wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 12:53 PM EST

PDB ID	:	7MUQ
EMDB ID	:	EMD-24018
Title	:	Reconstruction of the Legionella pneumophila Dot/Icm T4SS 3DVA Map 1
Authors	:	Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.
Deposited on	:	2021-05-14
Resolution	:	4.60 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:

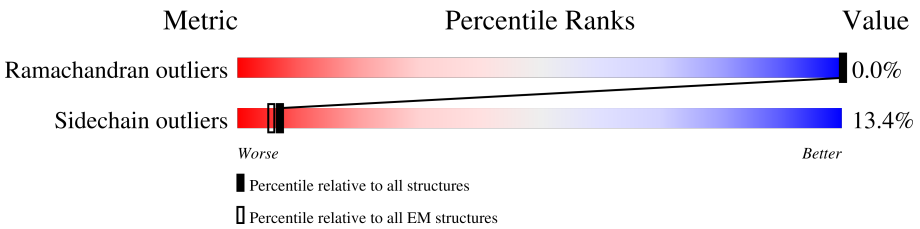
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.60 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)
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	AG	1048	13% • 84%
1	Ag	1048	• 97%
1	BG	1048	13% • 84%
1	Bg	1048	• • 97%
1	CG	1048	13% • 84%
1	Cg	1048	• • 97%
1	DG	1048	14% • 84%
1	Dg	1048	• • 97%
1	EG	1048	13% • 84%

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Mol	Chain	Length	Quality of chain
1	Eg	1048	97%
1	FG	1048	14% 84%
1	Fg	1048	97%
1	GG	1048	14% 84%
1	Gg	1048	97%
1	HG	1048	14% 84%
1	Hg	1048	97%
1	IG	1048	15% 84%
1	Ig	1048	97%
1	JG	1048	14% 84%
1	Jg	1048	97%
1	KG	1048	14% 84%
1	Kg	1048	97%
1	LG	1048	14% 84%
1	Lg	1048	97%
1	MG	1048	13% 84%
1	Mg	1048	97%
1	NG	1048	13% 84%
1	OG	1048	14% 84%
1	PG	1048	14% 84%
1	VG	1048	97%
1	WG	1048	97%
1	XG	1048	97%
1	YG	1048	97%
1	ZG	1048	97%

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Mol	Chain	Length	Quality of chain
2	AC	303	60% 9% 31%
2	BC	303	60% 9% 31%
2	CC	303	59% 10% 31%
2	DC	303	72% 8% 20%
2	EC	303	61% 8% 31%
2	FC	303	59% 10% 31%
2	GC	303	61% 8% 31%
2	HC	303	73% 8% 20%
2	IC	303	72% 9% 20%
2	JC	303	60% 9% 31%
2	KC	303	58% 11% 31%
2	LC	303	75% 6% 20%
2	MC	303	72% 8% 20%
3	AF	269	19% 5% 77%
3	Af	269	17% 78%
3	BF	269	21% 77%
3	Bf	269	20% 78%
3	CF	269	20% 77%
3	Cf	269	18% 78%
3	DF	269	21% 77%
3	Df	269	21% 78%
3	EF	269	21% 77%
3	Ef	269	19% 78%
3	FF	269	21% 77%
3	Ff	269	19% 78%

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Mol	Chain	Length	Quality of chain
3	GF	269	21% 77%
3	Gf	269	20% 78%
3	HF	269	21% 77%
3	Hf	269	19% 78%
3	IF	269	20% 77%
3	If	269	18% 78%
3	JF	269	20% 77%
3	Jf	269	18% 78%
3	KF	269	21% 77%
3	Kf	269	20% 78%
3	LF	269	21% 77%
3	Lf	269	20% 78%
3	MF	269	21% 77%
3	Mf	269	20% 78%
3	VF	269	20% 77%
3	WF	269	20% 77%
3	XF	269	20% 77%
3	YF	269	21% 77%
3	ZF	269	20% 77%
4	AD	163	75% 11% 14%
4	Ad	163	76% 8% 16%
4	BD	163	77% 9% 14%
4	Bd	163	73% 11% 16%
4	CD	163	74% 12% 14%
4	Cd	163	76% 8% 16%

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Mol	Chain	Length	Quality of chain
4	DD	163	77% 9% 14%
4	Dd	163	74% 10% 16%
4	ED	163	79% 7% 14%
4	Ed	163	75% 9% 16%
4	FD	163	76% 10% 14%
4	Fd	163	75% 9% 16%
4	GD	163	76% 10% 14%
4	Gd	163	75% 9% 16%
4	HD	163	80% 6% 14%
4	Hd	163	76% 8% 16%
4	ID	163	80% 6% 14%
4	Id	163	75% 9% 16%
4	JD	163	78% 8% 14%
4	Jd	163	78% 6% 16%
4	KD	163	81% 5% 14%
4	Kd	163	77% 7% 16%
4	LD	163	76% 10% 14%
4	Ld	163	77% 7% 16%
4	MD	163	80% 6% 14%
4	Md	163	76% 8% 16%
5	AH	361	63% 8% 29%
5	BH	361	63% 8% 29%
5	CH	361	63% 8% 29%
5	DH	361	64% 7% 29%
5	EH	361	62% 10% 29%

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Mol	Chain	Length	Quality of chain
5	FH	361	63% 8% 29%
5	GH	361	65% 6% 29%
5	HH	361	63% 9% 29%
5	IH	361	64% 7% 29%
5	JH	361	66% 5% 29%
5	KH	361	66% 6% 29%
5	LH	361	64% 7% 29%
5	MH	361	64% 7% 29%
5	VH	361	7% 60% 7% 33%
5	WH	361	14% 60% 7% 33%
5	XH	361	21% 59% 8% 33%
5	YH	361	6% 60% 7% 33%
5	ZH	361	23% 59% 8% 33%
6	AK	189	69% 11% 20%
6	BK	189	74% 6% 20%
6	CK	189	70% 10% 20%
6	DK	189	72% 7% 20%
6	EK	189	68% 12% 20%
6	FK	189	69% 11% 20%
6	GK	189	73% 7% 20%
6	HK	189	70% 10% 20%
6	IK	189	76% 20%
6	JK	189	69% 11% 20%
6	KK	189	69% 11% 20%
6	LK	189	70% 10% 20%

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Mol	Chain	Length	Quality of chain
6	MK	189	71% 8% 20%
7	AL	249	64% 5% 31%
7	BL	249	64% 5% 31%
7	CL	249	62% 8% 31%
7	DL	249	61% 8% 31%
7	EL	249	65% 31%
7	FL	249	61% 8% 31%
7	GL	249	63% 7% 31%
7	HL	249	64% 6% 31%
7	IL	249	63% 6% 31%
7	JL	249	63% 6% 31%
7	KL	249	61% 8% 31%
7	LL	249	63% 6% 31%
7	ML	249	63% 6% 31%
8	AM	320	58% 7% 35%
8	BM	320	56% 9% 35%
8	CM	320	56% 9% 35%
8	DM	320	58% 7% 35%
8	EM	320	56% 9% 35%
8	FM	320	57% 8% 35%
8	GM	320	58% 7% 35%
8	HM	320	56% 9% 35%
8	IM	320	57% 8% 35%
8	JM	320	58% 7% 35%
8	KM	320	58% 8% 35%

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Mol	Chain	Length	Quality of chain
8	LM	320	58% 8% 35%
8	MM	320	56% 9% 35%
9	AN	124	58% 5% 37%
9	BN	124	56% 6% 37%
9	CN	124	56% 7% 37%
9	DN	124	56% 7% 37%
9	EN	124	54% 9% 37%
9	FN	124	51% 12% 37%
9	GN	124	55% 8% 37%
9	HN	124	56% 6% 37%
9	IN	124	6% 56% 7% 37%
9	JN	124	55% 8% 37%
9	KN	124	54% 9% 37%
9	LN	124	56% 7% 37%
9	MN	124	56% 7% 37%
10	AU	9	100%
10	BU	9	100%
10	CU	9	100%
10	DU	9	100%
10	EU	9	100%
10	FU	9	100%
10	GU	9	100%
10	HU	9	100%
10	IU	9	100%
10	JU	9	100%

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Mol	Chain	Length	Quality of chain
10	KU	9	100%
10	LU	9	100%
10	MU	9	100%
11	AX	48	35% 100%
11	BX	48	44% 100%
11	CX	48	23% 100%
11	DX	48	29% 100%
11	EX	48	25% 100%
11	FX	48	35% 100%
11	GX	48	21% 100%
11	HX	48	31% 100%
11	IX	48	27% 100%
11	JX	48	31% 100%
11	KX	48	31% 100%
11	LX	48	35% 100%
11	MX	48	38% 100%
11	VX	48	29% 100%
11	WX	48	27% 100%
11	XX	48	25% 100%
11	YX	48	33% 100%
11	ZX	48	17% 100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 192370 atoms, of which 0 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 IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	Gg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Hg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	BG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	Bg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Ig	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Jg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	CG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	Kg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Lg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	DG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	Cg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Mg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Ag	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	VG	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	WG	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	EG	165	1229	780	203	242	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	XG	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	YG	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	ZG	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	FG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	Dg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	GG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	Eg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	Fg	34	276	168	47	60	1	0	0
			Total	C	N	O	S		
1	HG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	IG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	JG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	KG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	LG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	MG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	NG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	OG	165	1229	780	203	242	4	0	0
			Total	C	N	O	S		
1	PG	165	1229	780	203	242	4	0	0

- Molecule 2 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BC	209	1667	1061	292	309	5	0	0
			Total	C	N	O	S		
2	EC	209	1667	1061	292	309	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CC	209	1667	1061	292	309	5	0	0
			Total	C	N	O	S		
2	DC	243	1921	1216	340	357	8	0	0
			Total	C	N	O	S		
2	FC	209	1667	1061	292	309	5	0	0
			Total	C	N	O	S		
2	GC	209	1667	1061	292	309	5	0	0
			Total	C	N	O	S		
2	IC	243	1921	1216	340	357	8	0	0
			Total	C	N	O	S		
2	JC	209	1667	1061	292	309	5	0	0
			Total	C	N	O	S		
2	KC	209	1667	1061	292	309	5	0	0
			Total	C	N	O	S		
2	MC	243	1921	1216	340	357	8	0	0
			Total	C	N	O	S		
2	HC	243	1921	1216	340	357	8	0	0
			Total	C	N	O	S		
2	LC	243	1921	1216	340	357	8	0	0
			Total	C	N	O	S		
2	AC	209	1667	1061	292	309	5	0	0

- Molecule 3 is a protein called DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	GF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Gf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	HF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Hf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	IF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	If	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	JF	63	483	308	84	90	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Jf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	KF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Kf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	LF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Lf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	MF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Mf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	VF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	WF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	XF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	YF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Df	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	ZF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Af	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	BF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	CF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Bf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	Cf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	DF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	EF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Ef	59	449	290	77	81	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	FF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Ff	59	449	290	77	81	1	0	0

- Molecule 4 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	GD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Gd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	HD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Hd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	ID	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Dd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	Id	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	JD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Jd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	KD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Kd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	LD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Ld	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	MD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Md	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	CD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Ad	137	1058	672	182	202	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Bd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	AD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Cd	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	DD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	ED	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Ed	137	1058	672	182	202	2	0	0
			Total	C	N	O	S		
4	FD	140	1086	692	185	206	3	0	0
			Total	C	N	O	S		
4	Fd	137	1058	672	182	202	2	0	0

- Molecule 5 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	GH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	HH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	IH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	JH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	AH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	KH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	LH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	MH	258	1983	1268	336	371	8	0	0
			Total	C	N	O	S		
5	VH	243	1875	1201	319	348	7	0	0
			Total	C	N	O	S		
5	WH	243	1875	1201	319	348	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	XH	243	1875	1201	319	348	7	0	0
5	YH	243	1875	1201	319	348	7	0	0
5	ZH	243	1875	1201	319	348	7	0	0
5	BH	258	1983	1268	336	371	8	0	0
5	CH	258	1983	1268	336	371	8	0	0
5	DH	258	1983	1268	336	371	8	0	0
5	EH	258	1983	1268	336	371	8	0	0
5	FH	258	1983	1268	336	371	8	0	0

- Molecule 6 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	GK	151	1175	747	209	215	4	0	0
6	HK	151	1175	747	209	215	4	0	0
6	IK	151	1175	747	209	215	4	0	0
6	JK	151	1175	747	209	215	4	0	0
6	KK	151	1175	747	209	215	4	0	0
6	LK	151	1175	747	209	215	4	0	0
6	AK	151	1175	747	209	215	4	0	0
6	MK	151	1175	747	209	215	4	0	0
6	BK	151	1175	747	209	215	4	0	0
6	CK	151	1175	747	209	215	4	0	0
6	DK	151	1175	747	209	215	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	EK	151	1175	747	209	215	4	0	0
			Total	C	N	O	S		
6	FK	151	1175	747	209	215	4	0	0

- Molecule 7 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	GL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	HL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	IL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	JL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	KL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	LL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	ML	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	AL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	BL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	CL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	DL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	EL	173	1388	877	253	253	5	0	0
			Total	C	N	O	S		
7	FL	173	1388	877	253	253	5	0	0

- Molecule 8 is a protein called DUF2807 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	GM	208	1650	1046	293	308	3	0	0
			Total	C	N	O	S		
8	HM	208	1650	1046	293	308	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	IM	208	1650	1046	293	308	3	0	0
8	JM	208	1650	1046	293	308	3	0	0
8	KM	208	1650	1046	293	308	3	0	0
8	LM	208	1650	1046	293	308	3	0	0
8	MM	208	1650	1046	293	308	3	0	0
8	AM	208	1650	1046	293	308	3	0	0
8	BM	208	1650	1046	293	308	3	0	0
8	CM	208	1650	1046	293	308	3	0	0
8	DM	208	1650	1046	293	308	3	0	0
8	EM	208	1650	1046	293	308	3	0	0
8	FM	208	1650	1046	293	308	3	0	0

- Molecule 9 is a protein called Neurogenic locus notch.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	GN	78	582	357	99	113	13	0	0
9	HN	78	582	357	99	113	13	0	0
9	IN	78	582	357	99	113	13	0	0
9	JN	78	582	357	99	113	13	0	0
9	KN	78	582	357	99	113	13	0	0
9	LN	78	582	357	99	113	13	0	0
9	MN	78	582	357	99	113	13	0	0
9	AN	78	582	357	99	113	13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	BN	78	582	357	99	113	13	0	0
9	CN	78	582	357	99	113	13	0	0
9	DN	78	582	357	99	113	13	0	0
9	EN	78	582	357	99	113	13	0	0
9	FN	78	582	357	99	113	13	0	0

- Molecule 10 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	GU	9	45	27	9	9	0	0
10	HU	9	45	27	9	9	0	0
10	IU	9	45	27	9	9	0	0
10	JU	9	45	27	9	9	0	0
10	KU	9	45	27	9	9	0	0
10	LU	9	45	27	9	9	0	0
10	MU	9	45	27	9	9	0	0
10	AU	9	45	27	9	9	0	0
10	BU	9	45	27	9	9	0	0
10	CU	9	45	27	9	9	0	0
10	DU	9	45	27	9	9	0	0
10	EU	9	45	27	9	9	0	0
10	FU	9	45	27	9	9	0	0

- Molecule 11 is a protein called Unknown protein fragment.

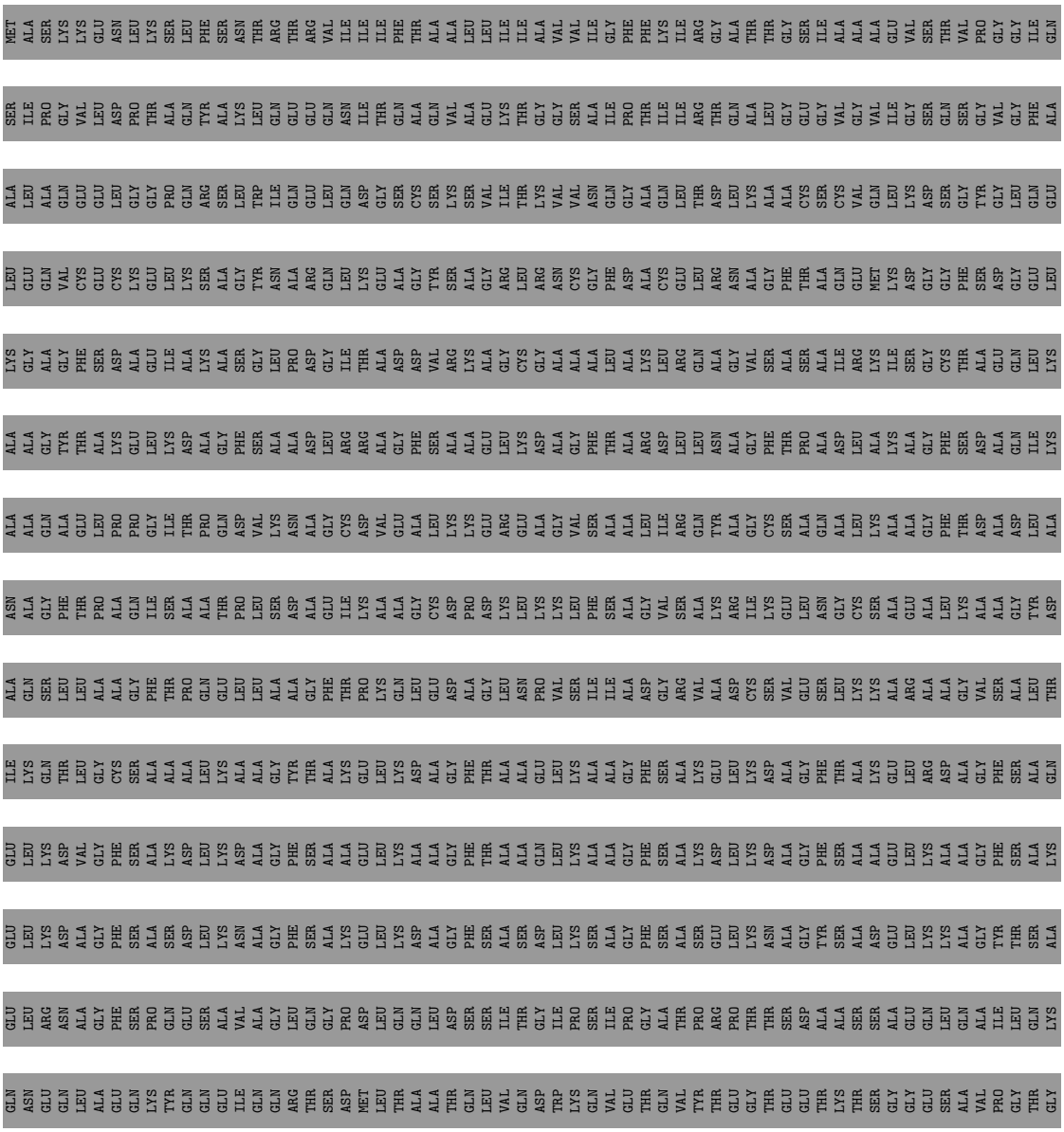
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	GX	48	240	144	48	48	0	0
11	DX	48	240	144	48	48	0	0
11	HX	48	240	144	48	48	0	0
11	IX	48	240	144	48	48	0	0
11	JX	48	240	144	48	48	0	0
11	KX	48	240	144	48	48	0	0
11	LX	48	240	144	48	48	0	0
11	MX	48	240	144	48	48	0	0
11	VX	48	240	144	48	48	0	0
11	WX	48	240	144	48	48	0	0
11	XX	48	240	144	48	48	0	0
11	YX	48	240	144	48	48	0	0
11	ZX	48	240	144	48	48	0	0
11	AX	48	240	144	48	48	0	0
11	BX	48	240	144	48	48	0	0
11	CX	48	240	144	48	48	0	0
11	EX	48	240	144	48	48	0	0
11	FX	48	240	144	48	48	0	0

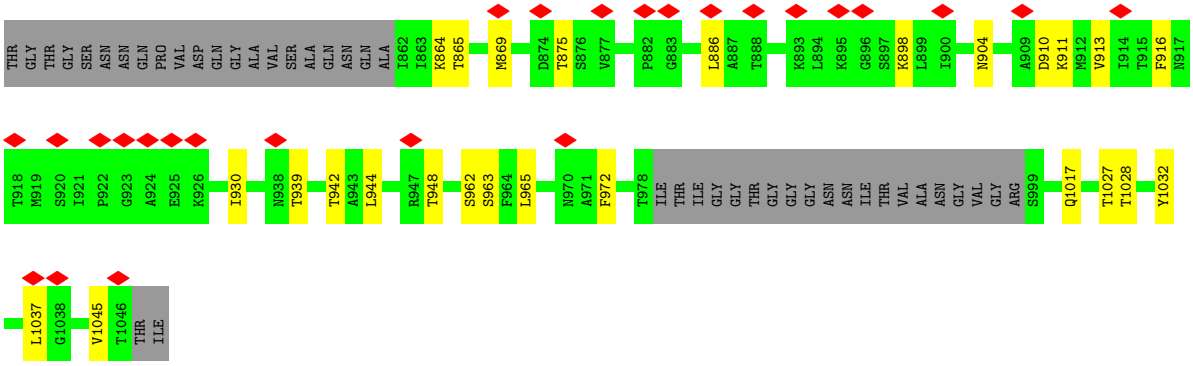
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: IcmE protein

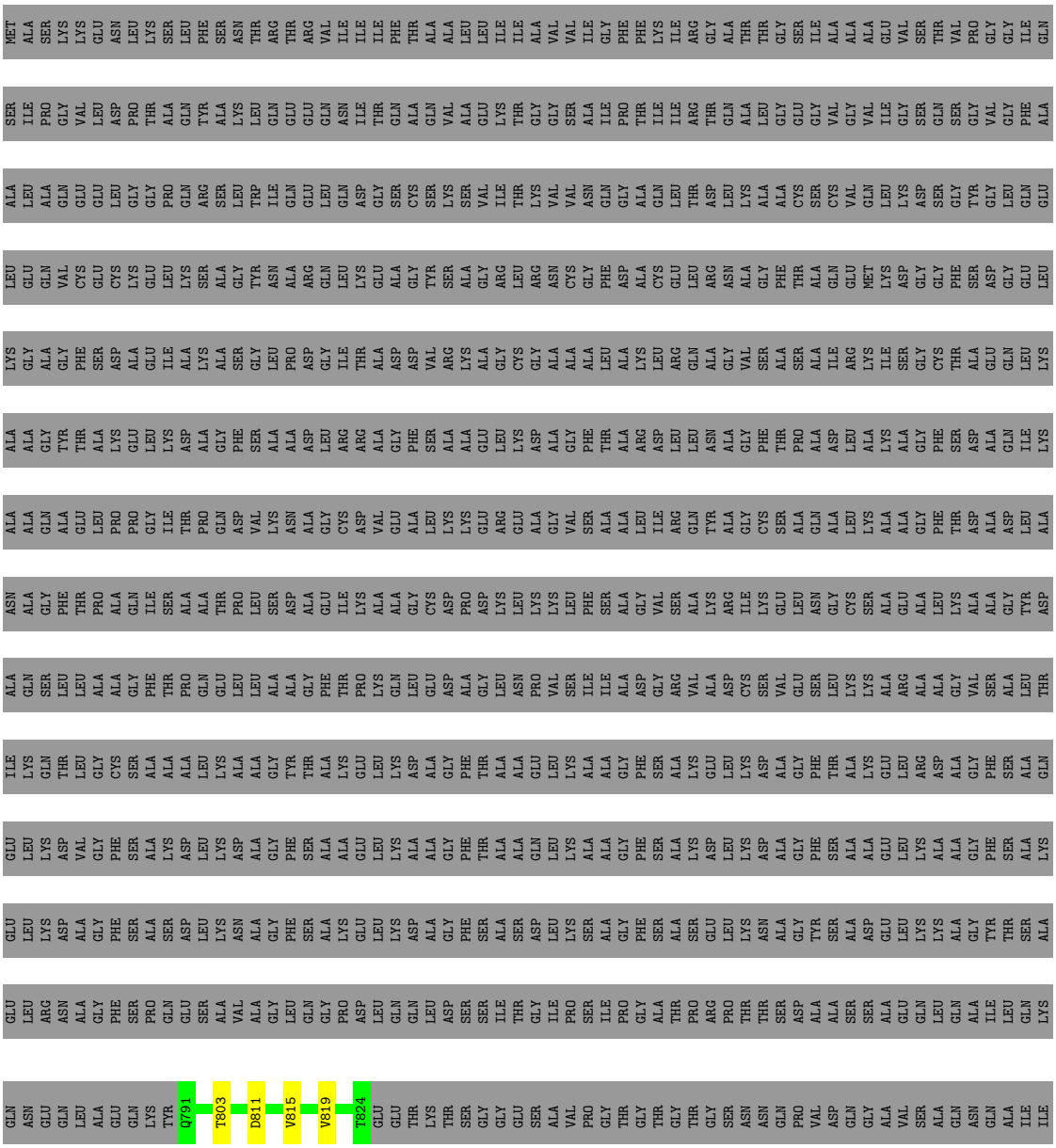
Chain AG:

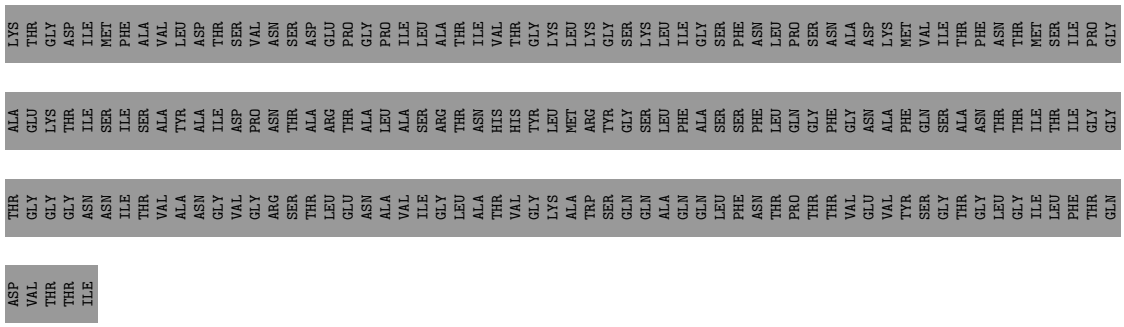




- Molecule 1: IcmE protein

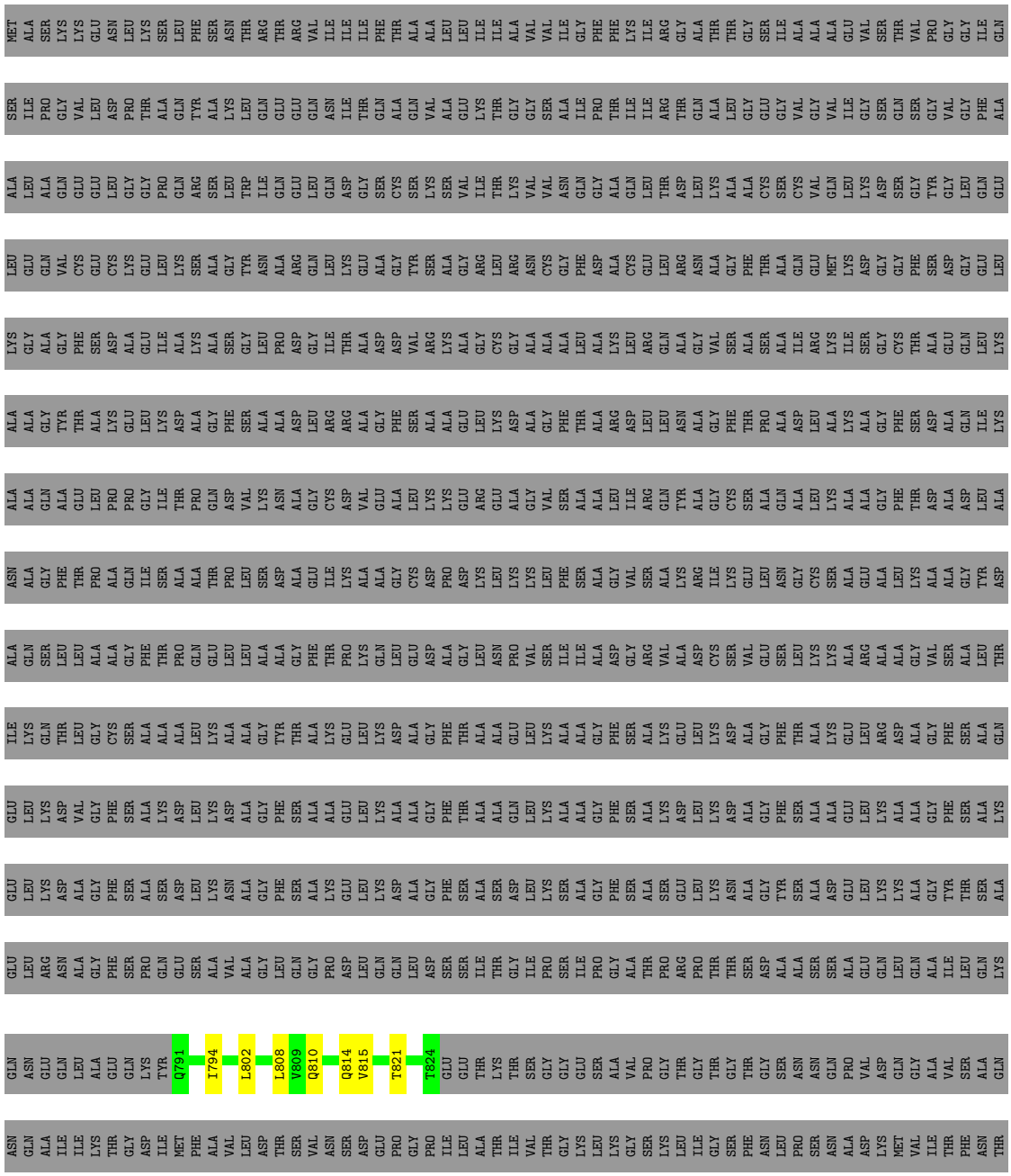
Chain Gg: 97%

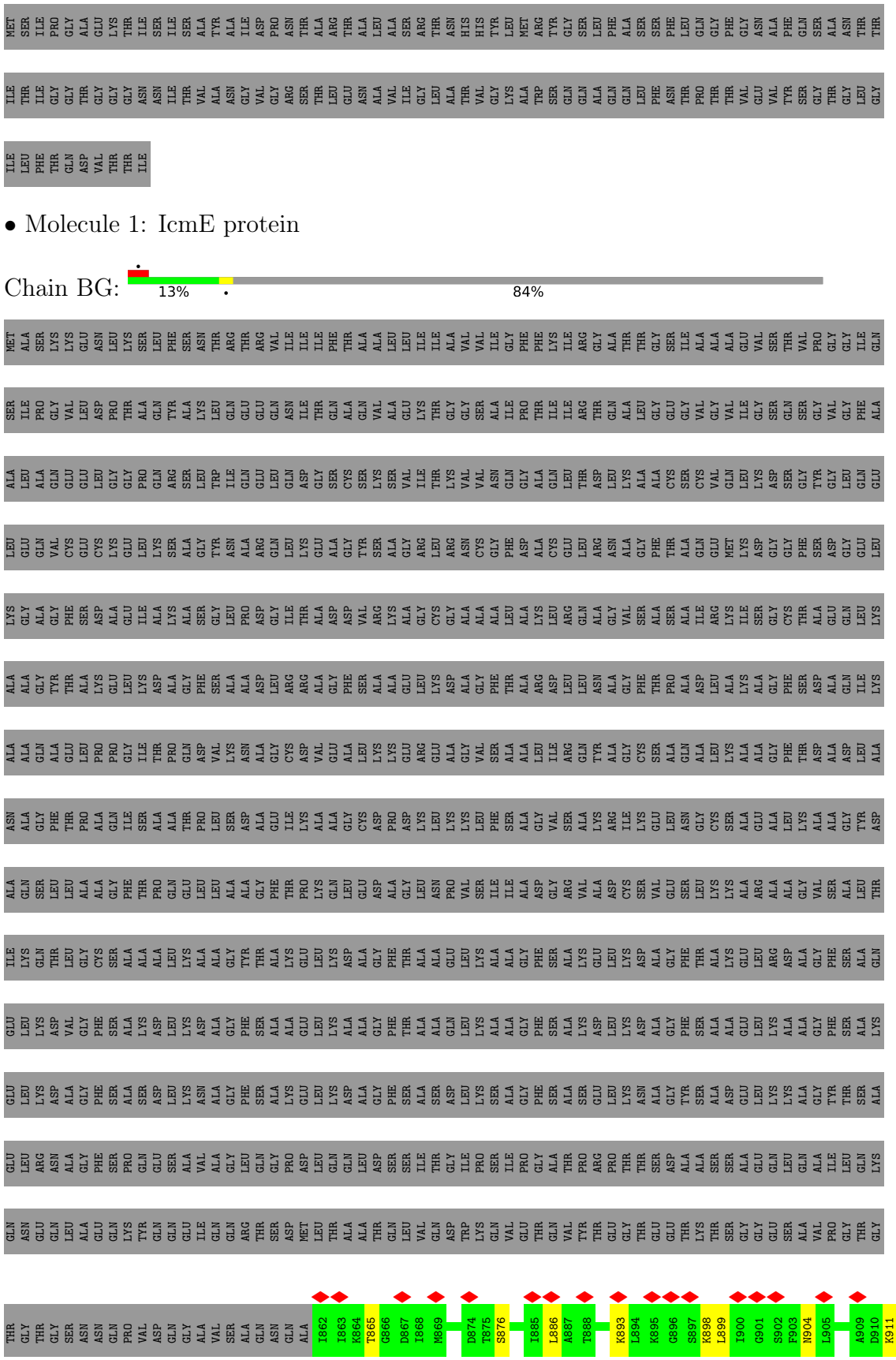


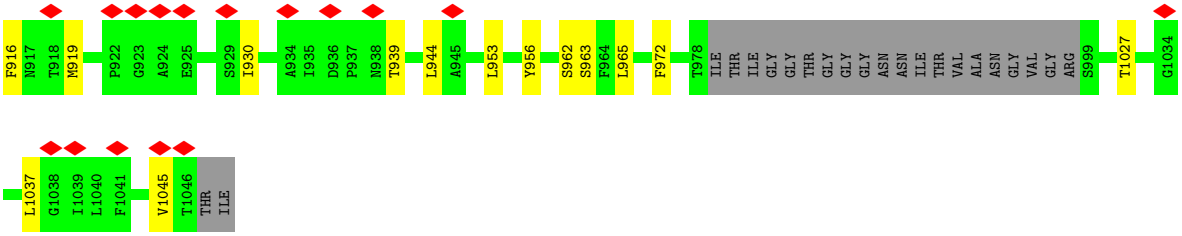


- Molecule 1: IcmE protein

Chain Hg: 97%

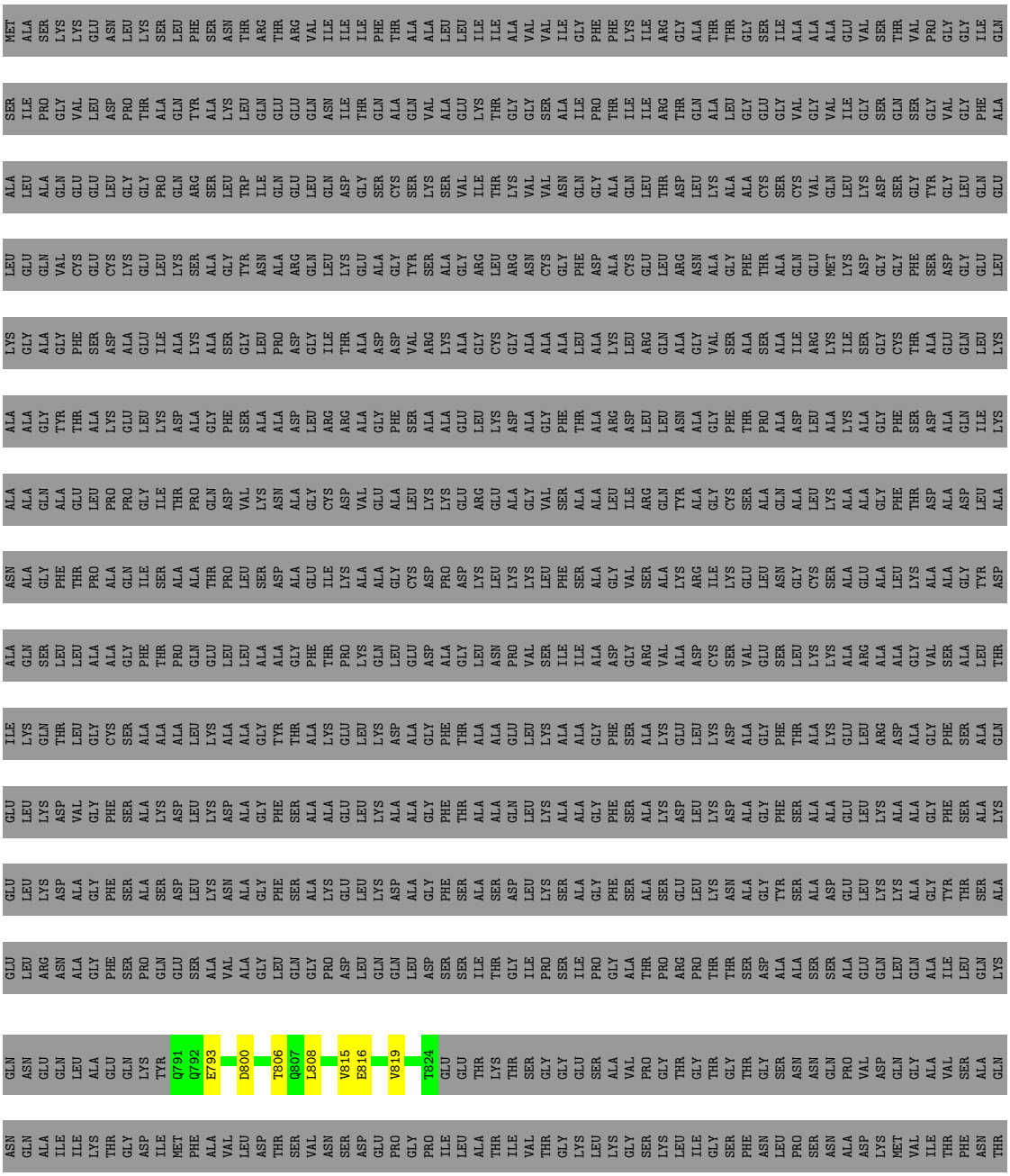


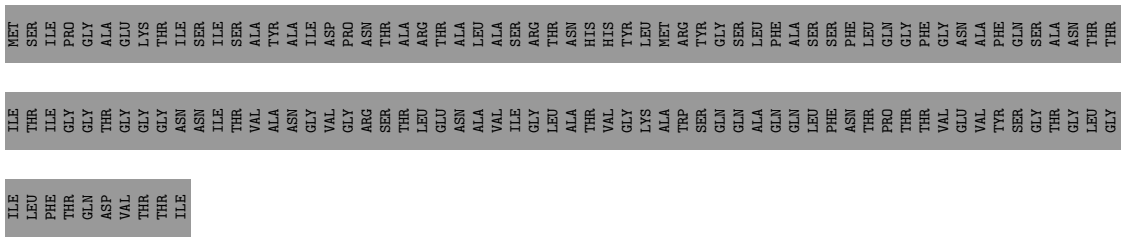

MET SER ILE PRO GLY ALA GLU LYS THR ILE SER ILE SER ALA TYR ALA ILE ASP PRO ASN THR ALA ARG THR ALA LEU ALA SER ARG THR ASN HIS HIS TYR LEU MET ARG TYR GLY SER LEU PHE ALA SER SER PHE LEU GLN GLY PHE GLY ASN ALA PHE GLN SER ALA ASN THR THR
ILE THR ILE GLY GLY THR GLY GLY GLY ASN ASN ILE THR VAL ALA ASN GLY VAL GLY ARG SER THR LEU GLU ASN ALA VAL ILE GLY LEU ALA THR VAL GLY LYS ALA TRP SER GLN GLN ALA GLN GLN LEU PHE ASN THR PRO THR THR VAL GLU VAL TYR SER GLY THR GLY LEU GLY
ILE LEU PHE THR GLN ASP VAL THR THR ILE
• Molecule 1: IcmE protein
Chain BG: 13% 84%
MET ALA SER LYS LYS GLU ASN LEU LYS SER LEU PHE SER ASN THR ARG THR ARG VAL ILE ILE ILE PHE PHE THR ALA ALA LEU LEU ILE ILE ALA VAL VAL ILE GLY PHE PHE LYS ILE ARG GLY ALA THR THR GLY SER ILE ALA ALA ALA GLU VAL SER THR VAL PRO GLY GLY ILE GLN
SER ILE PRO GLY VAL LEU ASP PRO THR ALA GLN TYR ALA LYS LEU GLN GLU GLU GLN ASN ILE THR GLN ALA GLN VAL ALA GLU LYS THR GLY GLY SER ALA ILE PRO THR ILE ILE ARG THR GLN ALA LEU GLY GLU GLY VAL GLY VAL ILE GLY SER GLN SER GLY VAL GLY PHE ALA
ALA LEU ALA GLN GLU GLU LEU GLY GLY PRO GLN ARG SER LEU TRP ILE GLN GLU LEU GLN ASP GLY SER CYS SER LYS SER VAL ILE THR LYS VAL VAL ASN GLN GLY ALA GLN LEU THR ASP LEU LYS ALA ALA CYS SER CYS VAL GLN LEU LYS ASP SER GLY TYR GLY LEU GLN GLU
LEU GLU GLN VAL CYS GLU CYS LYS GLU LEU LYS SER ALA GLY TYR ASN ALA ARG GLN LEU LYS GLU ALA GLY TYR SER ALA GLY ARG LEU ARG ASN CYS GLY PHE ASP ALA CYS GLU LEU ARG ASN ALA GLY PHE THR ALA GLN GLU MET LYS ASP GLY GLY PHE SER ASP GLY GLU LEU
LYS GLY ALA GLY PHE SER ASP ALA GLU ILE ALA LYS ALA SER GLY LEU PRO ASP GLY ILE THR ALA ASP ASP VAL ARG LYS ALA GLY CYS GLY ALA ALA ALA LEU ALA LYS LEU ARG GLN ALA ALA GLY VAL SER ALA SER ALA ILE ARG LYS ILE SER GLY CYS THR ALA GLU GLN LEU LYS
ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA ASP LEU ARG ARG ALA GLY PHE SER ALA ALA GLU LEU LYS ASP ALA GLY PHE THR ALA ALA ARG ASP LEU LEU ASN ALA GLY PHE THR PRO ALA ASP LEU ALA LYS ALA SER ASP ALA GLN ILE LYS
ALA ALA GLN ALA GLU LEU PRO PRO GLY ILE THR PRO GLN ASP VAL LYS ASN ALA GLY CYS ASP VAL GLU ALA LEU LYS LYS GLU ARG GLU ALA GLY VAL SER ALA ALA ALA GLN TYR ALA GLY CYS SER ALA GLN ALA LEU LYS ALA ALA GLY PHE THR ASP ALA ASP LEU ALA
ASN ALA GLY PHE THR PRO ALA GLN ILE SER ALA ALA THR PRO LEU SER ASP ALA GLU ILE LYS ALA ALA GLY CYS ASP PRO ASP ASP LYS LEU LYS LYS LEU PHE SER ALA GLY VAL SER ALA LYS ARG ILE LYS GLU LEU ASN GLY CYS CYS SER ALA GLU ALA LEU LYS LYS GLU GLU ALA GLY PHE THR ALA ALA LYS ALA GLU
ALA GLN SER LEU LEU ALA ALA GLY PHE THR PRO GLN GLU LEU LEU ALA ALA GLY PHE THR PRO LYS GLN LEU GLU ASP ALA GLY LEU ASN PRO VAL SER ILE ILE ALA ASP GLY ARG VAL ALA ASP CYS SER VAL GLU SER LEU LYS LYS ALA ARG ALA ALA LEU GLY PHE THR ALA LYS
ILE LYS GLN THR LEU GLY CYS SER ALA ALA ALA LEU LYS ALA ALA ALA GLY TYR THR ALA LYS GLU LEU ASP ALA ALA GLY PHE THR ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA LYS GLU LEU ALA LYS ALA ALA GLN
GLU LEU LYS ASP VAL GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA ALA ALA GLN LEU LYS ASP ALA GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA LYS
GLU LEU LYS ASP ALA GLY PHE SER SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER SER ALA ALA ALA GLN LEU LYS ASP ALA GLY PHE SER SER ALA ALA ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY TYR THR SER ALA
GLU LEU ARG ASN ALA GLY PHE SER PRO GLN GLU SER ALA VAL ALA GLY PRO ASP LEU GLN GLN LEU ASP SER SER ILE THR GLY ILE PRO SER ILE PRO GLY ALA THR PRO ARG PRO THR THR SER ALA ASP GLU LEU GLN GLN ALA ILE LEU GLN LYS
GLN ASN GLU GLN LEU ALA GLU GLN LYS TYR GLN GLN GLU ILE GLN GLN ARG THR SER ASP MET LEU THR ALA ALA THR GLN LEU VAL GLN ASP TRP LYS GLN VAL GLU THR GLN VAL TYR THR GLU GLY THR THR GLU GLU THR LYS THR SER GLY GLY GLU SER ALA VAL PRO GLY THR GLY
THR GLY THR GLY SER ASN ASN GLN PRO VAL ASP GLN GLY ALA VAL SER ALA GLN ASN GLN ALA I862 I863 K864 T865 G866 D867 I868 M869 D874 T875 S876 I885 L886 A887 T888 K893 L894 K895 G896 S897 K898 L899 I900 G901 S902 F903 N904 L905 A909 D910 K911 M912 V913 I914 T915



