wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 09:17 PM EST

PDB ID	:	7MUY
EMDB ID	:	EMD-24026
Title	:	Reconstruction of the Legionella pneumophila Dot/Icm T4SS 3DVA Map 5
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:

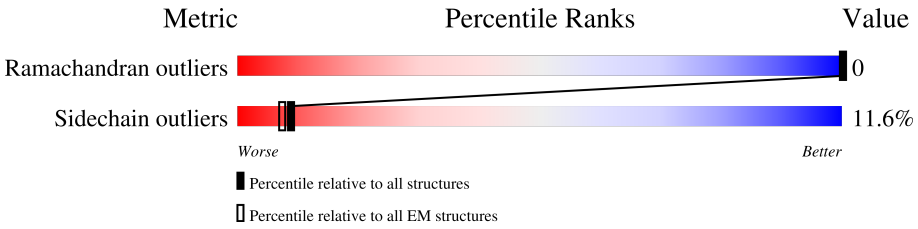
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	14% 84%
1	Ag	1048	97%
1	BG	1048	14% 84%
1	Bg	1048	97%
1	CG	1048	5% 14% 84%
1	Cg	1048	97%
1	DG	1048	6% 14% 84%
1	Dg	1048	97%
1	EG	1048	5% 14% 84%

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Mol	Chain	Length	Quality of chain
1	Eg	1048	97%
1	FG	1048	5% 14% 84%
1	Fg	1048	97%
1	GG	1048	5% 14% 84%
1	Gg	1048	97%
1	HG	1048	5% 14% 84%
1	Hg	1048	97%
1	IG	1048	5% 14% 84%
1	Ig	1048	97%
1	JG	1048	5% 14% 84%
1	Jg	1048	97%
1	KG	1048	5% 14% 84%
1	Kg	1048	97%
1	LG	1048	14% 84%
1	Lg	1048	97%
1	MG	1048	14% 84%
1	Mg	1048	97%
1	NG	1048	15% 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	AD	163	77% 9% 14%
2	Ad	163	77% 7% 16%
2	BD	163	81% 5% 14%
2	Bd	163	77% 7% 16%
2	CD	163	76% 10% 14%
2	Cd	163	75% 9% 16%
2	DD	163	80% 6% 14%
2	Dd	163	77% 7% 16%
2	ED	163	82% 14%
2	Ed	163	77% 7% 16%
2	FD	163	76% 10% 14%
2	Fd	163	79% 6% 16%
2	GD	163	79% 7% 14%
2	Gd	163	77% 7% 16%
2	HD	163	79% 7% 14%
2	Hd	163	79% 5% 16%
2	ID	163	80% 6% 14%
2	Id	163	78% 6% 16%
2	JD	163	80% 6% 14%
2	Jd	163	79% 5% 16%
2	KD	163	79% 7% 14%
2	Kd	163	78% 6% 16%
2	LD	163	77% 9% 14%
2	Ld	163	78% 6% 16%
2	MD	163	77% 9% 14%

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Mol	Chain	Length	Quality of chain
2	Md	163	77% 7% 16%
3	AF	269	21% 77%
3	Af	269	20% 78%
3	BF	269	20% 77%
3	Bf	269	20% 78%
3	CF	269	22% 77%
3	Cf	269	19% 78%
3	DF	269	20% 77%
3	Df	269	21% 78%
3	EF	269	21% 77%
3	Ef	269	22% 78%
3	FF	269	20% 77%
3	Ff	269	20% 78%
3	GF	269	21% 77%
3	Gf	269	20% 78%
3	HF	269	20% 77%
3	Hf	269	20% 78%
3	IF	269	21% 77%
3	If	269	20% 78%
3	JF	269	20% 77%
3	Jf	269	21% 78%
3	KF	269	22% 77%
3	Kf	269	21% 78%
3	LF	269	21% 77%
3	Lf	269	18% 78%

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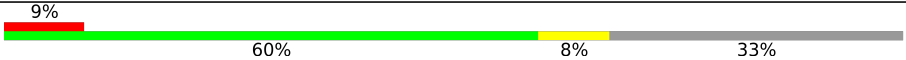
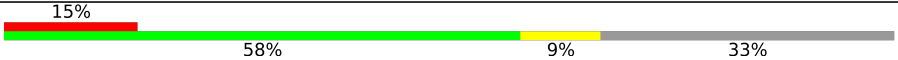
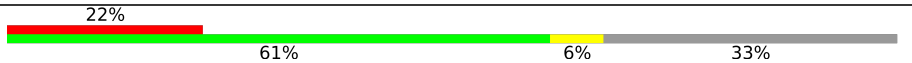
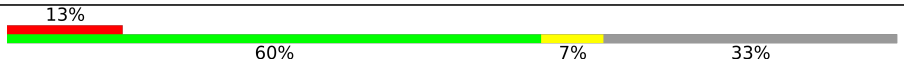
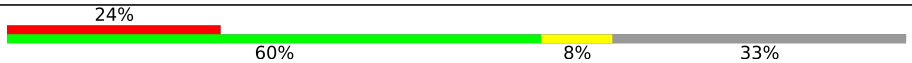
Mol	Chain	Length	Quality of chain
3	MF	269	
3	Mf	269	
3	VF	269	
3	WF	269	
3	XF	269	
3	YF	269	
3	ZF	269	
4	AH	361	
4	BH	361	
4	CH	361	
4	DH	361	
4	EH	361	
4	FH	361	
4	GH	361	
4	HH	361	
4	IH	361	
4	JH	361	
4	KH	361	
4	LH	361	
4	MH	361	
4	VH	361	
4	WH	361	
4	XH	361	
4	YH	361	
4	ZH	361	

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Mol	Chain	Length	Quality of chain
5	AK	189	70% 10% 20%
5	BK	189	71% 9% 20%
5	CK	189	74% 6% 20%
5	DK	189	76% 20%
5	EK	189	74% 6% 20%
5	FK	189	73% 7% 20%
5	GK	189	76% 20%
5	HK	189	75% 5% 20%
5	IK	189	71% 8% 20%
5	JK	189	75% 5% 20%
5	KK	189	72% 8% 20%
5	LK	189	74% 6% 20%
5	MK	189	72% 8% 20%
6	AL	249	64% 6% 31%
6	BL	249	62% 7% 31%
6	CL	249	63% 6% 31%
6	DL	249	65% 31%
6	EL	249	63% 7% 31%
6	FL	249	63% 6% 31%
6	GL	249	63% 6% 31%
6	HL	249	63% 6% 31%
6	IL	249	64% 6% 31%
6	JL	249	63% 6% 31%
6	KL	249	64% 6% 31%
6	LL	249	65% 5% 31%

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Mol	Chain	Length	Quality of chain
6	ML	249	63% 6% 31%
7	AM	320	60% 5% 35%
7	BM	320	56% 9% 35%
7	CM	320	57% 8% 35%
7	DM	320	58% 7% 35%
7	EM	320	57% 8% 35%
7	FM	320	58% 7% 35%
7	GM	320	58% 7% 35%
7	HM	320	58% 7% 35%
7	IM	320	57% 8% 35%
7	JM	320	58% 8% 35%
7	KM	320	57% 8% 35%
7	LM	320	58% 7% 35%
7	MM	320	60% 5% 35%
8	AN	124	58% 5% 37%
8	BN	124	5% 52% 10% 37%
8	CN	124	6% 60% 37%
8	DN	124	54% 9% 37%
8	EN	124	52% 10% 37%
8	FN	124	53% 10% 37%
8	GN	124	6% 56% 7% 37%
8	HN	124	5% 52% 10% 37%
8	IN	124	56% 7% 37%
8	JN	124	6% 58% 5% 37%
8	KN	124	7% 56% 6% 37%

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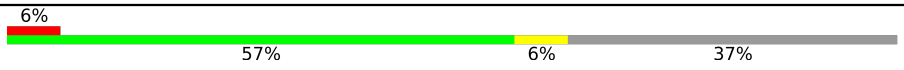
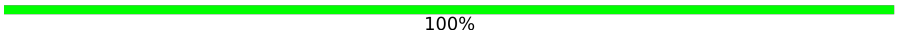
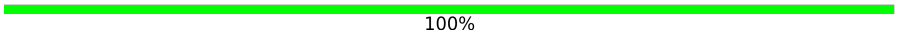
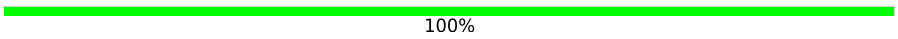
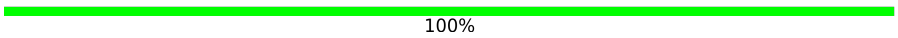
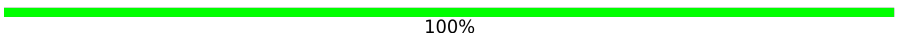
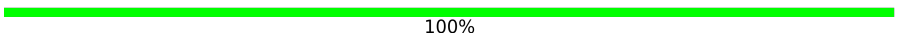
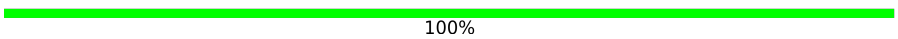
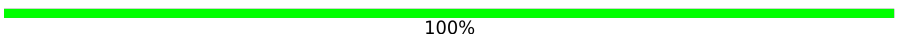
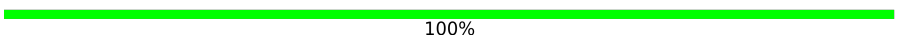
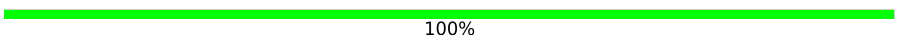
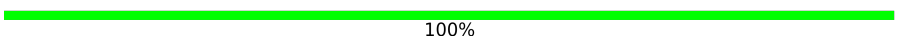
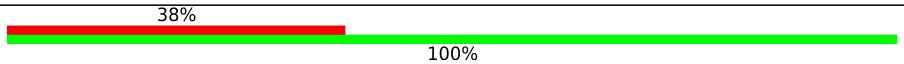
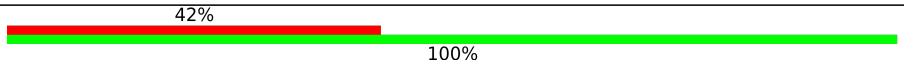
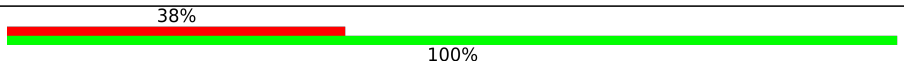
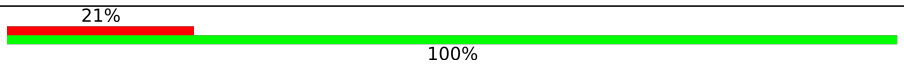
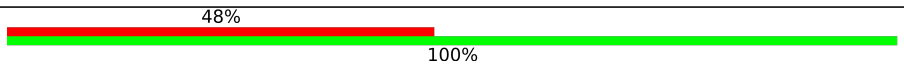
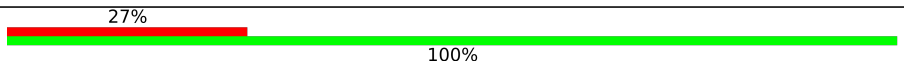
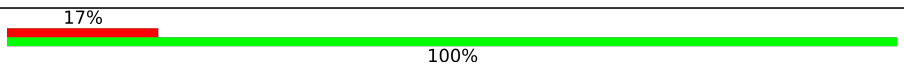
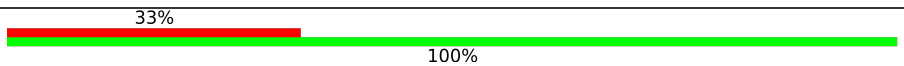
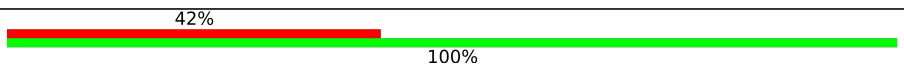
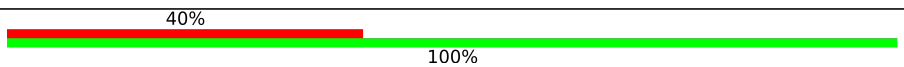
Mol	Chain	Length	Quality of chain
8	LN	124	
8	MN	124	
9	AU	9	
9	BU	9	
9	CU	9	
9	DU	9	
9	EU	9	
9	FU	9	
9	GU	9	
9	HU	9	
9	IU	9	
9	JU	9	
9	KU	9	
9	LU	9	
9	MU	9	
10	AX	48	
10	BX	48	
10	CX	48	
10	DX	48	
10	EX	48	
10	FX	48	
10	GX	48	
10	HX	48	
10	IX	48	
10	JX	48	

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Mol	Chain	Length	Quality of chain
10	KX	48	38% 100%
10	LX	48	46% 100%
10	MX	48	29% 100%
10	VX	48	38% 100%
10	WX	48	33% 100%
10	XX	48	21% 100%
10	YX	48	27% 100%
10	ZX	48	35% 100%
11	AC	303	64% 5% 31%
11	BC	303	73% 7% 20%
11	CC	303	5% 71% 10% 20%
11	DC	303	61% 8% 31%
11	EC	303	64% 5% 31%
11	FC	303	73% 7% 20%
11	GC	303	6% 73% 8% 20%
11	HC	303	63% 6% 31%
11	IC	303	59% 10% 31%
11	JC	303	63% 6% 31%
11	KC	303	6% 70% 10% 20%
11	LC	303	63% 6% 31%
11	MC	303	61% 8% 31%

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
1	AG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Eg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Fg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	BG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Gg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Hg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	CG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Bg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Ig	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Jg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	DG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Kg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Lg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	EG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Mg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	VG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	WG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

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

- Molecule 2 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	ED	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
2	Ed	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	DD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		
2	Dd	137	Total	C	N	O	S	0	0
			1058	672	182	202	2		
2	AD	140	Total	C	N	O	S	0	0
			1086	692	185	206	3		

- Molecule 3 is a protein called DotF.

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

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

- Molecule 4 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	EH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	FH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	GH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	HH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	IH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	JH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	AH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	KH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	LH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	MH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	VH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
4	WH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
4	XH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
4	YH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
4	ZH	243	Total	C	N	O	S	0	0
			1875	1201	319	348	7		
4	BH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	CH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		
4	DH	258	Total	C	N	O	S	0	0
			1983	1268	336	371	8		

- Molecule 5 is a protein called Inner membrane lipoprotein YiaD.

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

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

- Molecule 6 is a protein called Outer membrane protein, OmpA family protein.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	CL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		
6	DL	173	Total	C	N	O	S	0	0
			1388	877	253	253	5		

- Molecule 7 is a protein called DUF2807 domain-containing protein.

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

- Molecule 8 is a protein called Neurogenic locus notch.

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

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

- Molecule 9 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	EU	9	Total	C	N	O	0	0
			45	27	9	9		
9	FU	9	Total	C	N	O	0	0
			45	27	9	9		
9	GU	9	Total	C	N	O	0	0
			45	27	9	9		
9	HU	9	Total	C	N	O	0	0
			45	27	9	9		
9	IU	9	Total	C	N	O	0	0
			45	27	9	9		
9	JU	9	Total	C	N	O	0	0
			45	27	9	9		
9	KU	9	Total	C	N	O	0	0
			45	27	9	9		
9	LU	9	Total	C	N	O	0	0
			45	27	9	9		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	MU	9	Total	C	N	O	0	0
			45	27	9	9		
9	AU	9	Total	C	N	O	0	0
			45	27	9	9		
9	BU	9	Total	C	N	O	0	0
			45	27	9	9		
9	CU	9	Total	C	N	O	0	0
			45	27	9	9		
9	DU	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 10 is a protein called Unknown protein fragment.

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	AX	48	Total	C	N	O	0	0
			240	144	48	48		
10	BX	48	Total	C	N	O	0	0
			240	144	48	48		
10	CX	48	Total	C	N	O	0	0
			240	144	48	48		
10	DX	48	Total	C	N	O	0	0
			240	144	48	48		

- Molecule 11 is a protein called DotC.

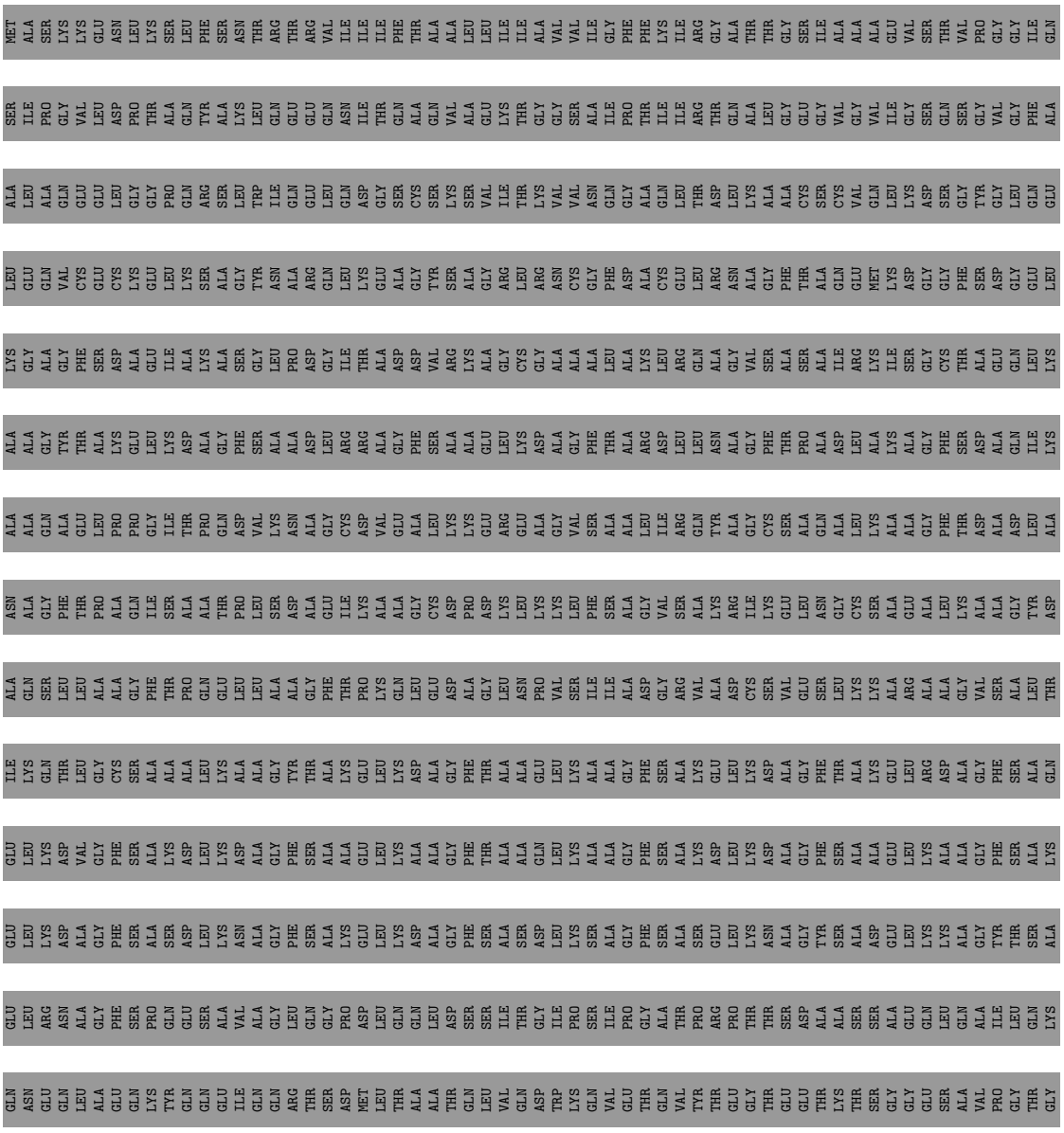
Mol	Chain	Residues	Atoms					AltConf	Trace
11	CC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	BC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	GC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	KC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	DC	209	Total	C	N	O	S	0	0
			1667	1061	292	309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

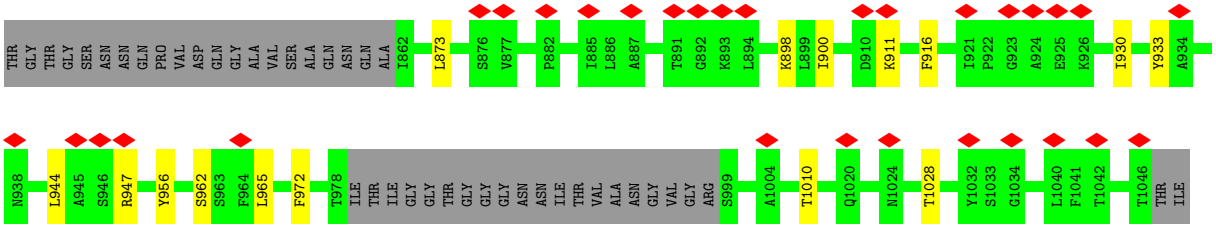
3 Residue-property plots (i)

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

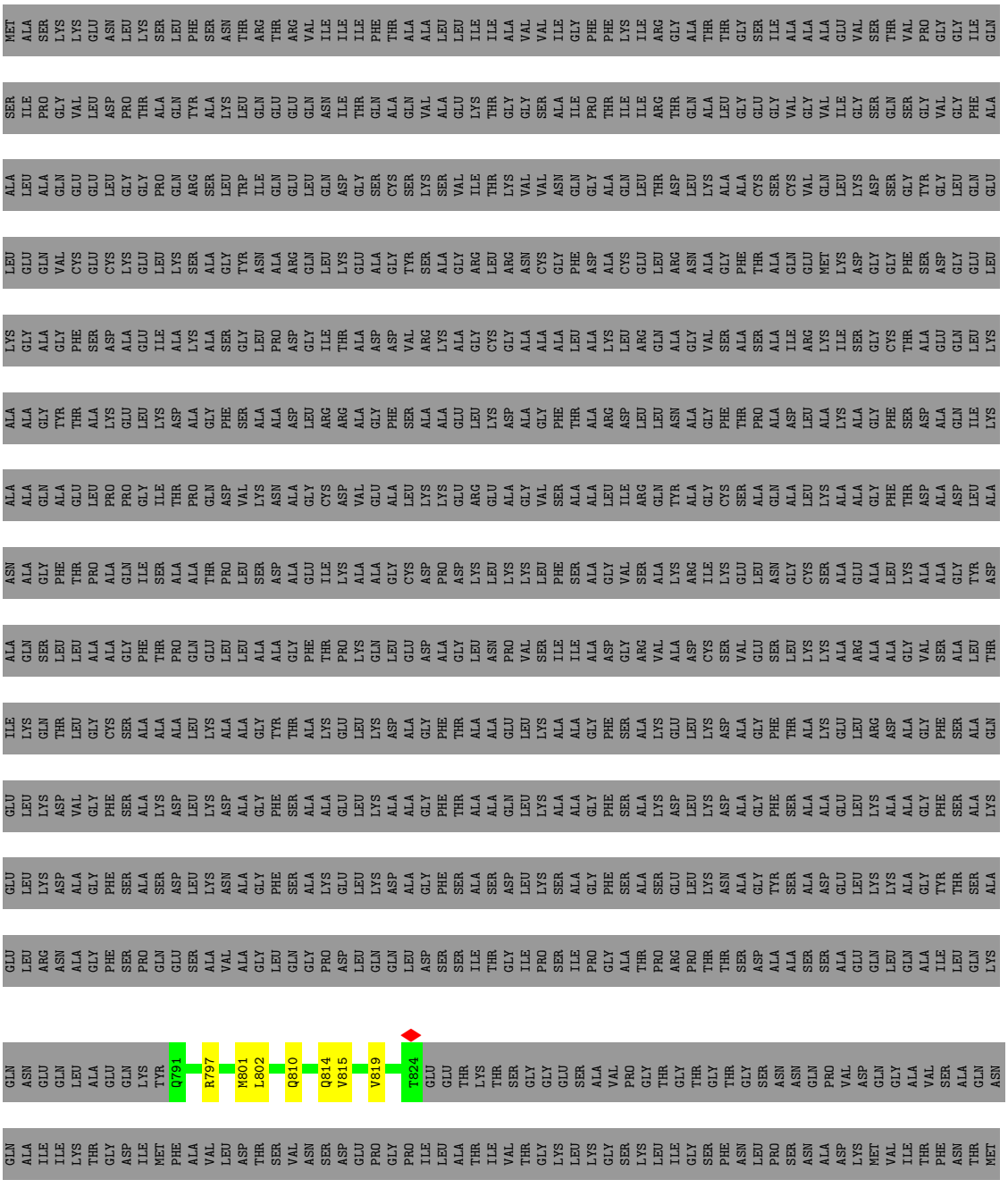
Chain AG:

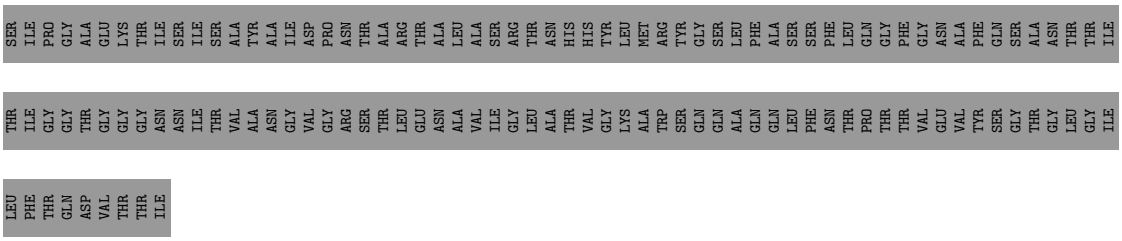




• Molecule 1: IcmE protein

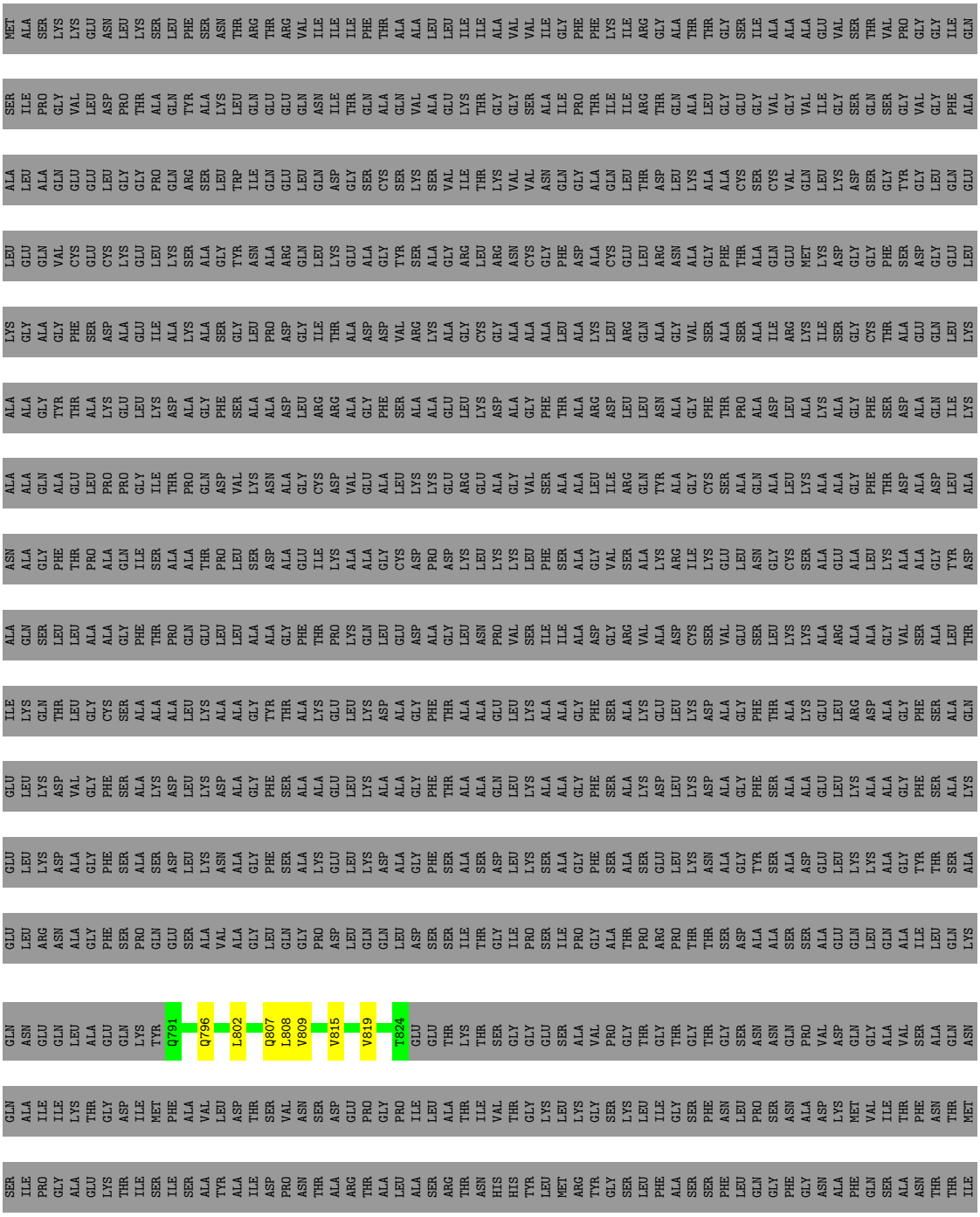
Chain Eg: 97%

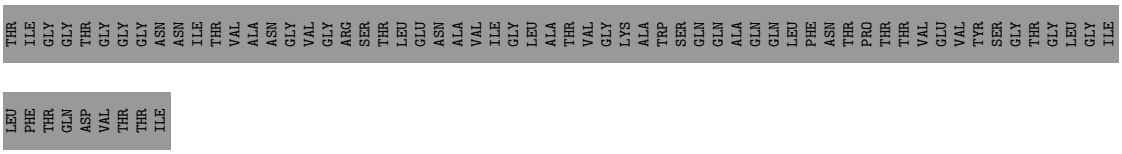




• Molecule 1: IcmE protein

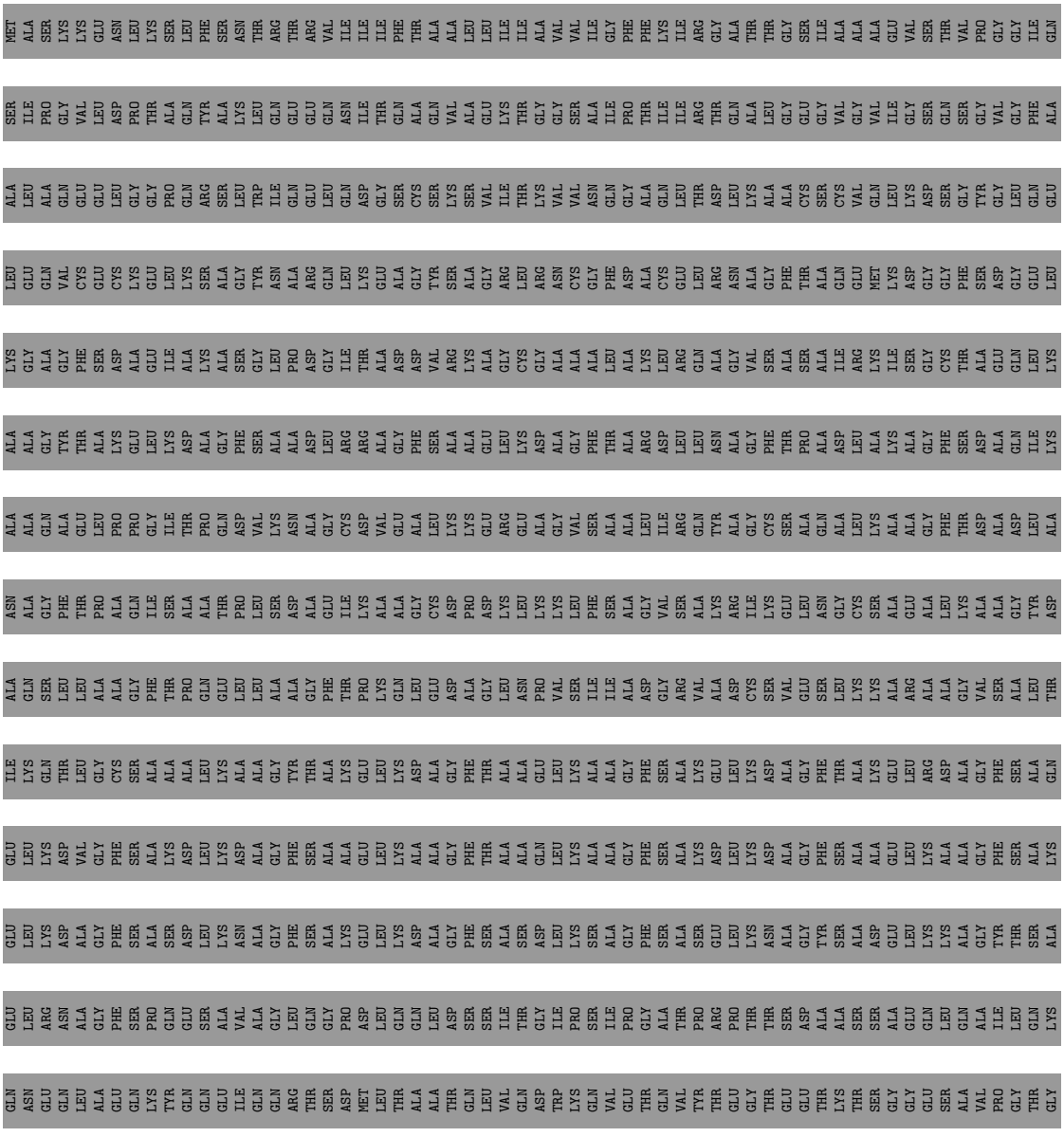
Chain Fg: 97%

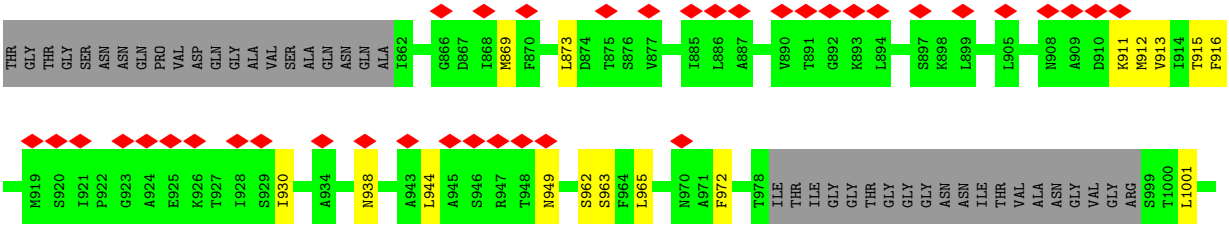


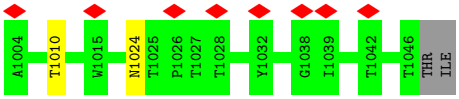


• Molecule 1: IcmE protein

Chain BG:

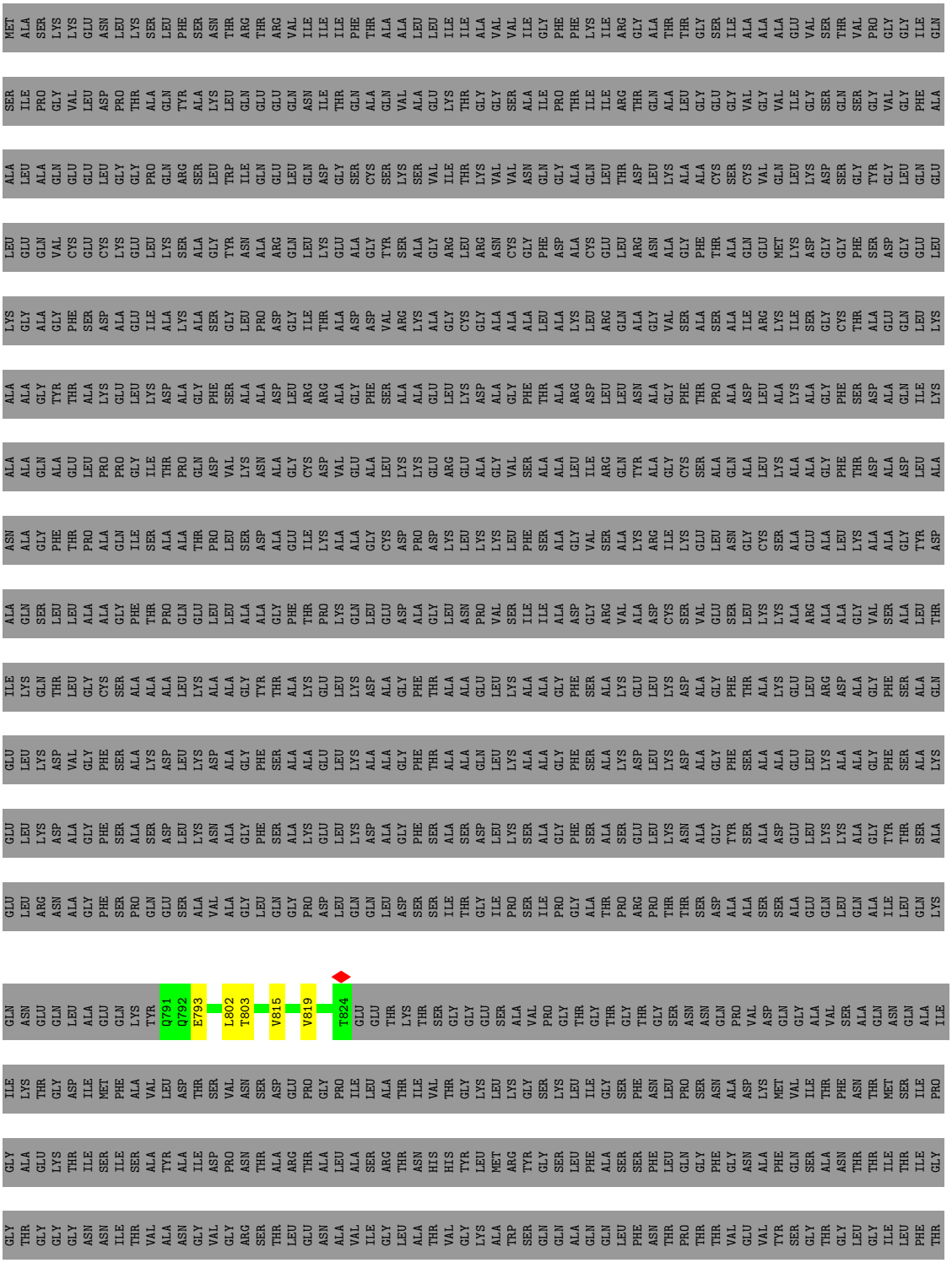






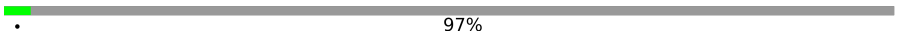
• Molecule 1: IcmE protein

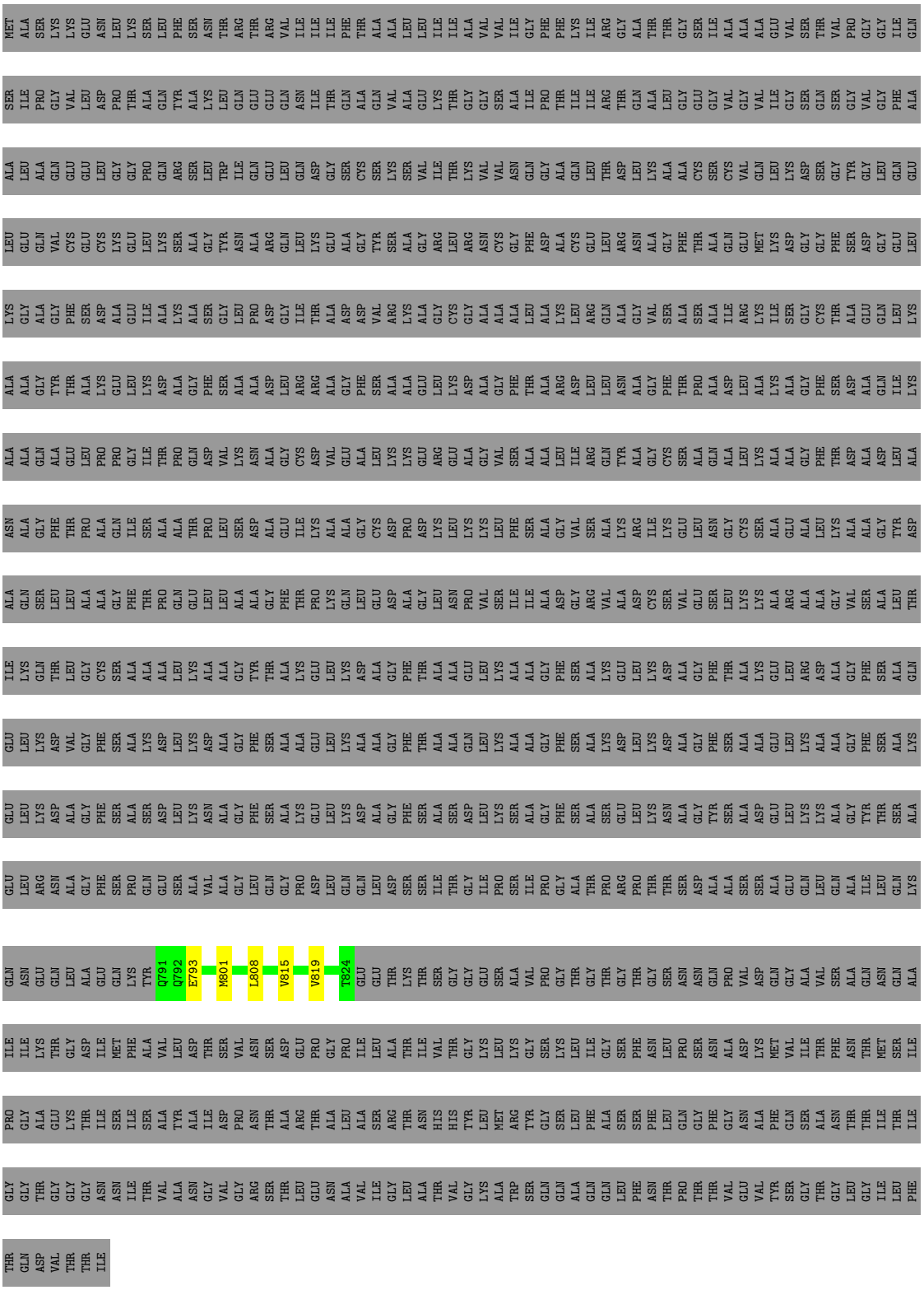
Chain Gg: 97%



• Molecule 1: IcmE protein

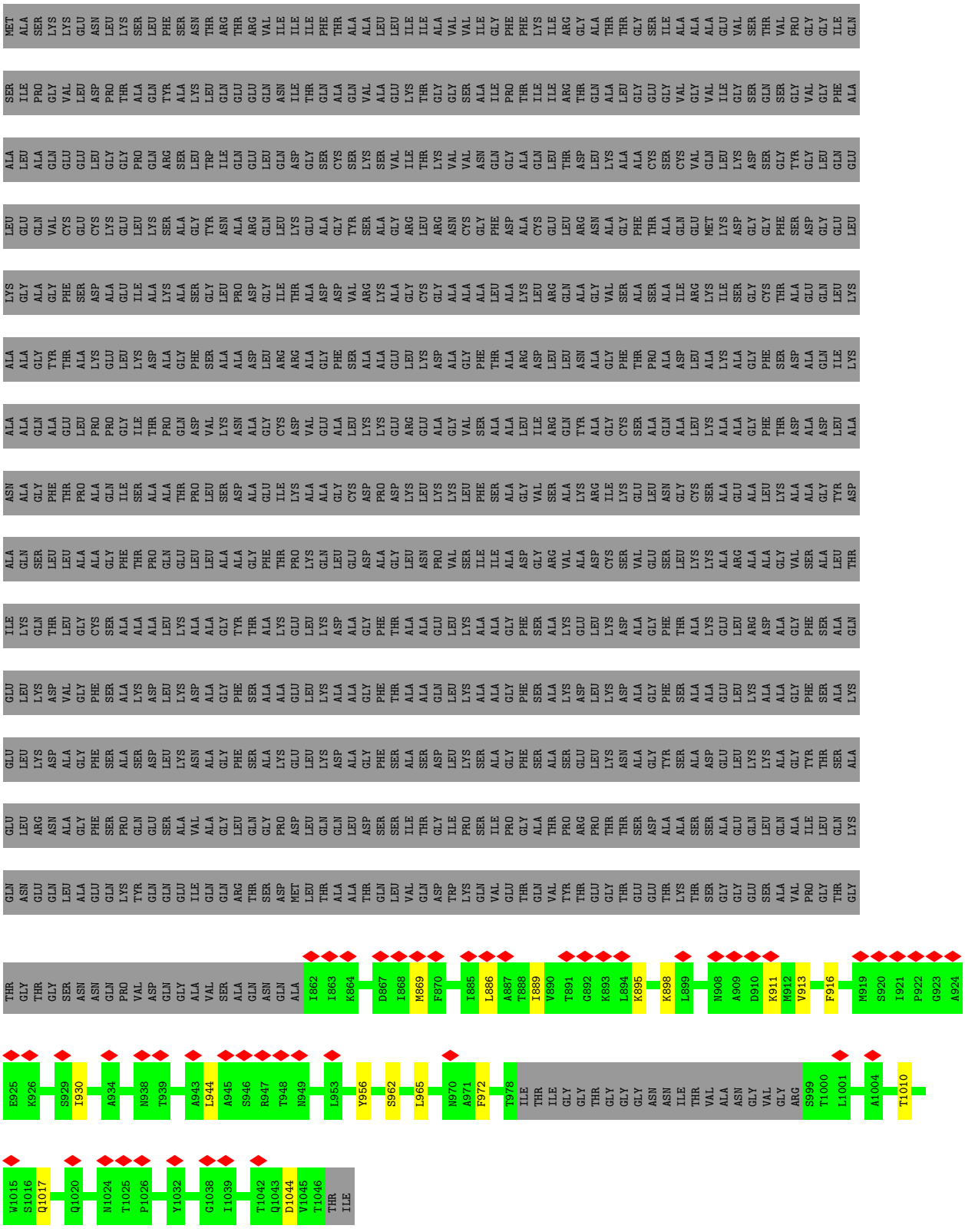
Chain Hg:





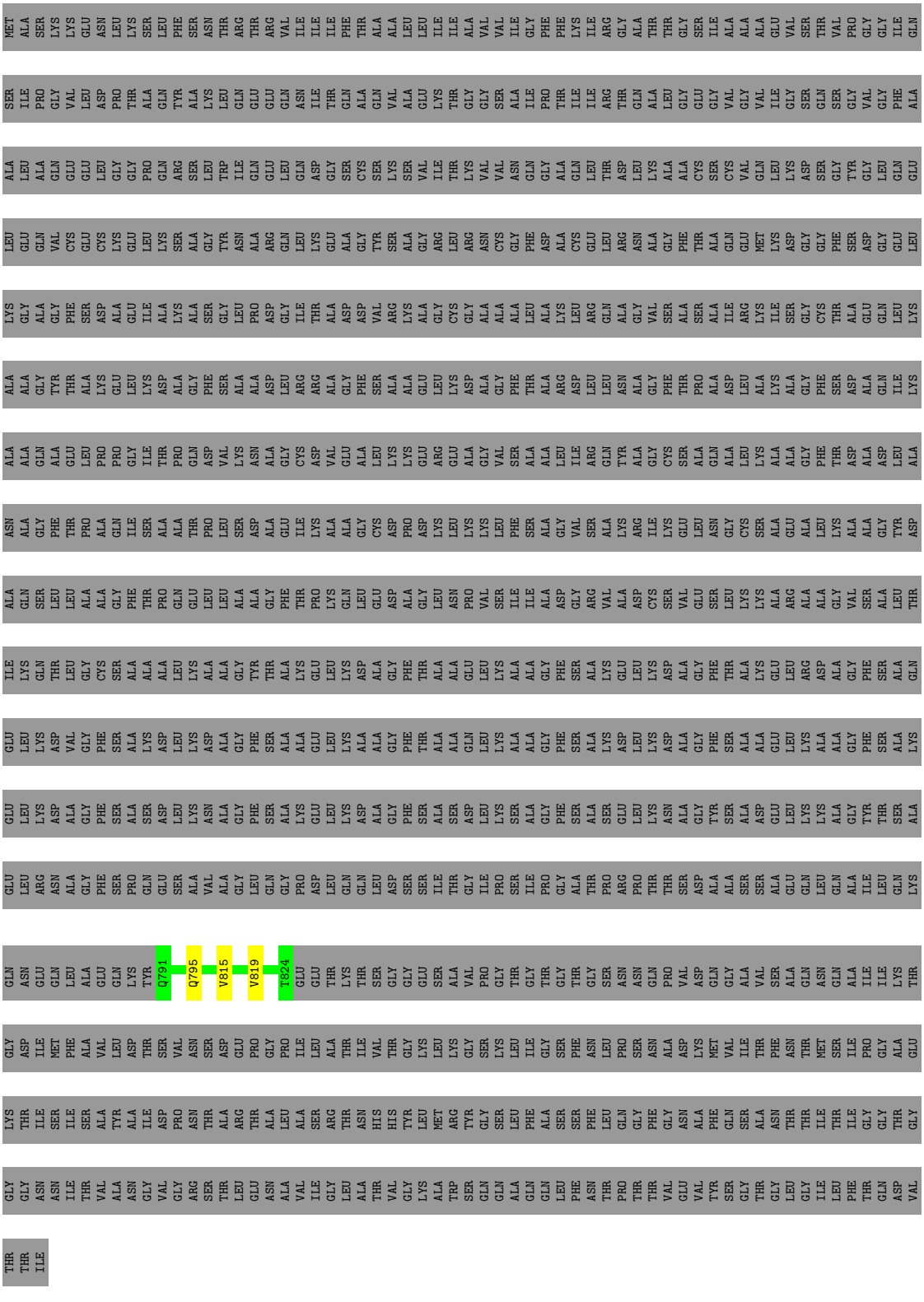
• Molecule 1: IcmE protein

Chain CG:



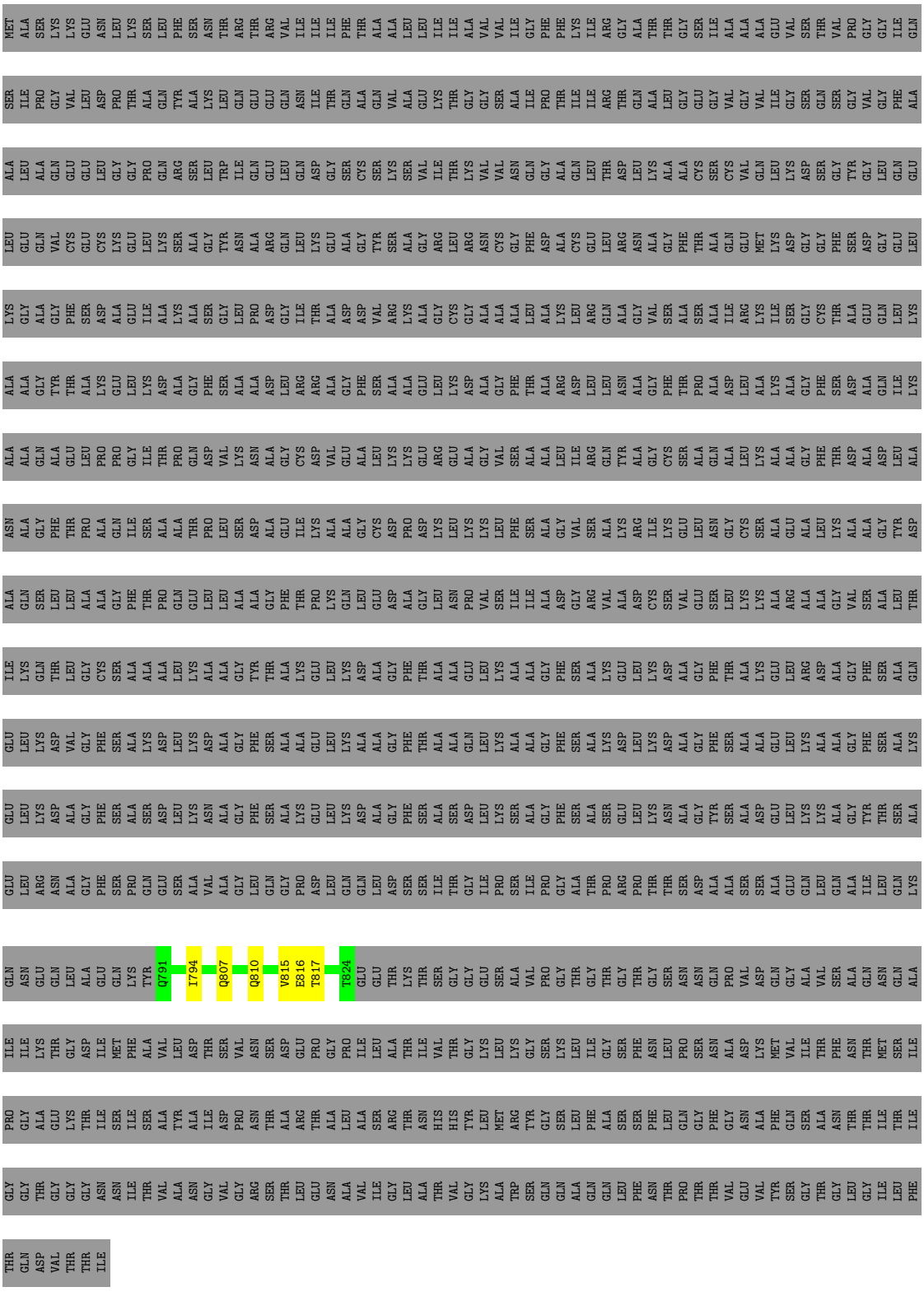
• Molecule 1: IcmE protein

Chain Bg: 97%



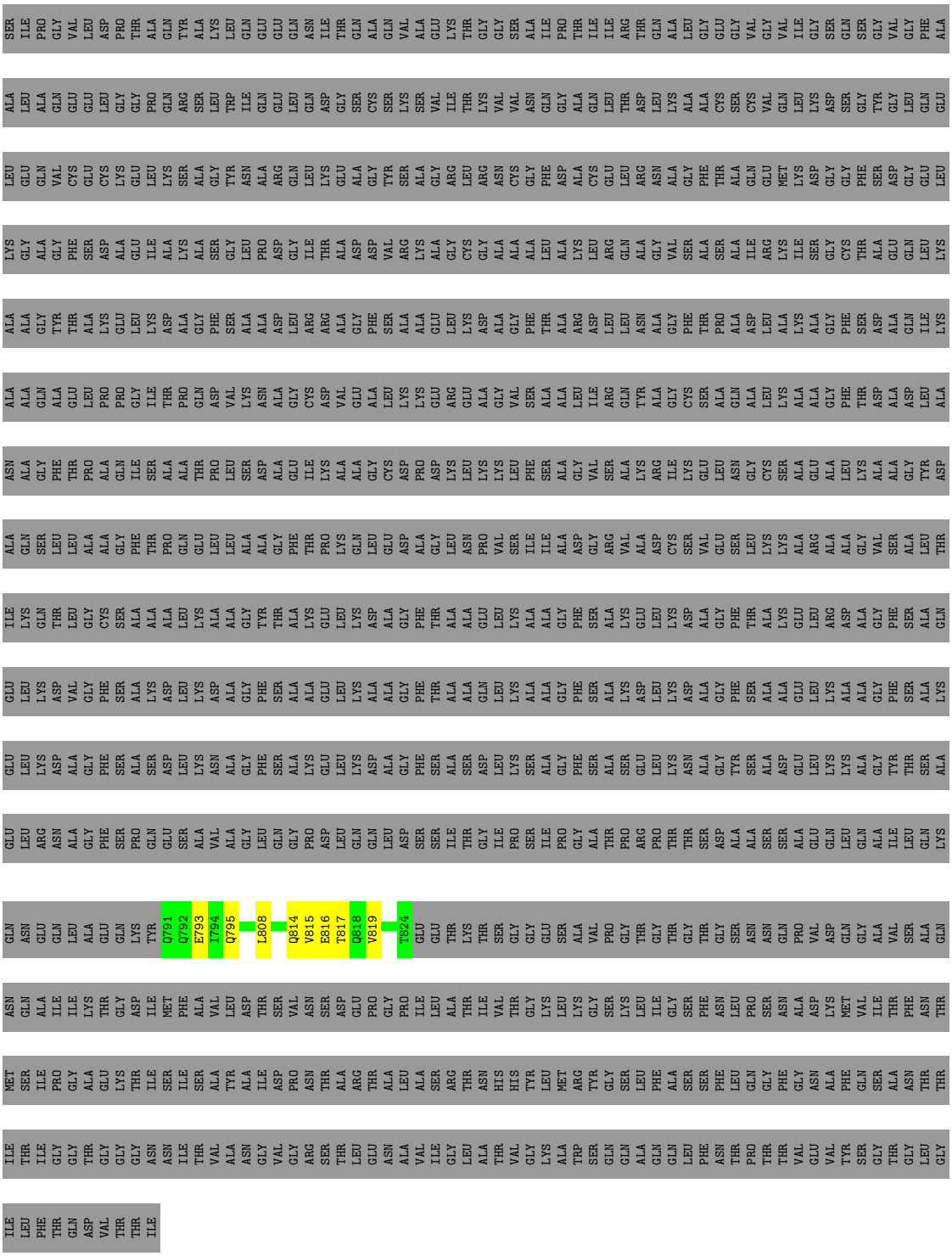
• Molecule 1: IcmE protein

Chain Ig: 97%



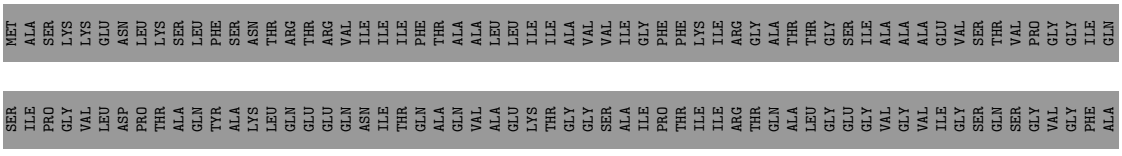
• Molecule 1: IcmE protein

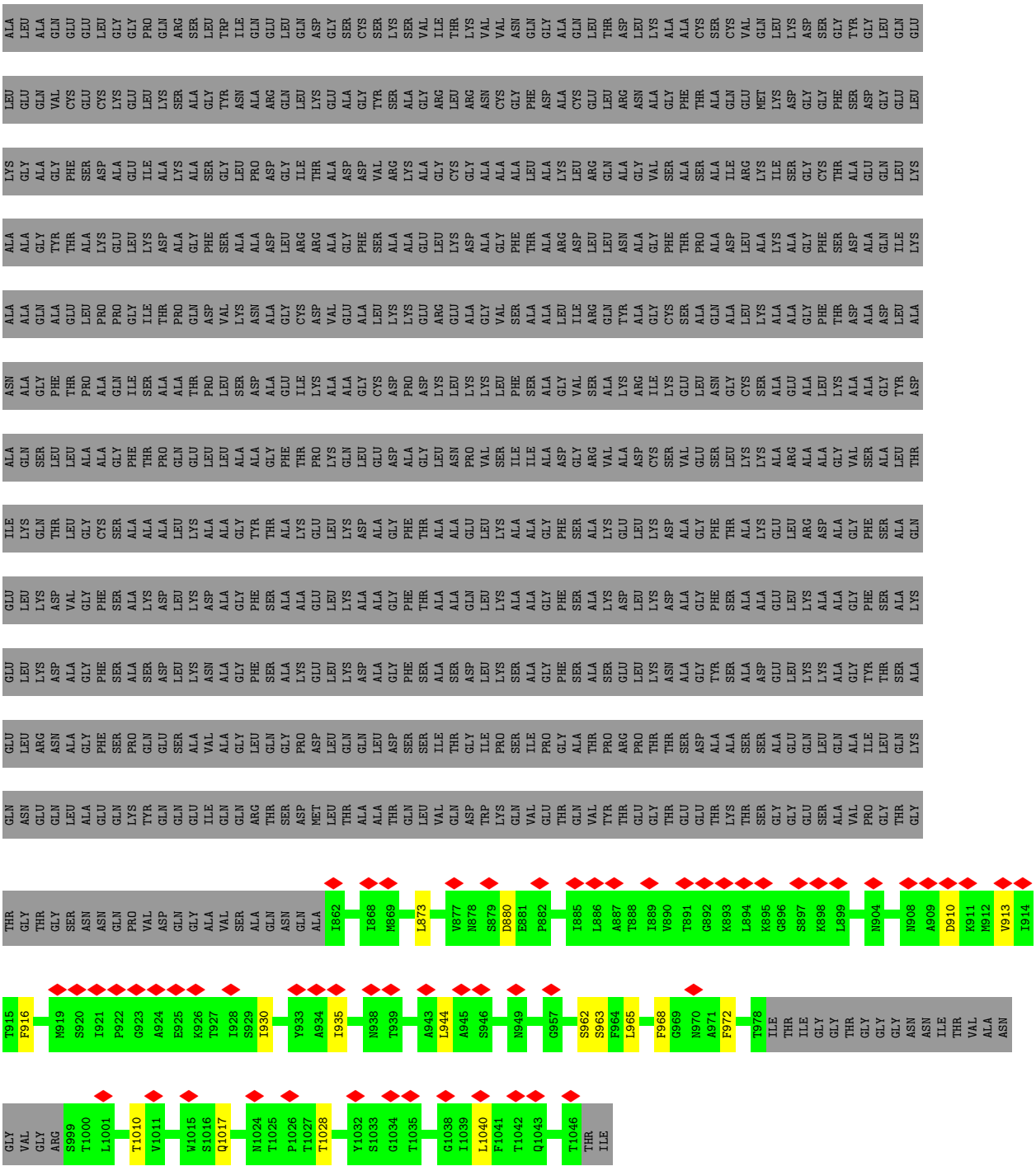
Chain Jg: 97%



• Molecule 1: IcmE protein

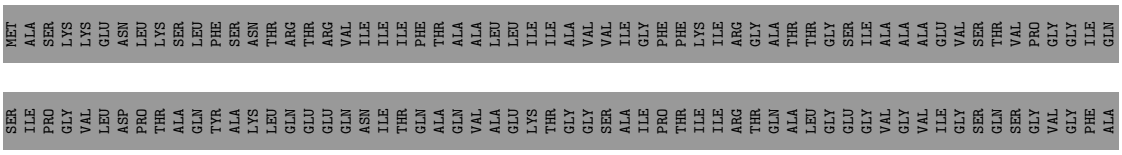
Chain DG:

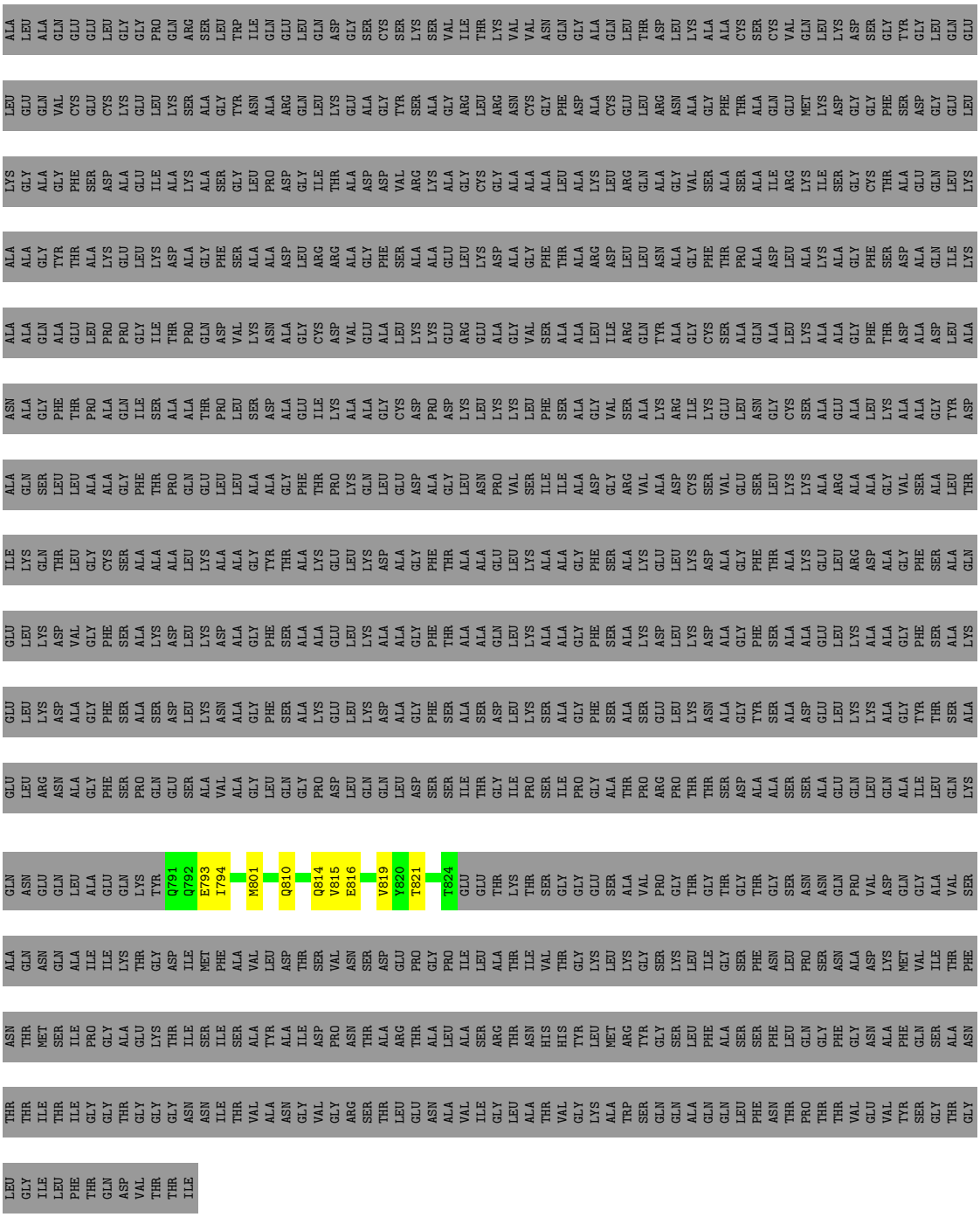




• Molecule 1: IcmE protein

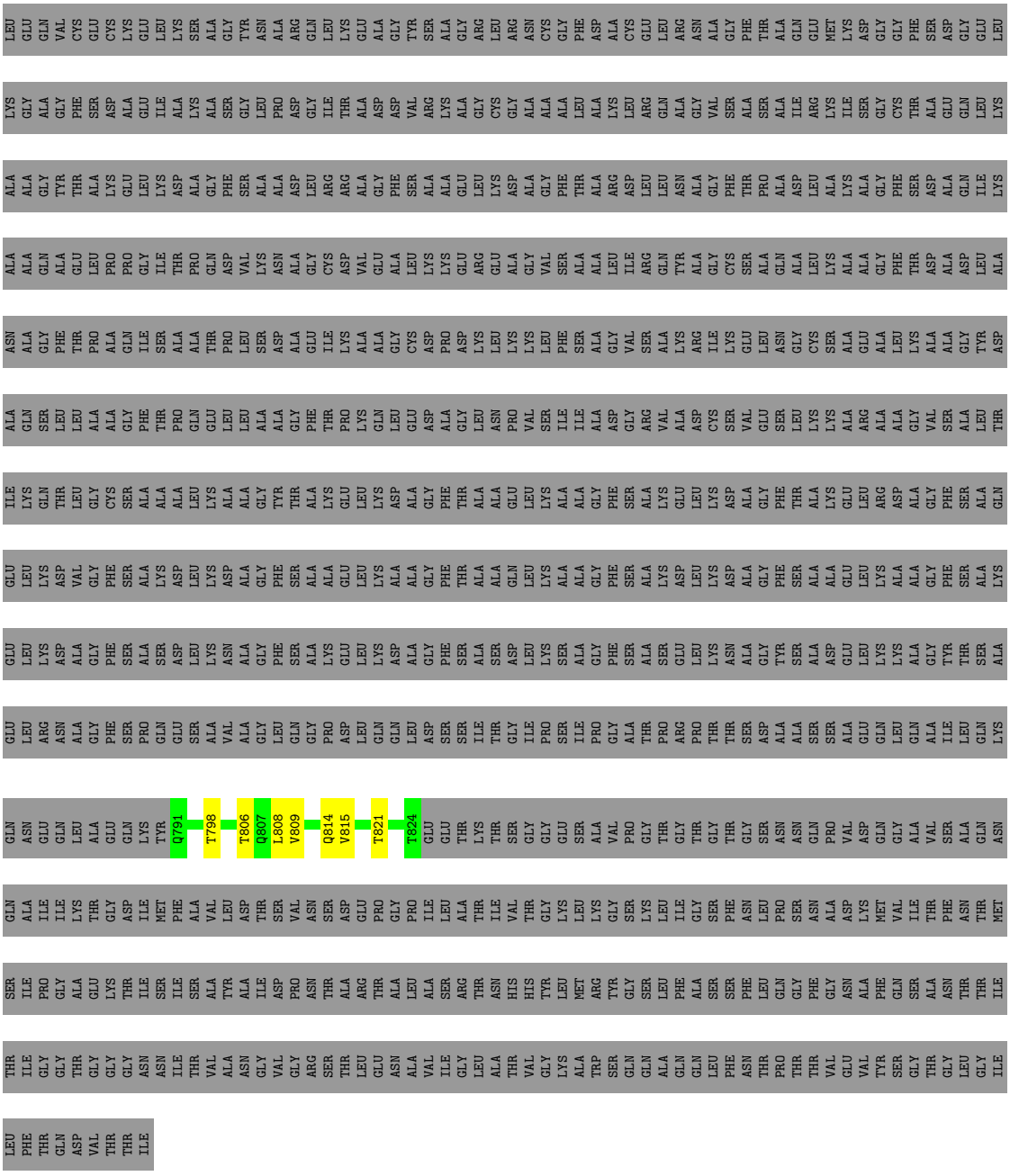
Chain Kg: 97%





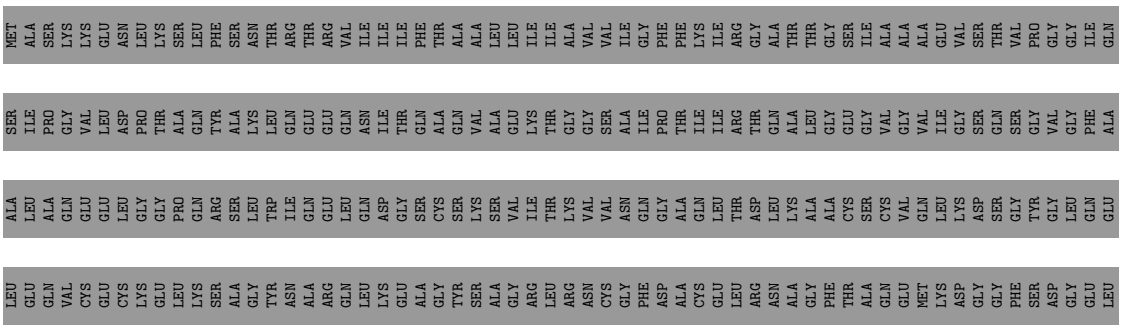
• Molecule 1: IcmE protein

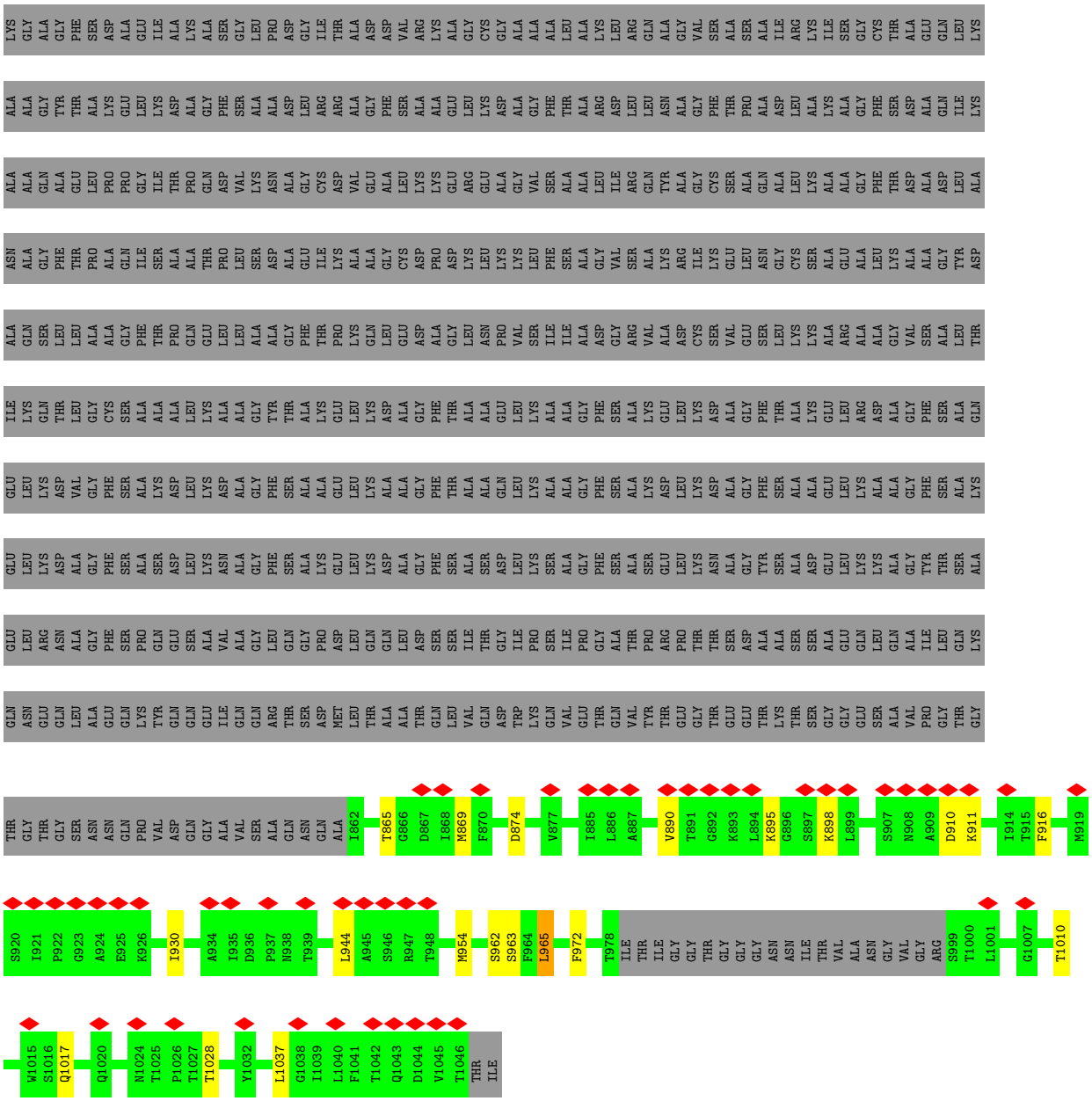
Chain Lg: 97%



• Molecule 1: IcmE protein

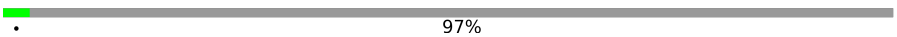
Chain EG:

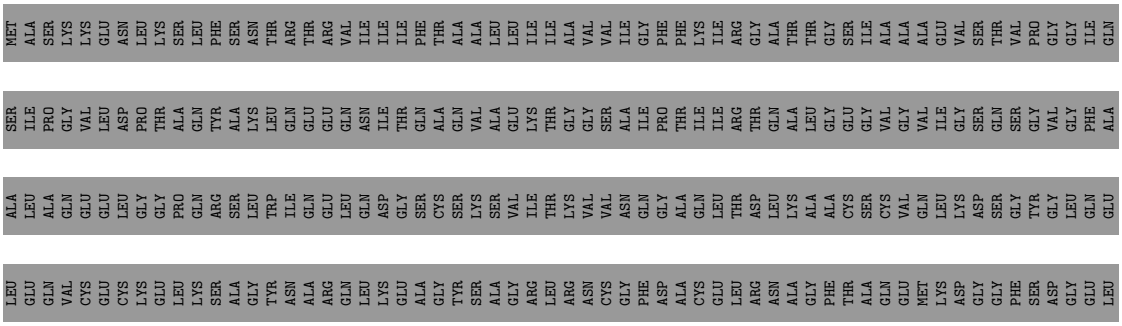


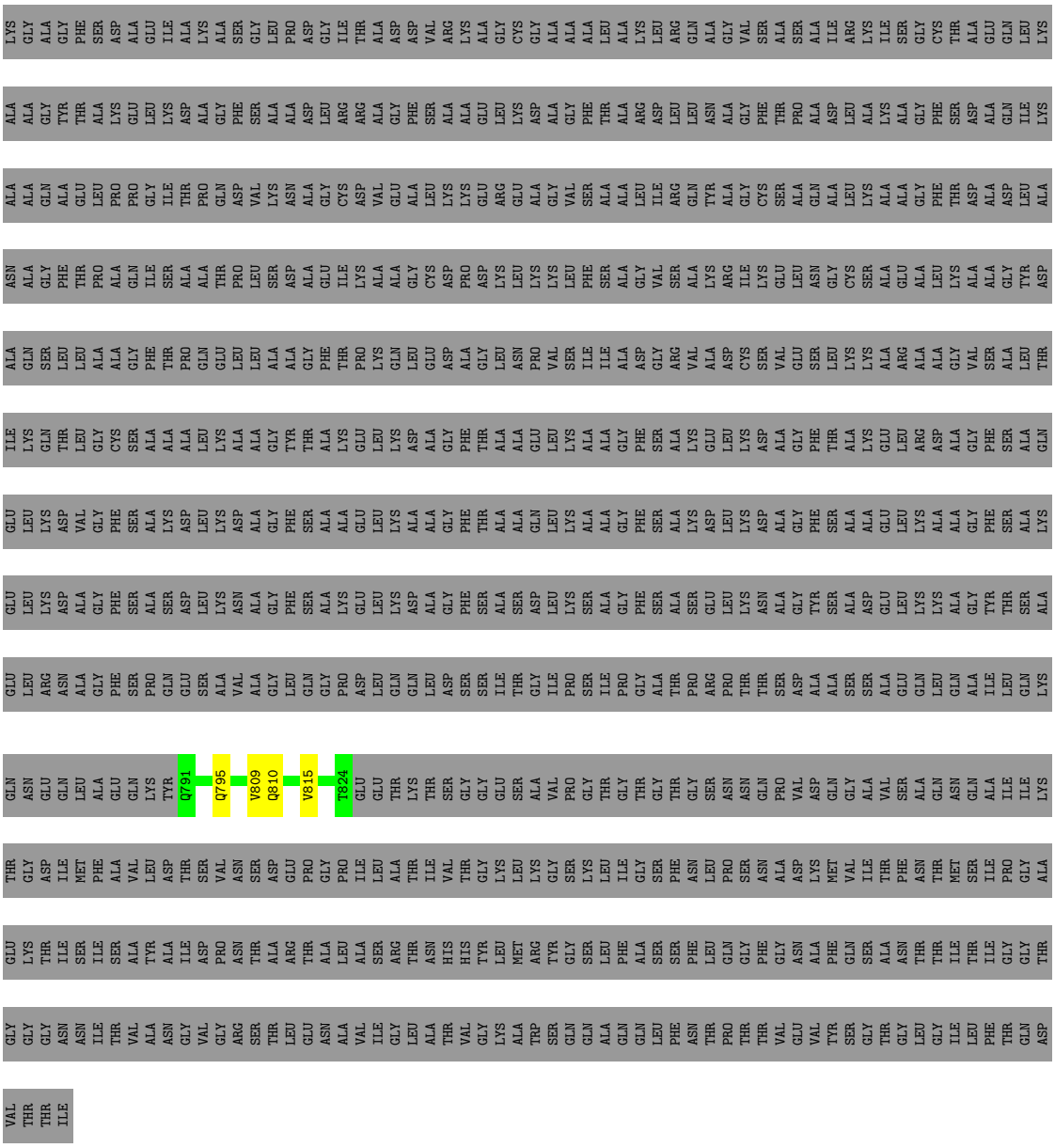


• Molecule 1: IcmE protein

Chain Mg:

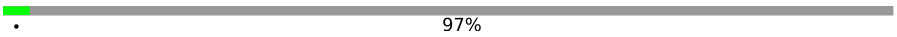


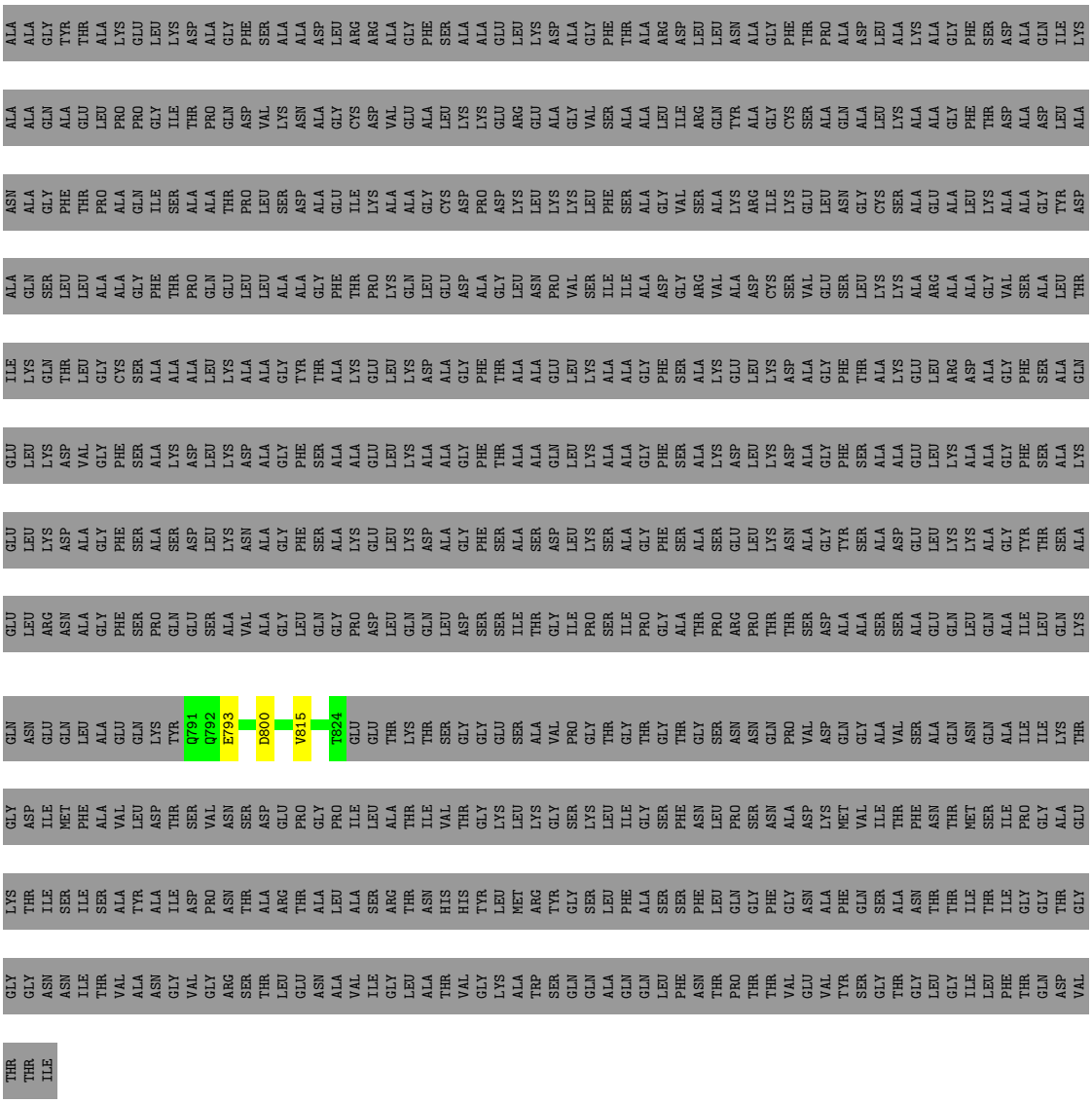




• Molecule 1: IcmE protein

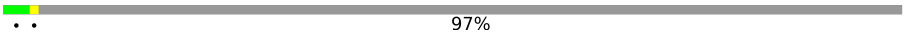
Chain VG:

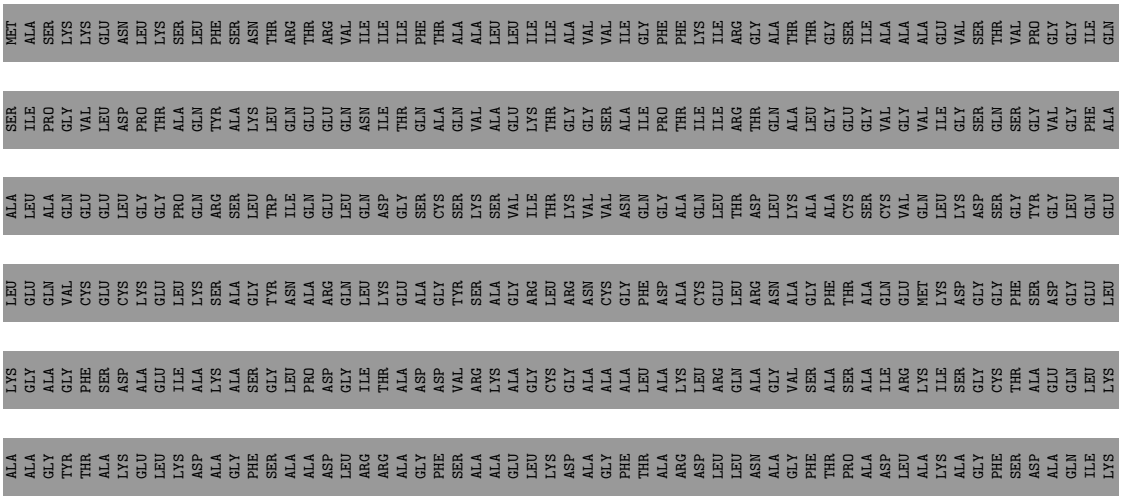


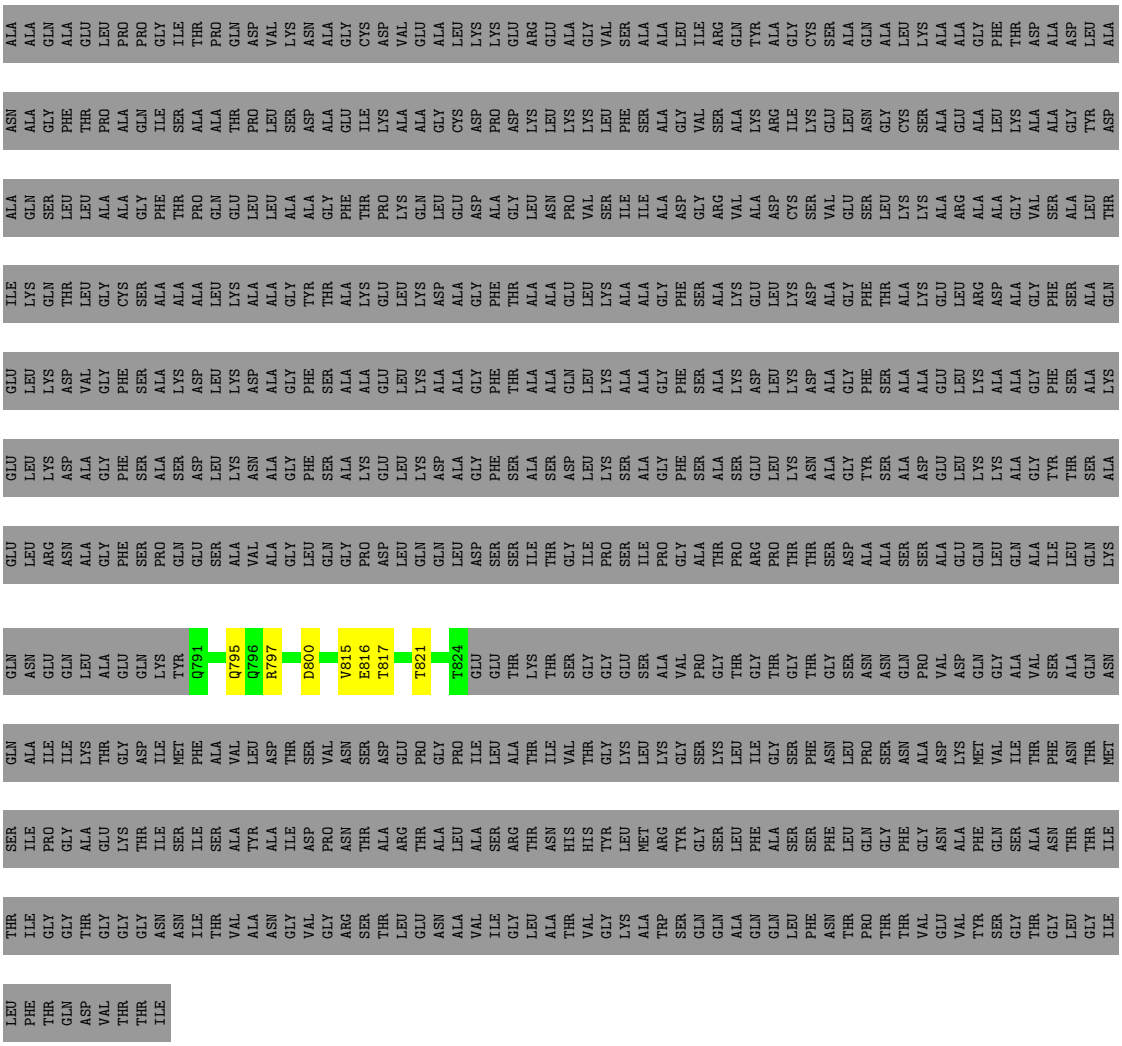


• Molecule 1: IcmE protein

Chain WG:

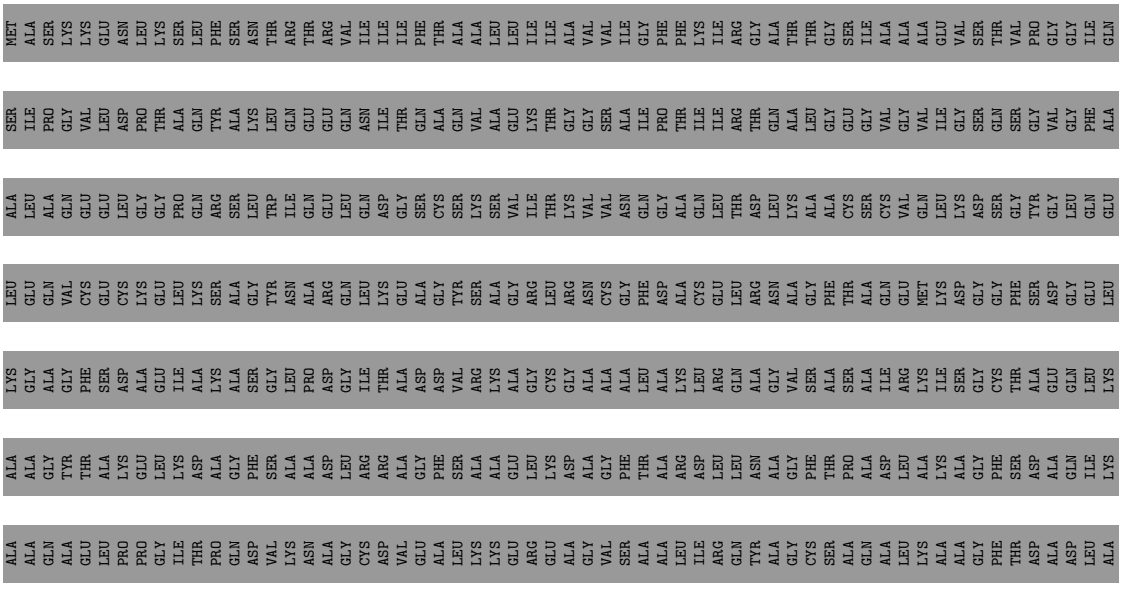






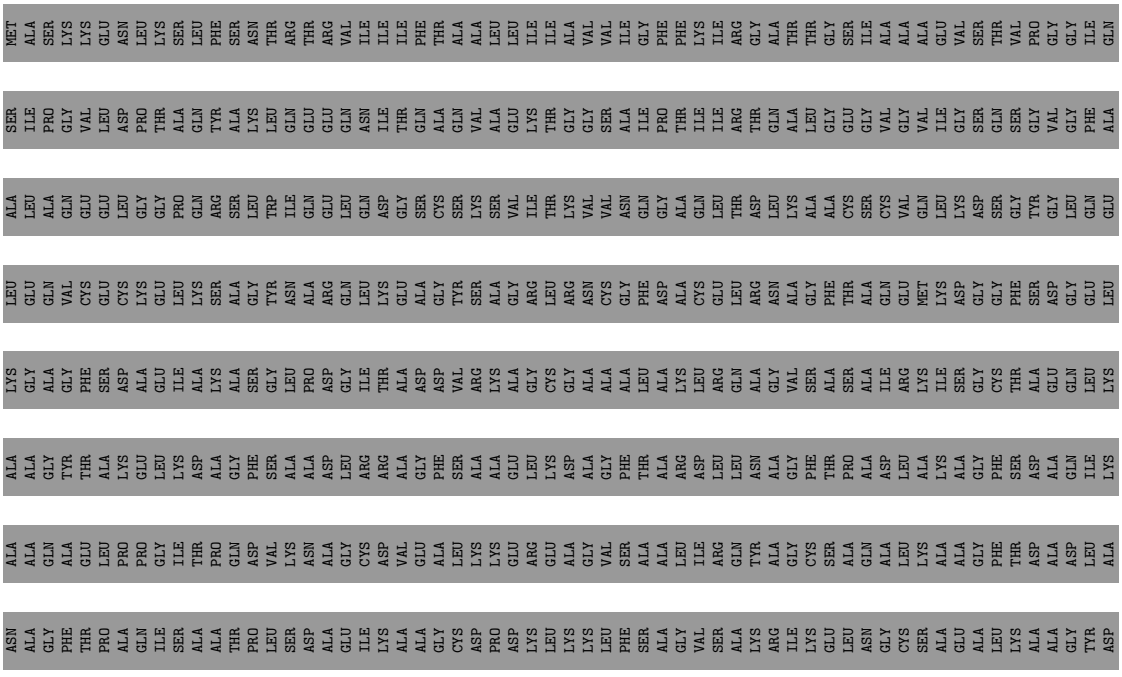
• Molecule 1: IcmE protein

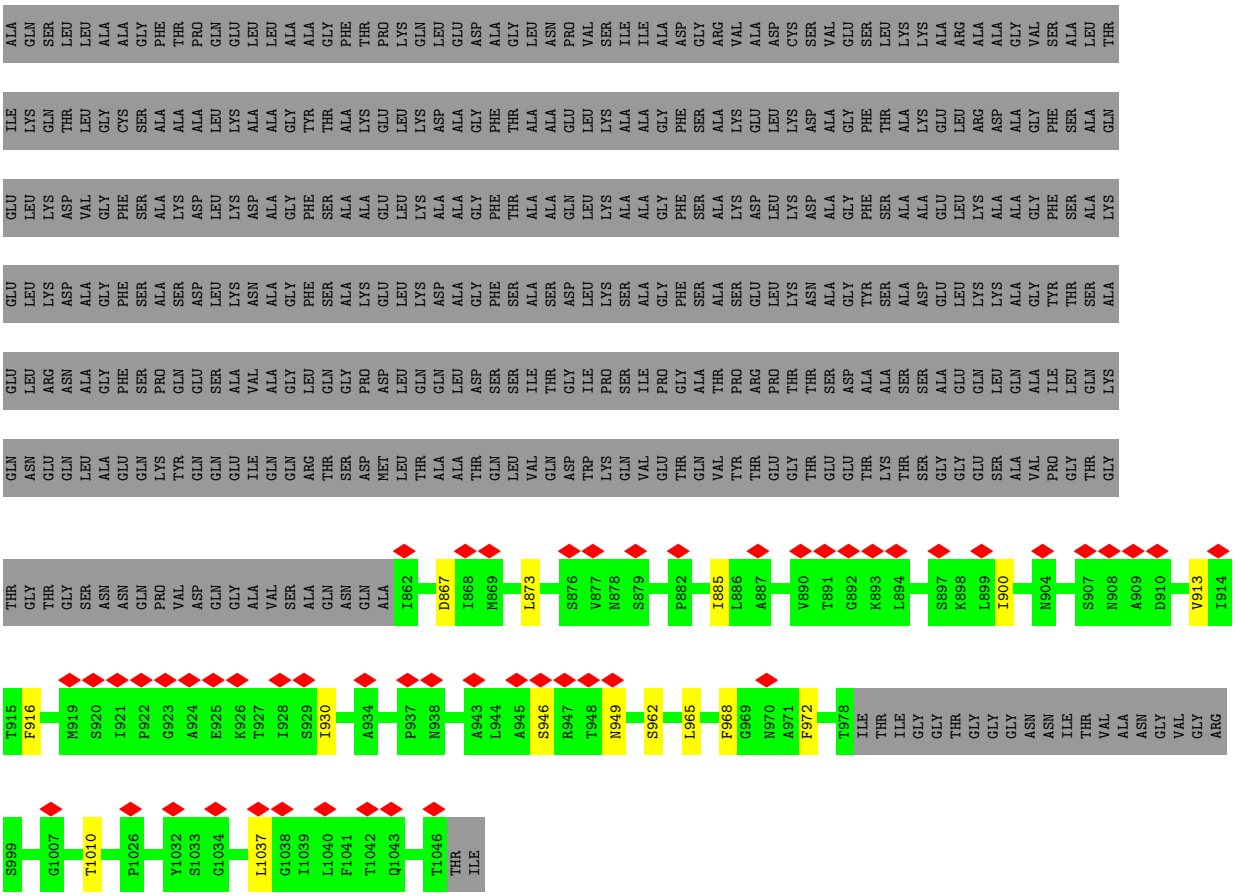
Chain XG: 97%



• Molecule 1: IcmE protein

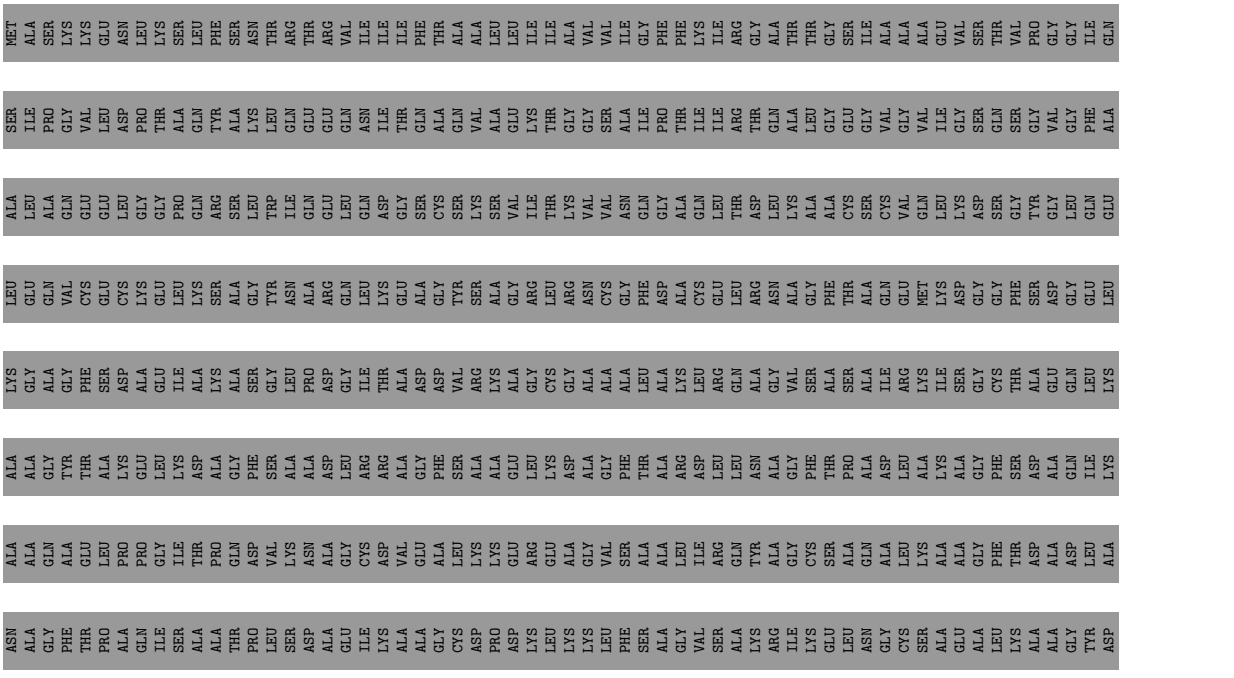
Chain FG:





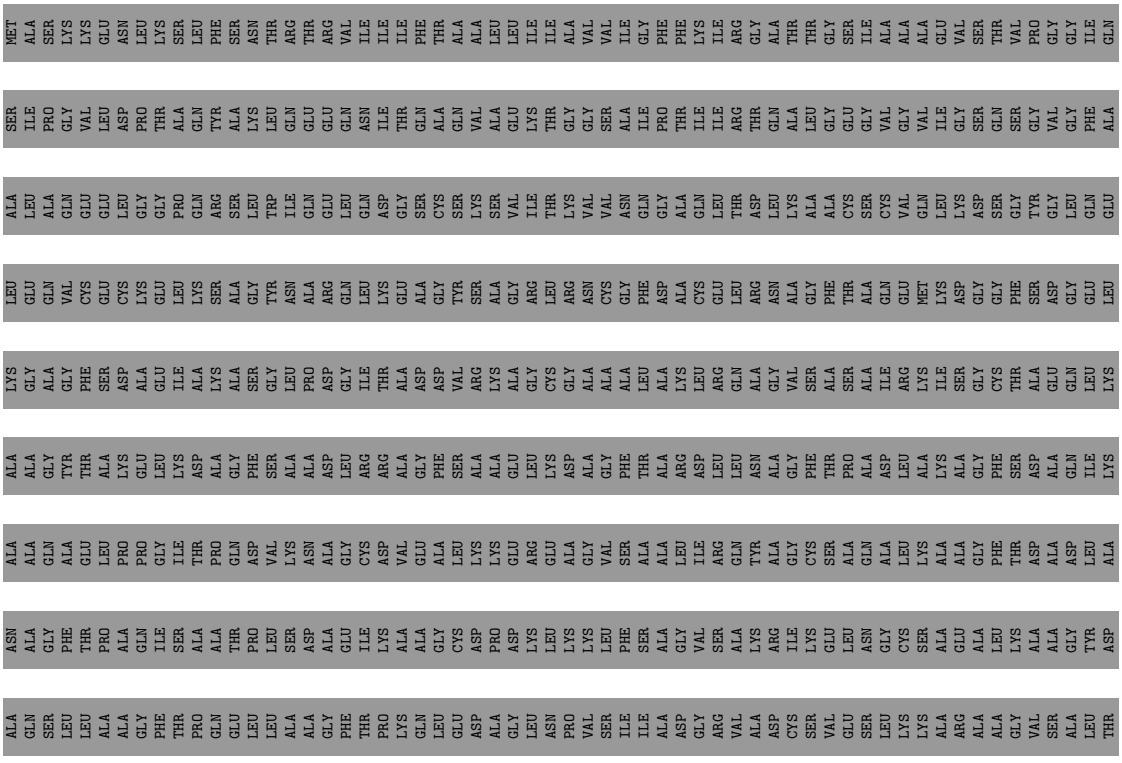
• Molecule 1: IcmE protein

Chain YG: 97%



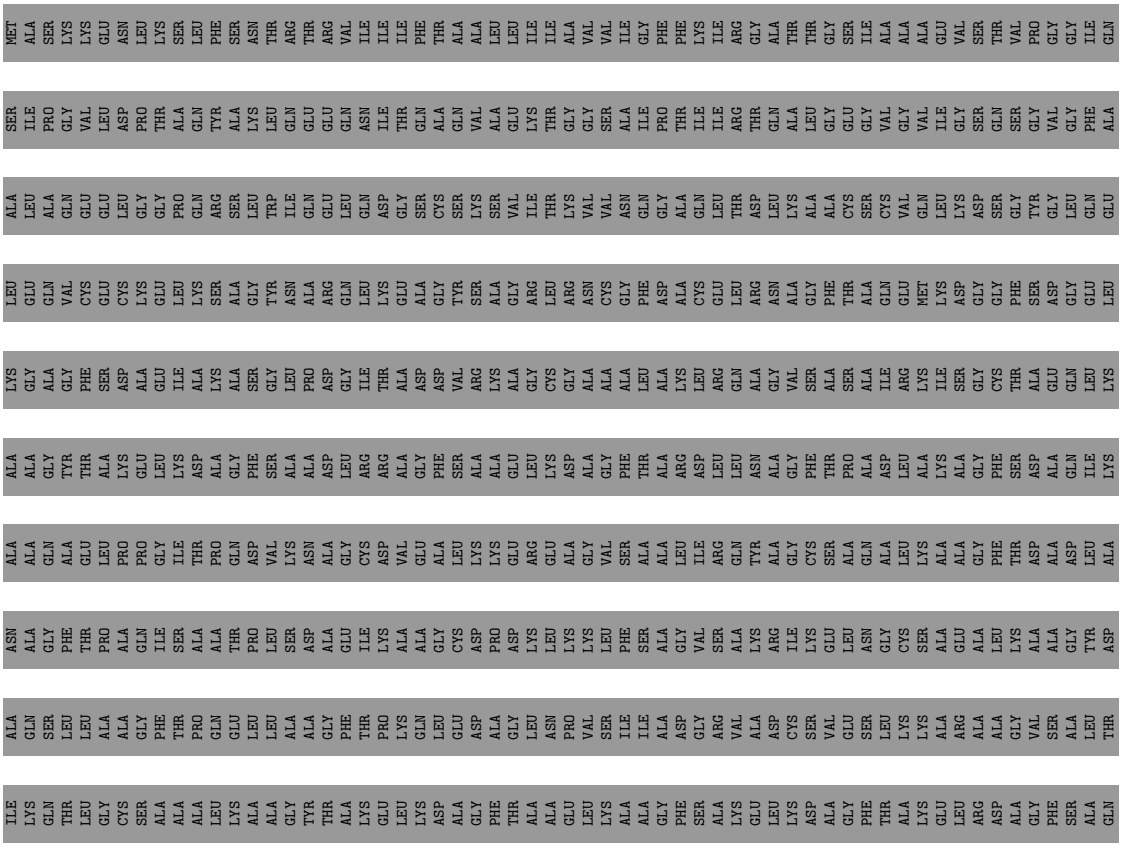
• Molecule 1: IcmE protein

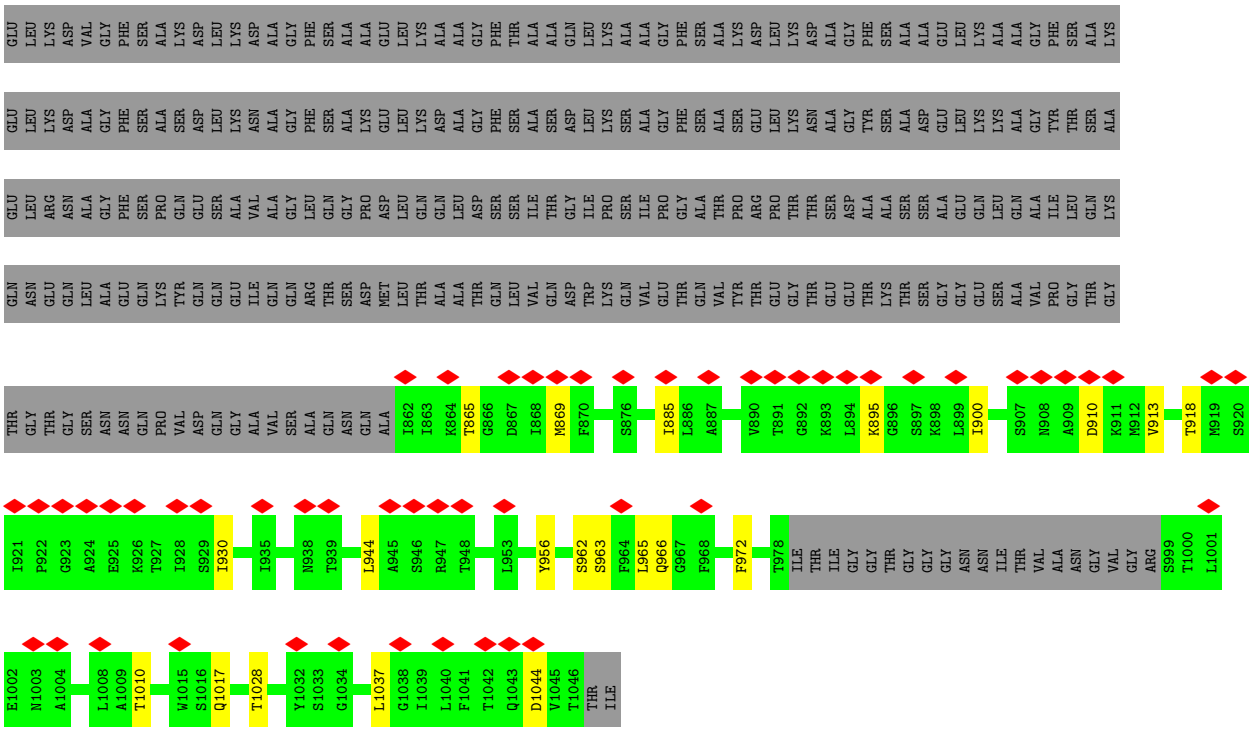
Chain ZG: 97%



• Molecule 1: IcmE protein

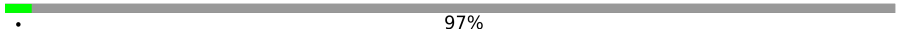
Chain GG:

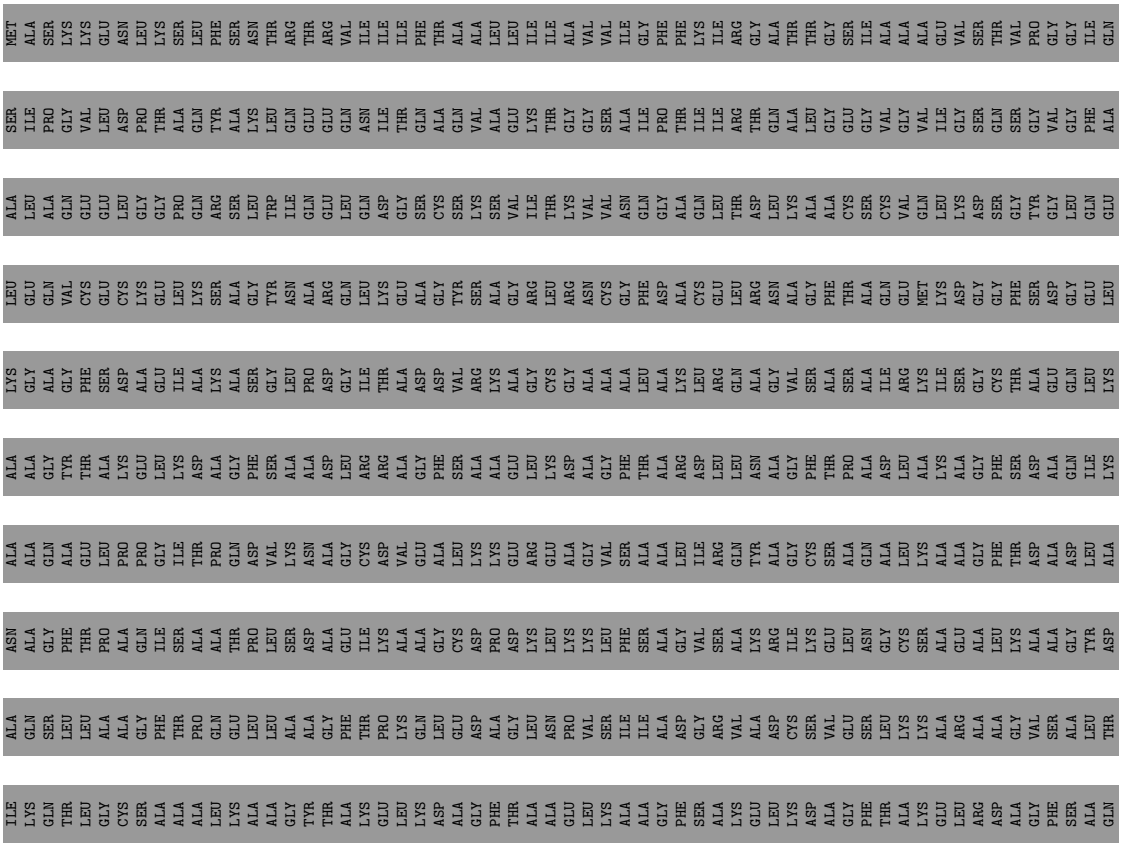


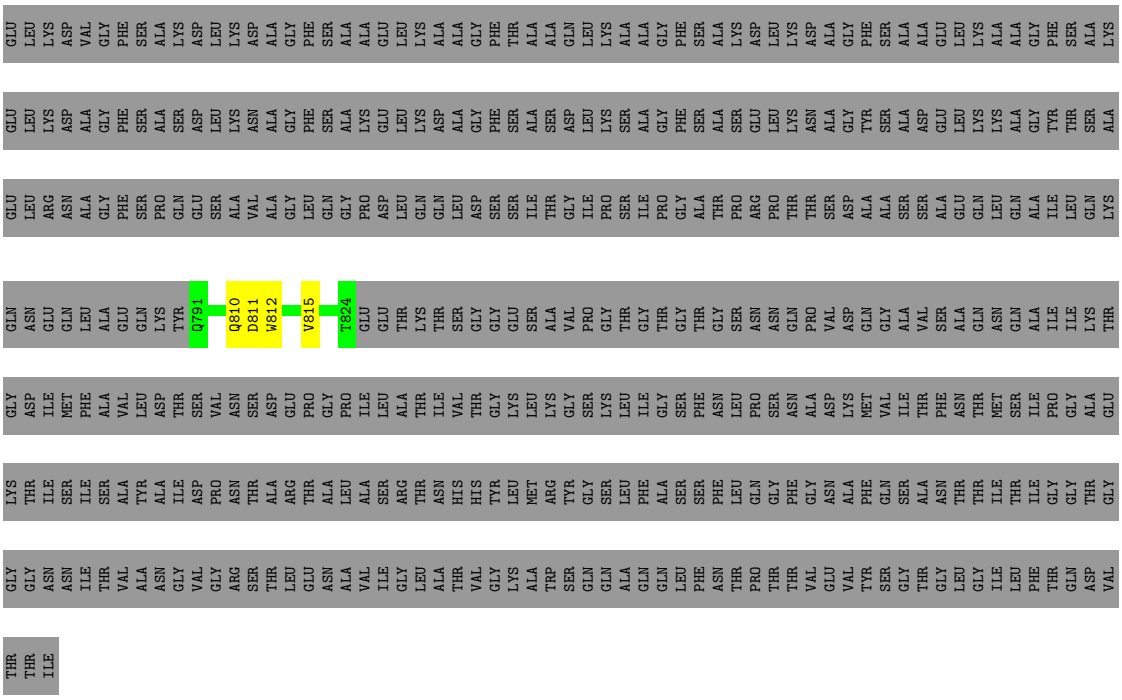


• Molecule 1: IcmE protein

Chain Cg:

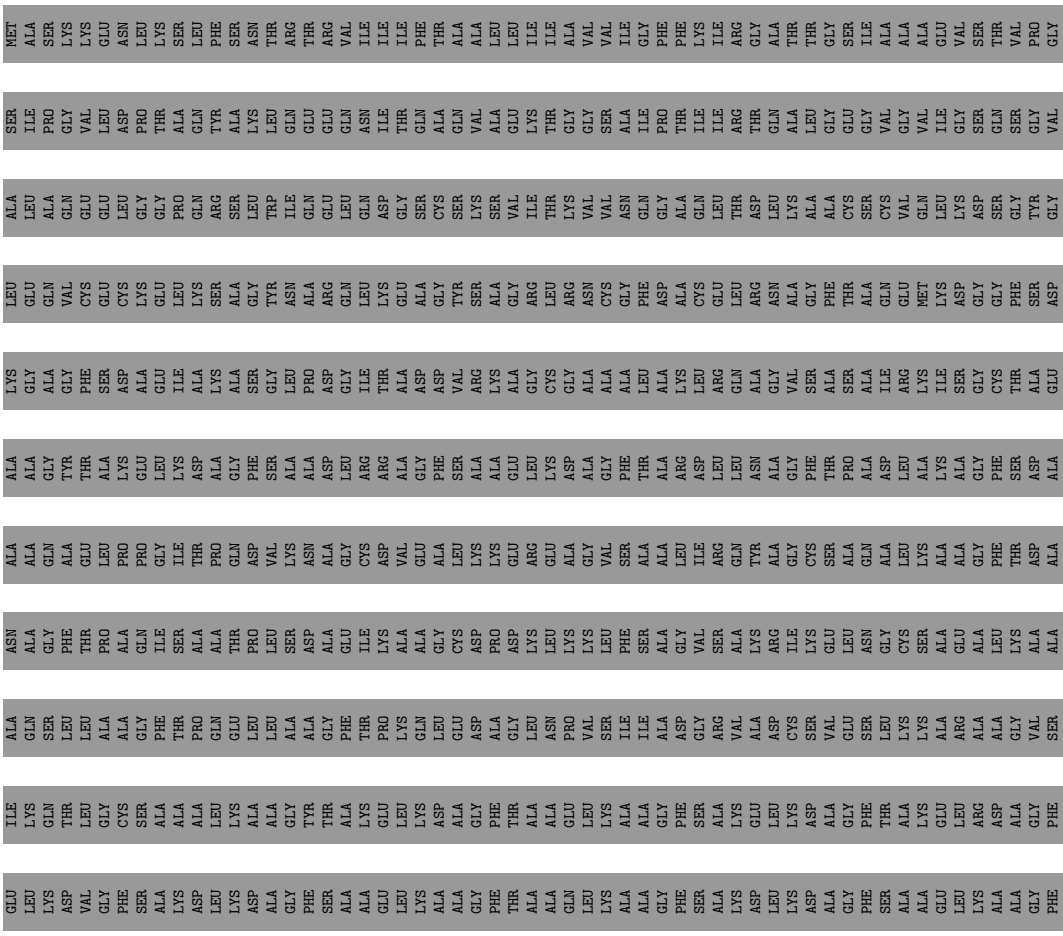


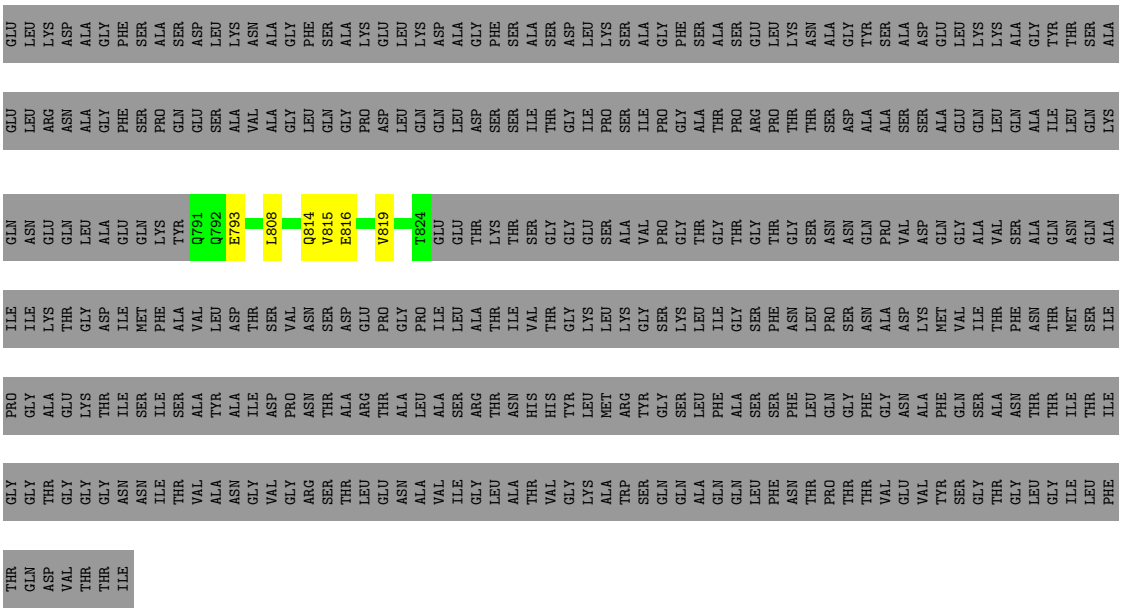




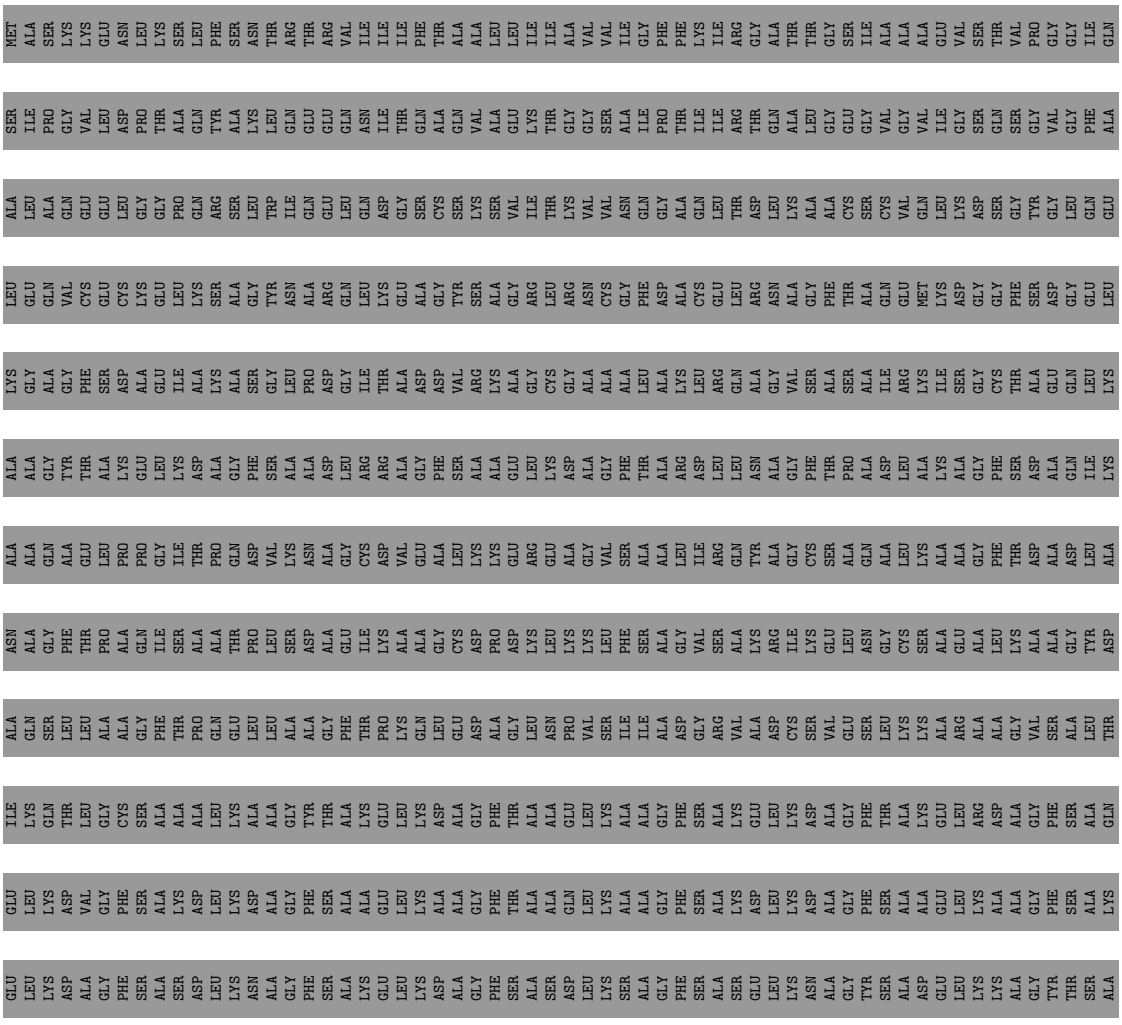
• Molecule 1: IcmE protein

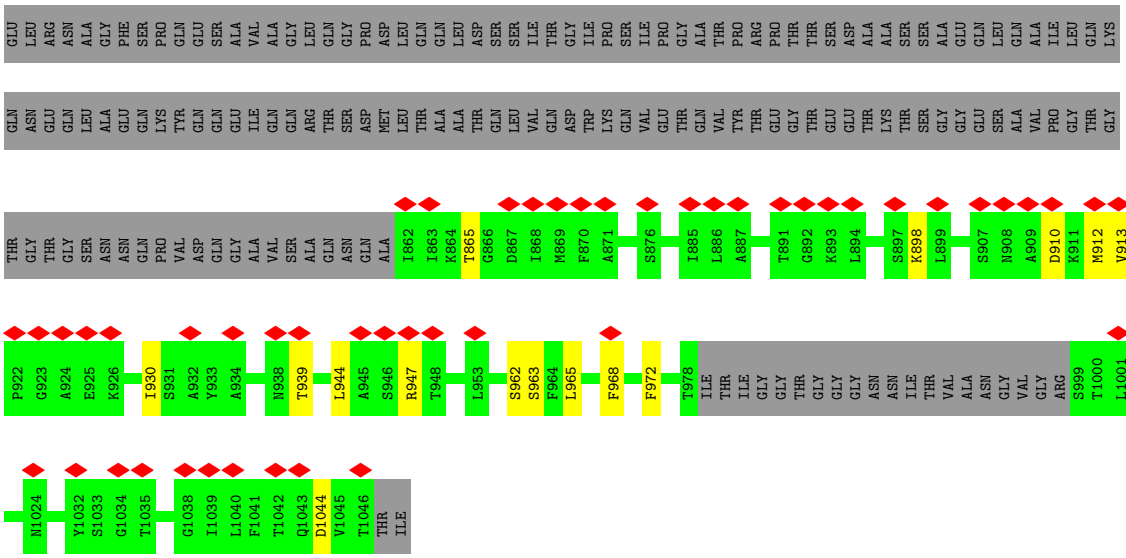
Chain Dg: 97%





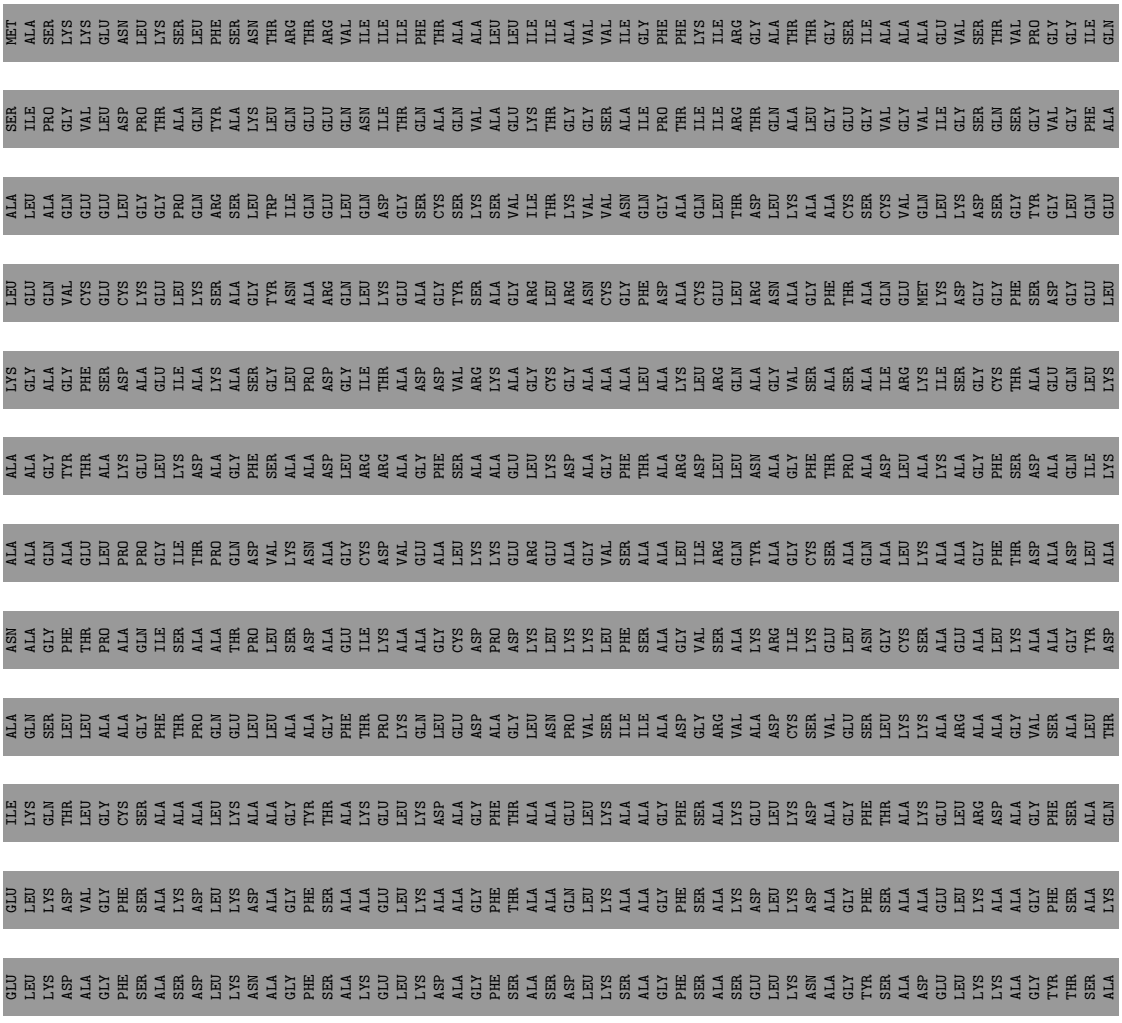
• Molecule 1: IcmE protein

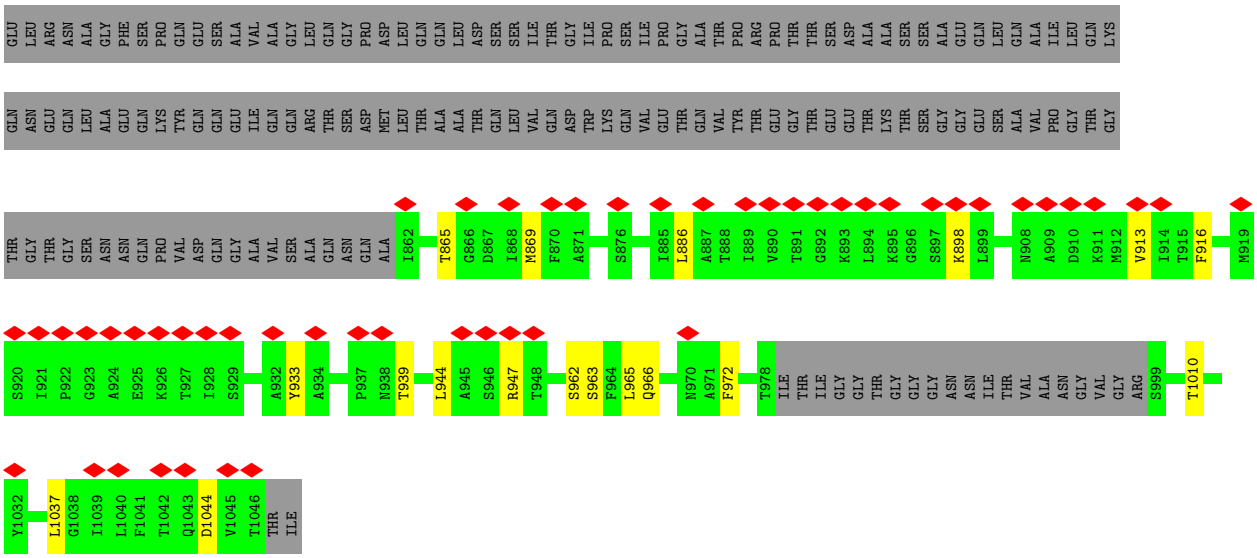




• Molecule 1: IcmE protein

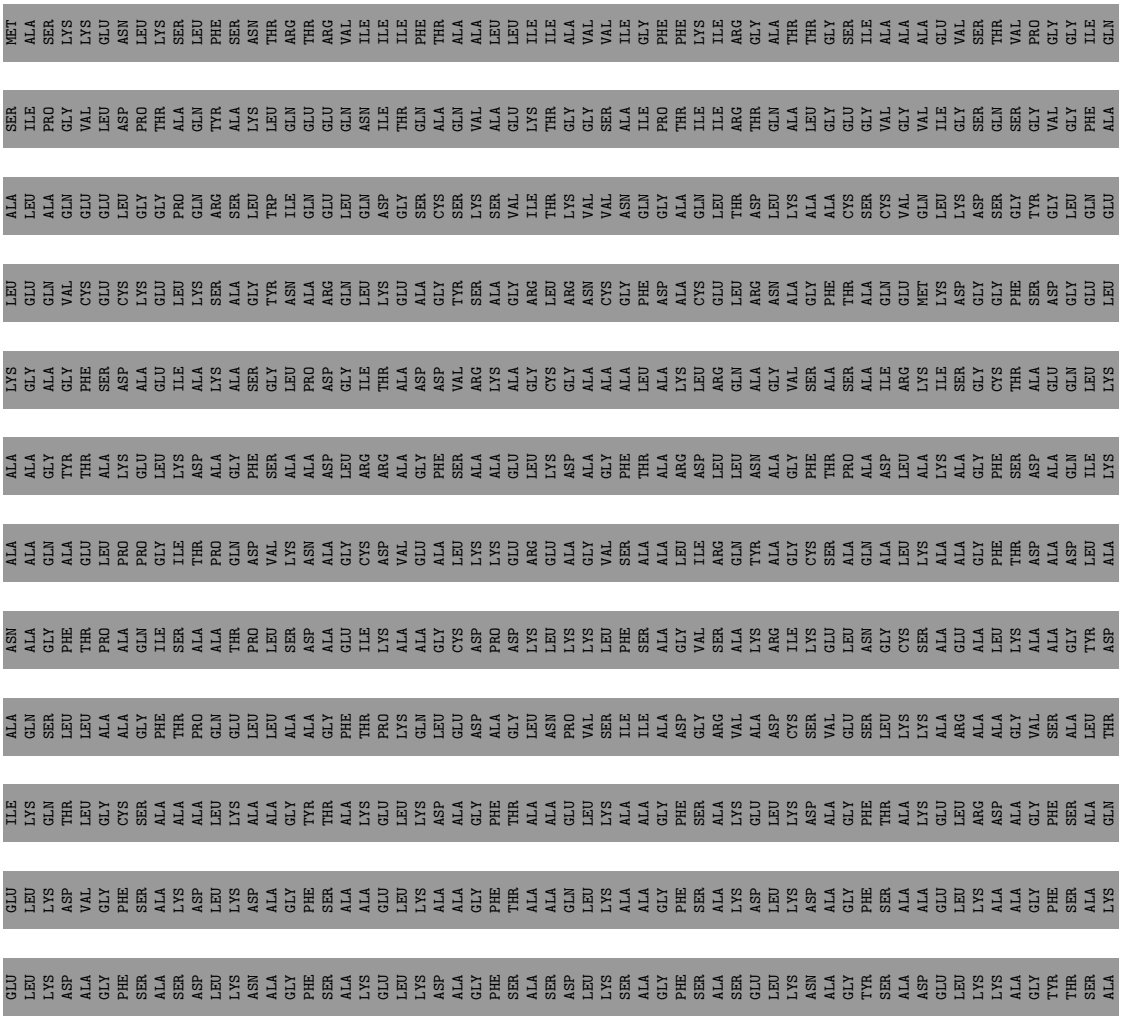
Chain IG:

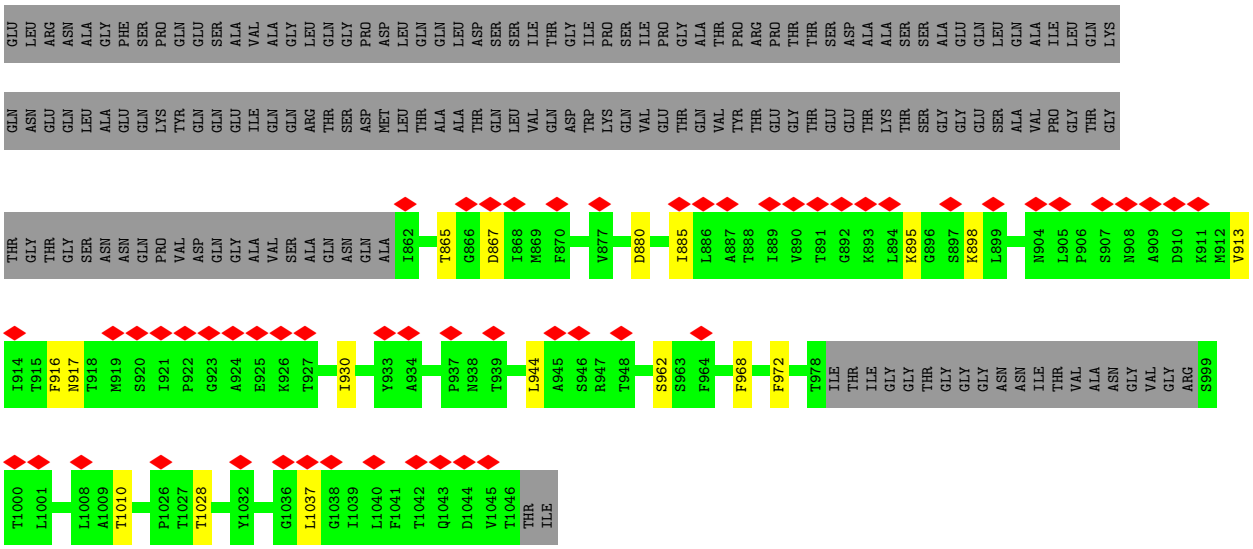


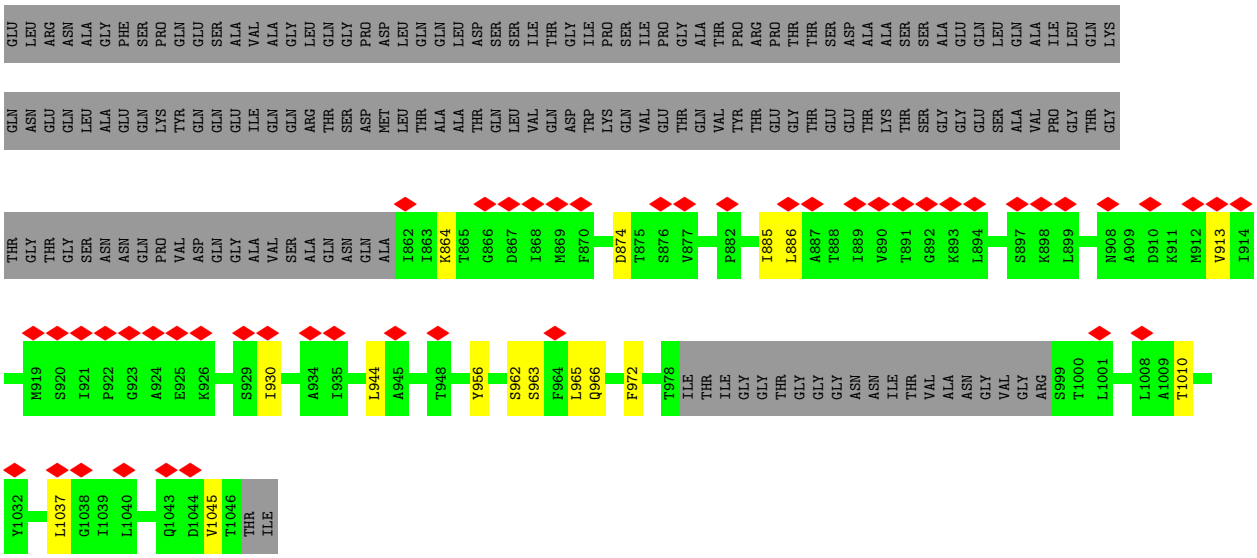


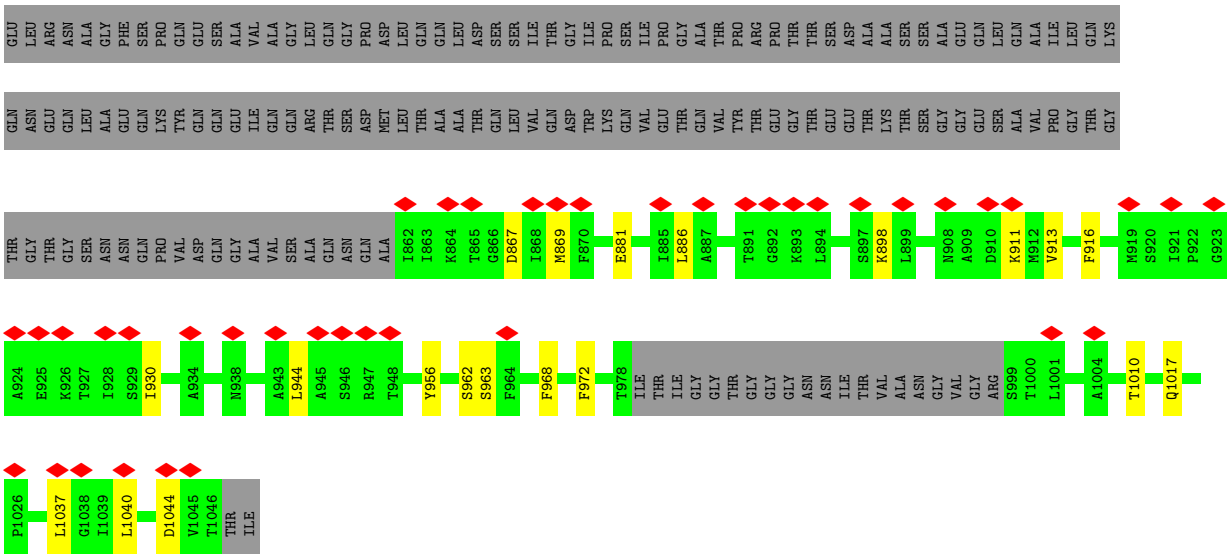
• Molecule 1: IcmE protein

Chain JG:



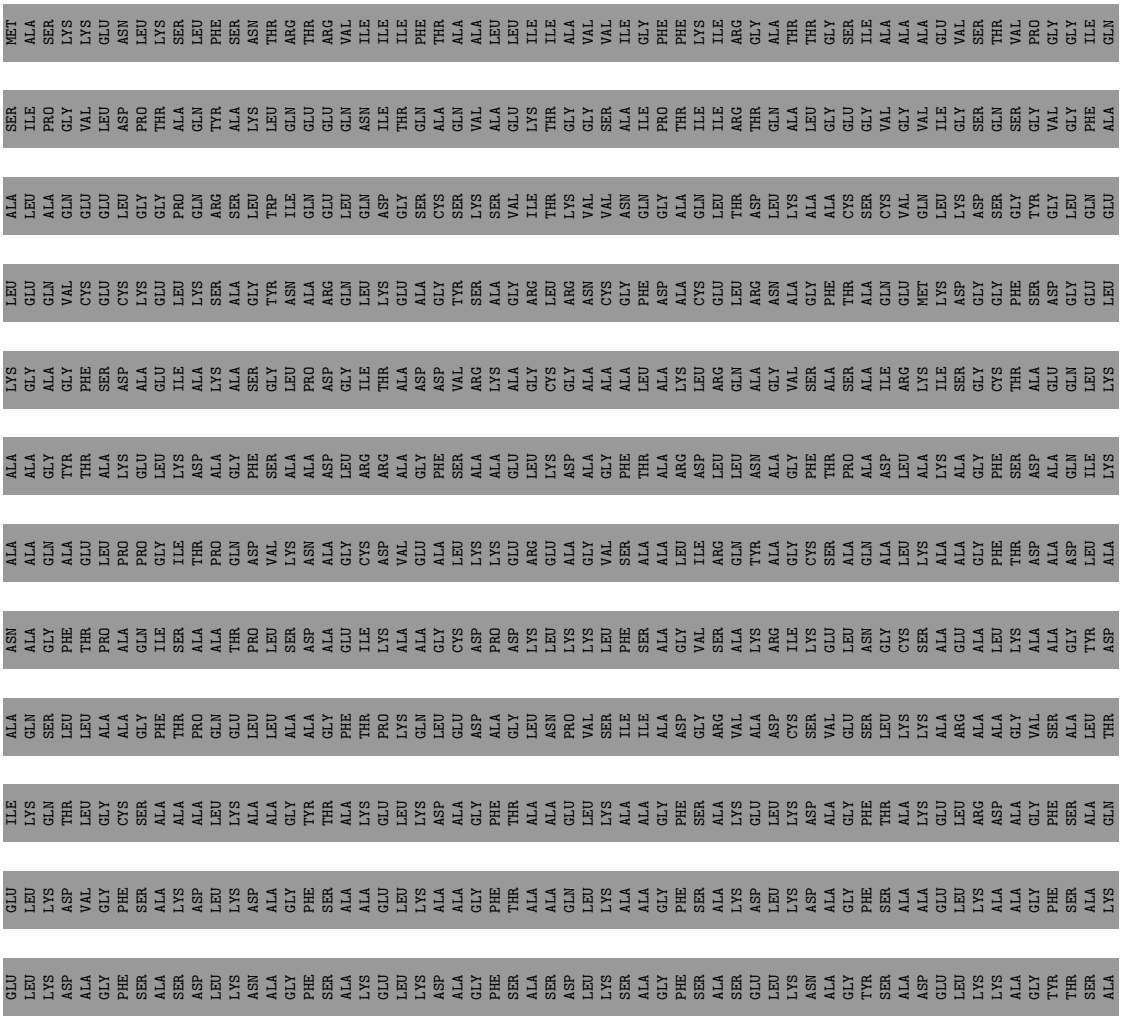


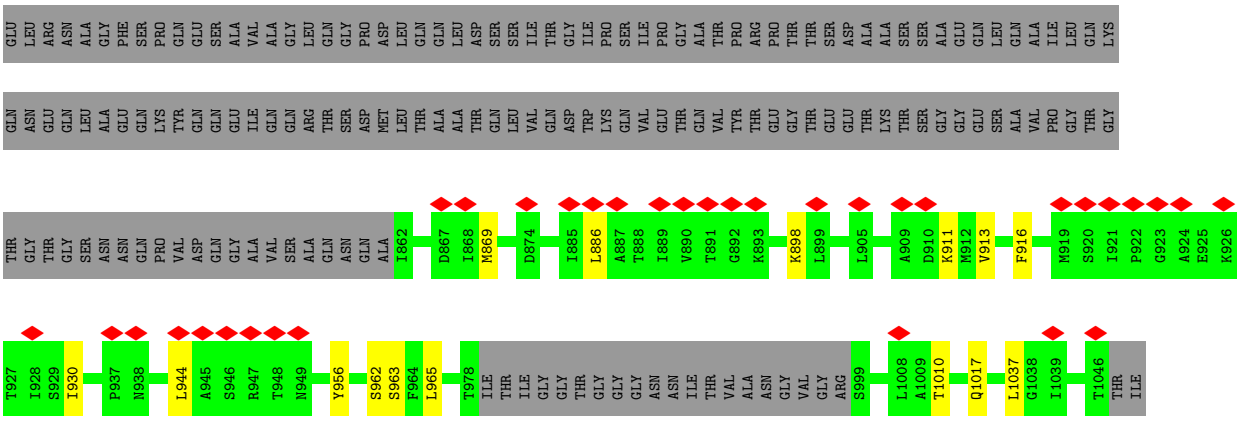




• Molecule 1: IcmE protein

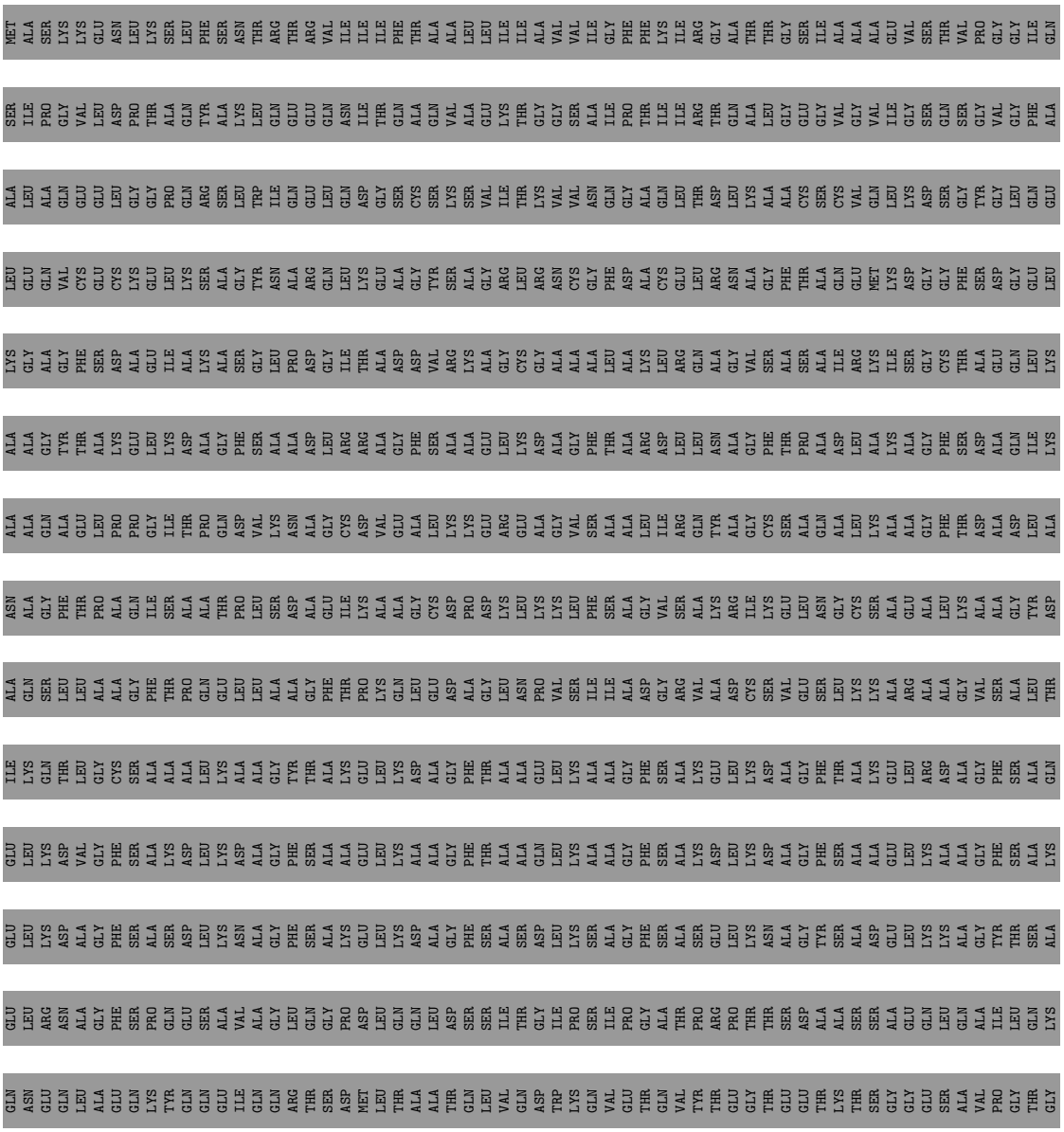
Chain MG:

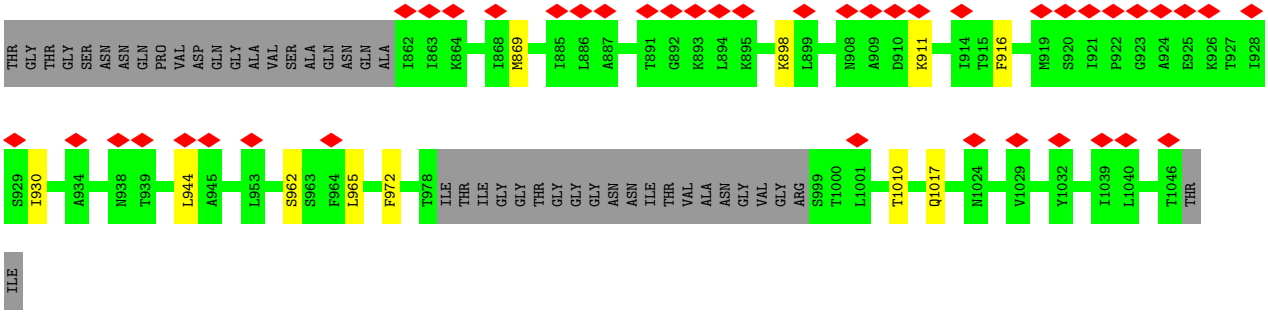




• Molecule 1: IcmE protein

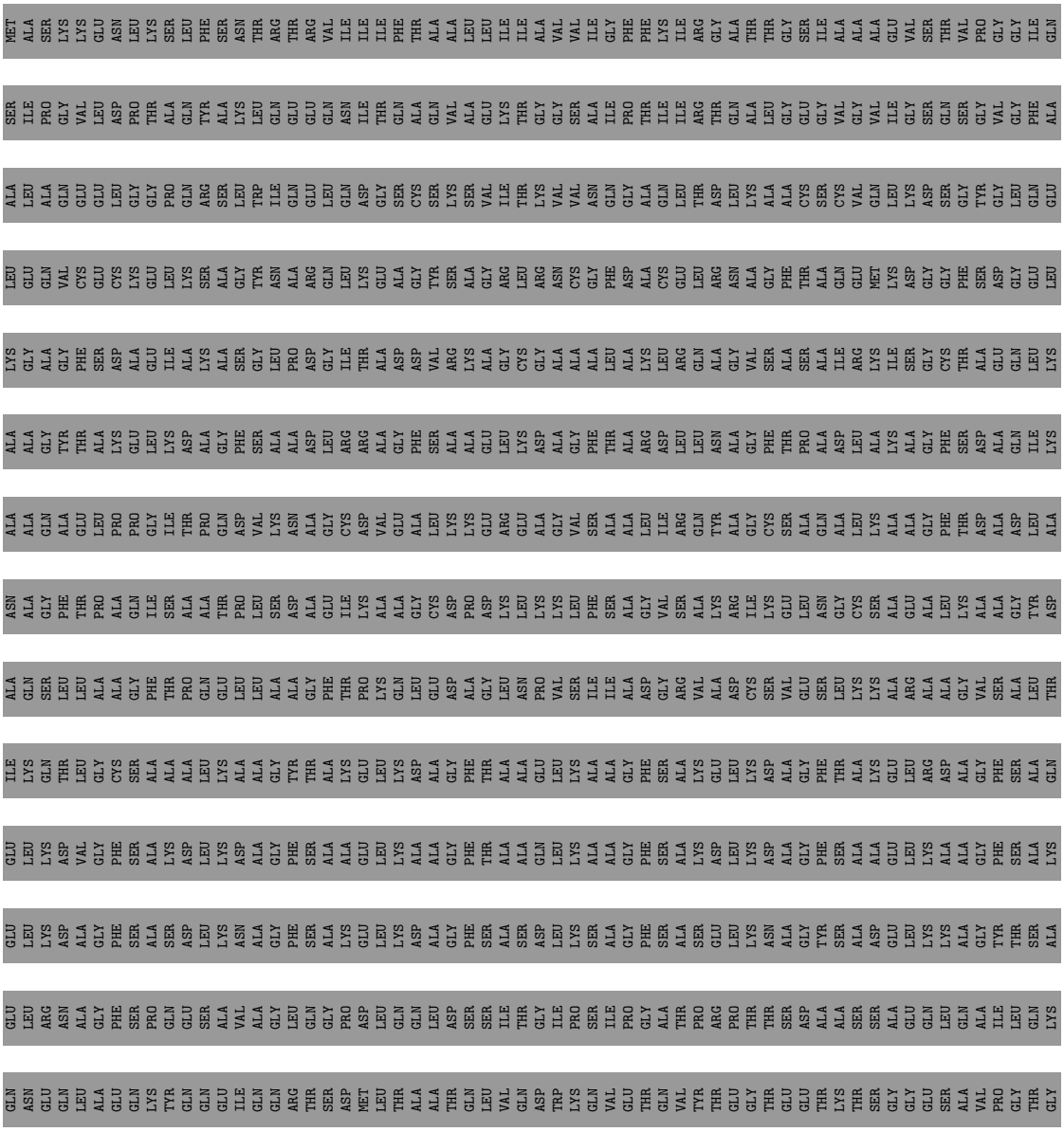
Chain NG:

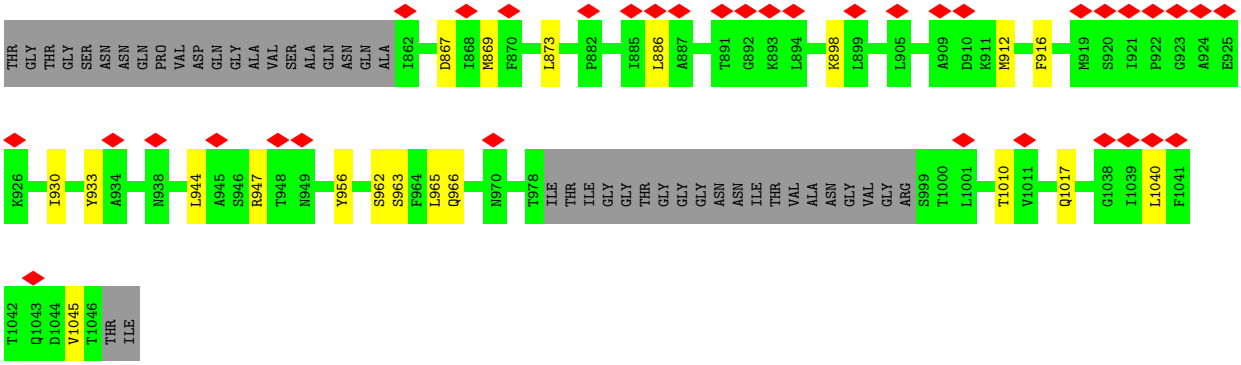




- Molecule 1: IcmE protein

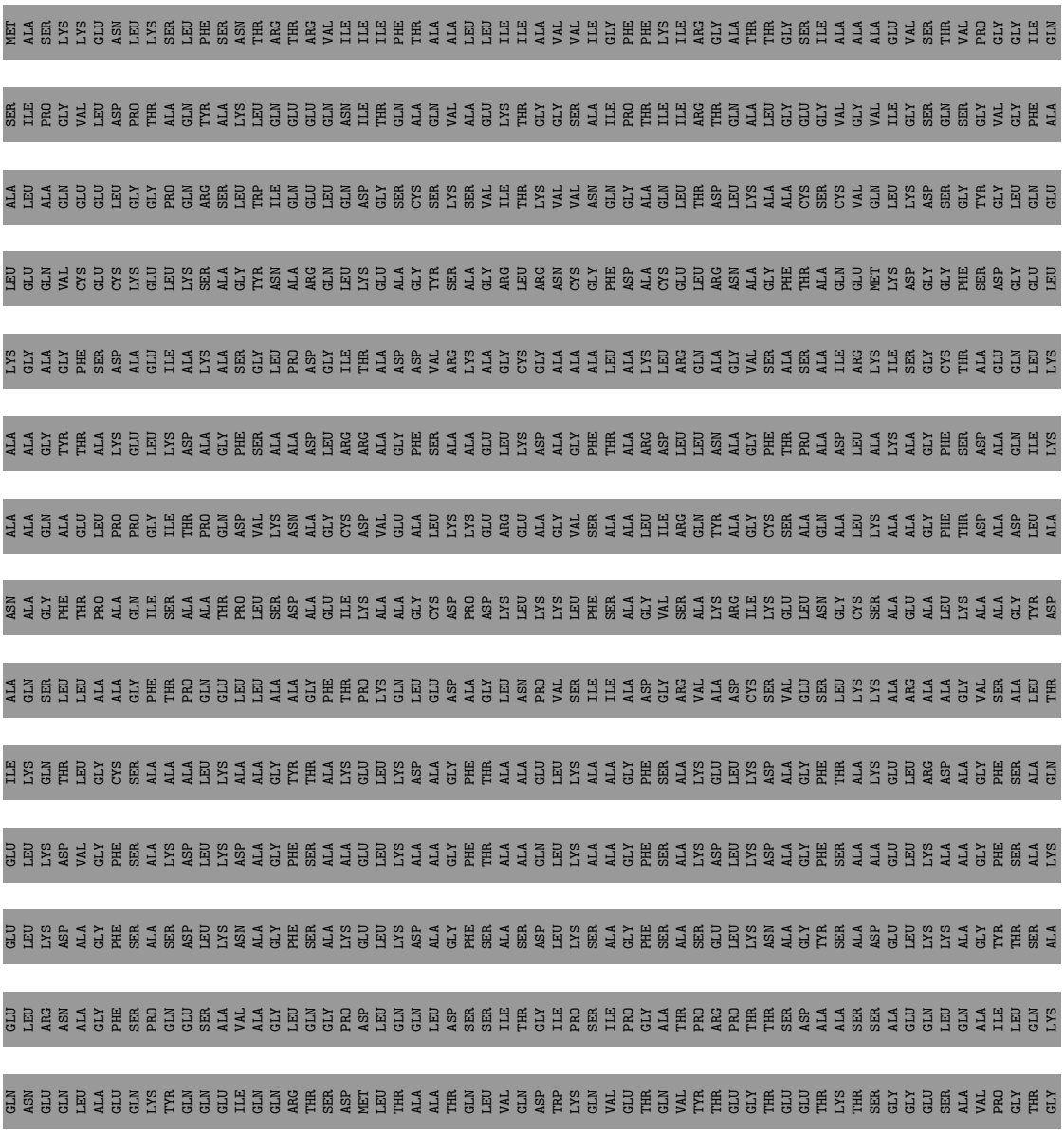
Chain OG:

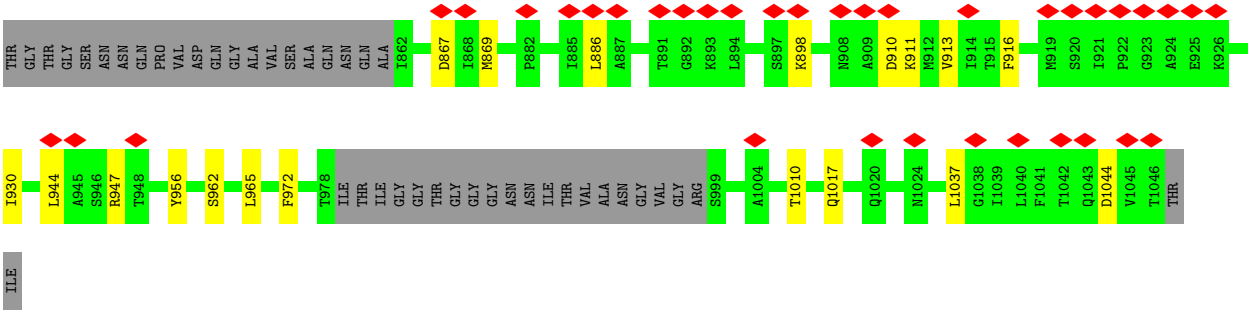




- Molecule 1: IcmE protein

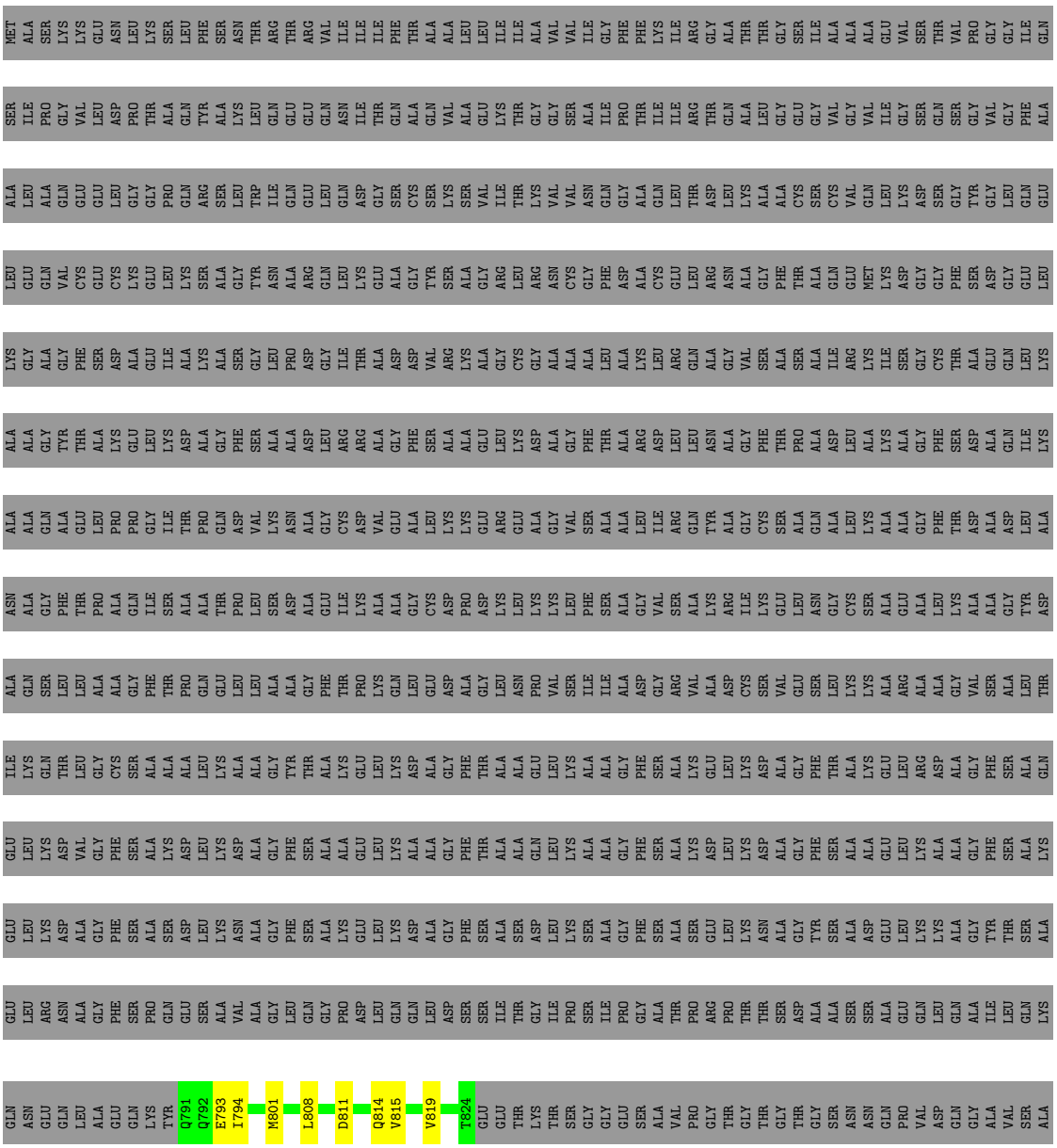
Chain PG:

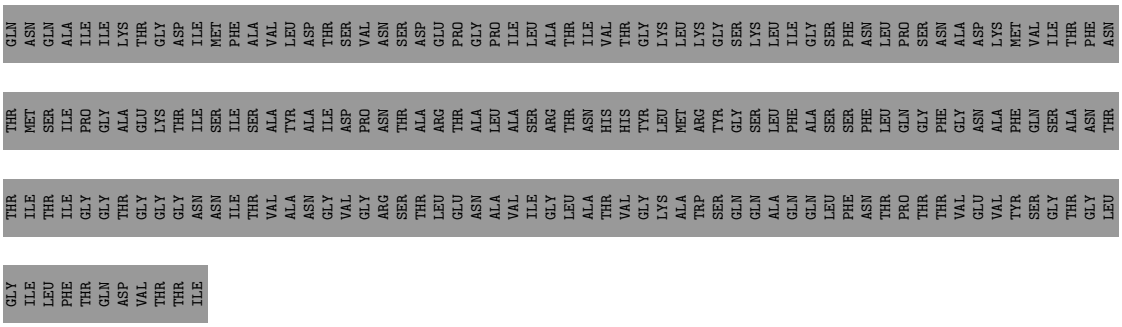




- Molecule 1: IcmE protein

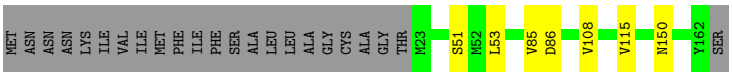
Chain Ag: 97%





• Molecule 2: DotD

Chain ED:



• Molecule 2: DotD

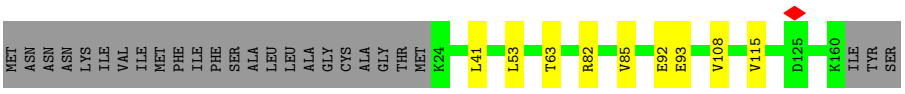
Chain Ed:

• Molecule 2: DotD

Chain FD:

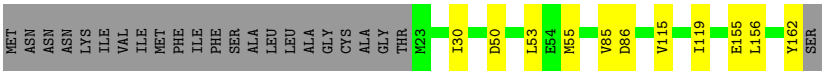
• Molecule 2: DotD

Chain Fd:



• Molecule 2: DotD

Chain GD:



• Molecule 2: DotD

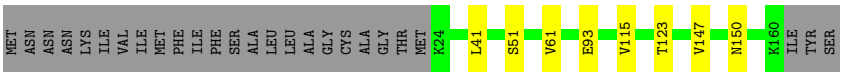
Chain Gd:

• Molecule 2: DotD

Chain HD:

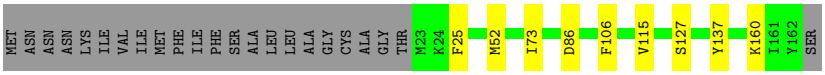
• Molecule 2: DotD

Chain Hd:



• Molecule 2: DotD

Chain ID:



• Molecule 2: DotD

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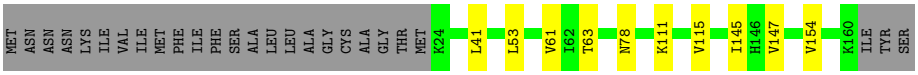

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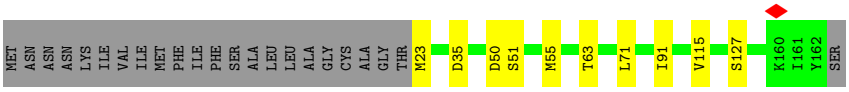
Chain JD:



• Molecule 2: DotD

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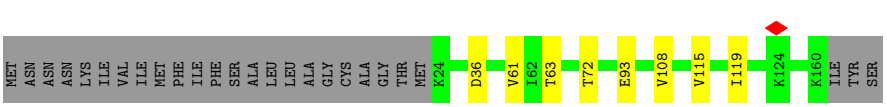

• Molecule 2: DotD

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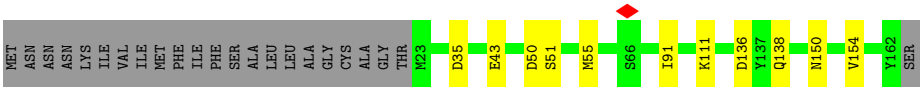
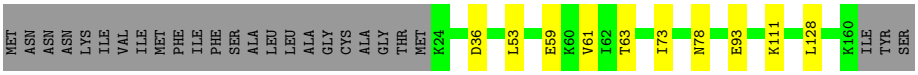


• Molecule 2: DotD

Chain Kd:

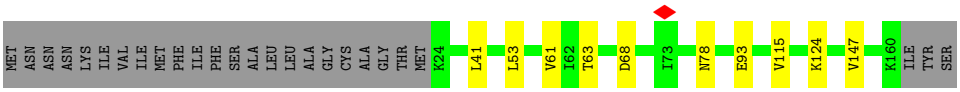


• Molecule 2: DotD

Chain LD:

• Molecule 2: DotD

Chain Ld:



• Molecule 2: DotD

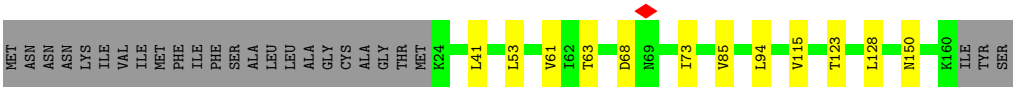
Chain MD:

• Molecule 2: DotD

Chain Md:

• Molecule 2: DotD

Chain Ad:



• Molecule 2: DotD

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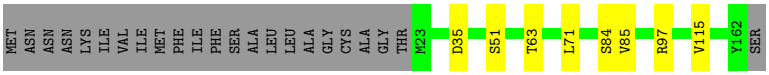
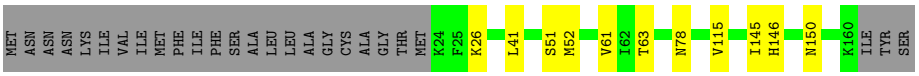


• Molecule 2: DotD

Chain Bd:



• Molecule 2: DotD

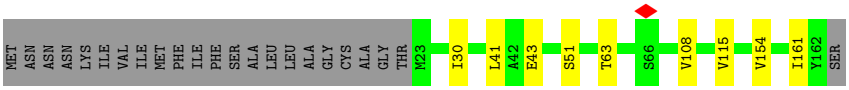
Chain CD:

• Molecule 2: DotD

Chain Cd:

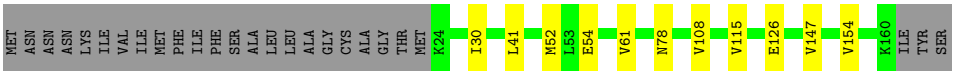
• Molecule 2: DotD

Chain DD:



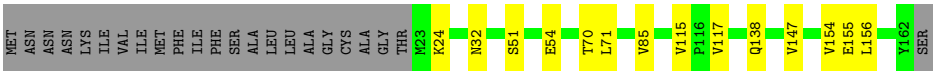
• Molecule 2: DotD

Chain Dd:



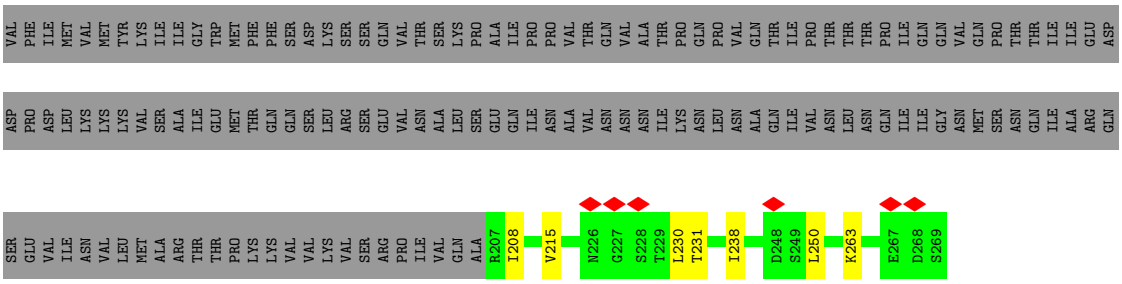
• Molecule 2: DotD

Chain AD:



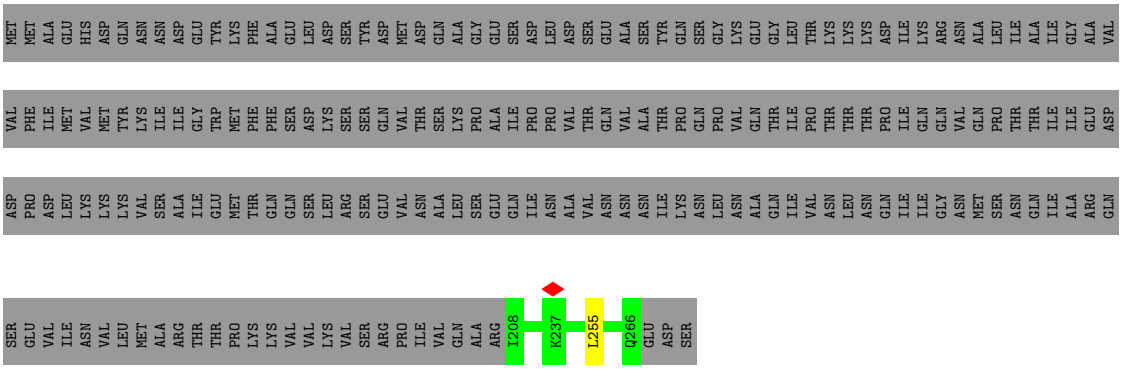
• Molecule 3: DotF

Chain EF:



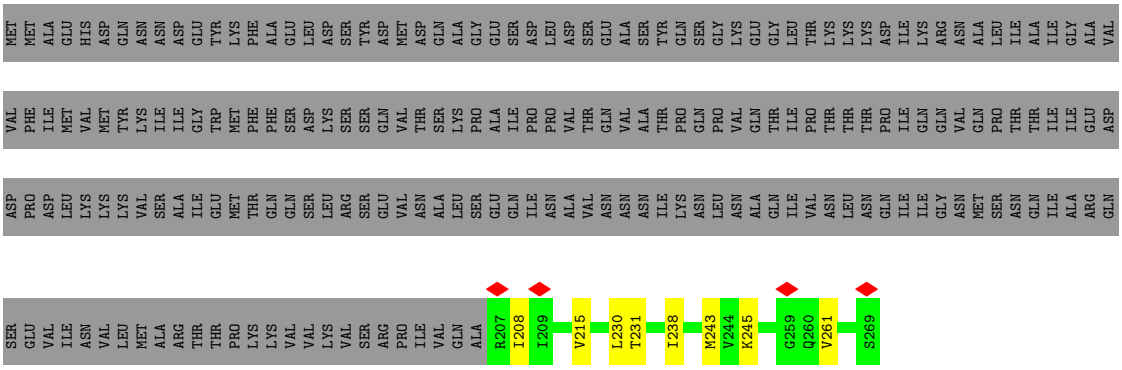
• Molecule 3: DotF

Chain Ef:



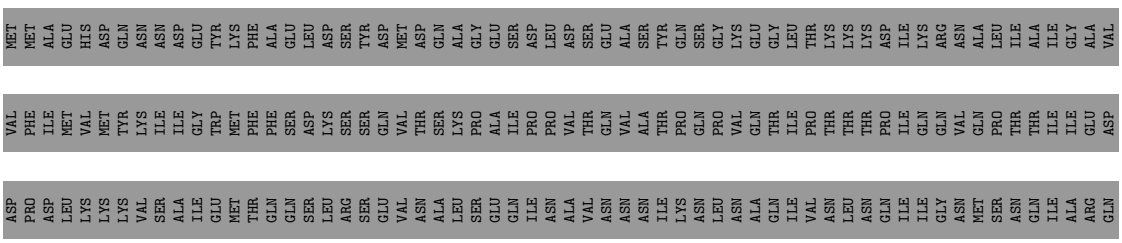
• Molecule 3: DotF

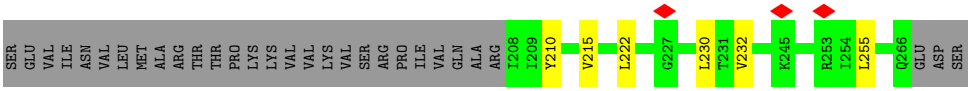
Chain FF:



• Molecule 3: DotF

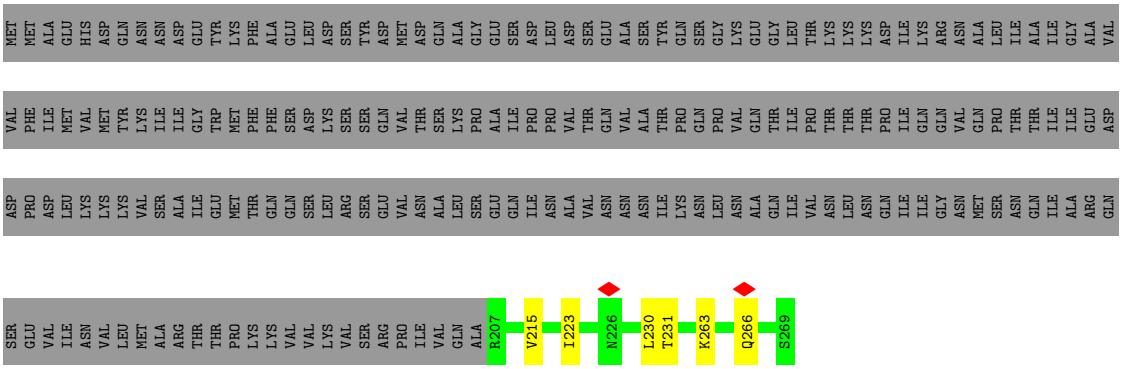
Chain Ff:





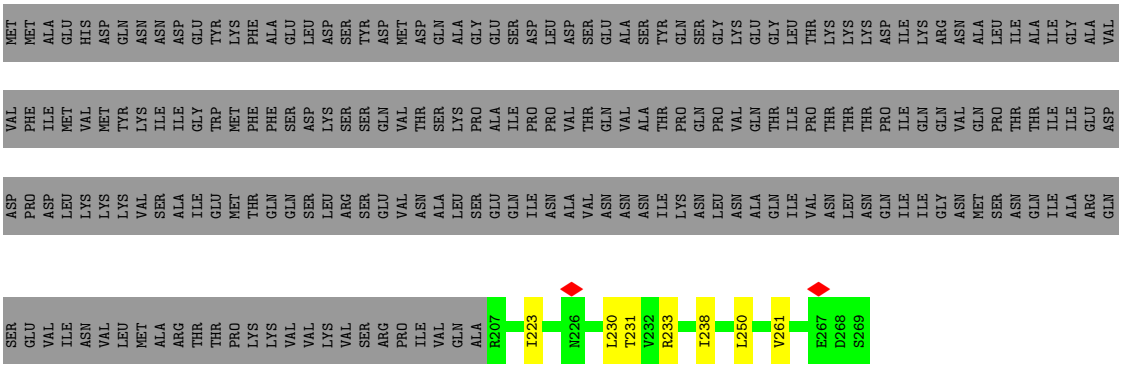
• Molecule 3: DotF

Chain AF:



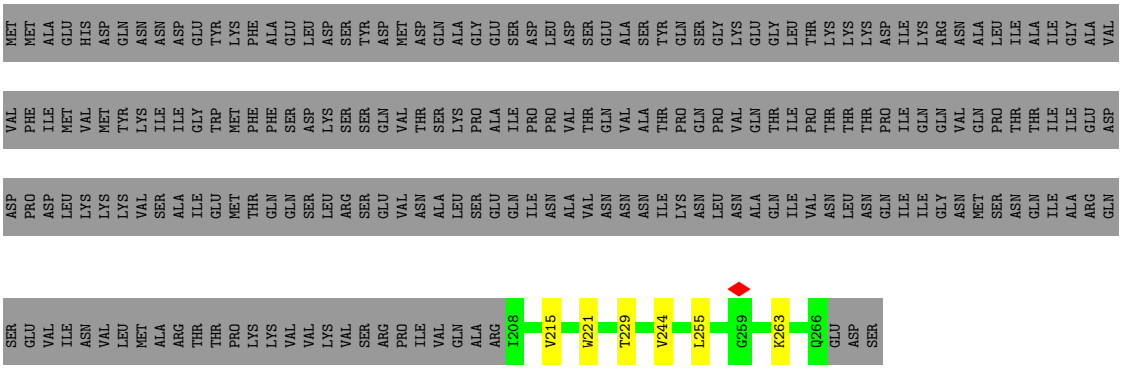
• Molecule 3: DotF

Chain GF:



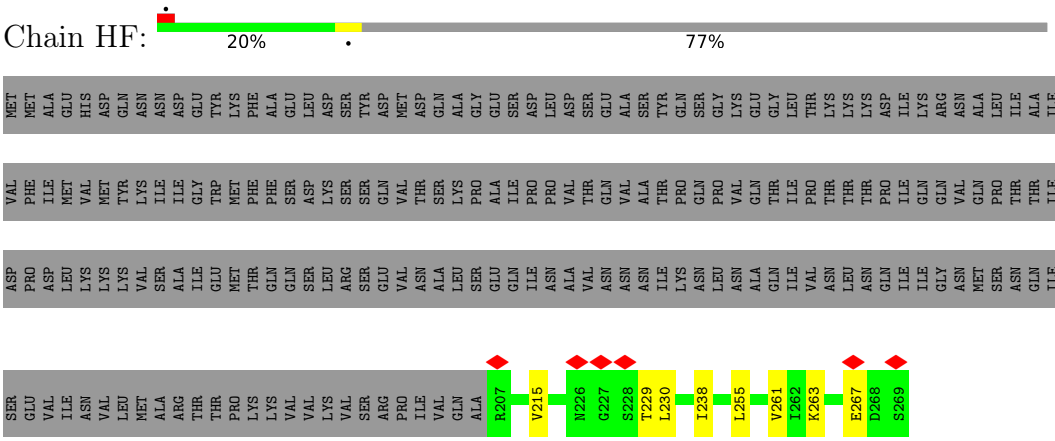
• Molecule 3: DotF

Chain Gf:



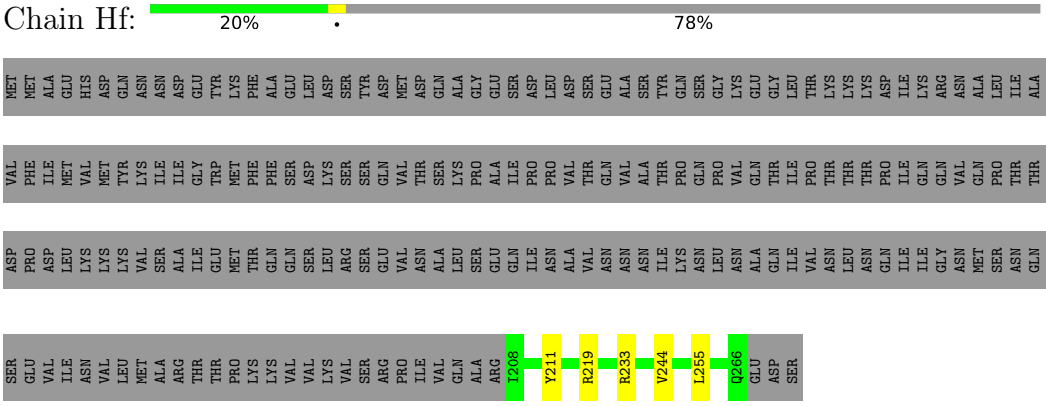
• Molecule 3: DotF

Chain HF:



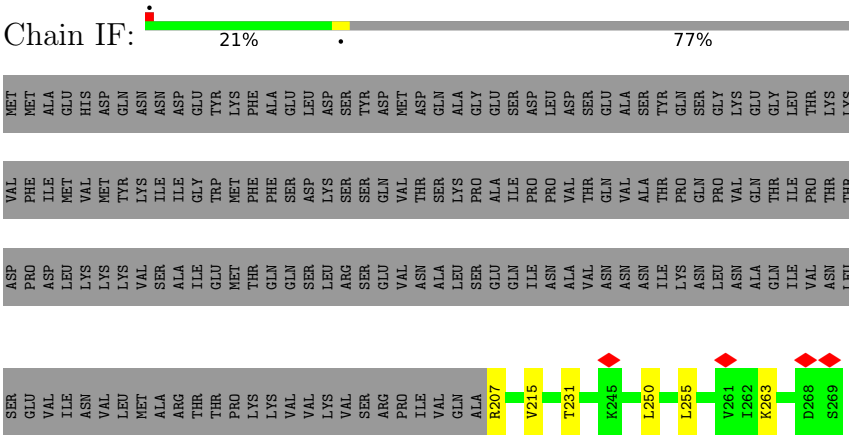
• Molecule 3: DotF

Chain Hf:



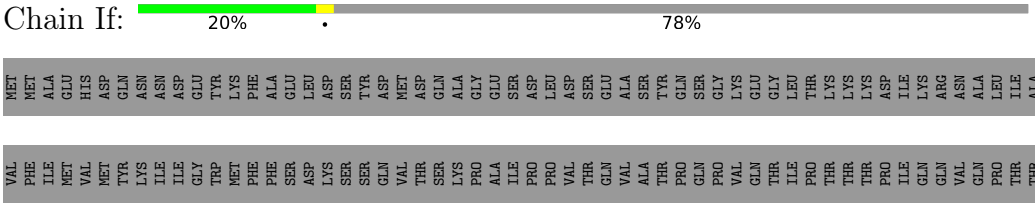
• Molecule 3: DotF

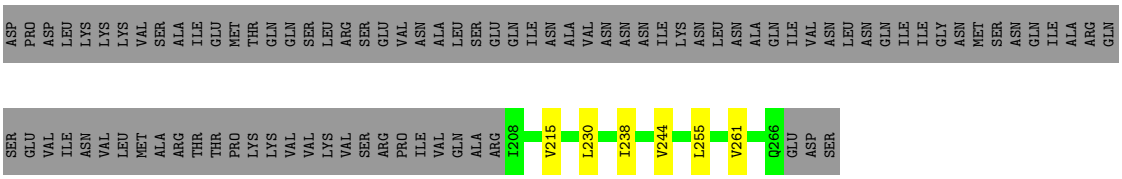
Chain IF:



• Molecule 3: DotF

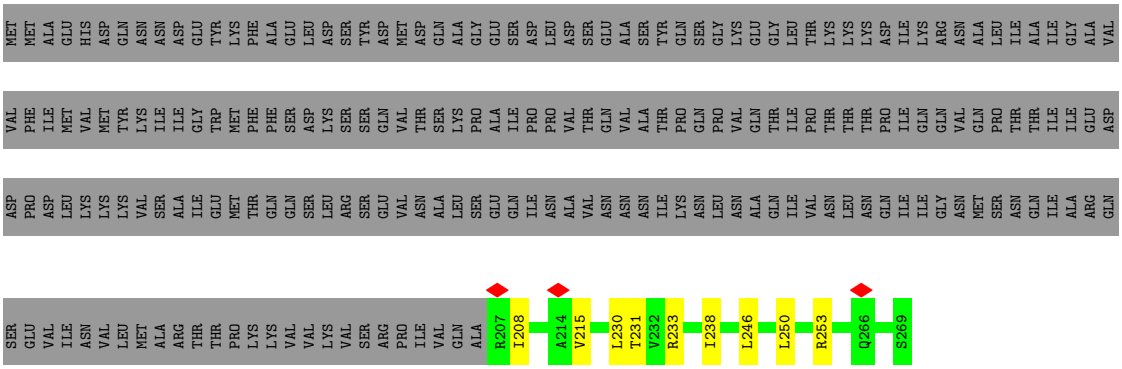
Chain If:





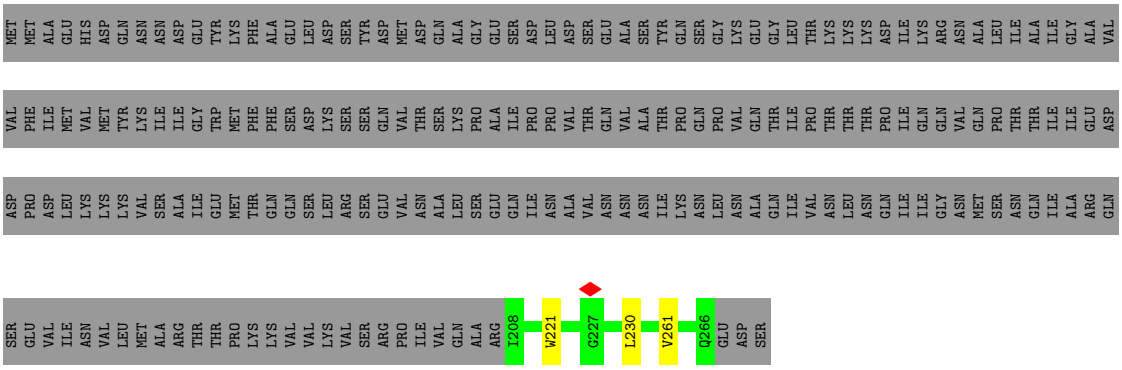
• Molecule 3: DotF

Chain JF:



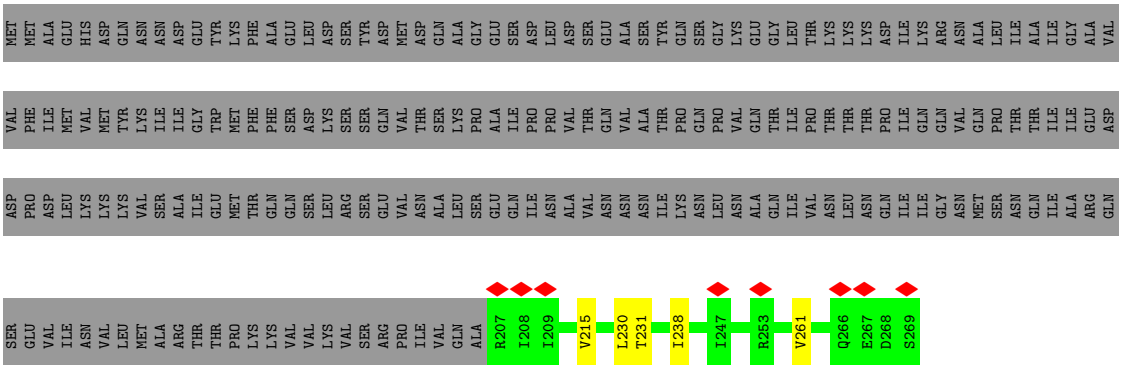
• Molecule 3: DotF

Chain Jf:



• Molecule 3: DotF

Chain KF:



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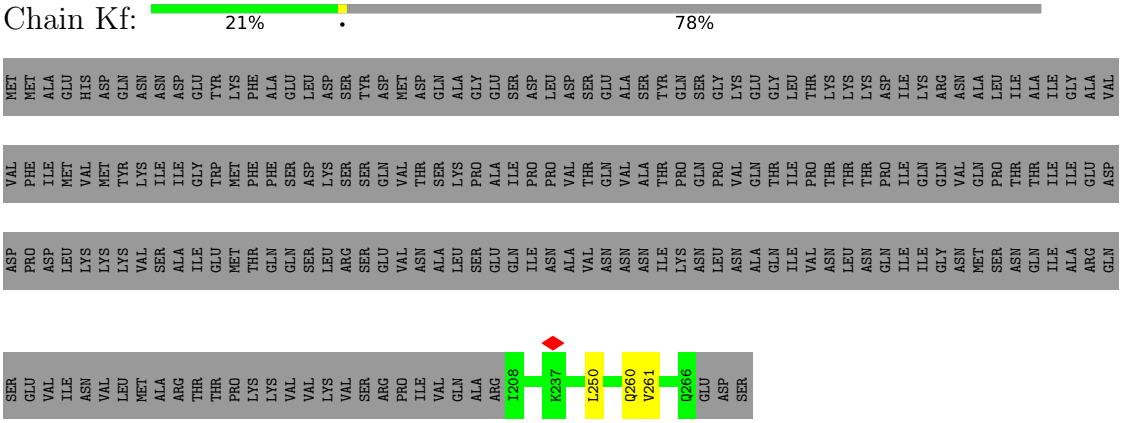
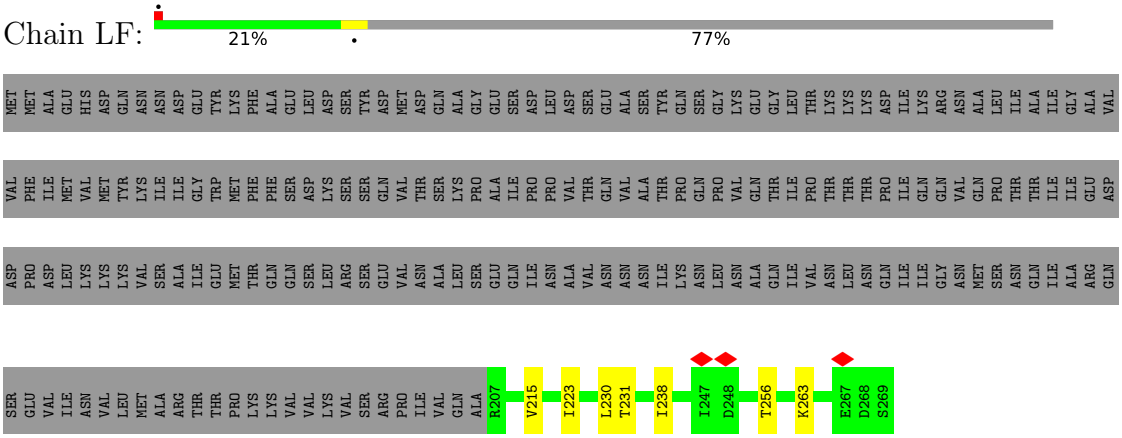
Chain Kf:



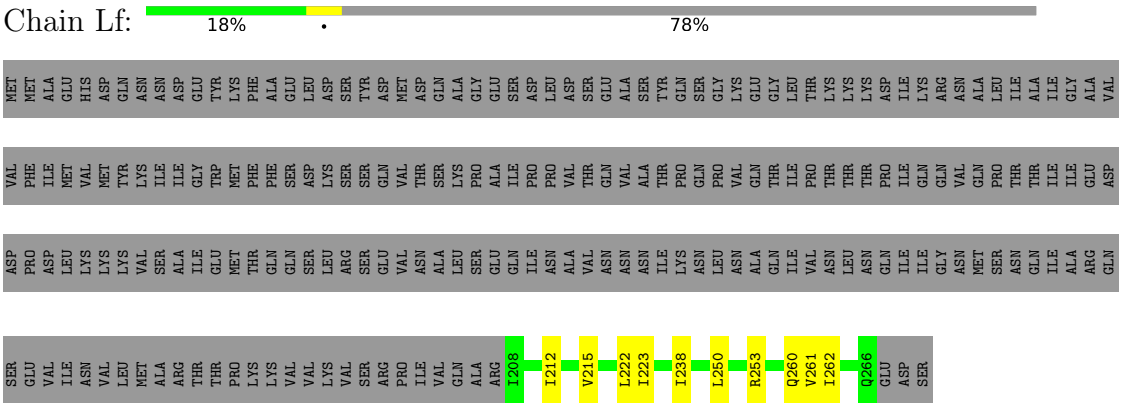
• Molecule 3: DotF

Chain LF:



• Molecule 3: DotF

Chain Lf:



• Molecule 3: DotF

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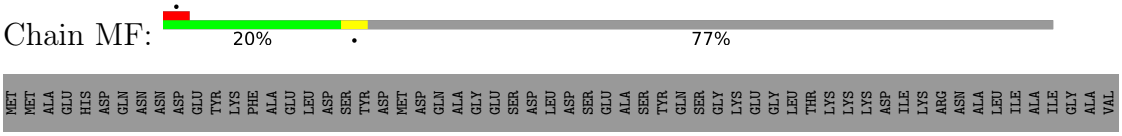

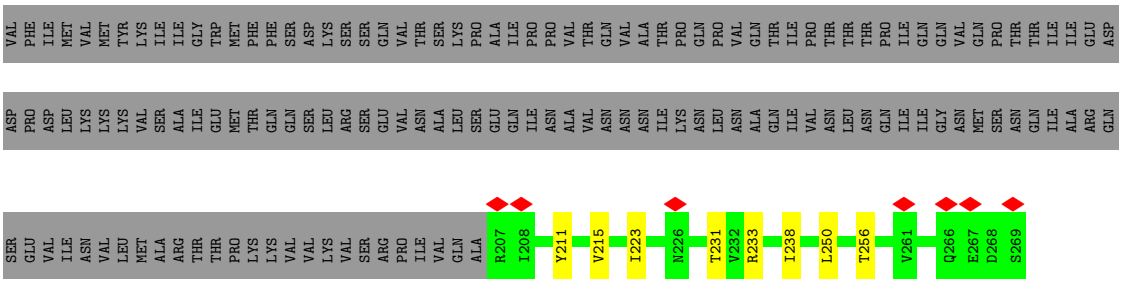

• Molecule 3: DotF

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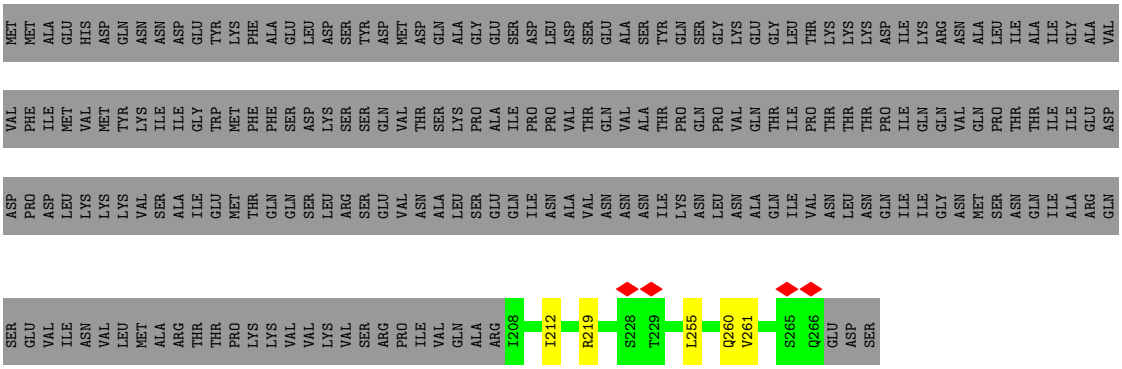
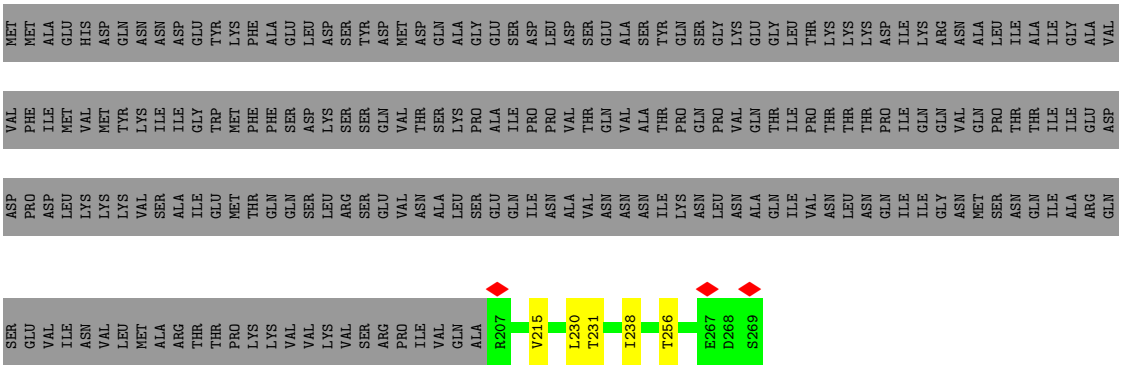


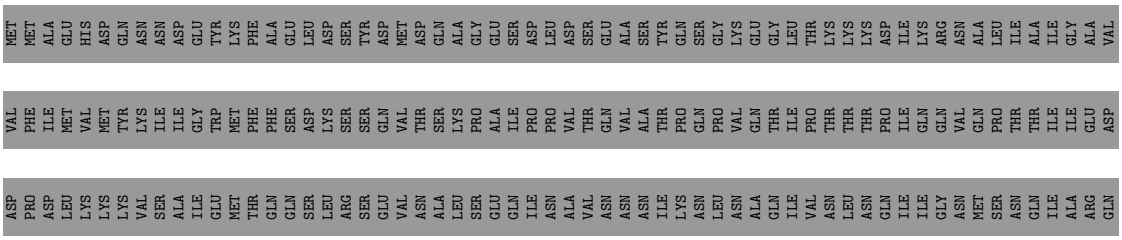
• Molecule 3: DotF

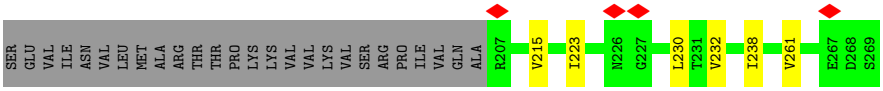
Chain VF:



• Molecule 3: DotF

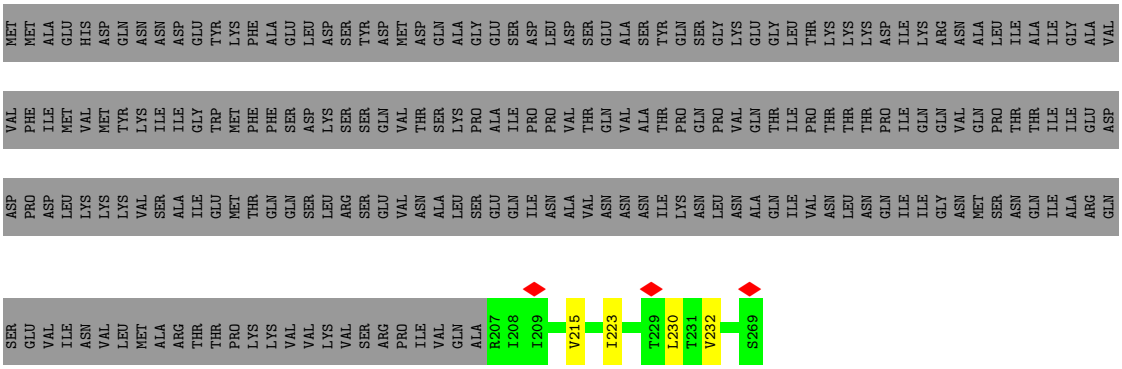
Chain WF:





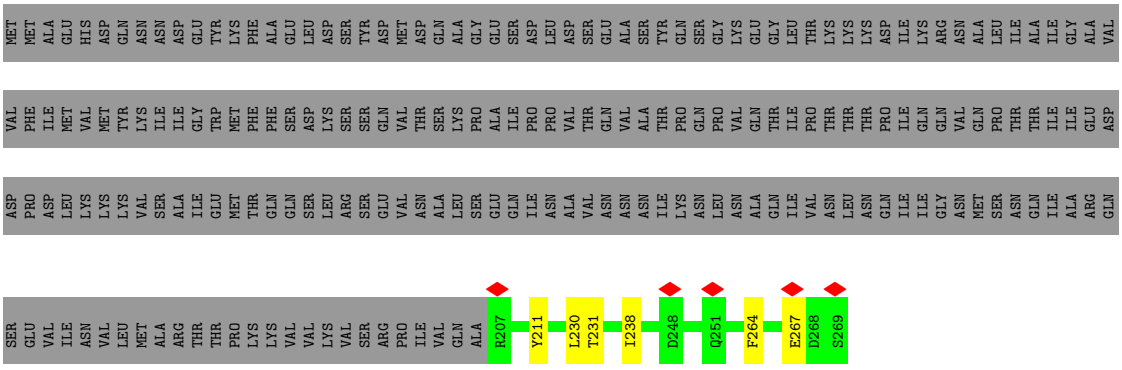
• Molecule 3: DotF

Chain XF:



• Molecule 3: DotF

Chain YF:



• Molecule 3: DotF

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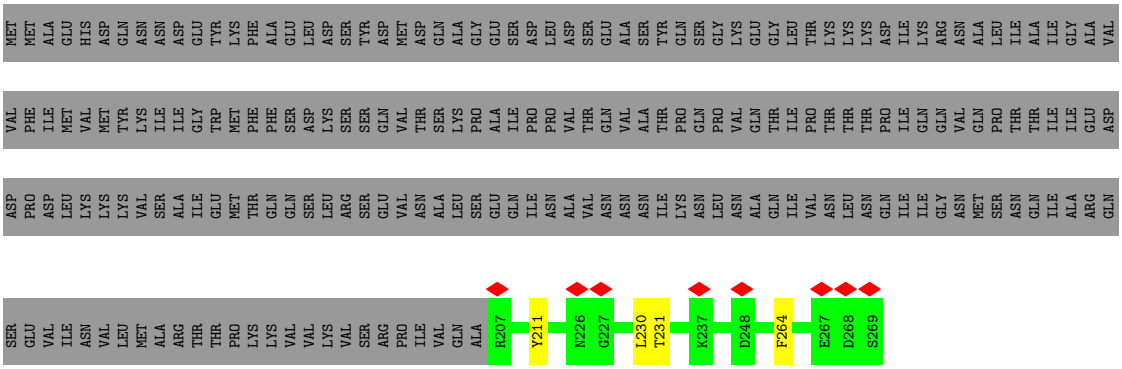
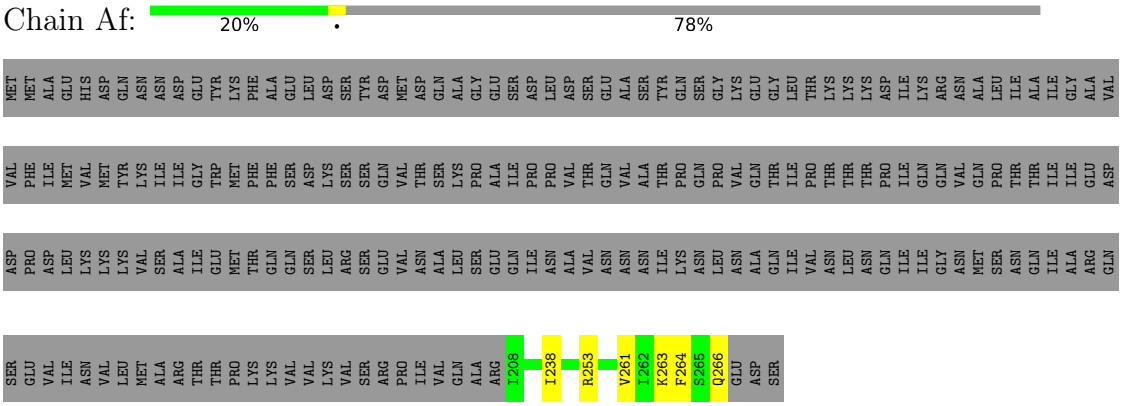


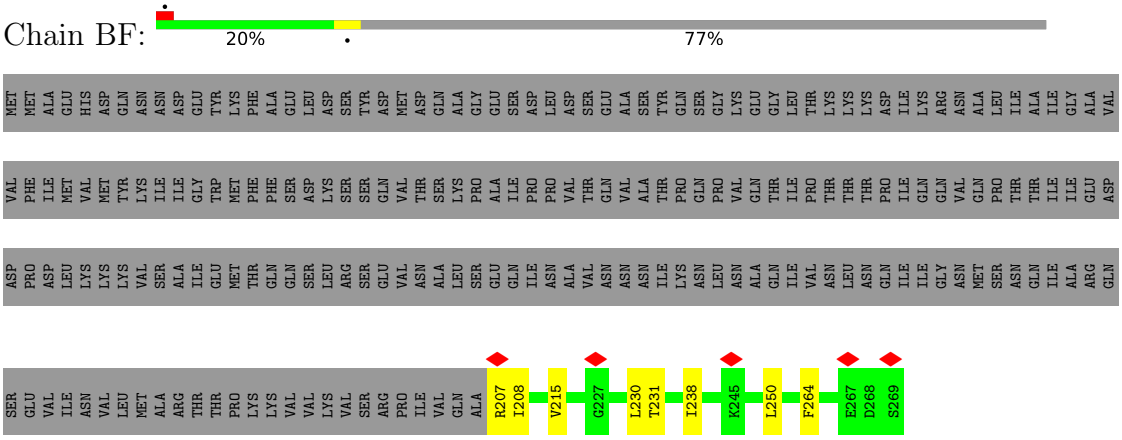
• Molecule 3: DotF

Chain Af:



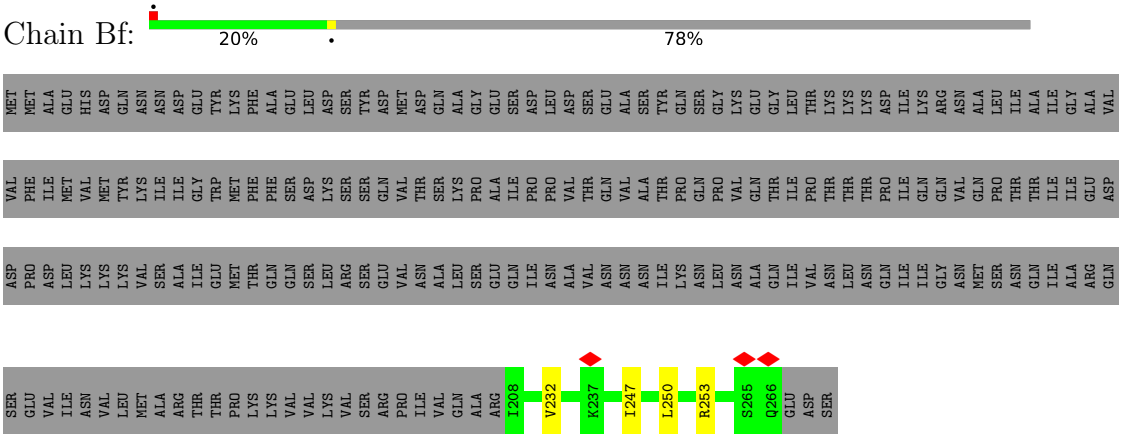
• Molecule 3: DotF

Chain BF:



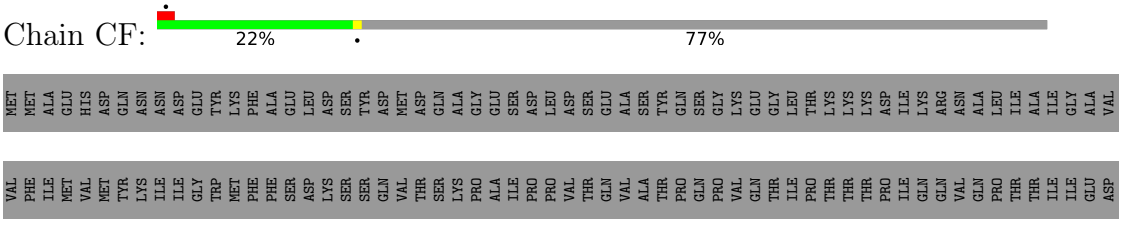
• Molecule 3: DotF

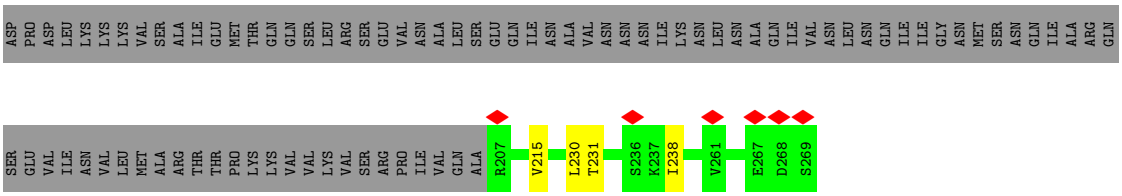
Chain Bf:



• Molecule 3: DotF

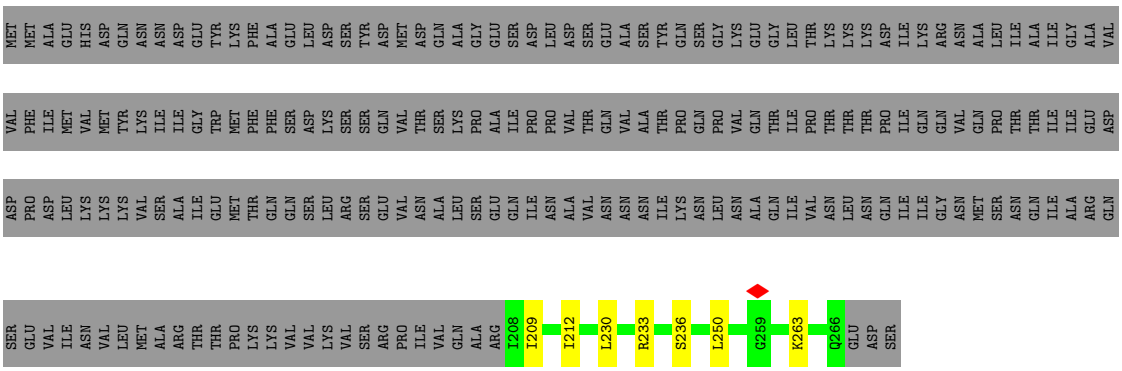
Chain CF:





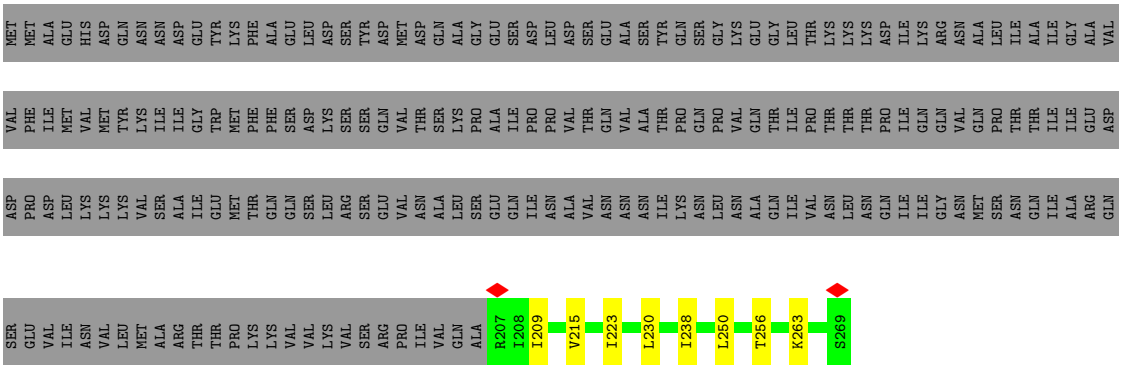
• Molecule 3: DotF

Chain Cf:



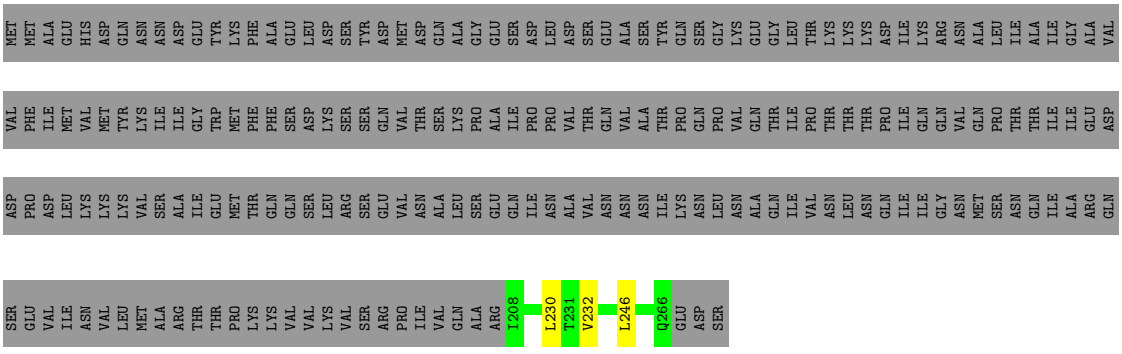
• Molecule 3: DotF

Chain DF:



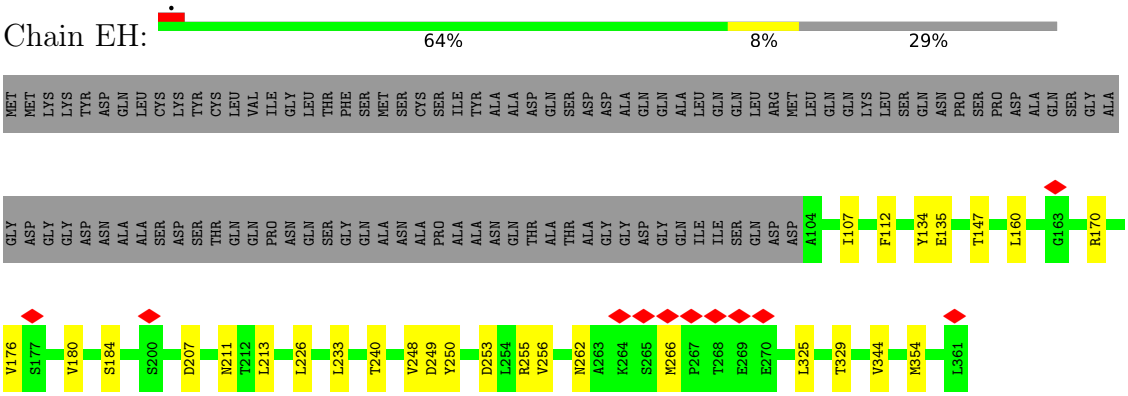
• Molecule 3: DotF

Chain Df:



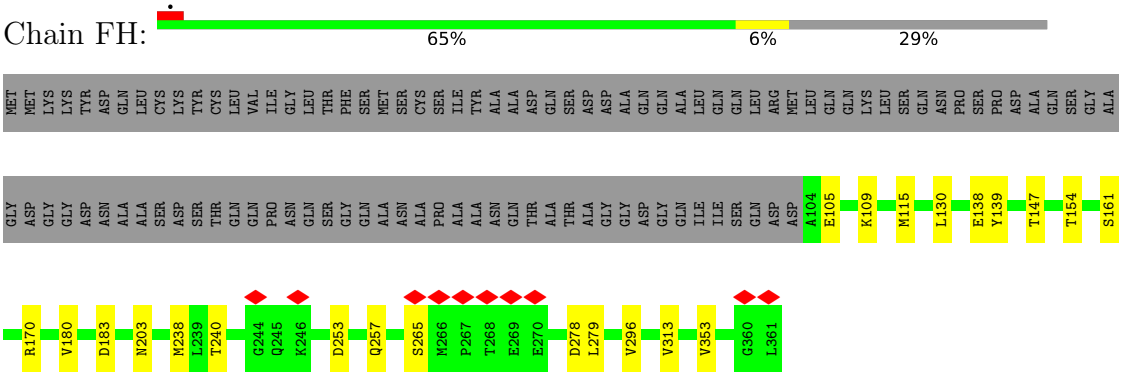
• Molecule 4: Type IV secretion protein IcmK

Chain EH:



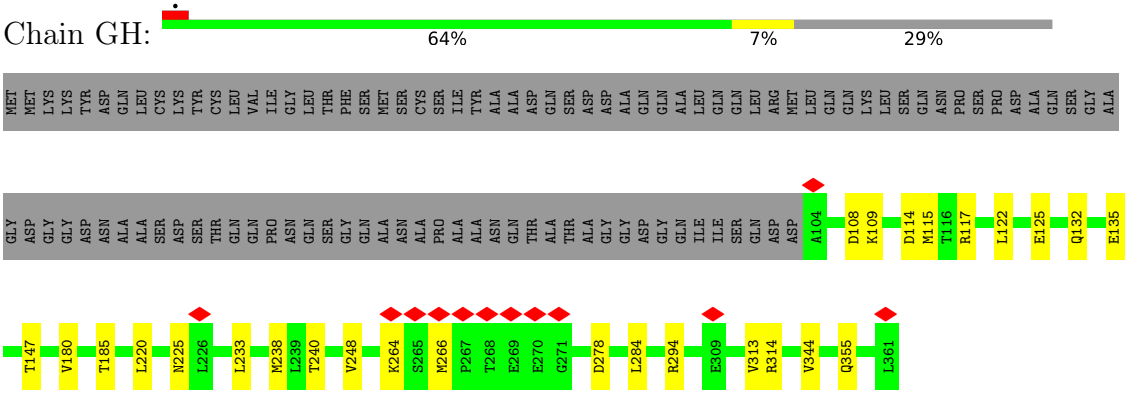
• Molecule 4: Type IV secretion protein IcmK

Chain FH:



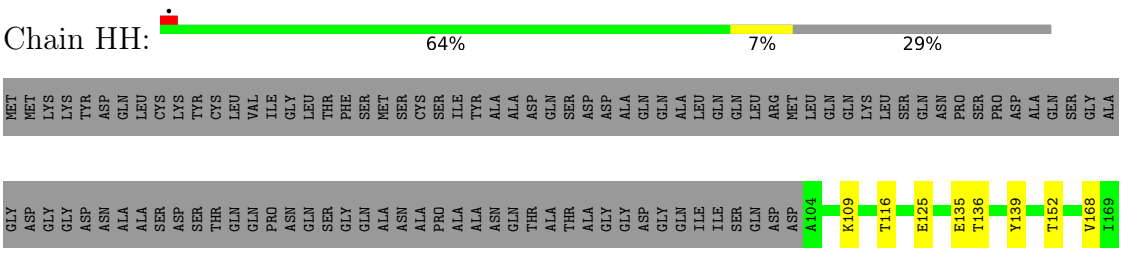
• Molecule 4: Type IV secretion protein IcmK

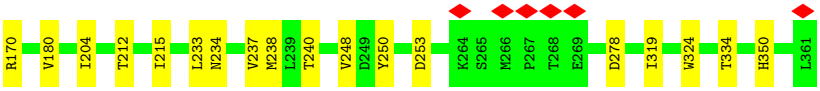
Chain GH:



• Molecule 4: Type IV secretion protein IcmK

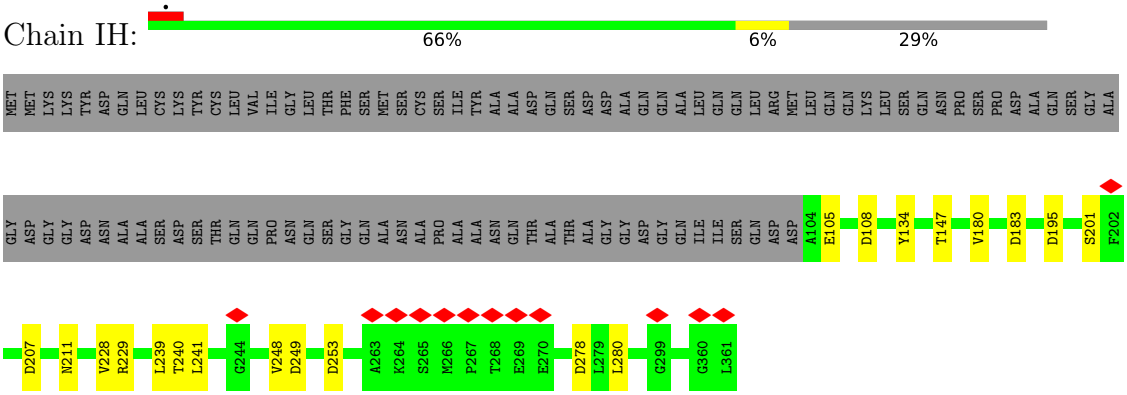
Chain HH:





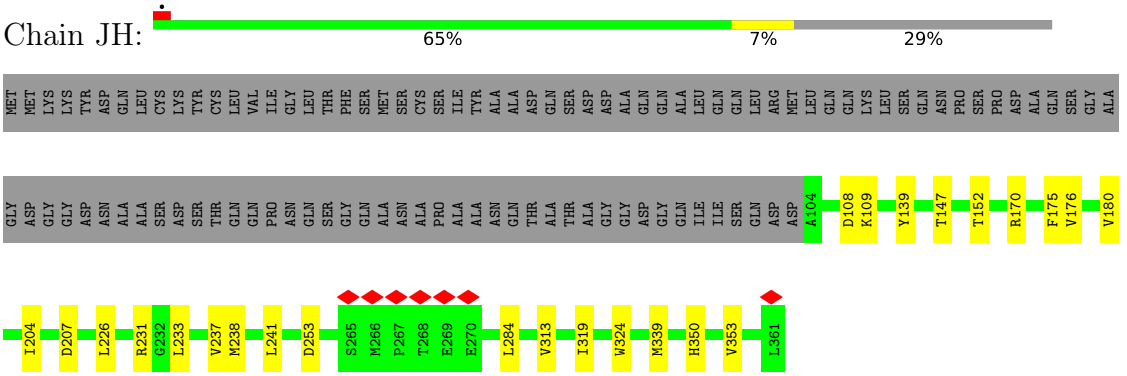
• Molecule 4: Type IV secretion protein IcmK

Chain IH:



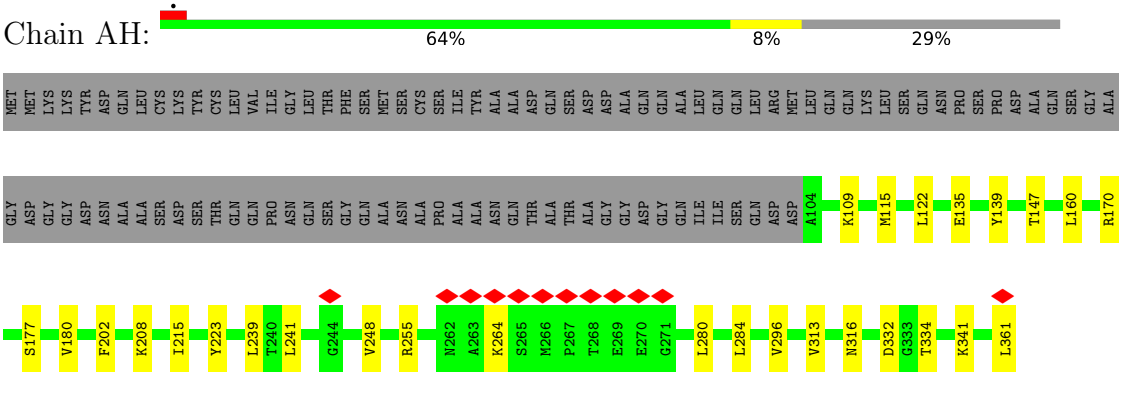
• Molecule 4: Type IV secretion protein IcmK

Chain JH:



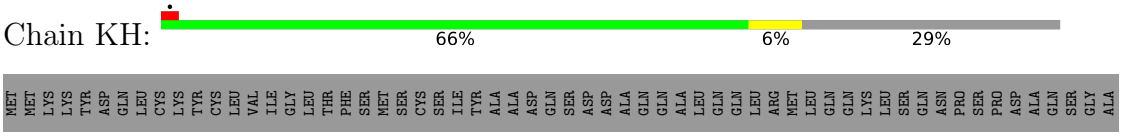
• Molecule 4: Type IV secretion protein IcmK

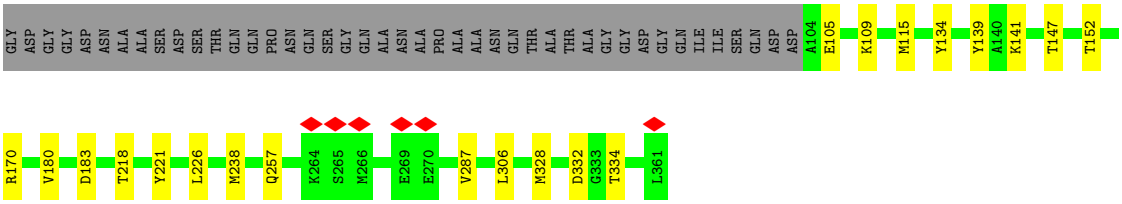
Chain AH:



• Molecule 4: Type IV secretion protein IcmK

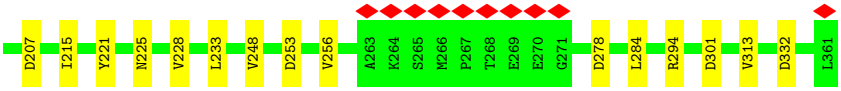
Chain KH:





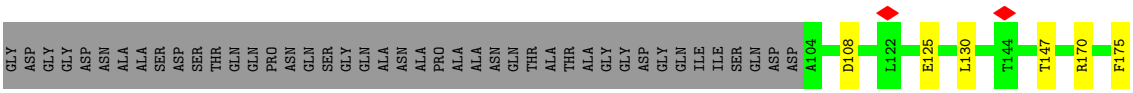
• Molecule 4: Type IV secretion protein IcmK

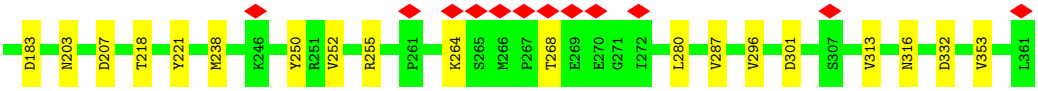
Chain LH:



• Molecule 4: Type IV secretion protein IcmK

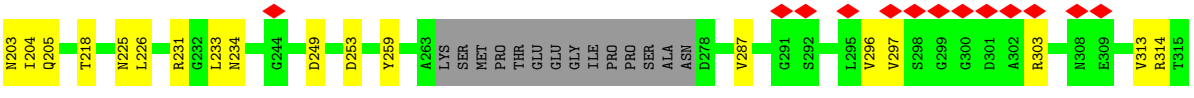
Chain MH:

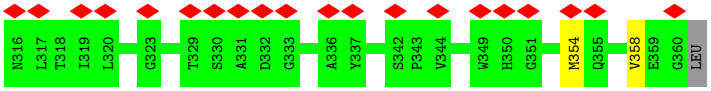




• Molecule 4: Type IV secretion protein IcmK

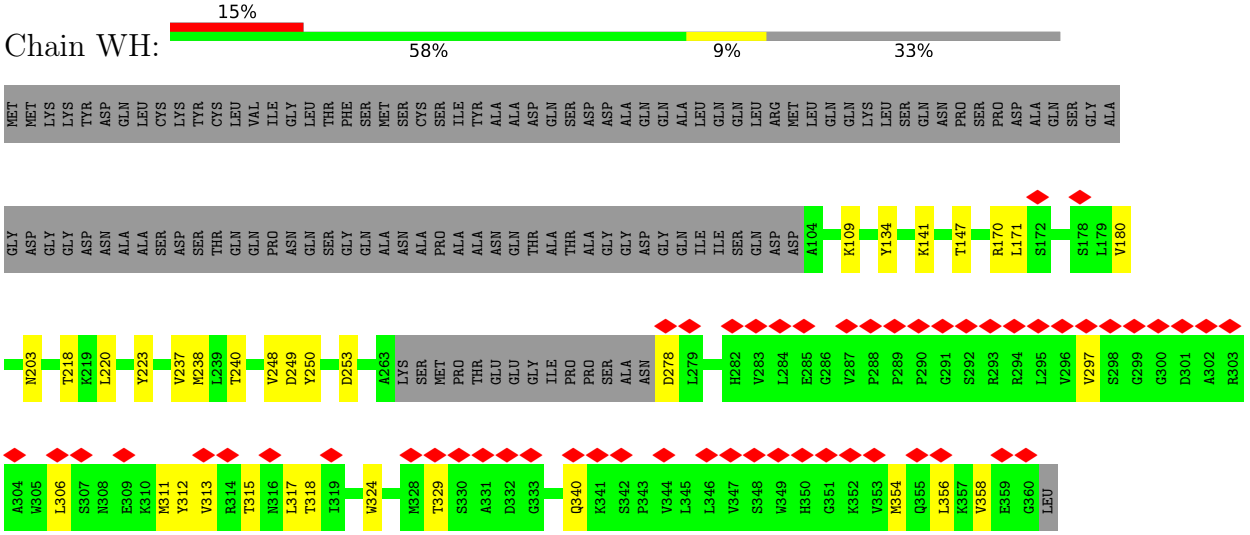
Chain VH:





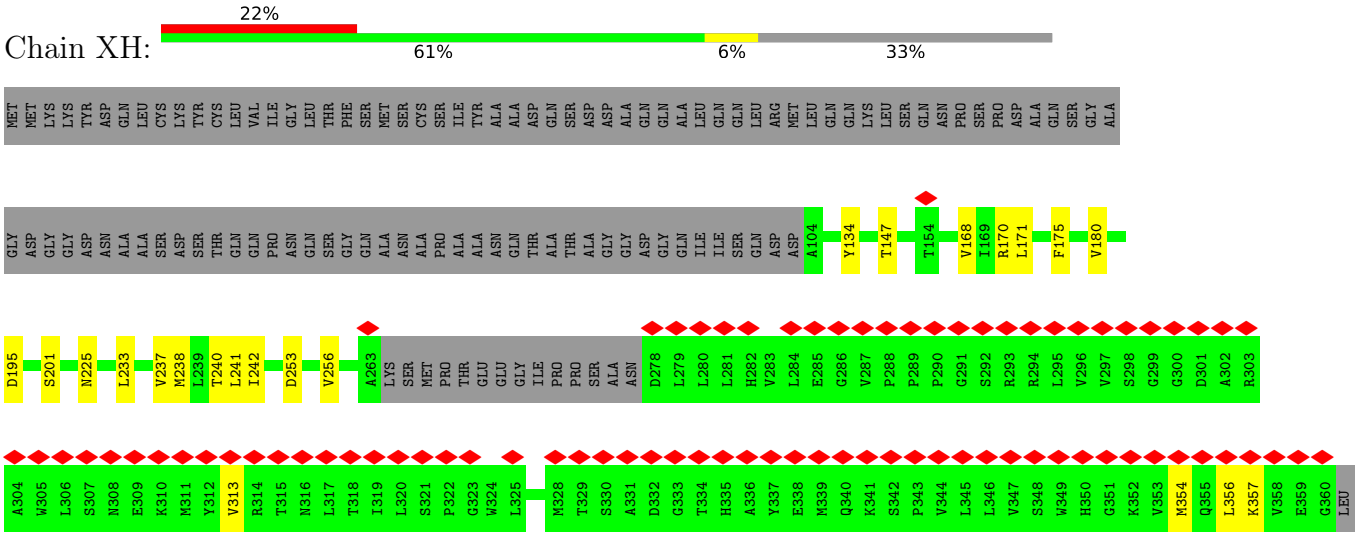
• Molecule 4: Type IV secretion protein IcmK

Chain WH:



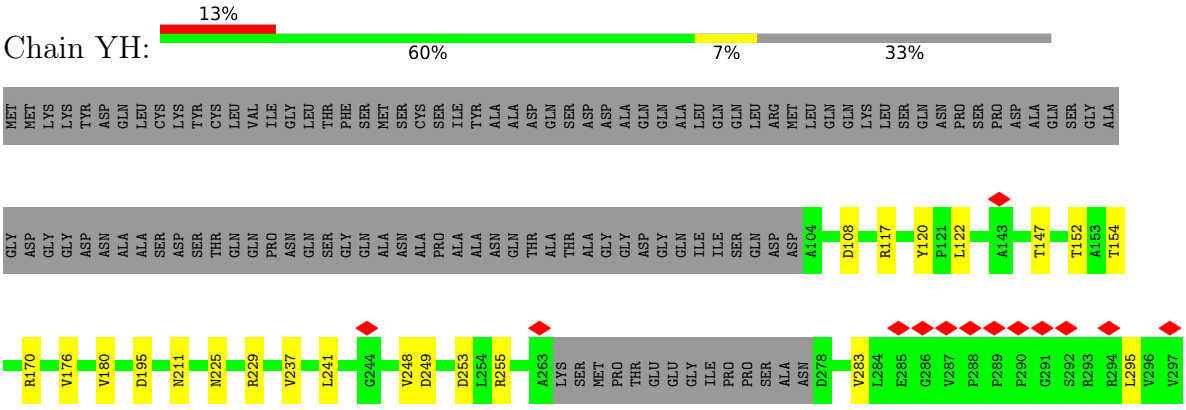
• Molecule 4: Type IV secretion protein IcmK

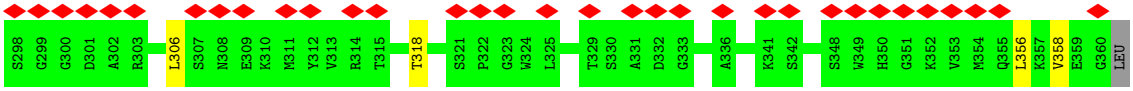
Chain XH:



• Molecule 4: Type IV secretion protein IcmK

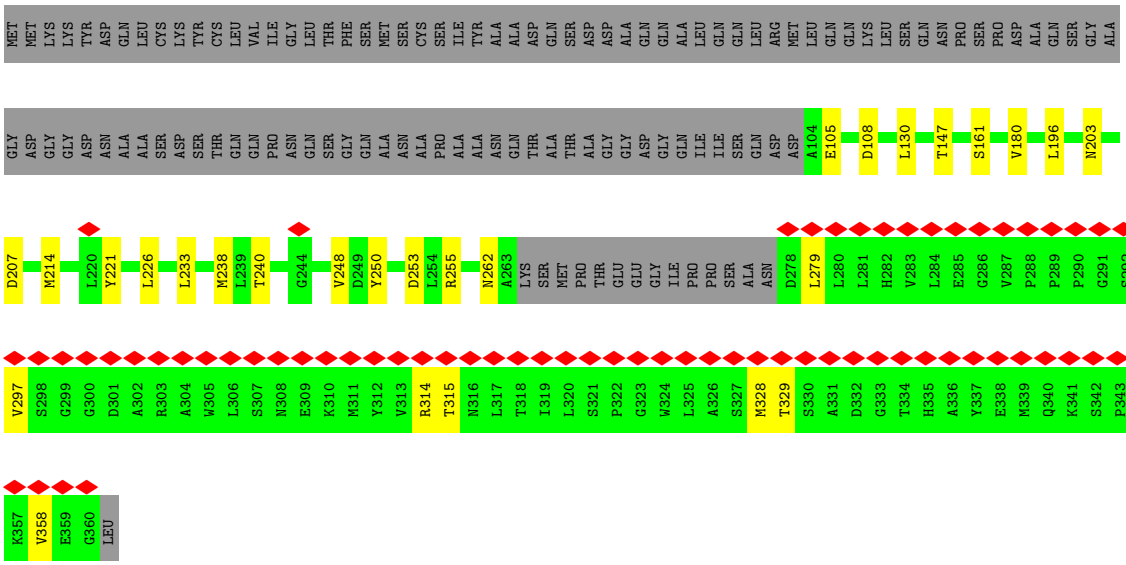
Chain YH:





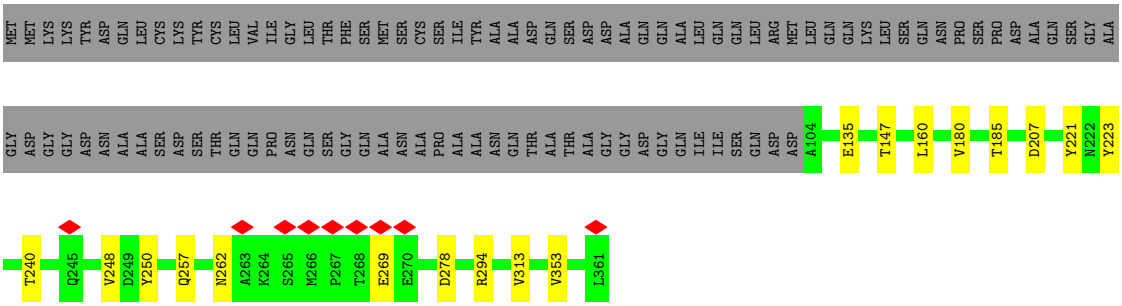
• Molecule 4: Type IV secretion protein IcmK

Chain ZH:



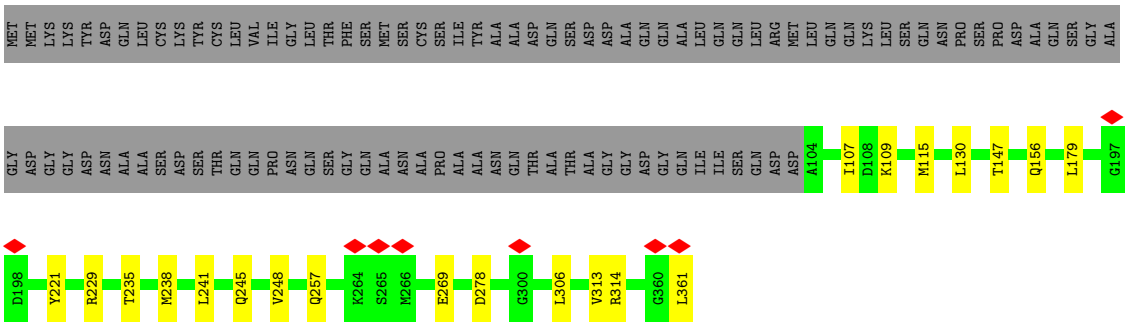
• Molecule 4: Type IV secretion protein IcmK

Chain BH:



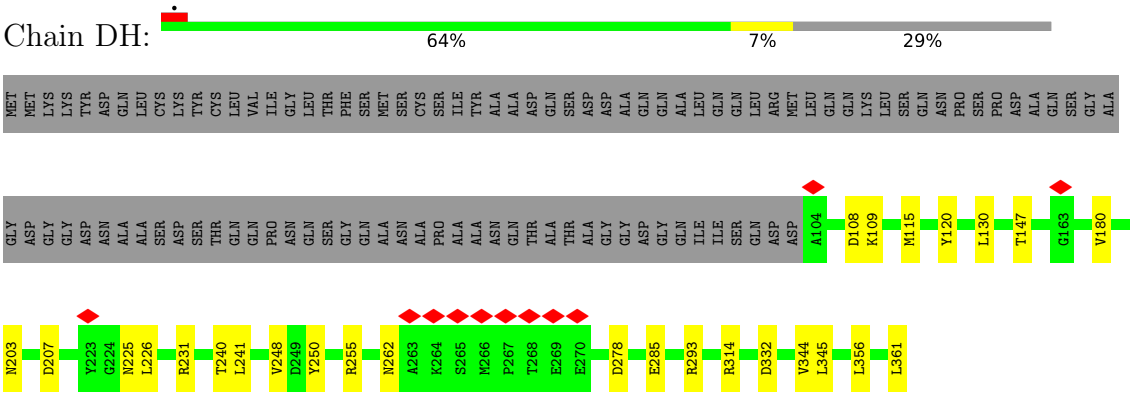
• Molecule 4: Type IV secretion protein IcmK

Chain CH:



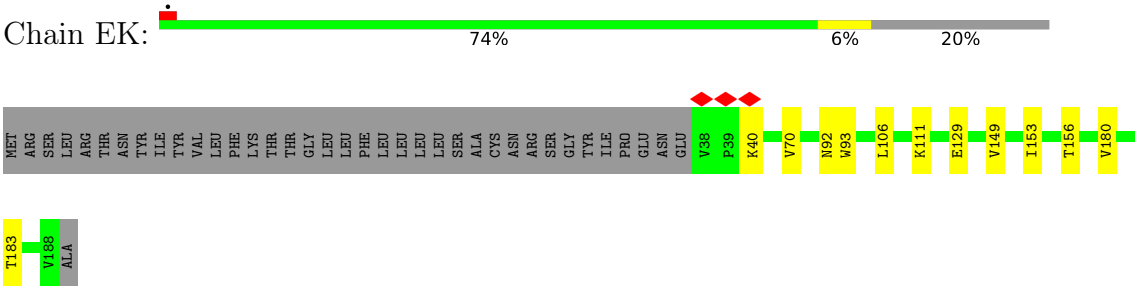
• Molecule 4: Type IV secretion protein IcmK

Chain DH:



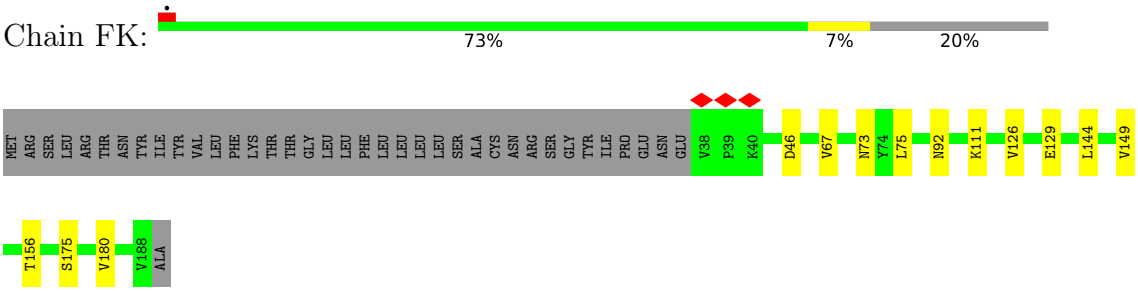
• Molecule 5: Inner membrane lipoprotein YiaD

Chain EK:



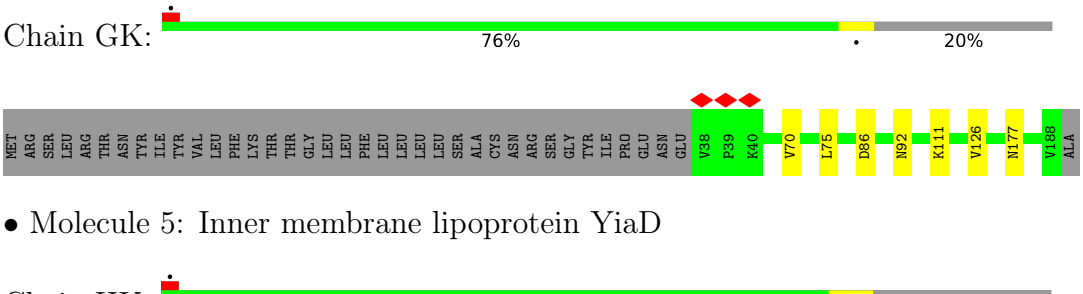
• Molecule 5: Inner membrane lipoprotein YiaD

Chain FK:



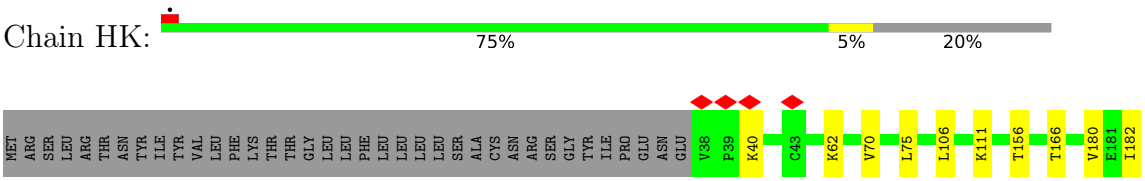
• Molecule 5: Inner membrane lipoprotein YiaD

Chain GK:



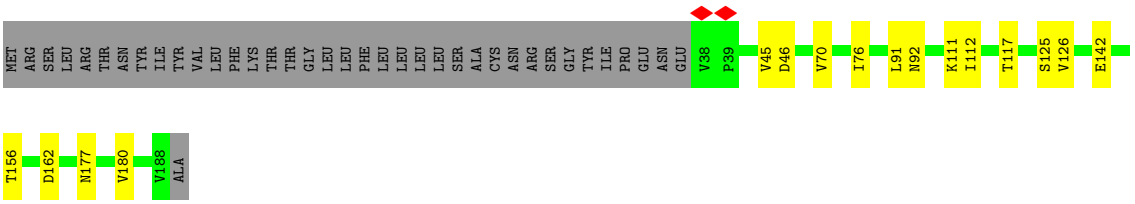
• Molecule 5: Inner membrane lipoprotein YiaD

Chain HK:



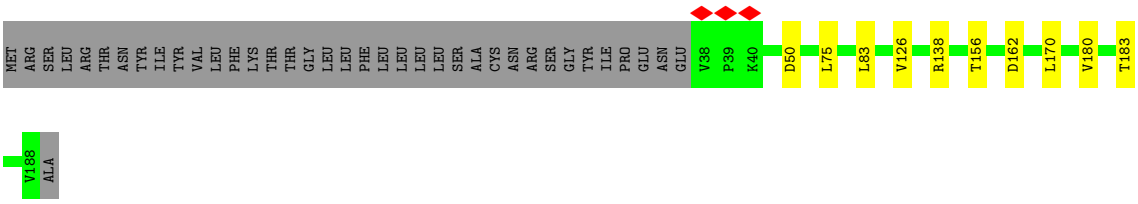
• Molecule 5: Inner membrane lipoprotein YiaD

Chain IK:



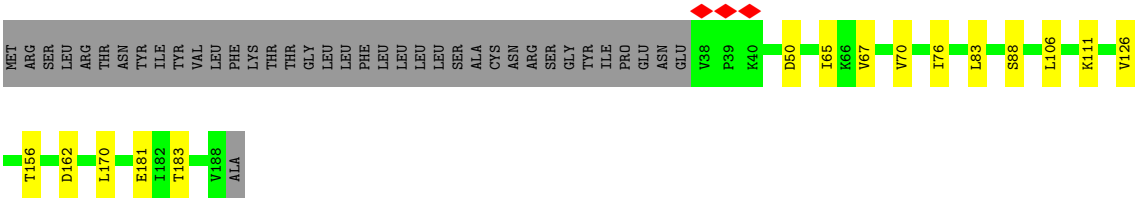
• Molecule 5: Inner membrane lipoprotein YiaD

Chain JK:



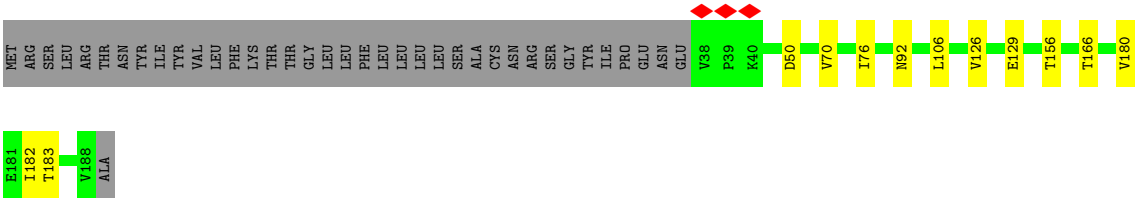
• Molecule 5: Inner membrane lipoprotein YiaD

Chain KK:



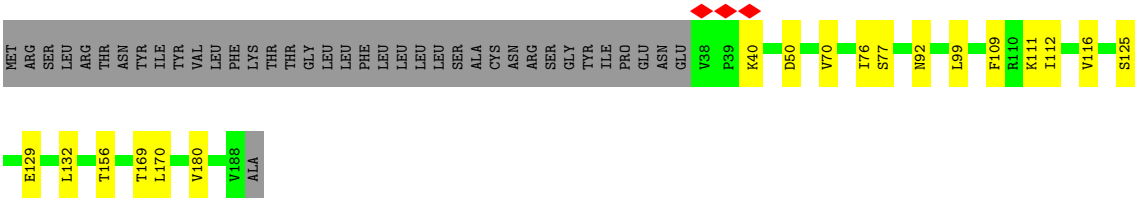
• Molecule 5: Inner membrane lipoprotein YiaD

Chain LK:



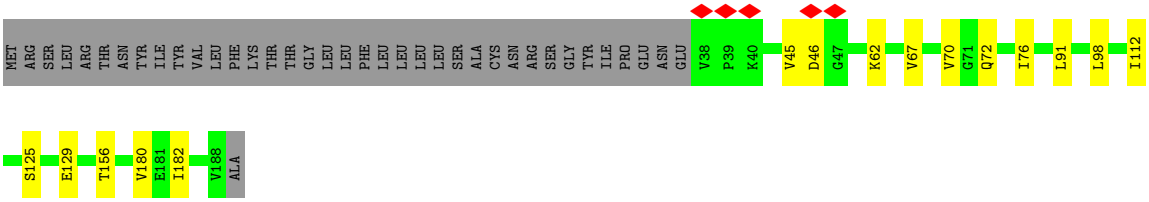
• Molecule 5: Inner membrane lipoprotein YiaD

Chain AK:



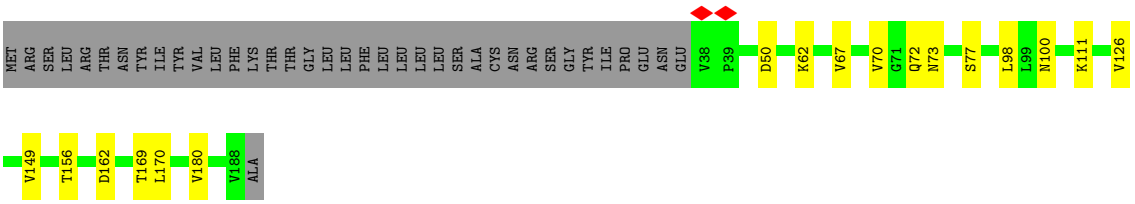
• Molecule 5: Inner membrane lipoprotein YiaD

Chain MK:



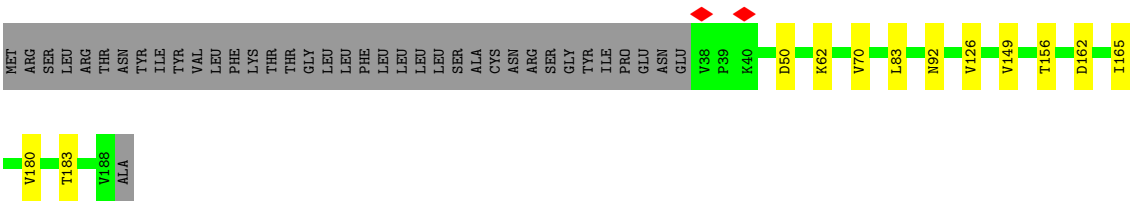
• Molecule 5: Inner membrane lipoprotein YiaD

Chain BK:



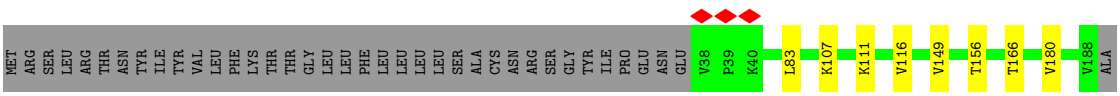
• Molecule 5: Inner membrane lipoprotein YiaD

Chain CK:



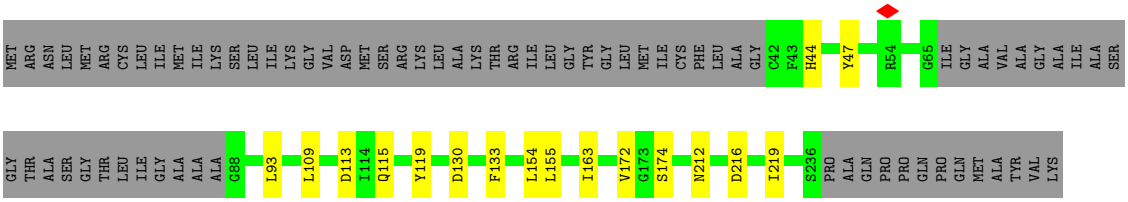
• Molecule 5: Inner membrane lipoprotein YiaD

Chain DK:



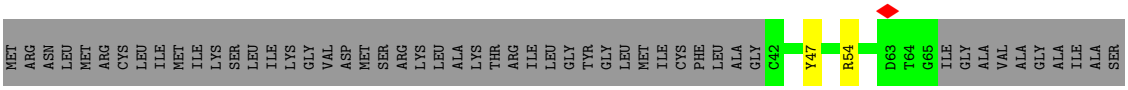
• Molecule 6: Outer membrane protein, OmpA family protein

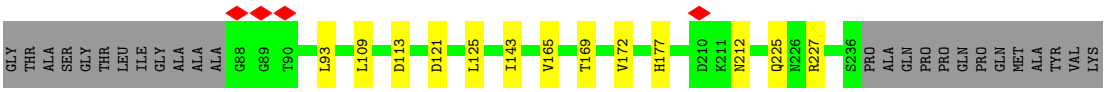
Chain EL:



• Molecule 6: Outer membrane protein, OmpA family protein

Chain FL:



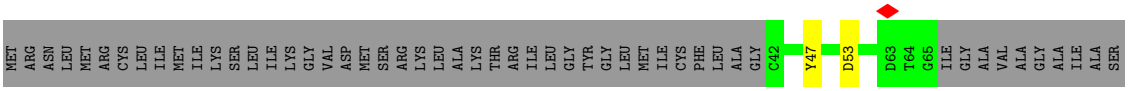


• Molecule 6: Outer membrane protein, OmpA family protein

Chain GL:

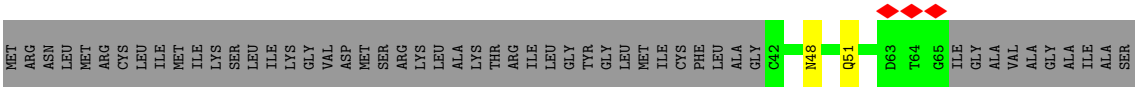
• Molecule 6: Outer membrane protein, OmpA family protein

Chain HL:



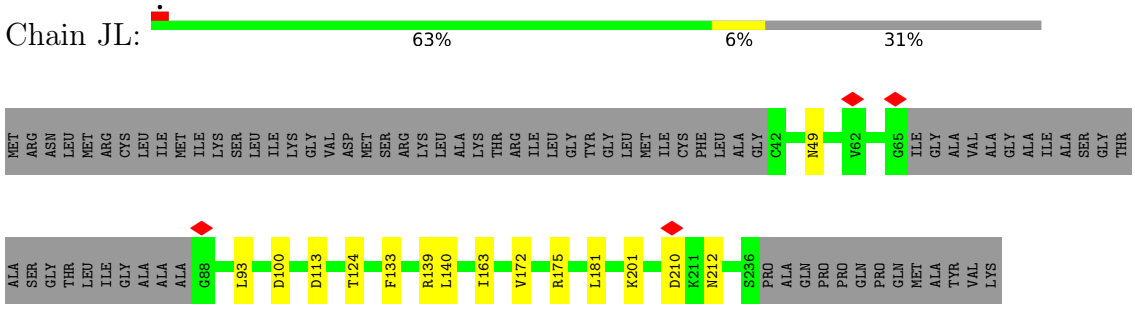
• Molecule 6: Outer membrane protein, OmpA family protein

Chain IL:



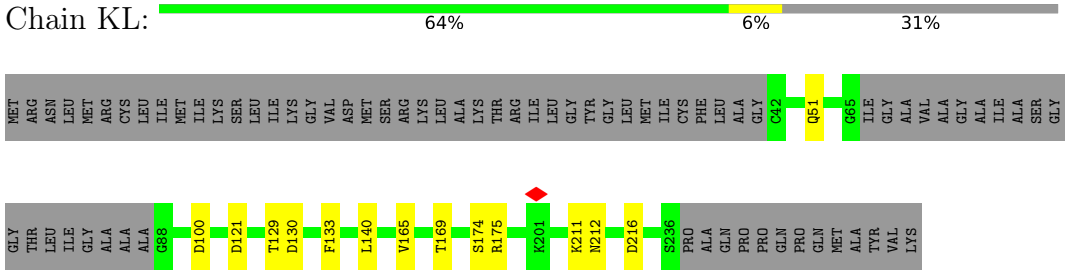
• Molecule 6: Outer membrane protein, OmpA family protein

Chain JL:



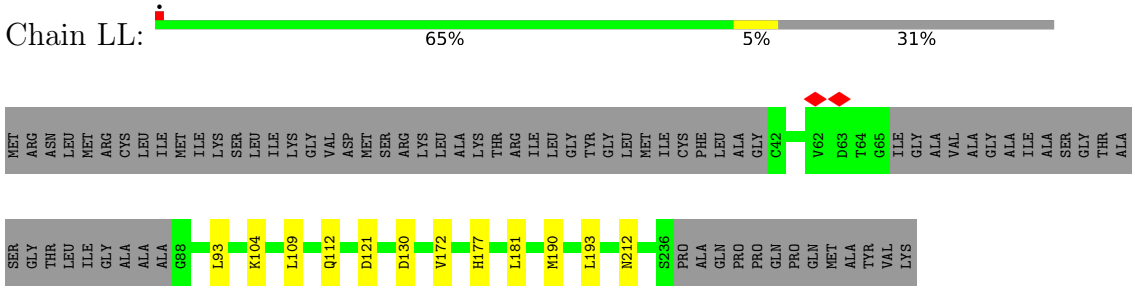
• Molecule 6: Outer membrane protein, OmpA family protein

Chain KL:



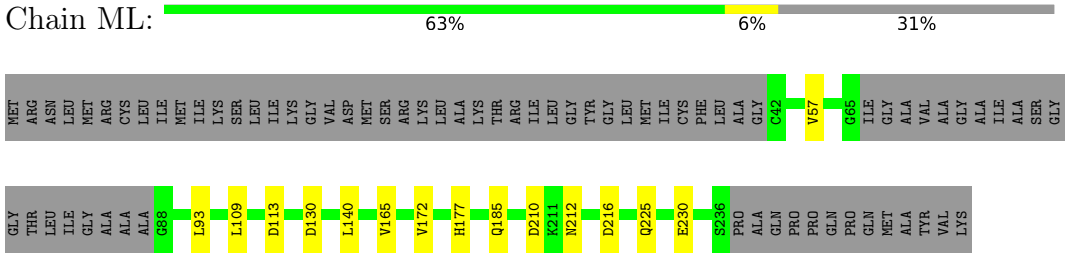
• Molecule 6: Outer membrane protein, OmpA family protein

Chain LL:



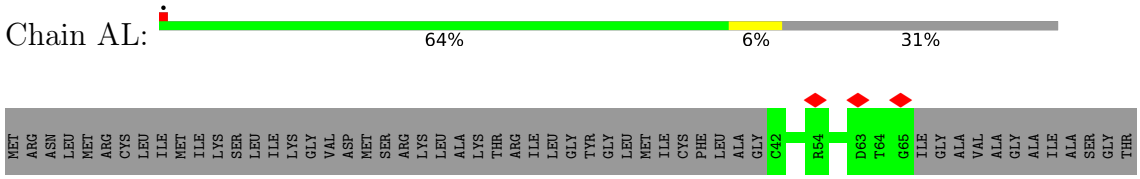
• Molecule 6: Outer membrane protein, OmpA family protein

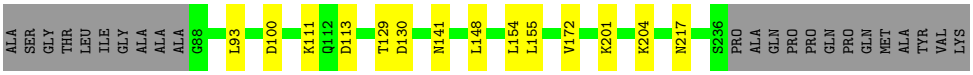
Chain ML:



• Molecule 6: Outer membrane protein, OmpA family protein

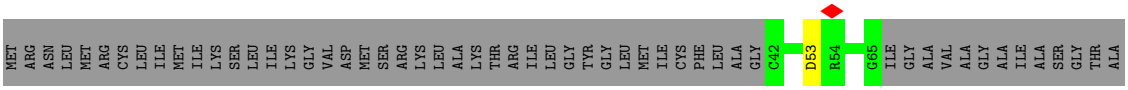
Chain AL:





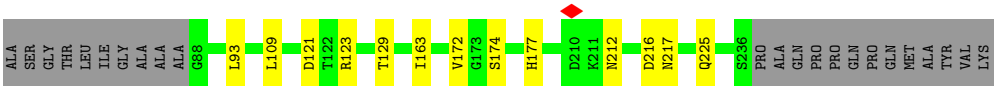
• Molecule 6: Outer membrane protein, OmpA family protein

Chain BL:



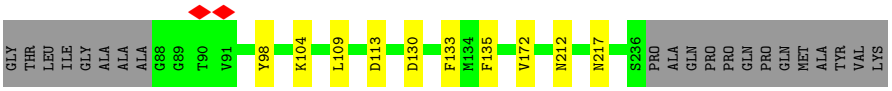
• Molecule 6: Outer membrane protein, OmpA family protein

Chain CL:



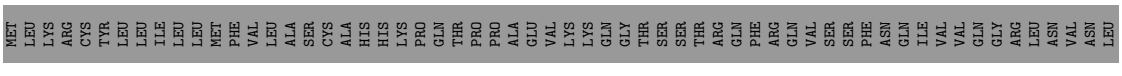
• Molecule 6: Outer membrane protein, OmpA family protein

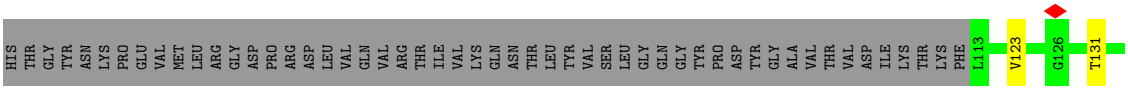
Chain DL:

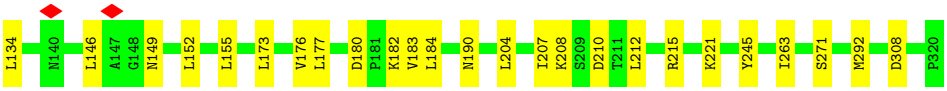


• Molecule 7: DUF2807 domain-containing protein

Chain EM:

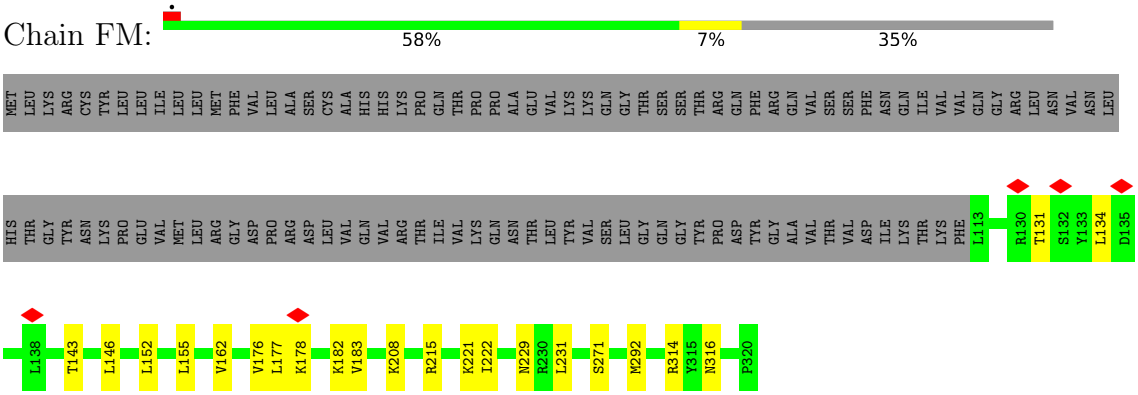






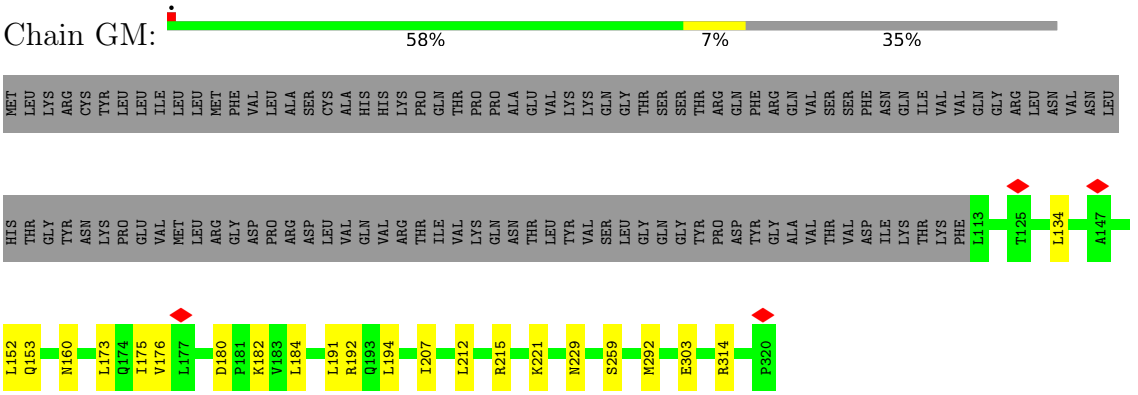
• Molecule 7: DUF2807 domain-containing protein

