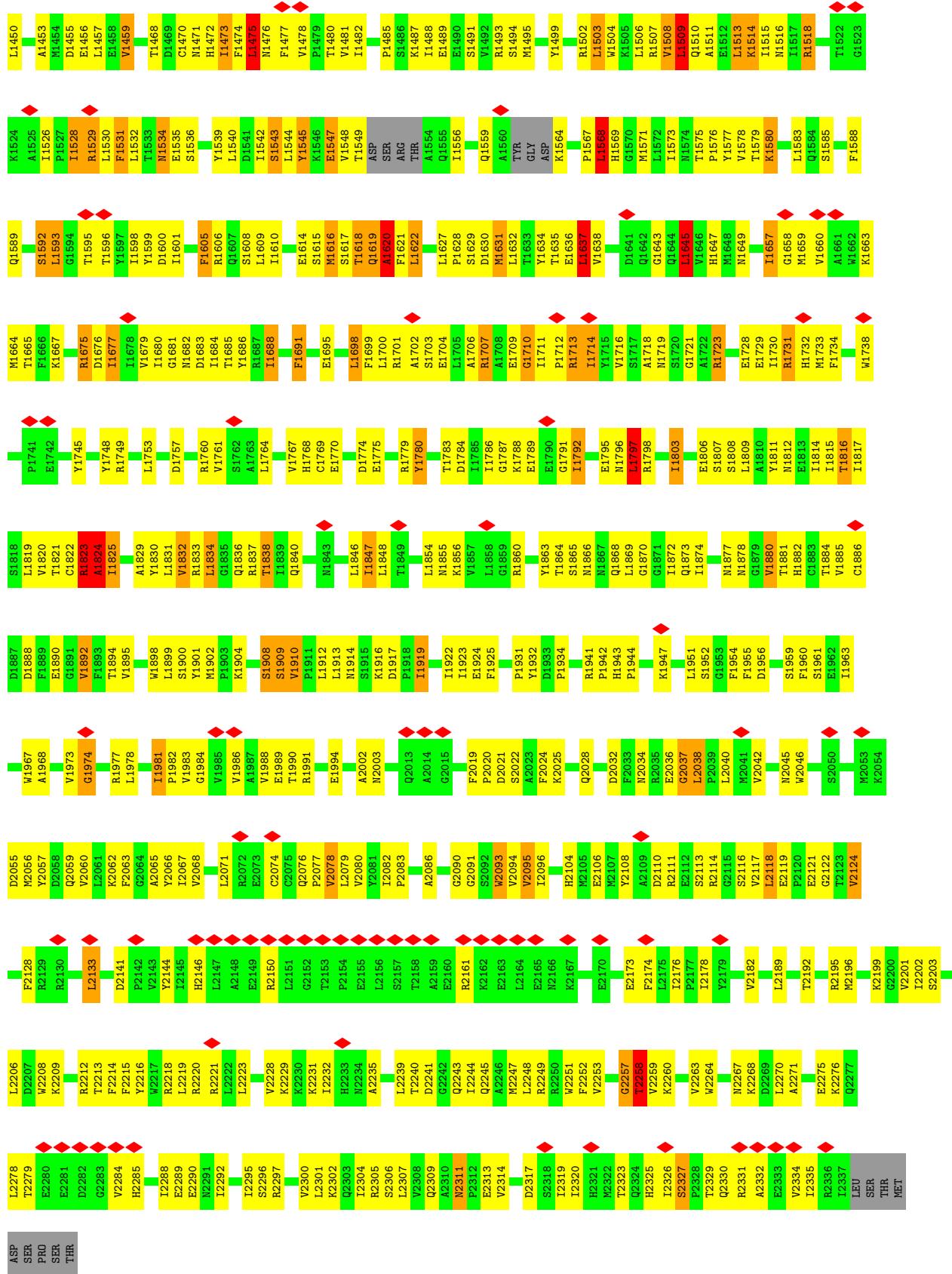
### 3 Residue-property plots

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.