- Molecule 1: IcmE protein

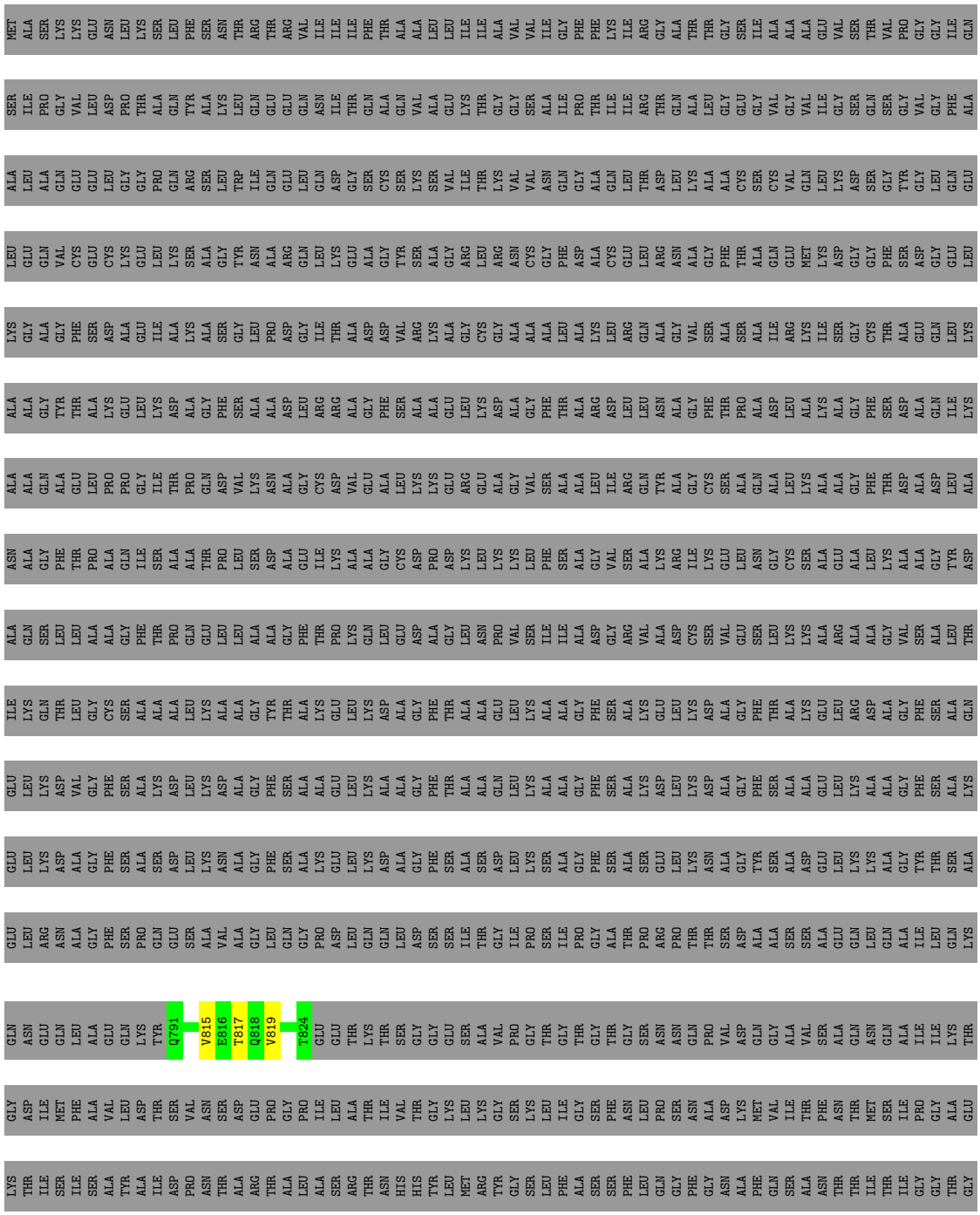
Chain Bg: 97%

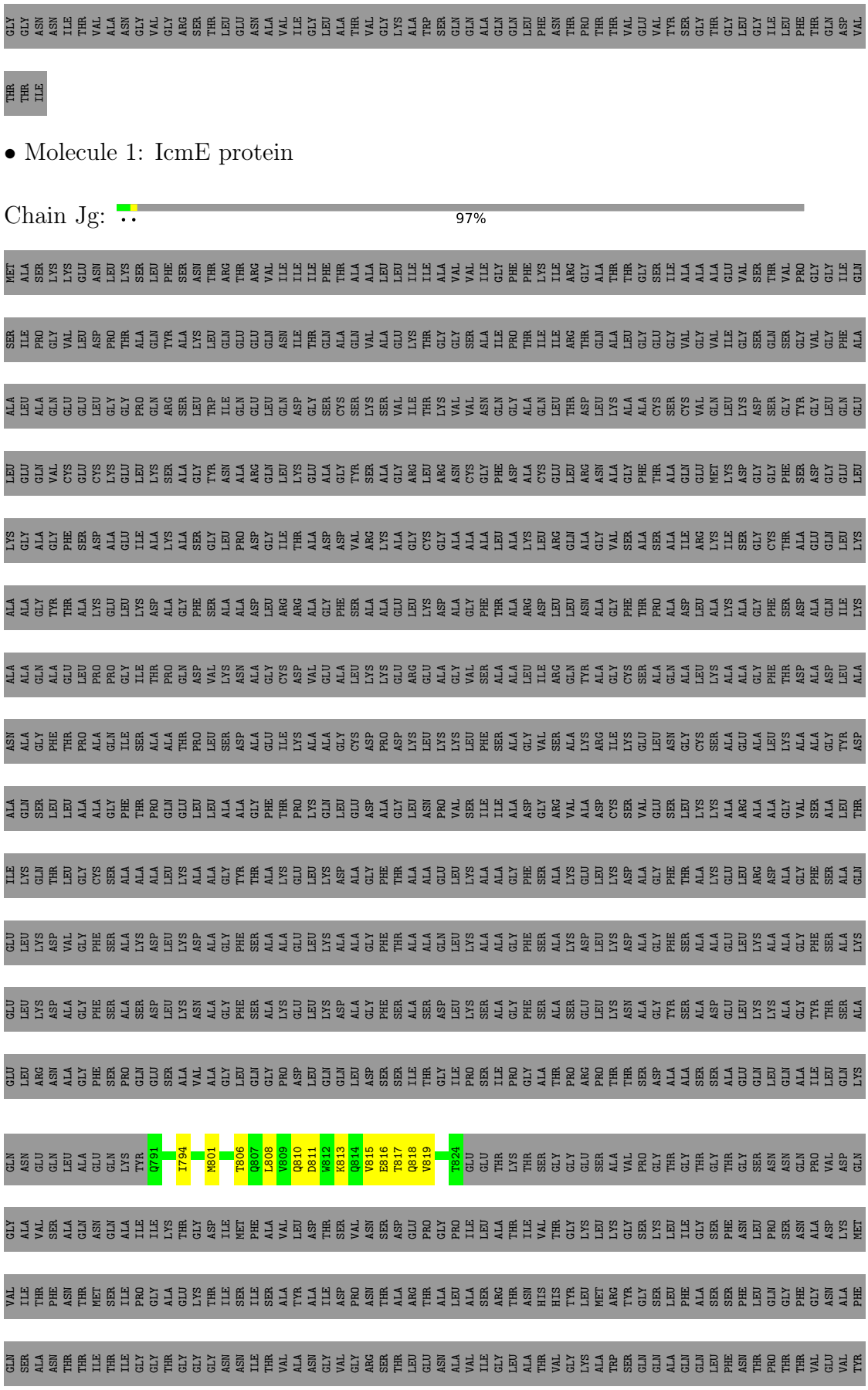




• Molecule 1: IcmE protein

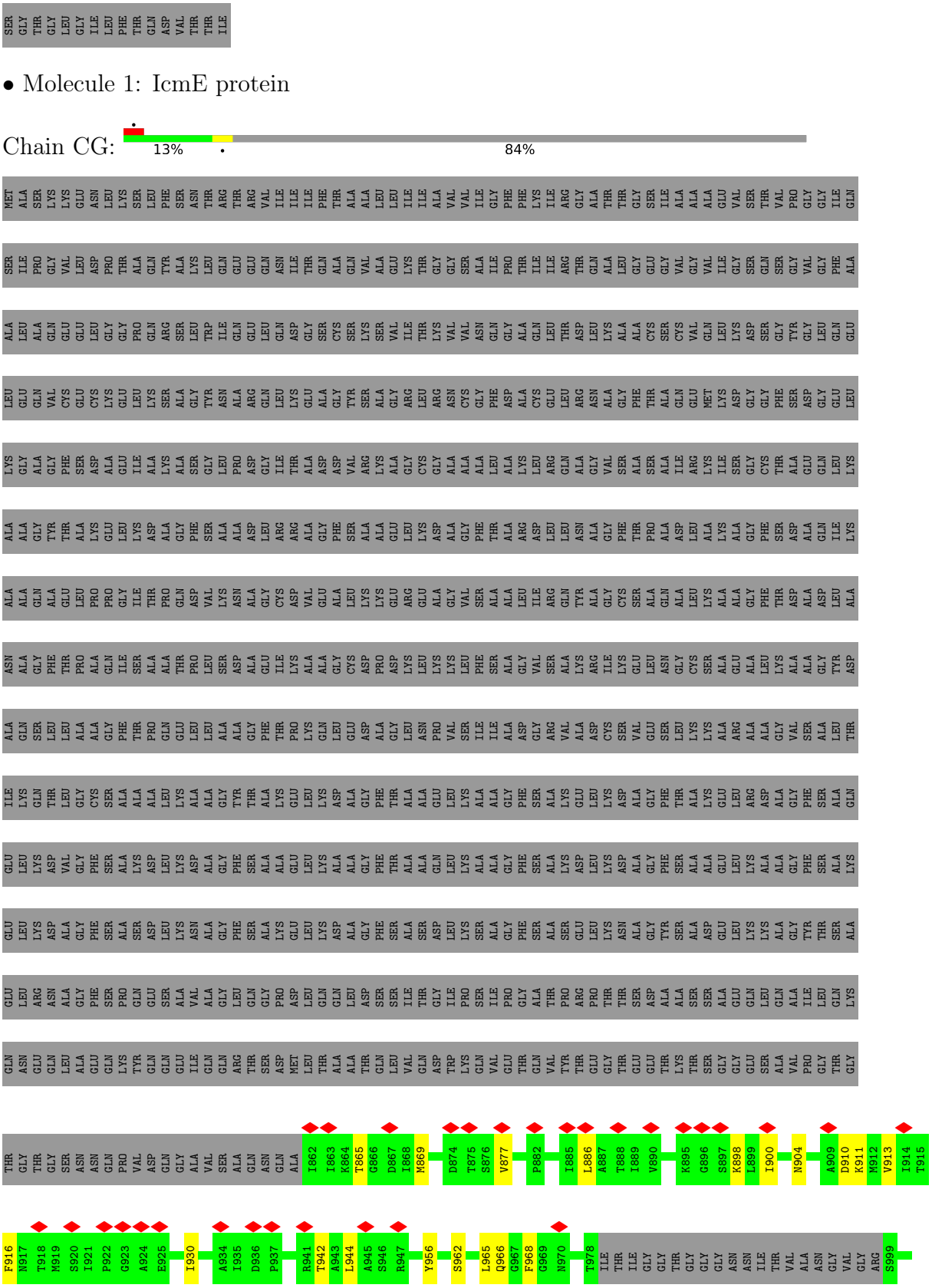
Chain Ig: 97%

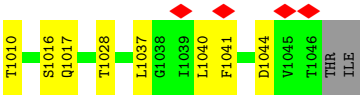




- Molecule 1: IcmE protein

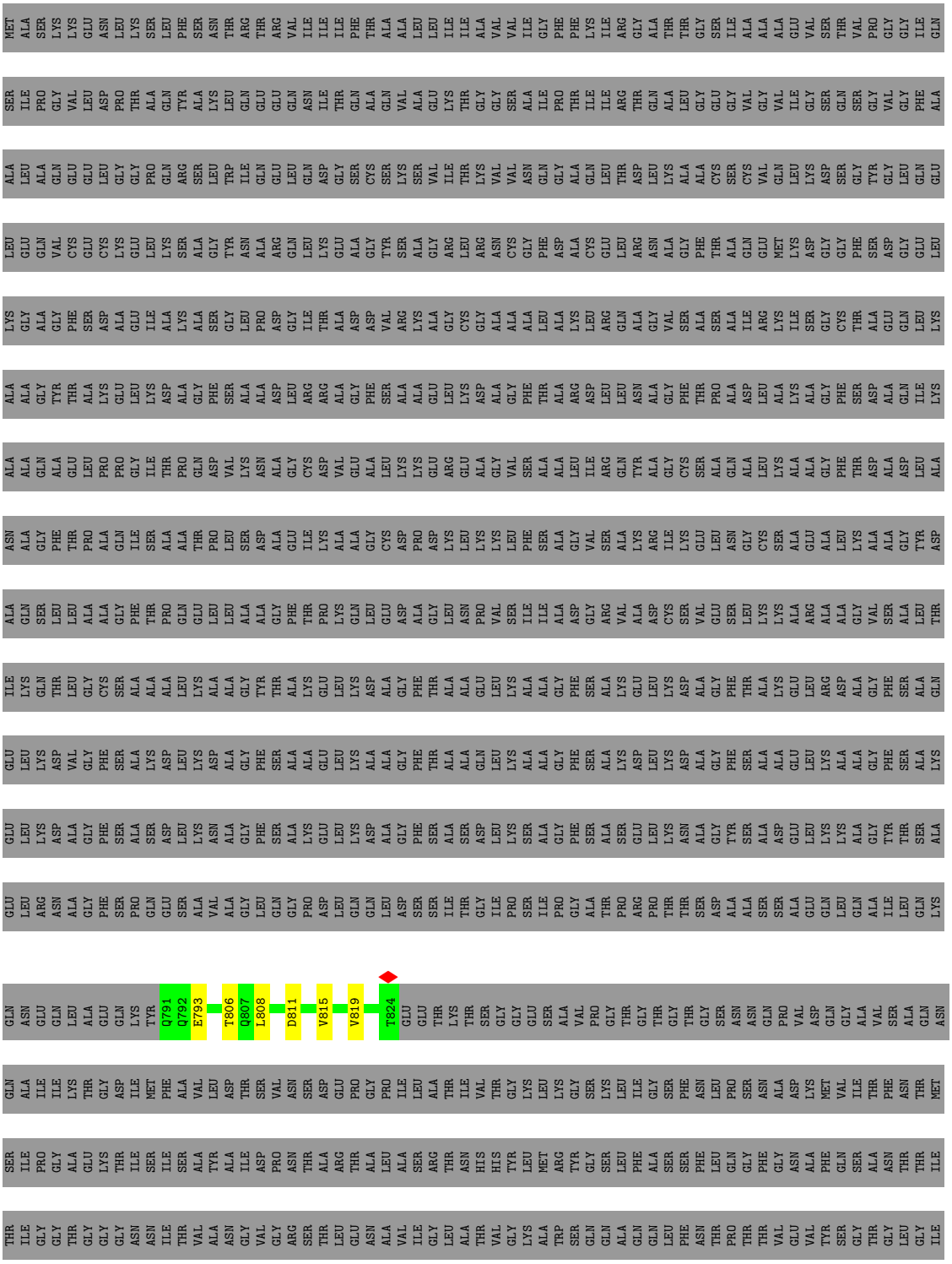
Chain Jg: 97%

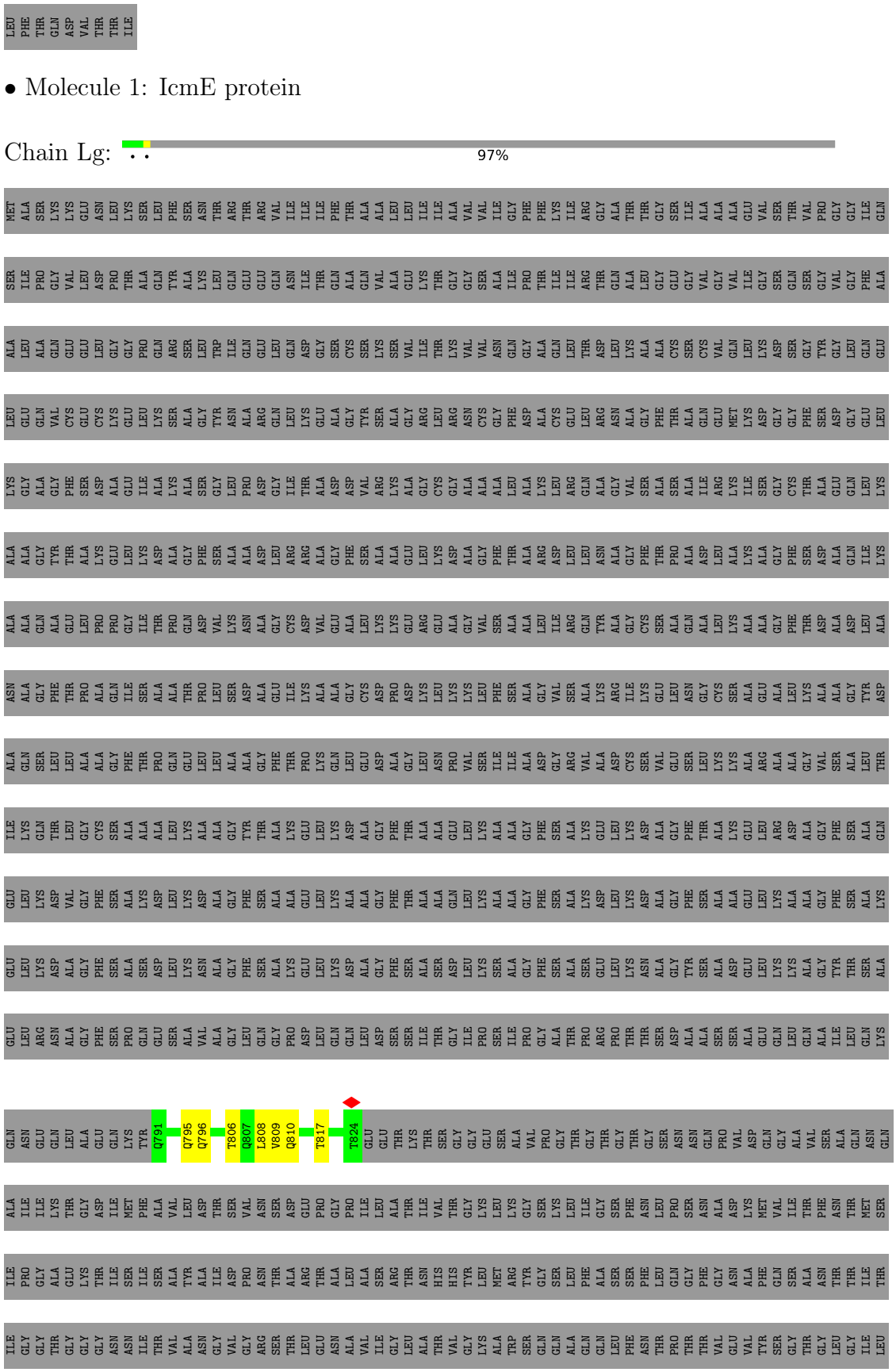

SER GLY THR GLY LEU GLY ILE LEU PHE THR GLN ASP VAL THR THR ILE
• Molecule 1: IcmE protein
Chain CG:
13%
84%
I862 I863 K864 T865 G866 D867 I868 M869 D874 T875 S876 V877 P882 I885 L886 A887 T888 I889 V890 K895 G896 S897 K898 L899 I900 N904 A909 D910 K911 M912 V913 I914 T915
F916 N917 T918 M919 S920 I921 P922 G923 A924 E925 I930 A934 I935 D936 P937 R941 T942 A943 L944 A945 S946 R947 Y956 S962 L965 Q966 G967 F968 G969 N970 T978 ILE THR ILE GLY GLY THR GLY GLY GLY ASN ASN ILE THR VAL ALA ASN GLY VAL GLY ARG S999

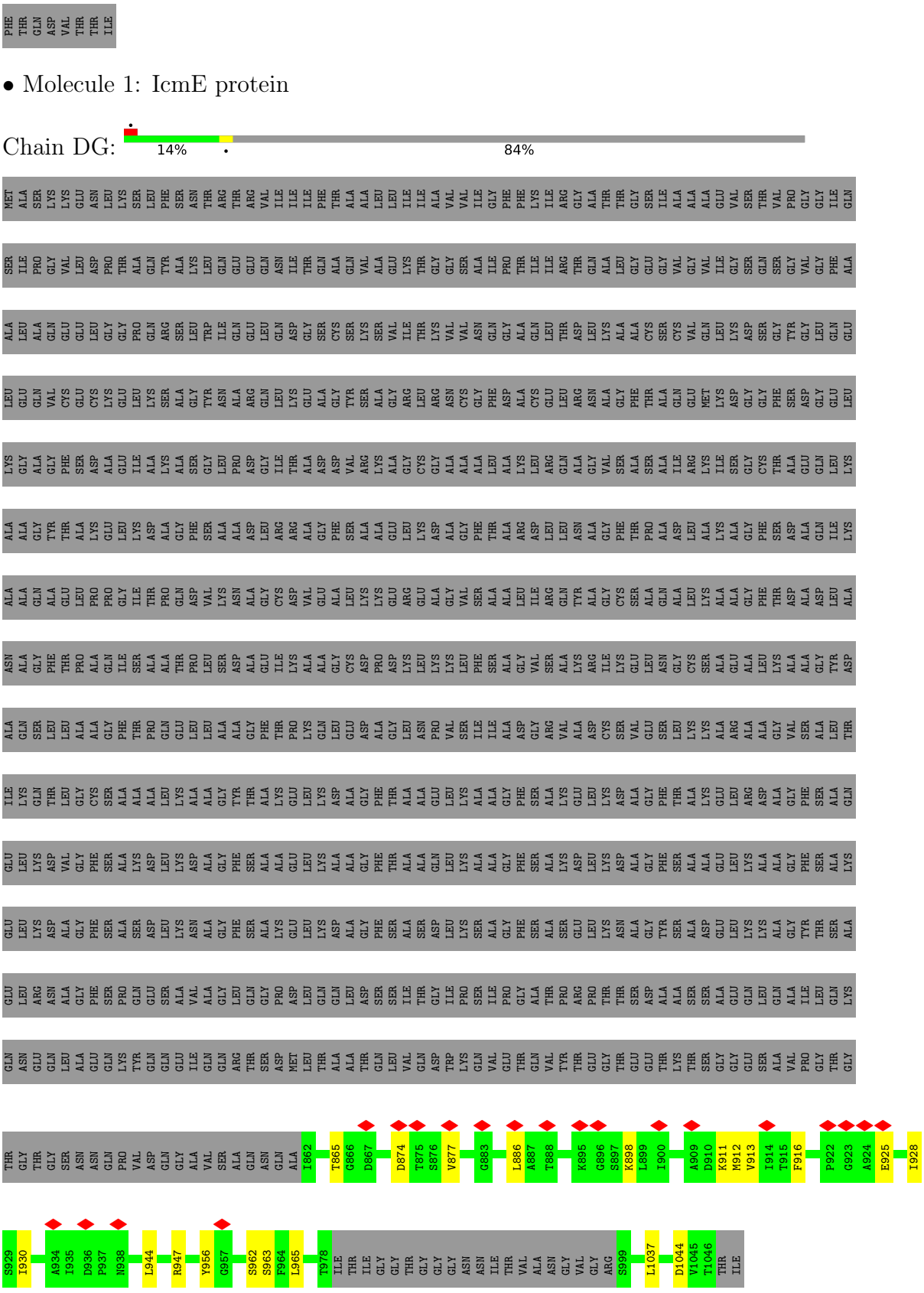


- Molecule 1: IcmE protein

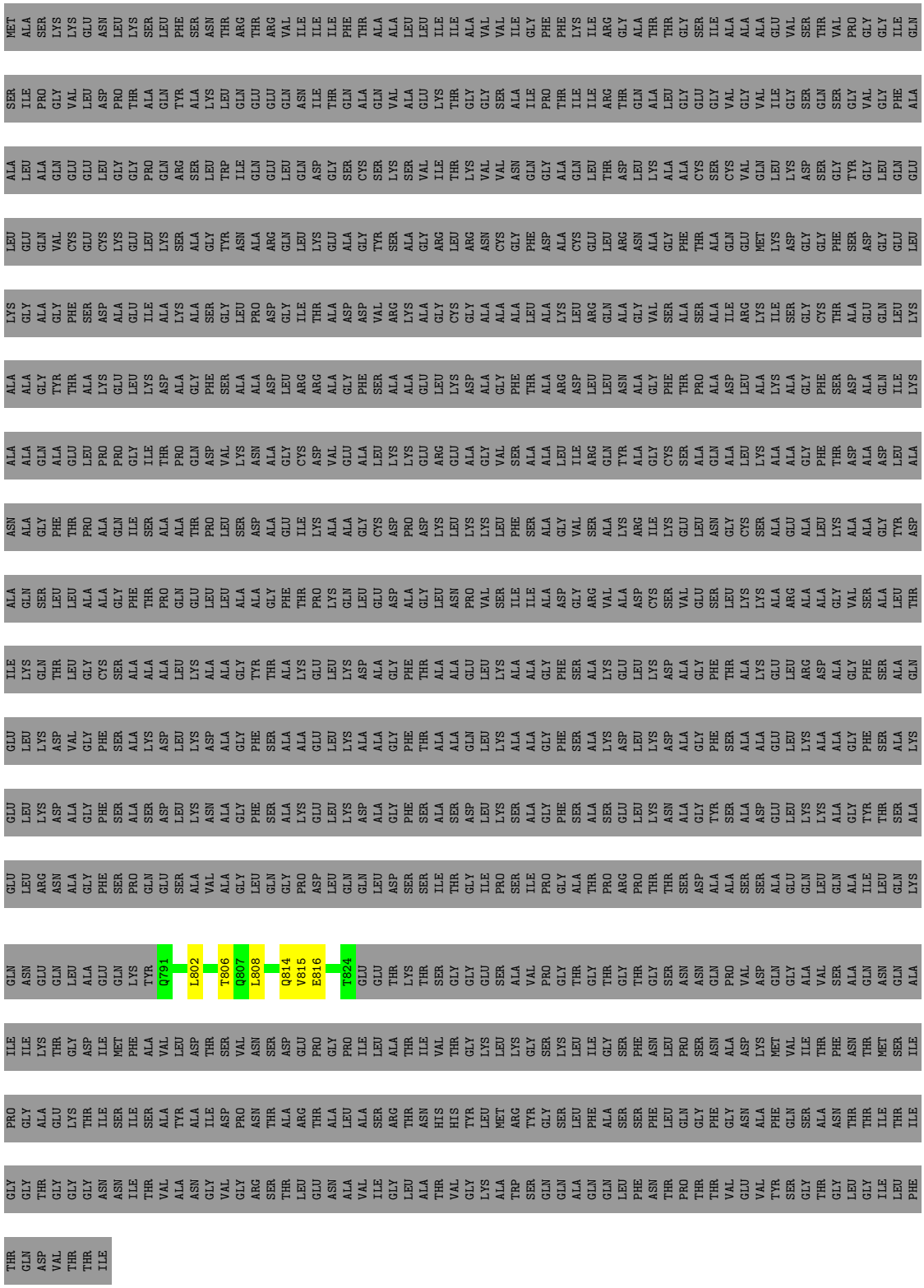
Chain Kg: 97%




LEU PHE THR GLN ASP VAL THR THR ILE
• Molecule 1: IcmE protein
Chain Lg:
97%
Q791
Q795
Q796
T806
Q807
L808
V809
Q810
T817
T824

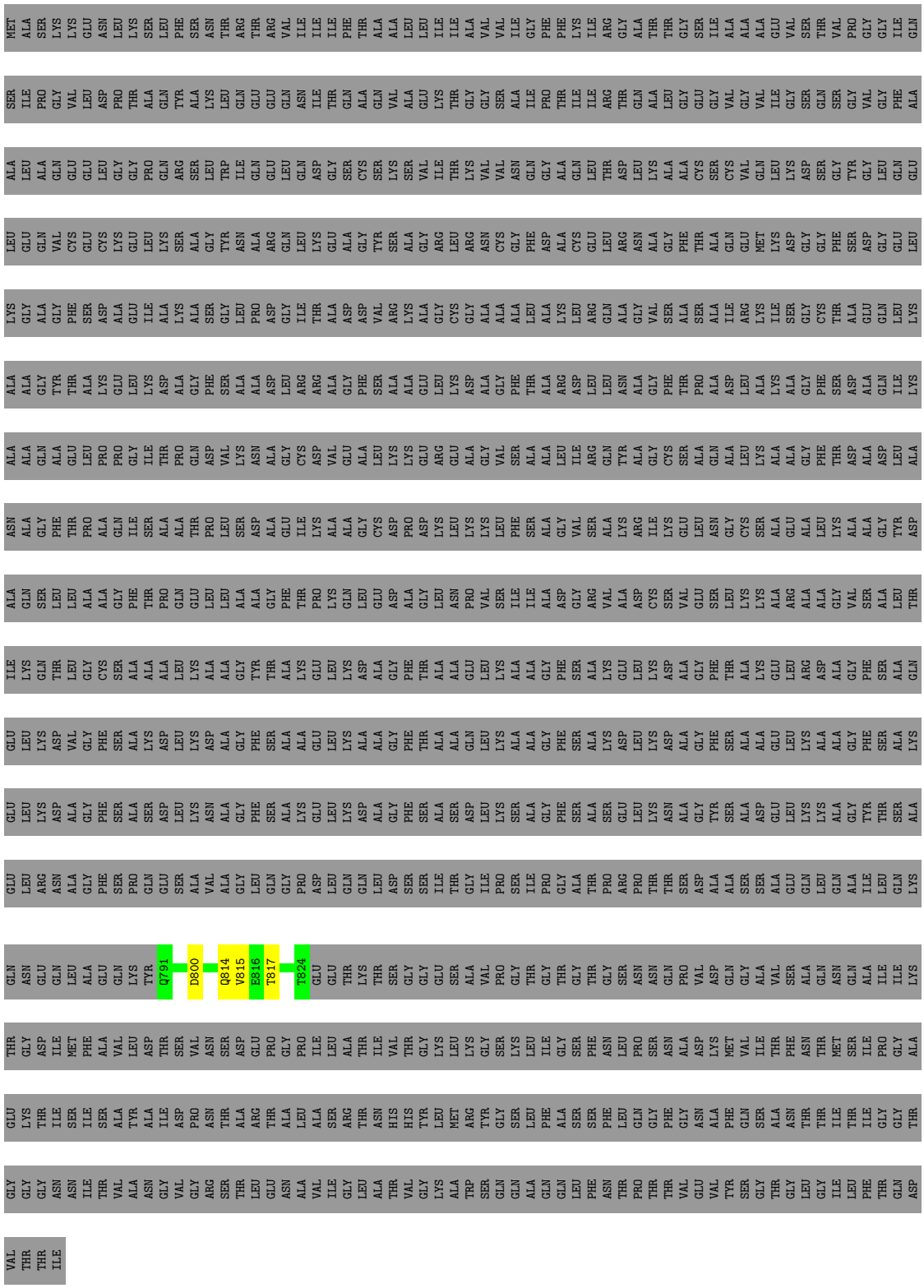

PHE THR GLN ASP VAL THR THR ILE
• Molecule 1: IcmE protein
Chain DG:
14%
84%
MET ALA SER LYS LYS GLU ASN LEU LYS SER LEU PHE SER ASN THR ARG THR ARG VAL ILE ILE ILE PHE THR ALA ALA LEU LEU LEU ILE ILE ALA VAL VAL ILE GLY PHE PHE LYS ILE ARG GLY ALA THR THR GLY SER ILE ALA ALA ALA GLU VAL SER THR VAL PRO GLY GLY ILE GLN
SER ILE PRO GLY VAL LEU ASP PRO THR ALA GLN TYR ALA LYS LEU GLN GLU GLU GLN ASN ILE THR GLN ALA GLN VAL ALA ALA GLU LYS THR GLY GLY SER ALA ILE ILE PRO THR ILE ILE ARG THR GLN ALA LEU GLY GLU GLY VAL GLY VAL ILE GLY SER GLN SER GLY VAL GLY PHE ALA
ALA LEU ALA GLN GLU GLU LEU GLY GLY PRO GLN ARG SER LEU TRP ILE GLN GLU LEU GLN ASP GLY SER CYS SER LYS SER VAL ILE THR LYS VAL VAL ASN GLN GLY ALA GLN LEU THR ASP LEU LYS ALA ALA CYS SER CYS VAL GLN GLU LEU LYS ASP SER GLY TYR GLY LEU GLN GLU
LEU GLU GLN VAL CYS GLU CYS LYS GLU LEU LYS SER ALA GLY TYR ASN ALA ARG GLN LEU LYS GLU ALA GLY TYR SER ALA GLY ARG LEU ARG ASN CYS GLY PHE ASP ALA CYS GLU LEU ARG ASN ALA GLY PHE THR ALA GLN GLU MET LYS ASP GLY GLY PHE SER ASP GLY GLU LEU
LYS GLY ALA GLY PHE SER ASP ALA GLU ILE ALA LYS ALA SER GLY LEU PRO ASP GLY ILE THR ALA ASP ASP VAL ARG LYS ALA GLY CYS GLY ALA ALA ALA LYS LEU ARG GLN ALA GLY VAL SER ALA SER ALA ILE ARG ALA SER GLY CYS THR ALA GLU GLN LEU LYS
ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA ASP LEU ARG ARG ALA GLY PHE SER ALA ALA GLU LEU LYS ASP ALA GLY PHE THR ALA ARG ASP LEU LEU ASN ALA GLY PHE THR PRO ALA ASP LEU ARG ALA ALA LYS ILE ALA GLN ILE LYS
ALA ALA GLN ALA GLU LEU PRO PRO GLY ILE THR PRO GLN ASP VAL LYS ASN ALA GLY CYS ASP VAL GLU ALA LEU LYS LYS GLU ARG GLU ALA GLY VAL SER ALA ALA ALA GLN TYR ALA GLY CYS SER ALA GLN ALA LEU LYS ALA ALA GLY PHE THR ASP ALA ASP LEU GLN ILE
ASN ALA GLY PHE THR PRO ALA GLN ILE SER ALA ALA THR PRO LEU SER ASP ALA GLU ILE LYS ALA ALA GLY CYS ASP PRO ASP LYS LEU LYS ASP SER ALA GLY VAL SER ALA LYS ARG ILE LYS GLU LEU ASN GLY CYS SER ALA GLU ALA ALA LEU ASP ALA GLY GLY
ALA GLN SER LEU LEU ALA ALA GLY PHE THR PRO GLN GLU LEU LEU ALA ALA GLY PHE THR PRO LYS GLN LEU GLU ASP ALA GLY LEU ASN PRO VAL SER ILE ILE ALA ASP GLY ARG VAL ALA ASP CYS SER VAL GLU SER LEU LYS LYS ALA ARG ALA ALA GLY VAL SER ALA LEU THR
ILE LYS GLN THR LEU GLY CYS SER ALA ALA LEU LYS ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA GLN
GLU LEU LYS ASP VAL GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA ALA GLU LEU LYS ASP ALA ALA GLY PHE THR ALA ALA ALA GLN LEU LEU LYS ASP ALA GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS
GLU LEU LYS ASP ALA GLY PHE SER ALA SER ASP LEU LYS ASN ALA GLY PHE SER ALA SER ASP LEU LYS SER ALA ALA GLY PHE SER ALA SER GLU LEU LYS ASN ALA GLY PHE SER ALA SER GLU LEU LYS ASP ALA GLY PHE SER ALA SER GLU LEU LYS ASN ALA GLY TYR THR SER ALA
GLU LEU ARG ASN ALA GLY PHE SER PRO GLN GLU SER ALA VAL ALA GLY LEU GLN GLY PRO ASP LEU GLN GLN GLN LEU ASP SER SER ILE THR GLY ILE PRO SER ILE PRO GLY ALA THR PRO ARG PRO THR THR SER ASP ALA ALA SER GLU LEU GLN LEU LYS GLU GLN LYS
GLN ASN GLU GLN GLU ALA GLU GLN LYS TYR GLN GLN GLN GLU ILE GLN ARG THR SER ASP PRO GLN ALA ALA ALA ALA MET LEU THR ALA ALA THR GLN LEU VAL GLN ASP TRP LYS GLN VAL GLU THR GLN VAL TYR THR GLU GLY THR GLU GLU THR LYS THR SER GLY GLY GLU SER ALA GLN GLY THR GLY
THR GLY THR GLY SER ASN ASN GLN PRO VAL ASP GLN GLY ALA VAL SER ALA GLN ASN GLN ALA I862 T865 G866 D867 D874 T875 S876 V877 G883 L886 A887 T888 K895 G896 S897 K898 L899 I900 A909 D910 K911 M912 V913 I914 T915 F916 P922 G923 A924 E925 I928
S929 I930 A934 I935 D936 P937 N938 L944 R947 Y956 G957 S962 S963 F964 L965 T978 ILE THR ILE GLY GLY THR GLY GLY GLY ASN ASN ILE THR VAL ALA ALA ASN GLY VAL GLY ARG S999 L1037 D1044 V1045 T1046 THR ILE
• Molecule 1: IcmE protein