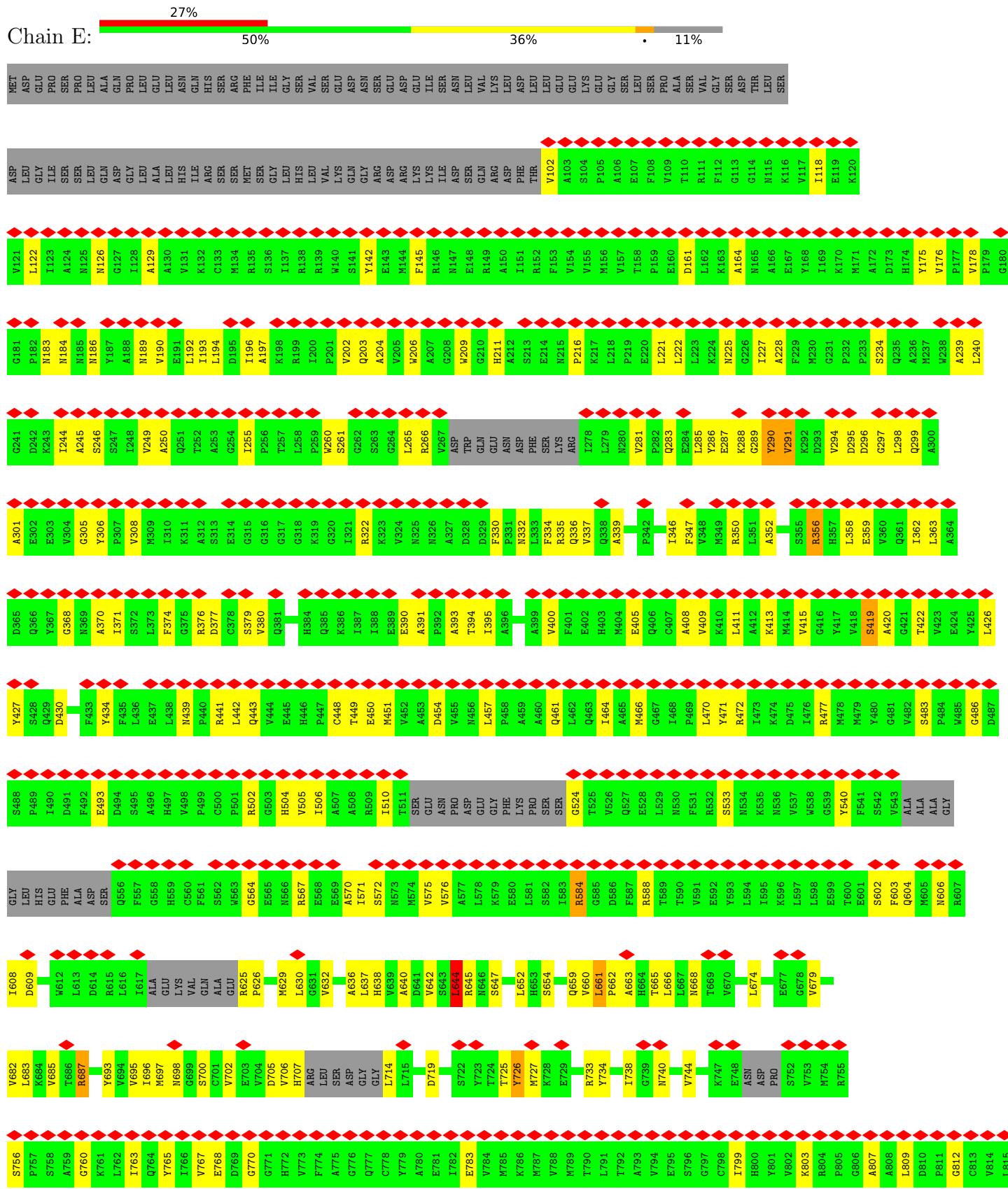
- Molecule 1: Acetyl-CoA carboxylase 1

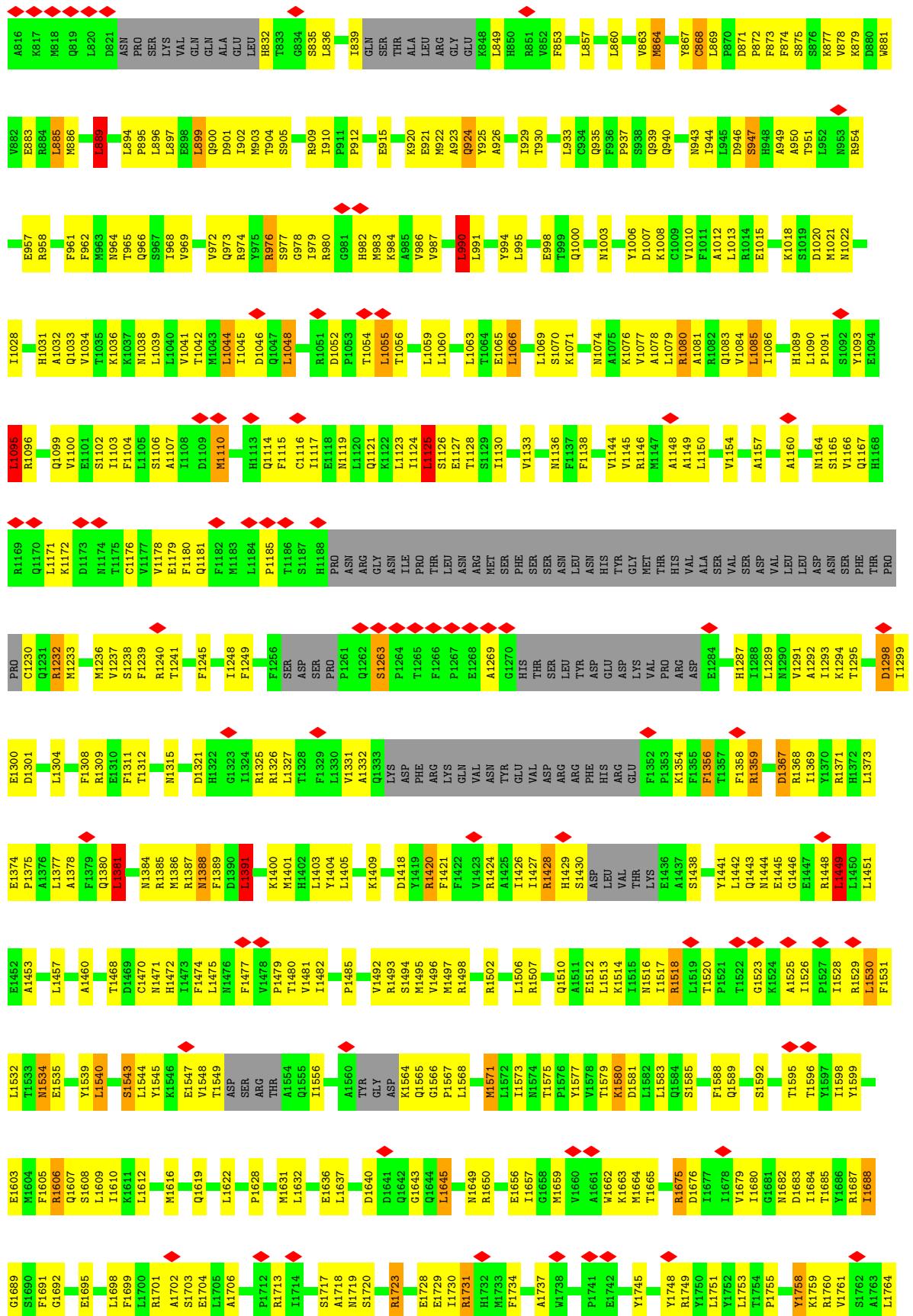


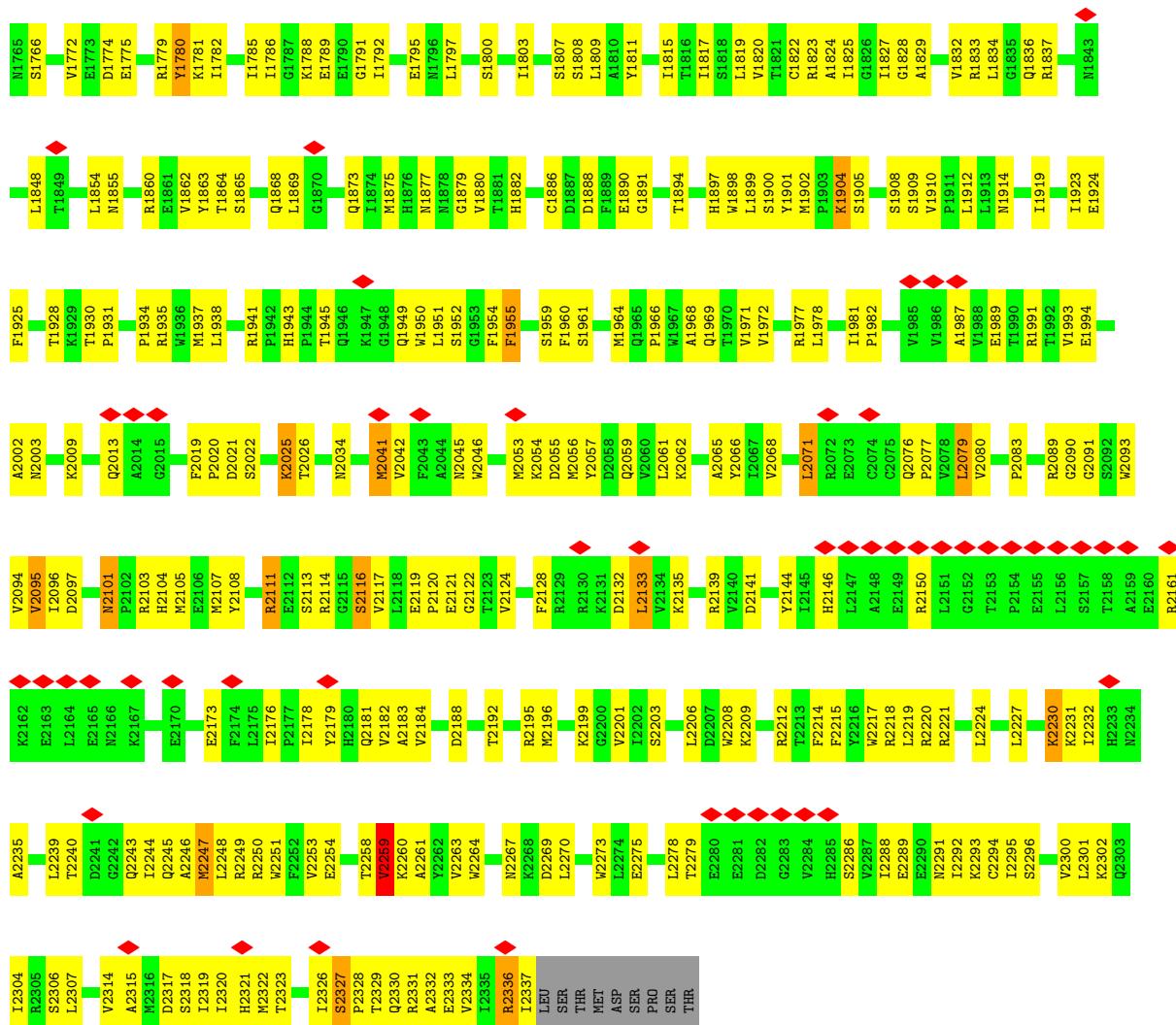




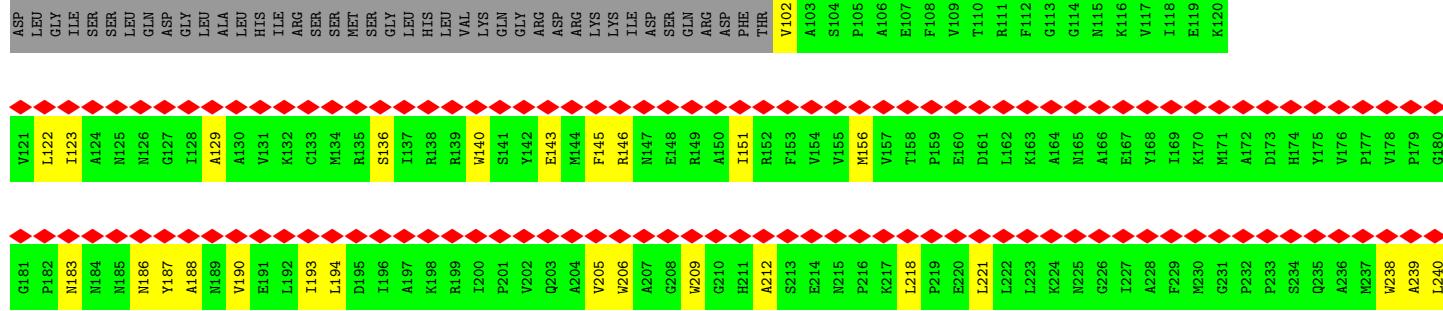
- Molecule 1: Acetyl-CoA carboxylase 1



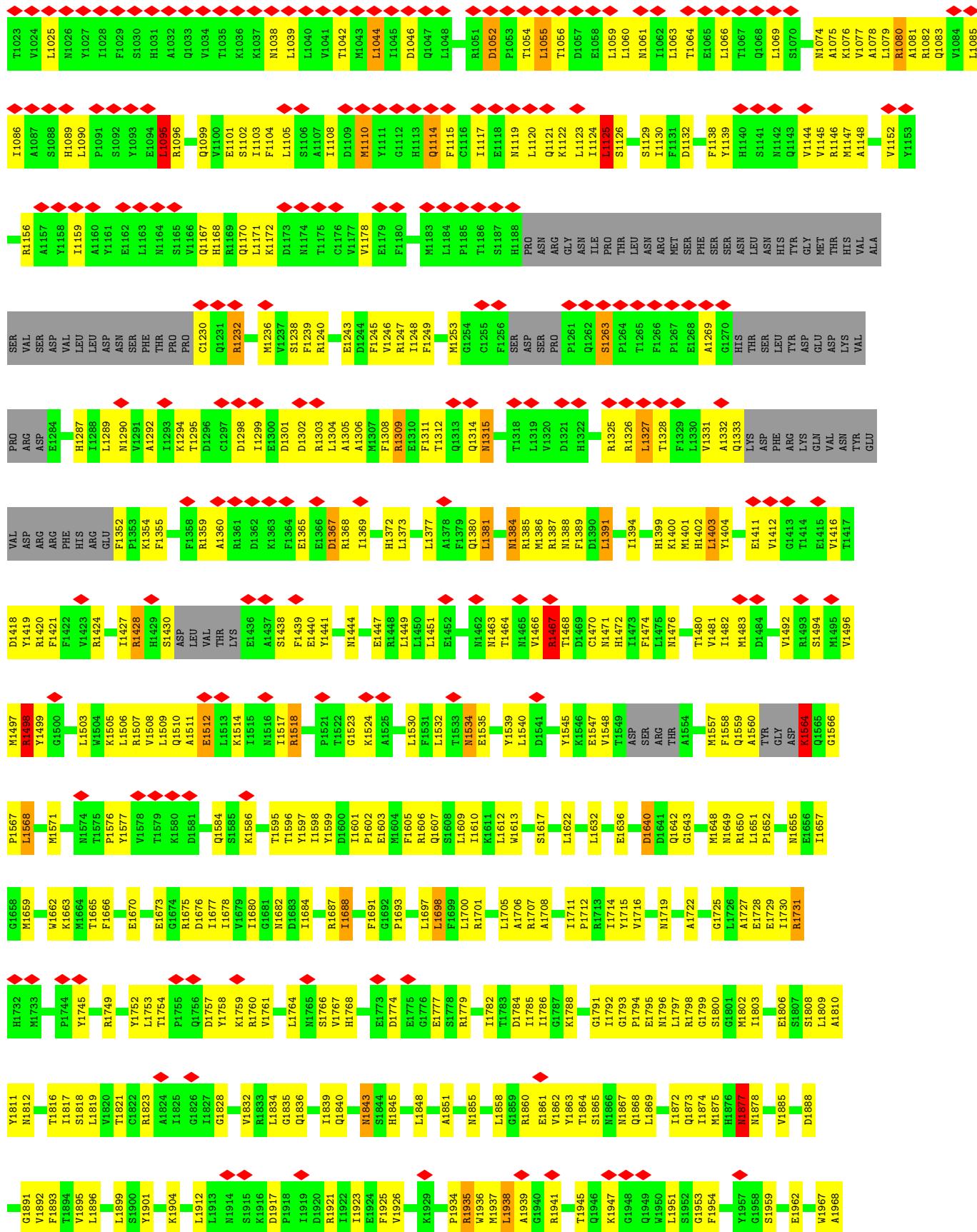


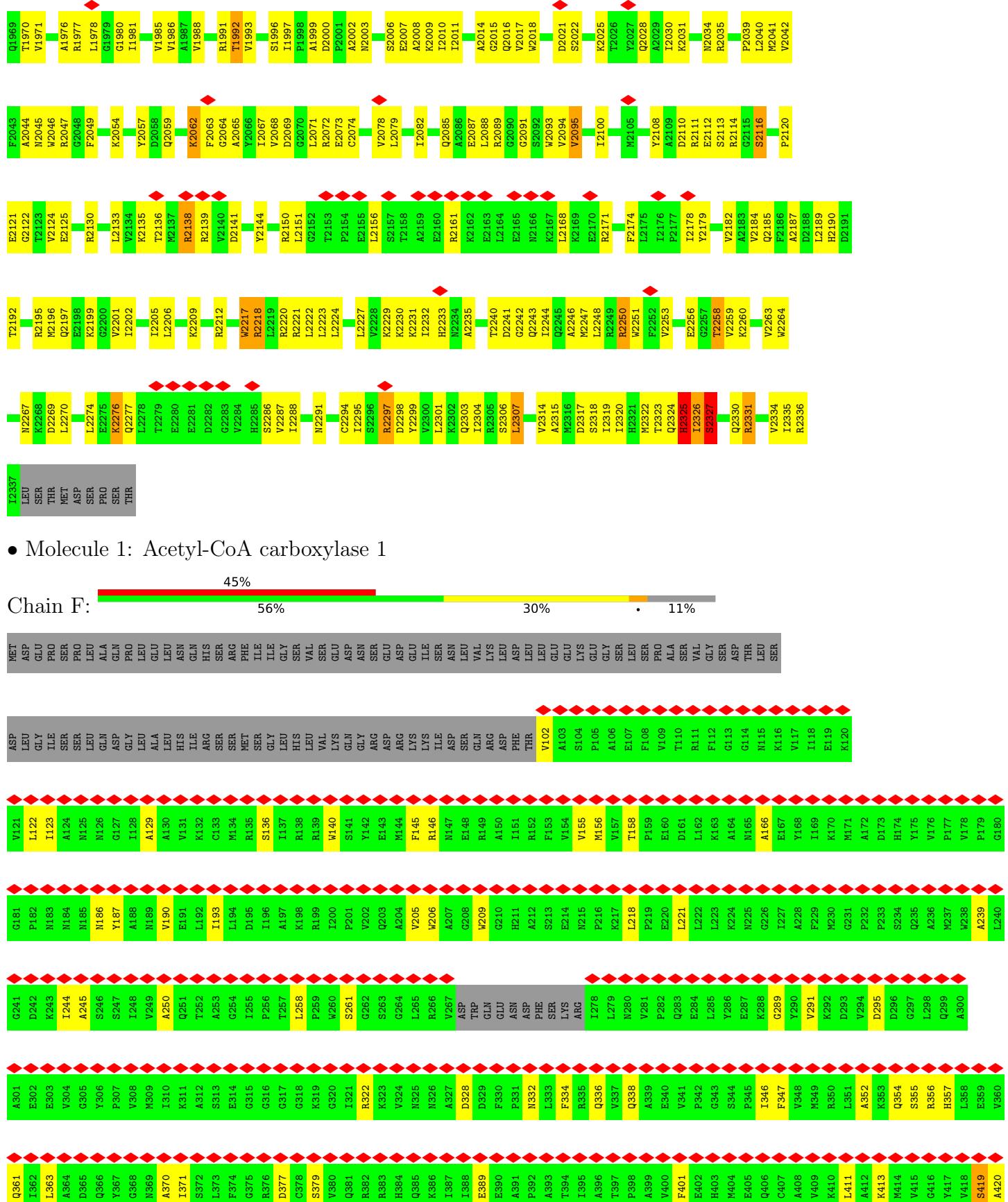


- Molecule 1: Acetyl-CoA carboxylase 1

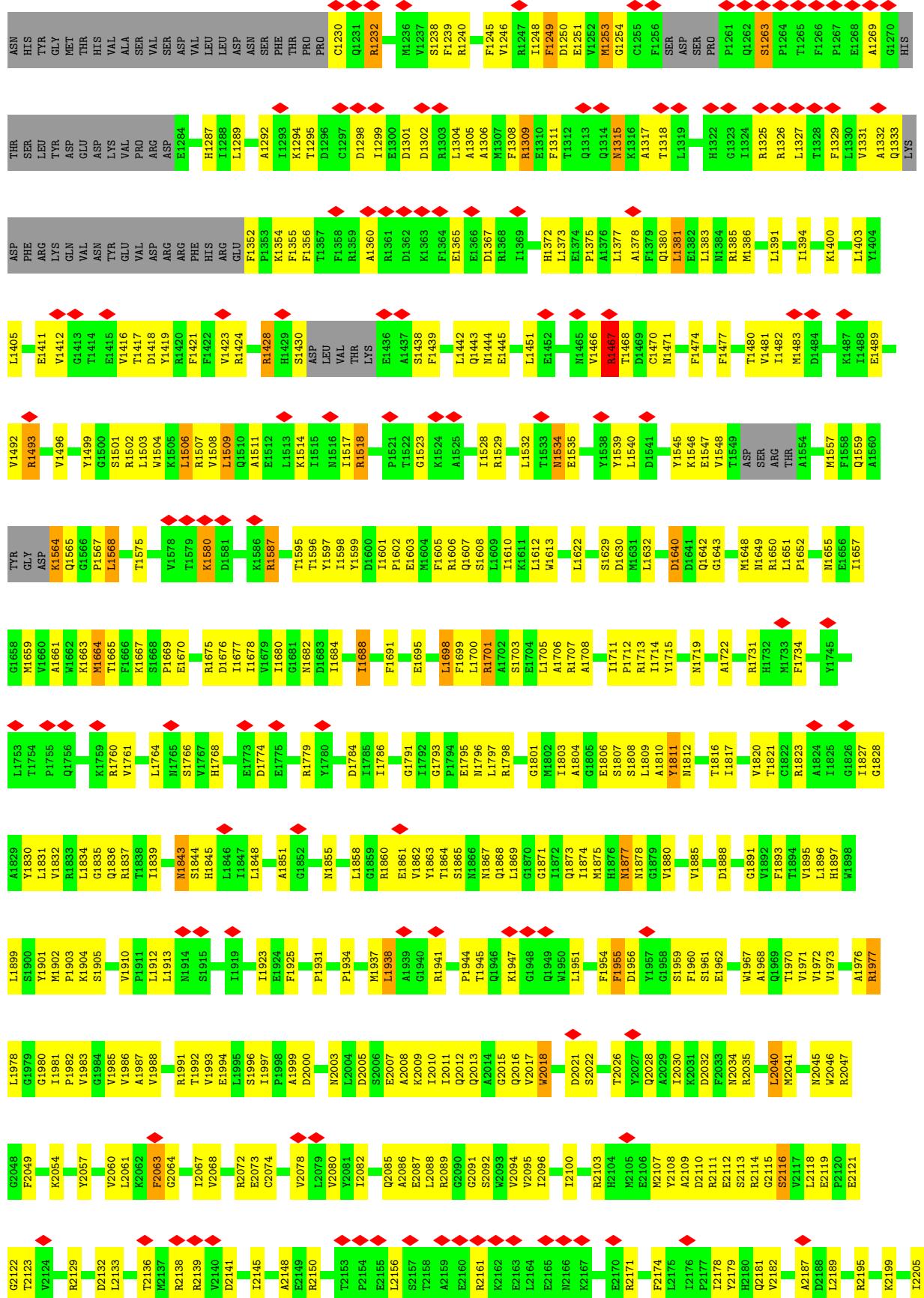


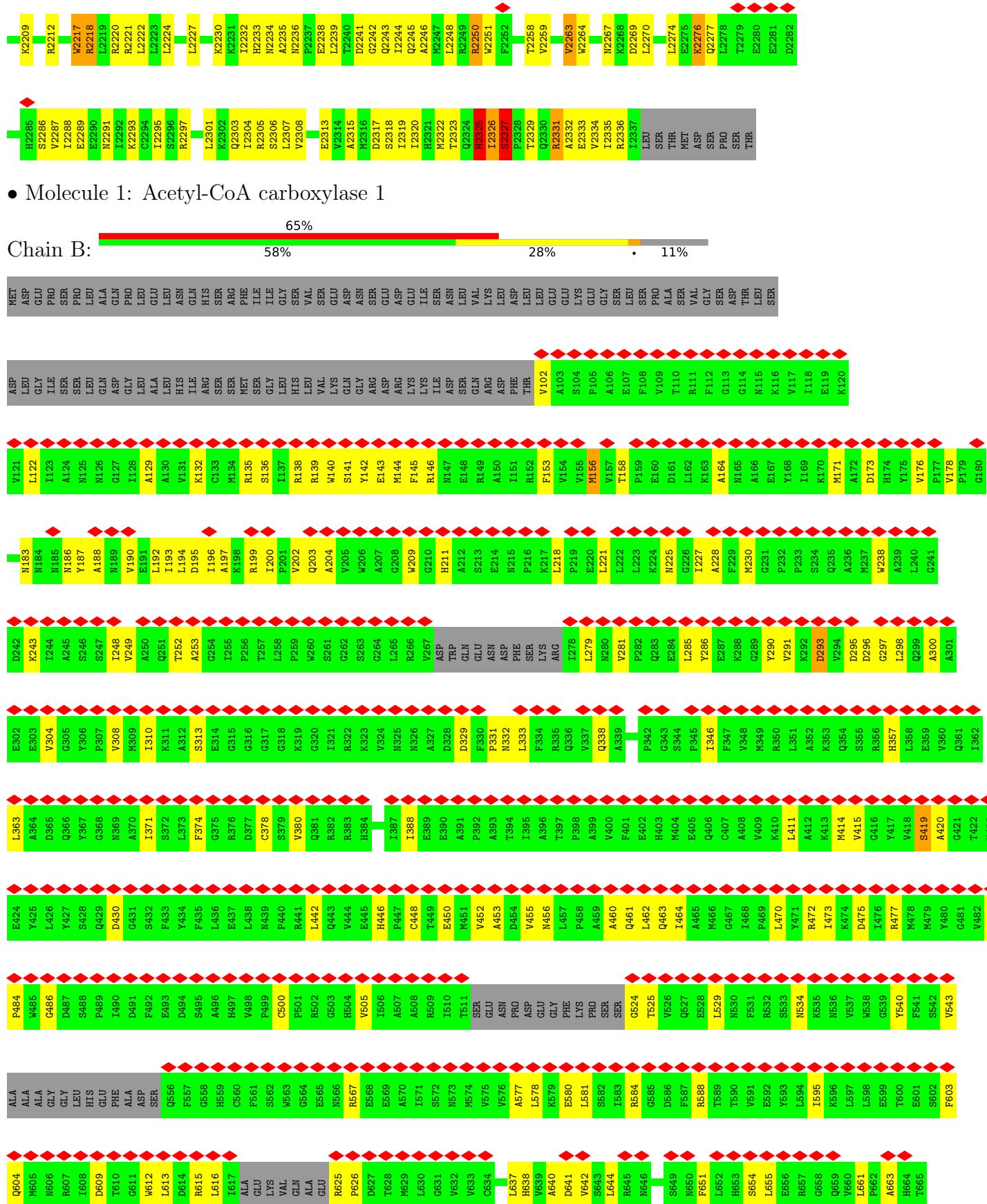
D901	SER	S721	E601	F541	G481	Q361	G241
I902	THR	S722	F602	S542	V482	T362	D242
M903	ALA	Y723	F603	V543	S483	L363	K243
T904	ARG	V784	T724	H664	P484	E424	I244
GLY	GLY	Y785	T725	M605	W485	Y425	A245
GLU	GLU	Y786	T726	M606	G486	Y426	S246
K846	K846	M787	T727	R607	GLY	D487	S247
L849	L849	V788	K728	N608	LEU	S488	I248
G908	G908	R850	N789	D609	HIS	P489	V249
R909	R909	R851	T790	T610	GLU	P490	A250
I910	I910	V852	L791	G611	PHE	D490	A250
F911	F911	F853	D854	W612	ALA	G491	Q251
P912	P912	D732	E733	E613	ASP	F492	T252
M913	M913	A793	V794	D614	SER	B493	T252
V914	V914	V855	V794	R615	GLU	F493	A252
V856	V856	E915	E795	G586	GLU	D494	I253
K916	K916	L857	I795	H589	GLU	F494	G254
S917	S917	I917	I796	L616	GLN	G495	C254
I918	I918	N859	E796	E617	GLN	L496	G255
R919	R919	L860	C798	E617	GLN	P496	I255
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K920	K920	N862	V740	E619	GLU	D497	P256
E921	E921	D855	V740	G620	GLU	F498	T256
A922	M922	V863	V741	V581	GLN	G499	S256
A923	A923	R864	V742	V682	GLN	R500	V257
N924	N924	N865	C743	E621	GLU	R501	A257
Y925	Y925	R866	V744	E622	GLU	R502	G252
M926	A926	V867	F745	D623	GLU	R503	S252
I927	S927	I927	E746	E624	GLU	R504	L255
A928	A928	R868	A808	E625	GLU	R505	R256
I929	I929	P870	L809	P626	GLU	R506	R256
R929	R929	D871	D810	D627	GLU	R507	R256
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S931	S931	V868	A807	E629	GLU	R509	R256
V932	V932	R869	A808	E630	GLU	R510	R256
I933	I933	N869	A809	E631	GLU	R511	R256
C934	C934	R870	D810	E632	GLU	R512	R256
Y935	Y935	P871	P812	E633	GLU	R513	R256
I936	I936	V872	A807	E634	GLU	R514	R256
V937	V937	P873	V753	E635	GLU	R515	R256
A938	A938	V874	V754	E636	GLU	R516	R256
I939	I939	S875	V755	E637	GLU	R517	R256
C939	C939	V876	V756	E638	GLU	R518	R256
Y940	Y940	V877	A816	E639	GLU	R519	R256
I941	I941	K878	V817	E640	GLU	R520	R256
D946	D946	M880	M818	A640	GLU	R521	R256
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N943	N943	W881	W881	V642	GLU	R523	R256
I1003	I1003	V882	A821	L762	GLU	R524	R256
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H1005	H1005	R884	V817	V763	GLU	R526	R256
F1006	F1006	D885	M818	A759	GLU	R527	R256
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D1007	D1007	Q887	Q819	V641	GLU	R529	R256
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A949	A949	I1004	I944	V642	GLU	R531	R256
A950	A950	F1011	I945	V643	GLU	R532	R256
T951	T951	A1012	L952	V644	GLU	R533	R256
D946	D946	A1013	N953	V645	GLU	R534	R256
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N943	N943	A954	I1004	V647	GLU	R536	R256
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A956	A956	T951	E1015	T644	GLU	R539	R256
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D946	D946	A1012	A1016	V646	GLU	R541	R256
A942	A942	A1013	N953	V647	GLU	R542	R256
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C1009	C1009	A955	F1010	S649	GLU	R544	R256
I1010	I1010	S956	A1015	T644	GLU	R545	R256
A956	A956	T951	E1016	T645	GLU	R546	R256
I1011	I1011	L952	A1017	V646	GLU	R547	R256
D946	D946	A1012	N1017	V647	GLU	R548	R256
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A956	A956	T951	A1015	V646	GLU	R567	R256
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N943	N943	R954	F1010	S649	GLU	R571	R256
C1009	C1009	A955	A1014	T644	GLU	R572	R256
I1010	I1010	S956	F1011	T645	GLU	R573	R256
A956	A956	T951	A1015	V646	GLU	R574	R256
I1011	I1011	L952	E1016	V647	GLU	R575	R256
D946	D946	A1012	A1017	V648	GLU	R576	R256
A942	A942	A1013	N1019	V649	GLU	R577	R256
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C1009	C1009	A955	A1014	T644	GLU	R579	R256
I1010	I1010	S956	F1011	T645	GLU	R580	R256
A956	A956	T951	A1015	V646	GLU	R581	R256
I1011	I1011	L952	E1016	V647	GLU	R582	R256
D946	D946	A1012	A1017	V648	GLU	R583	R256
A942	A942	A1013	N1019	V649	GLU	R584	R256
N943	N943	R954	F1010	S649	GLU	R585	R256
C1009	C1009	A955	A1014	T644	GLU	R586	R256
I1010	I1010	S956	F1011	T645	GLU	R587	R256
A956	A956	T951	A1015	V646	GLU	R588	R256
I1011	I1011	L952	E1016	V647	GLU	R589	R256
D946	D946	A1012	A1017	V648	GLU	R590	R256
A942	A942	A1013	N1019	V649	GLU	R591	R256
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A956	A956	T951	A1015	V646	GLU	R595	R256
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D946	D946	A1012	A1017	V648	GLU	R597	R256
A942	A942	A1013	N1019	V649	GLU	R598	R256
N943	N943	R954	F1010	S649	GLU	R599	R256
C1009	C1009	A955	A1014	T644	GLU	R600	R256
I1010	I1010	S956	F1011	T645	GLU	R601	R256
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D946	D946	A1012	A1017	V648	GLU	R604	R256
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I1010	I1010	S956	F1011	T645	GLU	R608	R256
A956	A956	T951	A1015	V646	GLU	R609	R256
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D946	D946	A1012	A1017	V648	GLU	R611	R256
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A956	A956	T951	A1015	V646	GLU	R616	R256
I1011	I1011	L952	E1016	V647	GLU	R617	R256
D946	D946	A1012	A1017	V648	GLU	R618	R256
A942	A942	A1013	N1019	V649	GLU	R619	R256
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A956	A956	T951	A1015	V646	GLU	R623	R256
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A942	A942	A1013	N1019	V649	GLU	R626	R256
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C1009	C1009	A955	A1014	T644	GLU	R628	R256
I1010	I1010	S956	F1011	T645	GLU	R629	R256
A956	A956	T951	A1015	V646	GLU	R630	R256
I1011	I1011	L952	E1016	V647	GLU	R631	R256
D946	D946	A1012	A1017	V648	GLU	R632	R256
A942	A942	A1013	N1019	V649	GLU	R633	R256
N943	N943	R954	F1010	S649	GLU	R634	R256
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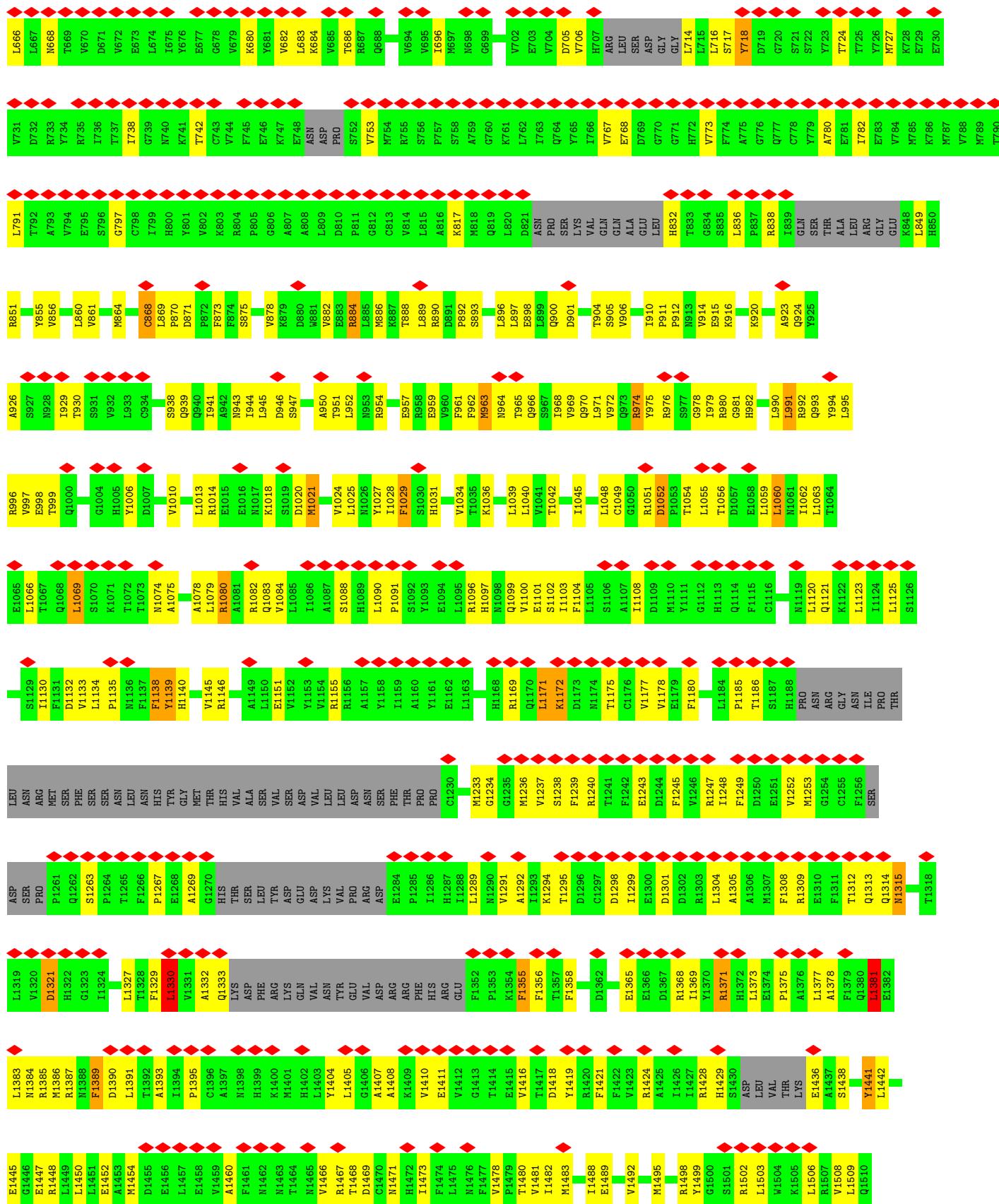






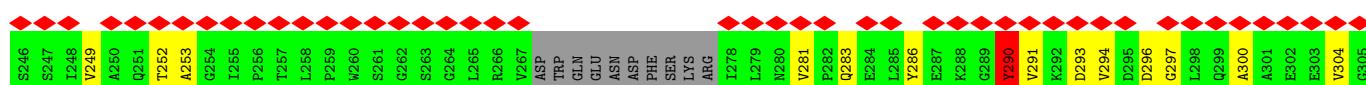
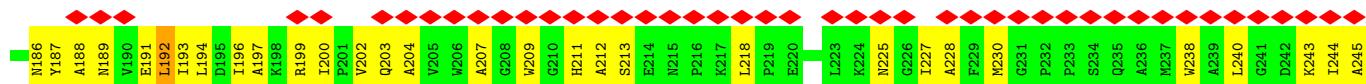