Chain Cg: 97%



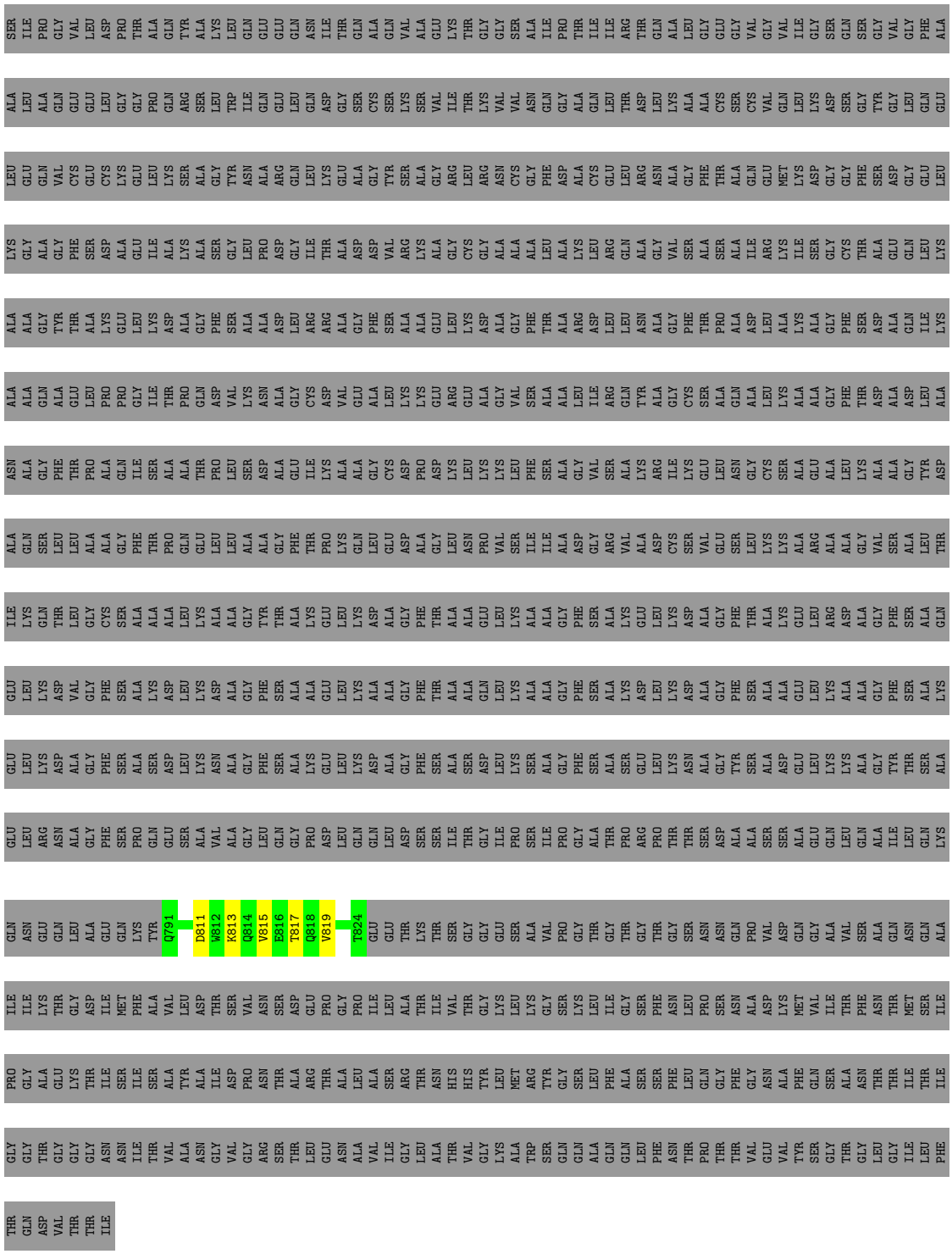
- Molecule 1: IcmE protein

Chain Mg: 97%



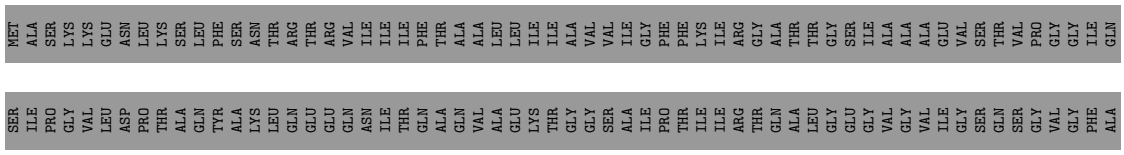
- Molecule 1: IcmE protein

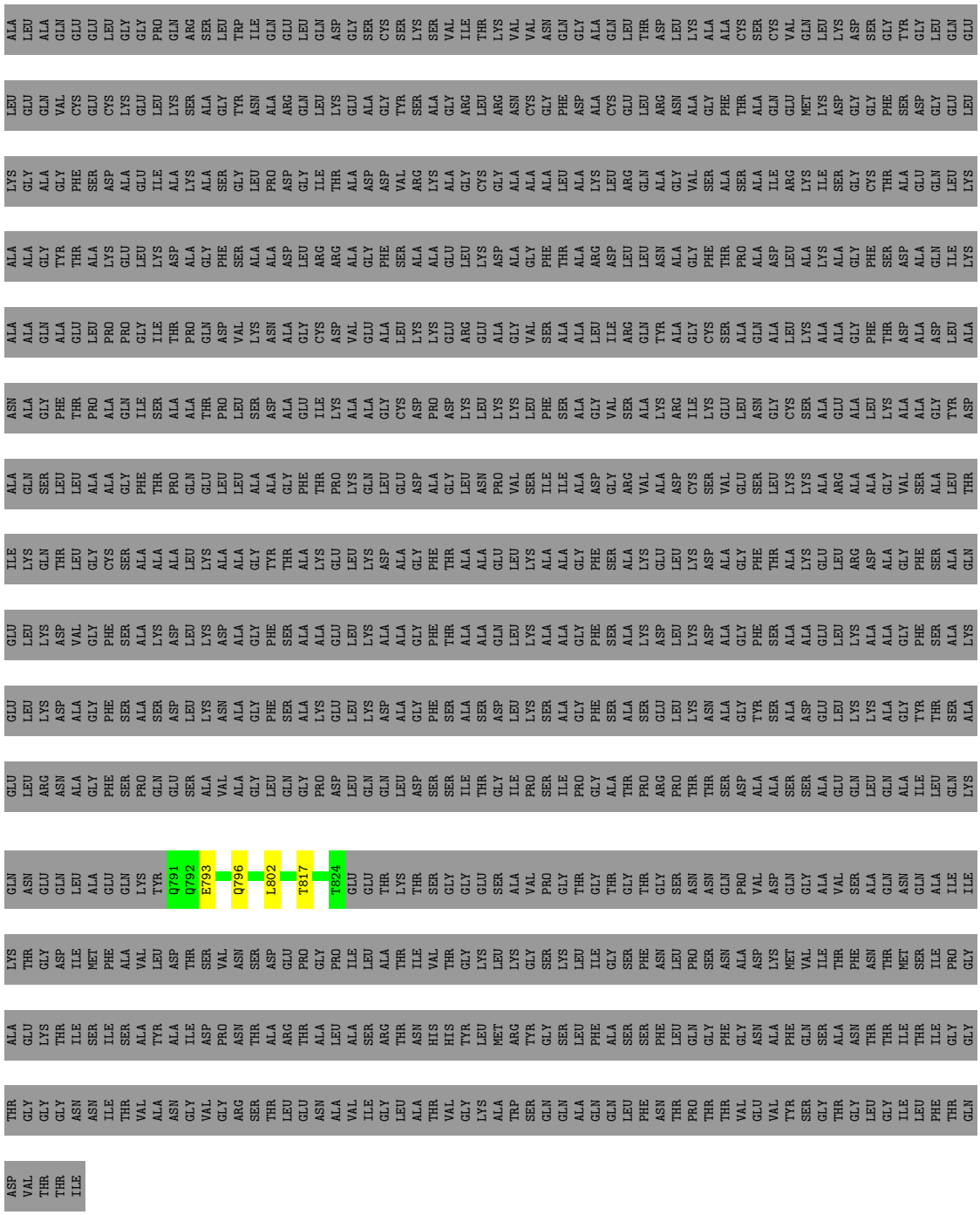
Chain Ag: 97%



• Molecule 1: IcmE protein

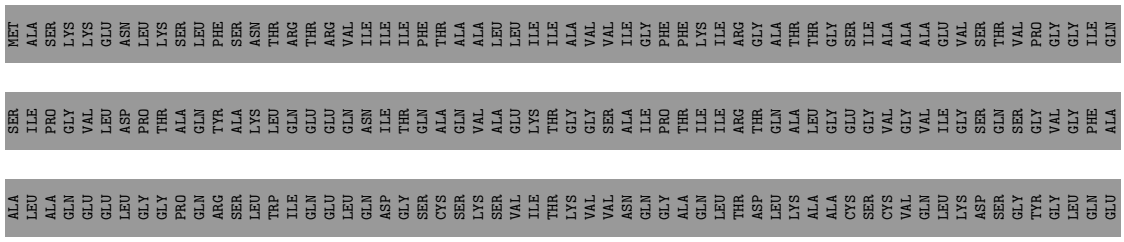
Chain VG: 97%

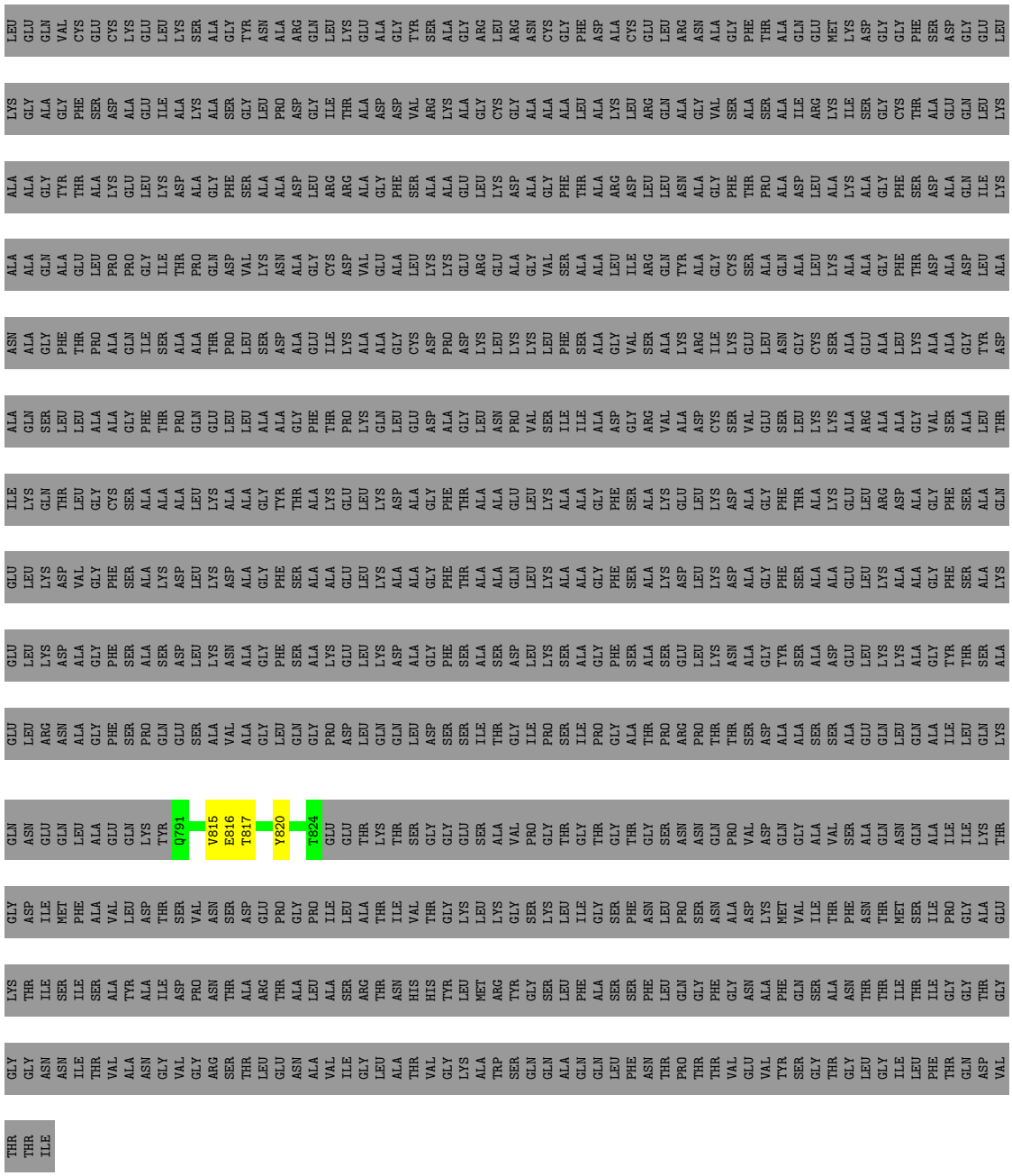




- Molecule 1: IcmE protein

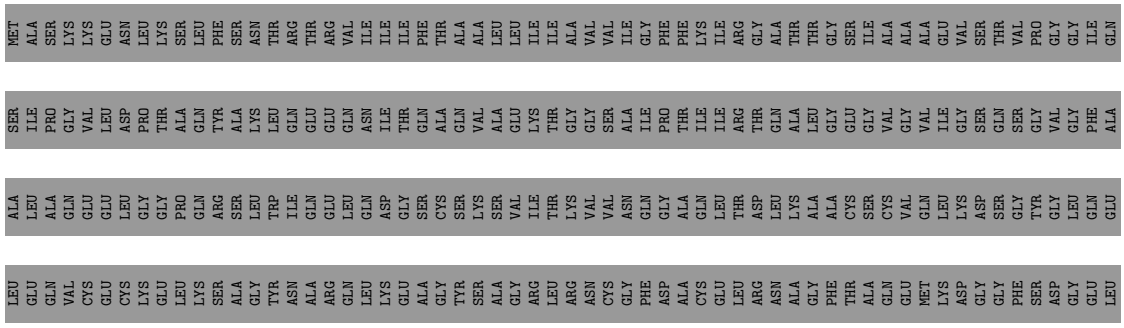
Chain WG: 97%

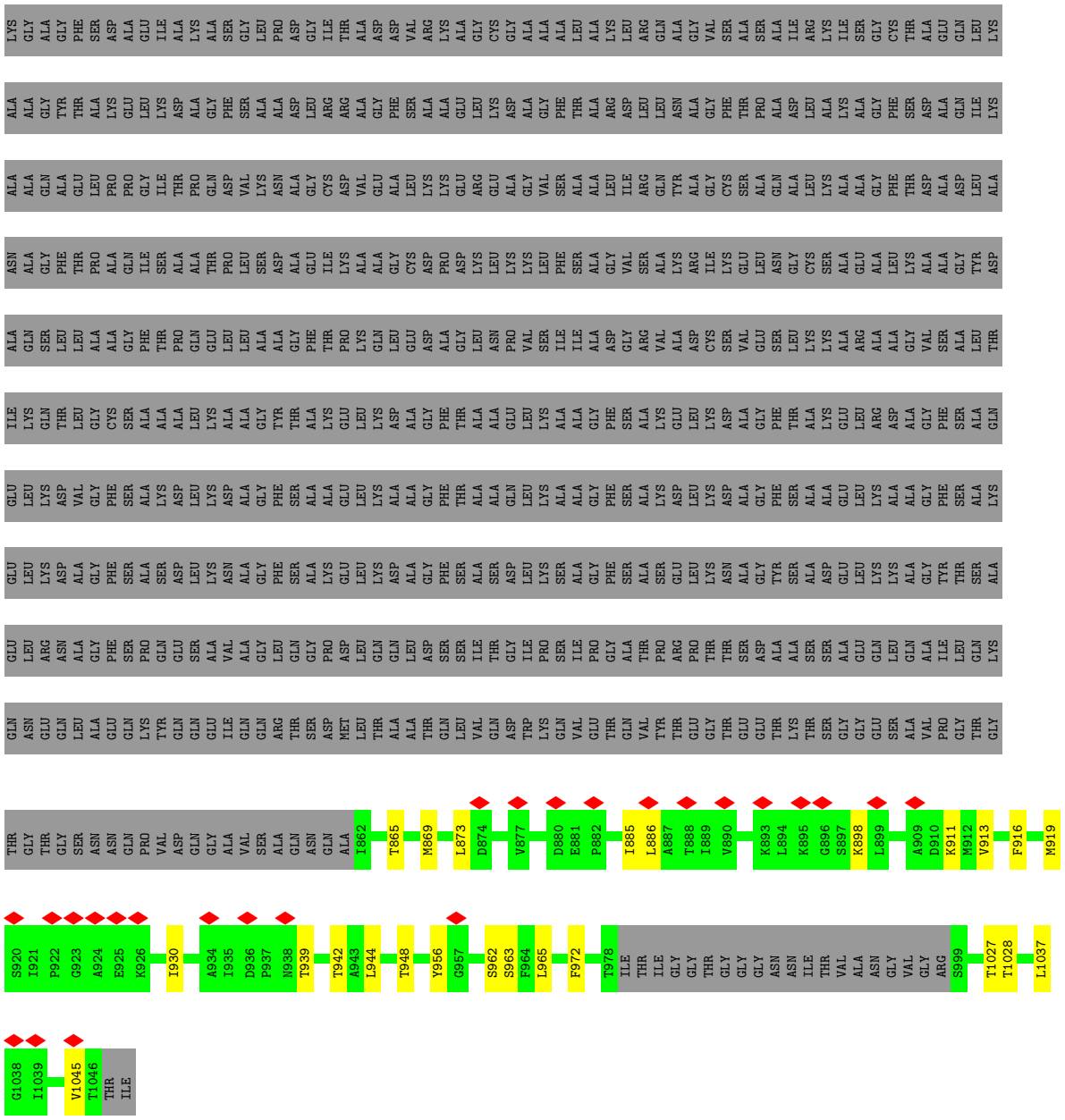




- Molecule 1: IcmE protein

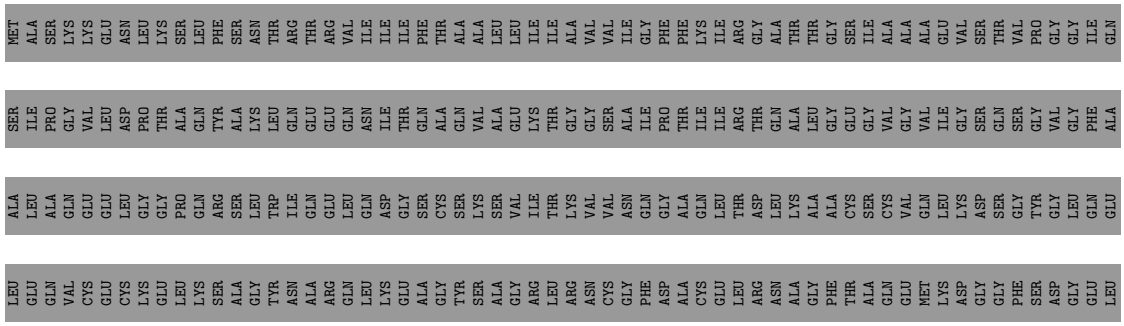
Chain EG:

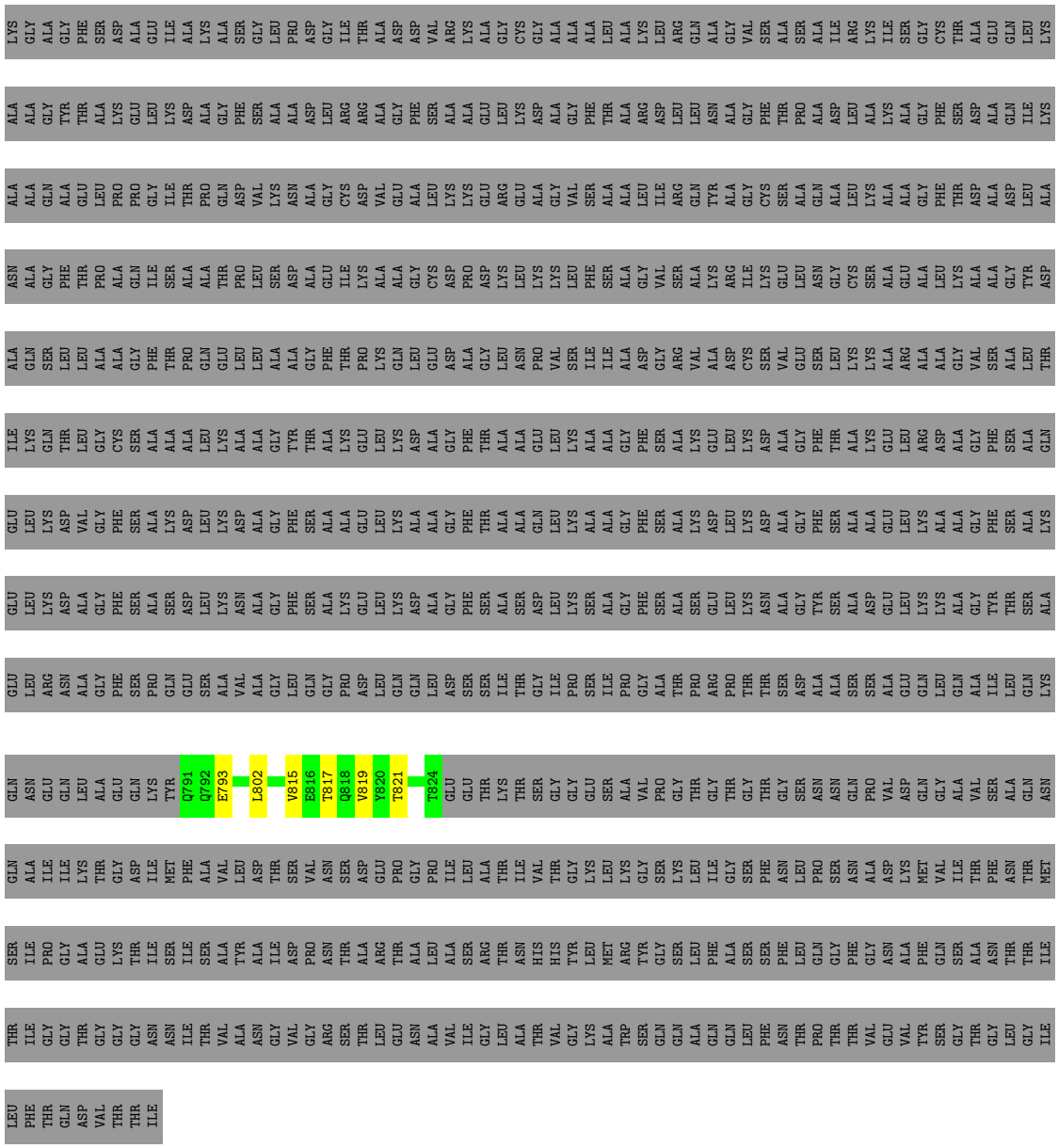




- Molecule 1: IcmE protein

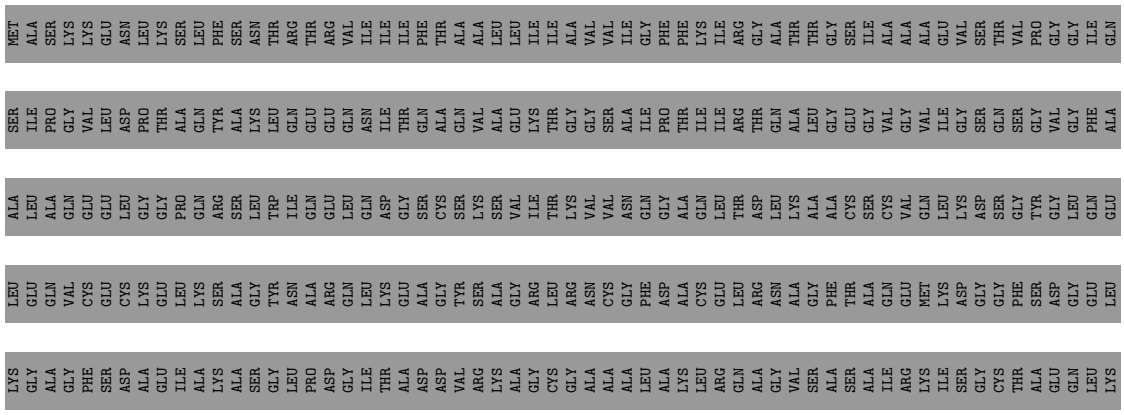
Chain XG: 97%

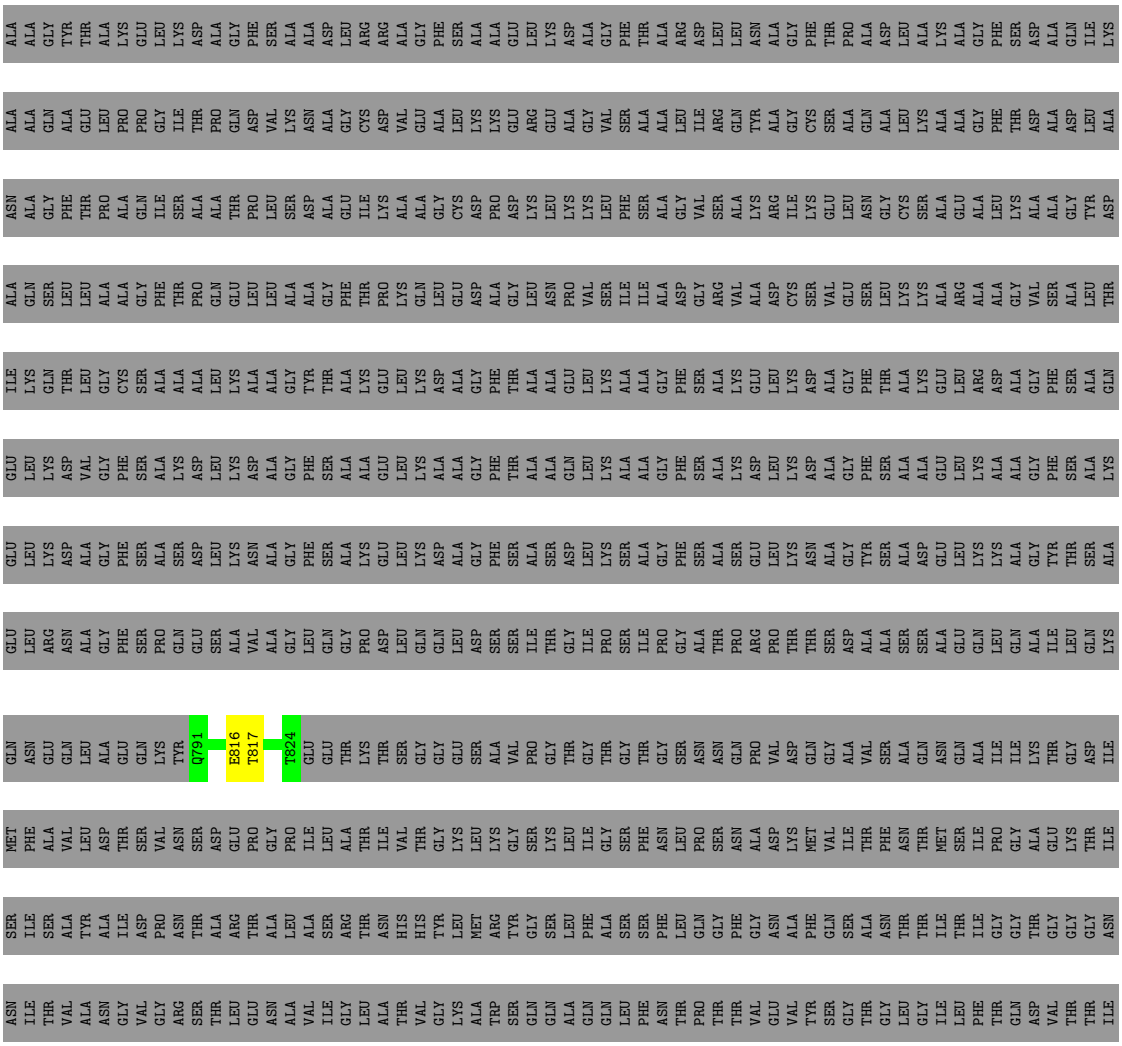




- Molecule 1: IcmE protein

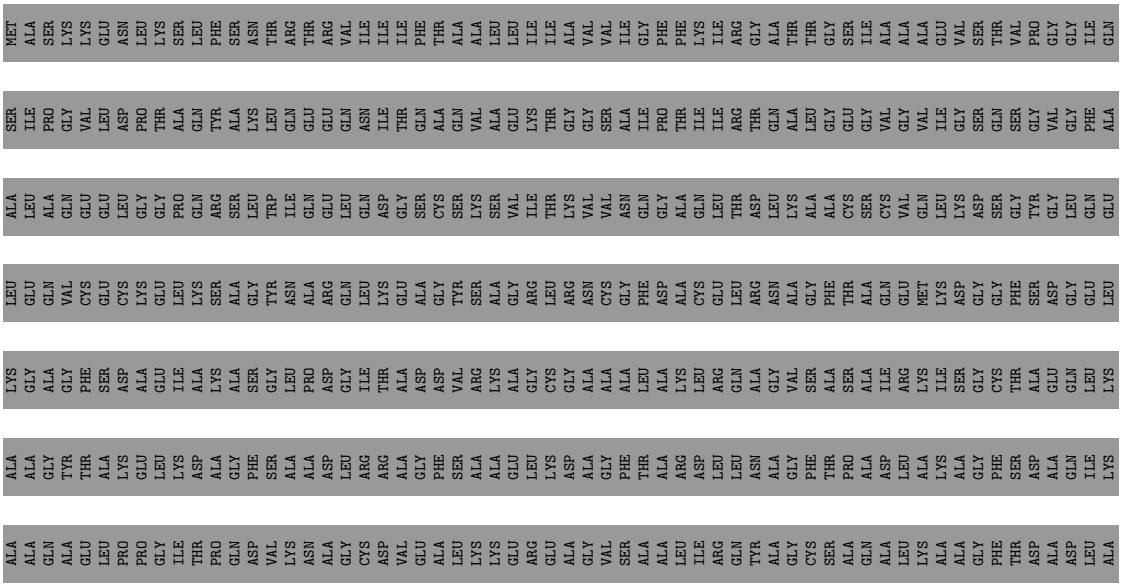
Chain YG: 97%

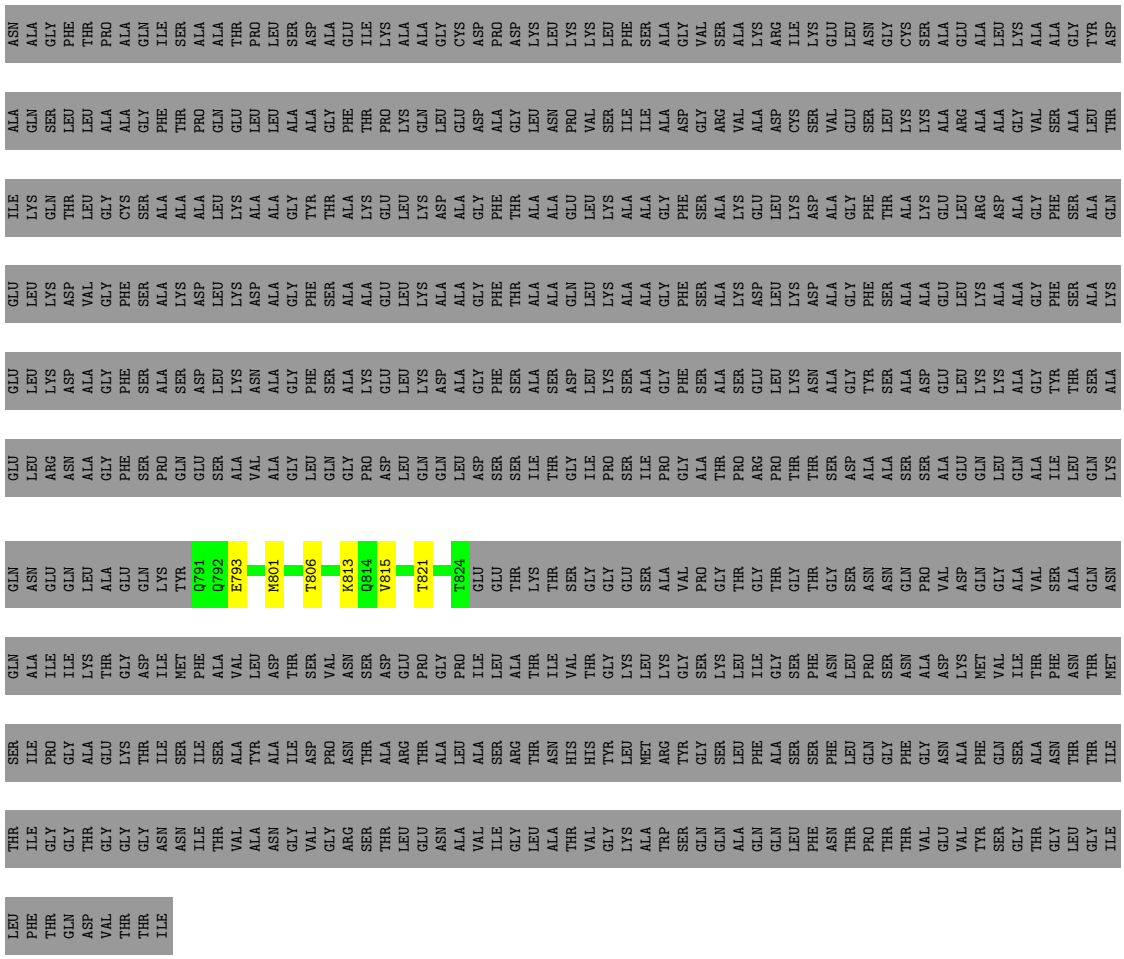




• Molecule 1: IcmE protein

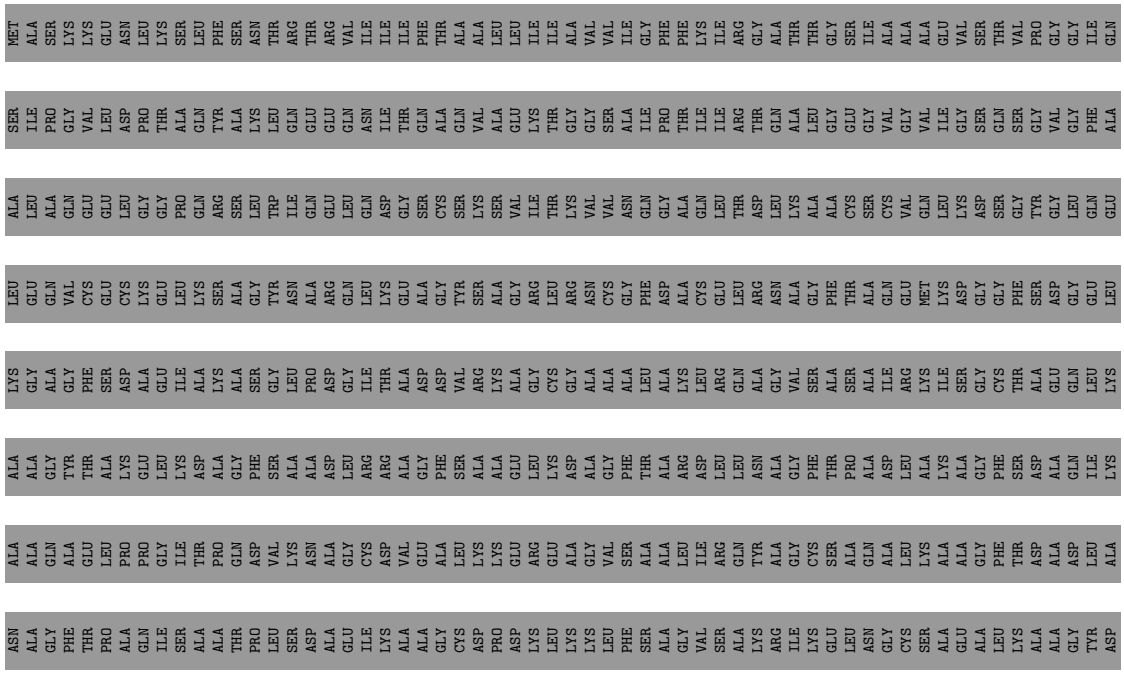
Chain ZG: 97%

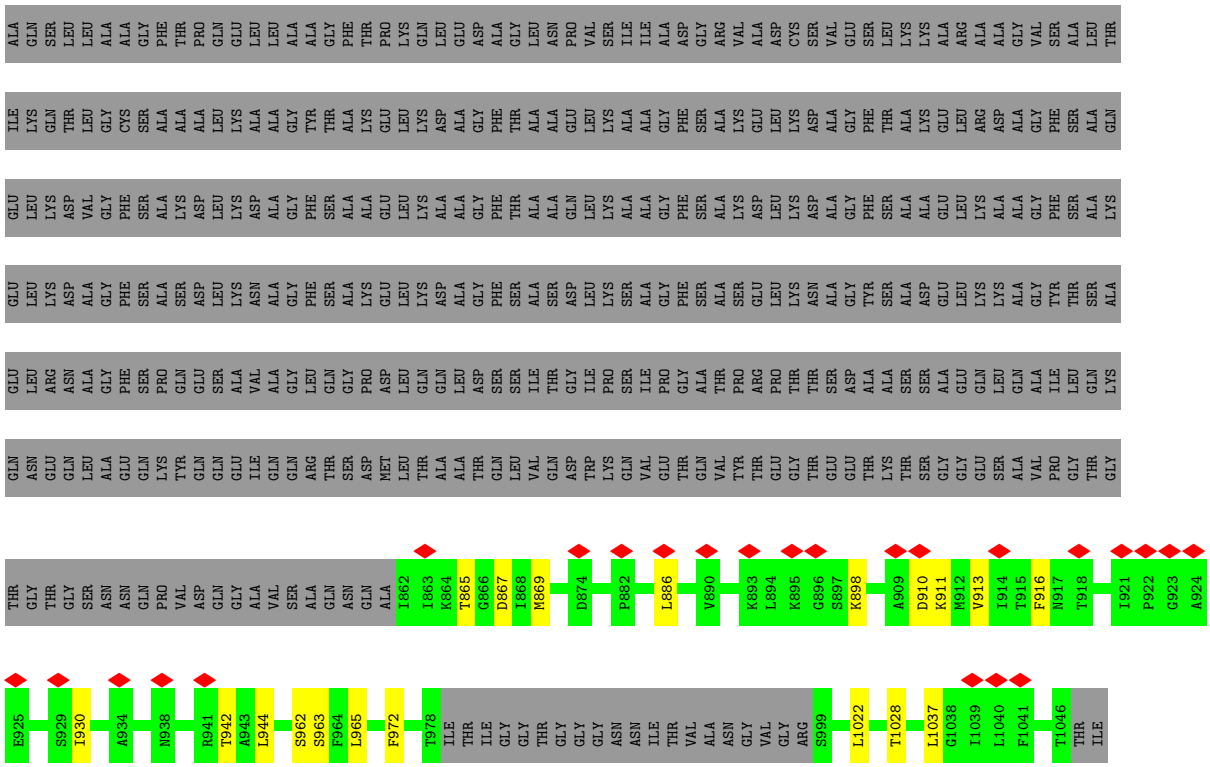




• Molecule 1: IcmE protein

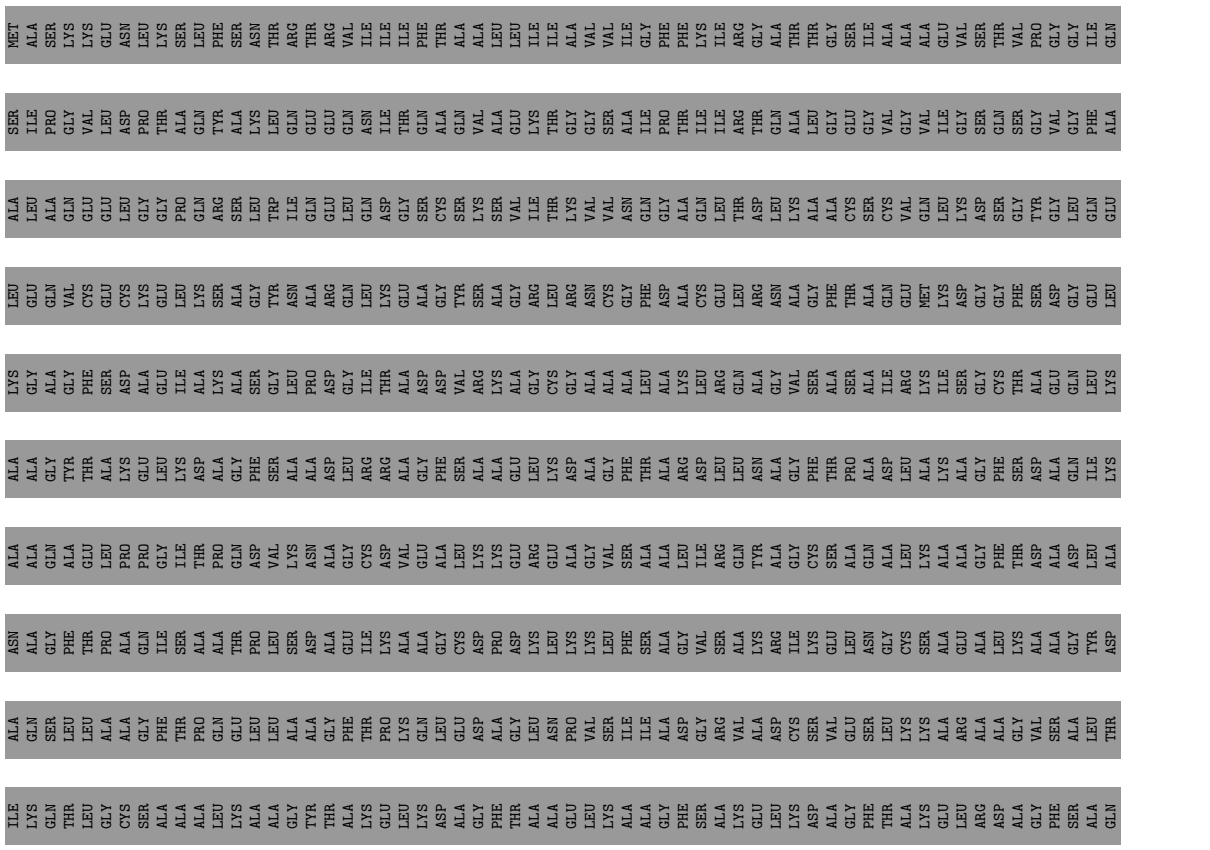
Chain FG:





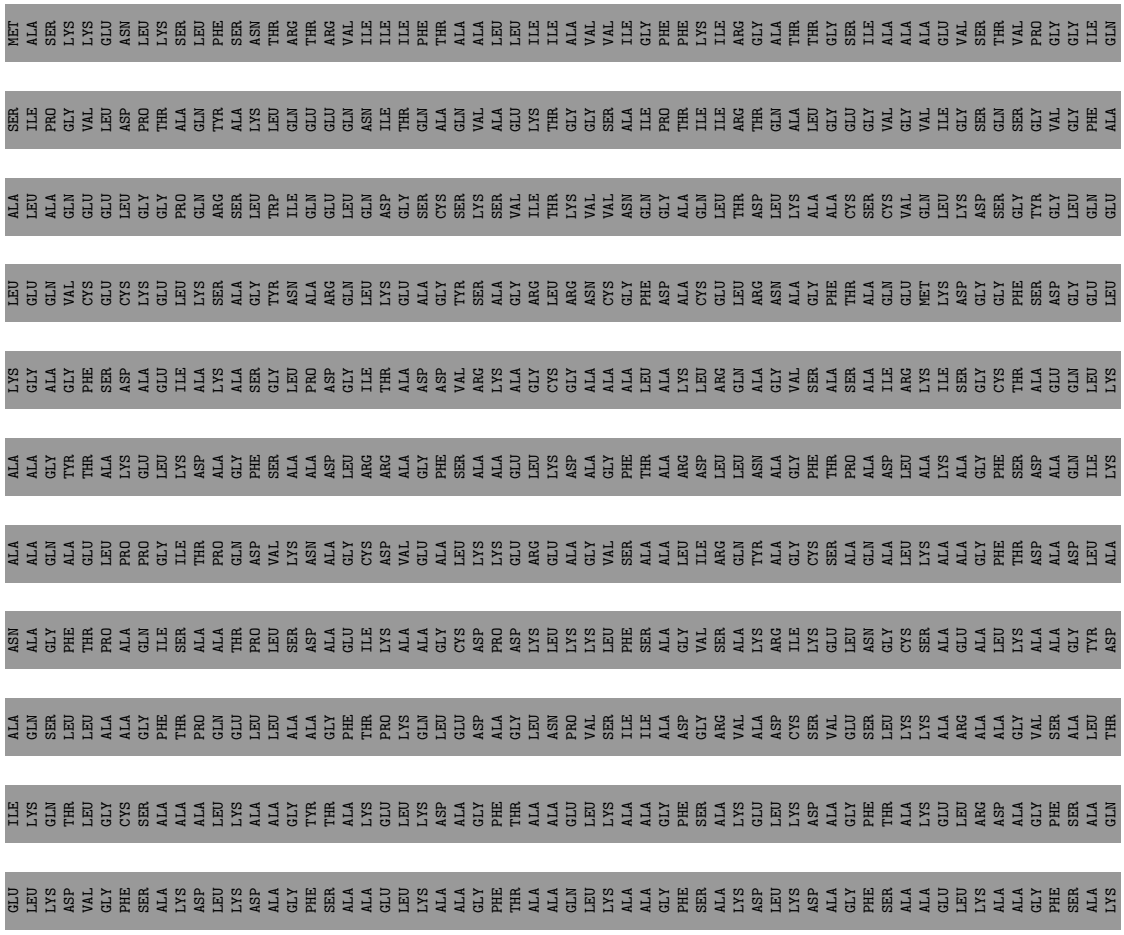
- Molecule 1: IcmE protein

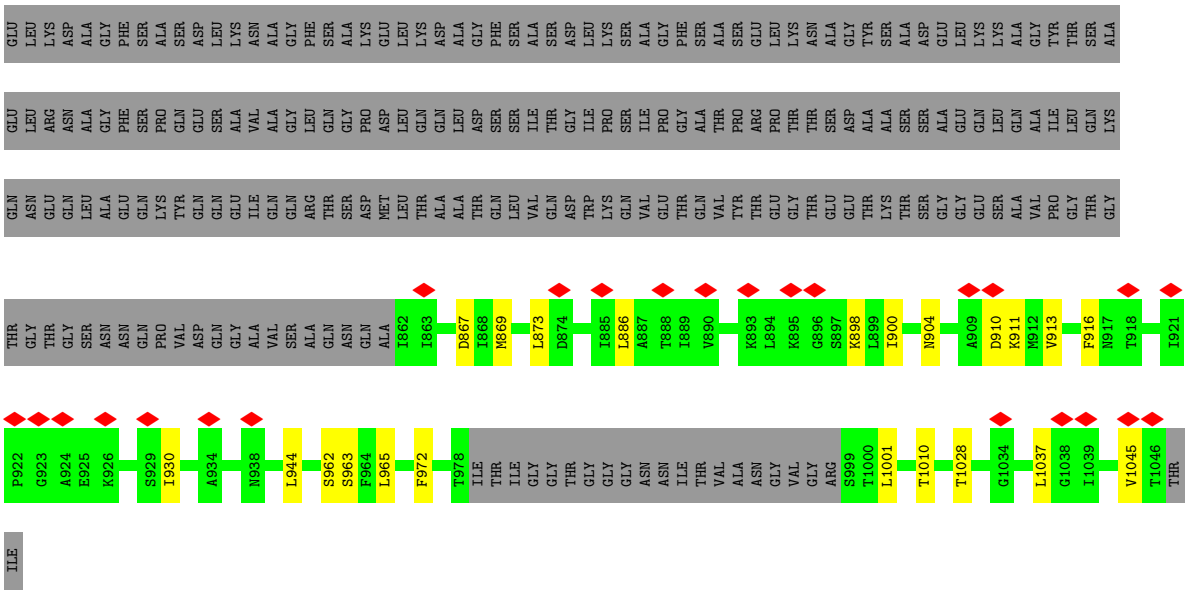
Chain Dg: 97%



- Molecule 1: IcmE protein

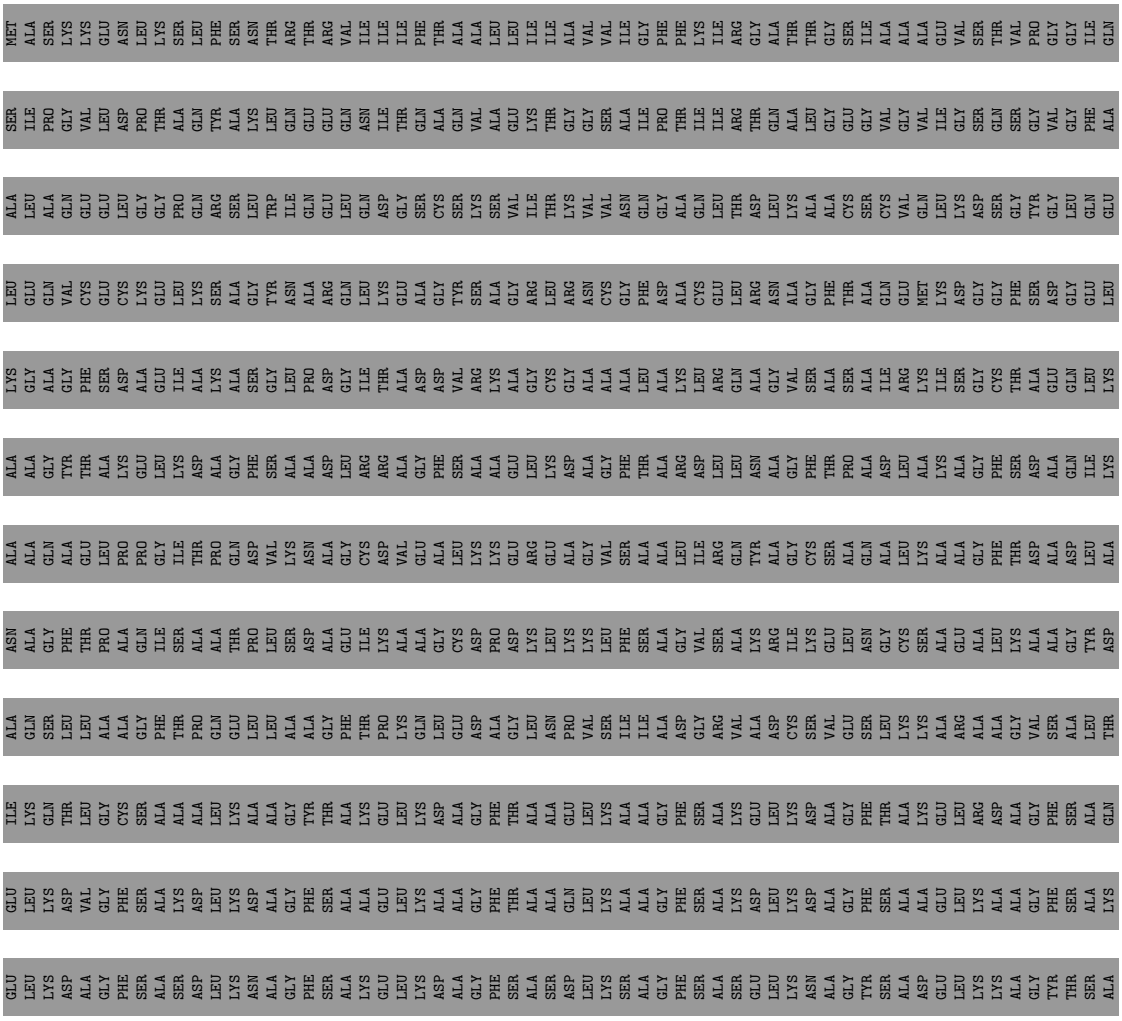
Chain GG:





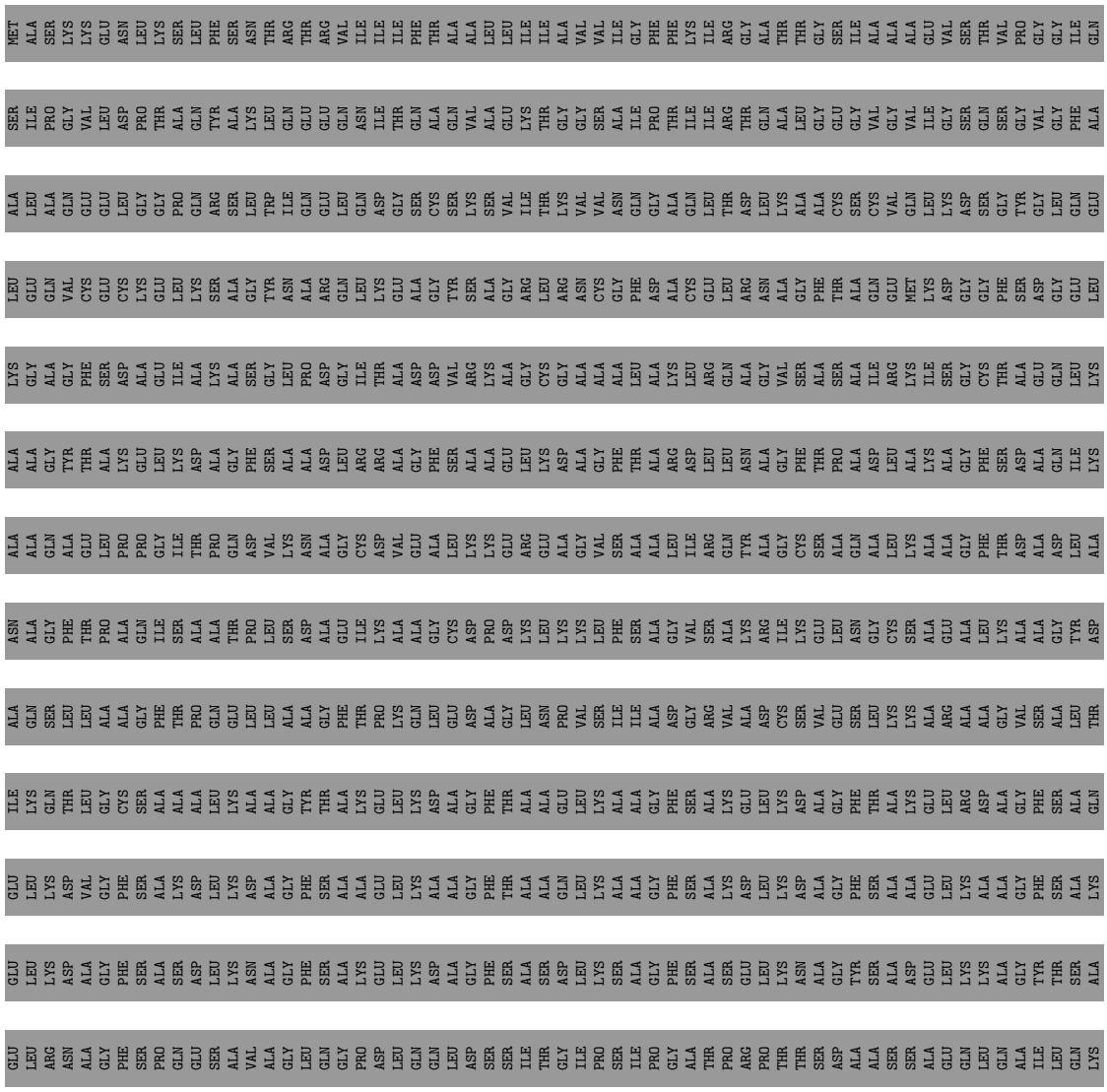
- Molecule 1: IcmE protein

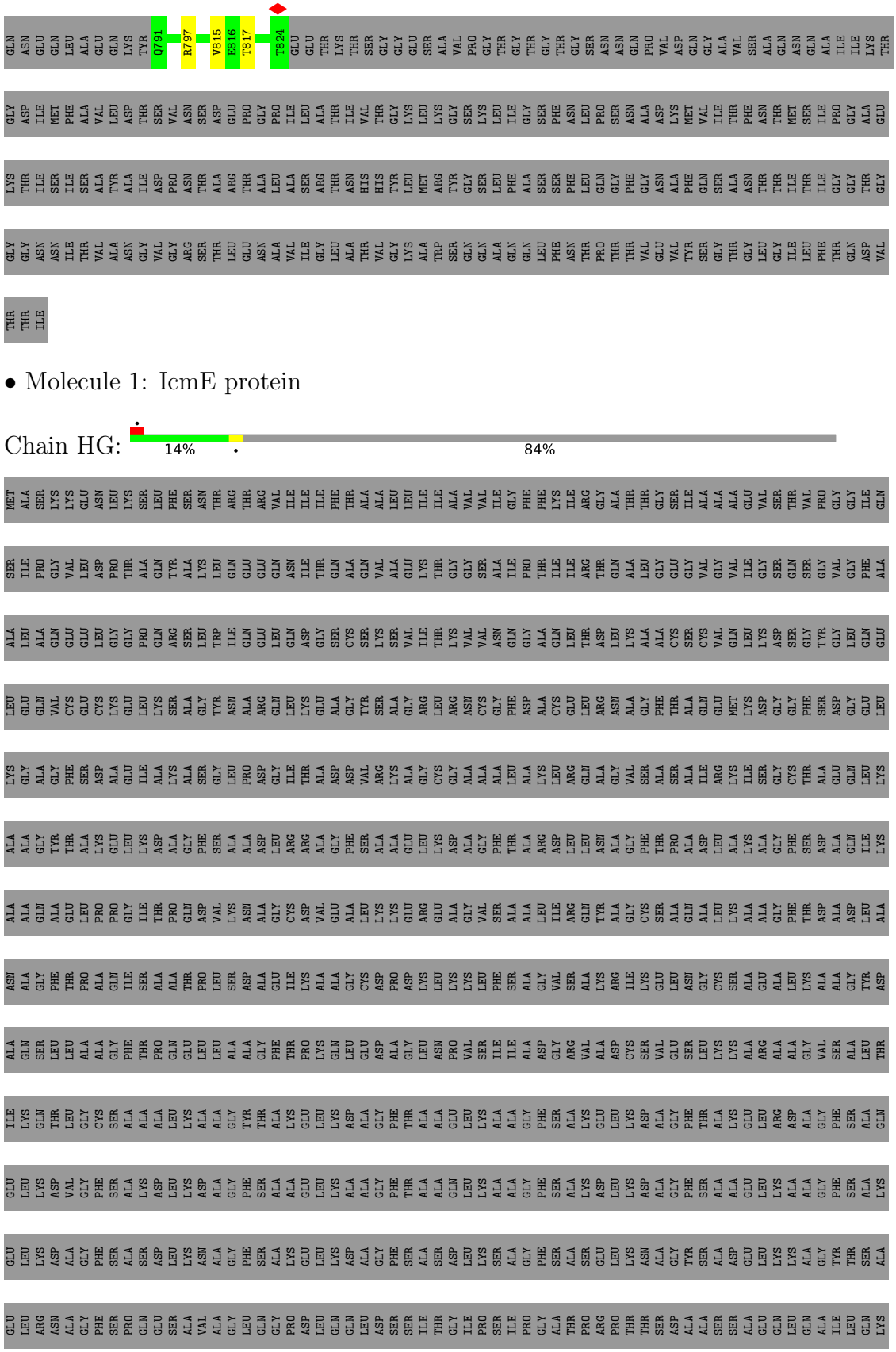
Chain Eg: 97%



- Molecule 1: IcmE protein

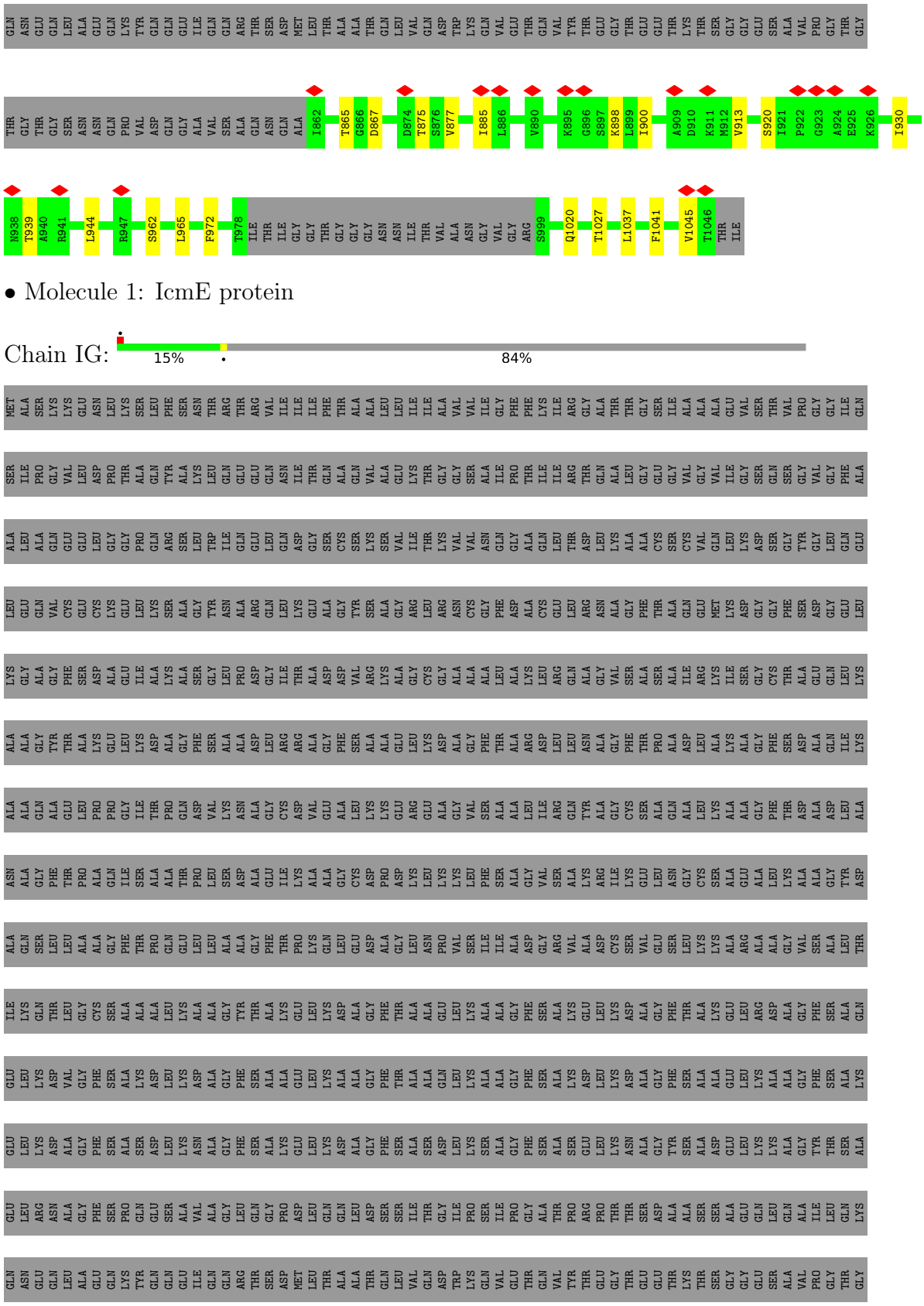
Chain Fg: 97%





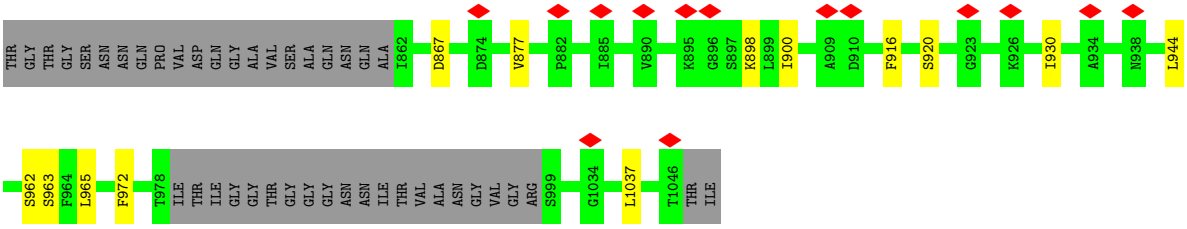
- Molecule 1: IcmE protein

Chain HG:



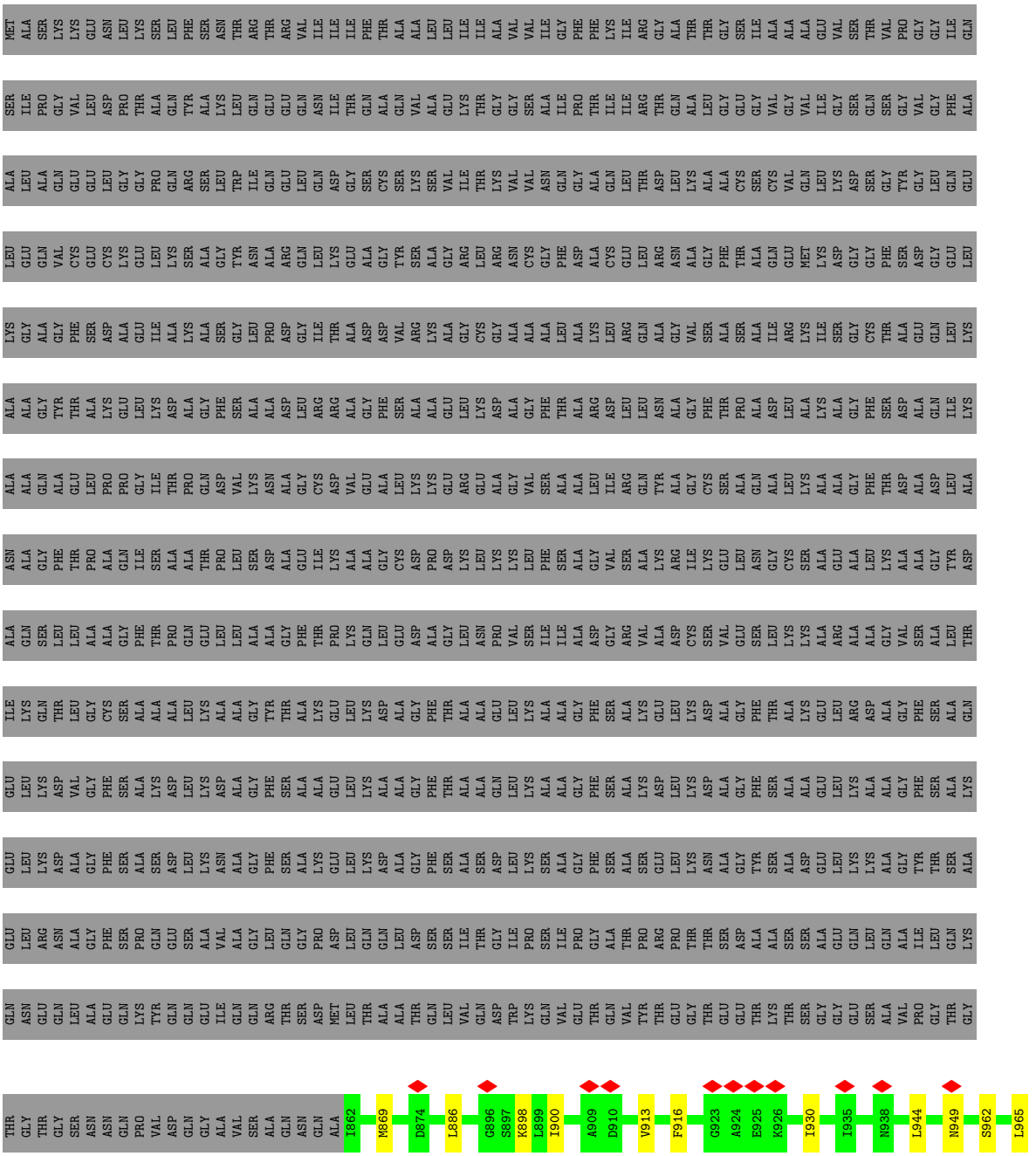
• Molecule 1: IcmE protein

Chain IG:



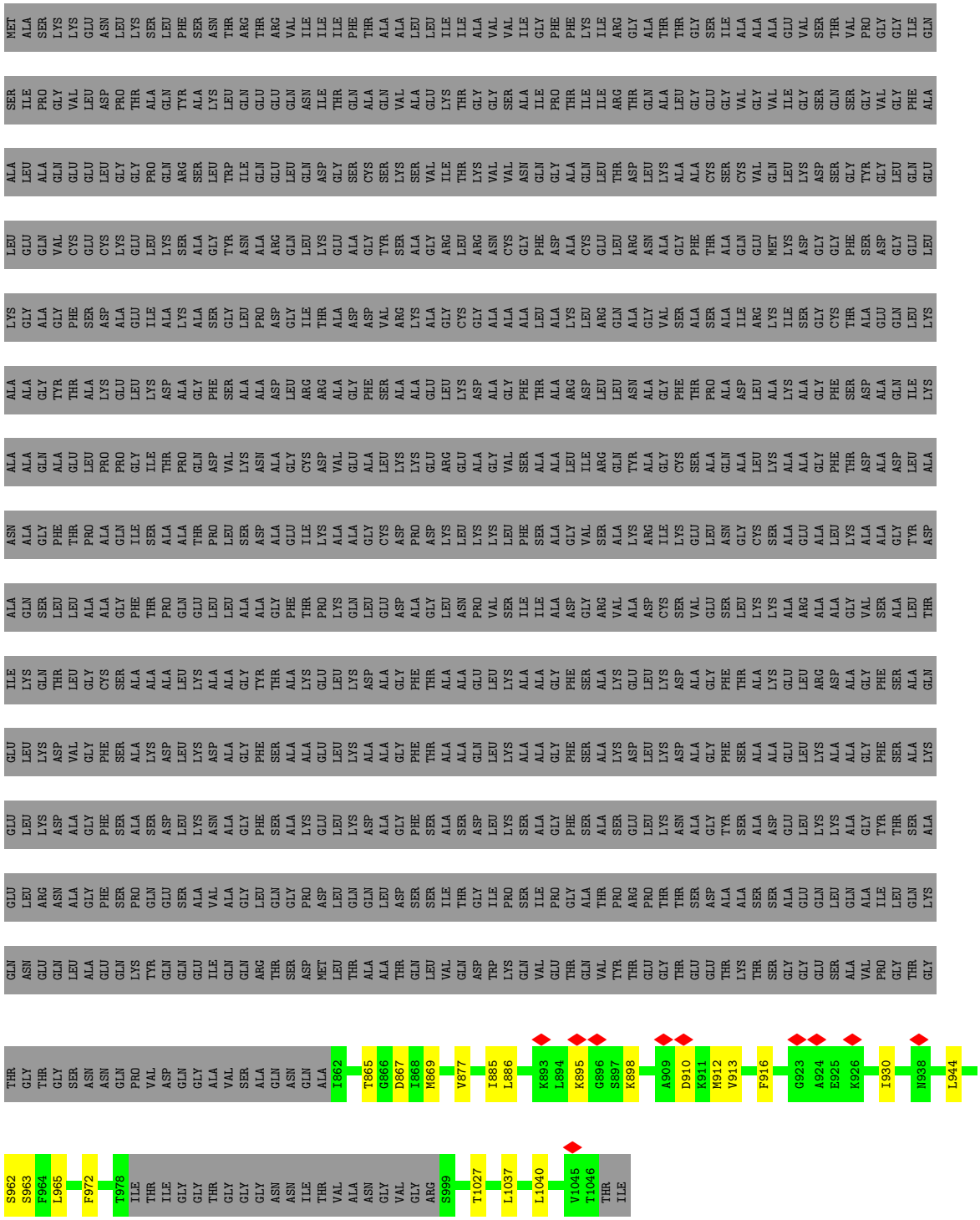
- Molecule 1: IcmE protein

Chain JG:



• Molecule 1: IcmE protein

Chain KG:



• Molecule 1: IcmE protein

Chain LG: 14% 84%

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

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

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

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

LYS GLY ALA GLY PHE SER ASP ALA GLU ILE ALA LYS ALA SER GLY LEU PRO ASP GLY ILE THR ALA ASP ASP VAL ARG LYS ALA GLY CYS GLY ALA ALA ALA ALA LYS LEU ARG GLN ALA GLY VAL SER ALA SER ALA ILE ARG LYS ILE SER GLY CYS THR ALA GLU GLN ILE LEU

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

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

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

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

ILE LYS GLN THR LEU GLY CYS SER ALA ALA LEU LYS ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA LYS GLU LEU LYS ALA GLU LEU ARG ASP ALA GLN

GLU LEU LYS ASP VAL GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA ALA GLU LEU LYS ALA ALA GLY PHE THR ALA ALA ALA GLN LEU LYS ALA ALA GLY PHE SER ALA LYS ASP LEU LEU LYS ASP ALA GLY PHE SER ALA ALA LYS

GLU LEU LYS ASP ALA GLY PHE SER ALA SER ASP LEU LYS ASN ALA GLY PHE SER ALA SER ASP LEU LYS ASP ALA GLY PHE SER ALA SER GLU LEU LYS ASN ALA GLY TYR SER ALA ASP GLU LEU LYS ALA ALA GLY TYR THR SER ALA

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

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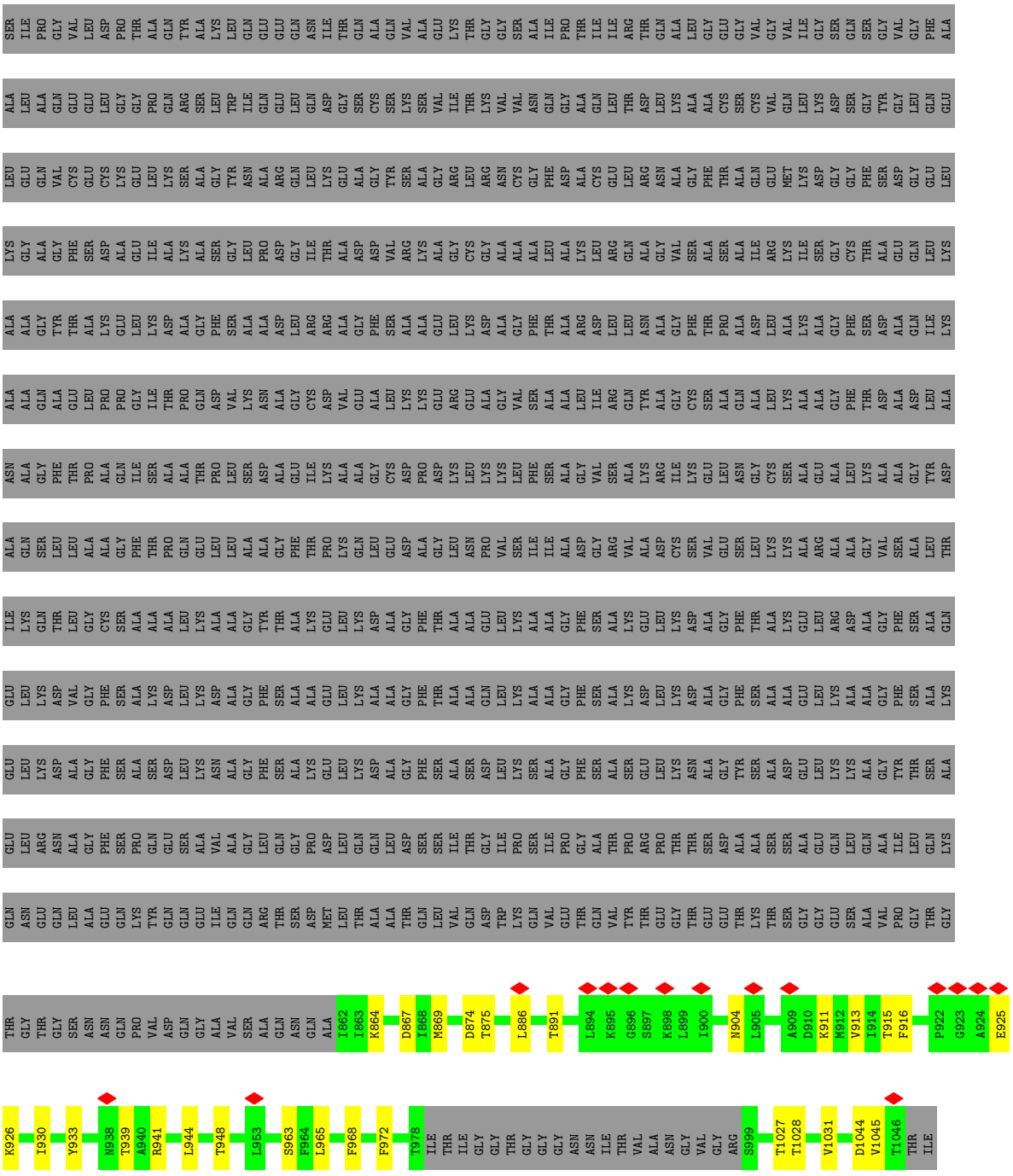
THR GLY THR GLY SER ASN ASN GLN PRO VAL ASP GLN GLY ALA VAL SER ALA GLN ASN GLN ALA I862 T865 K895 K898 A909 D910 K911 M912 V913 S920 G923 I930 I935 N938 T939 L944 R947 T948 N949 L965 F972 T978 ILE THR ILE

GLY GLY THR GLY GLY GLY ASN ASN ILE THR VAL ALA ASN GLY VAL GLY ARG S999 Q1020 Y1032 L1037 L1040 V1045 T1046 THR ILE

- Molecule 1: IcmE protein

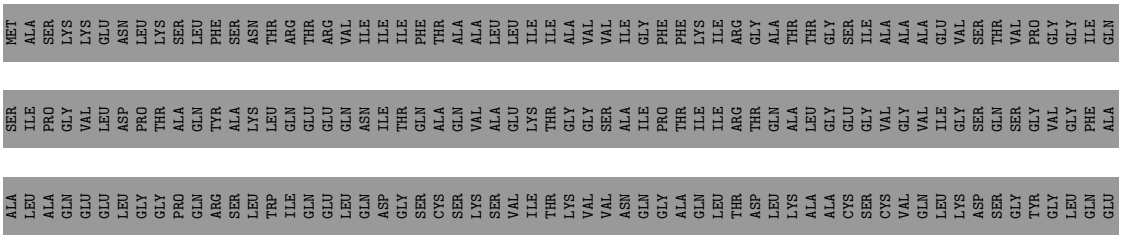
Chain MG: 13% 84%

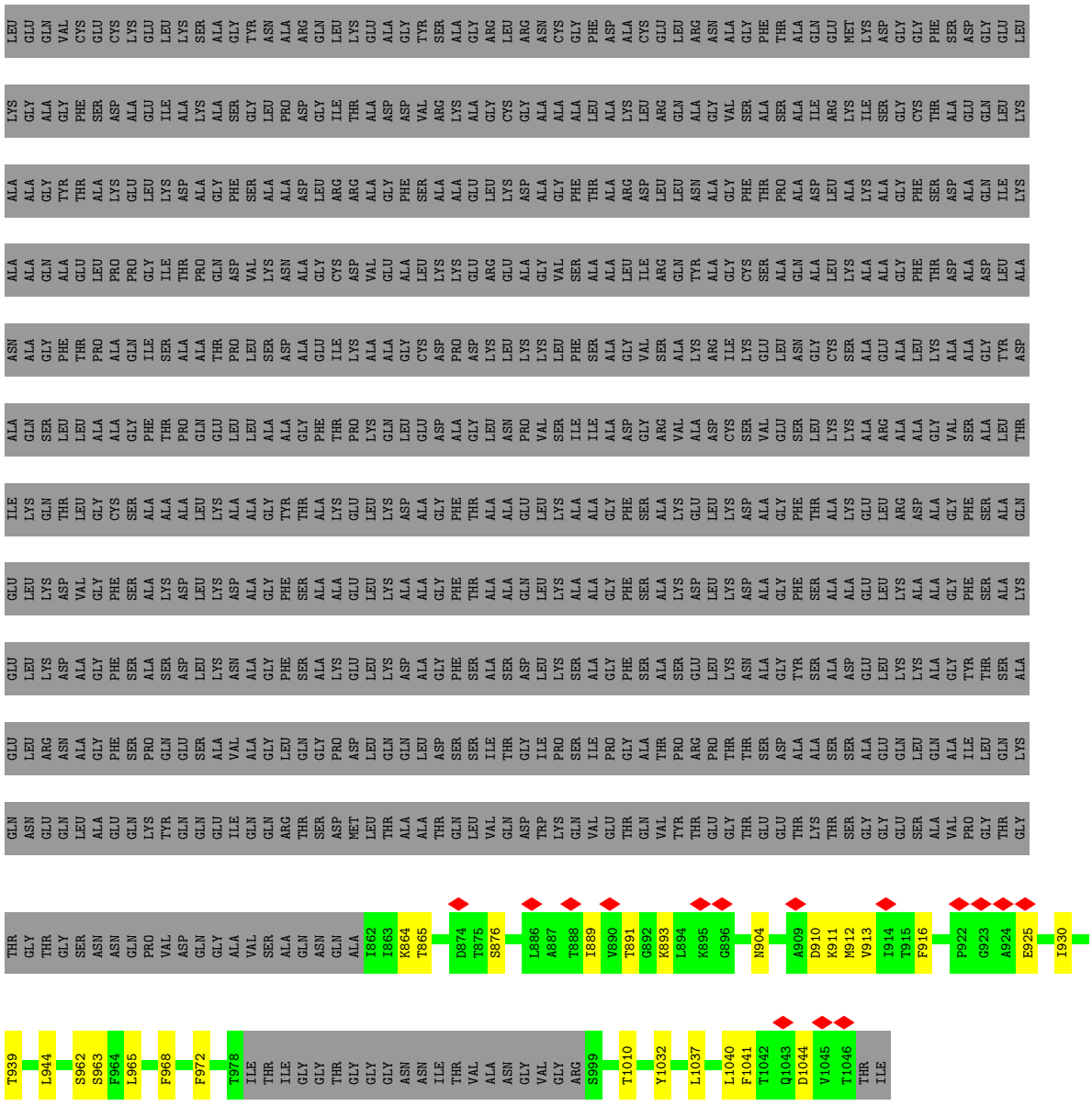
MET ALA SER LYS LYS GLU ASN LEU LYS SER LEU PHE SER ASN THR ARG THR ARG VAL ILE ILE ILE PHE THR ALA ALA LEU LEU ILE ILE ALA VAL VAL ILE GLY PHE PHE LYS ILE ARG GLY ALA THR THR GLY SER ILE ALA ALA ALA GLU VAL SER THR VAL PRO GLY GLY ILE GLN



- Molecule 1: IcmE protein

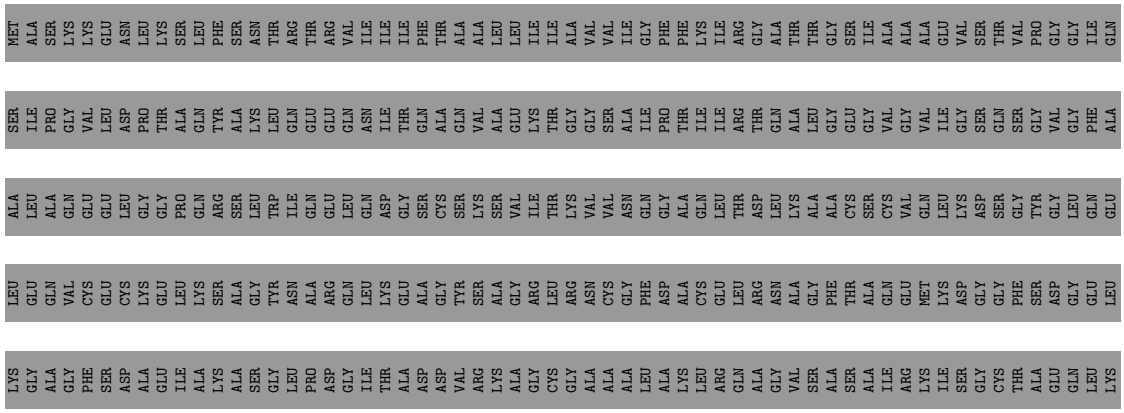
Chain NG:

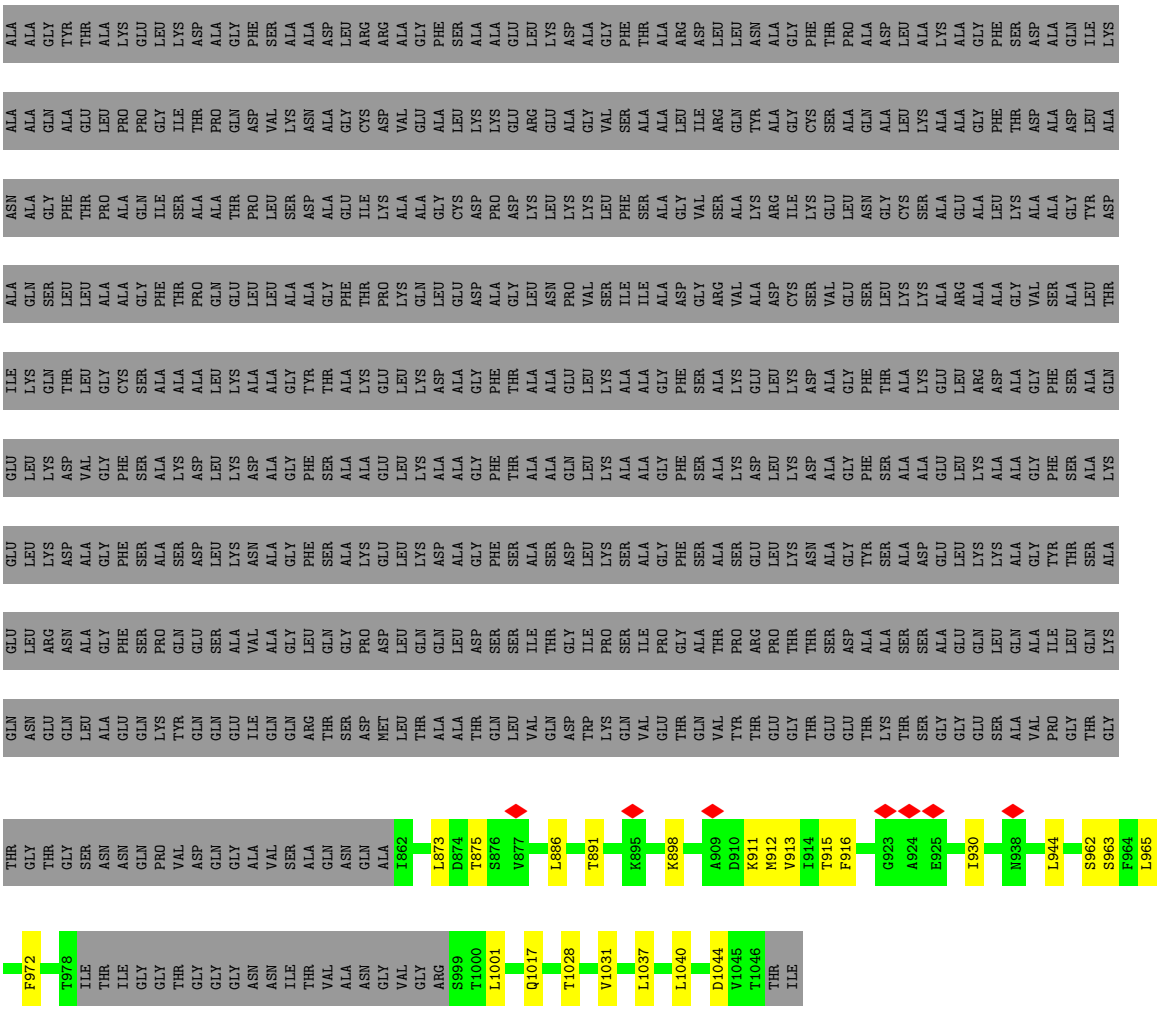


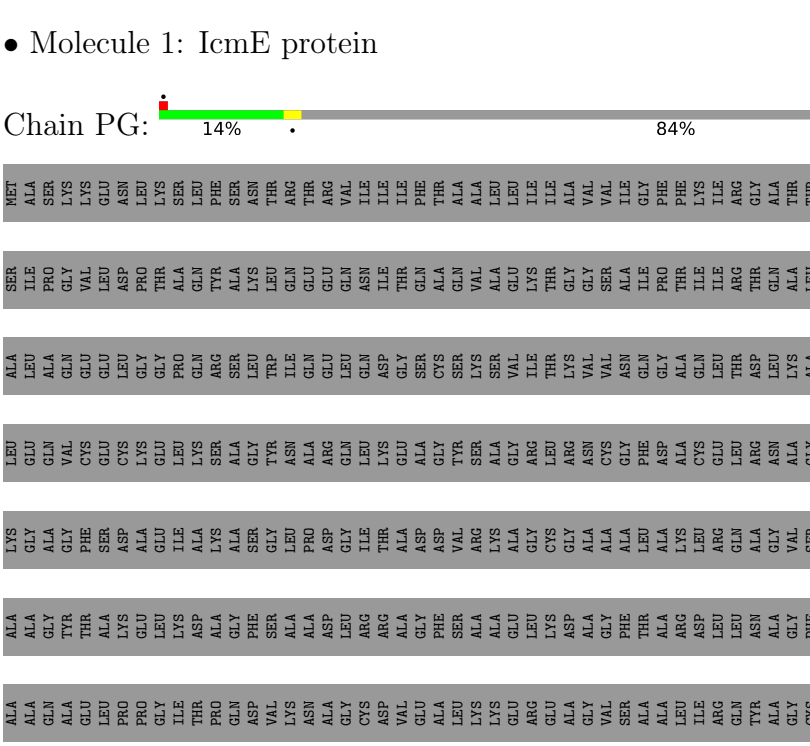


- Molecule 1: IcmE protein

Chain OG:

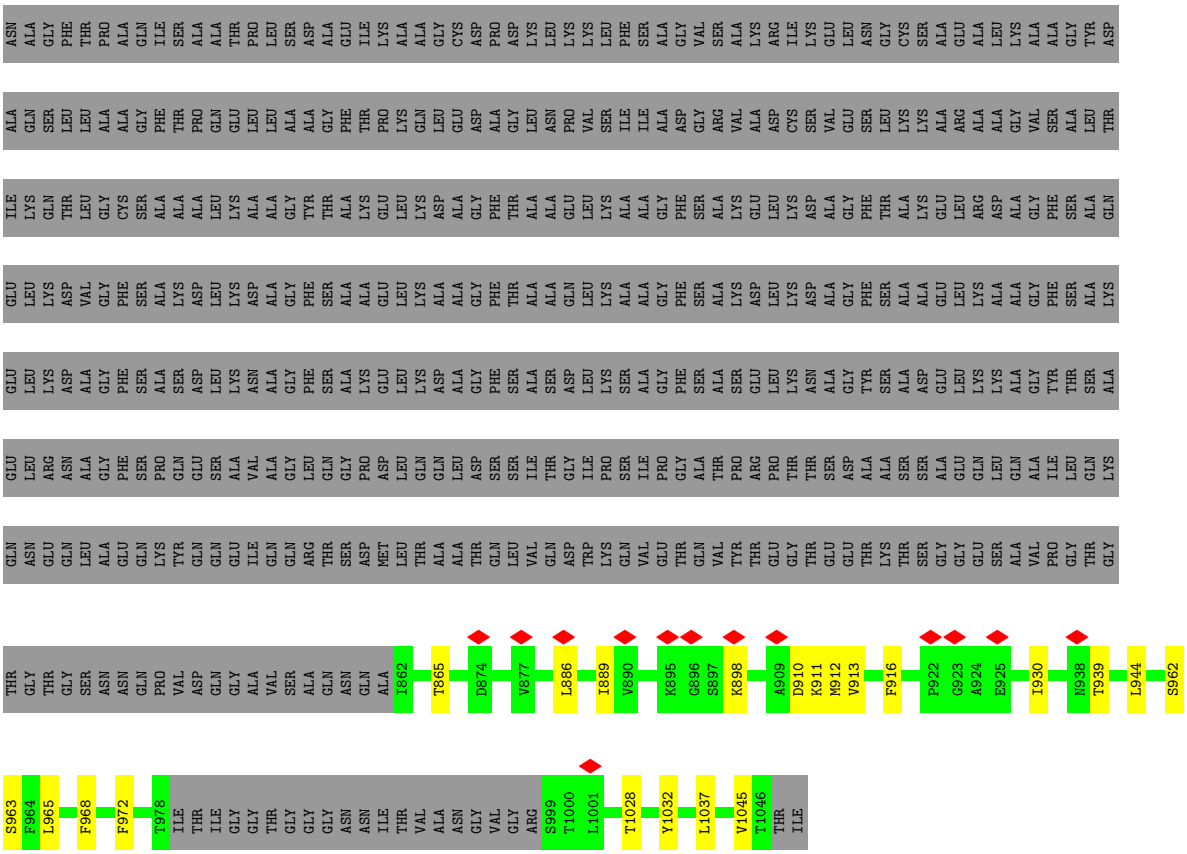






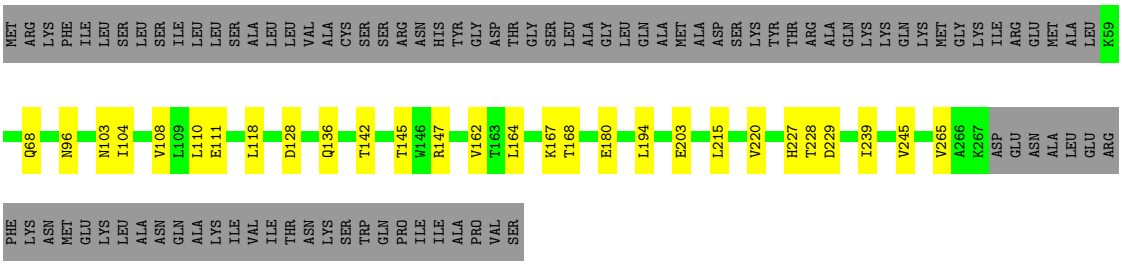
- Molecule 1: IcmE protein

Chain PG:



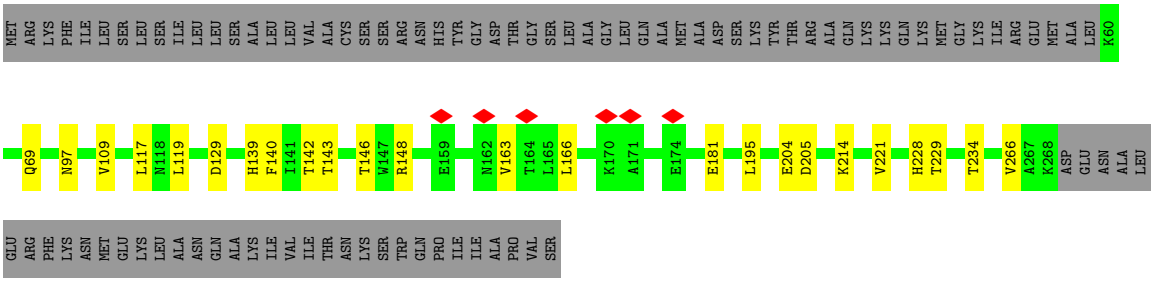
• Molecule 2: DotC

Chain BC:



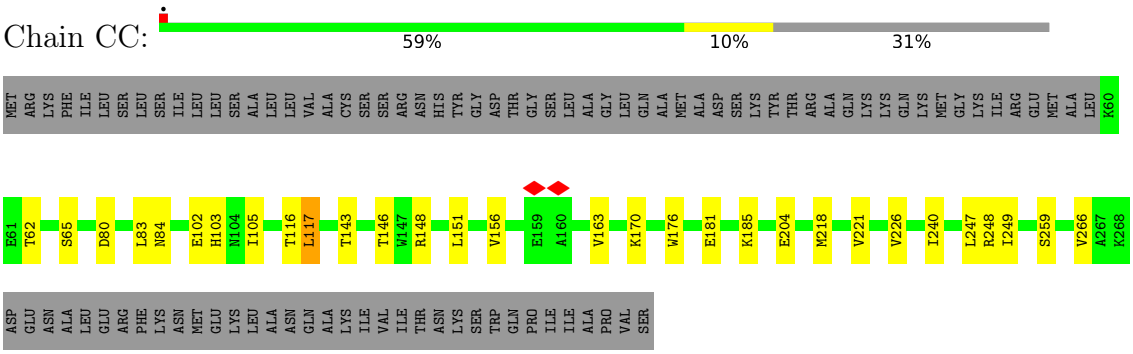
• Molecule 2: DotC

Chain EC:



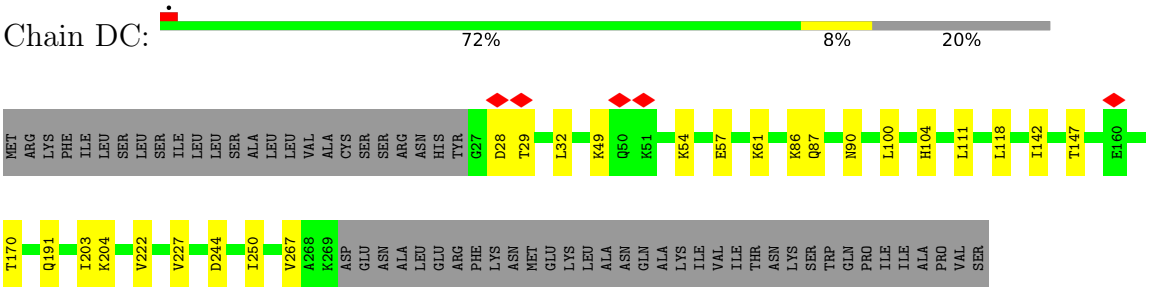
• Molecule 2: DotC

Chain CC:



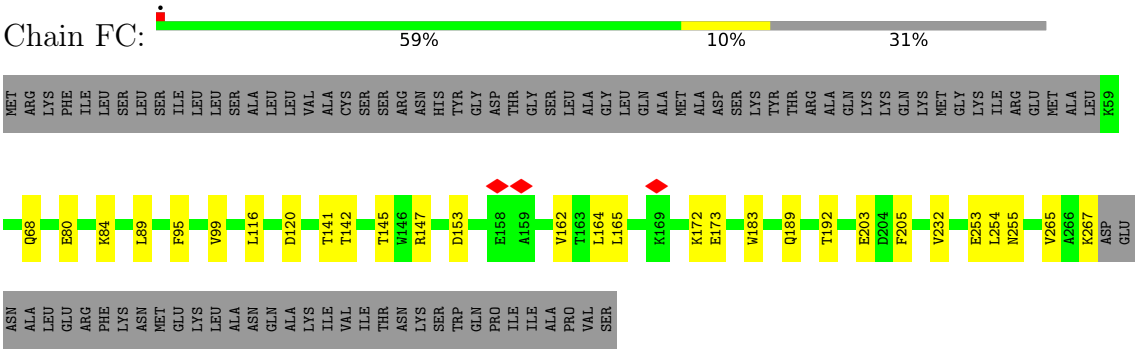
- Molecule 2: DotC

Chain DC:



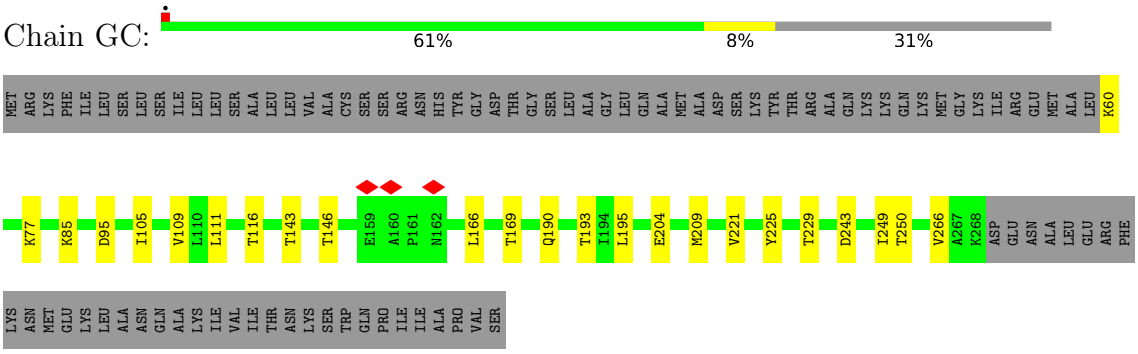
- Molecule 2: DotC

Chain FC:



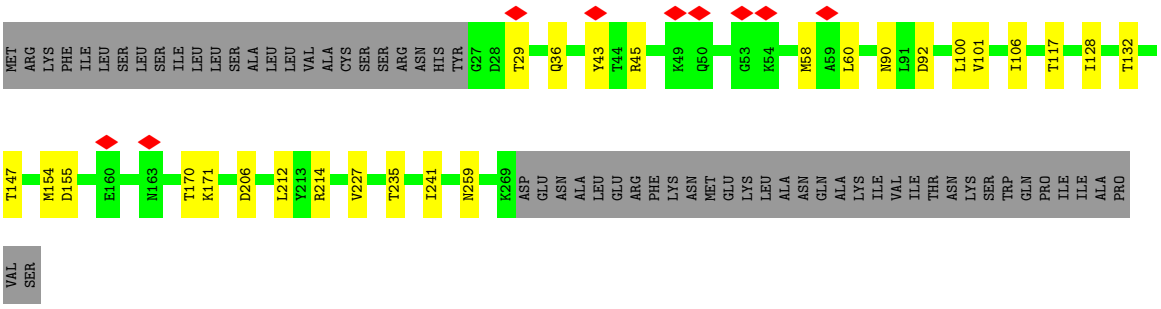
- Molecule 2: DotC

Chain GC:



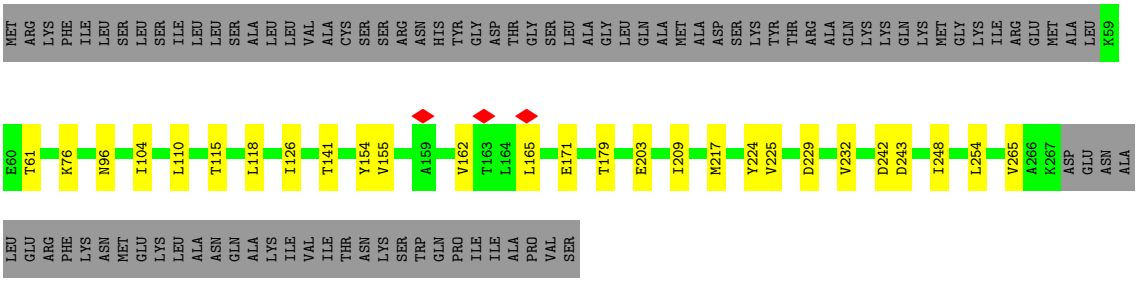
- Molecule 2: DotC

Chain IC:



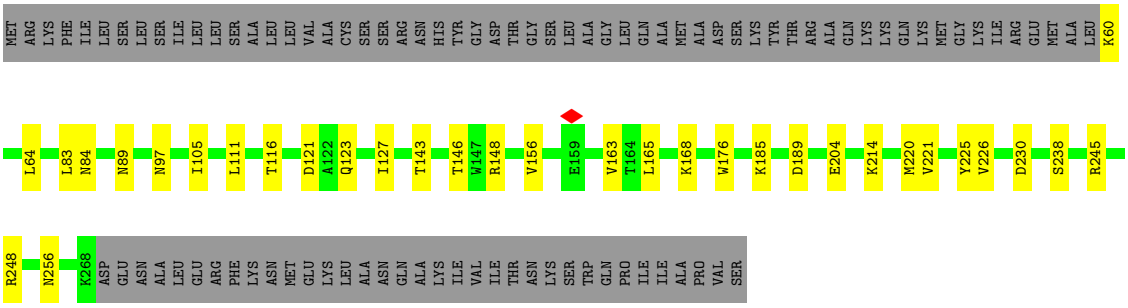
- Molecule 2: DotC

Chain JC:



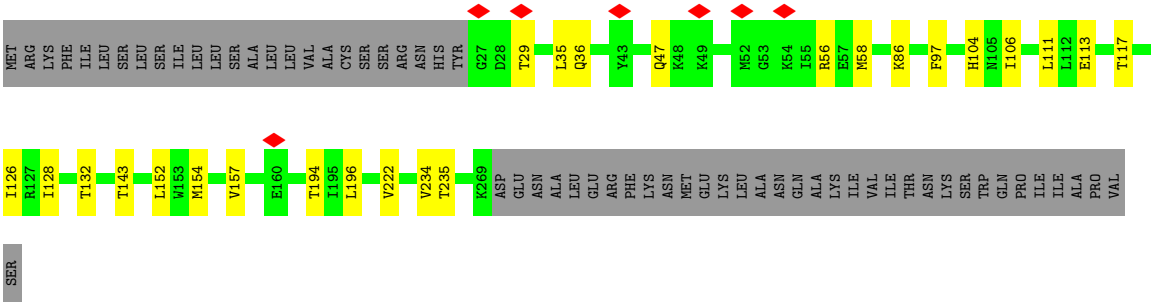
- Molecule 2: DotC

Chain KC:



- Molecule 2: DotC

Chain MC:



- Molecule 2: DotC

Chain HC: 73% 8% 20%

MET ARG LYS PHE ILE LEU SER LEU SER ILE LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR G27 D28 T29 D40 Y43 Q47 K48 K49 Q50 K51 M52 E57 L84 H104 T143 T144 L152 D155 E160 K169 T170 K171 D190

D206 K215 V222 V227 D231 T235 D244 E255 L256 K269 ASP GLU ASN ALA LEU GLU ARG PHE LYS ASN MET GLU LYS LEU ALA ASN GLN ALA LYS ILE VAL ILE THR ASN LYS SER TRP GLN PRO ILE ILE ALA PRO VAL SER

- Molecule 2: DotC

Chain LC: 75% 6% 20%

MET ARG LYS PHE ILE LEU SER LEU SER ILE LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR G27 D28 T29 G30 Q36 A37 M38 A39 D40 S41 K48 K49 M52 G53 R56 L84 V101 H104 F141 T147 E160 N163 V164

K171 T181 D206 K215 V227 D244 L256 K269 ASP GLU ASN ALA LEU GLU ARG PHE LYS ASN MET GLU LYS LEU ALA ASN GLN ALA LYS ILE VAL ILE THR ASN LYS SER TRP GLN PRO ILE ILE ALA PRO VAL SER