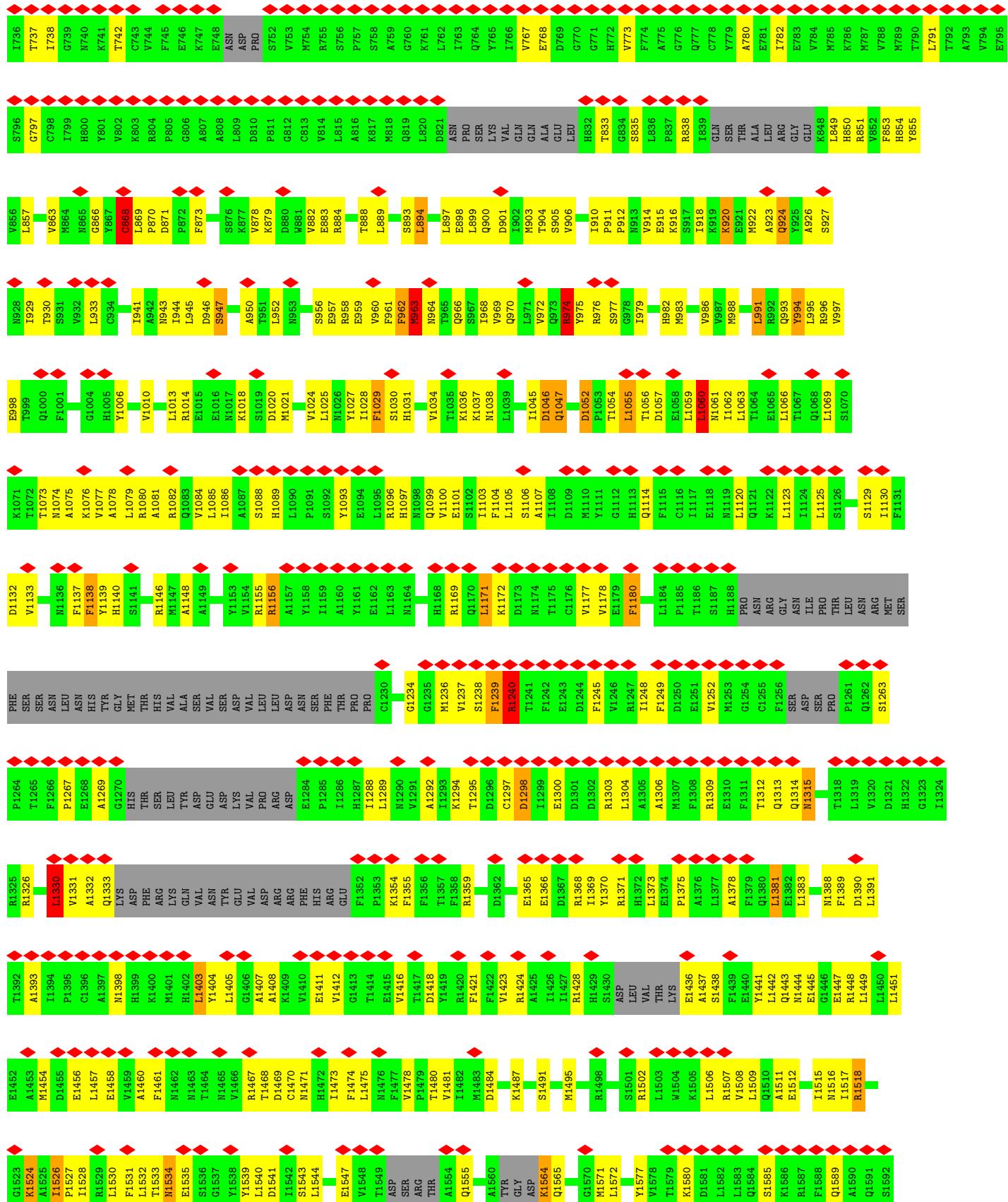






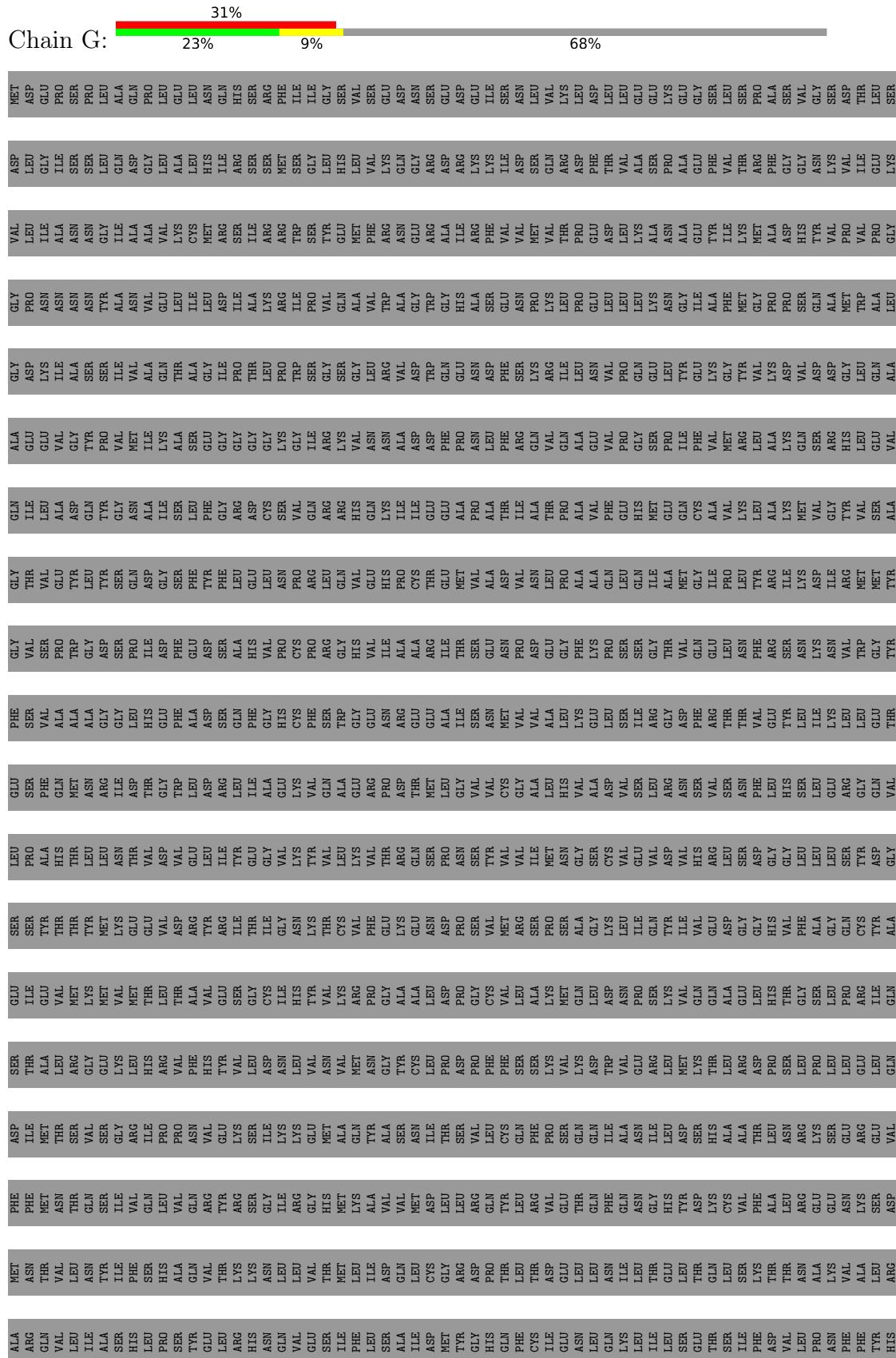
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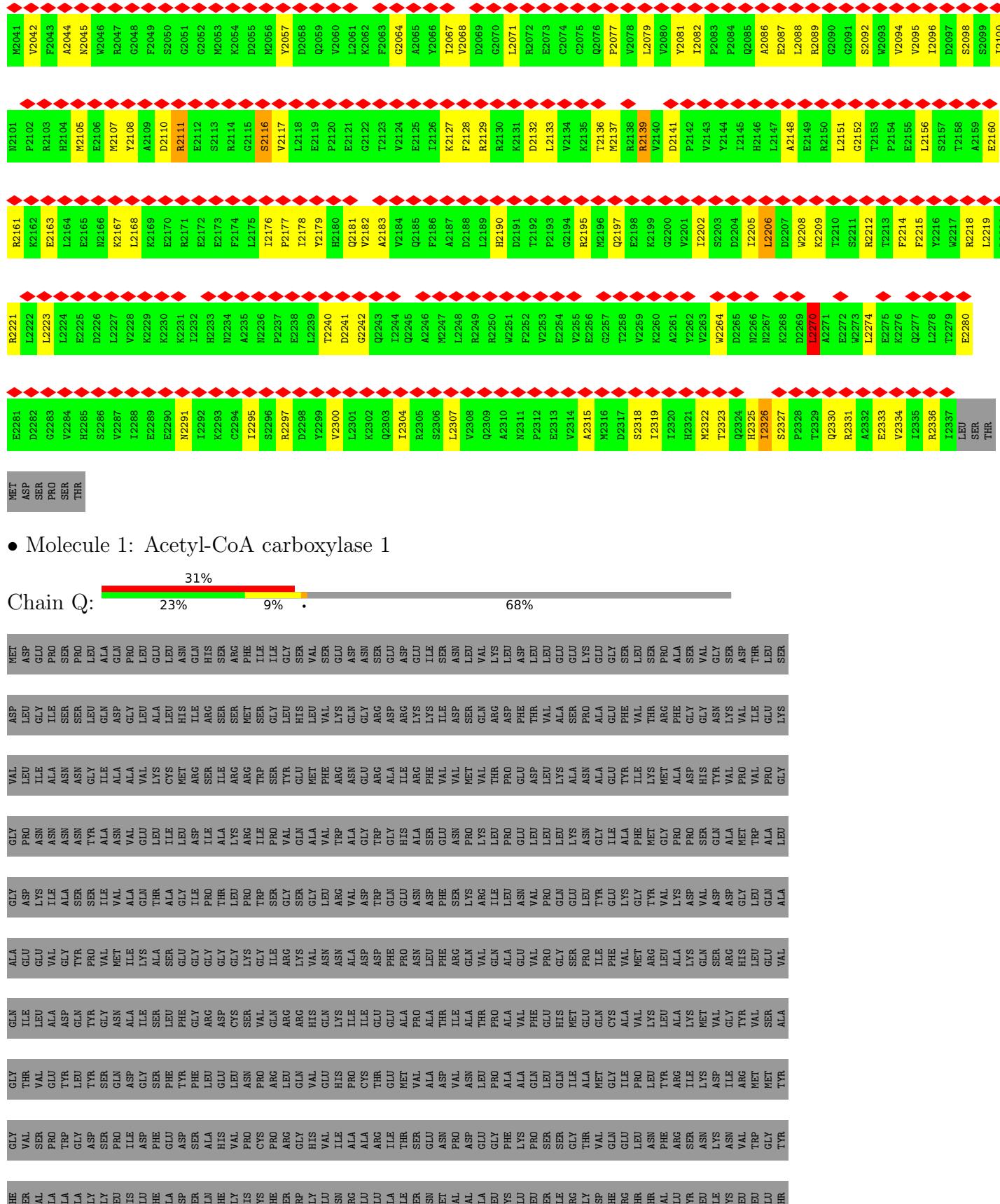


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D2265	Q2330	V2018	Y1857	M1655	T1.596
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A2332	L2274	V2140	S1900	M1658	I.1598
R2334	E2275	D2141	S1961	K1781	M1.599
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C2209	R2302	V2182	V2088	V1973	I1848
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M2209	R2340	G2193	V2088	V1973	I1848
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K2209	R2342	T2193	V2088	V1973	I1848
J2209	R2343	V2193	V2088	V1973	I1848
I2209	R2344	G2194	V2088	V1973	I1848
H2209	R2345	E2194	V2088	V1973	I1848
G2209	R2346	T2194	V2088	V1973	I1848
F2209	R2347	V2194	V2088	V1973	I1848
E2209	R2348	G2195	V2088	V1973	I1848
D2209	R2349	E2195	V2088	V1973	I1848
C2209	R2350	T2195	V2088	V1973	I1848
B2209	R2351	V2195	V2088	V1973	I1848
A2209	R2352	G2196	V2088	V1973	I1848
Z2209	R2353	E2196	V2088	V1973	I1848
Y2209	R2354	T2196	V2088	V1973	I1848
X2209	R2355	V2196	V2088	V1973	I1848
W2209	R2356	G2197	V2088	V1973	I1848
V2209	R2357	E2197	V2088	V1973	I1848
U2209	R2358	T2197	V2088	V1973	I1848
T2209	R2359	V2197	V2088	V1973	I1848
S2209	R2360	G2198	V2088	V1973	I1848
R2209	R2361	E2198	V2088	V1973	I1848
P2209	R2362	T2198	V2088	V1973	I1848
N2209	R2363	V2198	V2088	V1973	I1848
M2209	R2364	G2199	V2088	V1973	I1848
L2209	R2365	E2199	V2088	V1973	I1848
K2209	R2366	T2199	V2088	V1973	I1848
J2209	R2367	V2199	V2088	V1973	I1848
I2209	R2368	G2200	V2088	V1973	I1848
H2209	R2369	E2200	V2088	V1973	I1848
G2209	R2370	T2200	V2088	V1973	I1848
F2209	R2371	V2200	V2088	V1973	I1848
E2209	R2372	G2201	V2088	V1973	I1848
D2209	R2373	E2201	V2088	V1973	I1848
C2209	R2374	T2201	V2088	V1973	I1848
B2209	R2375	V2201	V2088	V1973	I1848
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V2209	R2381	E2203	V2088	V1973	I1848
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D2209	R2397	E2207	V2088	V1973	I1848
C2209	R2398	T2207	V2088	V1973	I1848
B2209	R2399	V2207	V2088	V1973	I1848
A2209	R2400	G2208	V2088	V1973	I1848
Z2209</td					

- Molecule 1: Acetyl-CoA carboxylase 1



SER	PRO	SER	ASN	GLN	GLN	GLN	VAL
M1861	F1621	G1681	Y1862	M1622	L1622	A1622	VAL
V1862	M1802	N1682	E1742	I1803	D1683	E1743	VAL
Y1863	V1863	F1925	T1926	T1929	T1930	P1931	VAL
I1923	I1924	F1925	V1926	K1927	P1927	P1932	VAL
C1984	E1985	V1985	V1986	A1804	S1885	P1808	VAL
V1985	V1986	F1925	V1926	A1804	S1885	S1808	VAL
A1887	A1887	V1926	V1926	A1804	S1885	S1808	VAL
A1887	A1887	T1928	T1928	T1809	I1889	R1873	VAL
V1988	V1988	T1928	T1928	T1809	I1889	R1873	VAL
E1989	E1989	K1929	K1929	T1749	T1750	T1873	VAL
T1990	T1990	T1929	T1929	R1873	I1889	I1874	VAL
R1991	R1991	P1932	P1932	I1873	I1874	I1874	VAL
T1992	T1992	Y1932	Y1932	I1873	I1874	I1874	VAL
V1993	V1993	D1933	D1933	I1873	I1874	I1874	VAL
E1994	E1994	P1933	P1933	I1873	I1874	I1874	VAL
L1995	L1995	R1935	R1935	I1873	I1875	I1875	VAL
S1996	S1996	W1936	W1936	I1873	I1875	I1875	VAL
I1997	I1997	M1937	M1937	I1873	I1875	I1875	VAL
P1998	P1998	L1938	L1938	I1873	I1875	I1875	VAL
A1999	A1999	A1939	A1939	I1873	I1875	I1875	VAL
D2000	D2000	P1940	P1940	I1873	I1875	I1875	VAL
P2001	P2001	R1941	R1941	T1881	T1881	T1881	VAL
M2002	M2002	P1942	P1942	H1882	C1883	C1883	VAL
N2003	N2003	H1943	H1943	D1883	R1823	A1823	VAL
L2004	L2004	P1944	P1944	T1884	A1824	A1824	VAL
D2005	D2005	T1945	T1945	V1884	I1825	I1825	VAL
T2010	T2010	W1950	W1950	V1885	T1880	T1880	VAL
S2006	S2006	Q1946	Q1946	C1886	C1826	C1822	VAL
E2007	E2007	K1947	K1947	H1882	I1827	I1827	VAL
A2008	A2008	G1948	G1948	D1888	C1828	C1828	VAL
K2009	K2009	Q1949	Q1949	F1889	A1829	A1829	VAL
T2011	T2011	T1945	T1945	E1889	V1885	V1885	VAL
I2014	I2014	L1951	L1951	G1881	C1881	C1881	VAL
Q2012	Q2012	S1952	S1952	V1892	V1893	V1893	VAL
Q2013	Q2013	G1953	G1953	F1893	R1893	R1893	VAL
A2014	A2014	F1954	F1954	T1894	I1834	I1834	VAL
G2015	G2015	F1955	F1955	V1895	G1935	G1935	VAL
Q2016	Q2016	D1956	D1956	L1896	Q1836	Q1836	VAL
Q2017	Q2017	Y1957	Y1957	H1897	R1837	R1837	VAL
W2018	W2018	G1958	G1958	W1888	T1838	T1838	VAL
F2019	F2019	F1954	F1954	T1894	I1839	I1839	VAL
P2020	P2020	S1959	S1959	V1899	T1899	T1899	VAL
K2025	K2025	F1960	F1960	S1900	Q1840	Y1780	VAL
D2021	D2021	S1961	S1961	V1901	K1901	K1901	VAL
S2022	S2022	E1962	E1962	M1902	I1841	G1721	VAL
A2023	A2023	V1963	V1963	S1908	E1842	I1782	VAL
F2024	F2024	A1968	A1968	S1908	I1847	K1667	VAL
I2030	I2030	M1964	M1964	K1904	N1843	T1773	VAL
K2025	K2025	Q1985	Q1985	S1905	S1905	M1663	VAL
T2026	T2026	P1986	P1986	V1906	V1906	S1664	VAL
Y2027	Y2027	W1967	W1967	H1897	E1842	P1602	VAL
Q2028	Q2028	V1972	V1972	A1968	I1783	K1667	VAL
A2029	A2029	V1973	V1973	P1969	I1783	T1773	VAL
R2035	R2035	G1974	G1974	N1914	L1854	P1794	VAL
E2036	E2036	B1975	B1975	S1915	N1855	E1795	VAL
G2037	G2037	A1976	A1976	K1916	K1916	M1616	VAL
L2038	L2038	R1977	R1977	D1917	D1917	S1617	VAL
P2039	P2039	L1978	L1978	P1918	L1858	R1798	VAL
L2040	L2040	G1979	G1979	I1919	G1859	T1799	VAL
						G1860	VAL

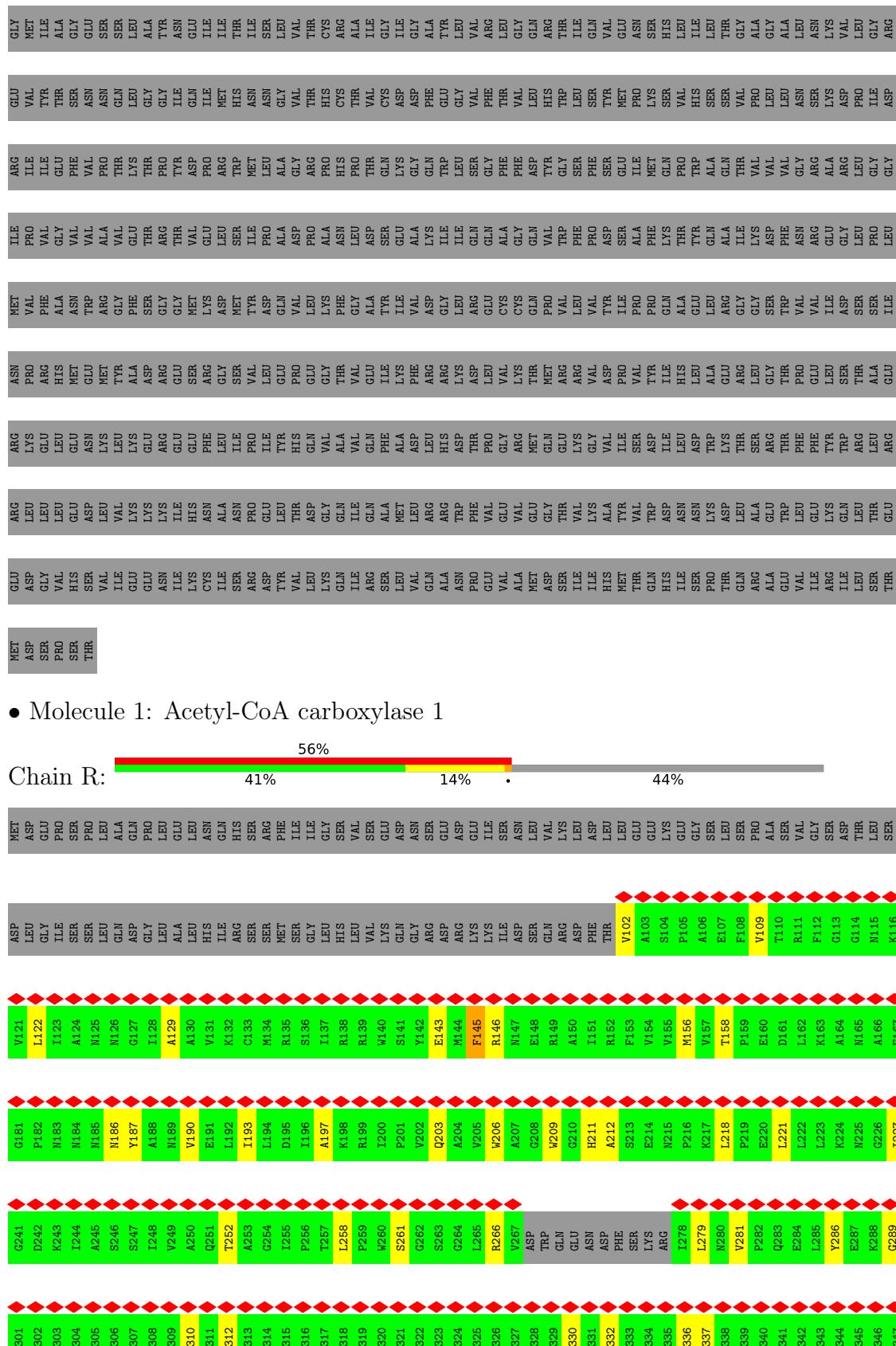




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ASP	GLY	I2424	I2425	ASP	GLY	E2245	E2246	V1986
ASP	GLY	I2425	I					

SER	E781	S721	T782	P662	E601	G481	G241	V121
THR	I792	S722	I783	P663	S602	V442	P182	L122
ALA	M903	E783	ARG	V854	K603	A663	N183	N123
LEU	T904	V784	GLY	Q604	H664	T724	E422	D242
GLU	S905	M785	GLY	M605	T665	T725	V423	K243
VAL	V906	K786	GLY	N606	L666	Y726	V423	V304
ASP	K848	M787	GLY	R607	L667	M727	P424	A364
S907	L849	V788	GLY	R608	N668	K728	P425	Y425
G908	H850	H851	GLY	T608	H715	K738	W426	Y426
R909	R851	T790	ASP	D609	T669	T729	W427	Y427
I910	V852	L791	SER	T610	V670	V730	W428	Y428
P911	F853	P792	ASP	G611	D671	D732	W429	Y429
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V914	V856	V794	SER	D614	L674	V734	P432	Y432
E915	E795	E795	ASP	R615	I675	T735	E433	Y433
K916	K857	S796	SER	L616	Y676	V736	E434	Y434
S917	N859	G797	ASP	I617	E677	T737	F435	Y435
I918	L860	C798	SER	R618	G678	V738	F436	Y436
K919	V861	I799	ASP	D619	V679	T739	F437	Y437
L857	I857	T736	SER	N740	K680	N740	F438	Y438
K916	K916	D858	ASP	H681	V681	V681	F439	Y439
E921	V862	V863	SER	K741	T682	T742	F440	Y440
M922	M864	V864	ASP	V802	T682	R683	F441	Y441
A923	N865	R803	SER	C743	L683	R625	F442	Y442
Q924	Q866	R804	ASP	V744	K684	P626	F443	Y443
Y925	Y867	P805	SER	F745	T685	D627	F444	Y444
A926	A926	G806	ASP	E746	T686	T628	F445	Y445
S927	S927	A807	SER	K747	R687	M629	F446	Y446
M928	L869	A808	ASP	E748	Q688	A629	F447	Y447
I929	P870	L809	PRO	R749	V689	R630	F448	Y448
T930	D871	D810	ASP	P690	A691	V632	F449	Y449
S931	C838	P872	PRO	N691	S633	T511	F450	Y450
F873	M864	P811	ASP	S752	S692	M574	F451	Y451
V932	V933	V933	SER	V753	C634	V575	S693	Y452
S875	C834	C834	ASP	M754	G635	V576	A694	Y453
Q934	Q935	S876	SER	R755	T636	A577	V694	Y454
K877	K877	A816	ASP	P756	S695	A578	T695	Y455
F878	F878	P757	SER	T757	M697	A579	V695	Y456
V936	V937	K817	ASP	S758	V698	A580	S699	Y457
K879	M818	V813	SER	A759	V699	P759	V699	Y458
M880	M880	V814	ASP	G760	V699	A581	V699	Y459
Q939	Q939	Q819	SER	T760	D641	S582	V699	Y460
K881	K881	M896	ASP	V765	S642	V699	S699	Y461
Q940	Q940	V822	SER	T766	S647	S647	E528	Y462
I941	E883	A821	ASP	D767	C701	S648	G524	Y463
D946	A942	A821	ASP	V768	V702	T649	G584	Y464
S947	S948	L839	ASP	T769	E703	V649	G585	Y465
N943	L838	R830	SER	A770	V704	V649	D586	Y466
L944	I944	M836	ASP	T771	D705	V649	V656	Y467
M945	L945	V835	SER	V772	V706	V649	V657	Y468
K887	K887	GLN	ASP	T773	V707	V649	V658	Y469
GLN	GLN	GLN	SER	A774	E707	V649	V659	Y470
ALA	ALA	ALA	ASP	T775	V708	V649	V660	Y471
GLU	GLU	GLU	SER	A776	V709	V649	V661	Y472
LEU	LEU	LEU	ASP	D777	V710	V649	V662	Y473
P832	P832	P832	SER	F778	V711	V649	V663	Y474
T833	S833	S833	ASP	V779	E712	V649	V664	Y475
G834	S834	S834	SER	V780	V713	V649	V665	Y476
L835	L835	L835	ASP	V781	V714	V649	V666	Y477
H836	L836	L836	SER	V782	V715	V649	V667	Y478
P837	P837	P837	ASP	V783	V716	V649	V668	Y479
L838	L838	L838	SER	V784	V717	V649	V669	Y480
R839	R839	R839	ASP	V785	V718	V649	V670	Y481
E836	E836	E836	SER	V786	V719	V649	V671	Y482
B839	B839	B839	ASP	V787	V779	V649	V672	Y483
GLN	GLN	GLN	SER	V788	V779	V649	V673	Y484
Q900	Q900	Q900	ASP	V789	V779	V649	V674	Y485

PRO	PHE	Y1441	D1321	P1261	S1141	F961
	GLU	R1502	E1382	H322	N1442	F962
	ASN	I1442	R1383	G1323	N1443	H963
	ASP	Q1443	G1383	G1323	Q1443	T1023
	PRO	K1564	M1504	M1384	P1264	V1084
	THR	TYR	LYS	R1385	R1324	L1085
	LEU	TYR	ARG	R1386	R1325	R1086
	ILE	TYR	TYR	R1387	L1327	M1447
	PRO	PRO	GLN	R1388	T1328	A1087
	GLY	GLY	GLU	R1389	E1268	A1088
	SER	SER	ASP	D1390	F1329	H1089
	ASP	ASP	TYR	M1391	L1330	L1090
	LEU	LEU	LEU	A1391	V1331	V1091
	ILE	ILE	ILE	A1392	A1332	A1092
	PRO	PRO	GLU	A1393	Q1333	V1093
	GLN	ASP	ASP	M1394	Y1333	V1093
	ASP	ASP	TYR	R1395	Y1334	V1094
	LEU	LEU	LEU	P1395	R1334	R1094
	ILE	ILE	ILE	R1396	E1267	L1095
	PRO	VAL	VAL	R1397	T1328	A1096
	GLN	ASP	ASP	A1398	E1268	A1097
	ASP	ASP	TYR	R1399	F1329	H1098
	LEU	LEU	LEU	M1400	L1330	V1098
	ILE	ILE	ILE	A1400	V1331	V1099
	PRO	VAL	VAL	R1401	A1332	V1099
	GLU	ASP	ASP	M1401	Q1333	V1099
	ASP	ASP	TYR	R1402	E1268	V1099
	LEU	LEU	LEU	M1402	F1329	H1099
	ILE	ILE	ILE	A1402	L1330	V1099
	PRO	VAL	VAL	R1402	V1331	V1099
	GLU	ASP	ASP	M1403	E1268	V1099
	ASP	ASP	TYR	R1404	F1329	H1099
	LEU	LEU	LEU	M1404	L1330	V1099
	ILE	ILE	ILE	A1404	V1331	V1099
	PRO	VAL	VAL	R1405	A1332	V1099
	GLN	ASP	ASP	M1405	Q1333	V1099
	ASP	ASP	TYR	R1406	E1268	H1098
	LEU	LEU	LEU	M1406	F1329	V1098
	ILE	ILE	ILE	A1406	L1330	V1098
	PRO	VAL	VAL	R1406	V1331	V1098
	GLN	ASP	ASP	M1407	E1268	H1098
	ASP	ASP	TYR	R1407	F1329	V1098
	LEU	LEU	LEU	M1407	L1330	V1098
	ILE	ILE	ILE	A1407	V1331	V1098
	PRO	VAL	VAL	R1408	A1332	V1098
	GLN	ASP	ASP	M1408	Q1333	V1098
	ASP	ASP	TYR	R1409	E1268	H1098
	LEU	LEU	LEU	M1409	F1329	V1098
	ILE	ILE	ILE	A1409	L1330	V1098
	PRO	VAL	VAL	R1410	V1331	V1098
	GLN	ASP	ASP	M1410	A1332	V1098
	ASP	ASP	TYR	R1411	Q1333	V1098
	LEU	LEU	LEU	M1411	E1332	V1098
	ILE	ILE	ILE	A1411	Q1333	V1098
	PRO	VAL	VAL	R1411	F1329	H1098
	GLN	ASP	ASP	M1412	L1330	V1098
	ASP	ASP	TYR	R1412	V1331	V1098
	LEU	LEU	LEU	M1412	E1268	H1098
	ILE	ILE	ILE	A1412	Q1333	V1098
	PRO	VAL	VAL	R1412	F1329	H1098
	GLN	ASP	ASP	M1413	L1330	V1098
	ASP	ASP	TYR	R1413	V1331	V1098
	LEU	LEU	LEU	M1413	E1268	H1098
	ILE	ILE	ILE	A1413	Q1333	V1098
	PRO	VAL	VAL	R1413	F1329	H1098
	GLN	ASP	ASP	M1414	L1330	V1098
	ASP	ASP	TYR	R1414	V1331	V1098
	LEU	LEU	LEU	M1414	E1268	H1098
	ILE	ILE	ILE	A1414	Q1333	V1098
	PRO	VAL	VAL	R1414	F1329	H1098
	GLN	ASP	ASP	M1415	L1330	V1098
	ASP	ASP	TYR	R1415	V1331	V1098
	LEU	LEU	LEU	M1415	E1268	H1098
	ILE	ILE	ILE	A1415	Q1333	V1098
	PRO	VAL	VAL	R1415	F1329	H1098
	GLN	ASP	ASP	M1416	L1330	V1098
	ASP	ASP	TYR	R1416	V1331	V1098
	LEU	LEU	LEU	M1416	E1268	H1098
	ILE	ILE	ILE	A1416	Q1333	V1098
	PRO	VAL	VAL	R1416	F1329	H1098
	GLN	ASP	ASP	M1417	L1330	V1098
	ASP	ASP	TYR	R1417	V1331	V1098
	LEU	LEU	LEU	M1417	E1268	H1098
	ILE	ILE	ILE	A1417	Q1333	V1098
	PRO	VAL	VAL	R1417	F1329	H1098
	GLN	ASP	ASP	M1418	L1330	V1098
	ASP	ASP	TYR	R1418	V1331	V1098
	LEU	LEU	LEU	M1418	E1268	H1098
	ILE	ILE	ILE	A1418	Q1333	V1098
	PRO	VAL	VAL	R1418	F1329	H1098
	GLN	ASP	ASP	M1419	L1330	V1098
	ASP	ASP	TYR	R1419	V1331	V1098
	LEU	LEU	LEU	M1419	E1268	H1098
	ILE	ILE	ILE	A1419	Q1333	V1098
	PRO	VAL	VAL	R1419	F1329	H1098
	GLN	ASP	ASP	M1420	L1330	V1098
	ASP	ASP	TYR	R1420	V1331	V1098
	LEU	LEU	LEU	M1420	E1268	H1098
	ILE	ILE	ILE	A1420	Q1333	V1098
	PRO	VAL	VAL	R1420	F1329	H1098
	GLN	ASP	ASP	M1421	L1330	V1098
	ASP	ASP	TYR	R1421	V1331	V1098
	LEU	LEU	LEU	M1421	E1268	H1098
	ILE	ILE	ILE	A1421	Q1333	V1098
	PRO	VAL	VAL	R1421	F1329	H1098
	GLN	ASP	ASP	M1422	L1330	V1098
	ASP	ASP	TYR	R1422	V1331	V1098
	LEU	LEU	LEU	M1422	E1268	H1098
	ILE	ILE	ILE	A1422	Q1333	V1098
	PRO	VAL	VAL	R1422	F1329	H1098
	GLN	ASP	ASP	M1423	L1330	V1098
	ASP	ASP	TYR	R1423	V1331	V1098
	LEU	LEU	LEU	M1423	E1268	H1098
	ILE	ILE	ILE	A1423	Q1333	V1098
	PRO	VAL	VAL	R1423	F1329	H1098
	GLN	ASP	ASP	M1424	L1330	V1098
	ASP	ASP	TYR	R1424	V1331	V1098
	LEU	LEU	LEU	M1424	E1268	H1098
	ILE	ILE	ILE	A1424	Q1333	V1098
	PRO	VAL	VAL	R1424	F1329	H1098
	GLN	ASP	ASP	M1425	L1330	V1098
	ASP	ASP	TYR	R1425	V1331	V1098
	LEU	LEU	LEU	M1425	E1268	H1098
	ILE	ILE	ILE	A1425	Q1333	V1098
	PRO	VAL	VAL	R1425	F1329	H1098
	GLN	ASP	ASP	M1426	L1330	V1098
	ASP	ASP	TYR	R1426	V1331	V1098
	LEU	LEU	LEU	M1426	E1268	H1098
	ILE	ILE	ILE	A1426	Q1333	V1098
	PRO	VAL	VAL	R1426	F1329	H1098
	GLN	ASP	ASP	M1427	L1330	V1098
	ASP	ASP	TYR	R1427	V1331	V1098
	LEU	LEU	LEU	M1427	E1268	H1098
	ILE	ILE	ILE	A1427	Q1333	V1098
	PRO	VAL	VAL	R1427	F1329	H1098
	GLN	ASP	ASP	M1428	L1330	V1098
	ASP	ASP	TYR	R1428	V1331	V1098
	LEU	LEU	LEU	M1428	E1268	H1098
	ILE	ILE	ILE	A1428	Q1333	V1098
	PRO	VAL	VAL	R1428	F1329	H1098
	GLN	ASP	ASP	M1429	L1330	V1098
	ASP	ASP	TYR	R1429	V1331	V1098
	LEU	LEU	LEU	M1429	E1268	H1098
	ILE	ILE	ILE	A1429	Q1333	V1098
	PRO	VAL	VAL	R1429	F1329	H1098
	GLN	ASP	ASP	M1430	L1330	V1098
	ASP	ASP	TYR	R1430	V1331	V1098
	LEU	LEU	LEU	M1430	E1268	H1098
	ILE	ILE	ILE	A1430	Q1333	V1098
	PRO	VAL	VAL	R1430	F1329	H1098
	GLN	ASP	ASP	M1431	L1330	V1098
	ASP	ASP	TYR	R1431	V1331	V1098
	LEU	LEU	LEU	M1431	E1268	H1098
	ILE	ILE	ILE	A1431	Q1333	V1098
	PRO	VAL	VAL	R1431	F1329	H1098
	GLN	ASP	ASP	M1432	L1330	V1098
	ASP	ASP	TYR	R1432	V1331	V1098
	LEU	LEU	LEU	M1432	E1268	H1098
	ILE	ILE	ILE	A1432	Q1333	V1098
	PRO	VAL	VAL	R1432	F1329	H1098
	GLN	ASP	ASP	M1433	L1330	V1098
	ASP	ASP	TYR	R1433	V1331	V1098
	LEU	LEU	LEU	M1433	E1268	H1098
	ILE	ILE	ILE	A1433	Q1333	V1098
	PRO	VAL	VAL	R1433	F1329	H1098
	GLN	ASP	ASP	M1434	L1330	V1098
	ASP	ASP	TYR	R1434	V1331	V1098
	LEU	LEU	LEU	M1434	E1268	H1098
	ILE	ILE	ILE	A1434	Q1333	V1098
	PRO	VAL	VAL	R1434	F1329	H1098
	GLN	ASP	ASP	M1435	L1330	V1098
	ASP	ASP	TYR	R1435	V1331	V1098
	LEU	LEU	LEU	M1435	E1268	H1098
	ILE	ILE	ILE	A1435	Q1333	V1098
	PRO	VAL	VAL	R1435	F1329	H1098
	GLN	ASP	ASP	M1436	L1330	V1098
	ASP	ASP	TYR	R1436	V1331	V1098
	LEU	LEU	LEU	M1436	E1268	H1098
	ILE	ILE	ILE	A1436	Q1333	V1098
	PRO	VAL	VAL	R1436	F1329	H1098
	GLN	ASP	ASP	M1437	L1330	V1098
	ASP	ASP	TYR	R1437	V1331	V1098
	LEU	LEU	LEU	M1437	E1268	H1098
	ILE	ILE	ILE	A1437	Q1333	V1098
	PRO	VAL	VAL	R1437	F1329	H1098
	GLN	ASP	ASP	M1438	L1330	V1098
	ASP	ASP	TYR	R1438	V1331	V1098
	LEU	LEU	LEU	M1438	E1268	H1098
	ILE	ILE	ILE	A1438	Q1333	V1098
	PRO	VAL	VAL	R1438	F1329	H1098
	GLN	ASP	ASP	M1439	L1330	V1098
	ASP	ASP	TYR	R1439	V1331	V1098
	LEU	LEU	LEU	M1439	E1268	H1098
	ILE	ILE	ILE	A1439	Q1333	V1098
	PRO	VAL	VAL	R1439	F1329	H1098
	GLN	ASP	ASP	M1440	L1330	V1098
	ASP	ASP	TYR	R1440	V1331	V1098
	LEU	LEU	LEU	M1440	E1268	H1098
	ILE	ILE	ILE	A1440	Q1333	V1098
	PRO	VAL	VAL	R1440	F1329	H1098
	GLN	ASP	ASP	M1441	L1330	V1098
	ASP	ASP	TYR	R1441	V1331	V1098
	LEU	LEU	LEU	M144		