- Molecule 2: DotC

Chain AC: 60% 9% 31%

MET ARG LYS PHE ILE LEU SER LEU SER ILE LEU LEU SER ALA LEU LEU VAL ALA CYS SER SER ARG ASN HIS TYR GLY ASP THR GLY SER LEU ALA GLY LEU GLN ALA MET ALA ASP SER LYS TYR THR ARG ALA GLN LYS LYS GLN LYS MET GLY LYS ILE ARG GLU MET ALA LEU K59

D79 N96 E101 H102 N103 V108 E111 T115 L118 I124 R125 I126 F139 T142 T145 W146 R147 D153 E158 V162 T163 L164 A170 E180 R181 E203 D204 F205 K213 L214 L215 V220 H227 D242 D243 V265 A266 K267

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

- Molecule 3: DotF

Chain AF: 19% 5% 77%

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

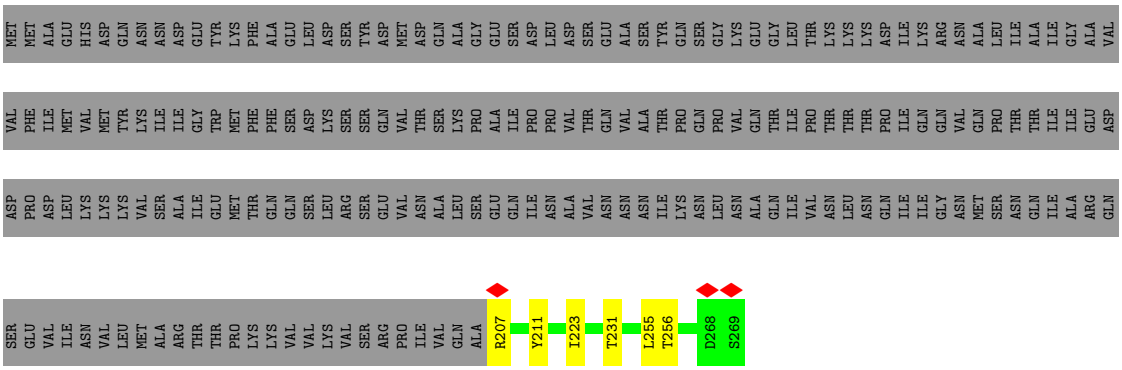
VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

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

SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I208 I209 V215 G227 S228 T229 L230 T231 I238 L250 R253 T256 S257 S258 K263 E267 D268 S269

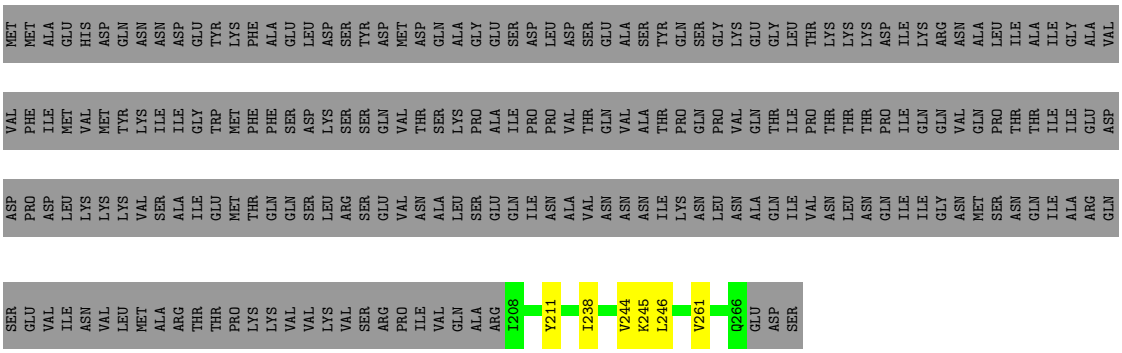
- Molecule 3: DotF

Chain GF: 21% 77%



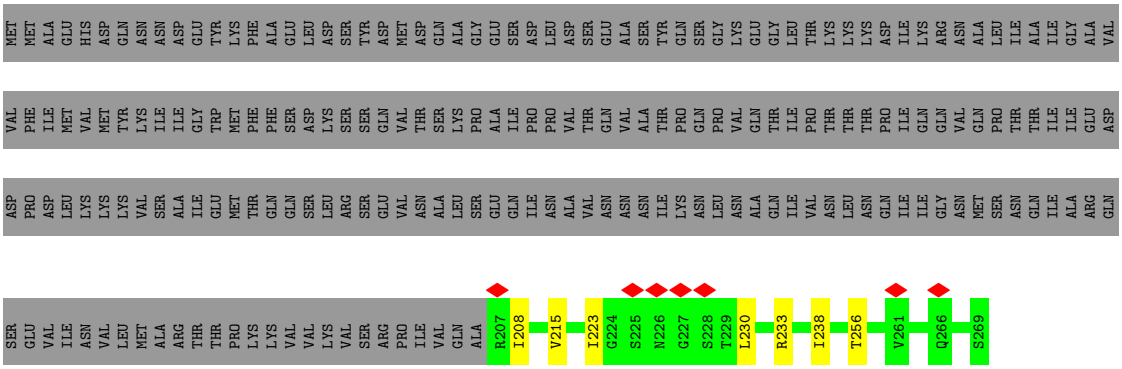
- Molecule 3: DotF

Chain Gf:



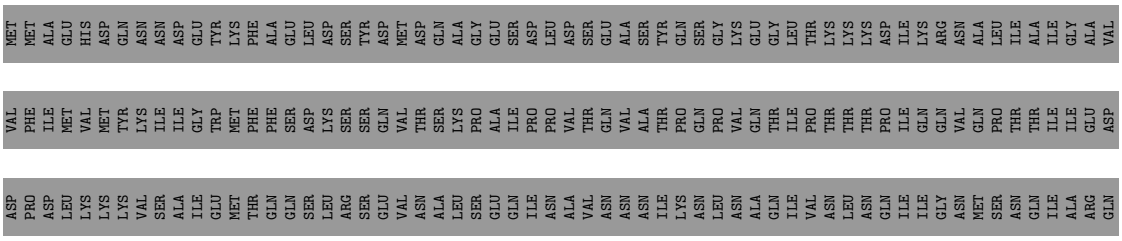
- Molecule 3: DotF

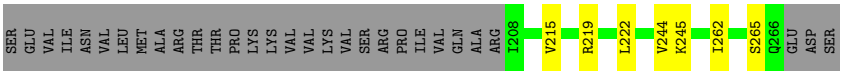
Chain HF:



- Molecule 3: DotF

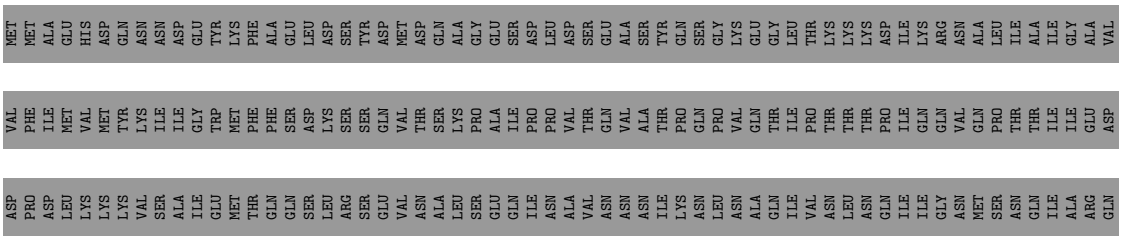
Chain Hf:

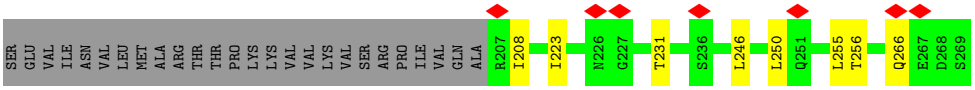




• Molecule 3: DotF

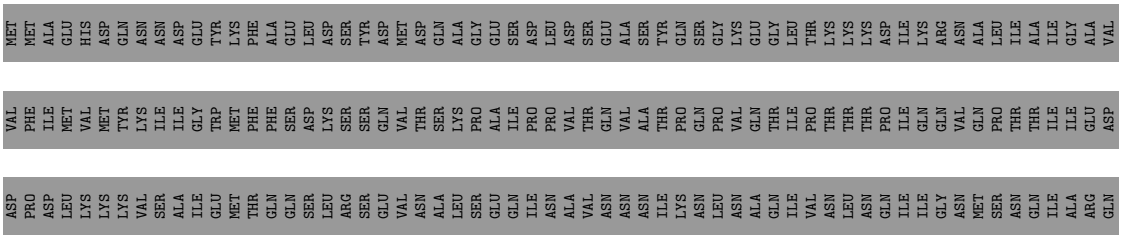
Chain IF:





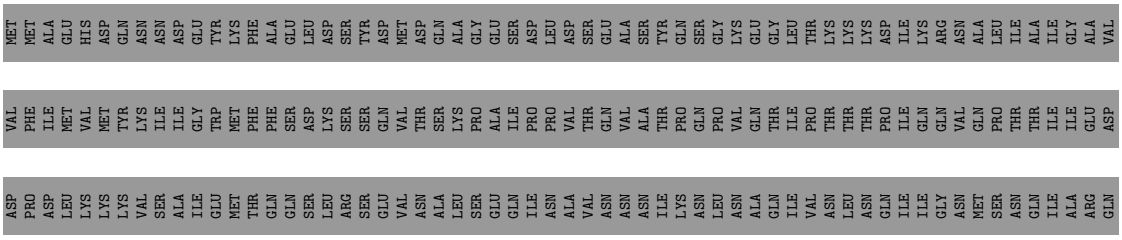
• Molecule 3: DotF

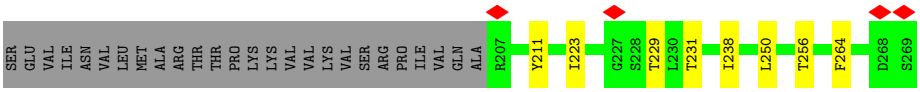
Chain If:



• Molecule 3: DotF

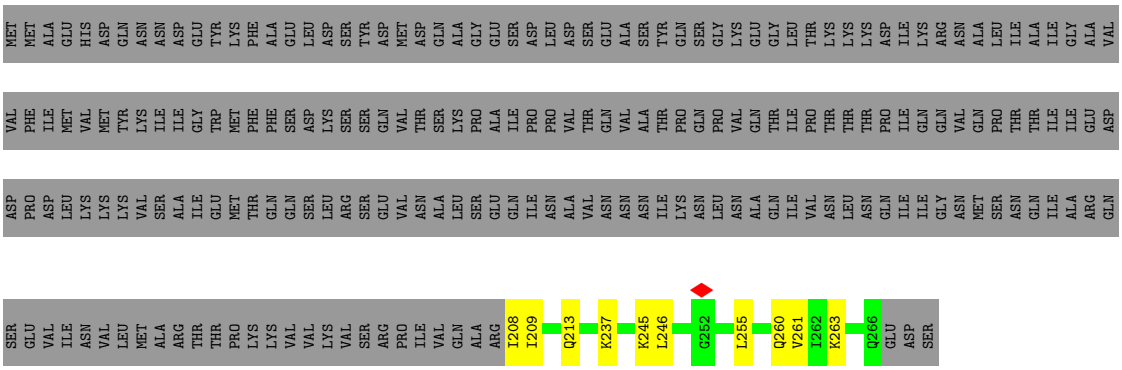
Chain JF:





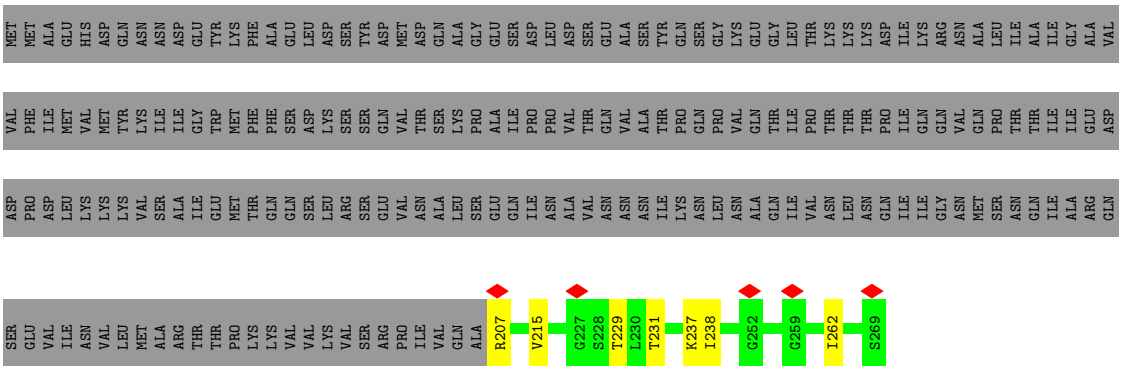
• Molecule 3: DotF

Chain Jf:



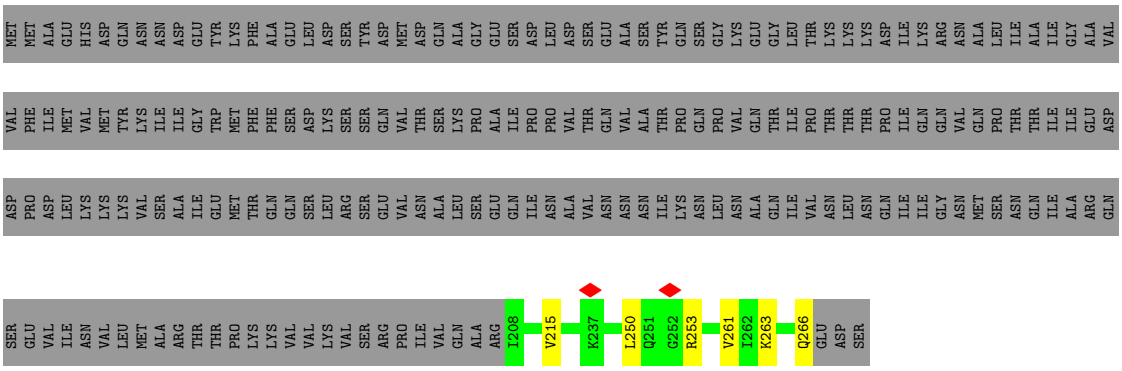
- Molecule 3: DotF

Chain KF:



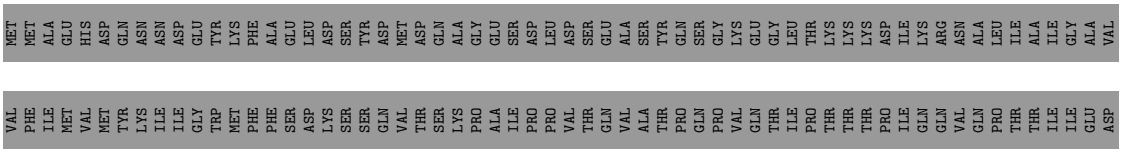
- Molecule 3: DotF

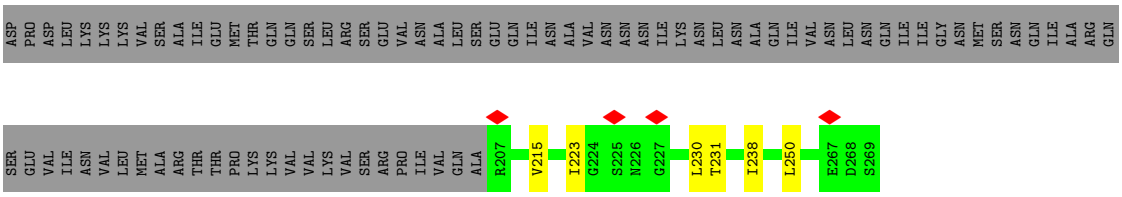
Chain Kf:



- Molecule 3: DotF

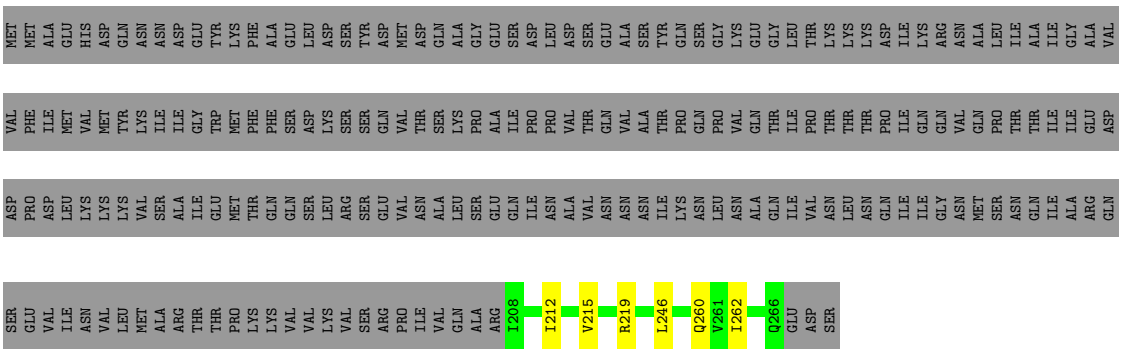
Chain LF:





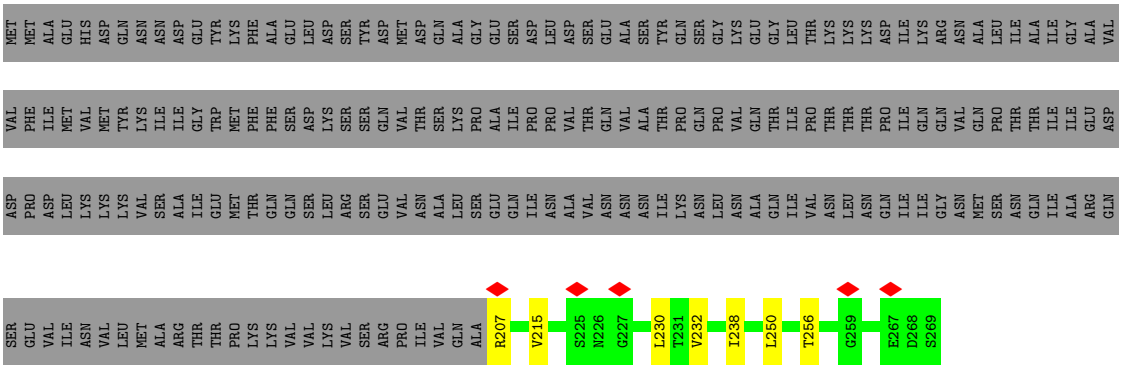
• Molecule 3: DotF

Chain Lf:



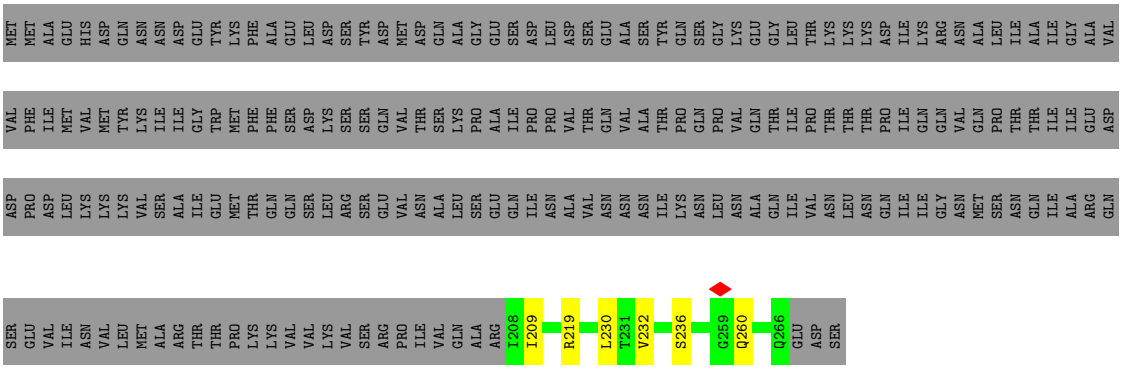
• Molecule 3: DotF

Chain MF:



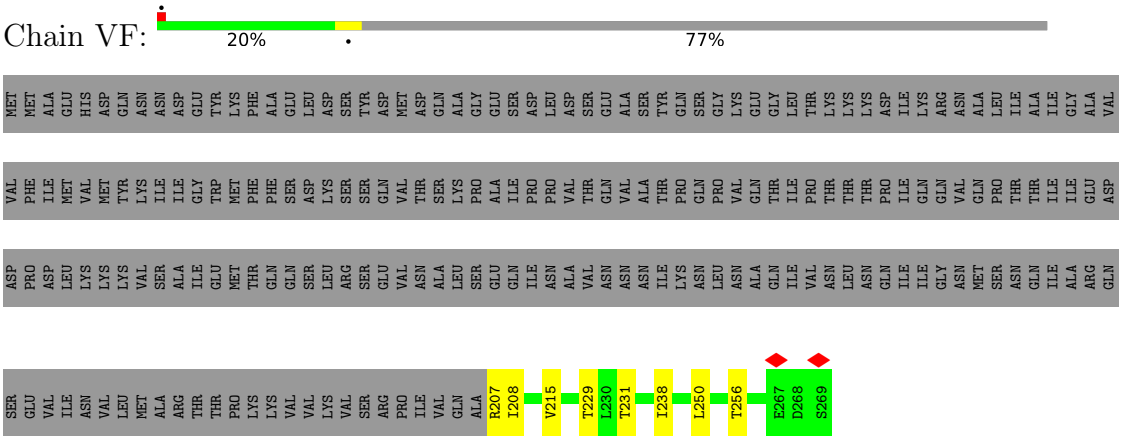
• Molecule 3: DotF

Chain Mf:



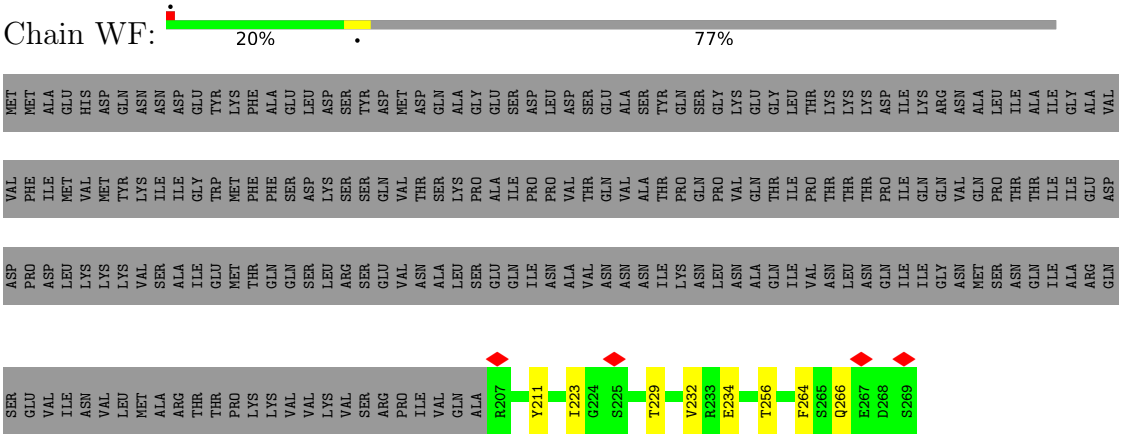
- Molecule 3: DotF

Chain VF:



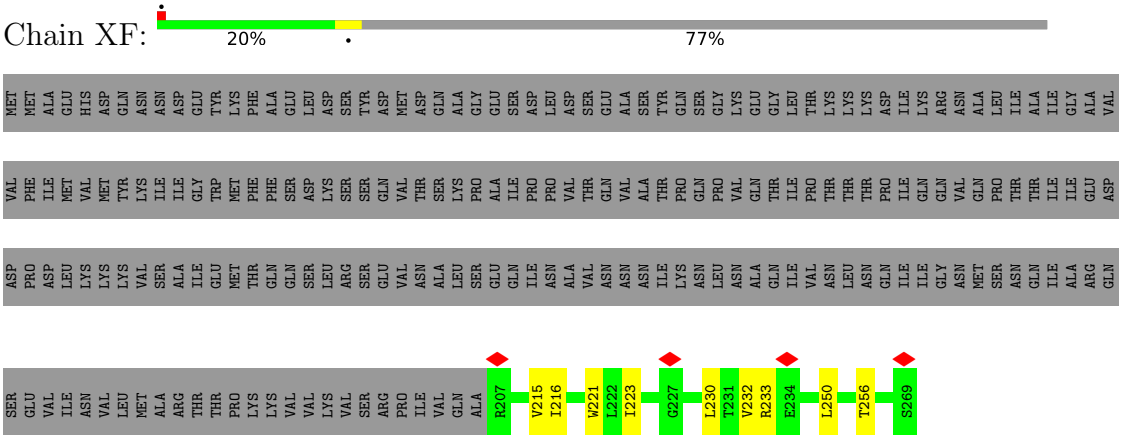
- Molecule 3: DotF

Chain WF:



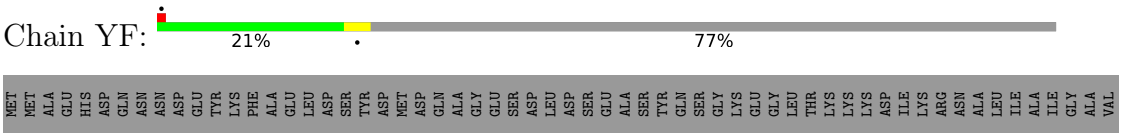
- Molecule 3: DotF

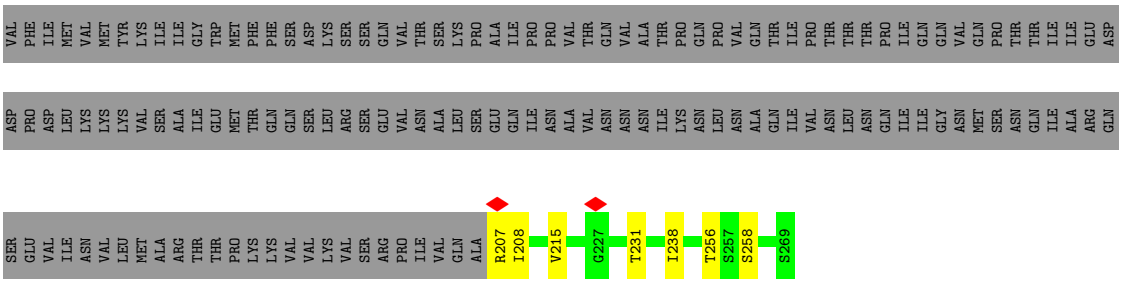
Chain XF:



- Molecule 3: DotF

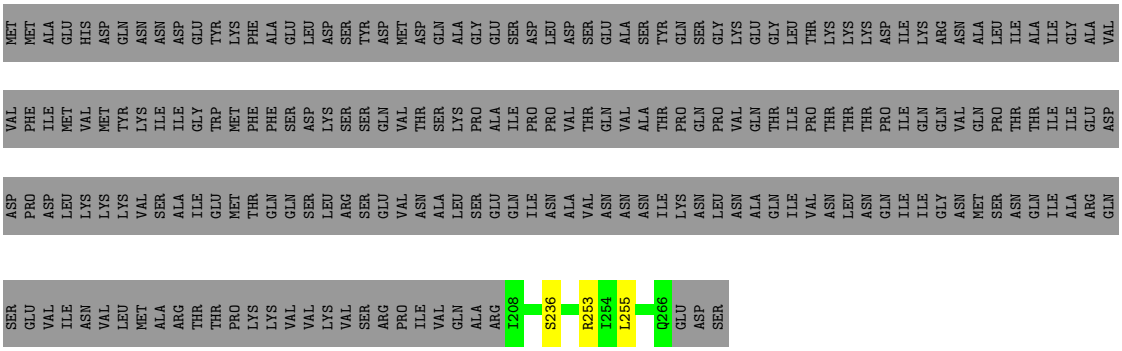
Chain YF:





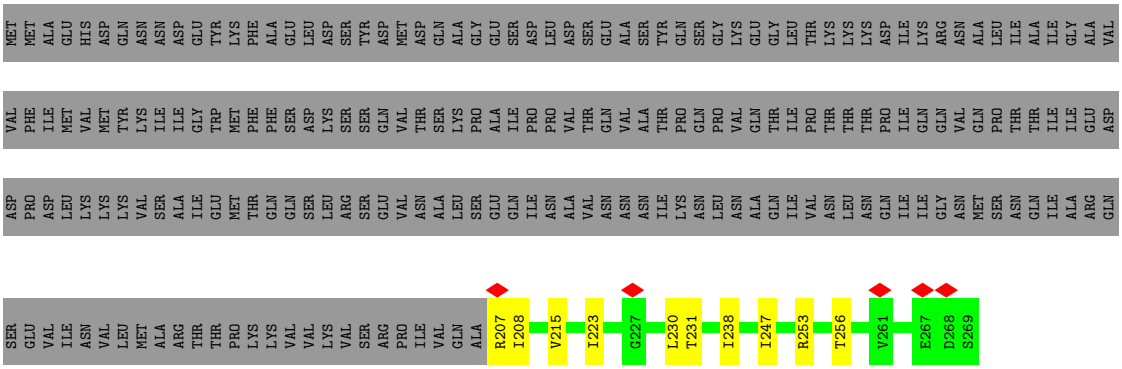
• Molecule 3: DotF

Chain Df:



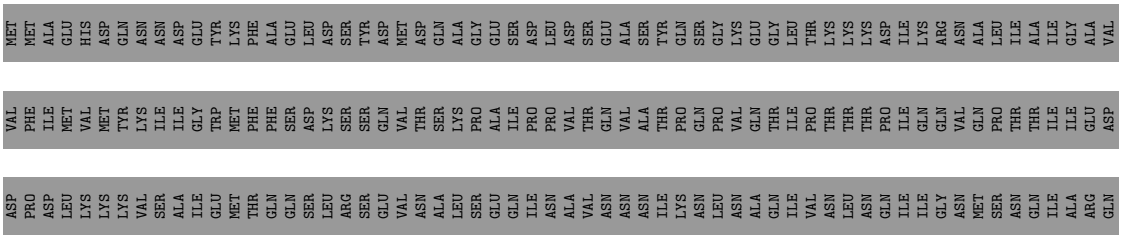
• Molecule 3: DotF

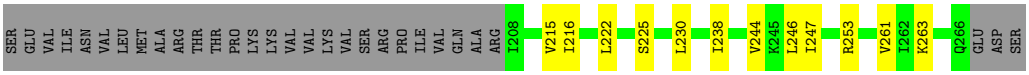
Chain ZF:



• Molecule 3: DotF

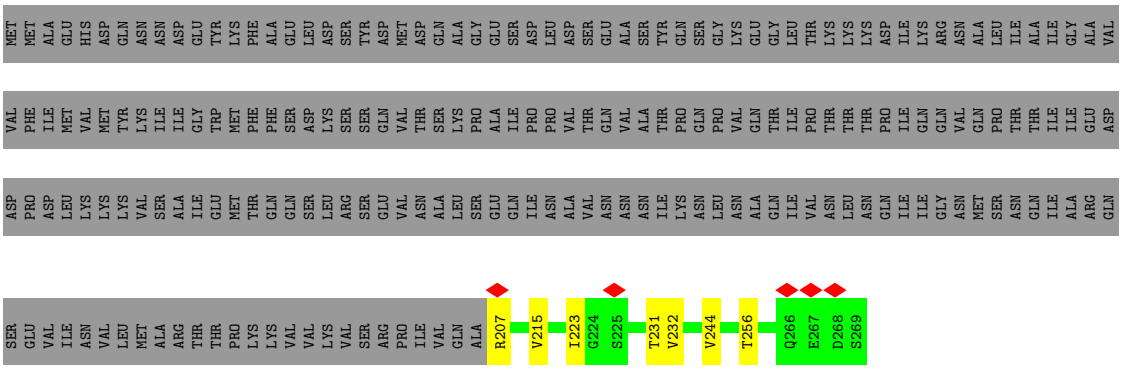
Chain Af:





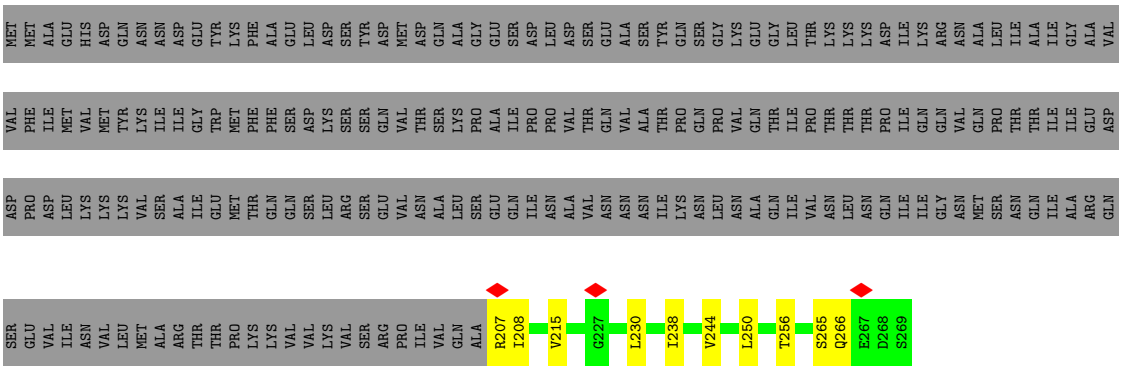
• Molecule 3: DotF

Chain BF: 21% 77%



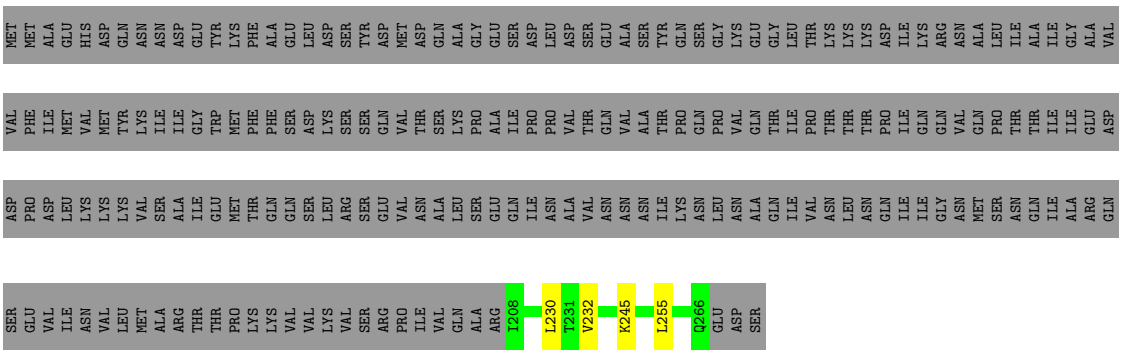
• Molecule 3: DotF

Chain CF: 20% 77%



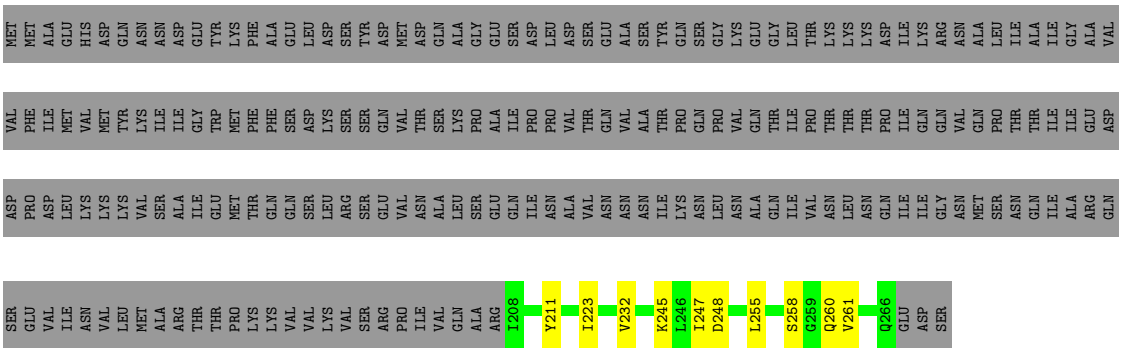
• Molecule 3: DotF

Chain Bf: 20% 78%



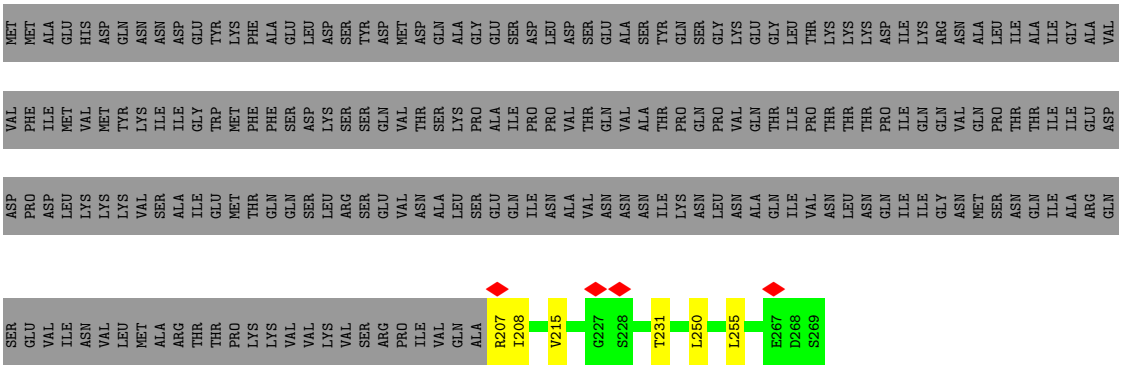
• Molecule 3: DotF

Chain Cf: 18% 78%



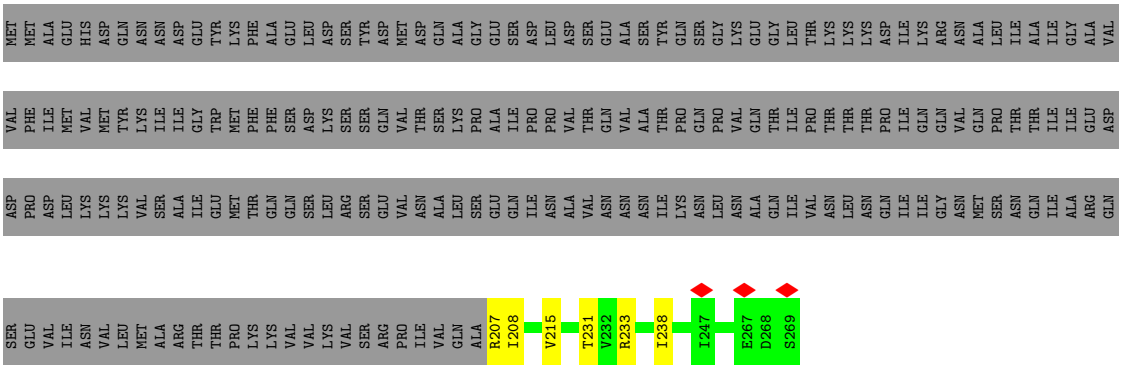
- Molecule 3: DotF

Chain DF:



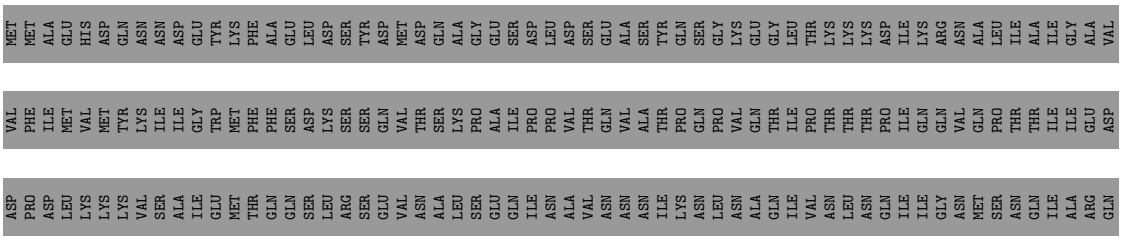
- Molecule 3: DotF

Chain EF:



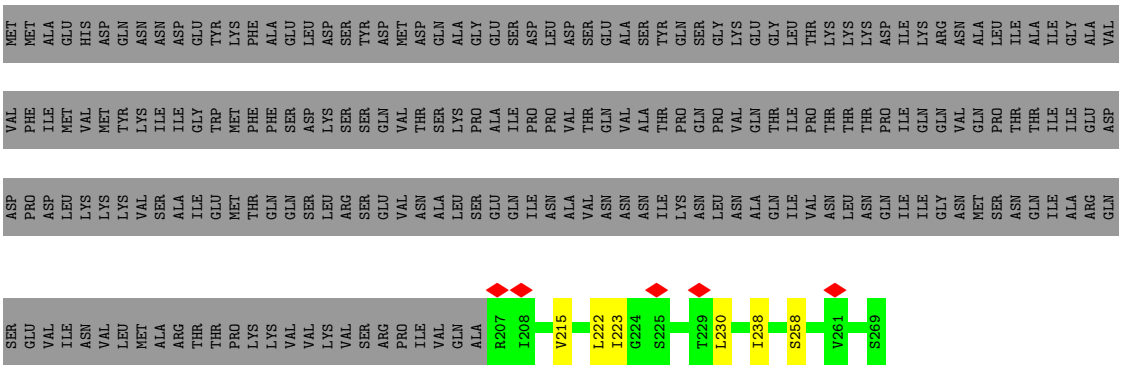
- Molecule 3: DotF

Chain Ef:



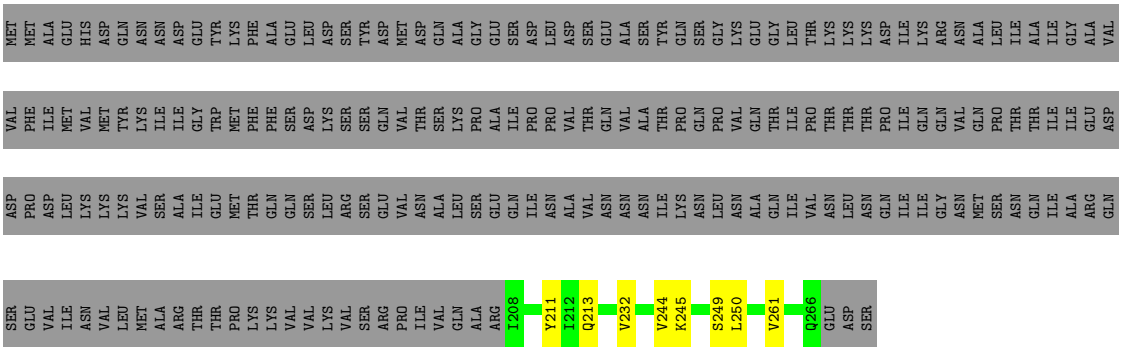
- Molecule 3: DotF

Chain FF:



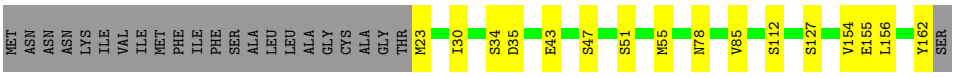
- Molecule 3: DotF

Chain Ff:



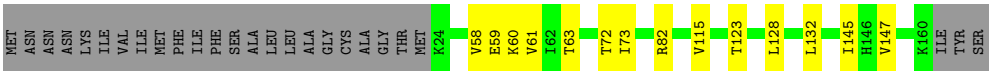
- Molecule 4: DotD

Chain GD:



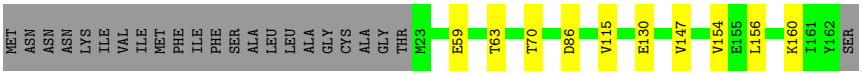
- Molecule 4: DotD

Chain Gd:



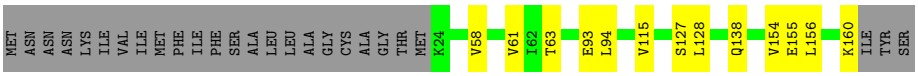
- Molecule 4: DotD

Chain HD:



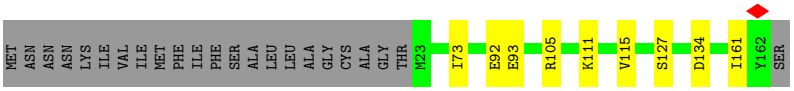
• Molecule 4: DotD

Chain Hd:



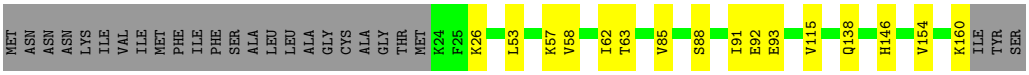
• Molecule 4: DotD

Chain ID:



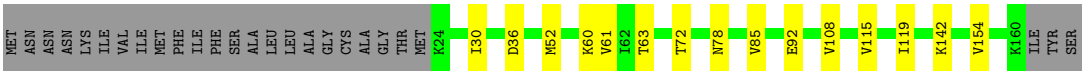
• Molecule 4: DotD

Chain Dd:



• Molecule 4: DotD

Chain Id:



• Molecule 4: DotD

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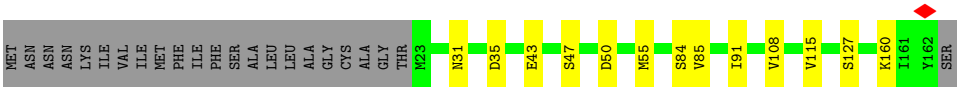
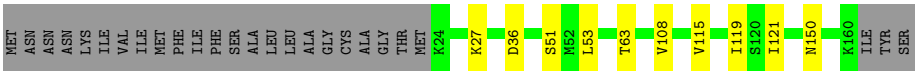


• Molecule 4: DotD

Chain Jd:

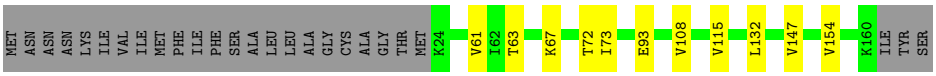


• Molecule 4: DotD

Chain KD:

• Molecule 4: DotD

Chain Kd:



• Molecule 4: DotD

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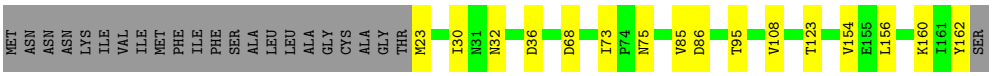

• Molecule 4: DotD

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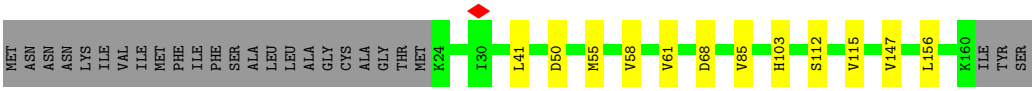
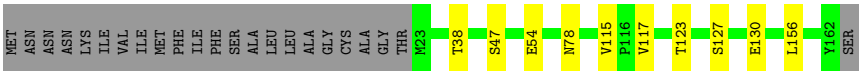


• Molecule 4: DotD

Chain MD:



• Molecule 4: DotD

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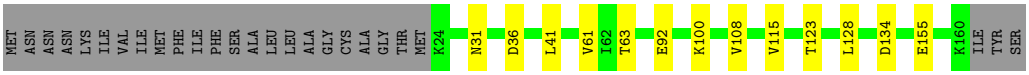

• Molecule 4: DotD

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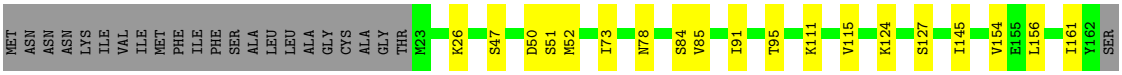