	Q361	G421	G431	F541	S452	P462	T422	T422	I362	M1021	F961	L661	S721	S722	I752	A663	A663	A663	A663	R1081	R1082	R1083	R1084	
	Q362	G422	G432	F542	S453	P463	T423	T423	I363	M1022	F962	L662	S722	S723	I753	A664	A664	A664	A664	R1085	R1086	R1087	R1088	
	Q363	G423	G433	F543	S454	P464	T424	T424	I364	M1023	F963	L663	S723	S724	I754	A665	A665	A665	A665	R1089	R1090	R1091	R1092	
	Q364	G424	G434	F544	S455	P465	T425	T425	I365	M1024	F964	L664	S724	S725	I755	A666	A666	A666	A666	R1093	R1094	R1095	R1096	
	Q365	G425	G435	F545	S456	P466	T426	T426	I366	M1025	F965	L665	S725	S726	I756	A667	A667	A667	A667	R1097	R1098	R1099	R1100	
	Q366	G426	G436	F546	S457	P467	T427	T427	I367	M1026	F966	L666	S726	S727	I757	A668	A668	A668	A668	R1101	R1102	R1103	R1104	
	Q367	G427	G437	F547	S458	P468	T428	T428	I368	M1027	F967	L667	S727	S728	I758	A669	A669	A669	A669	R1105	R1106	R1107	R1108	
	Q368	G428	G438	F548	S459	P469	T429	T429	I369	M1028	F968	L668	S728	S729	I759	A670	A670	A670	A670	R1109	R1110	R1111	R1112	
	Q369	G429	G439	F549	S460	P470	T430	T430	I370	M1029	F969	L669	S729	S730	I750	A671	A671	A671	A671	R1113	R1114	R1115	R1116	
	Q370	G430	G440	F550	S461	P471	T431	T431	I371	M1030	F970	L670	S730	S731	I751	A672	A672	A672	A672	R1117	R1118	R1119	R1120	
	Q371	G431	G441	F551	S462	P472	T432	T432	I372	M1031	F971	L671	S731	S732	I752	A673	A673	A673	A673	R1121	R1122	R1123	R1124	
	Q372	G432	G442	F552	S463	P473	T433	T433	I373	M1032	F972	L672	S732	S733	I753	A674	A674	A674	A674	R1125	R1126	R1127	R1128	
	Q373	G433	G443	F553	S464	P474	T434	T434	I374	M1033	F973	L673	S733	S734	I754	A675	A675	A675	A675	R1129	R1130	R1131	R1132	
	Q374	G434	G444	F554	S465	P475	T435	T435	I375	M1034	F974	L674	S734	S735	I755	A676	A676	A676	A676	R1133	R1134	R1135	R1136	
	Q375	G435	G445	F555	S466	P476	T436	T436	I376	M1035	F975	L675	S735	S736	I756	A677	A677	A677	A677	R1137	R1138	R1139	R1140	
	Q376	G436	G446	F556	S467	P477	T437	T437	I377	M1036	F976	L676	S736	S737	I757	A678	A678	A678	A678	R1141	R1142	R1143	R1144	
	Q377	G437	G447	F557	S468	P478	T438	T438	I378	M1037	F977	L677	S737	S738	I758	A679	A679	A679	A679	R1145	R1146	R1147	R1148	
	Q378	G438	G448	F558	S469	P479	T439	T439	I379	M1038	F978	L678	S738	S739	I759	A680	A680	A680	A680	R1149	R1150	R1151	R1152	
	Q379	G439	G449	F559	S470	P480	T440	T440	I380	M1039	F979	L679	S739	S740	I760	A681	A681	A681	A681	R1153	R1154	R1155	R1156	
	Q380	G440	G450	F560	S471	P481	T441	T441	I381	M1040	F980	L680	S740	S741	I761	A682	A682	A682	A682	R1157	R1158	R1159	R1160	
	Q381	G441	G451	F561	S472	P482	T442	T442	I382	M1041	F981	L681	S741	S742	I762	A683	A683	A683	A683	R1161	R1162	R1163	R1164	
	Q382	G442	G452	F562	S473	P483	T443	T443	I383	M1042	F982	L682	S742	S743	I763	A684	A684	A684	A684	R1165	R1166	R1167	R1168	
	Q383	G443	G453	F563	S474	P484	T444	T444	I384	M1043	F983	L683	S743	S744	I764	A685	A685	A685	A685	R1171	R1172	R1173	R1174	
	Q384	G444	G454	F564	S475	P485	T445	T445	I385	M1044	F984	L684	S744	S745	I765	A686	A686	A686	A686	R1175	R1176	R1177	R1178	
	Q385	G445	G455	F565	S476	P486	T446	T446	I386	M1045	F985	L685	S745	S746	I766	A687	A687	A687	A687	R1179	R1180	R1181	R1182	
	Q386	G446	G456	F566	S477	P487	T447	T447	I387	M1046	F986	L686	S746	S747	I767	A688	A688	A688	A688	R1183	R1184	R1185	R1186	
	Q387	G447	G457	F567	S478	P488	T448	T448	I388	M1047	F987	L687	S747	S748	I768	A689	A689	A689	A689	R1187	R1188	R1189	R1190	
	Q388	G448	G458	F568	S479	P489	T449	T449	I389	M1048	F988	L688	S748	S749	I769	A690	A690	A690	A690	R1191	R1192	R1193	R1194	
	Q389	G449	G459	F569	S480	P490	T450	T450	I390	M1049	F989	L689	S749	S750	I770	A691	A691	A691	A691	R1195	R1196	R1197	R1198	
	Q390	G450	G460	F570	S481	P491	T451	T451	I391	M1050	F990	L690	S750	S751	I771	A692	A692	A692	A692	R1199	R1200	R1201	R1202	
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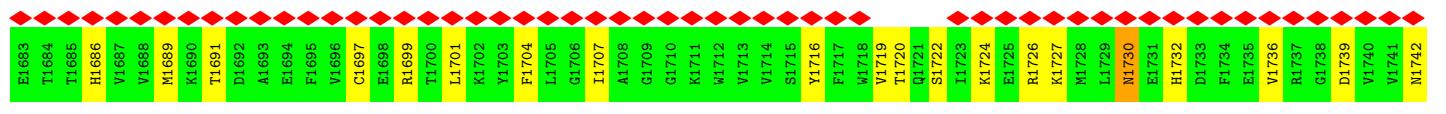
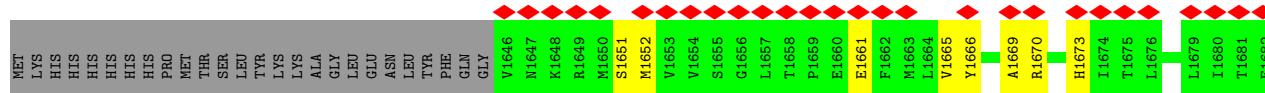
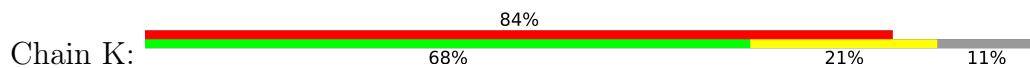
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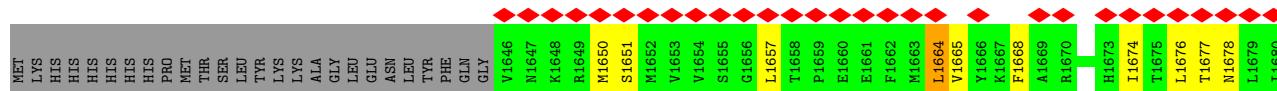


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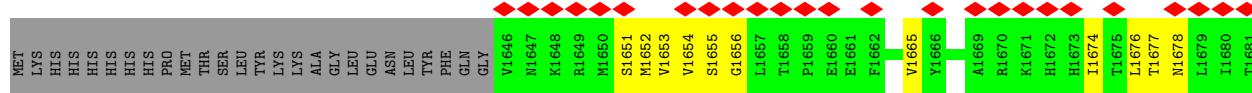
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Chain M: 



- Molecule 2: Breast cancer type 1 susceptibility protein

Chain O: 



- Molecule 2: Breast cancer type 1 susceptibility protein

Chain S: 



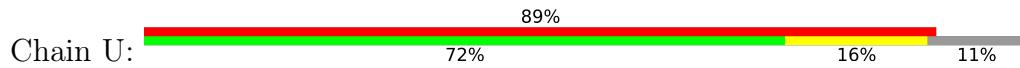
- Molecule 2: Breast cancer type 1 susceptibility protein

Chain T: 



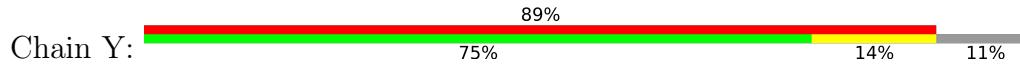
V1740	I1680	MET
V1741	G1801	LYS
T1682	HIS	HIS
E1682	HIS	HIS
N1742	HIS	HIS
G1803	E1683	HIS
T1802	T1682	HIS
N1743	G1803	G1743
E1683	T1682	E1683
H1804	V1804	R1744
M1744	HIS	HIS
T1684	HIS	HIS
H1805	HIS	HIS
M1745	HIS	HIS
P1806	P1806	H1746
H1746	PRO	PRO
H1806	P1806	H1746
M1747	MET	MET
I1807	Q1747	Q1747
V1808	T1808	T1808
V1809	V1809	V1809
V1810	V1810	K1750
R1751	R1751	V1691
Q1811	Q1811	Q1756
P1812	P1812	A1752
D1813	D1813	D1753
A1693	A1693	A1694
E1694	E1694	E1754
F1695	F1695	S1755
W1815	ASN	ASN
T1816	LEU	LEU
V1696	LYS	LYS
T1697	TYR	TYR
C1697	C1697	D1757
D1818	D1818	R1758
A1814	A1814	E1694
N1819	N1819	K1759
G1820	T1760	T1760
F1821	F1821	F1761
H1822	H1822	A1701
R1753	K1648	K1702
G1753	Y1703	G1763
A1649	R1649	R1649
M1650	M1650	F1704
S1651	S1651	L1764
L1765	L1765	E1765
E1765	E1765	G1766
G1825	G1825	Q1826
E1826	E1826	M1652
C1766	C1766	M1827
G1767	G1767	C1767
I1767	I1767	C1768
A1768	A1768	E1829
M1768	M1768	A1830
F1769	F1769	A1830
G1769	G1769	P1831
T1770	T1770	P1831
G1770	G1770	P1832
K1771	K1771	V1832
P1772	P1772	V1832
V1773	V1773	V1833
T1773	T1773	P1659
N1774	N1774	T1834
E1660	E1660	N1774
G1656	G1656	M1775
E1661	E1661	R1835
S1715	S1715	E1836
Y1716	Y1716	P1776
F1717	F1717	V1837
T1777	T1777	V1837
D1778	D1778	V1838
L1839	L1839	V1838
Q1779	Q1779	V1718
V1718	V1718	D1778
V1719	V1719	Q1779
V1720	V1720	Q1779
Y1666	Y1666	D1840
K1721	K1721	S1841
S1722	S1722	V1842
M1723	M1723	A1843
A1669	A1669	L1844
K1724	K1724	Y1845
R1670	R1670	Y1845
E1725	E1725	K1671
K1671	K1671	E1726
H1672	H1672	H1672
K1727	K1727	K1727
H1673	H1673	H1673
M1728	M1728	M1728
T1674	T1674	T1674
T1675	T1675	T1675
K1676	K1676	K1676
N1730	N1730	N1730
L1677	T1677	T1677
V1791	E1731	E1731
C1847	C1847	C1847
H1792	H1792	H1792
H1793	H1793	H1793
D1793	D1793	D1793
L1679	L1679	L1679
E1734	E1734	E1734
F1734	F1734	F1734
L1795	E1735	E1735
S1796	V1736	V1736
V1797	R1737	R1737
G1738	F1798	F1798
I1858	P1856	P1856
Q1857	Q1857	Q1857
I1858	P1859	P1859

- Molecule 2: Breast cancer type 1 susceptibility protein



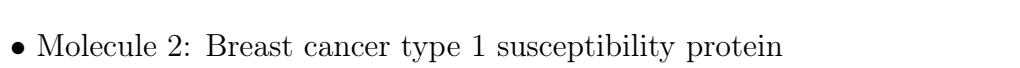
V1740	I1680	MET
V1741	G1801	LYS
T1682	HIS	HIS
E1682	HIS	HIS
N1742	HIS	HIS
G1803	E1683	G1743
T1802	T1682	E1683
N1743	G1803	T1684
E1683	T1682	T1684
H1804	V1804	M1745
M1744	HIS	HIS
T1684	HIS	HIS
H1805	HIS	HIS
M1745	HIS	HIS
P1806	P1806	H1746
H1746	PRO	PRO
H1806	P1806	H1746
M1747	MET	MET
I1807	Q1747	Q1747
V1808	T1808	T1808
V1809	V1809	V1809
V1810	V1810	K1750
R1751	R1751	V1691
Q1811	Q1811	Q1756
P1812	P1812	A1752
D1813	D1813	D1753
A1693	A1693	A1694
E1694	E1694	E1754
F1695	F1695	S1755
W1815	ASN	ASN
T1816	LEU	LEU
V1696	LYS	LYS
T1697	TYR	TYR
C1697	C1697	D1757
D1818	D1818	R1758
A1814	A1814	E1694
N1819	N1819	K1759
G1820	T1760	T1760
F1821	F1821	F1761
H1822	H1822	A1701
R1753	K1648	K1702
G1753	Y1703	G1763
A1649	R1649	R1649
M1650	M1650	F1704
S1651	S1651	L1764
L1765	L1765	E1765
E1825	E1825	G1766
Q1826	Q1826	Q1826
M1827	M1827	C1767
C1766	C1766	A1708
V1653	V1653	A1708
V1654	V1654	V1654
E1828	E1828	C1768
S1655	S1655	G1769
E1829	E1829	V1769
A1830	A1830	G1770
P1831	P1831	K1711
V1832	V1832	F1772
V1833	V1833	W1712
V1773	V1773	V1713
P1659	P1659	V1713
T1774	T1774	V1714
N1774	N1774	M1775
E1660	E1660	R1835
G1656	G1656	E1836
E1661	E1661	P1776
S1715	S1715	V1837
Y1716	Y1716	V1837
F1717	F1717	V1838
T1777	T1777	D1778
D1778	D1778	Q1779
L1839	L1839	D1840
Q1779	Q1779	S1841
V1718	V1718	V1842
V1719	V1719	A1843
V1720	V1720	L1844
Y1666	Y1666	Y1845
K1721	K1721	K1667
S1722	S1722	F1668
M1723	M1723	M1669
A1669	A1669	K1724
K1724	K1724	R1670
R1670	R1670	E1725
E1725	E1725	K1671
K1671	K1671	R1726
H1672	H1672	H1672
K1727	K1727	K1727
H1673	H1673	H1673
M1728	M1728	M1728
T1674	T1674	T1674
T1675	T1675	T1675
K1676	K1676	K1676
N1730	N1730	N1730
L1677	T1677	T1677
V1791	E1731	E1731
C1847	C1847	C1847
H1792	H1792	H1792
H1793	H1793	H1793
D1793	D1793	D1793
L1679	L1679	L1679
E1734	E1734	E1734
F1734	F1734	F1734
L1795	E1735	E1735
S1796	V1736	V1736
V1797	R1737	R1737
G1738	F1798	F1798
I1858	P1856	P1856
Q1857	Q1857	Q1857
I1858	P1859	P1859

- Molecule 2: Breast cancer type 1 susceptibility protein



V1740	I1680	MET
V1741	G1801	LYS
T1682	HIS	HIS
E1682	HIS	HIS
N1742	HIS	HIS
G1803	E1683	G1743
T1802	T1682	E1683
N1743	G1803	T1684
E1683	T1682	T1684
H1804	V1804	M1745
M1744	HIS	HIS
T1684	HIS	HIS
H1805	HIS	HIS
M1745	HIS	HIS
P1806	P1806	H1746
H1746	PRO	PRO
H1806	P1806	H1746
M1747	MET	MET
I1807	Q1747	Q1747
V1808	T1808	T1808
V1809	V1809	V1809
V1810	V1810	K1750
R1751	R1751	V1691
Q1811	Q1811	Q1756
P1812	P1812	A1752
D1813	D1813	D1753
A1693	A1693	A1694
E1694	E1694	E1754
F1695	F1695	S1755
W1815	ASN	ASN
T1816	LEU	LEU
V1696	LYS	LYS
T1697	TYR	TYR
C1697	C1697	D1757
D1818	D1818	R1758
A1814	A1814	E1694
N1819	N1819	K1759
G1820	T1760	T1760
F1821	F1821	F1761
H1822	H1822	A1701
R1753	K1648	K1702
G1753	Y1703	G1763
A1649	R1649	R1649
M1650	M1650	F1704
S1651	S1651	L1764
L1765	L1765	E1765
E1825	E1825	G1766
Q1826	Q1826	Q1826
M1827	M1827	C1767
C1766	C1766	A1708
V1653	V1653	A1708
V1654	V1654	V1654
E1828	E1828	C1768
S1655	S1655	G1769
E1829	E1829	V1769
A1830	A1830	G1770
P1831	P1831	K1711
V1832	V1832	F1772
V1833	V1833	W1712
V1773	V1773	V1713
P1659	P1659	V1713
T1774	T1774	V1714
N1774	N1774	M1775
E1660	E1660	R1835
G1656	G1656	E1836
E1661	E1661	P1776
S1715	S1715	V1837
Y1716	Y1716	V1837
F1717	F1717	V1838
T1777	T1777	D1778
D1778	D1778	Q1779
L1839	L1839	D1840
Q1779	Q1779	S1841
V1718	V1718	V1842
V1719	V1719	A1843
V1720	V1720	L1844
Y1666	Y1666	Y1845
K1721	K1721	K1667
S1722	S1722	F1668
M1723	M1723	M1669
A1669	A1669	K1724
K1724	K1724	R1670
R1670	R1670	E1725
E1725	E1725	K1671
K1671	K1671	R1726
H1672	H1672	H1672
K1727	K1727	K1727
H1673	H1673	H1673
M1728	M1728	M1728
T1674	T1674	T1674
T1675	T1675	T1675
K1676	K1676	K1676
N1730	N1730	N1730
L1677	T1677	T1677
V1791	E1731	E1731
C1847	C1847	C1847
H1792	H1792	H1792
H1793	H1793	H1793
D1793	D1793	D1793
L1679	L1679	L1679
E1734	E1734	E1734
F1734	F1734	F1734
L1795	E1735	E1735
S1796	V1736	V1736
V1797	R1737	R1737
G1738	F1798	F1798
I1858	P1856	P1856
Q1857	Q1857	Q1857
I1858	P1859	P1859

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L1800	V174

MET	I1680	V1740	T1681	T1681	LYS
G1801	V1741	N1742	E1682	HIS	HIS
T1802		G1743	E1683	HIS	HIS
G1803		R1744	T1684	HIS	HIS
V1804		N1745	T1685	HIS	HIS
H1805		H1746	H1686	PRO	PRO
P1806				MET	MET
T1807		Q1747	V1687	THR	THR
V1808		G1748	V1688	SER	SER
V1809		P1749	M1689	LEU	LEU
V1810		K1750	K1690	TYR	TYR
		Q1811	R1751	T1691	LYS
			P1812	D1692	ALA
L1820		D1813	R1753	A1693	GLY
		A1814	E1754	E1694	LEU
		W1815	S1755	F1695	GLU
		T1816	Q1756	V1696	ASN
		E1817	D1757	C1697	TYR
		D1818	R1758	E1698	PHE
		N1819	K1759	R1699	GLN
		G1820	I1760	T1700	GLY
		F1821	F1761	L1701	
		H1822	R1762	K1702	
		A1823	G1763	Y1703	
		I1824	L1764	F1704	
		G1825	E1765	L1705	
		Q1826	I1766	G1706	
		M1827	C1767	I1707	
		C1828	C1768	A1708	
		E1829	Y1769	G1709	
		A1830	G1770	G1710	
		P1831	P1771	K1711	
		V1832	F1772	W1712	
		V1833	T1773	V1713	
		T1834	N1774	V1714	
		R1835	M1775	S1715	
		E1836	P1776	Y1716	
		W1837	T1777	F1717	
		V1838	D1778	W1718	
		L1839	Q1779	V1719	
		D1840	L1780	T1720	
		S1841	E1781	Q1721	
		V1842	W1782	S1722	
		A1843	M1783	I1723	
		L1844	V1784	K1724	
		Y1845	Q1785	E1725	
		Q1846	L1786	R1726	
		C1847	C1787	K1727	
		Q1848	G1788	M1728	
		E1849	A1789	L1729	
		L1850	S1790	N1730	
		D1851	V1791	E1731	
		Y1852	V1792	H1732	
		Y1853	K1793	D1733	
		L1854	E1794	F1734	
		I1855	L1795	E1735	
		P1856	S1796	V1736	
		Q1857	S1797	R1737	
		I1858	F1798	G1738	
			T1799	D1739	

## 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 ( $e^-/\text{\AA}^2$ )	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 i

### 5.1 Standard geometry i

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

*Continued on next page...*

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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(°)	Ideal(°)
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

*Continued on next page...*

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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...*

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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(°)	Ideal(°)
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.

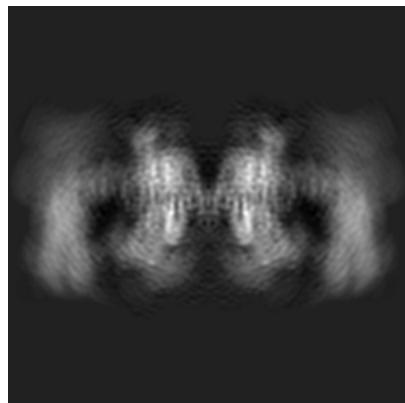
## 6 Map visualisation i

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.

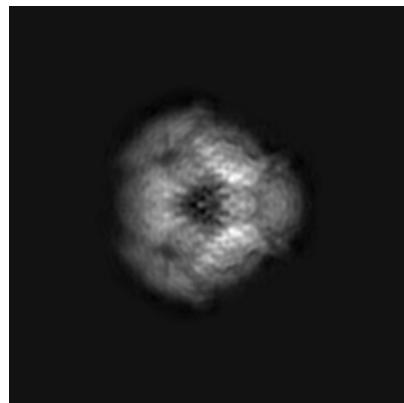
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections i

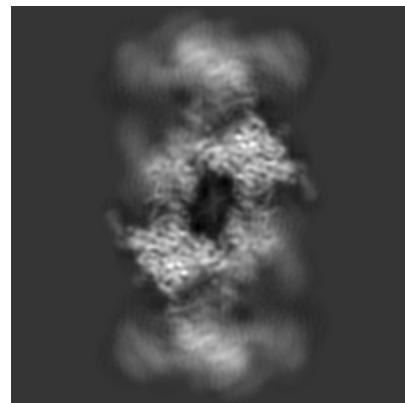
#### 6.1.1 Primary map



X



Y

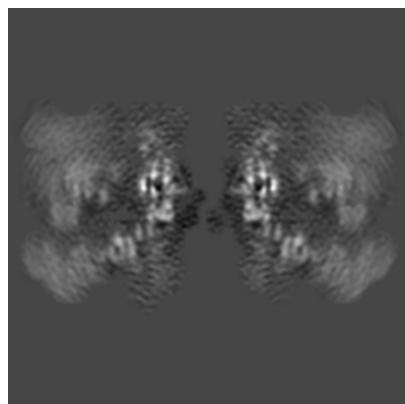


Z

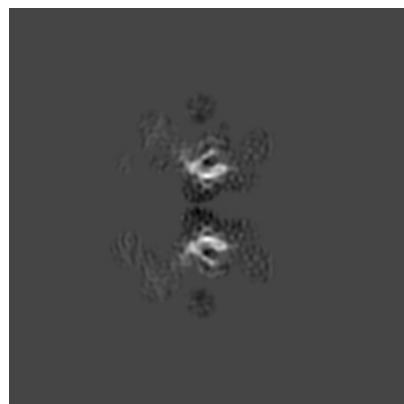
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices i

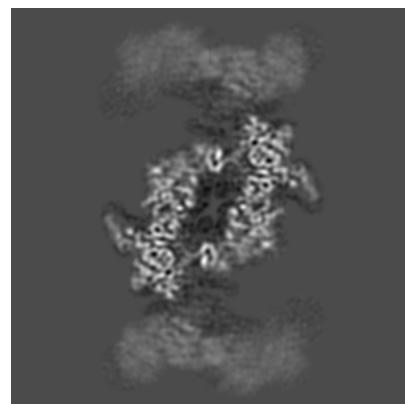
#### 6.2.1 Primary map



X Index: 188



Y Index: 188

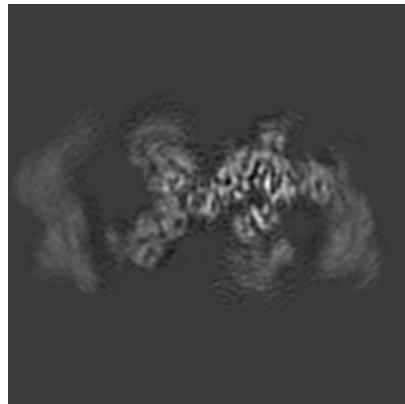


Z Index: 188

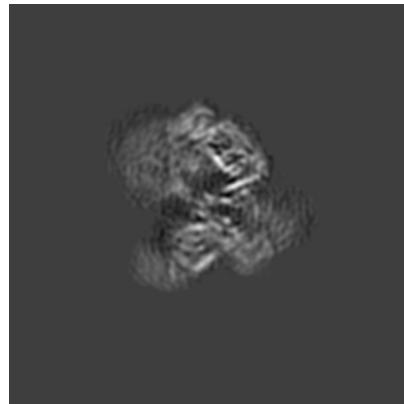
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices [\(i\)](#)

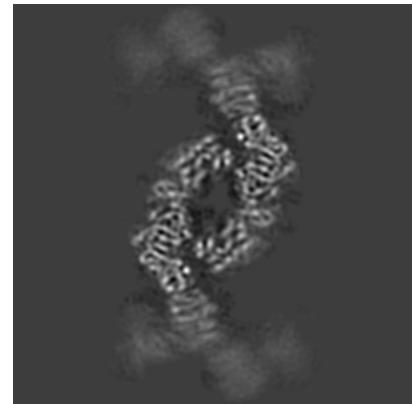
#### 6.3.1 Primary map



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.