• Molecule 4: DotD

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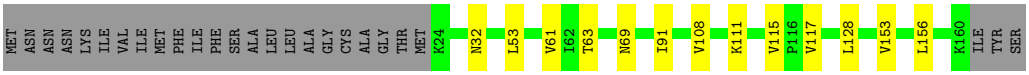

• Molecule 4: DotD

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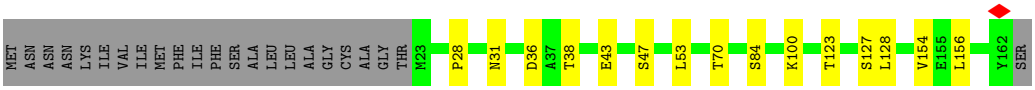
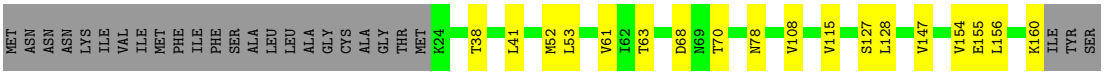


• Molecule 4: DotD

Chain Bd:

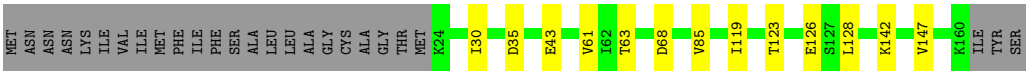


• Molecule 4: DotD

Chain AD:

• Molecule 4: DotD

Chain Cd:



• Molecule 4: DotD

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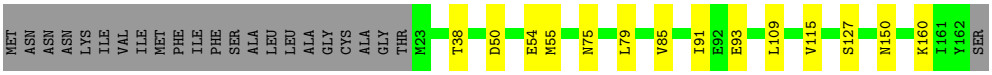

• Molecule 4: DotD

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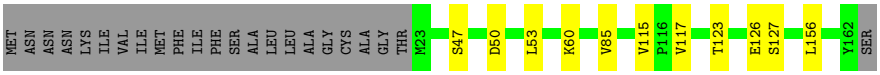
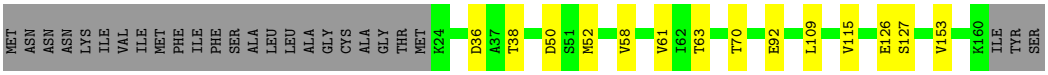


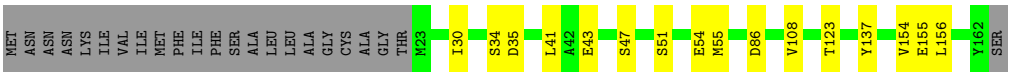
• Molecule 4: DotD

Chain Ed:



- Molecule 4: DotD

Chain FD:

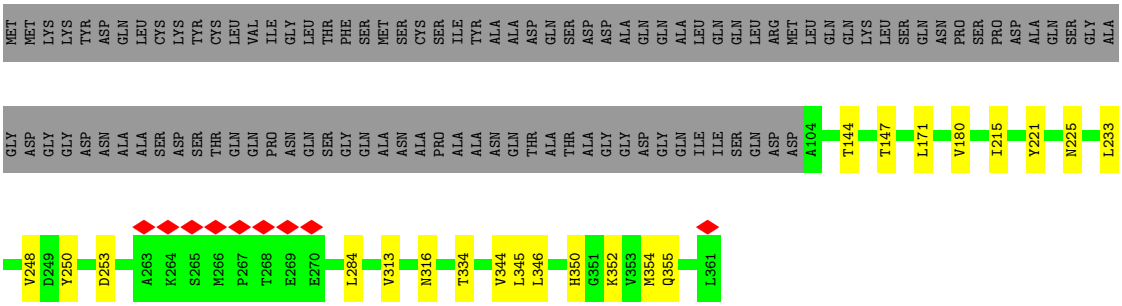


- Molecule 4: DotD

Chain Fd:

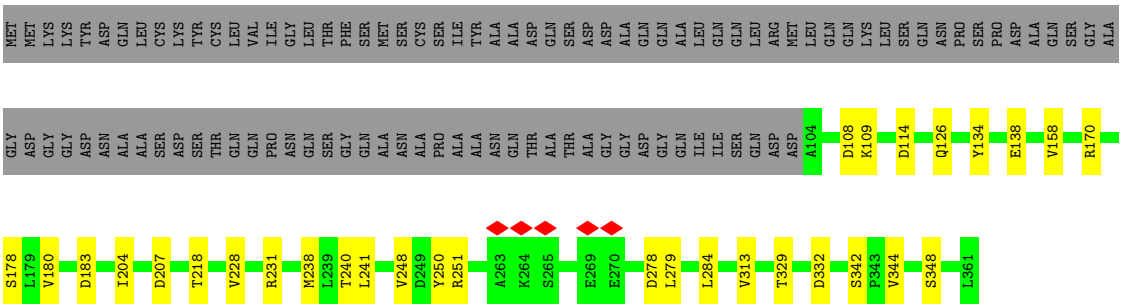
- Molecule 5: Type IV secretion protein IcmK

Chain GH:



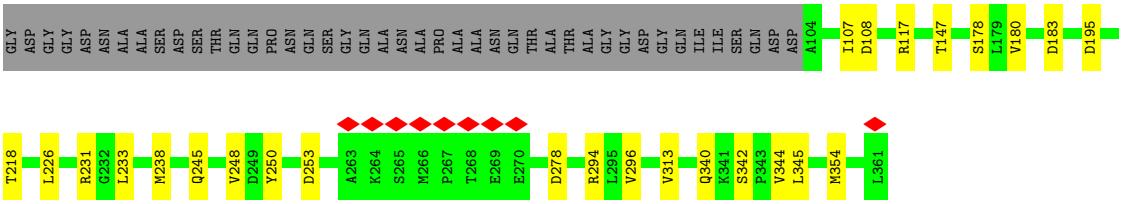
- Molecule 5: Type IV secretion protein IcmK

Chain HH:



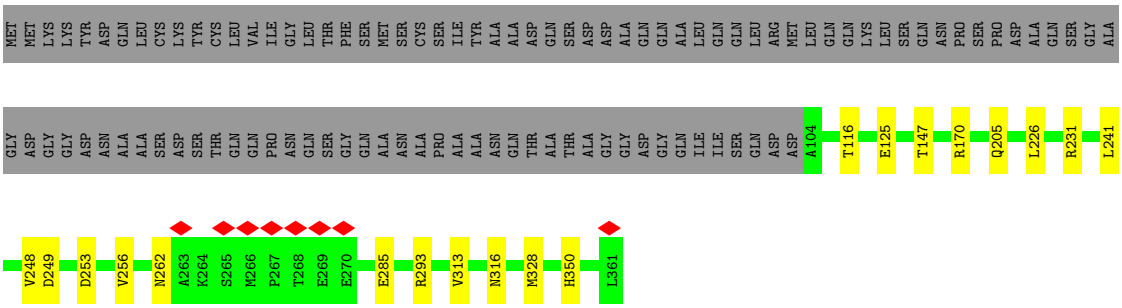
- Molecule 5: Type IV secretion protein IcmK

Chain IH:



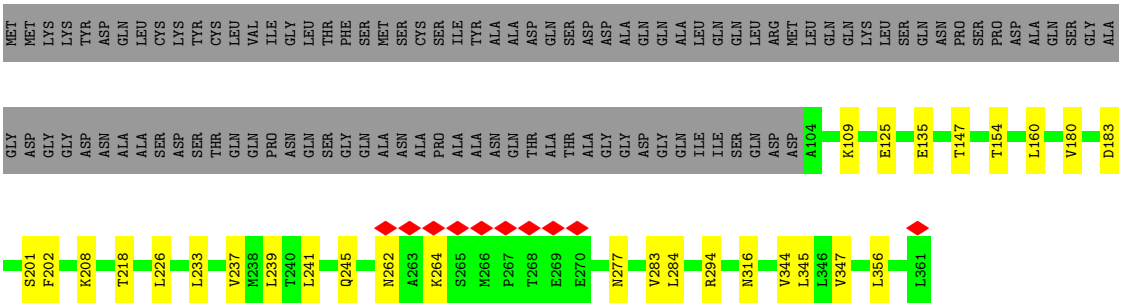
- Molecule 5: Type IV secretion protein IcmK

Chain JH:



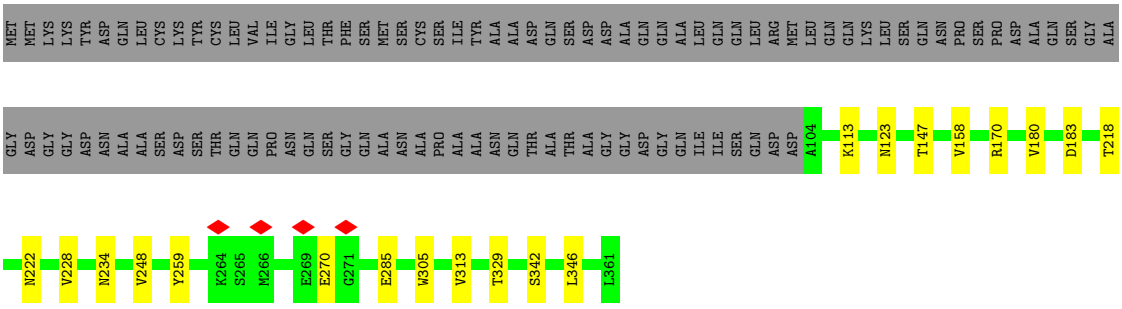
- Molecule 5: Type IV secretion protein IcmK

Chain AH:



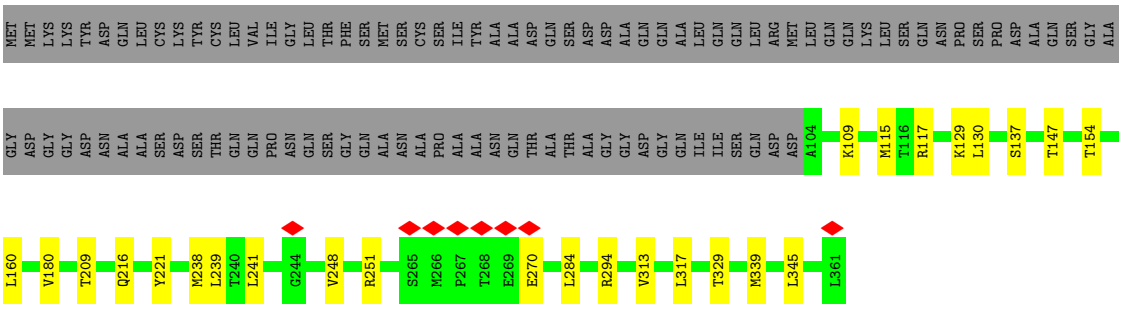
- Molecule 5: Type IV secretion protein IcmK

Chain KH:



- Molecule 5: Type IV secretion protein IcmK

Chain LH:



- Molecule 5: Type IV secretion protein IcmK

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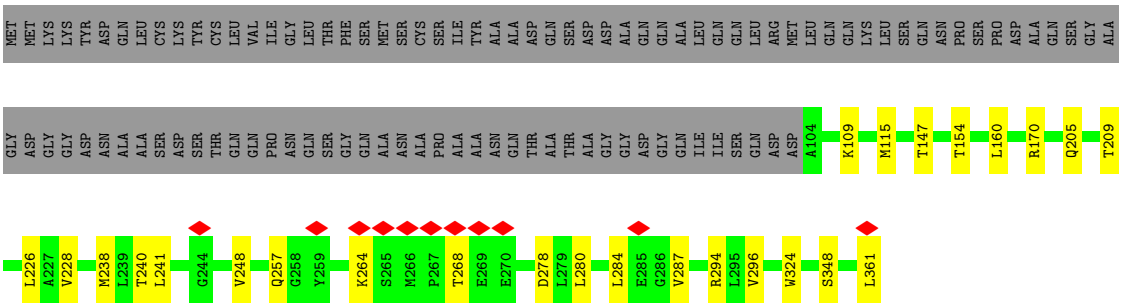
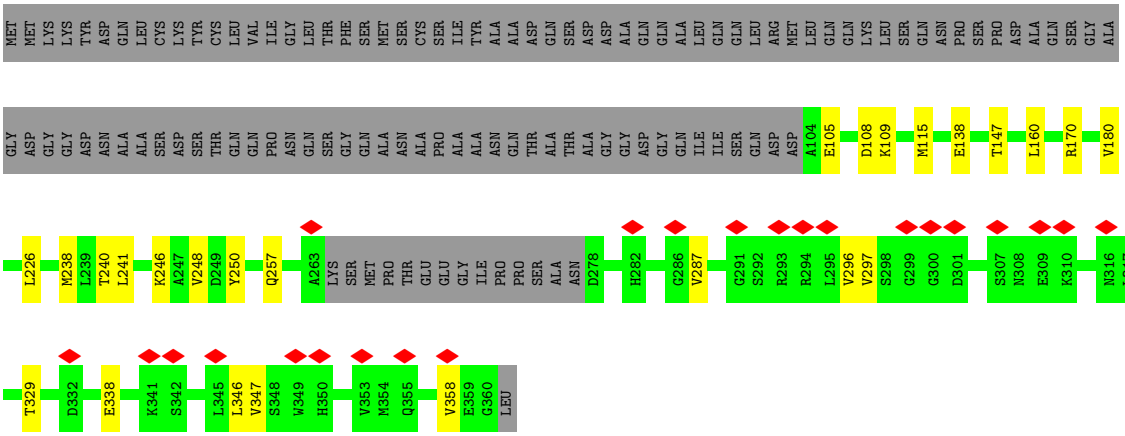


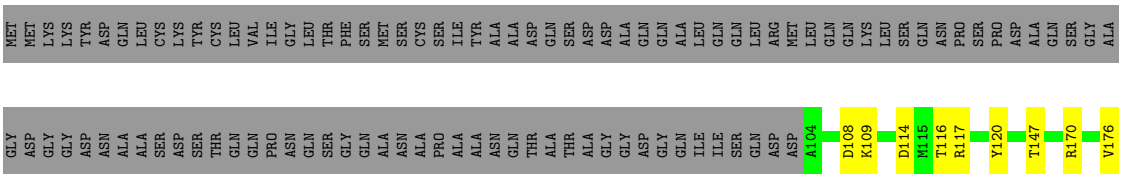
- Molecule 5: Type IV secretion protein IcmK

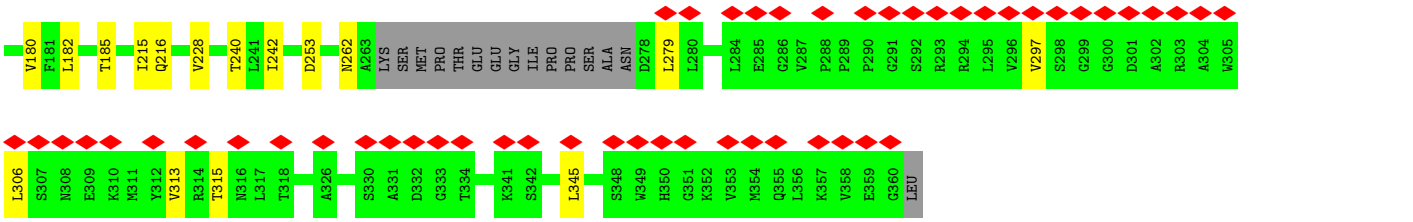
Chain VH:



- Molecule 5: Type IV secretion protein IcmK

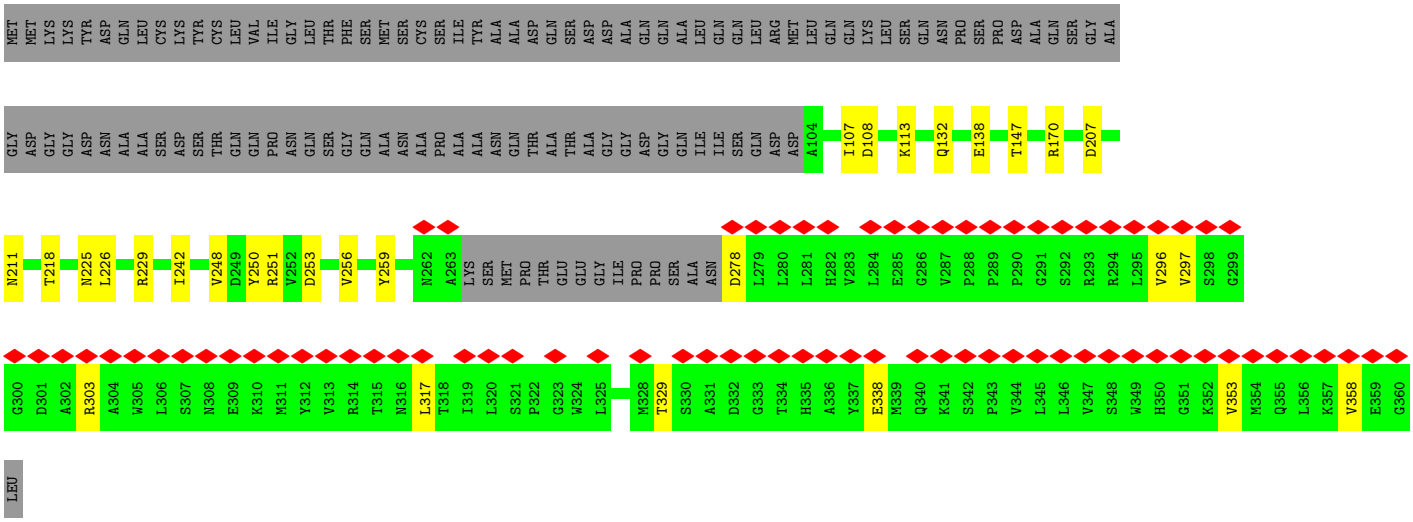
Chain WH:





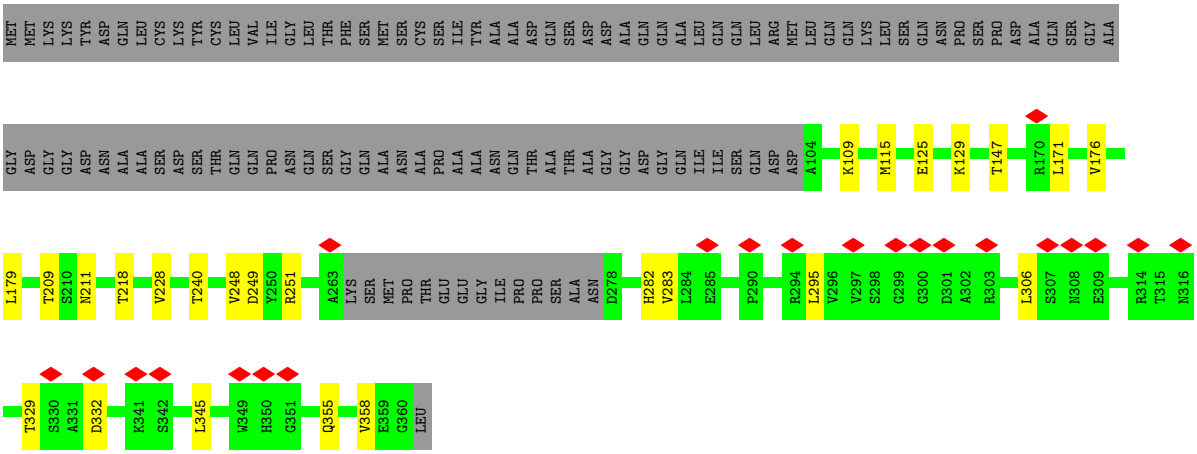
• Molecule 5: Type IV secretion protein IcmK

Chain XH:



• Molecule 5: Type IV secretion protein IcmK

Chain YH:



• Molecule 5: Type IV secretion protein IcmK

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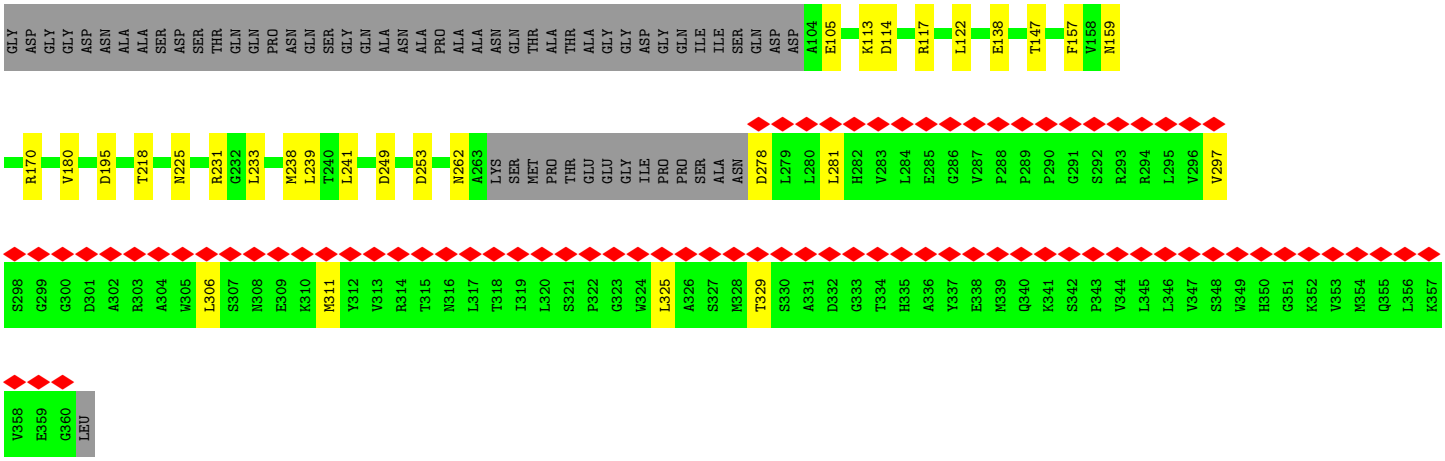
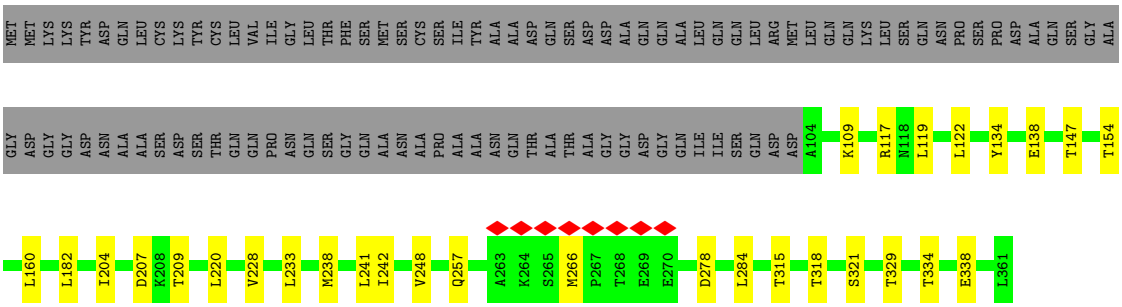


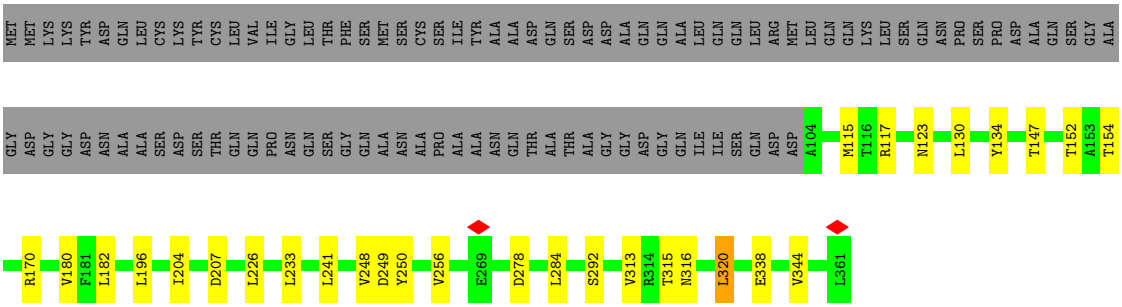
- Molecule 5: Type IV secretion protein IcmK

Chain BH:



- Molecule 5: Type IV secretion protein IcmK

Chain CH:



- Molecule 5: Type IV secretion protein IcmK

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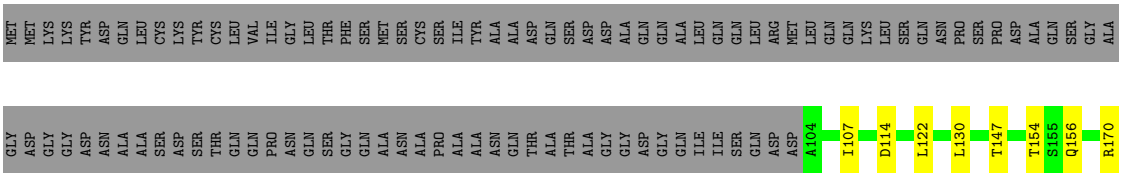
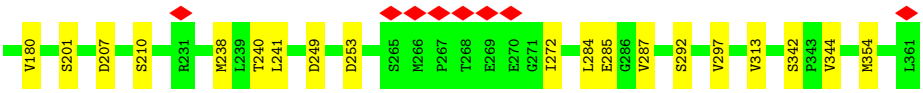
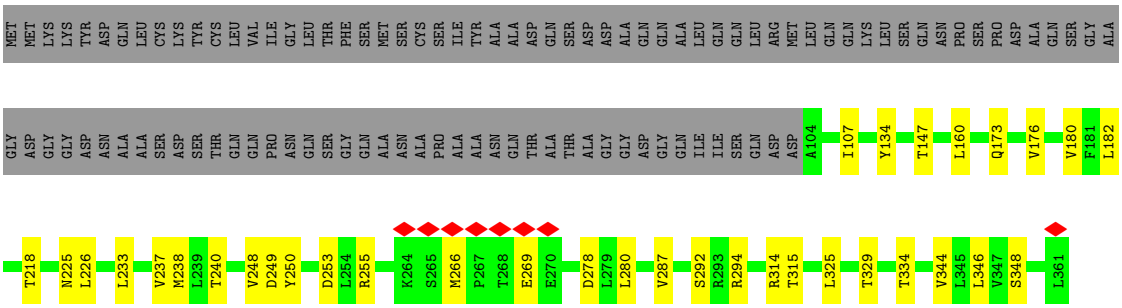




• Molecule 5: Type IV secretion protein IcmK

Chain EH:



• Molecule 5: Type IV secretion protein IcmK

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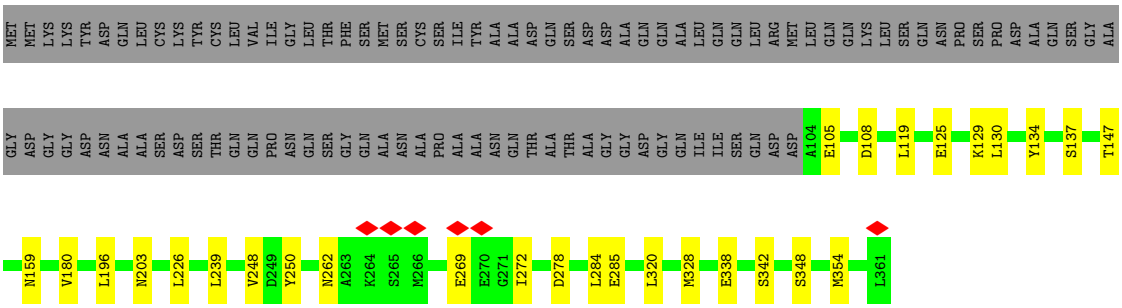
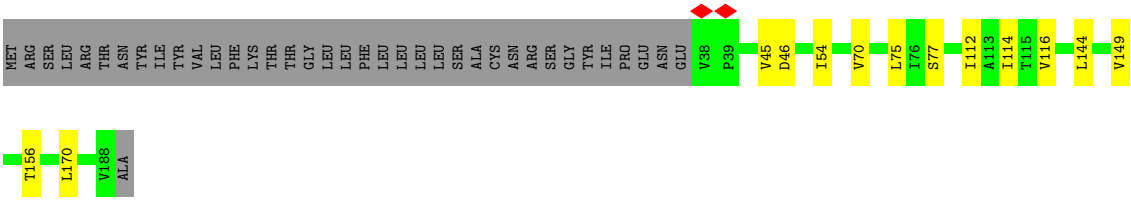


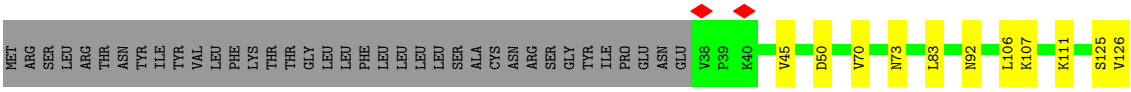
• Molecule 6: Inner membrane lipoprotein YiaD

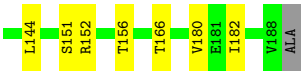
Chain GK:



• Molecule 6: Inner membrane lipoprotein YiaD

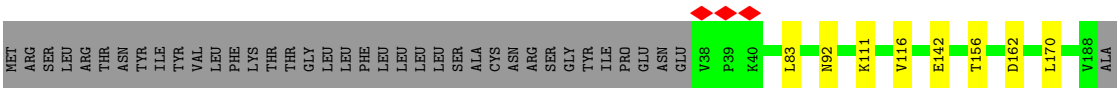
Chain HK:





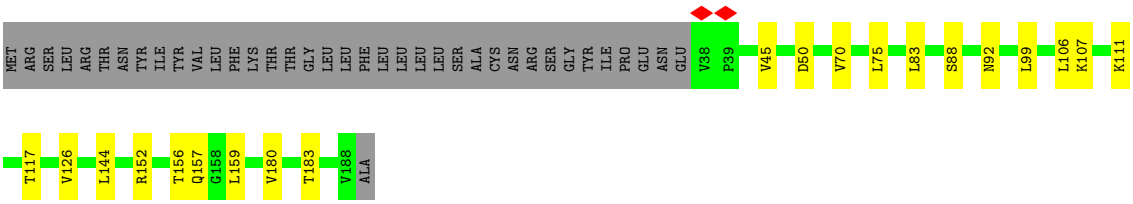
• Molecule 6: Inner membrane lipoprotein YiaD

Chain IK:



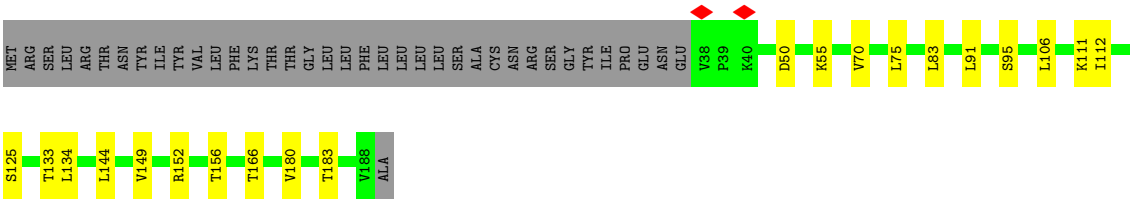
• Molecule 6: Inner membrane lipoprotein YiaD

Chain JK:



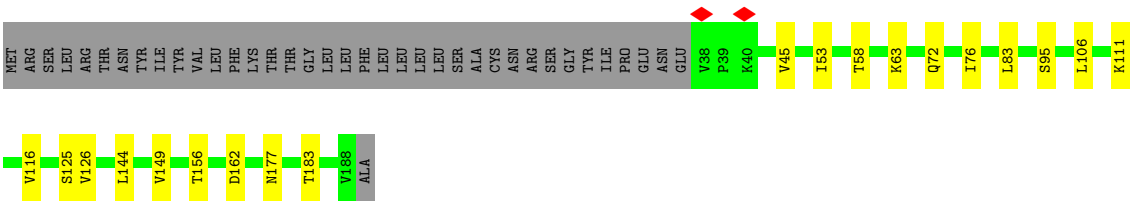
• Molecule 6: Inner membrane lipoprotein YiaD

Chain KK:



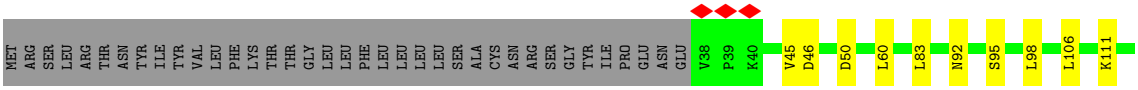
• Molecule 6: Inner membrane lipoprotein YiaD

Chain LK:



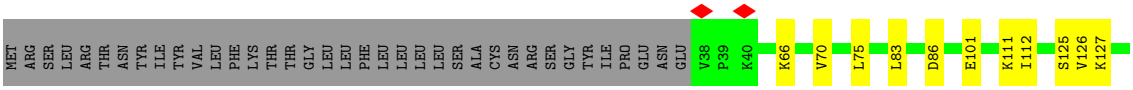
• Molecule 6: Inner membrane lipoprotein YiaD

Chain AK:



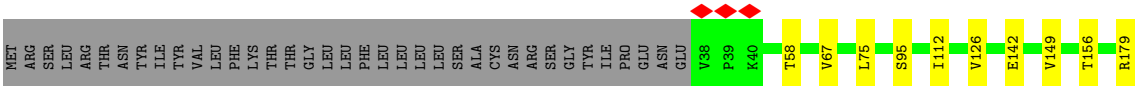
• Molecule 6: Inner membrane lipoprotein YiaD

Chain MK:



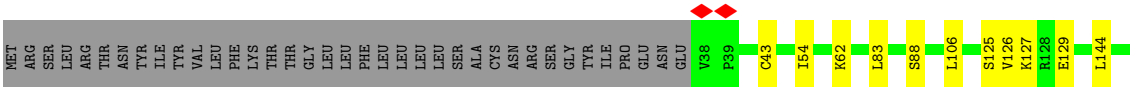
• Molecule 6: Inner membrane lipoprotein YiaD

Chain BK:



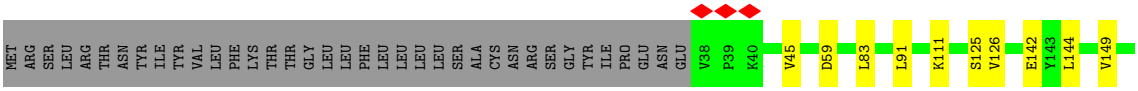
• Molecule 6: Inner membrane lipoprotein YiaD

Chain CK:



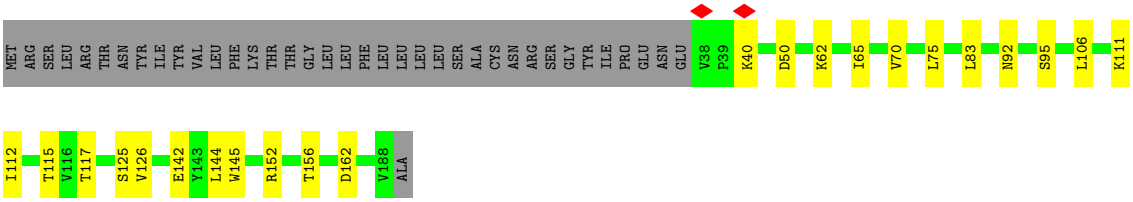
• Molecule 6: Inner membrane lipoprotein YiaD

Chain DK:



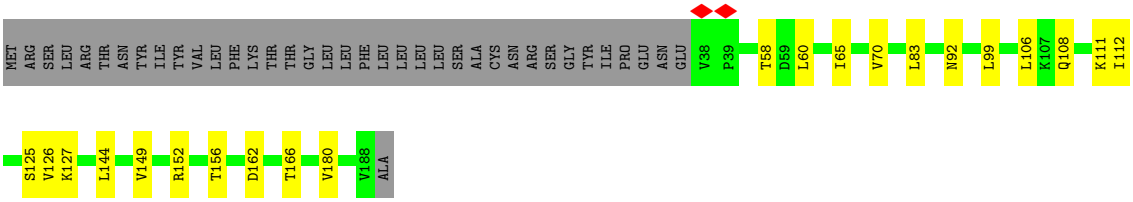
• Molecule 6: Inner membrane lipoprotein YiaD

Chain EK:



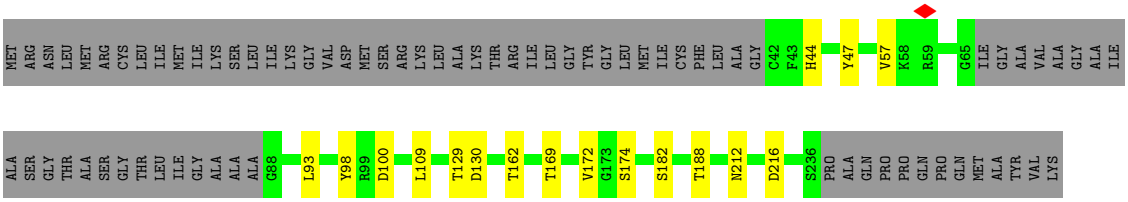
• Molecule 6: Inner membrane lipoprotein YiaD

Chain FK:



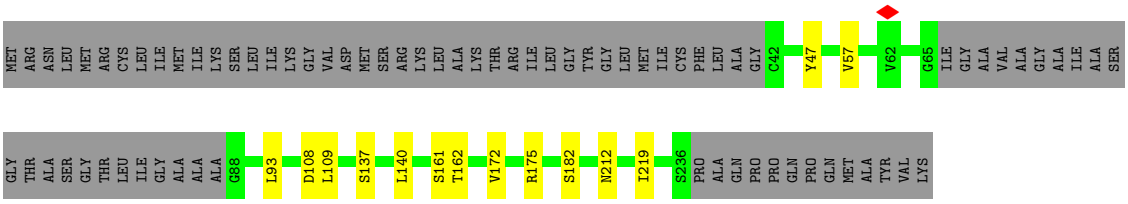
• Molecule 7: Outer membrane protein, OmpA family protein

Chain GL:



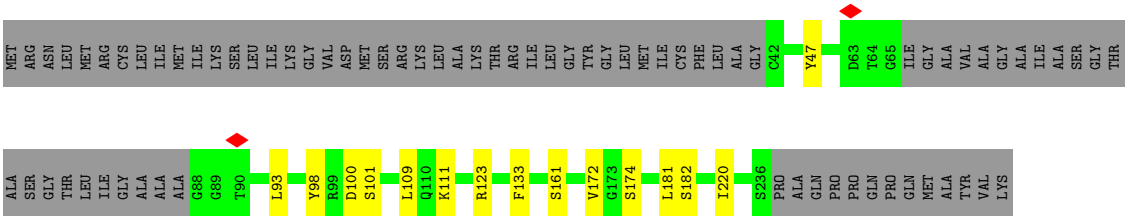
• Molecule 7: Outer membrane protein, OmpA family protein

Chain HL:



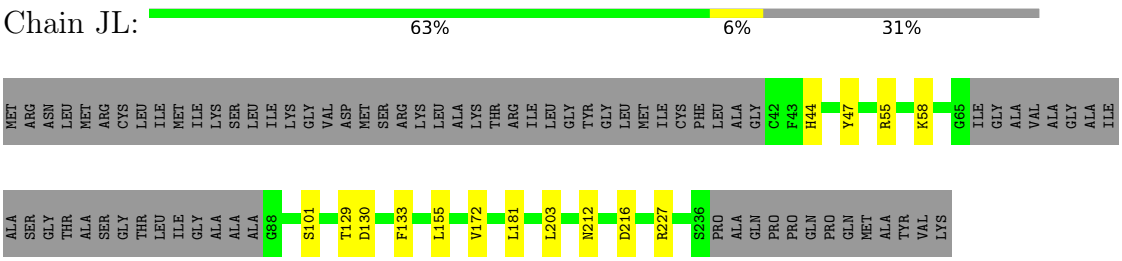
• Molecule 7: Outer membrane protein, OmpA family protein

Chain IL:



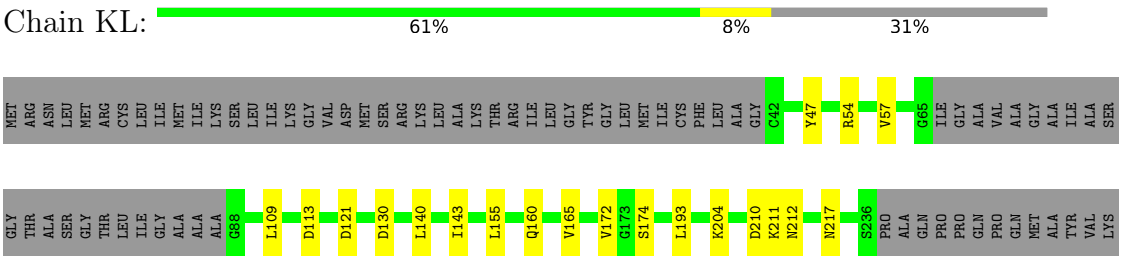
• Molecule 7: Outer membrane protein, OmpA family protein

Chain JL:



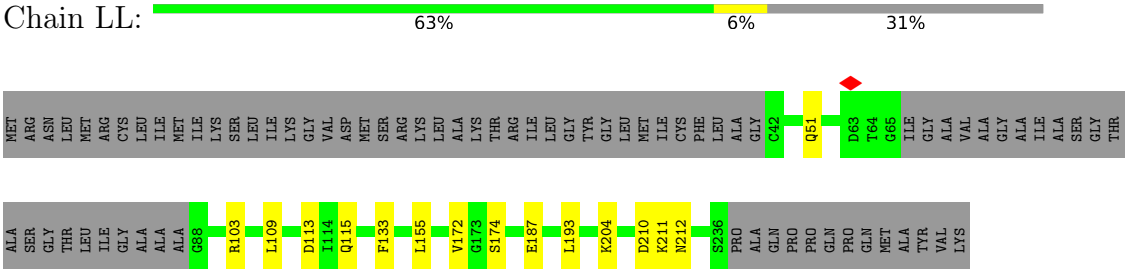
• Molecule 7: Outer membrane protein, OmpA family protein

Chain KL:



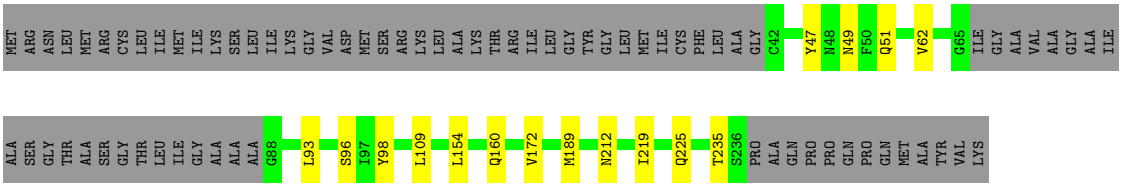
• Molecule 7: Outer membrane protein, OmpA family protein

Chain LL:



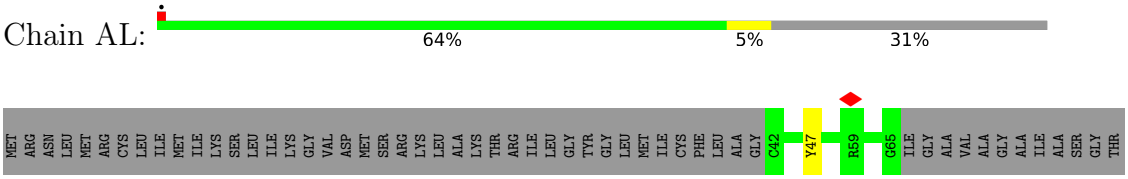
• Molecule 7: Outer membrane protein, OmpA family protein

Chain ML:



• Molecule 7: Outer membrane protein, OmpA family protein

Chain AL:

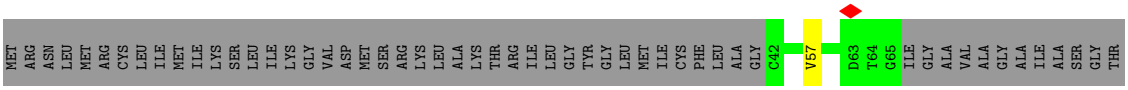


• Molecule 7: Outer membrane protein, OmpA family protein

Chain BL:

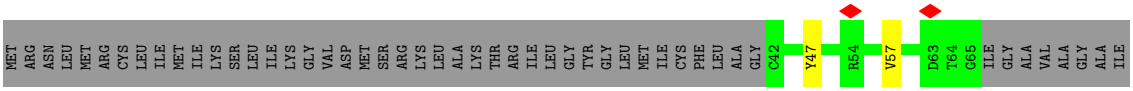
• Molecule 7: Outer membrane protein, OmpA family protein

Chain CL:



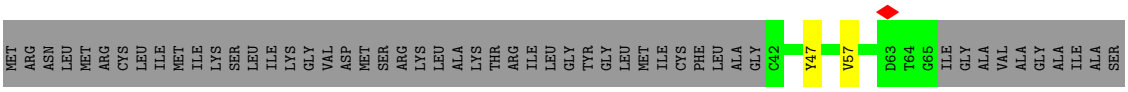
• Molecule 7: Outer membrane protein, OmpA family protein

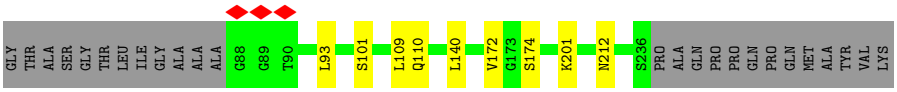
Chain DL:



• Molecule 7: Outer membrane protein, OmpA family protein

Chain EL:





• Molecule 7: Outer membrane protein, OmpA family protein

Chain FL: 61% 8% 31%

MET ARG ASN LEU MET ARG CYS LEU ILE MET ILE LYS SER LEU ILE LYS GLY VAL ASP MET SER ARG LYS LEU ALA LYS THR ARG ILE LEU GLY TYR GLY LEU MET ILE CYS PHE LEU ALA GLY C42 Y47 Q51 V57 K58 G65 ILE GLY ALA VAL ALA GLY ALA ILE ALA

SER GLY THR ALA SER GLY THR LEU ILE GLY ALA ALA ALA G38 Y98 L109 L125 F133 L140 L155 I163 V172 G173 S174 H177 K204 D210 K211 N212 N217 Q225 E230 S236 PRO ALA GLN PRO PRO GLN PRO GLN MET ALA TYR VAL

LYS

- Molecule 8: DUF2807 domain-containing protein

Chain GM: 58% 7% 35%

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

HIS THR GLY TYR ASN LYS PRO GLU VAL MET LEU ARG GLY ASP PRO ARG ASP LEU VAL GLN VAL ARG THR ILE VAL LYS GLN ASN THR LEU TYR VAL SER LEU GLY GLN GLY TYR PRO ASP TYR GLY ALA VAL THR VAL ASP ILE LYS THR LYS PHE L113 N114 T131 L134 L146

A147 G148 N149 L152 Q153 V162 I175 K182 V183 L184 F188 V189 N190 L191 R192 K199 I207 L212 Y245 S259 I263 S271 S277 L299 P320

- Molecule 8: DUF2807 domain-containing protein

Chain HM: 56% 9% 35%

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

HIS THR GLY TYR ASN LYS PRO GLU VAL MET LEU ARG GLY ASP PRO ARG ASP LEU VAL GLN VAL ARG THR ILE VAL LYS GLN ASN THR LEU TYR VAL SER LEU GLY GLN GLY TYR PRO ASP TYR GLY ALA VAL THR VAL ASP ILE LYS THR LYS PHE L113 A121 T131 Y137

N140 L146 N149 L152 N160 G161 V162 S170 V176 L177 K178 G179 D180 L184 L194 T201 D210 T211 L212 I222 L231 D237 K242 S251 S259 E262 Q269 S277 L284 M292 V298 E303 P320

- Molecule 8: DUF2807 domain-containing protein

Chain IM: 57% 8% 35%

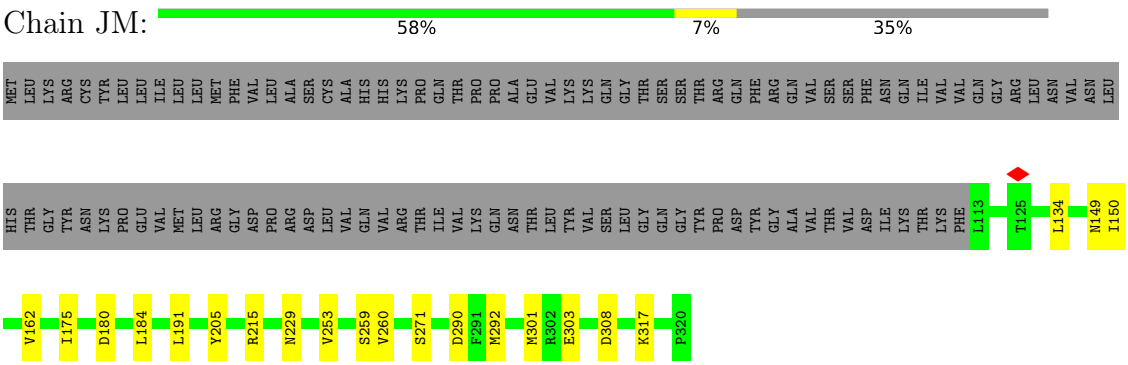
MET LEU LYS ARG CYS TYR LEU LEU ILE LEU LEU MET PHE VAL LEU ALA SER CYS ALA HIS HIS LYS PRO GLN THR PRO PRO ALA GLU VAL LYS LYS GLN GLY THR SER SER THR ARG GLN PHE ARG GLN VAL SER SER PHE ASN GLN ILE VAL VAL GLN GLY ARG LEU ASN VAL ASN LEU

HIS THR GLY TYR ASN LYS PRO GLU VAL MET LEU ARG GLY ASP PRO ARG ASP LEU VAL GLN VAL ARG THR ILE VAL LYS GLN ASN THR LEU TYR VAL SER LEU GLY GLN GLY TYR PRO ASP TYR GLY ALA VAL THR VAL ASP ILE LYS THR LYS PHE L113 N114 R115 L129 L134

T144 N149 L152 N160 R171 I175 V176 L177 D180 V183 L184 L191 L202 I222 Q223 L224 V233 V253 E262 I263 M292 S297 D300 M301 R302 E303 P320

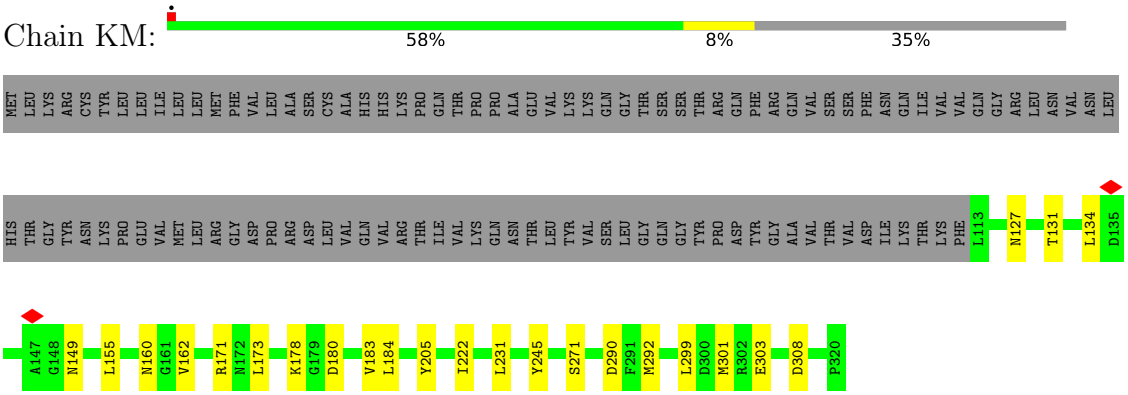
- Molecule 8: DUF2807 domain-containing protein

Chain JM:



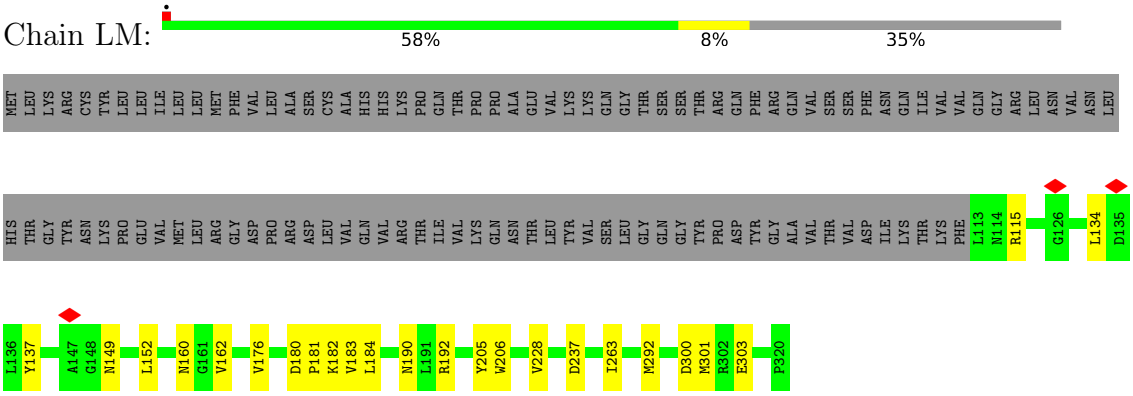
- Molecule 8: DUF2807 domain-containing protein

Chain KM:



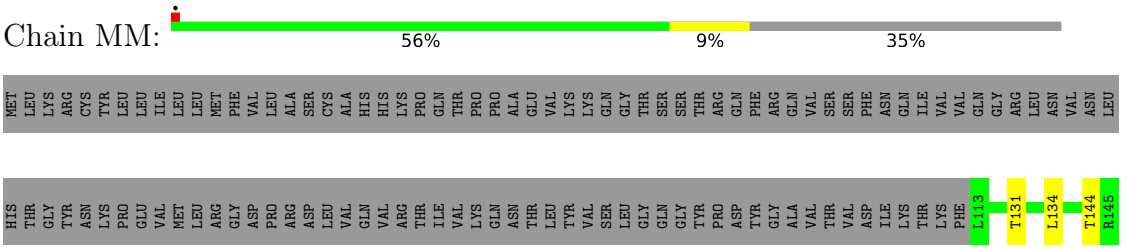
- Molecule 8: DUF2807 domain-containing protein

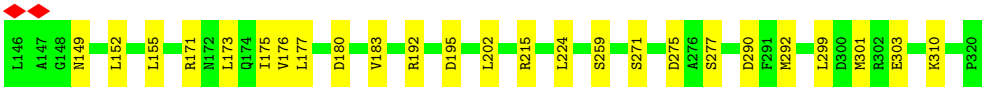
Chain LM:



- Molecule 8: DUF2807 domain-containing protein

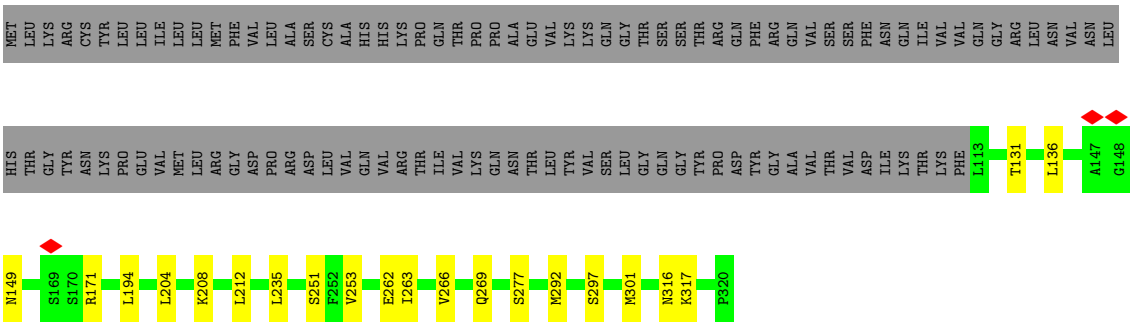
Chain MM:





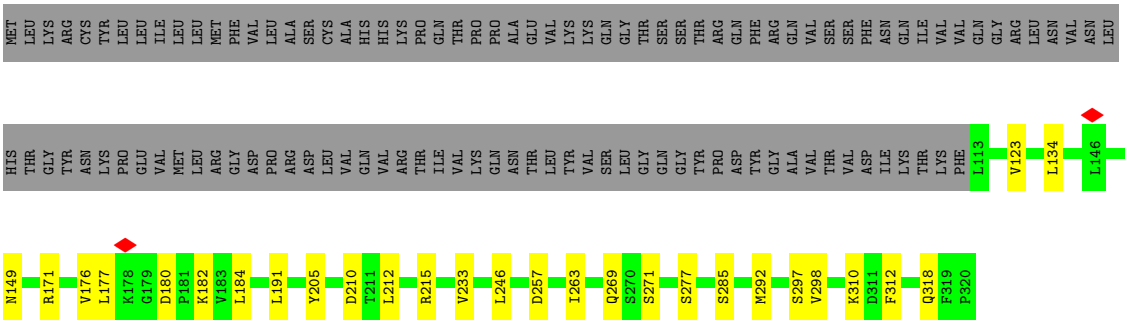
• Molecule 8: DUF2807 domain-containing protein

Chain AM:



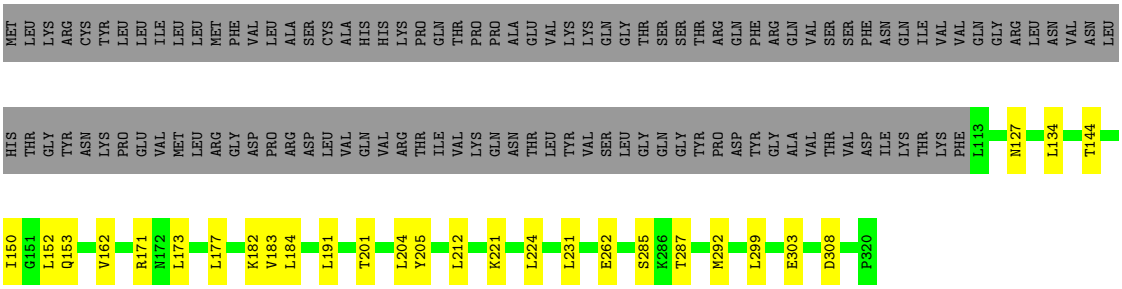
• Molecule 8: DUF2807 domain-containing protein

Chain BM:



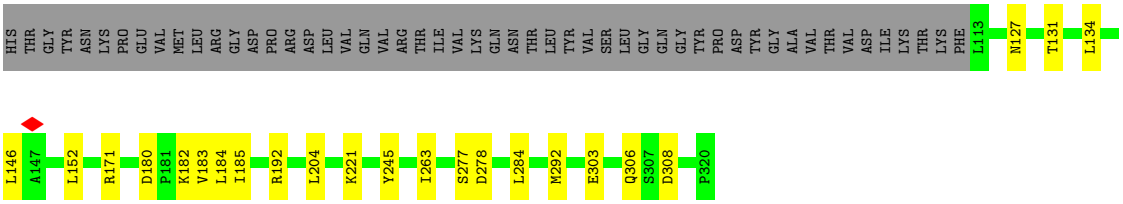
• Molecule 8: DUF2807 domain-containing protein

Chain CM:



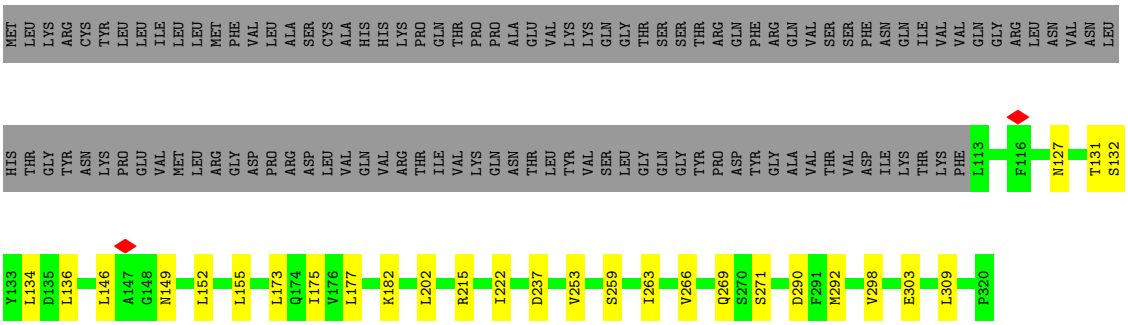
• Molecule 8: DUF2807 domain-containing protein

Chain DM:



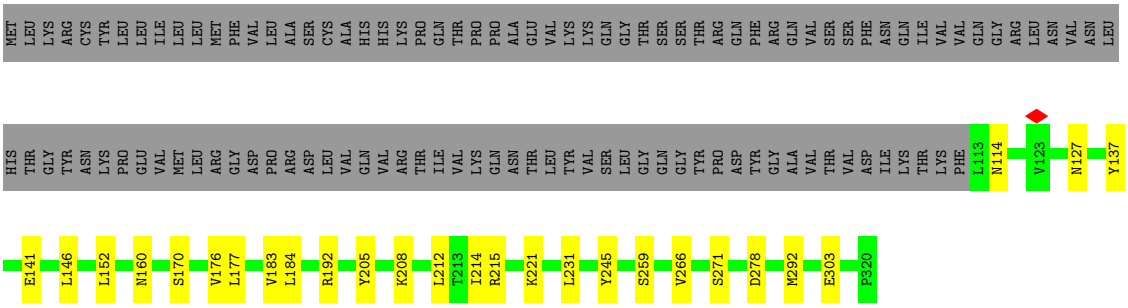
- Molecule 8: DUF2807 domain-containing protein

Chain EM:



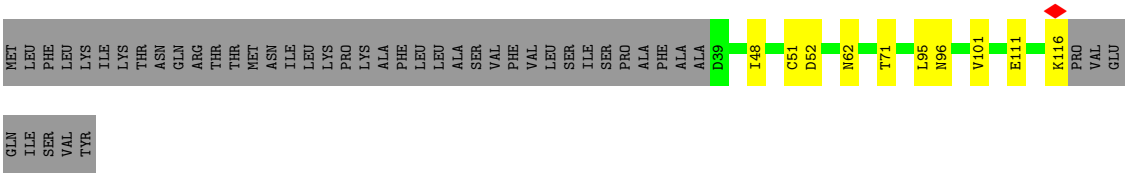
- Molecule 8: DUF2807 domain-containing protein

Chain FM:



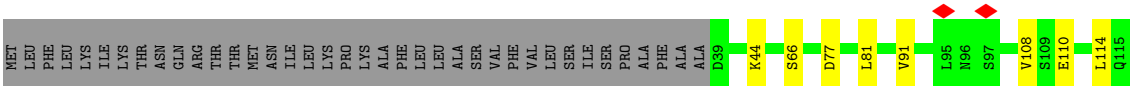
- Molecule 9: Neurogenic locus notch

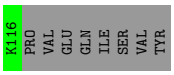
Chain GN:



- Molecule 9: Neurogenic locus notch

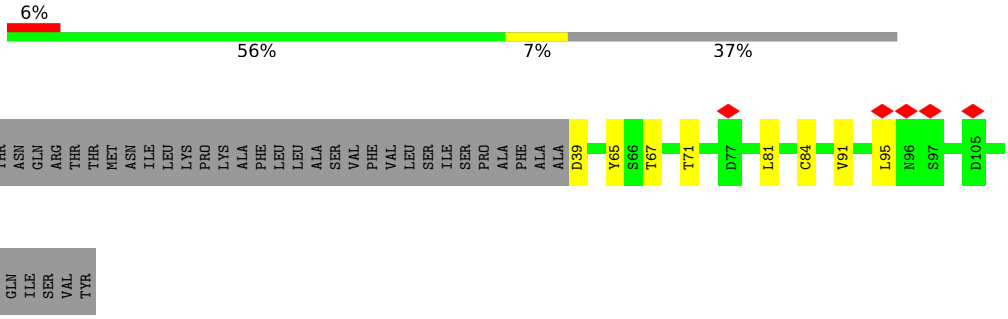
Chain HN:





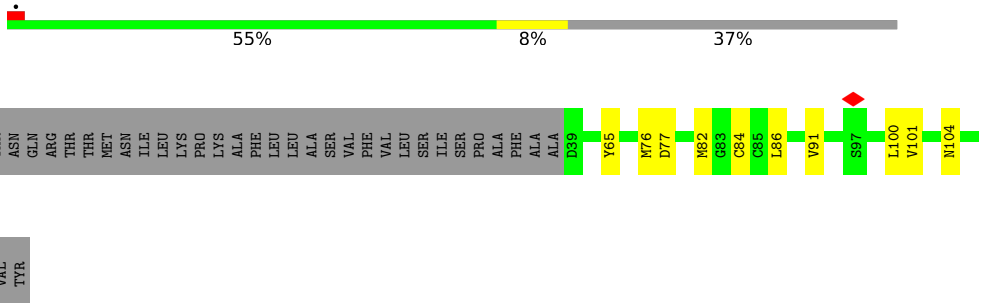
• Molecule 9: Neurogenic locus notch

Chain IN:



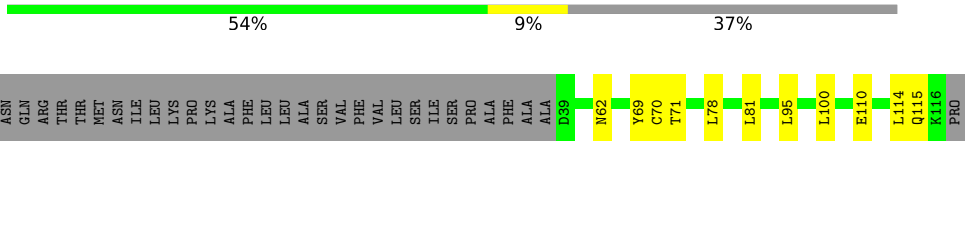
• Molecule 9: Neurogenic locus notch

Chain JN:



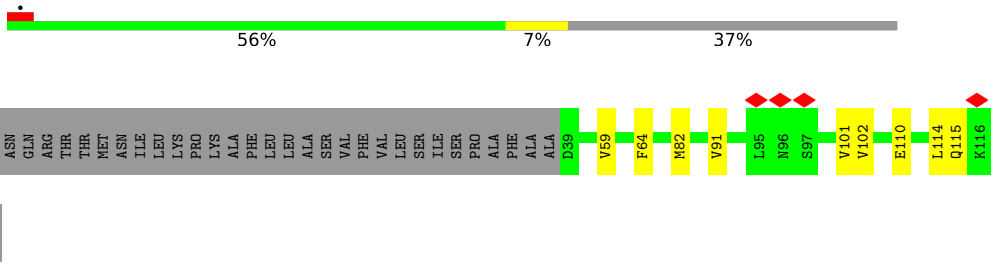
• Molecule 9: Neurogenic locus notch

Chain KN:



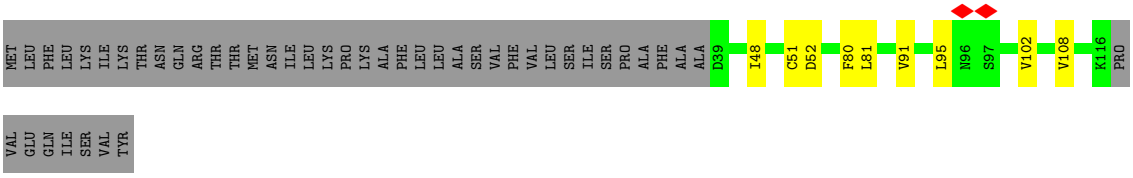
• Molecule 9: Neurogenic locus notch

Chain LN:



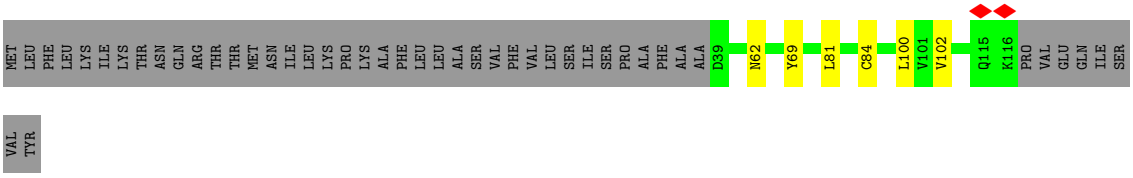
• Molecule 9: Neurogenic locus notch

Chain MN:



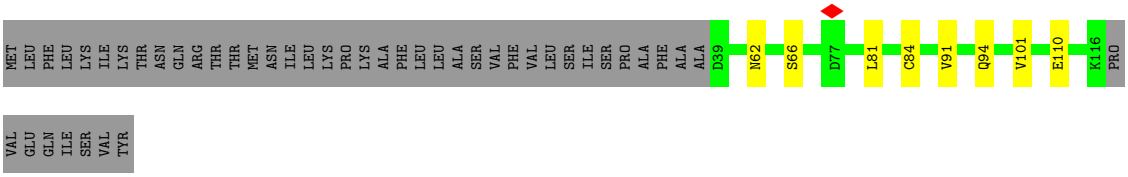
• Molecule 9: Neurogenic locus notch

Chain AN:



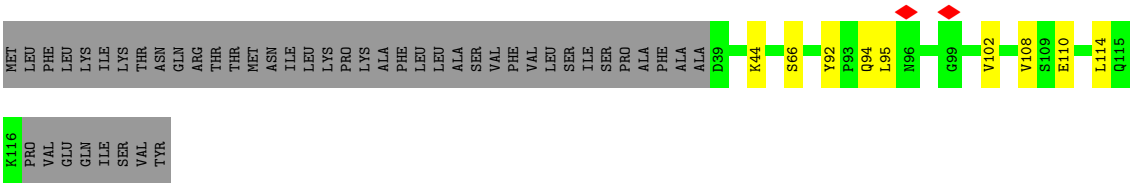
• Molecule 9: Neurogenic locus notch

Chain BN:



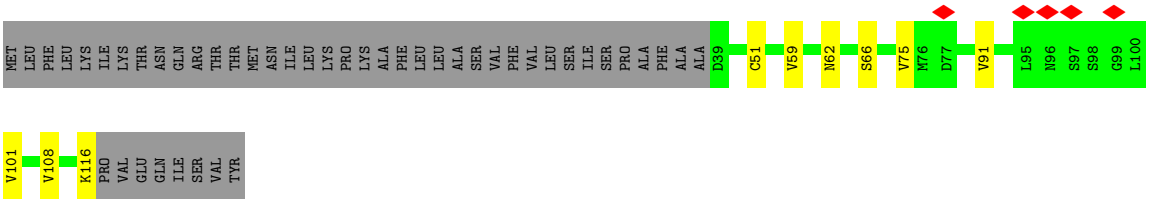
• Molecule 9: Neurogenic locus notch

Chain CN:



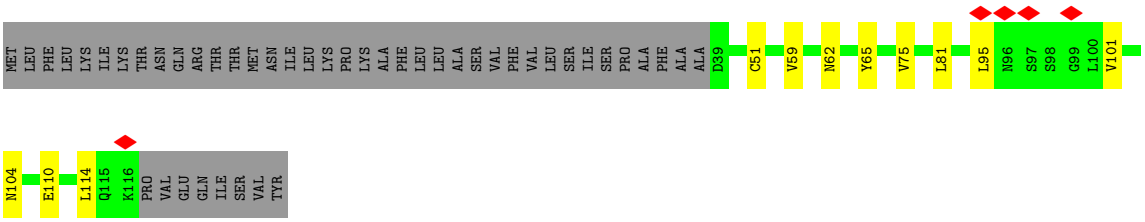
• Molecule 9: Neurogenic locus notch

Chain DN:



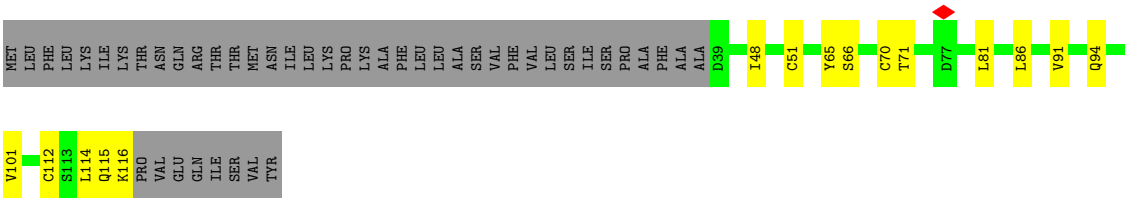
• Molecule 9: Neurogenic locus notch

Chain EN:



• Molecule 9: Neurogenic locus notch

Chain FN:



• Molecule 10: Unknown protein fragment

Chain GU:

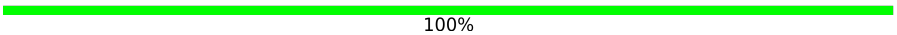
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain HU:

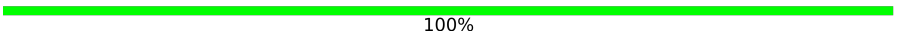
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain IU: 

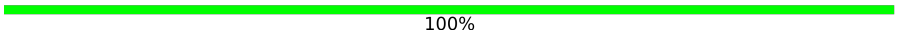
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain JU: 

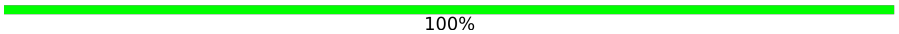
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain KU: 

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain LU: 

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain MU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain AU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain BU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain CU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain DU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain EU: 100%

There are no outlier residues recorded for this chain.

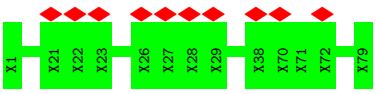
• Molecule 10: Unknown protein fragment

Chain FU: 100%

There are no outlier residues recorded for this chain.

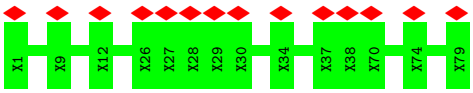
• Molecule 11: Unknown protein fragment

Chain GX: 21% 100%



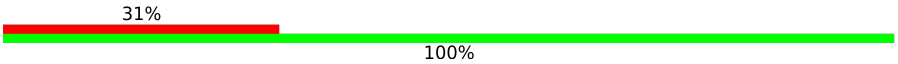
• Molecule 11: Unknown protein fragment

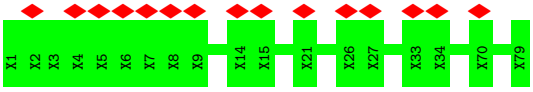
Chain DX: 29% 100%



• Molecule 11: Unknown protein fragment

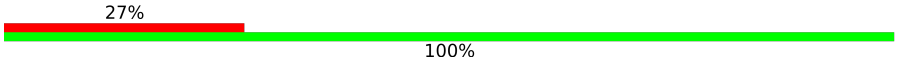
Chain HX:

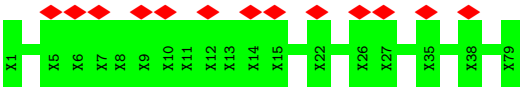




• Molecule 11: Unknown protein fragment

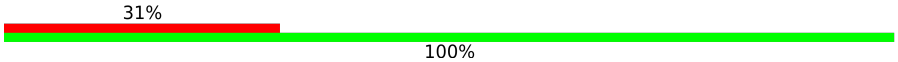
Chain IX:

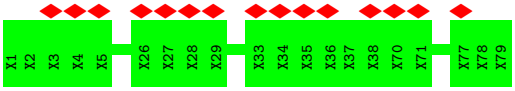




• Molecule 11: Unknown protein fragment

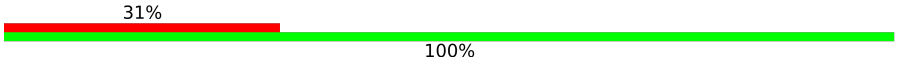
Chain JX:

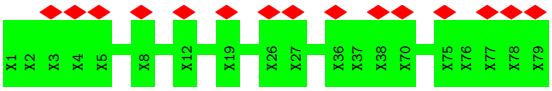




• Molecule 11: Unknown protein fragment

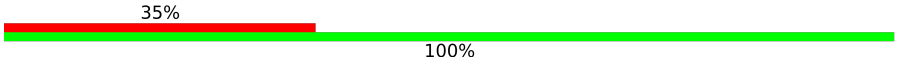
Chain KX:

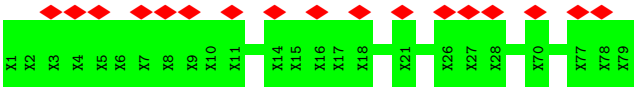




• Molecule 11: Unknown protein fragment

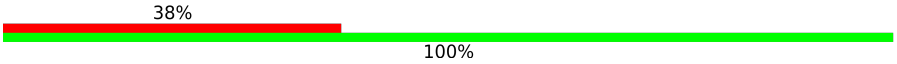
Chain LX:

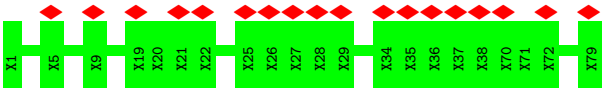




• Molecule 11: Unknown protein fragment

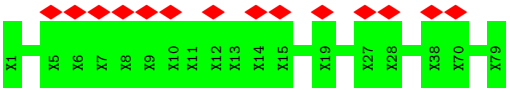
Chain MX:





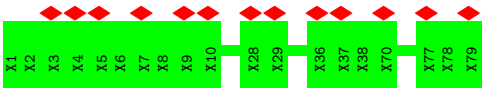
• Molecule 11: Unknown protein fragment

Chain VX: 29% 100%



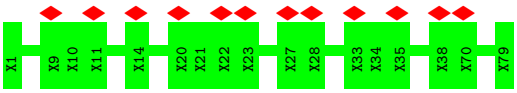
• Molecule 11: Unknown protein fragment

Chain WX: 27% 100%



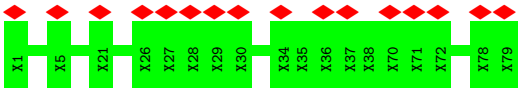
• Molecule 11: Unknown protein fragment

Chain XX: 25% 100%



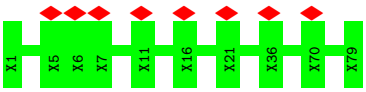
• Molecule 11: Unknown protein fragment

Chain YX: 33% 100%



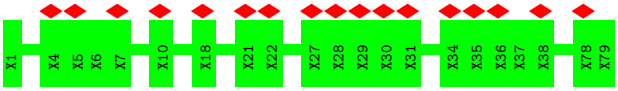
• Molecule 11: Unknown protein fragment

Chain ZX: 17% 100%



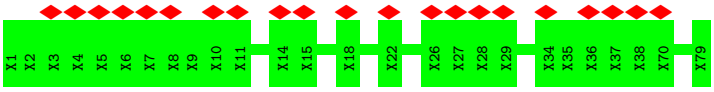
• Molecule 11: Unknown protein fragment

Chain AX: 35% 100%



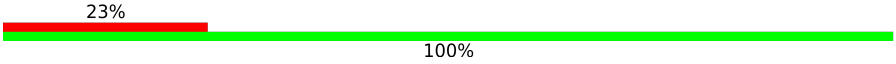
• Molecule 11: Unknown protein fragment

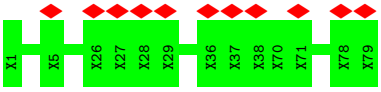
Chain BX: 44% 100%



- Molecule 11: Unknown protein fragment

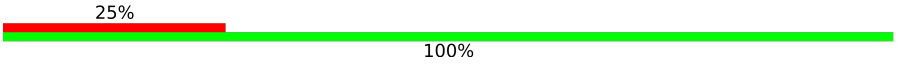
Chain CX:

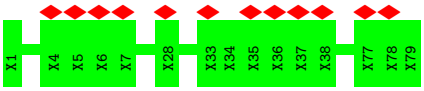




- Molecule 11: Unknown protein fragment

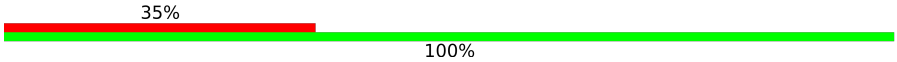
Chain EX:

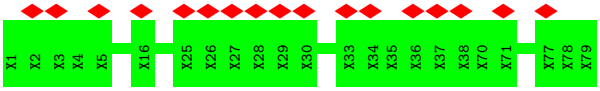




- Molecule 11: Unknown protein fragment

Chain FX:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79720	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.547	Depositor
Minimum map value	-4.150	Depositor
Average map value	0.089	Depositor
Map value standard deviation	0.575	Depositor
Recommended contour level	2.25	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.244, 2.244, 2.244	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	AG	0.32	0/1250	0.57	0/1699
1	Ag	0.31	0/278	0.46	0/377
1	BG	0.32	0/1250	0.58	0/1699
1	Bg	0.29	0/278	0.48	0/377
1	CG	0.33	0/1250	0.57	0/1699
1	Cg	0.28	0/278	0.47	0/377
1	DG	0.32	0/1250	0.56	0/1699
1	Dg	0.30	0/278	0.48	0/377
1	EG	0.31	0/1250	0.57	0/1699
1	Eg	0.30	0/278	0.46	0/377
1	FG	0.31	0/1250	0.56	0/1699
1	Fg	0.30	0/278	0.47	0/377
1	GG	0.32	0/1250	0.56	0/1699
1	Gg	0.31	0/278	0.50	0/377
1	HG	0.31	0/1250	0.56	0/1699
1	Hg	0.29	0/278	0.48	0/377
1	IG	0.32	0/1250	0.56	0/1699
1	Ig	0.31	0/278	0.48	0/377
1	JG	0.32	0/1250	0.56	0/1699
1	Jg	0.31	0/278	0.50	0/377
1	KG	0.33	0/1250	0.59	0/1699
1	Kg	0.31	0/278	0.48	0/377
1	LG	0.34	0/1250	0.56	0/1699
1	Lg	0.31	0/278	0.50	0/377
1	MG	0.33	0/1250	0.58	0/1699
1	Mg	0.32	0/278	0.48	0/377
1	NG	0.34	0/1250	0.58	0/1699
1	OG	0.34	0/1250	0.58	0/1699
1	PG	0.32	0/1250	0.58	0/1699
1	VG	0.31	0/278	0.52	0/377
1	WG	0.30	0/278	0.52	0/377
1	XG	0.32	0/278	0.51	0/377
1	YG	0.34	0/278	0.48	0/377
1	ZG	0.30	0/278	0.52	0/377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AC	0.38	0/1702	0.55	0/2315
2	BC	0.39	0/1702	0.57	0/2315
2	CC	0.39	0/1702	0.59	1/2315 (0.0%)
2	DC	0.38	0/1957	0.55	0/2651
2	EC	0.39	0/1702	0.55	0/2315
2	FC	0.39	0/1702	0.57	0/2315
2	GC	0.39	0/1702	0.55	0/2315
2	HC	0.38	0/1957	0.54	0/2651
2	IC	0.37	0/1957	0.53	0/2651
2	JC	0.39	0/1702	0.56	0/2315
2	KC	0.40	0/1702	0.57	0/2315
2	LC	0.38	0/1957	0.55	0/2651
2	MC	0.36	0/1957	0.54	0/2651
3	AF	0.28	0/490	0.55	0/660
3	Af	0.32	0/456	0.54	0/615
3	BF	0.29	0/490	0.54	0/660
3	Bf	0.30	0/456	0.54	0/615
3	CF	0.28	0/490	0.57	0/660
3	Cf	0.31	0/456	0.53	0/615
3	DF	0.29	0/490	0.54	0/660
3	Df	0.31	0/456	0.54	0/615
3	EF	0.28	0/490	0.53	0/660
3	Ef	0.30	0/456	0.56	0/615
3	FF	0.28	0/490	0.55	0/660
3	Ff	0.33	0/456	0.52	0/615
3	GF	0.30	0/490	0.55	0/660
3	Gf	0.30	0/456	0.54	0/615
3	HF	0.28	0/490	0.55	0/660
3	Hf	0.31	0/456	0.53	0/615
3	IF	0.30	0/490	0.54	0/660
3	If	0.31	0/456	0.57	0/615
3	JF	0.31	0/490	0.54	0/660
3	Jf	0.31	0/456	0.55	0/615
3	KF	0.28	0/490	0.54	0/660
3	Kf	0.31	0/456	0.55	0/615
3	LF	0.28	0/490	0.54	0/660
3	Lf	0.30	0/456	0.54	0/615
3	MF	0.27	0/490	0.55	0/660
3	Mf	0.30	0/456	0.56	0/615
3	VF	0.29	0/490	0.57	0/660
3	WF	0.30	0/490	0.56	0/660
3	XF	0.29	0/490	0.55	0/660
3	YF	0.29	0/490	0.54	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	ZF	0.29	0/490	0.54	0/660
4	AD	0.37	0/1107	0.56	0/1502
4	Ad	0.36	0/1078	0.52	0/1463
4	BD	0.38	0/1107	0.57	0/1502
4	Bd	0.37	0/1078	0.54	0/1463
4	CD	0.38	0/1107	0.58	0/1502
4	Cd	0.36	0/1078	0.54	0/1463
4	DD	0.38	0/1107	0.57	0/1502
4	Dd	0.35	0/1078	0.53	0/1463
4	ED	0.37	0/1107	0.56	0/1502
4	Ed	0.35	0/1078	0.52	0/1463
4	FD	0.37	0/1107	0.56	0/1502
4	Fd	0.35	0/1078	0.52	0/1463
4	GD	0.36	0/1107	0.56	0/1502
4	Gd	0.36	0/1078	0.52	0/1463
4	HD	0.38	0/1107	0.55	0/1502
4	Hd	0.35	0/1078	0.54	0/1463
4	ID	0.37	0/1107	0.55	0/1502
4	Id	0.36	0/1078	0.54	0/1463
4	JD	0.38	0/1107	0.55	0/1502
4	Jd	0.35	0/1078	0.51	0/1463
4	KD	0.39	0/1107	0.55	0/1502
4	Kd	0.35	0/1078	0.52	0/1463
4	LD	0.36	0/1107	0.54	0/1502
4	Ld	0.36	0/1078	0.55	0/1463
4	MD	0.38	0/1107	0.56	0/1502
4	Md	0.34	0/1078	0.52	0/1463
5	AH	0.35	0/2033	0.55	0/2775
5	BH	0.35	0/2033	0.57	0/2775
5	CH	0.35	0/2033	0.56	0/2775
5	DH	0.35	0/2033	0.54	0/2775
5	EH	0.34	0/2033	0.54	0/2775
5	FH	0.34	0/2033	0.55	0/2775
5	GH	0.35	0/2033	0.55	0/2775
5	HH	0.35	0/2033	0.55	0/2775
5	IH	0.34	0/2033	0.55	0/2775
5	JH	0.34	0/2033	0.55	0/2775
5	KH	0.34	0/2033	0.54	0/2775
5	LH	0.35	0/2033	0.55	0/2775
5	MH	0.36	0/2033	0.55	0/2775
5	VH	0.30	0/1921	0.52	0/2620
5	WH	0.29	0/1921	0.53	0/2620
5	XH	0.29	0/1921	0.53	0/2620

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	YH	0.31	0/1921	0.53	0/2620
5	ZH	0.30	0/1921	0.55	0/2620
6	AK	0.38	0/1195	0.56	0/1616
6	BK	0.40	0/1195	0.58	0/1616
6	CK	0.38	0/1195	0.56	0/1616
6	DK	0.39	0/1195	0.56	0/1616
6	EK	0.39	0/1195	0.58	0/1616
6	FK	0.38	0/1195	0.57	0/1616
6	GK	0.39	0/1195	0.57	0/1616
6	HK	0.39	0/1195	0.57	0/1616
6	IK	0.39	0/1195	0.56	0/1616
6	JK	0.40	0/1195	0.57	0/1616
6	KK	0.41	0/1195	0.56	0/1616
6	LK	0.37	0/1195	0.58	0/1616
6	MK	0.39	0/1195	0.56	0/1616
7	AL	0.37	0/1417	0.58	0/1912
7	BL	0.36	0/1417	0.59	0/1912
7	CL	0.38	0/1417	0.59	0/1912
7	DL	0.36	0/1417	0.59	0/1912
7	EL	0.38	0/1417	0.59	0/1912
7	FL	0.39	0/1417	0.59	0/1912
7	GL	0.38	0/1417	0.57	0/1912
7	HL	0.38	0/1417	0.58	0/1912
7	IL	0.39	0/1417	0.60	0/1912
7	JL	0.39	0/1417	0.58	0/1912
7	KL	0.38	0/1417	0.60	0/1912
7	LL	0.38	0/1417	0.59	0/1912
7	ML	0.37	0/1417	0.59	0/1912
8	AM	0.35	0/1678	0.59	0/2262
8	BM	0.35	0/1678	0.60	0/2262
8	CM	0.34	0/1678	0.62	0/2262
8	DM	0.33	0/1678	0.58	0/2262
8	EM	0.33	0/1678	0.60	0/2262
8	FM	0.34	0/1678	0.58	0/2262
8	GM	0.34	0/1678	0.60	0/2262
8	HM	0.34	0/1678	0.58	0/2262
8	IM	0.34	0/1678	0.60	0/2262
8	JM	0.34	0/1678	0.61	1/2262 (0.0%)
8	KM	0.34	0/1678	0.59	0/2262
8	LM	0.34	0/1678	0.58	0/2262
8	MM	0.33	0/1678	0.60	0/2262
9	AN	0.39	0/593	0.55	0/799
9	BN	0.42	0/593	0.61	0/799

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	CN	0.42	0/593	0.54	0/799
9	DN	0.39	0/593	0.55	0/799
9	EN	0.40	0/593	0.55	0/799
9	FN	0.39	0/593	0.56	0/799
9	GN	0.42	0/593	0.54	0/799
9	HN	0.39	0/593	0.56	0/799
9	IN	0.40	0/593	0.57	0/799
9	JN	0.39	0/593	0.58	0/799
9	KN	0.41	0/593	0.59	0/799
9	LN	0.42	0/593	0.56	0/799
9	MN	0.39	0/593	0.57	0/799
All	All	0.35	0/191071	0.56	2/258997 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	LC	0	1
5	CH	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CC	117	LEU	CA-CB-CG	5.73	128.47	115.30
8	JM	134	LEU	CA-CB-CG	5.59	128.17	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	CH	320	LEU	Peptide
2	LC	30	GLY	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	AG	161/1048 (15%)	147 (91%)	14 (9%)	0	100	100
1	Ag	32/1048 (3%)	32 (100%)	0	0	100	100
1	BG	161/1048 (15%)	143 (89%)	18 (11%)	0	100	100
1	Bg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	CG	161/1048 (15%)	146 (91%)	15 (9%)	0	100	100
1	Cg	32/1048 (3%)	32 (100%)	0	0	100	100
1	DG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Dg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	EG	161/1048 (15%)	150 (93%)	11 (7%)	0	100	100
1	Eg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	FG	161/1048 (15%)	149 (92%)	12 (8%)	0	100	100
1	Fg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	GG	161/1048 (15%)	147 (91%)	14 (9%)	0	100	100
1	Gg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	HG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Hg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	IG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	Ig	32/1048 (3%)	32 (100%)	0	0	100	100
1	JG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Jg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	KG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Kg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	LG	161/1048 (15%)	150 (93%)	11 (7%)	0	100	100
1	Lg	32/1048 (3%)	32 (100%)	0	0	100	100
1	MG	161/1048 (15%)	147 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Mg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	NG	161/1048 (15%)	151 (94%)	10 (6%)	0	100	100
1	OG	161/1048 (15%)	148 (92%)	13 (8%)	0	100	100
1	PG	161/1048 (15%)	149 (92%)	12 (8%)	0	100	100
1	VG	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	WG	32/1048 (3%)	32 (100%)	0	0	100	100
1	XG	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	YG	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
2	AC	207/303 (68%)	191 (92%)	16 (8%)	0	100	100
2	BC	207/303 (68%)	195 (94%)	12 (6%)	0	100	100
2	CC	207/303 (68%)	188 (91%)	19 (9%)	0	100	100
2	DC	241/303 (80%)	229 (95%)	12 (5%)	0	100	100
2	EC	207/303 (68%)	192 (93%)	15 (7%)	0	100	100
2	FC	207/303 (68%)	189 (91%)	18 (9%)	0	100	100
2	GC	207/303 (68%)	192 (93%)	15 (7%)	0	100	100
2	HC	241/303 (80%)	227 (94%)	14 (6%)	0	100	100
2	IC	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
2	JC	207/303 (68%)	187 (90%)	20 (10%)	0	100	100
2	KC	207/303 (68%)	190 (92%)	17 (8%)	0	100	100
2	LC	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
2	MC	241/303 (80%)	229 (95%)	12 (5%)	0	100	100
3	AF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Af	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	BF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
3	Bf	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	CF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Cf	57/269 (21%)	51 (90%)	6 (10%)	0	100	100
3	DF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Df	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	EF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ef	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	FF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	Ff	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	GF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Gf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	HF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Hf	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	IF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	JF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Jf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	KF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
3	Kf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	LF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Lf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	MF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Mf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	VF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	WF	61/269 (23%)	54 (88%)	7 (12%)	0	100	100
3	XF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	YF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	ZF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
4	AD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
4	Ad	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
4	BD	138/163 (85%)	127 (92%)	10 (7%)	1 (1%)	22	62
4	Bd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
4	CD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
4	Cd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
4	DD	138/163 (85%)	127 (92%)	11 (8%)	0	100	100
4	Dd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
4	ED	138/163 (85%)	132 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Ed	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
4	FD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
4	Fd	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
4	GD	138/163 (85%)	128 (93%)	10 (7%)	0	100	100
4	Gd	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
4	HD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
4	Hd	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
4	ID	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
4	Id	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
4	JD	138/163 (85%)	129 (94%)	9 (6%)	0	100	100
4	Jd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
4	KD	138/163 (85%)	129 (94%)	9 (6%)	0	100	100
4	Kd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
4	LD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
4	Ld	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
4	MD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
4	Md	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
5	AH	256/361 (71%)	235 (92%)	21 (8%)	0	100	100
5	BH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
5	CH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	DH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
5	EH	256/361 (71%)	247 (96%)	9 (4%)	0	100	100
5	FH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
5	GH	256/361 (71%)	246 (96%)	10 (4%)	0	100	100
5	HH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	IH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
5	JH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
5	KH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	LH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100
5	MH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	VH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	WH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
5	XH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
5	YH	239/361 (66%)	230 (96%)	9 (4%)	0	100	100
5	ZH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
6	AK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
6	BK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
6	CK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
6	DK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
6	EK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
6	FK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
6	GK	149/189 (79%)	139 (93%)	10 (7%)	0	100	100
6	HK	149/189 (79%)	146 (98%)	3 (2%)	0	100	100
6	IK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	JK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	KK	149/189 (79%)	139 (93%)	10 (7%)	0	100	100
6	LK	149/189 (79%)	140 (94%)	9 (6%)	0	100	100
6	MK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
7	AL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
7	BL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	CL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	DL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
7	EL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	FL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
7	GL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
7	HL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
7	IL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	JL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
7	KL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	LL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	ML	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
8	AM	206/320 (64%)	190 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BM	206/320 (64%)	187 (91%)	19 (9%)	0	100	100
8	CM	206/320 (64%)	187 (91%)	19 (9%)	0	100	100
8	DM	206/320 (64%)	189 (92%)	17 (8%)	0	100	100
8	EM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
8	FM	206/320 (64%)	185 (90%)	21 (10%)	0	100	100
8	GM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
8	HM	206/320 (64%)	195 (95%)	11 (5%)	0	100	100
8	IM	206/320 (64%)	186 (90%)	20 (10%)	0	100	100
8	JM	206/320 (64%)	188 (91%)	18 (9%)	0	100	100
8	KM	206/320 (64%)	190 (92%)	16 (8%)	0	100	100
8	LM	206/320 (64%)	185 (90%)	21 (10%)	0	100	100
8	MM	206/320 (64%)	189 (92%)	17 (8%)	0	100	100
9	AN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	BN	76/124 (61%)	67 (88%)	9 (12%)	0	100	100
9	CN	76/124 (61%)	66 (87%)	10 (13%)	0	100	100
9	DN	76/124 (61%)	66 (87%)	10 (13%)	0	100	100
9	EN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	FN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	GN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
9	HN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
9	IN	76/124 (61%)	72 (95%)	4 (5%)	0	100	100
9	JN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
9	KN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	LN	76/124 (61%)	66 (87%)	10 (13%)	0	100	100
9	MN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
All	All	23724/70112 (34%)	22279 (94%)	1444 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	28	PRO