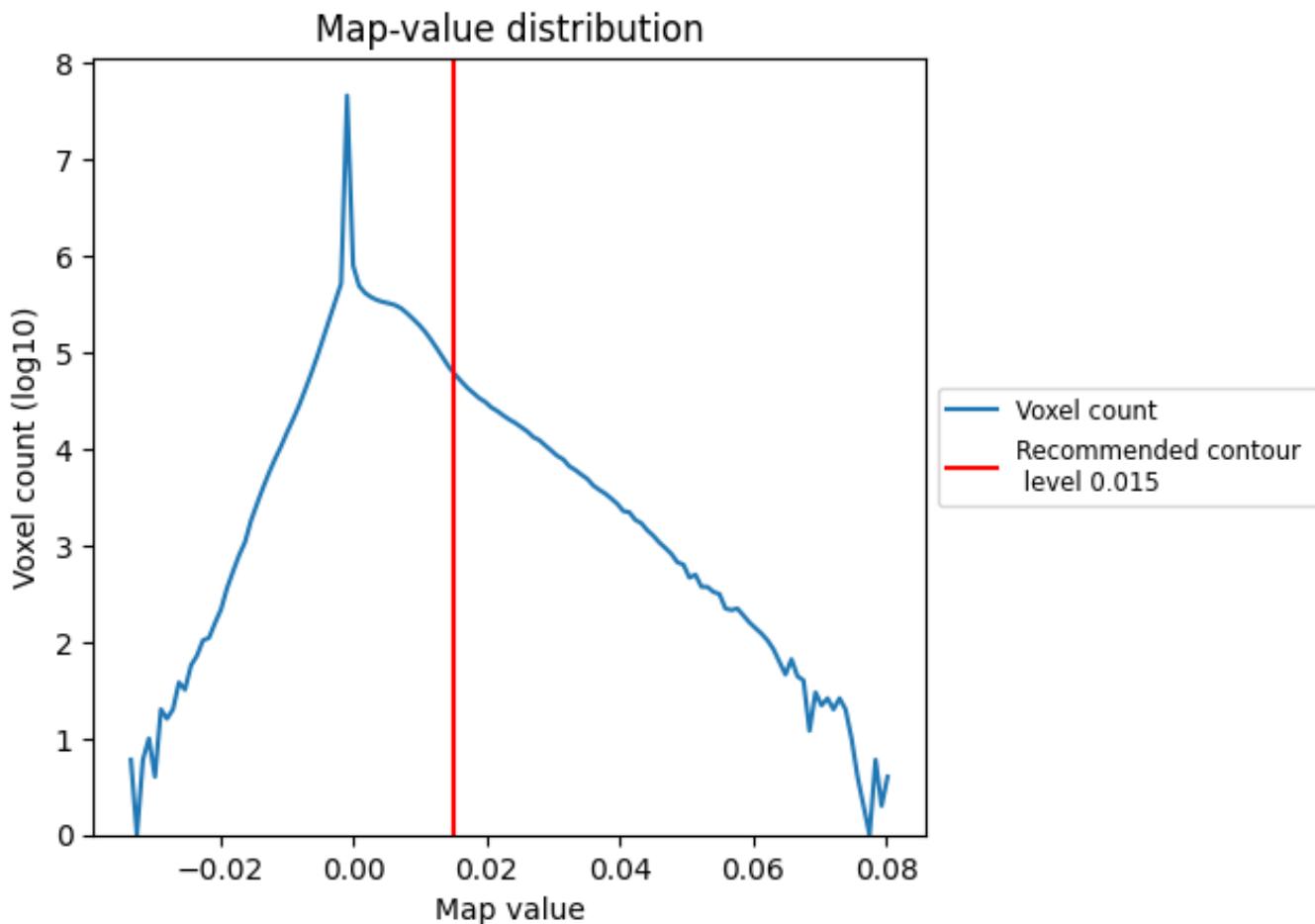
## 6.5 Mask visualisation

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

## 7 Map analysis (i)

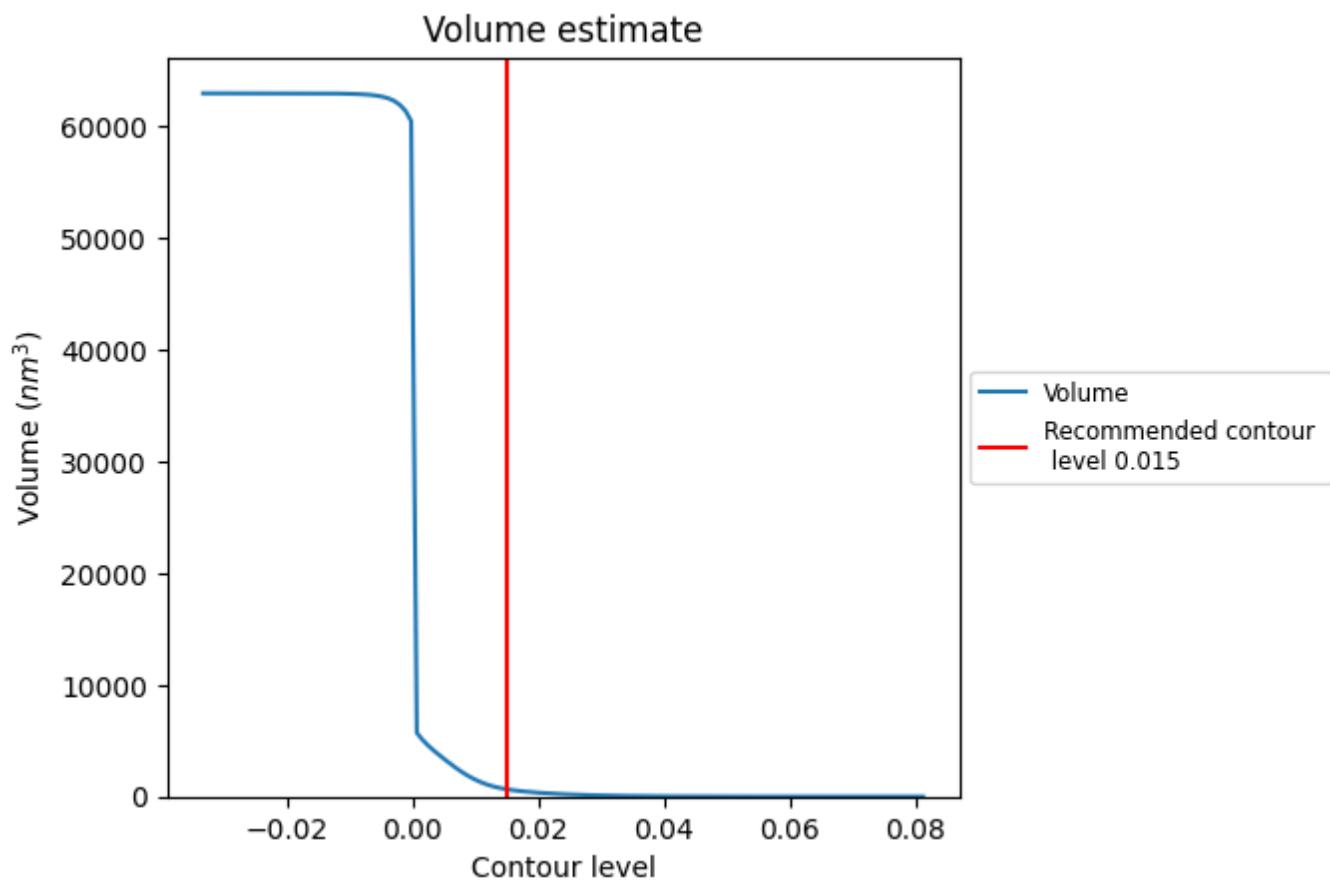
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution (i)



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.

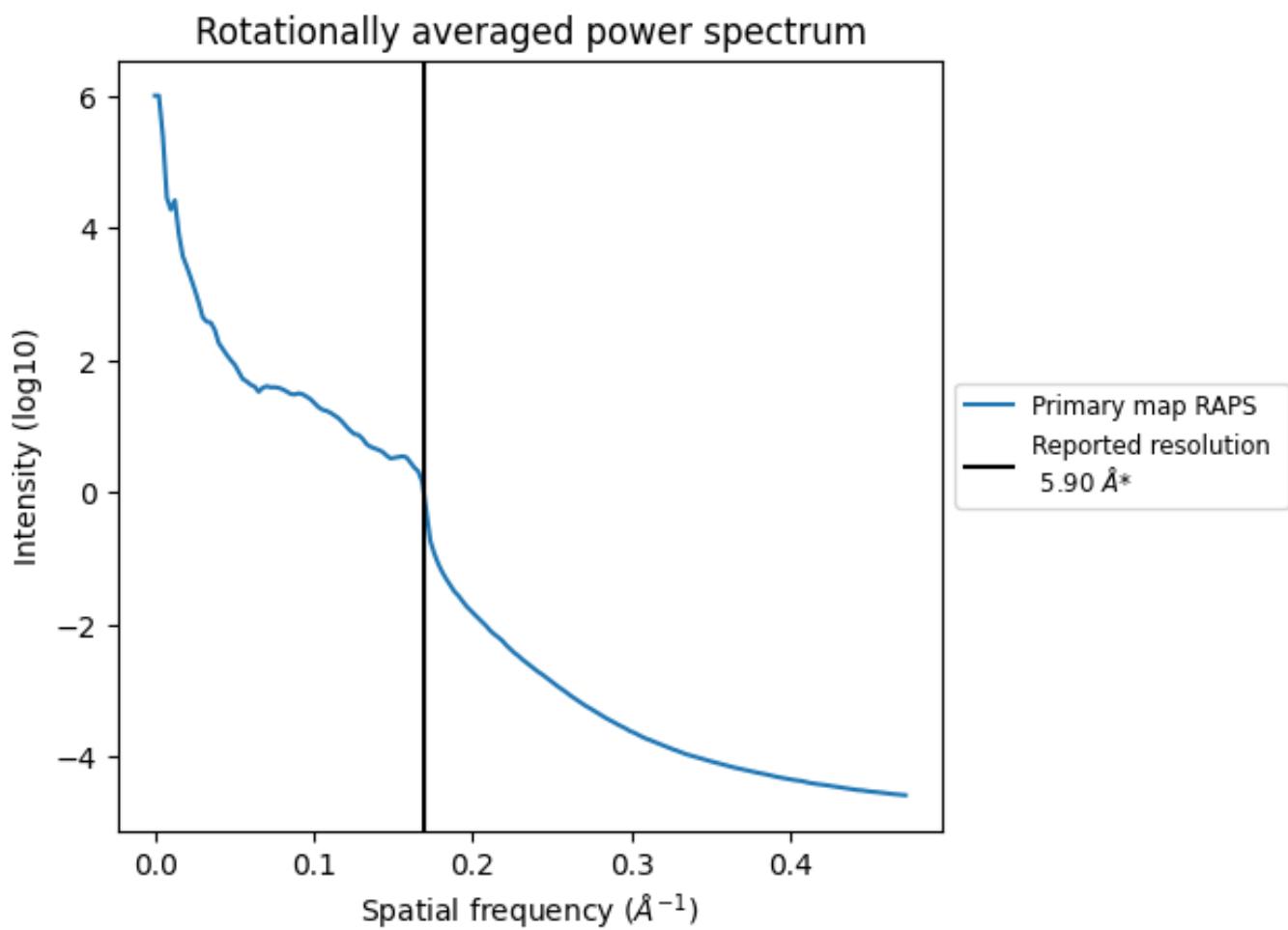
## 7.2 Volume estimate (i)



The volume at the recommended contour level is 649 nm<sup>3</sup>; 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  $0.169 \text{ \AA}^{-1}$

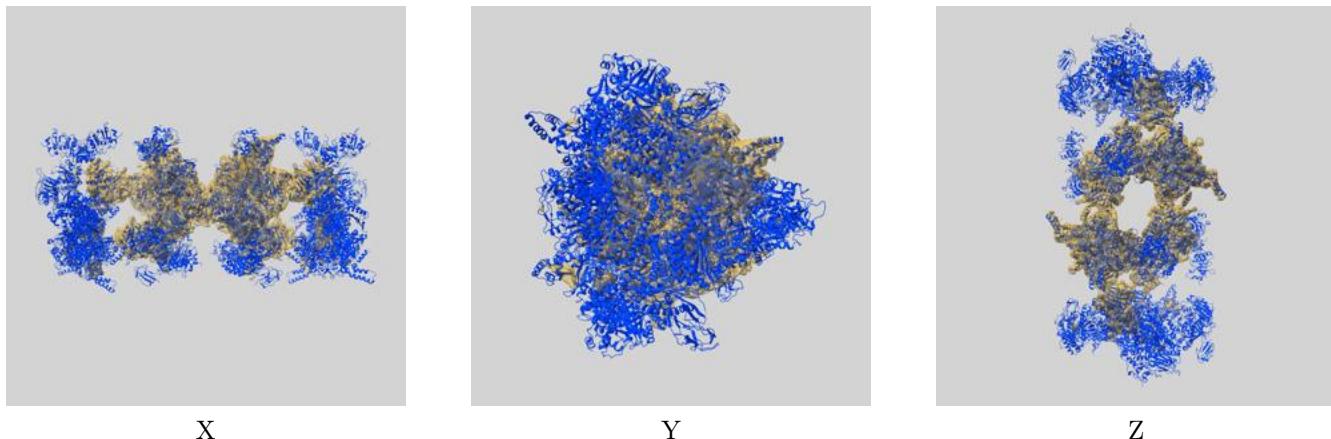
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [\(i\)](#)

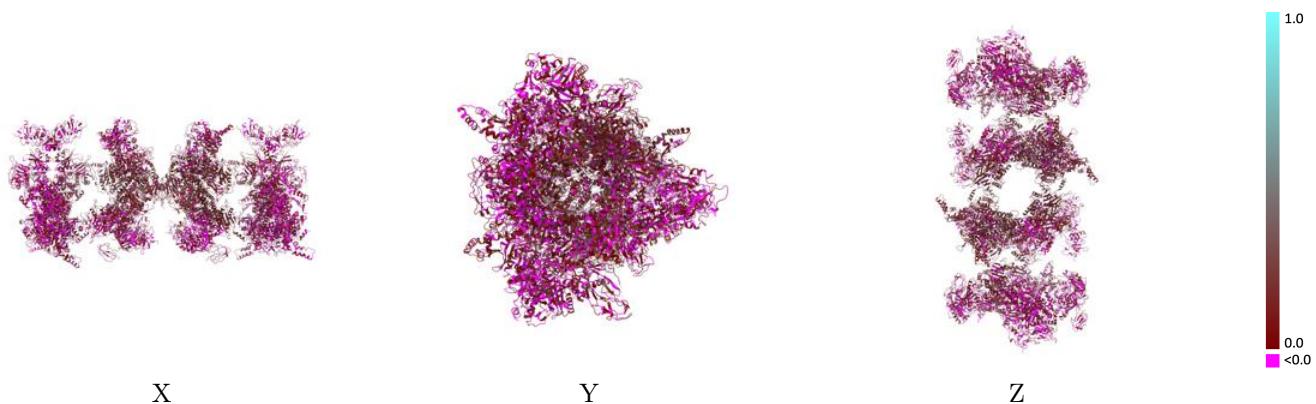
This section contains information regarding the fit between EMDB map EMD-4344 and PDB model 6G2I. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [\(i\)](#)



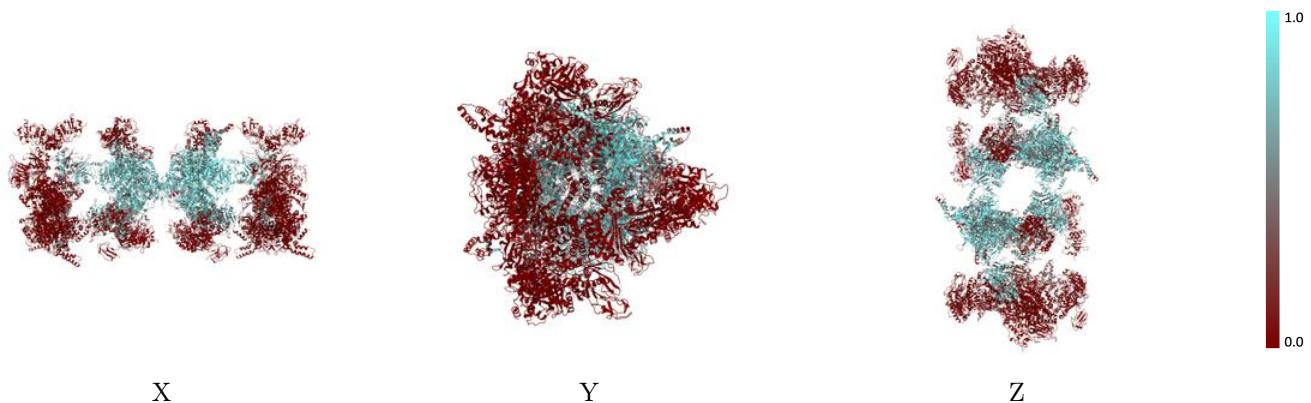
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



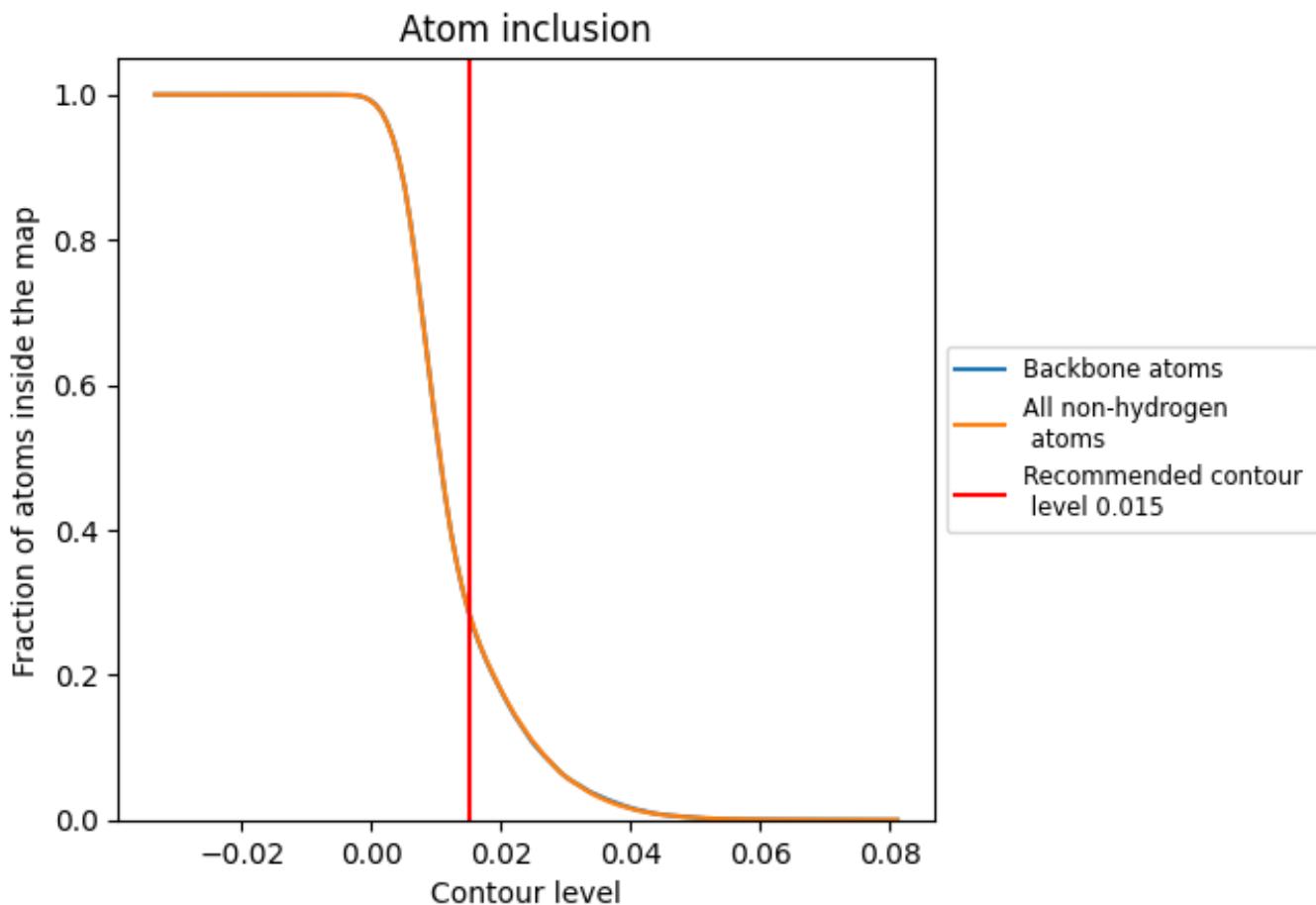
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [\(i\)](#)



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