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	AG	135/765 (18%)	109 (81%)	26 (19%)	1 9
1	Ag	31/765 (4%)	26 (84%)	5 (16%)	2 15
1	BG	135/765 (18%)	110 (82%)	25 (18%)	1 10
1	Bg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	CG	135/765 (18%)	108 (80%)	27 (20%)	1 8
1	Cg	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	DG	135/765 (18%)	115 (85%)	20 (15%)	3 17
1	Dg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	EG	135/765 (18%)	111 (82%)	24 (18%)	2 12
1	Eg	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	FG	135/765 (18%)	116 (86%)	19 (14%)	3 18
1	Fg	31/765 (4%)	28 (90%)	3 (10%)	8 29
1	GG	135/765 (18%)	113 (84%)	22 (16%)	2 14
1	Gg	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	HG	135/765 (18%)	115 (85%)	20 (15%)	3 17
1	Hg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	IG	135/765 (18%)	122 (90%)	13 (10%)	8 29
1	Ig	31/765 (4%)	28 (90%)	3 (10%)	8 29
1	JG	135/765 (18%)	117 (87%)	18 (13%)	4 20
1	Jg	31/765 (4%)	19 (61%)	12 (39%)	0 0
1	KG	135/765 (18%)	114 (84%)	21 (16%)	2 16
1	Kg	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	LG	135/765 (18%)	117 (87%)	18 (13%)	4 20
1	Lg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	MG	135/765 (18%)	106 (78%)	29 (22%)	1 6
1	Mg	31/765 (4%)	27 (87%)	4 (13%)	4 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NG	135/765 (18%)	108 (80%)	27 (20%)	1	8
1	OG	135/765 (18%)	112 (83%)	23 (17%)	2	13
1	PG	135/765 (18%)	114 (84%)	21 (16%)	2	16
1	VG	31/765 (4%)	27 (87%)	4 (13%)	4	20
1	WG	31/765 (4%)	27 (87%)	4 (13%)	4	20
1	XG	31/765 (4%)	25 (81%)	6 (19%)	1	9
1	YG	31/765 (4%)	29 (94%)	2 (6%)	17	44
1	ZG	31/765 (4%)	25 (81%)	6 (19%)	1	9
2	AC	178/257 (69%)	151 (85%)	27 (15%)	3	16
2	BC	178/257 (69%)	150 (84%)	28 (16%)	2	15
2	CC	178/257 (69%)	148 (83%)	30 (17%)	2	13
2	DC	203/257 (79%)	178 (88%)	25 (12%)	4	22
2	EC	178/257 (69%)	154 (86%)	24 (14%)	4	19
2	FC	178/257 (69%)	149 (84%)	29 (16%)	2	14
2	GC	178/257 (69%)	154 (86%)	24 (14%)	4	19
2	HC	203/257 (79%)	180 (89%)	23 (11%)	6	24
2	IC	203/257 (79%)	177 (87%)	26 (13%)	4	21
2	JC	178/257 (69%)	151 (85%)	27 (15%)	3	16
2	KC	178/257 (69%)	145 (82%)	33 (18%)	1	10
2	LC	203/257 (79%)	187 (92%)	16 (8%)	12	38
2	MC	203/257 (79%)	178 (88%)	25 (12%)	4	22
3	AF	53/237 (22%)	40 (76%)	13 (24%)	0	4
3	Af	49/237 (21%)	37 (76%)	12 (24%)	0	4
3	BF	53/237 (22%)	46 (87%)	7 (13%)	4	20
3	Bf	49/237 (21%)	45 (92%)	4 (8%)	11	36
3	CF	53/237 (22%)	43 (81%)	10 (19%)	1	9
3	Cf	49/237 (21%)	39 (80%)	10 (20%)	1	7
3	DF	53/237 (22%)	47 (89%)	6 (11%)	6	24
3	Df	49/237 (21%)	46 (94%)	3 (6%)	18	46
3	EF	53/237 (22%)	47 (89%)	6 (11%)	6	24
3	Ef	49/237 (21%)	42 (86%)	7 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FF	53/237 (22%)	47 (89%)	6 (11%)	6	24
3	Ff	49/237 (21%)	41 (84%)	8 (16%)	2	14
3	GF	53/237 (22%)	47 (89%)	6 (11%)	6	24
3	Gf	49/237 (21%)	43 (88%)	6 (12%)	5	22
3	HF	53/237 (22%)	46 (87%)	7 (13%)	4	20
3	Hf	49/237 (21%)	42 (86%)	7 (14%)	3	18
3	IF	53/237 (22%)	45 (85%)	8 (15%)	3	16
3	If	49/237 (21%)	38 (78%)	11 (22%)	1	6
3	JF	53/237 (22%)	45 (85%)	8 (15%)	3	16
3	Jf	49/237 (21%)	39 (80%)	10 (20%)	1	7
3	KF	53/237 (22%)	46 (87%)	7 (13%)	4	20
3	Kf	49/237 (21%)	43 (88%)	6 (12%)	5	22
3	LF	53/237 (22%)	47 (89%)	6 (11%)	6	24
3	Lf	49/237 (21%)	43 (88%)	6 (12%)	5	22
3	MF	53/237 (22%)	46 (87%)	7 (13%)	4	20
3	Mf	49/237 (21%)	43 (88%)	6 (12%)	5	22
3	VF	53/237 (22%)	45 (85%)	8 (15%)	3	16
3	WF	53/237 (22%)	45 (85%)	8 (15%)	3	16
3	XF	53/237 (22%)	44 (83%)	9 (17%)	2	13
3	YF	53/237 (22%)	46 (87%)	7 (13%)	4	20
3	ZF	53/237 (22%)	43 (81%)	10 (19%)	1	9
4	AD	121/139 (87%)	103 (85%)	18 (15%)	3	16
4	Ad	118/139 (85%)	105 (89%)	13 (11%)	6	25
4	BD	121/139 (87%)	107 (88%)	14 (12%)	5	23
4	Bd	118/139 (85%)	100 (85%)	18 (15%)	2	16
4	CD	121/139 (87%)	102 (84%)	19 (16%)	2	15
4	Cd	118/139 (85%)	105 (89%)	13 (11%)	6	25
4	DD	121/139 (87%)	107 (88%)	14 (12%)	5	23
4	Dd	118/139 (85%)	102 (86%)	16 (14%)	3	19
4	ED	121/139 (87%)	110 (91%)	11 (9%)	9	31
4	Ed	118/139 (85%)	104 (88%)	14 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	FD	121/139 (87%)	105 (87%)	16 (13%)	4	20
4	Fd	118/139 (85%)	103 (87%)	15 (13%)	4	21
4	GD	121/139 (87%)	105 (87%)	16 (13%)	4	20
4	Gd	118/139 (85%)	104 (88%)	14 (12%)	5	22
4	HD	121/139 (87%)	111 (92%)	10 (8%)	11	36
4	Hd	118/139 (85%)	105 (89%)	13 (11%)	6	25
4	ID	121/139 (87%)	112 (93%)	9 (7%)	13	40
4	Id	118/139 (85%)	103 (87%)	15 (13%)	4	21
4	JD	121/139 (87%)	108 (89%)	13 (11%)	6	26
4	Jd	118/139 (85%)	108 (92%)	10 (8%)	10	36
4	KD	121/139 (87%)	113 (93%)	8 (7%)	16	43
4	Kd	118/139 (85%)	107 (91%)	11 (9%)	9	30
4	LD	121/139 (87%)	105 (87%)	16 (13%)	4	20
4	Ld	118/139 (85%)	106 (90%)	12 (10%)	7	27
4	MD	121/139 (87%)	111 (92%)	10 (8%)	11	36
4	Md	118/139 (85%)	105 (89%)	13 (11%)	6	25
5	AH	220/300 (73%)	191 (87%)	29 (13%)	4	20
5	BH	220/300 (73%)	190 (86%)	30 (14%)	3	19
5	CH	220/300 (73%)	190 (86%)	30 (14%)	3	19
5	DH	220/300 (73%)	193 (88%)	27 (12%)	4	22
5	EH	220/300 (73%)	185 (84%)	35 (16%)	2	15
5	FH	220/300 (73%)	191 (87%)	29 (13%)	4	20
5	GH	220/300 (73%)	198 (90%)	22 (10%)	7	28
5	HH	220/300 (73%)	189 (86%)	31 (14%)	3	18
5	IH	220/300 (73%)	194 (88%)	26 (12%)	5	23
5	JH	220/300 (73%)	201 (91%)	19 (9%)	10	35
5	KH	220/300 (73%)	200 (91%)	20 (9%)	9	31
5	LH	220/300 (73%)	194 (88%)	26 (12%)	5	23
5	MH	220/300 (73%)	194 (88%)	26 (12%)	5	23
5	VH	207/300 (69%)	181 (87%)	26 (13%)	4	21
5	WH	207/300 (69%)	182 (88%)	25 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	XH	207/300 (69%)	178 (86%)	29 (14%)	3	19
5	YH	207/300 (69%)	182 (88%)	25 (12%)	5	22
5	ZH	207/300 (69%)	178 (86%)	29 (14%)	3	19
6	AK	129/163 (79%)	109 (84%)	20 (16%)	2	16
6	BK	129/163 (79%)	118 (92%)	11 (8%)	10	36
6	CK	129/163 (79%)	111 (86%)	18 (14%)	3	19
6	DK	129/163 (79%)	115 (89%)	14 (11%)	6	25
6	EK	129/163 (79%)	107 (83%)	22 (17%)	2	13
6	FK	129/163 (79%)	108 (84%)	21 (16%)	2	14
6	GK	129/163 (79%)	116 (90%)	13 (10%)	7	27
6	HK	129/163 (79%)	111 (86%)	18 (14%)	3	19
6	IK	129/163 (79%)	121 (94%)	8 (6%)	18	45
6	JK	129/163 (79%)	109 (84%)	20 (16%)	2	16
6	KK	129/163 (79%)	109 (84%)	20 (16%)	2	16
6	LK	129/163 (79%)	110 (85%)	19 (15%)	3	17
6	MK	129/163 (79%)	113 (88%)	16 (12%)	4	21
7	AL	148/203 (73%)	135 (91%)	13 (9%)	10	33
7	BL	148/203 (73%)	135 (91%)	13 (9%)	10	33
7	CL	148/203 (73%)	129 (87%)	19 (13%)	4	21
7	DL	148/203 (73%)	128 (86%)	20 (14%)	4	19
7	EL	148/203 (73%)	137 (93%)	11 (7%)	13	40
7	FL	148/203 (73%)	128 (86%)	20 (14%)	4	19
7	GL	148/203 (73%)	131 (88%)	17 (12%)	5	23
7	HL	148/203 (73%)	134 (90%)	14 (10%)	8	29
7	IL	148/203 (73%)	133 (90%)	15 (10%)	7	27
7	JL	148/203 (73%)	133 (90%)	15 (10%)	7	27
7	KL	148/203 (73%)	128 (86%)	20 (14%)	4	19
7	LL	148/203 (73%)	133 (90%)	15 (10%)	7	27
7	ML	148/203 (73%)	132 (89%)	16 (11%)	6	26
8	AM	175/276 (63%)	154 (88%)	21 (12%)	5	22
8	BM	175/276 (63%)	147 (84%)	28 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CM	175/276 (63%)	147 (84%)	28 (16%)	2	15
8	DM	175/276 (63%)	152 (87%)	23 (13%)	4	20
8	EM	175/276 (63%)	147 (84%)	28 (16%)	2	15
8	FM	175/276 (63%)	148 (85%)	27 (15%)	2	16
8	GM	175/276 (63%)	152 (87%)	23 (13%)	4	20
8	HM	175/276 (63%)	145 (83%)	30 (17%)	2	13
8	IM	175/276 (63%)	148 (85%)	27 (15%)	2	16
8	JM	175/276 (63%)	155 (89%)	20 (11%)	5	24
8	KM	175/276 (63%)	151 (86%)	24 (14%)	3	19
8	LM	175/276 (63%)	151 (86%)	24 (14%)	3	19
8	MM	175/276 (63%)	147 (84%)	28 (16%)	2	15
9	AN	66/107 (62%)	60 (91%)	6 (9%)	9	31
9	BN	66/107 (62%)	58 (88%)	8 (12%)	5	22
9	CN	66/107 (62%)	57 (86%)	9 (14%)	3	19
9	DN	66/107 (62%)	57 (86%)	9 (14%)	3	19
9	EN	66/107 (62%)	55 (83%)	11 (17%)	2	14
9	FN	66/107 (62%)	51 (77%)	15 (23%)	1	6
9	GN	66/107 (62%)	56 (85%)	10 (15%)	3	16
9	HN	66/107 (62%)	58 (88%)	8 (12%)	5	22
9	IN	66/107 (62%)	57 (86%)	9 (14%)	3	19
9	JN	66/107 (62%)	56 (85%)	10 (15%)	3	16
9	KN	66/107 (62%)	55 (83%)	11 (17%)	2	14
9	LN	66/107 (62%)	57 (86%)	9 (14%)	3	19
9	MN	66/107 (62%)	57 (86%)	9 (14%)	3	19
All	All	20484/55449 (37%)	17744 (87%)	2740 (13%)	7	20

5 of 2740 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	JC	248	ILE
9	EN	51	CYS
2	MC	157	VAL
2	JC	242	ASP
1	GG	1037	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
5	YH	159	ASN
9	FN	115	GLN
5	CH	205	GLN
1	NG	1020	GLN
2	JC	218	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	JX	1
11	BX	1
11	VX	1
11	KX	1
11	DX	1

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Mol	Chain	Number of breaks
11	YX	1
11	XX	1
11	ZX	1
11	LX	1
11	GX	1
11	EX	1
11	MX	1
11	WX	1
11	HX	1
11	CX	1
11	IX	1
11	FX	1
11	AX	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	JX	38:UNK	C	70:UNK	N	26.33
1	BX	38:UNK	C	70:UNK	N	25.95
1	VX	38:UNK	C	70:UNK	N	25.89
1	KX	38:UNK	C	70:UNK	N	25.61
1	DX	38:UNK	C	70:UNK	N	25.45

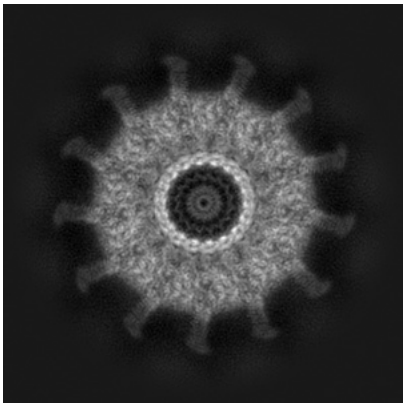
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24018. These allow visual inspection of the internal detail of the map and identification of artifacts.

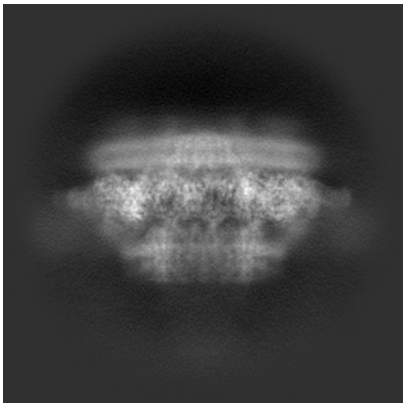
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

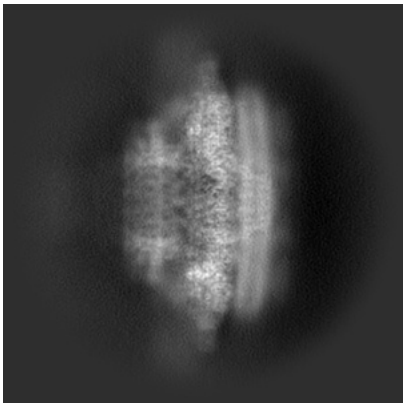
6.1.1 Primary map



X



Y

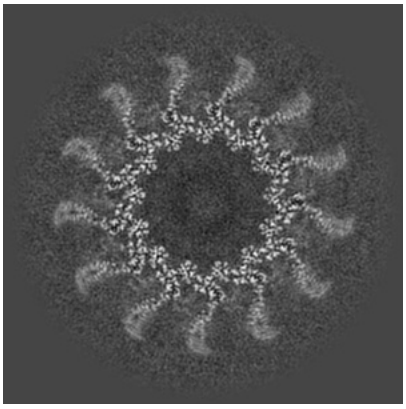


Z

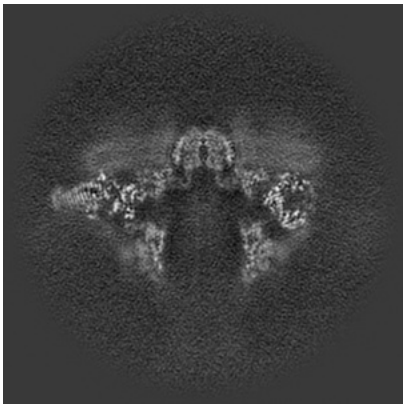
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 125



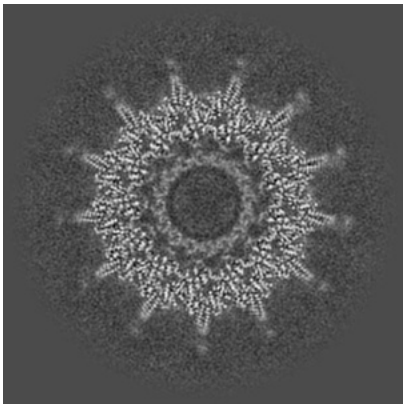
Y Index: 125

Z Index: 125

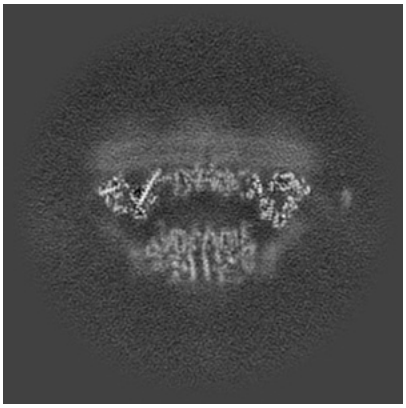
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

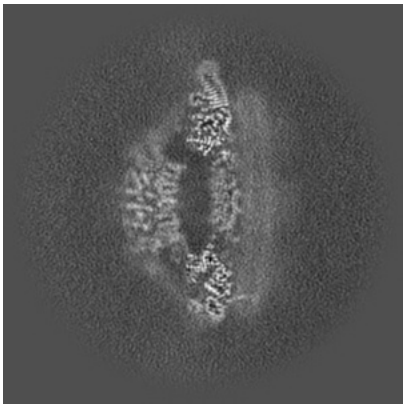
6.3.1 Primary map



X Index: 134



Y Index: 101



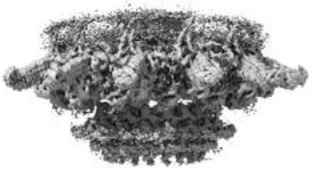
Z Index: 151

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 2.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

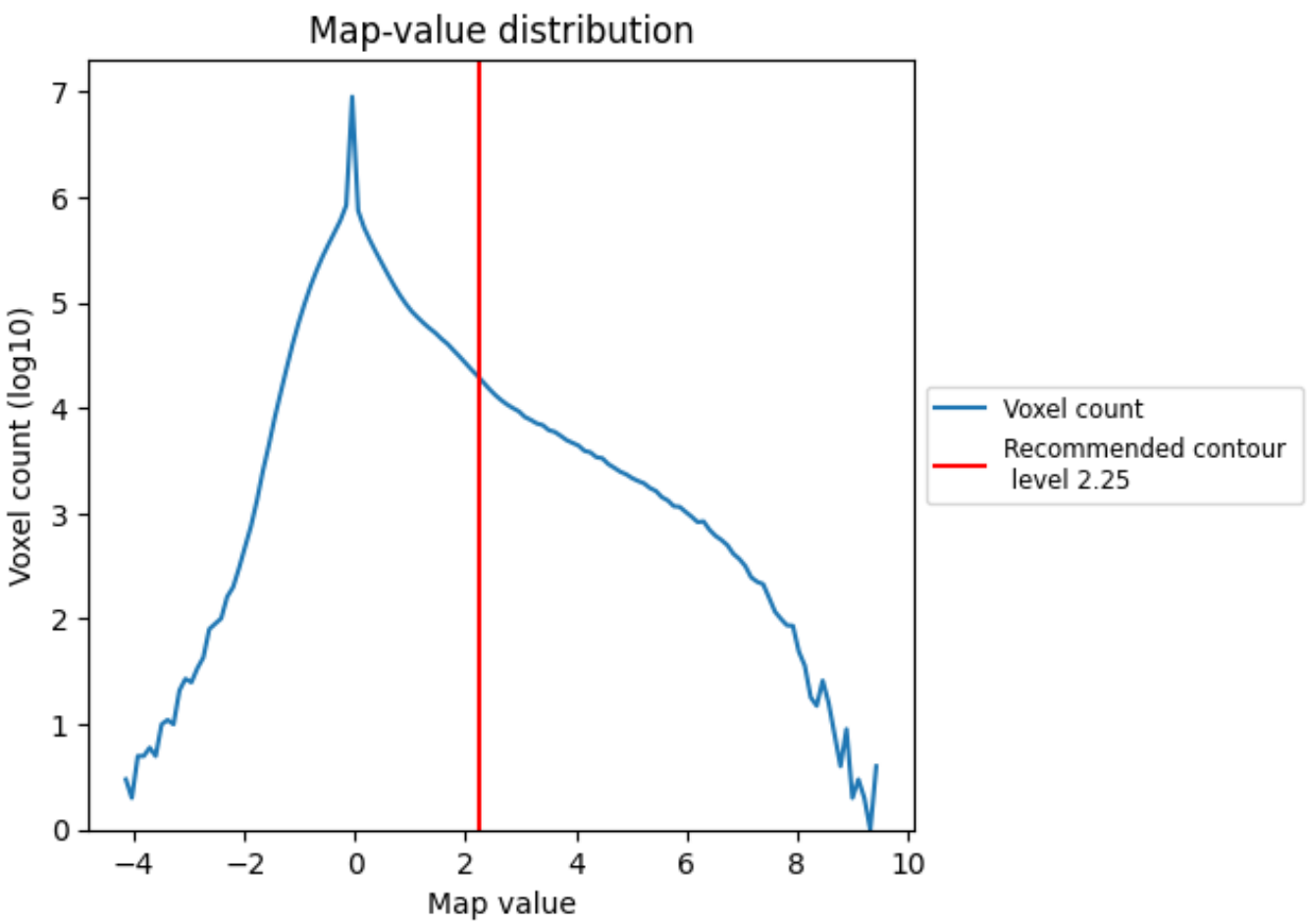
6.5 Mask visualisation (i)

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

7 Map analysis (i)

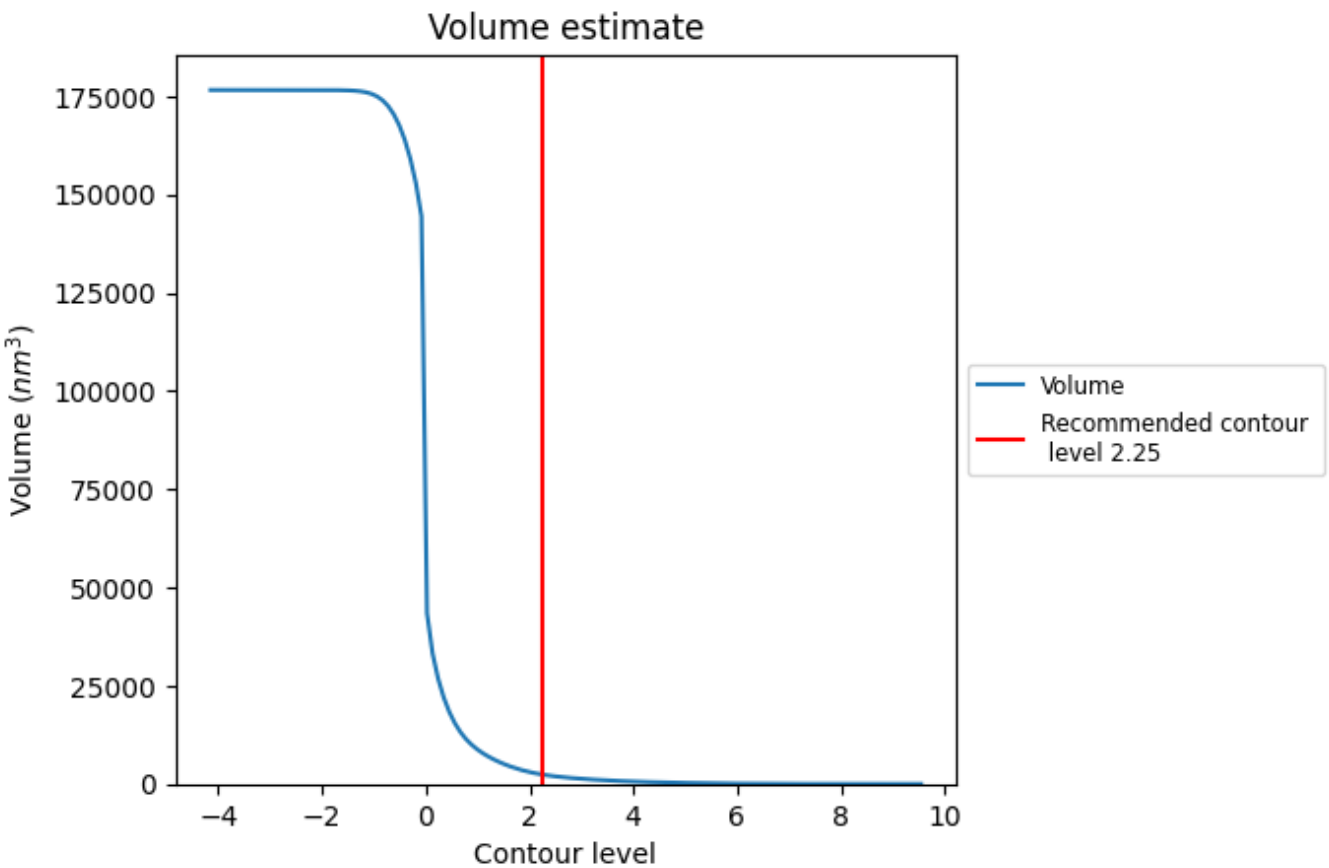
This section contains the results of statistical analysis of the map.

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.

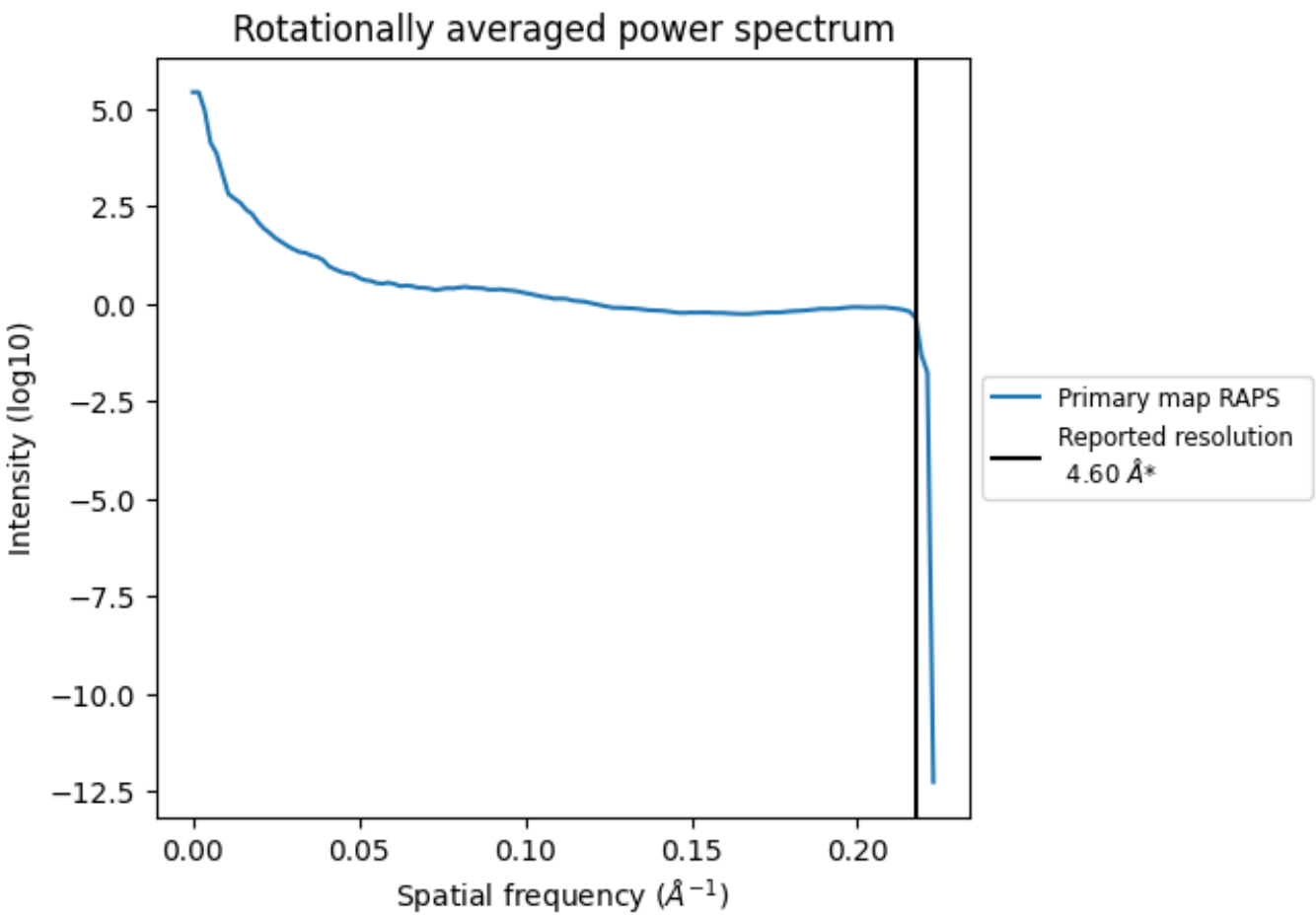
7.2 Volume estimate (i)



The volume at the recommended contour level is 2389 nm^3; this corresponds to an approximate mass of 2158 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 0.217 Å^{-1}

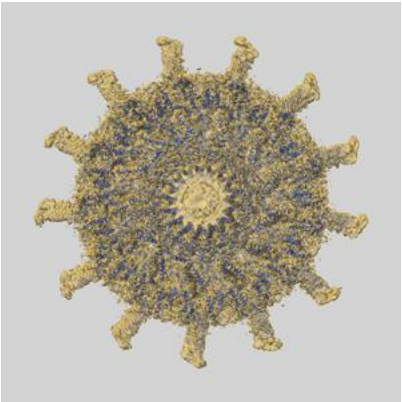
8 Fourier-Shell correlation (i)

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

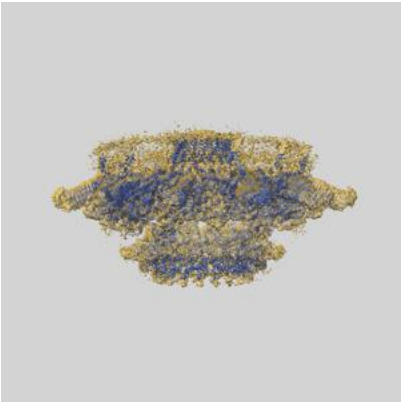
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24018 and PDB model 7MUQ. Per-residue inclusion information can be found in section 3 on page 22.

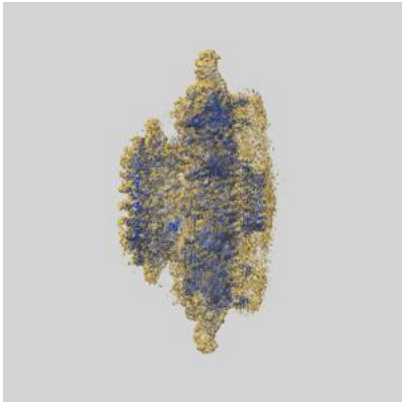
9.1 Map-model overlay (i)



X



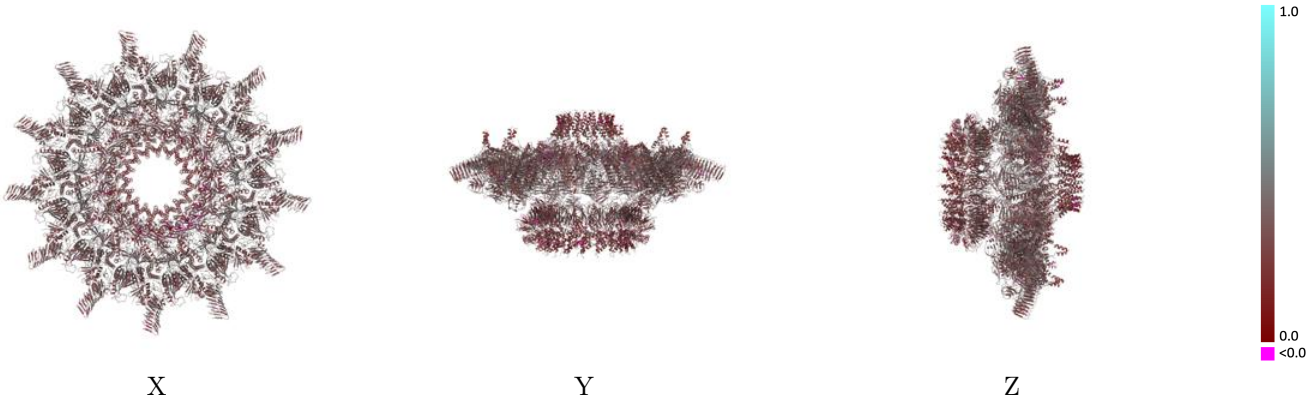
Y



Z

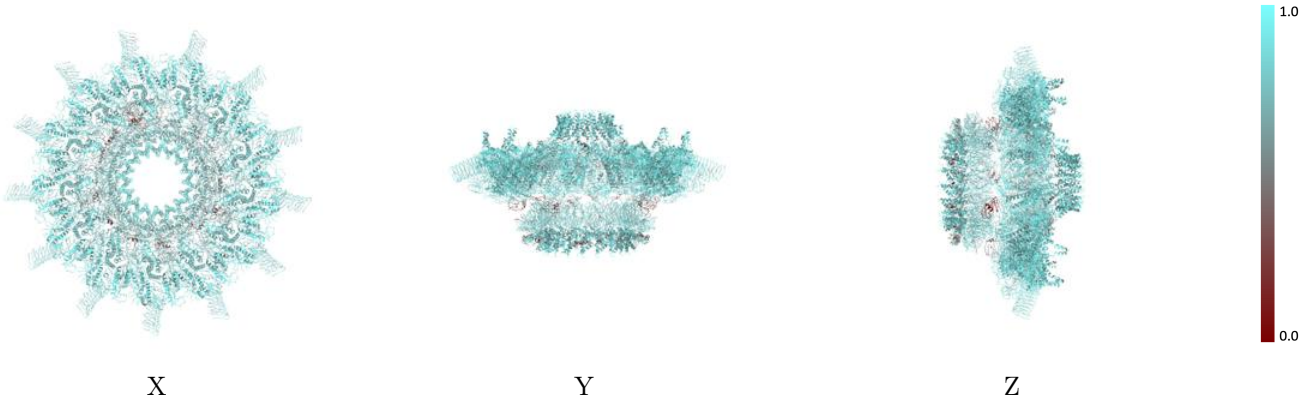
The images above show the 3D surface view of the map at the recommended contour level 2.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



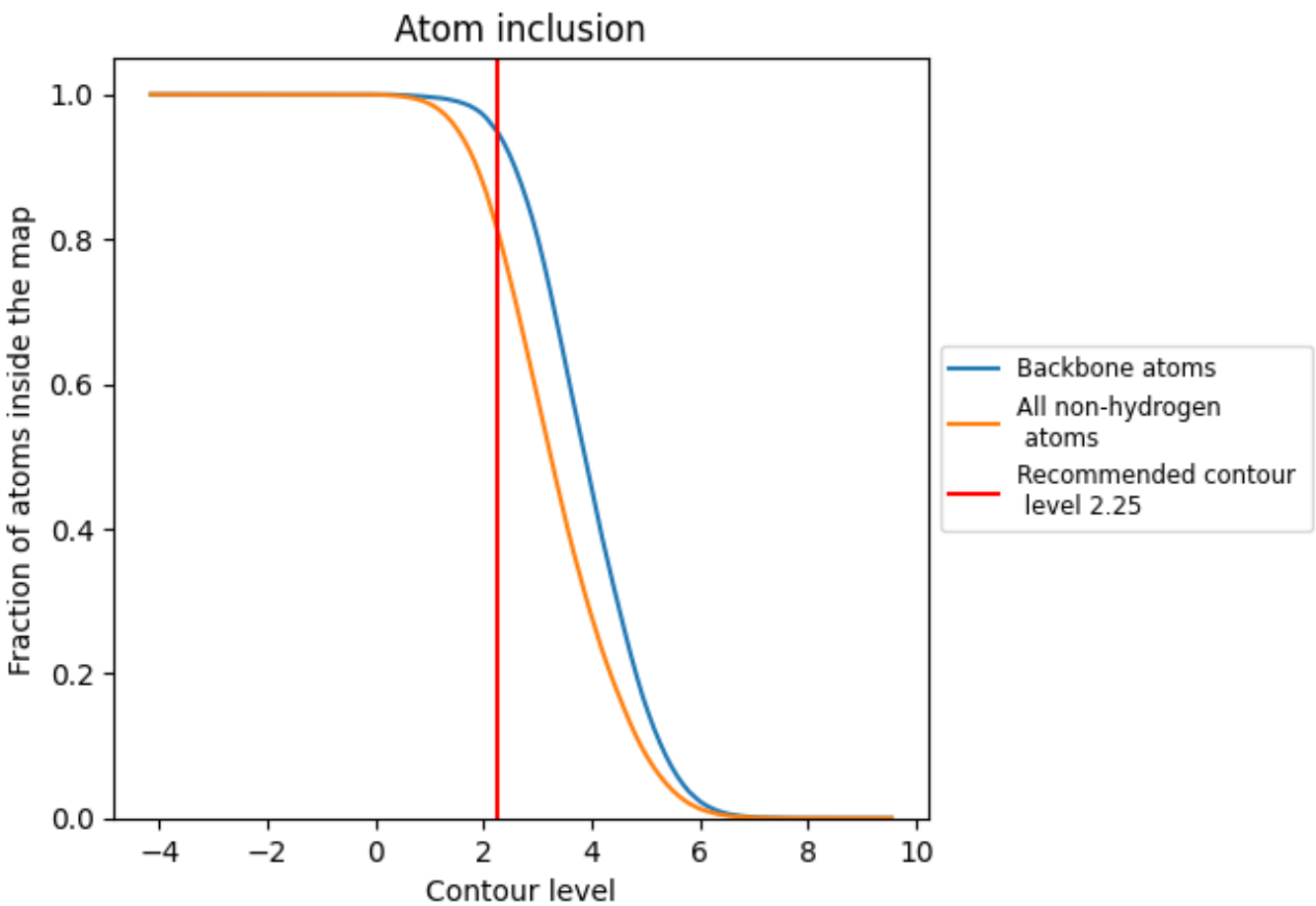
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.25).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8148	0.3350
AC	0.8595	0.3620
AD	0.8418	0.3710
AF	0.7792	0.2470
AG	0.7069	0.2330
AH	0.8126	0.3320
AK	0.8486	0.3780
AL	0.8629	0.3550
AM	0.8349	0.3520
AN	0.8024	0.3790
AU	1.0000	0.4870
AX	0.5667	0.2380
Ad	0.8569	0.3580
Af	0.8041	0.3300
Ag	0.8493	0.3040
BC	0.8730	0.3660
BD	0.8464	0.3790
BF	0.7792	0.2670
BG	0.6864	0.2220
BH	0.8101	0.3300
BK	0.8513	0.3730
BL	0.8643	0.3530
BM	0.8423	0.3600
BN	0.8549	0.3800
BU	1.0000	0.5100
BX	0.5583	0.2280
Bd	0.8453	0.3640
Bf	0.8405	0.3260
Bg	0.8235	0.3030
CC	0.8620	0.3660
CD	0.8652	0.3770
CF	0.7919	0.2800
CG	0.6741	0.2220
CH	0.8383	0.3380
CK	0.8609	0.3650

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Chain	Atom inclusion	Q-score
CL	0.8658	0.3510
CM	0.8535	0.3490
CN	0.8444	0.3790
CU	1.0000	0.4610
CX	0.7250	0.3180
Cd	0.8521	0.3640
Cf	0.8200	0.3220
Cg	0.8493	0.2960
DC	0.8100	0.3530
DD	0.8558	0.3670
DF	0.7643	0.2450
DG	0.7192	0.2400
DH	0.8280	0.3300
DK	0.8478	0.3720
DL	0.8540	0.3500
DM	0.8504	0.3510
DN	0.8182	0.3700
DU	1.0000	0.4710
DX	0.6167	0.2590
Dd	0.8655	0.3620
Df	0.8360	0.3250
Dg	0.8272	0.2810
EC	0.8380	0.3520
ED	0.8436	0.3740
EF	0.8132	0.2610
EG	0.7069	0.2470
EH	0.8311	0.3220
EK	0.8513	0.3730
EL	0.8473	0.3520
EM	0.8467	0.3520
EN	0.8112	0.3730
EU	1.0000	0.4780
EX	0.7208	0.2470
Ed	0.8444	0.3490
Ef	0.8246	0.3470
Eg	0.8051	0.2740
FC	0.8620	0.3580
FD	0.8436	0.3680
FF	0.7665	0.2560
FG	0.7176	0.2540
FH	0.8419	0.3240
FK	0.8583	0.3710

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Chain	Atom inclusion	Q-score
FL	0.8599	0.3500
FM	0.8547	0.3540
FN	0.8549	0.3970
FU	1.0000	0.5080
FX	0.5958	0.2440
Fd	0.8463	0.3530
Ff	0.8565	0.3430
Fg	0.7978	0.2630
GC	0.8552	0.3660
GD	0.8483	0.3710
GF	0.7962	0.2650
GG	0.7274	0.2700
GH	0.8208	0.3260
GK	0.8696	0.3790
GL	0.8755	0.3560
GM	0.8417	0.3520
GN	0.8531	0.3860
GU	0.9778	0.4780
GX	0.7333	0.2880
Gd	0.8559	0.3620
Gf	0.7995	0.3160
Gg	0.8566	0.2720
HC	0.8185	0.3550
HD	0.8399	0.3820
HF	0.7495	0.2500
HG	0.7406	0.2810
HH	0.8388	0.3350
HK	0.8574	0.3750
HL	0.8762	0.3540
HM	0.8523	0.3550
HN	0.8357	0.3850
HU	0.9778	0.5230
HX	0.6375	0.2570
Hd	0.8521	0.3510
Hf	0.8200	0.3240
Hg	0.8750	0.3090
IC	0.8057	0.3470
ID	0.8361	0.3690
IF	0.7601	0.2630
IG	0.7356	0.2920
IH	0.8208	0.3290
IK	0.8548	0.3760

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Chain	Atom inclusion	Q-score
IL	0.8554	0.3550
IM	0.8485	0.3540
IN	0.8112	0.3860
IU	1.0000	0.5190
IX	0.6792	0.2750
Id	0.8540	0.3610
If	0.8474	0.3300
Ig	0.8382	0.2770
JC	0.8472	0.3620
JD	0.8380	0.3750
JF	0.8025	0.2510
JG	0.7545	0.2950
JH	0.8255	0.3320
JK	0.8539	0.3750
JL	0.8614	0.3600
JM	0.8585	0.3540
JN	0.8252	0.3750
JU	0.9778	0.5050
JX	0.6250	0.2110
Jd	0.8501	0.3660
Jf	0.8178	0.3440
Jg	0.8382	0.2980
KC	0.8540	0.3650
KD	0.8418	0.3680
KF	0.7877	0.2610
KG	0.7545	0.3050
KH	0.8316	0.3340
KK	0.8688	0.3770
KL	0.8643	0.3520
KM	0.8318	0.3570
KN	0.8584	0.3910
KU	0.9778	0.4860
KX	0.6625	0.2820
Kd	0.8626	0.3620
Kf	0.7927	0.3310
Kg	0.8382	0.3100
LC	0.8153	0.3410
LD	0.8502	0.3630
LF	0.7919	0.2840
LG	0.7545	0.3100
LH	0.8152	0.3330
LK	0.8600	0.3690

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Chain	Atom inclusion	Q-score
LL	0.8755	0.3590
LM	0.8281	0.3450
LN	0.8374	0.3890
LU	1.0000	0.4790
LX	0.6375	0.2470
Ld	0.8636	0.3640
Lf	0.8497	0.3280
Lg	0.8456	0.2740
MC	0.8206	0.3530
MD	0.8455	0.3630
MF	0.7367	0.2480
MG	0.7348	0.2560
MH	0.8044	0.3280
MK	0.8591	0.3770
ML	0.8643	0.3650
MM	0.8430	0.3620
MN	0.8234	0.3820
MU	1.0000	0.4830
MX	0.5667	0.2530
Md	0.8521	0.3590
Mf	0.8269	0.3410
Mg	0.8382	0.2750
NG	0.7266	0.2380
OG	0.7791	0.2970
PG	0.7340	0.2450
VF	0.7983	0.2570
VG	0.7684	0.2800
VH	0.7212	0.3100
VX	0.6375	0.2660
WF	0.8047	0.2480
WG	0.7721	0.2560
WH	0.6652	0.3050
WX	0.6625	0.2720
XF	0.8132	0.2470
XG	0.7978	0.2560
XH	0.6065	0.2980
XX	0.6625	0.2760
YF	0.8089	0.2640
YG	0.8125	0.2890
YH	0.7272	0.3090
YX	0.6167	0.2650
ZF	0.7452	0.2580

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Chain	Atom inclusion	Q-score
ZG	0.7978	0.2780
ZH	0.5245	0.2790
ZX	0.7458	0.3150