Chain FM:



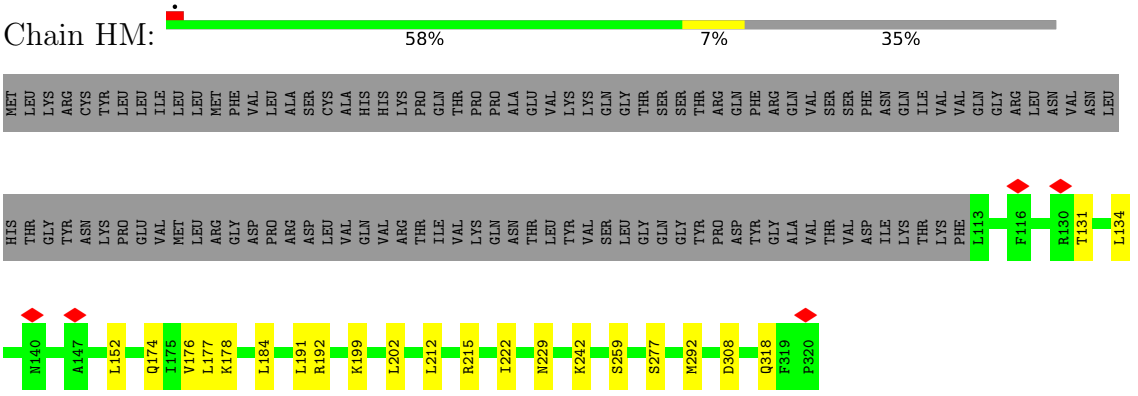
• Molecule 7: DUF2807 domain-containing protein

Chain GM:



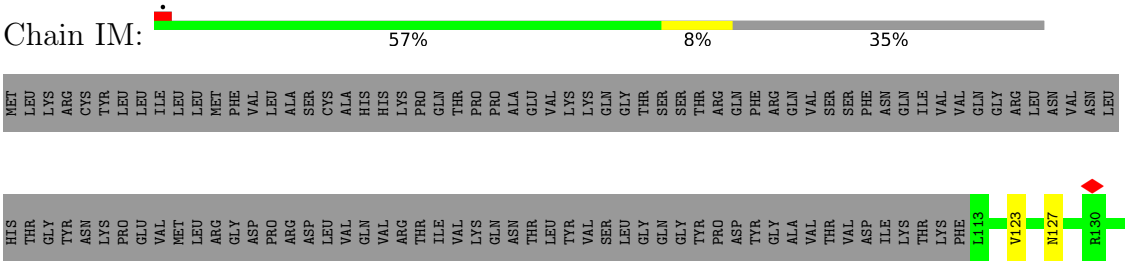
• Molecule 7: DUF2807 domain-containing protein

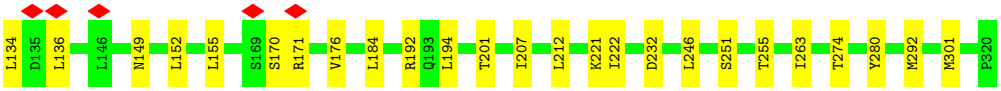
Chain HM:



• Molecule 7: DUF2807 domain-containing protein

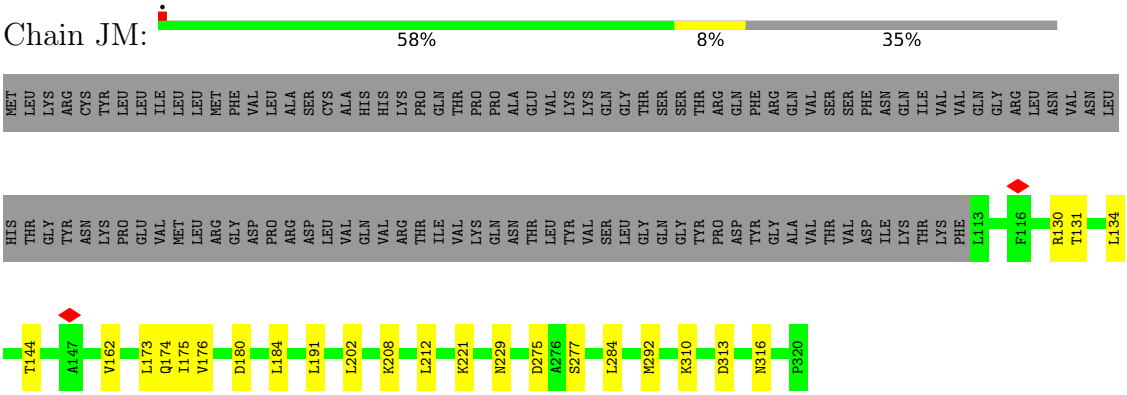
Chain IM:





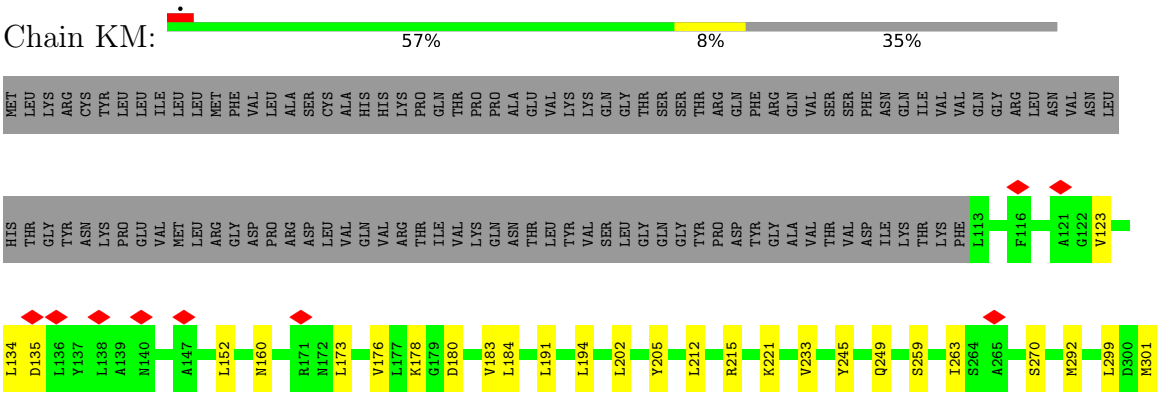
• Molecule 7: DUF2807 domain-containing protein

Chain JM:



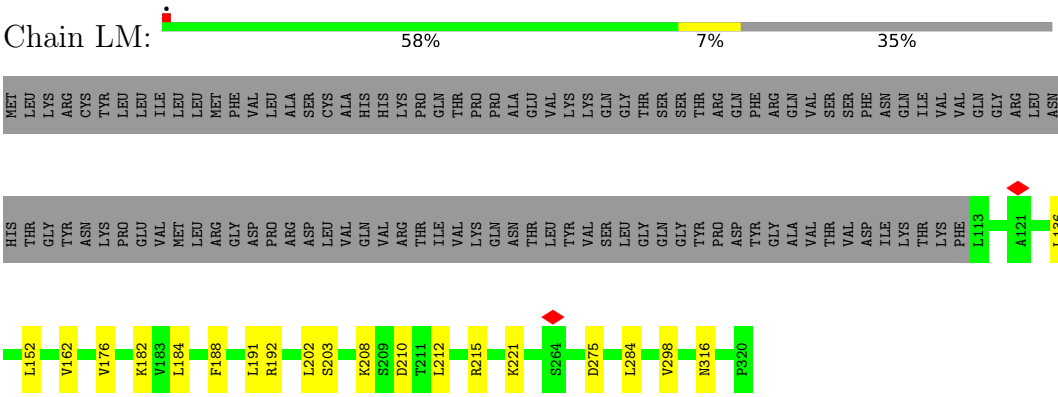
• Molecule 7: DUF2807 domain-containing protein

Chain KM:



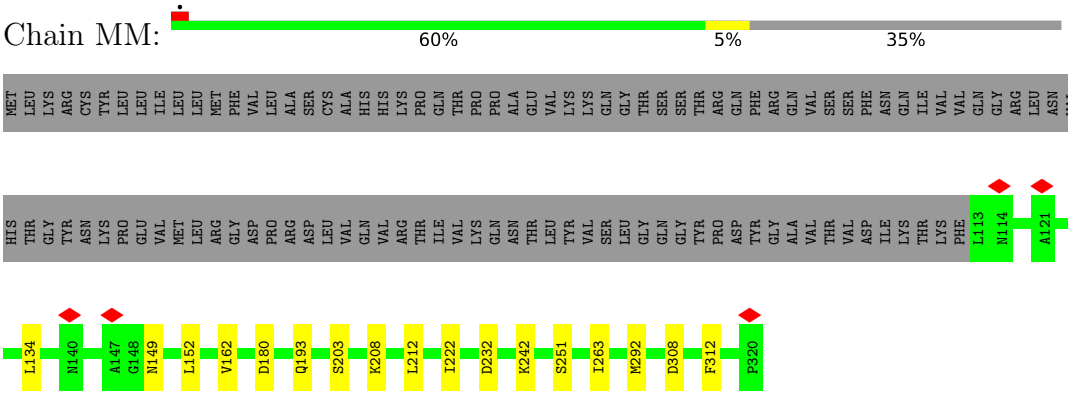
• Molecule 7: DUF2807 domain-containing protein

Chain LM:



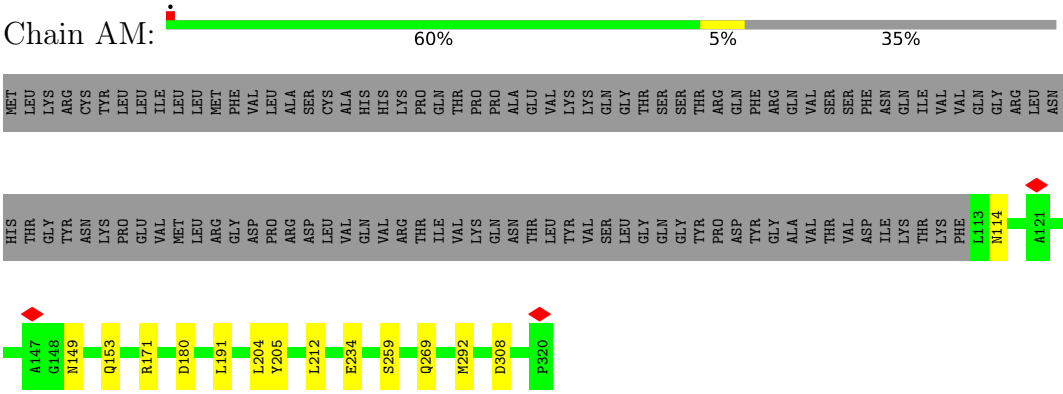
• Molecule 7: DUF2807 domain-containing protein

Chain MM:



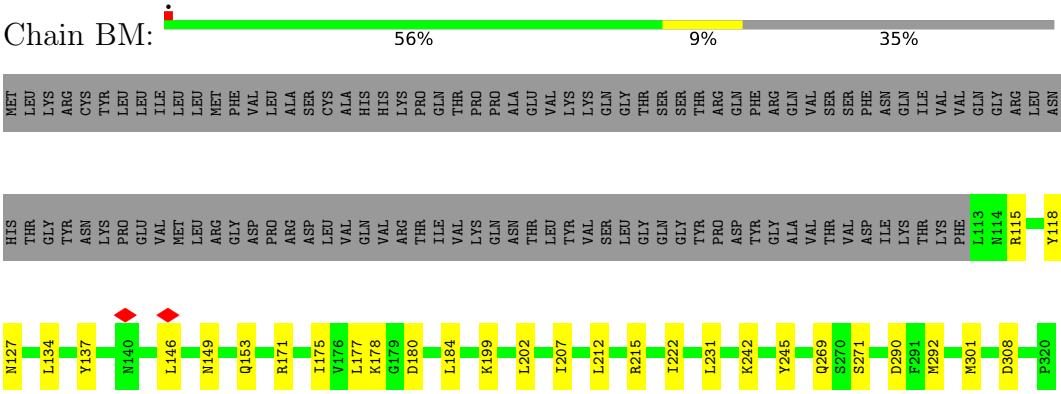
• Molecule 7: DUF2807 domain-containing protein

Chain AM:



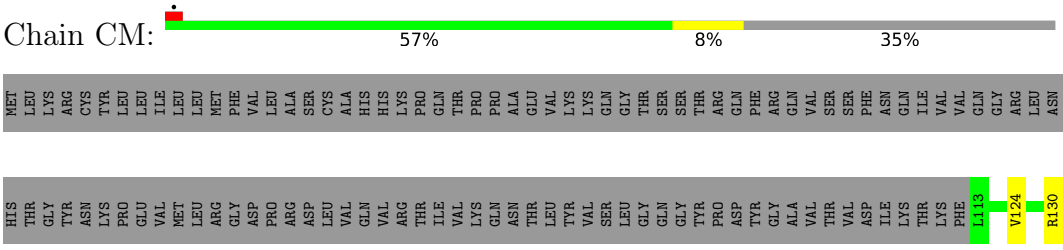
• Molecule 7: DUF2807 domain-containing protein

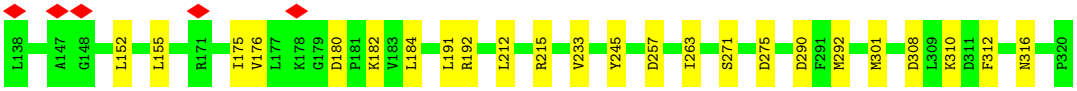
Chain BM:



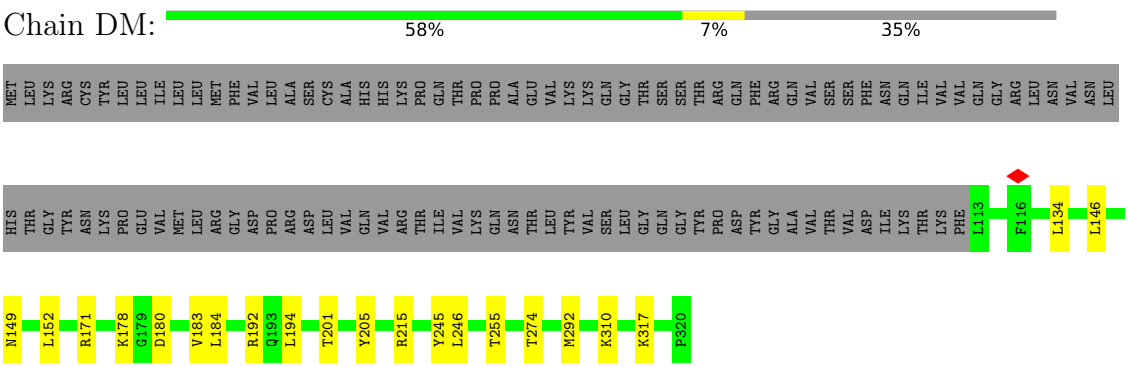
• Molecule 7: DUF2807 domain-containing protein

Chain CM:

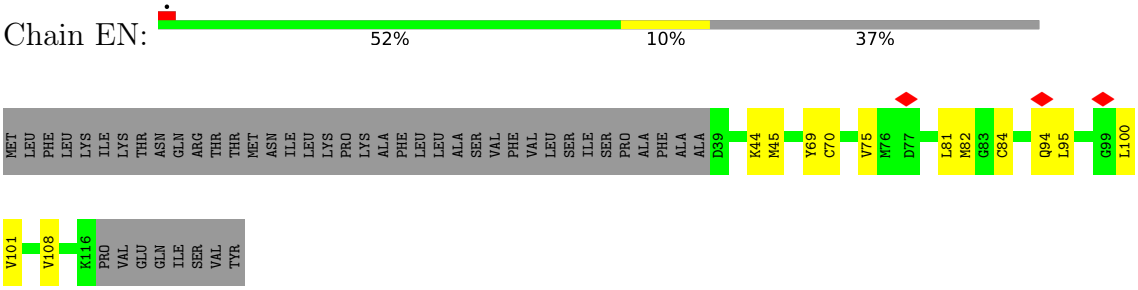




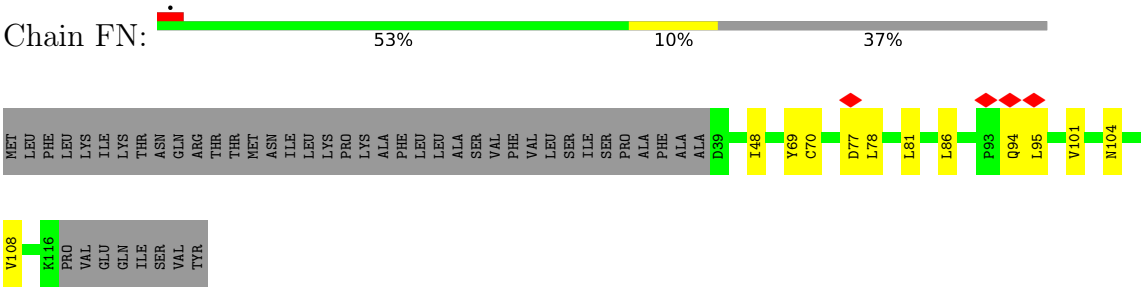
• Molecule 7: DUF2807 domain-containing protein



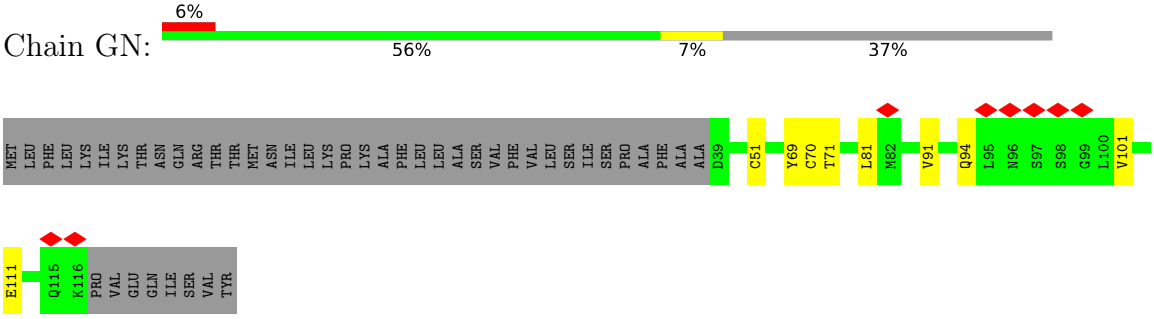
• Molecule 8: Neurogenic locus notch



• Molecule 8: Neurogenic locus notch

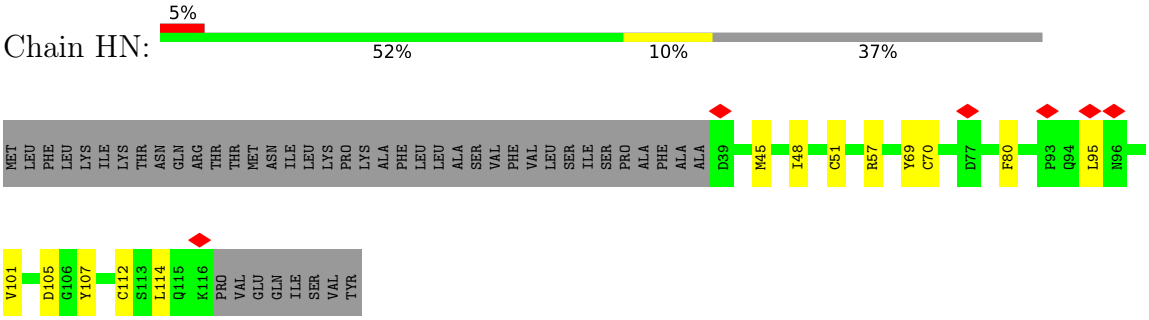


• Molecule 8: Neurogenic locus notch



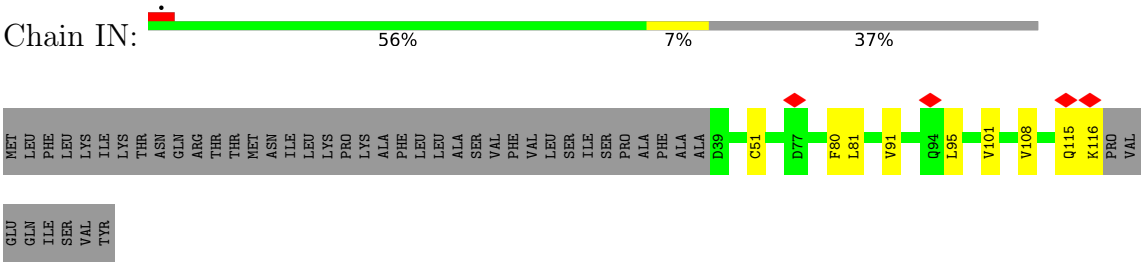
• Molecule 8: Neurogenic locus notch

Chain HN:



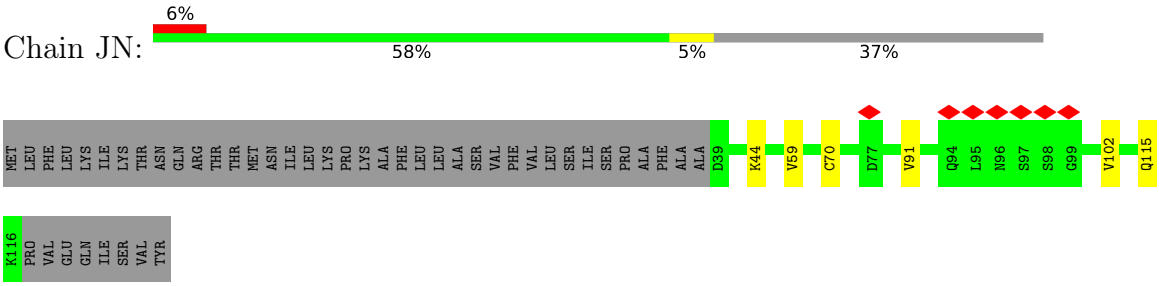
• Molecule 8: Neurogenic locus notch

Chain IN:



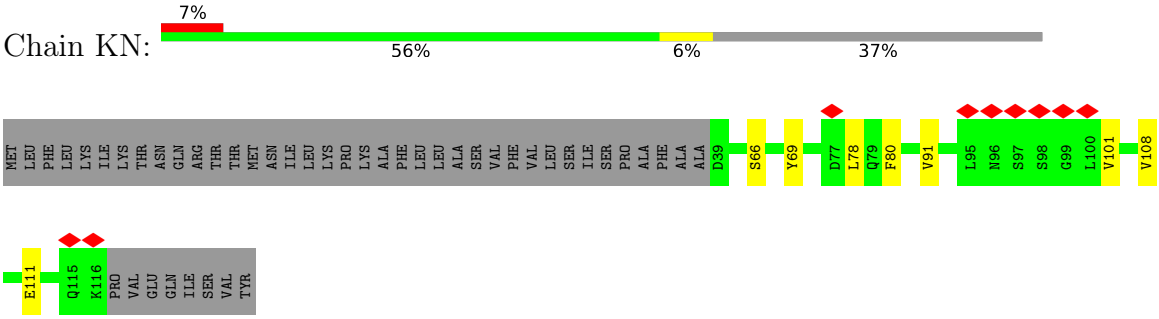
• Molecule 8: Neurogenic locus notch

Chain JN:



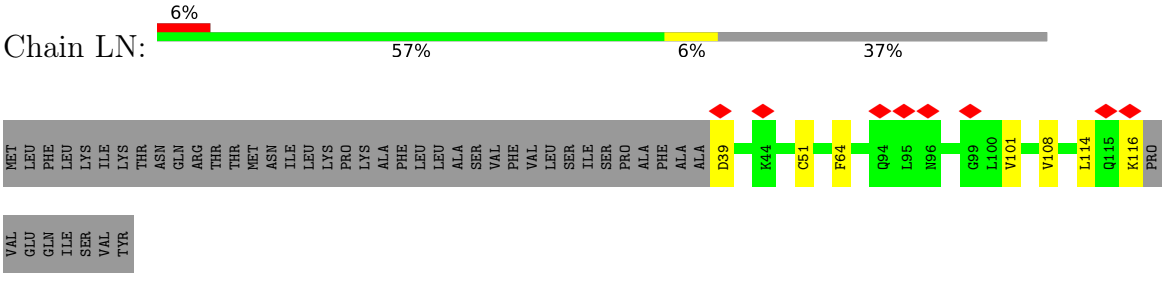
• Molecule 8: Neurogenic locus notch

Chain KN:



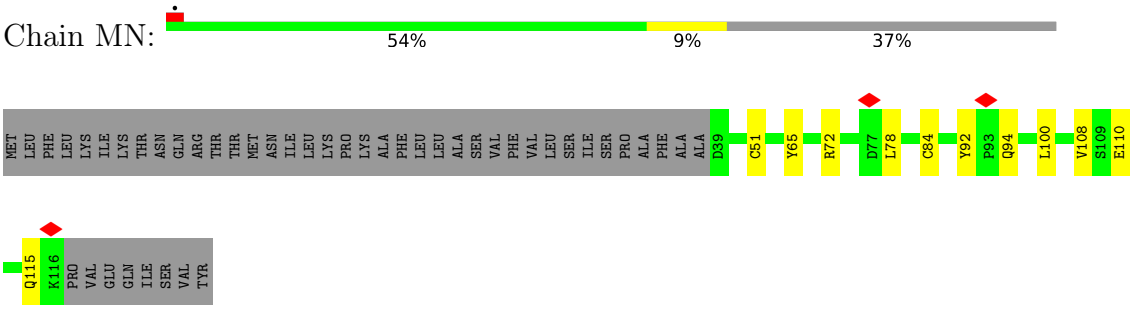
• Molecule 8: Neurogenic locus notch

Chain LN:



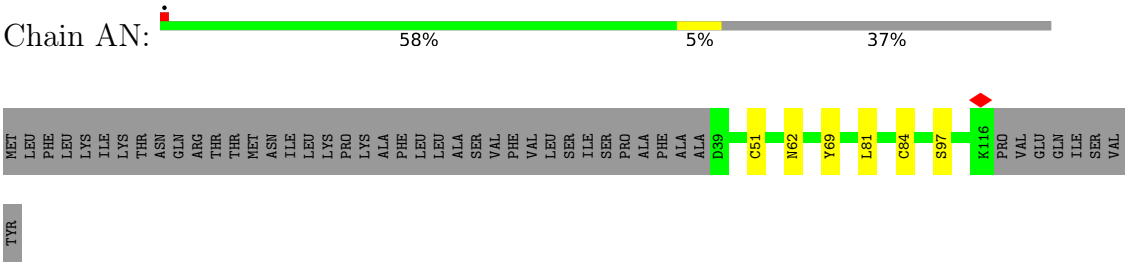
• Molecule 8: Neurogenic locus notch

Chain MN:



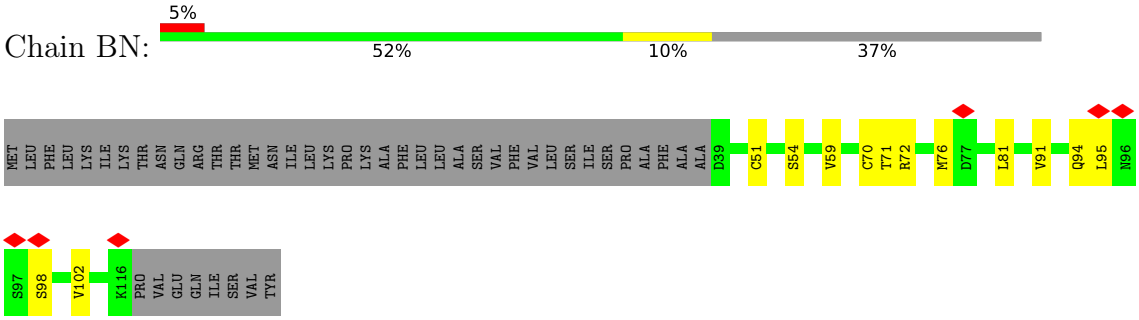
• Molecule 8: Neurogenic locus notch

Chain AN:



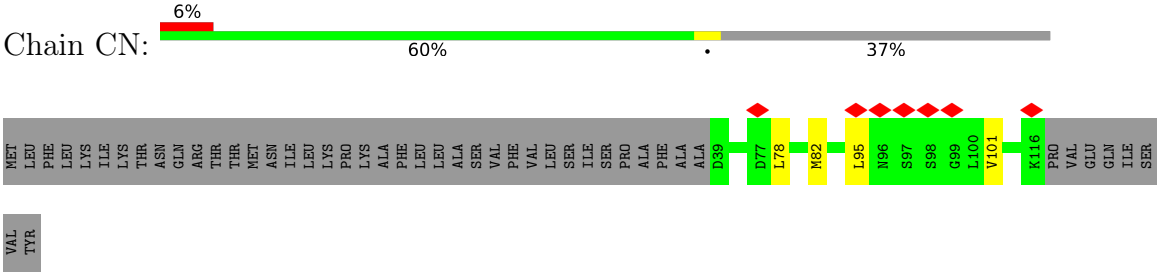
• Molecule 8: Neurogenic locus notch

Chain BN:



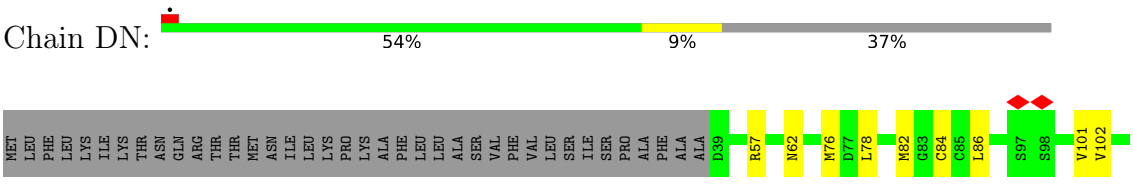
• Molecule 8: Neurogenic locus notch

Chain CN:



• Molecule 8: Neurogenic locus notch

Chain DN:



• Molecule 9: Unknown protein fragment

Chain EU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain FU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain GU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain HU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain IU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain JU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain KU: 100%

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain LU: 100%

There are no outlier residues recorded for this chain.

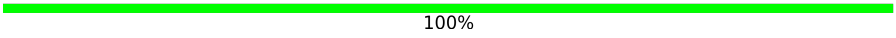
• Molecule 9: Unknown protein fragment

Chain MU:

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

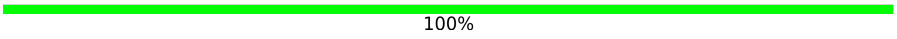
Chain AU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain BU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain CU:

There are no outlier residues recorded for this chain.

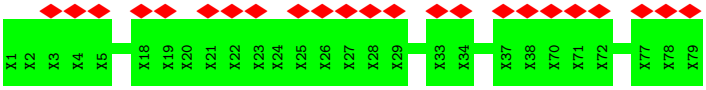
• Molecule 9: Unknown protein fragment

Chain DU:

There are no outlier residues recorded for this chain.

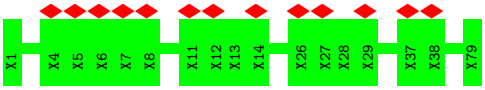
• Molecule 10: Unknown protein fragment

Chain EX:



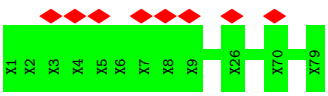
• Molecule 10: Unknown protein fragment

Chain FX:



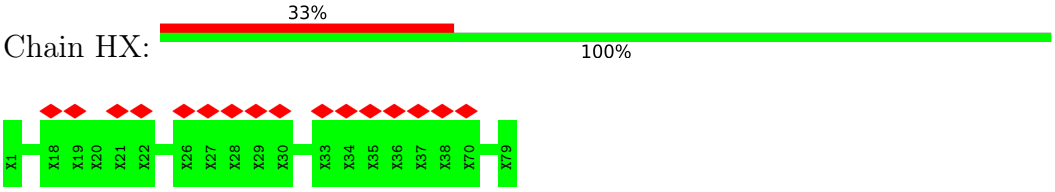
• Molecule 10: Unknown protein fragment

Chain GX:



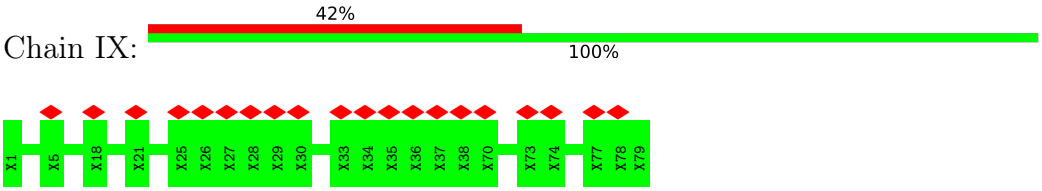
• Molecule 10: Unknown protein fragment

Chain HX:



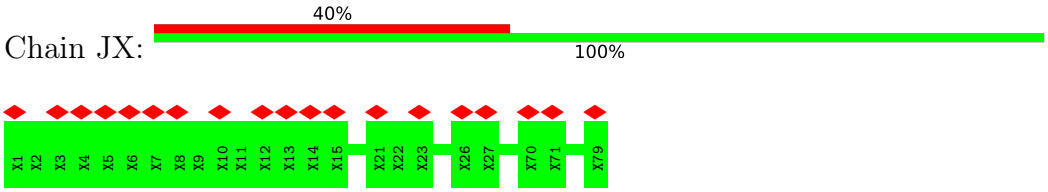
• Molecule 10: Unknown protein fragment

Chain IX:



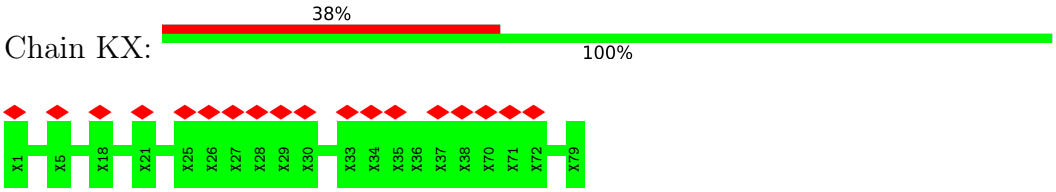
• Molecule 10: Unknown protein fragment

Chain JX:



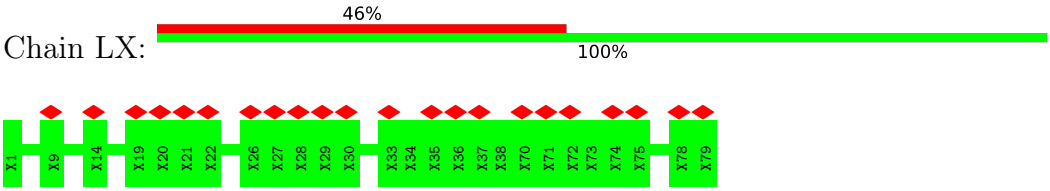
• Molecule 10: Unknown protein fragment

Chain KX:



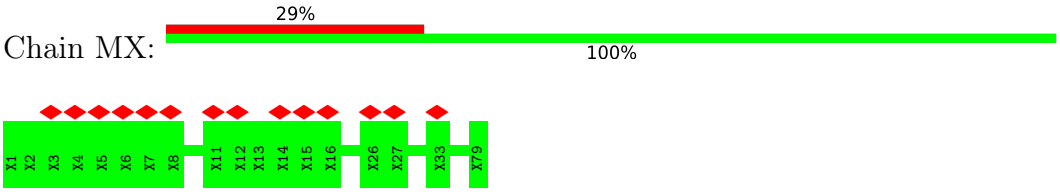
• Molecule 10: Unknown protein fragment

Chain LX:



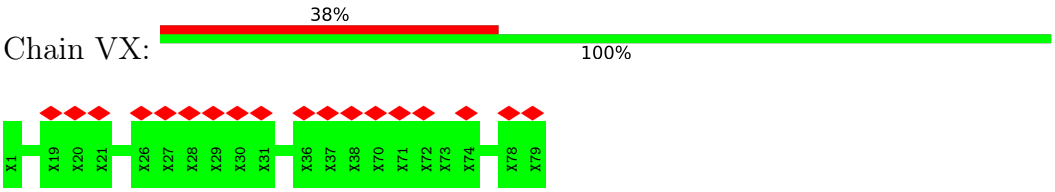
• Molecule 10: Unknown protein fragment

Chain MX:



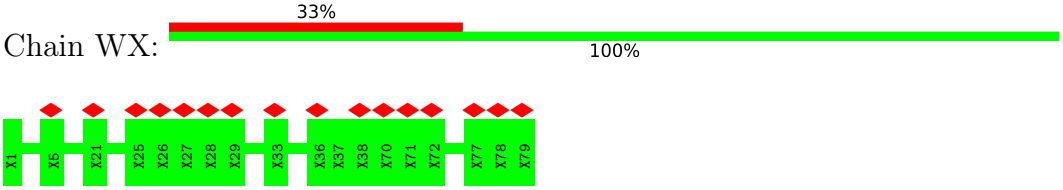
• Molecule 10: Unknown protein fragment

Chain VX:



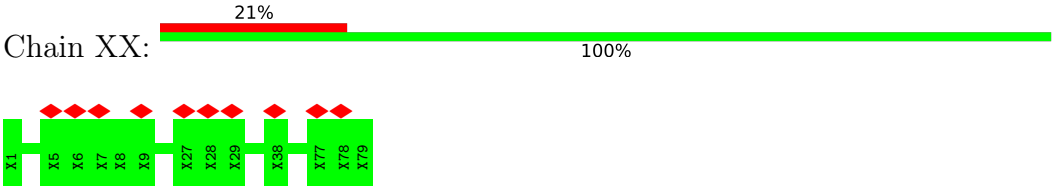
• Molecule 10: Unknown protein fragment

Chain WX:



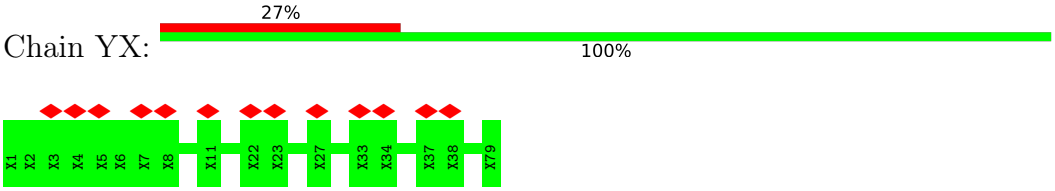
• Molecule 10: Unknown protein fragment

Chain XX:



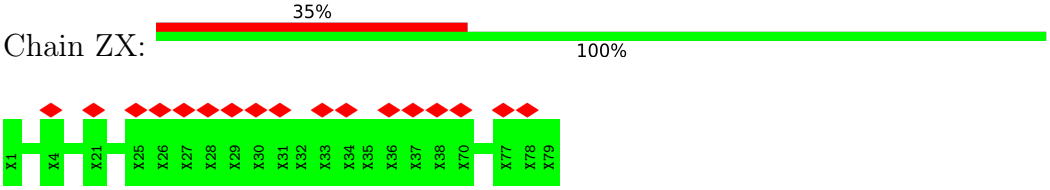
• Molecule 10: Unknown protein fragment

Chain YX:



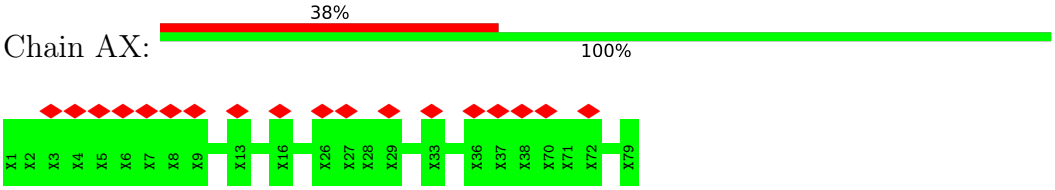
• Molecule 10: Unknown protein fragment

Chain ZX:



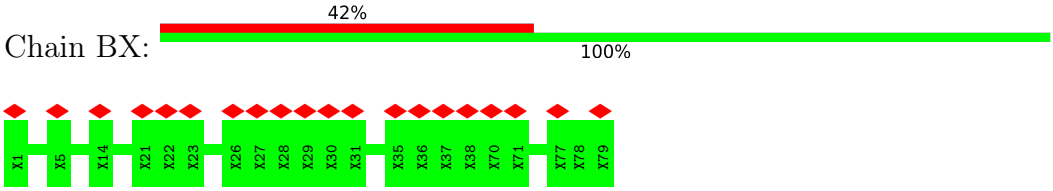
• Molecule 10: Unknown protein fragment

Chain AX:



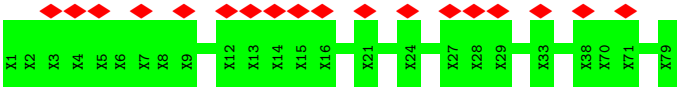
• Molecule 10: Unknown protein fragment

Chain BX:



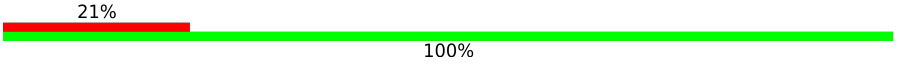
• Molecule 10: Unknown protein fragment

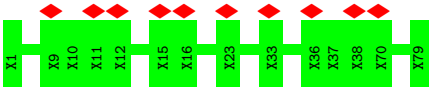
Chain CX:



• Molecule 10: Unknown protein fragment

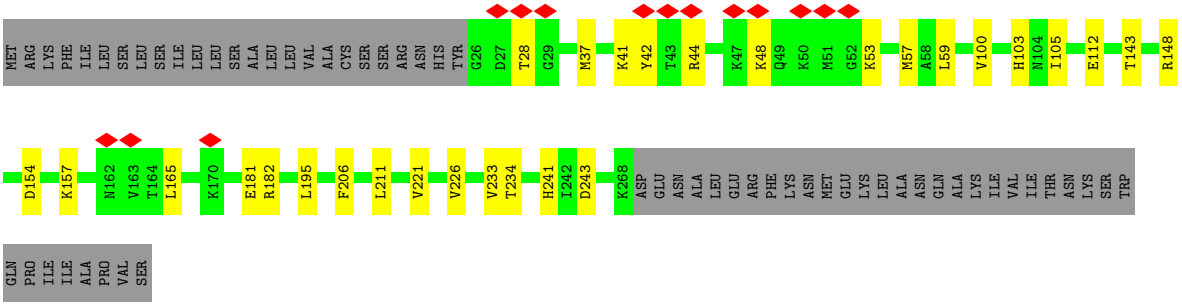
Chain DX:





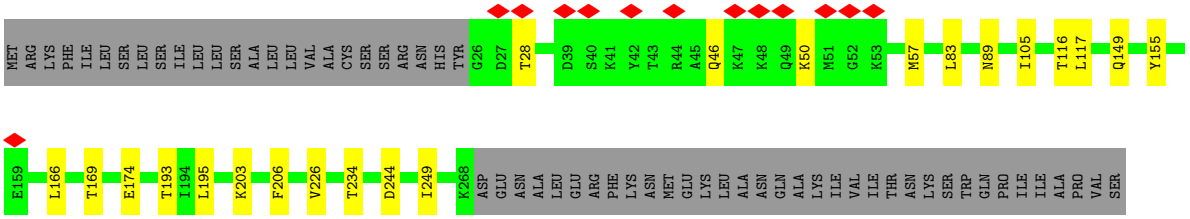
• Molecule 11: DotC

Chain CC:



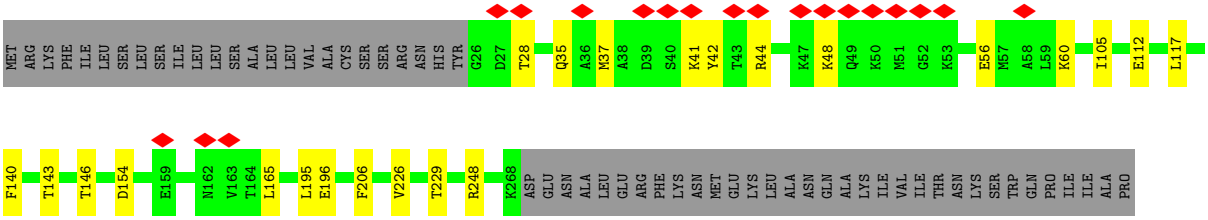
• Molecule 11: DotC

Chain BC:



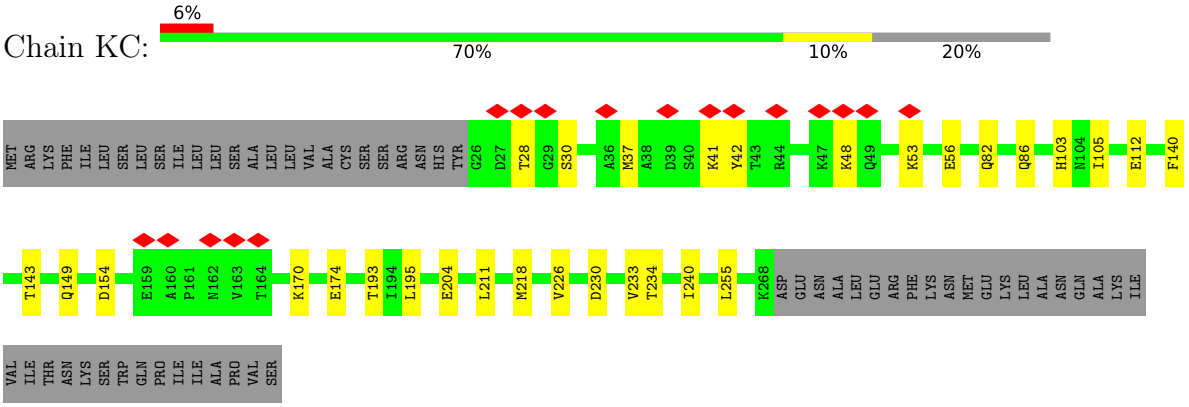
• Molecule 11: DotC

Chain GC:



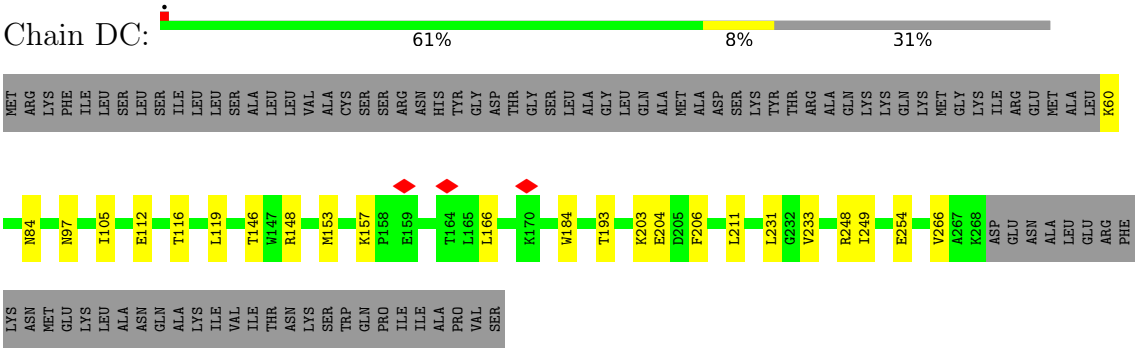
• Molecule 11: DotC

Chain KC:



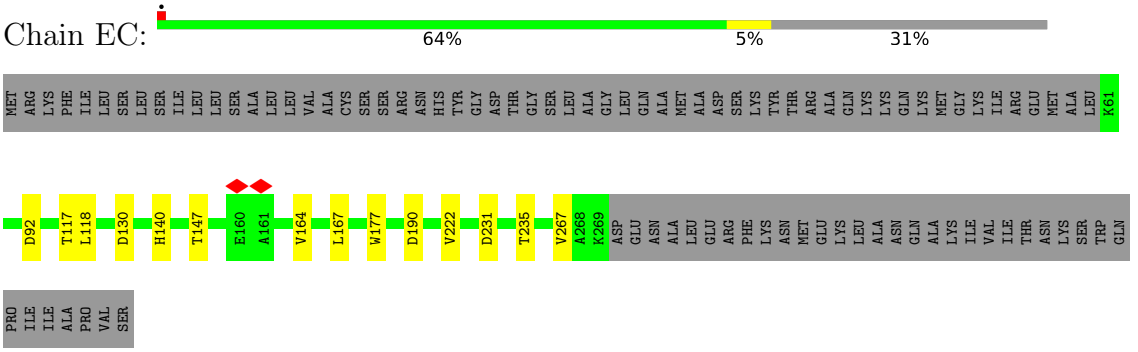
• Molecule 11: DotC

Chain DC:



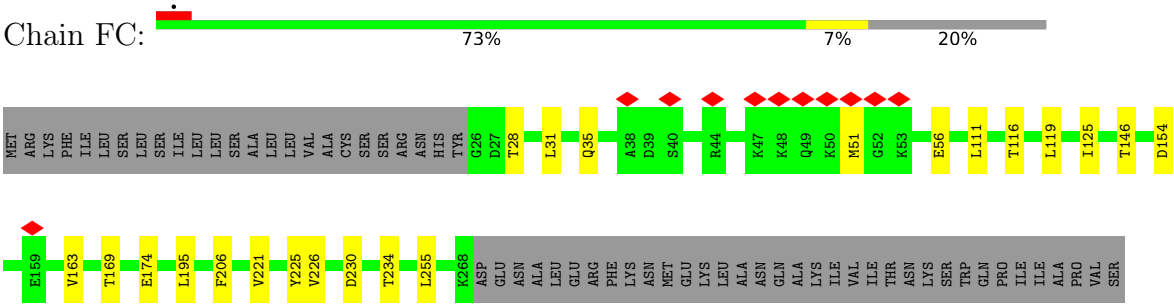
• Molecule 11: DotC

Chain EC:



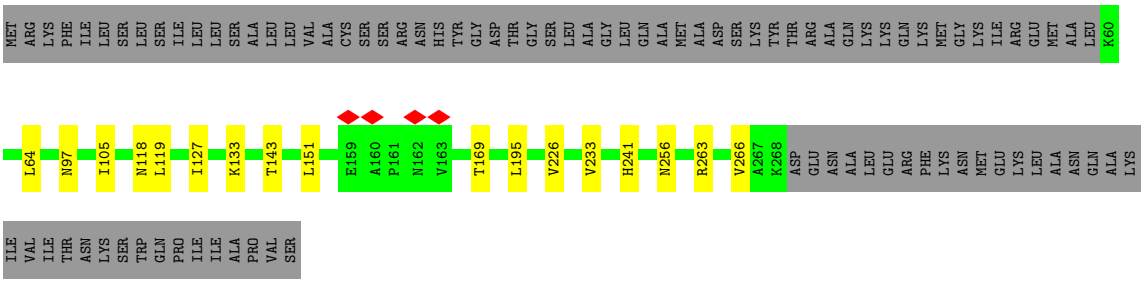
• Molecule 11: DotC

Chain FC:



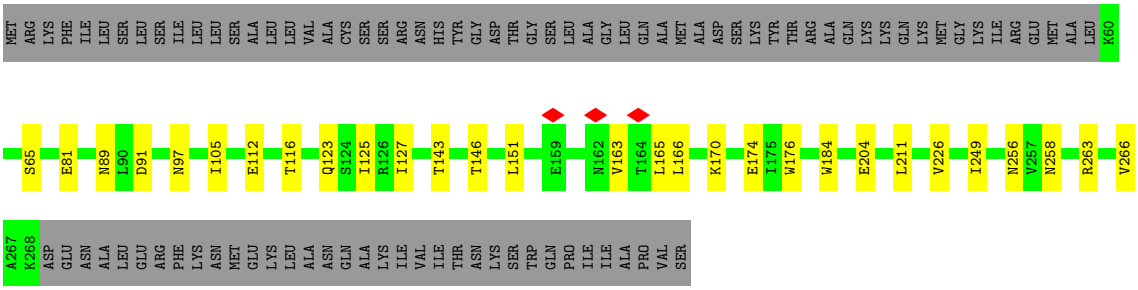
• Molecule 11: DotC

Chain HC:



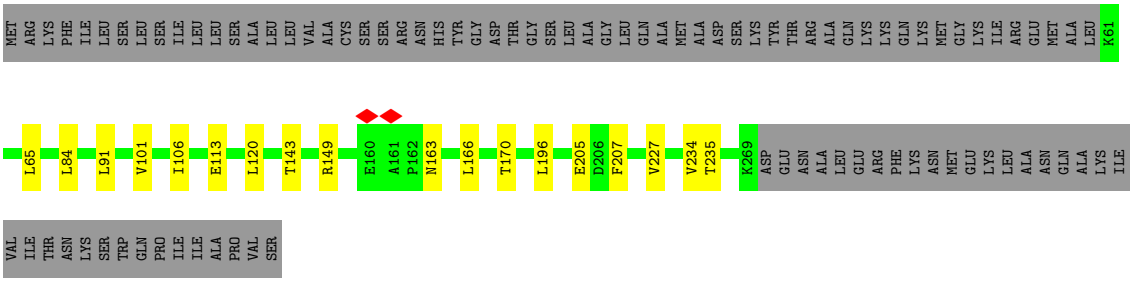
• Molecule 11: DotC

Chain IC:



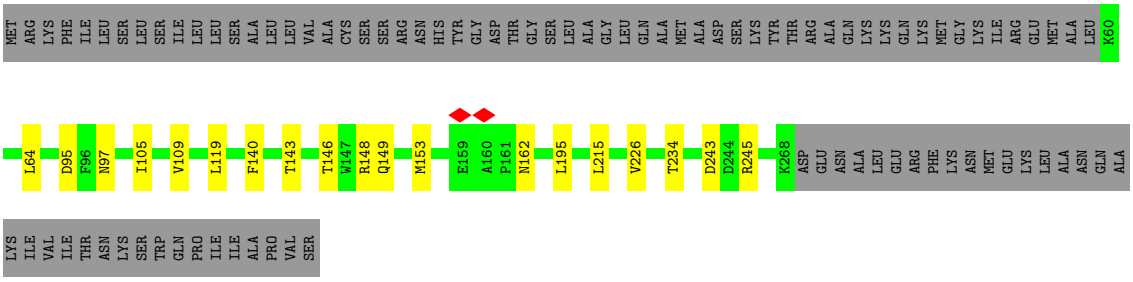
• Molecule 11: DotC

Chain JC:



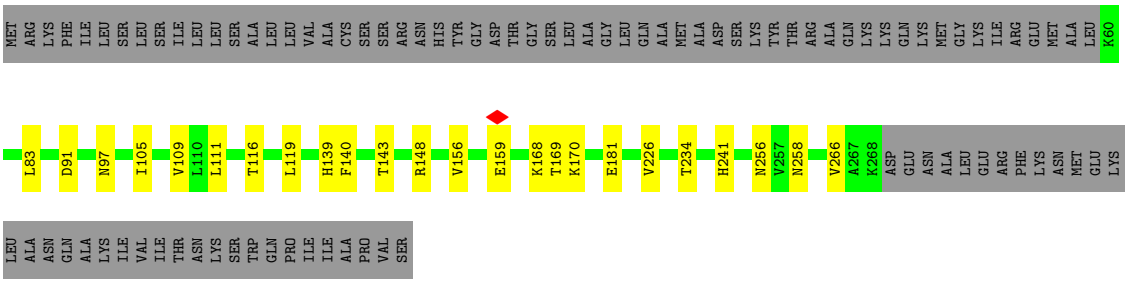
• Molecule 11: DotC

Chain LC:



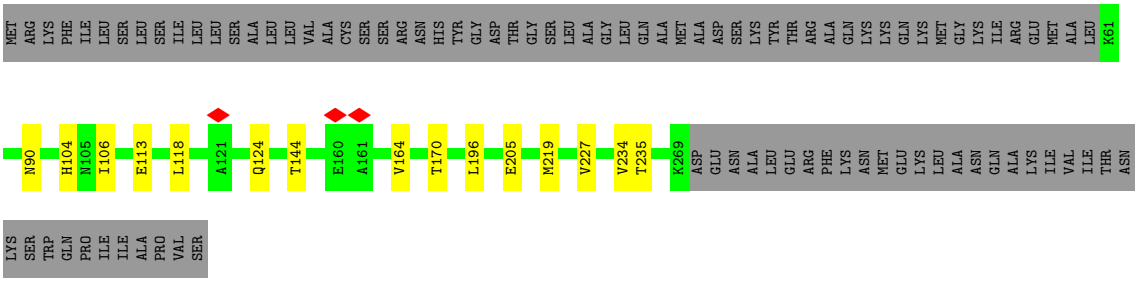
• Molecule 11: DotC

Chain MC:



• Molecule 11: DotC

Chain AC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41057	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	7.797	Depositor
Minimum map value	-2.782	Depositor
Average map value	0.094	Depositor
Map value standard deviation	0.545	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

5.1 Standard geometry

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	0.29	0/1250	0.56	0/1699
1	Ag	0.26	0/278	0.46	0/377
1	BG	0.29	0/1250	0.57	0/1699
1	Bg	0.25	0/278	0.48	0/377
1	CG	0.29	0/1250	0.57	0/1699
1	Cg	0.27	0/278	0.51	0/377
1	DG	0.28	0/1250	0.57	0/1699
1	Dg	0.27	0/278	0.47	0/377
1	EG	0.28	0/1250	0.58	1/1699 (0.1%)
1	Eg	0.26	0/278	0.48	0/377
1	FG	0.30	0/1250	0.57	0/1699
1	Fg	0.27	0/278	0.49	0/377
1	GG	0.29	0/1250	0.58	0/1699
1	Gg	0.26	0/278	0.48	0/377
1	HG	0.30	0/1250	0.58	0/1699
1	Hg	0.26	0/278	0.46	0/377
1	IG	0.29	0/1250	0.58	0/1699
1	Ig	0.26	0/278	0.48	0/377
1	JG	0.28	0/1250	0.57	0/1699
1	Jg	0.27	0/278	0.48	0/377
1	KG	0.29	0/1250	0.56	0/1699
1	Kg	0.25	0/278	0.48	0/377
1	LG	0.29	0/1250	0.57	1/1699 (0.1%)
1	Lg	0.27	0/278	0.49	0/377
1	MG	0.29	0/1250	0.56	0/1699
1	Mg	0.28	0/278	0.46	0/377
1	NG	0.29	0/1250	0.55	0/1699
1	OG	0.29	0/1250	0.56	0/1699
1	PG	0.29	0/1250	0.56	0/1699
1	VG	0.28	0/278	0.59	0/377
1	WG	0.26	0/278	0.52	0/377
1	XG	0.26	0/278	0.51	0/377
1	YG	0.28	0/278	0.51	0/377
1	ZG	0.28	0/278	0.50	0/377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	AD	0.30	0/1107	0.52	0/1502
2	Ad	0.29	0/1078	0.51	0/1463
2	BD	0.31	0/1107	0.53	0/1502
2	Bd	0.28	0/1078	0.49	0/1463
2	CD	0.30	0/1107	0.53	0/1502
2	Cd	0.28	0/1078	0.51	0/1463
2	DD	0.30	0/1107	0.53	0/1502
2	Dd	0.30	0/1078	0.49	0/1463
2	ED	0.32	0/1107	0.53	0/1502
2	Ed	0.30	0/1078	0.50	0/1463
2	FD	0.31	0/1107	0.52	0/1502
2	Fd	0.29	0/1078	0.49	0/1463
2	GD	0.30	0/1107	0.53	0/1502
2	Gd	0.29	0/1078	0.51	0/1463
2	HD	0.30	0/1107	0.52	0/1502
2	Hd	0.29	0/1078	0.50	0/1463
2	ID	0.30	0/1107	0.53	0/1502
2	Id	0.29	0/1078	0.50	0/1463
2	JD	0.31	0/1107	0.53	0/1502
2	Jd	0.29	0/1078	0.49	0/1463
2	KD	0.30	0/1107	0.53	0/1502
2	Kd	0.29	0/1078	0.50	0/1463
2	LD	0.29	0/1107	0.52	0/1502
2	Ld	0.29	0/1078	0.50	0/1463
2	MD	0.30	0/1107	0.53	0/1502
2	Md	0.28	0/1078	0.49	0/1463
3	AF	0.26	0/490	0.55	0/660
3	Af	0.28	0/456	0.54	0/615
3	BF	0.27	0/490	0.52	0/660
3	Bf	0.27	0/456	0.55	0/615
3	CF	0.27	0/490	0.54	0/660
3	Cf	0.28	0/456	0.53	0/615
3	DF	0.27	0/490	0.55	0/660
3	Df	0.27	0/456	0.53	0/615
3	EF	0.27	0/490	0.54	0/660
3	Ef	0.28	0/456	0.52	0/615
3	FF	0.26	0/490	0.53	0/660
3	Ff	0.29	0/456	0.52	0/615
3	GF	0.26	0/490	0.54	0/660
3	Gf	0.28	0/456	0.51	0/615
3	HF	0.27	0/490	0.54	0/660
3	Hf	0.28	0/456	0.54	0/615
3	IF	0.27	0/490	0.53	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	If	0.26	0/456	0.55	0/615
3	JF	0.26	0/490	0.54	0/660
3	Jf	0.28	0/456	0.53	0/615
3	KF	0.26	0/490	0.54	0/660
3	Kf	0.27	0/456	0.54	0/615
3	LF	0.27	0/490	0.55	0/660
3	Lf	0.27	0/456	0.53	0/615
3	MF	0.27	0/490	0.54	0/660
3	Mf	0.28	0/456	0.52	0/615
3	VF	0.27	0/490	0.51	0/660
3	WF	0.27	0/490	0.55	0/660
3	XF	0.27	0/490	0.54	0/660
3	YF	0.25	0/490	0.55	0/660
3	ZF	0.27	0/490	0.53	0/660
4	AH	0.29	0/2033	0.52	0/2775
4	BH	0.30	0/2033	0.53	0/2775
4	CH	0.29	0/2033	0.51	0/2775
4	DH	0.29	0/2033	0.51	0/2775
4	EH	0.29	0/2033	0.51	0/2775
4	FH	0.29	0/2033	0.52	0/2775
4	GH	0.29	0/2033	0.51	0/2775
4	HH	0.30	0/2033	0.52	0/2775
4	IH	0.29	0/2033	0.52	0/2775
4	JH	0.29	0/2033	0.51	0/2775
4	KH	0.30	0/2033	0.53	0/2775
4	LH	0.29	0/2033	0.52	0/2775
4	MH	0.30	0/2033	0.53	0/2775
4	VH	0.27	0/1921	0.51	0/2620
4	WH	0.27	0/1921	0.54	0/2620
4	XH	0.27	0/1921	0.52	0/2620
4	YH	0.27	0/1921	0.53	0/2620
4	ZH	0.27	0/1921	0.52	0/2620
5	AK	0.30	0/1195	0.54	0/1616
5	BK	0.31	0/1195	0.55	0/1616
5	CK	0.30	0/1195	0.54	0/1616
5	DK	0.31	0/1195	0.54	0/1616
5	EK	0.29	0/1195	0.54	0/1616
5	FK	0.29	0/1195	0.55	0/1616
5	GK	0.30	0/1195	0.53	0/1616
5	HK	0.32	0/1195	0.55	0/1616
5	IK	0.29	0/1195	0.54	0/1616
5	JK	0.30	0/1195	0.53	0/1616
5	KK	0.30	0/1195	0.54	0/1616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	LK	0.31	0/1195	0.54	0/1616
5	MK	0.30	0/1195	0.54	0/1616
6	AL	0.30	0/1417	0.54	0/1912
6	BL	0.30	0/1417	0.55	0/1912
6	CL	0.30	0/1417	0.54	0/1912
6	DL	0.30	0/1417	0.54	0/1912
6	EL	0.30	0/1417	0.54	0/1912
6	FL	0.30	0/1417	0.55	0/1912
6	GL	0.30	0/1417	0.55	0/1912
6	HL	0.30	0/1417	0.55	0/1912
6	IL	0.29	0/1417	0.56	0/1912
6	JL	0.30	0/1417	0.54	0/1912
6	KL	0.29	0/1417	0.56	0/1912
6	LL	0.31	0/1417	0.54	0/1912
6	ML	0.30	0/1417	0.55	0/1912
7	AM	0.29	0/1678	0.58	0/2262
7	BM	0.29	0/1678	0.58	0/2262
7	CM	0.29	0/1678	0.57	0/2262
7	DM	0.29	0/1678	0.57	0/2262
7	EM	0.28	0/1678	0.57	0/2262
7	FM	0.30	0/1678	0.58	0/2262
7	GM	0.29	0/1678	0.57	0/2262
7	HM	0.29	0/1678	0.58	0/2262
7	IM	0.29	0/1678	0.57	0/2262
7	JM	0.29	0/1678	0.57	0/2262
7	KM	0.28	0/1678	0.57	0/2262
7	LM	0.29	0/1678	0.58	0/2262
7	MM	0.28	0/1678	0.57	0/2262
8	AN	0.32	0/593	0.54	0/799
8	BN	0.31	0/593	0.56	0/799
8	CN	0.31	0/593	0.51	0/799
8	DN	0.31	0/593	0.53	0/799
8	EN	0.33	0/593	0.52	0/799
8	FN	0.33	0/593	0.52	0/799
8	GN	0.31	0/593	0.52	0/799
8	HN	0.31	0/593	0.53	0/799
8	IN	0.30	0/593	0.52	0/799
8	JN	0.31	0/593	0.53	0/799
8	KN	0.32	0/593	0.52	0/799
8	LN	0.32	0/593	0.51	0/799
8	MN	0.32	0/593	0.54	0/799
11	AC	0.30	0/1702	0.52	0/2315
11	BC	0.30	0/1957	0.52	0/2651

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	CC	0.29	0/1957	0.52	0/2651
11	DC	0.29	0/1702	0.51	0/2315
11	EC	0.30	0/1702	0.51	0/2315
11	FC	0.30	0/1957	0.50	0/2651
11	GC	0.29	0/1957	0.51	0/2651
11	HC	0.29	0/1702	0.50	0/2315
11	IC	0.29	0/1702	0.51	0/2315
11	JC	0.31	0/1702	0.52	0/2315
11	KC	0.29	0/1957	0.52	0/2651
11	LC	0.30	0/1702	0.55	0/2315
11	MC	0.30	0/1702	0.52	0/2315
All	All	0.29	0/191071	0.53	2/258997 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	LG	1040	LEU	CA-CB-CG	6.10	129.34	115.30
1	EG	965	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

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%)	154 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ag	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	BG	161/1048 (15%)	155 (96%)	6 (4%)	0	100	100
1	Bg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	CG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Cg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	DG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	Dg	32/1048 (3%)	32 (100%)	0	0	100	100
1	EG	161/1048 (15%)	156 (97%)	5 (3%)	0	100	100
1	Eg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	FG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Fg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	GG	161/1048 (15%)	151 (94%)	10 (6%)	0	100	100
1	Gg	32/1048 (3%)	32 (100%)	0	0	100	100
1	HG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Hg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	IG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Ig	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	JG	161/1048 (15%)	156 (97%)	5 (3%)	0	100	100
1	Jg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	KG	161/1048 (15%)	155 (96%)	6 (4%)	0	100	100
1	Kg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	LG	161/1048 (15%)	149 (92%)	12 (8%)	0	100	100
1	Lg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	MG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	Mg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	NG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	OG	161/1048 (15%)	157 (98%)	4 (2%)	0	100	100
1	PG	161/1048 (15%)	156 (97%)	5 (3%)	0	100	100
1	VG	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	WG	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	XG	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	YG	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
2	AD	138/163 (85%)	127 (92%)	11 (8%)	0	100	100
2	Ad	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
2	BD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Bd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
2	CD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Cd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	DD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Dd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ED	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Ed	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	FD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Fd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
2	GD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Gd	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
2	HD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Hd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ID	138/163 (85%)	127 (92%)	11 (8%)	0	100	100
2	Id	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
2	JD	138/163 (85%)	132 (96%)	6 (4%)	0	100	100
2	Jd	135/163 (83%)	126 (93%)	9 (7%)	0	100	100
2	KD	138/163 (85%)	126 (91%)	12 (9%)	0	100	100
2	Kd	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
2	LD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Ld	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	MD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Md	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
3	AF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	Af	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	BF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Bf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	CF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Cf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	DF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Df	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	EF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Ef	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	FF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
3	Ff	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	GF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Gf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	HF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	Hf	57/269 (21%)	51 (90%)	6 (10%)	0	100	100
3	IF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	If	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	JF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	Jf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	KF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Kf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	LF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Lf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	MF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
3	Mf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	VF	61/269 (23%)	61 (100%)	0	0	100	100
3	WF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	XF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
3	YF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	ZF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
4	AH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
4	BH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
4	CH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	DH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100
4	EH	256/361 (71%)	248 (97%)	8 (3%)	0	100	100
4	FH	256/361 (71%)	246 (96%)	10 (4%)	0	100	100
4	GH	256/361 (71%)	238 (93%)	18 (7%)	0	100	100
4	HH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
4	IH	256/361 (71%)	239 (93%)	17 (7%)	0	100	100
4	JH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
4	KH	256/361 (71%)	239 (93%)	17 (7%)	0	100	100
4	LH	256/361 (71%)	239 (93%)	17 (7%)	0	100	100
4	MH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
4	VH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
4	WH	239/361 (66%)	230 (96%)	9 (4%)	0	100	100
4	XH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
4	YH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
4	ZH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
5	AK	149/189 (79%)	145 (97%)	4 (3%)	0	100	100
5	BK	149/189 (79%)	145 (97%)	4 (3%)	0	100	100
5	CK	149/189 (79%)	141 (95%)	8 (5%)	0	100	100
5	DK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
5	EK	149/189 (79%)	146 (98%)	3 (2%)	0	100	100
5	FK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
5	GK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
5	HK	149/189 (79%)	140 (94%)	9 (6%)	0	100	100
5	IK	149/189 (79%)	141 (95%)	8 (5%)	0	100	100
5	JK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
5	KK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
5	LK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
5	MK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
6	AL	169/249 (68%)	165 (98%)	4 (2%)	0	100	100
6	BL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
6	CL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	DL	169/249 (68%)	158 (94%)	11 (6%)	0	100	100
6	EL	169/249 (68%)	158 (94%)	11 (6%)	0	100	100
6	FL	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
6	GL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
6	HL	169/249 (68%)	158 (94%)	11 (6%)	0	100	100
6	IL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
6	JL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
6	KL	169/249 (68%)	158 (94%)	11 (6%)	0	100	100
6	LL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
6	ML	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	AM	206/320 (64%)	190 (92%)	16 (8%)	0	100	100
7	BM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
7	CM	206/320 (64%)	194 (94%)	12 (6%)	0	100	100
7	DM	206/320 (64%)	196 (95%)	10 (5%)	0	100	100
7	EM	206/320 (64%)	193 (94%)	13 (6%)	0	100	100
7	FM	206/320 (64%)	188 (91%)	18 (9%)	0	100	100
7	GM	206/320 (64%)	193 (94%)	13 (6%)	0	100	100
7	HM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
7	IM	206/320 (64%)	188 (91%)	18 (9%)	0	100	100
7	JM	206/320 (64%)	189 (92%)	17 (8%)	0	100	100
7	KM	206/320 (64%)	189 (92%)	17 (8%)	0	100	100
7	LM	206/320 (64%)	192 (93%)	14 (7%)	0	100	100
7	MM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
8	AN	76/124 (61%)	66 (87%)	10 (13%)	0	100	100
8	BN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	CN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100
8	DN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
8	EN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	FN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	GN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
8	HN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	IN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
8	JN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	KN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100
8	LN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	MN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100
11	AC	207/303 (68%)	194 (94%)	13 (6%)	0	100	100
11	BC	241/303 (80%)	231 (96%)	10 (4%)	0	100	100
11	CC	241/303 (80%)	230 (95%)	11 (5%)	0	100	100
11	DC	207/303 (68%)	194 (94%)	13 (6%)	0	100	100
11	EC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
11	FC	241/303 (80%)	230 (95%)	11 (5%)	0	100	100
11	GC	241/303 (80%)	234 (97%)	7 (3%)	0	100	100
11	HC	207/303 (68%)	193 (93%)	14 (7%)	0	100	100
11	IC	207/303 (68%)	192 (93%)	15 (7%)	0	100	100
11	JC	207/303 (68%)	198 (96%)	9 (4%)	0	100	100
11	KC	241/303 (80%)	230 (95%)	11 (5%)	0	100	100
11	LC	207/303 (68%)	190 (92%)	17 (8%)	0	100	100
11	MC	207/303 (68%)	192 (93%)	15 (7%)	0	100	100
All	All	23724/70112 (34%)	22457 (95%)	1267 (5%)	0	100	100

There are no Ramachandran outliers to report.

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%)	120 (89%)	15 (11%)	6	25
1	Ag	31/765 (4%)	23 (74%)	8 (26%)	0	4
1	BG	135/765 (18%)	117 (87%)	18 (13%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Bg	31/765 (4%)	28 (90%)	3 (10%)	8 29
1	CG	135/765 (18%)	118 (87%)	17 (13%)	4 21
1	Cg	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	DG	135/765 (18%)	118 (87%)	17 (13%)	4 21
1	Dg	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	EG	135/765 (18%)	115 (85%)	20 (15%)	3 17
1	Eg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	FG	135/765 (18%)	120 (89%)	15 (11%)	6 25
1	Fg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	GG	135/765 (18%)	114 (84%)	21 (16%)	2 16
1	Gg	31/765 (4%)	26 (84%)	5 (16%)	2 15
1	HG	135/765 (18%)	117 (87%)	18 (13%)	4 20
1	Hg	31/765 (4%)	26 (84%)	5 (16%)	2 15
1	IG	135/765 (18%)	117 (87%)	18 (13%)	4 20
1	Ig	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	JG	135/765 (18%)	118 (87%)	17 (13%)	4 21
1	Jg	31/765 (4%)	23 (74%)	8 (26%)	0 4
1	KG	135/765 (18%)	119 (88%)	16 (12%)	5 22
1	Kg	31/765 (4%)	22 (71%)	9 (29%)	0 3
1	LG	135/765 (18%)	116 (86%)	19 (14%)	3 18
1	Lg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	MG	135/765 (18%)	120 (89%)	15 (11%)	6 25
1	Mg	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	NG	135/765 (18%)	124 (92%)	11 (8%)	11 37
1	OG	135/765 (18%)	115 (85%)	20 (15%)	3 17
1	PG	135/765 (18%)	116 (86%)	19 (14%)	3 18
1	VG	31/765 (4%)	28 (90%)	3 (10%)	8 29
1	WG	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	XG	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	YG	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	ZG	31/765 (4%)	27 (87%)	4 (13%)	4 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AD	121/139 (87%)	107 (88%)	14 (12%)	5 23
2	Ad	118/139 (85%)	106 (90%)	12 (10%)	7 27
2	BD	121/139 (87%)	113 (93%)	8 (7%)	16 43
2	Bd	118/139 (85%)	107 (91%)	11 (9%)	9 30
2	CD	121/139 (87%)	105 (87%)	16 (13%)	4 20
2	Cd	118/139 (85%)	104 (88%)	14 (12%)	5 22
2	DD	121/139 (87%)	112 (93%)	9 (7%)	13 40
2	Dd	118/139 (85%)	107 (91%)	11 (9%)	9 30
2	ED	121/139 (87%)	114 (94%)	7 (6%)	20 47
2	Ed	118/139 (85%)	106 (90%)	12 (10%)	7 27
2	FD	121/139 (87%)	105 (87%)	16 (13%)	4 20
2	Fd	118/139 (85%)	109 (92%)	9 (8%)	13 39
2	GD	121/139 (87%)	110 (91%)	11 (9%)	9 31
2	Gd	118/139 (85%)	106 (90%)	12 (10%)	7 27
2	HD	121/139 (87%)	109 (90%)	12 (10%)	8 28
2	Hd	118/139 (85%)	110 (93%)	8 (7%)	16 42
2	ID	121/139 (87%)	112 (93%)	9 (7%)	13 40
2	Id	118/139 (85%)	108 (92%)	10 (8%)	10 36
2	JD	121/139 (87%)	111 (92%)	10 (8%)	11 36
2	Jd	118/139 (85%)	110 (93%)	8 (7%)	16 42
2	KD	121/139 (87%)	110 (91%)	11 (9%)	9 31
2	Kd	118/139 (85%)	108 (92%)	10 (8%)	10 36
2	LD	121/139 (87%)	106 (88%)	15 (12%)	4 21
2	Ld	118/139 (85%)	108 (92%)	10 (8%)	10 36
2	MD	121/139 (87%)	107 (88%)	14 (12%)	5 23
2	Md	118/139 (85%)	106 (90%)	12 (10%)	7 27
3	AF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	Af	49/237 (21%)	43 (88%)	6 (12%)	5 22
3	BF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	Bf	49/237 (21%)	45 (92%)	4 (8%)	11 36
3	CF	53/237 (22%)	49 (92%)	4 (8%)	13 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Cf	49/237 (21%)	42 (86%)	7 (14%)	3 18
3	DF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	Df	49/237 (21%)	46 (94%)	3 (6%)	18 46
3	EF	53/237 (22%)	46 (87%)	7 (13%)	4 20
3	Ef	49/237 (21%)	48 (98%)	1 (2%)	55 73
3	FF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	Ff	49/237 (21%)	43 (88%)	6 (12%)	5 22
3	GF	53/237 (22%)	46 (87%)	7 (13%)	4 20
3	Gf	49/237 (21%)	43 (88%)	6 (12%)	5 22
3	HF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	Hf	49/237 (21%)	44 (90%)	5 (10%)	7 27
3	IF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	If	49/237 (21%)	43 (88%)	6 (12%)	5 22
3	JF	53/237 (22%)	44 (83%)	9 (17%)	2 13
3	Jf	49/237 (21%)	46 (94%)	3 (6%)	18 46
3	KF	53/237 (22%)	48 (91%)	5 (9%)	8 30
3	Kf	49/237 (21%)	46 (94%)	3 (6%)	18 46
3	LF	53/237 (22%)	46 (87%)	7 (13%)	4 20
3	Lf	49/237 (21%)	39 (80%)	10 (20%)	1 7
3	MF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	Mf	49/237 (21%)	44 (90%)	5 (10%)	7 27
3	VF	53/237 (22%)	48 (91%)	5 (9%)	8 30
3	WF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	XF	53/237 (22%)	49 (92%)	4 (8%)	13 40
3	YF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	ZF	53/237 (22%)	49 (92%)	4 (8%)	13 40
4	AH	220/300 (73%)	192 (87%)	28 (13%)	4 21
4	BH	220/300 (73%)	202 (92%)	18 (8%)	11 36
4	CH	220/300 (73%)	199 (90%)	21 (10%)	8 29
4	DH	220/300 (73%)	193 (88%)	27 (12%)	4 22
4	EH	220/300 (73%)	192 (87%)	28 (13%)	4 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	FH	220/300 (73%)	197 (90%)	23 (10%)	7	26
4	GH	220/300 (73%)	193 (88%)	27 (12%)	4	22
4	HH	220/300 (73%)	194 (88%)	26 (12%)	5	23
4	IH	220/300 (73%)	200 (91%)	20 (9%)	9	31
4	JH	220/300 (73%)	195 (89%)	25 (11%)	5	24
4	KH	220/300 (73%)	199 (90%)	21 (10%)	8	29
4	LH	220/300 (73%)	197 (90%)	23 (10%)	7	26
4	MH	220/300 (73%)	195 (89%)	25 (11%)	5	24
4	VH	207/300 (69%)	179 (86%)	28 (14%)	4	19
4	WH	207/300 (69%)	174 (84%)	33 (16%)	2	15
4	XH	207/300 (69%)	185 (89%)	22 (11%)	6	26
4	YH	207/300 (69%)	181 (87%)	26 (13%)	4	21
4	ZH	207/300 (69%)	179 (86%)	28 (14%)	4	19
5	AK	129/163 (79%)	111 (86%)	18 (14%)	3	19
5	BK	129/163 (79%)	112 (87%)	17 (13%)	4	20
5	CK	129/163 (79%)	117 (91%)	12 (9%)	9	30
5	DK	129/163 (79%)	121 (94%)	8 (6%)	18	45
5	EK	129/163 (79%)	117 (91%)	12 (9%)	9	30
5	FK	129/163 (79%)	116 (90%)	13 (10%)	7	27
5	GK	129/163 (79%)	122 (95%)	7 (5%)	22	49
5	HK	129/163 (79%)	119 (92%)	10 (8%)	12	38
5	IK	129/163 (79%)	113 (88%)	16 (12%)	4	21
5	JK	129/163 (79%)	119 (92%)	10 (8%)	12	38
5	KK	129/163 (79%)	114 (88%)	15 (12%)	5	23
5	LK	129/163 (79%)	117 (91%)	12 (9%)	9	30
5	MK	129/163 (79%)	114 (88%)	15 (12%)	5	23
6	AL	148/203 (73%)	134 (90%)	14 (10%)	8	29
6	BL	148/203 (73%)	130 (88%)	18 (12%)	5	22
6	CL	148/203 (73%)	133 (90%)	15 (10%)	7	27
6	DL	148/203 (73%)	137 (93%)	11 (7%)	13	40
6	EL	148/203 (73%)	131 (88%)	17 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	FL	148/203 (73%)	133 (90%)	15 (10%)	7 27
6	GL	148/203 (73%)	132 (89%)	16 (11%)	6 26
6	HL	148/203 (73%)	132 (89%)	16 (11%)	6 26
6	IL	148/203 (73%)	134 (90%)	14 (10%)	8 29
6	JL	148/203 (73%)	133 (90%)	15 (10%)	7 27
6	KL	148/203 (73%)	134 (90%)	14 (10%)	8 29
6	LL	148/203 (73%)	136 (92%)	12 (8%)	11 37
6	ML	148/203 (73%)	133 (90%)	15 (10%)	7 27
7	AM	175/276 (63%)	160 (91%)	15 (9%)	10 35
7	BM	175/276 (63%)	146 (83%)	29 (17%)	2 14
7	CM	175/276 (63%)	148 (85%)	27 (15%)	2 16
7	DM	175/276 (63%)	154 (88%)	21 (12%)	5 22
7	EM	175/276 (63%)	148 (85%)	27 (15%)	2 16
7	FM	175/276 (63%)	153 (87%)	22 (13%)	4 21
7	GM	175/276 (63%)	153 (87%)	22 (13%)	4 21
7	HM	175/276 (63%)	153 (87%)	22 (13%)	4 21
7	IM	175/276 (63%)	148 (85%)	27 (15%)	2 16
7	JM	175/276 (63%)	151 (86%)	24 (14%)	3 19
7	KM	175/276 (63%)	148 (85%)	27 (15%)	2 16
7	LM	175/276 (63%)	154 (88%)	21 (12%)	5 22
7	MM	175/276 (63%)	158 (90%)	17 (10%)	8 29
8	AN	66/107 (62%)	60 (91%)	6 (9%)	9 31
8	BN	66/107 (62%)	53 (80%)	13 (20%)	1 9
8	CN	66/107 (62%)	62 (94%)	4 (6%)	18 46
8	DN	66/107 (62%)	55 (83%)	11 (17%)	2 14
8	EN	66/107 (62%)	53 (80%)	13 (20%)	1 9
8	FN	66/107 (62%)	54 (82%)	12 (18%)	1 11
8	GN	66/107 (62%)	57 (86%)	9 (14%)	3 19
8	HN	66/107 (62%)	53 (80%)	13 (20%)	1 9
8	IN	66/107 (62%)	57 (86%)	9 (14%)	3 19
8	JN	66/107 (62%)	60 (91%)	6 (9%)	9 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	KN	66/107 (62%)	58 (88%)	8 (12%)	5 22
8	LN	66/107 (62%)	59 (89%)	7 (11%)	6 26
8	MN	66/107 (62%)	55 (83%)	11 (17%)	2 14
11	AC	178/257 (69%)	163 (92%)	15 (8%)	11 36
11	BC	203/257 (79%)	181 (89%)	22 (11%)	6 26
11	CC	203/257 (79%)	174 (86%)	29 (14%)	3 18
11	DC	178/257 (69%)	154 (86%)	24 (14%)	4 19
11	EC	178/257 (69%)	164 (92%)	14 (8%)	12 38
11	FC	203/257 (79%)	181 (89%)	22 (11%)	6 26
11	GC	203/257 (79%)	180 (89%)	23 (11%)	6 24
11	HC	178/257 (69%)	161 (90%)	17 (10%)	8 29
11	IC	178/257 (69%)	149 (84%)	29 (16%)	2 14
11	JC	178/257 (69%)	160 (90%)	18 (10%)	7 27
11	KC	203/257 (79%)	173 (85%)	30 (15%)	3 17
11	LC	178/257 (69%)	159 (89%)	19 (11%)	6 26
11	MC	178/257 (69%)	154 (86%)	24 (14%)	4 19
All	All	20484/55449 (37%)	18117 (88%)	2367 (12%)	9 23

5 of 2367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	IC	97	ASN
6	DL	113	ASP
11	LC	162	ASN
11	IC	89	ASN
1	Dg	808	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
4	WH	355	GLN
2	Ad	32	ASN
1	Ag	818	GLN
4	YH	205	GLN
4	ZH	205	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	JX	1
10	WX	1
10	YX	1
10	XX	1
10	GX	1
10	CX	1
10	MX	1
10	ZX	1
10	KX	1
10	HX	1
10	FX	1
10	EX	1
10	IX	1
10	DX	1
10	BX	1
10	AX	1

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Mol	Chain	Number of breaks
10	VX	1
10	LX	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	25.78
1	WX	38:UNK	C	70:UNK	N	25.34
1	YX	38:UNK	C	70:UNK	N	25.23
1	XX	38:UNK	C	70:UNK	N	25.08
1	GX	38:UNK	C	70:UNK	N	24.81

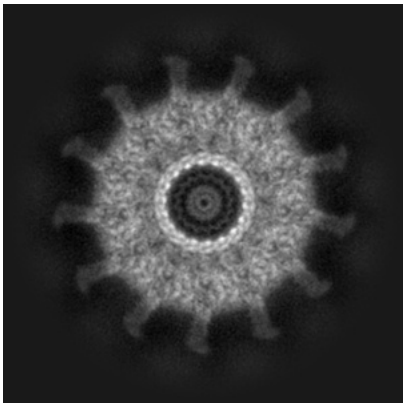
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24026. These allow visual inspection of the internal detail of the map and identification of artifacts.

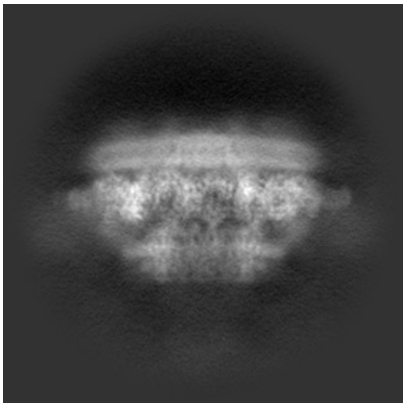
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

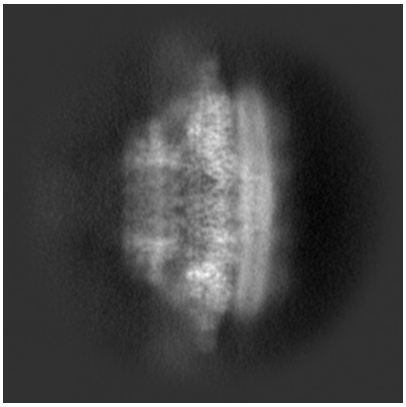
6.1.1 Primary map



X



Y

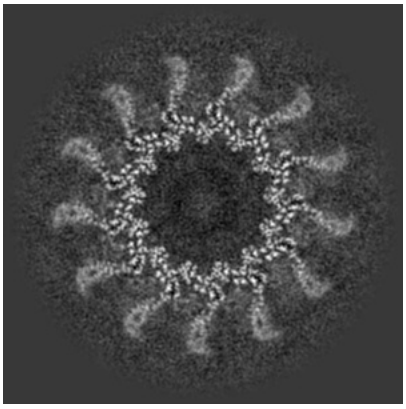


Z

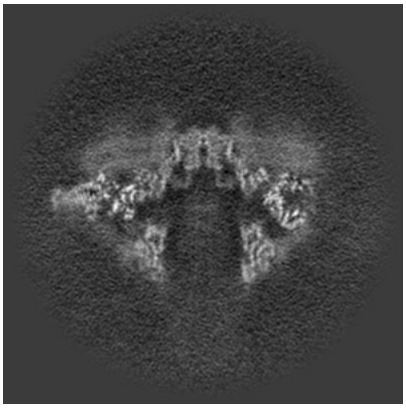
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 125



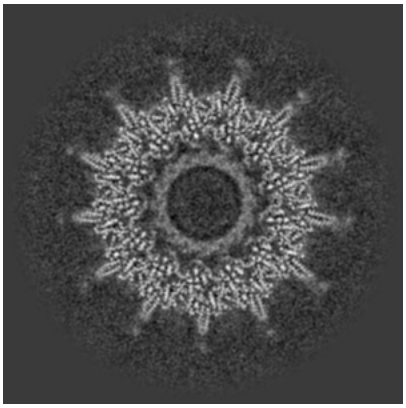
Y Index: 125

Z Index: 125

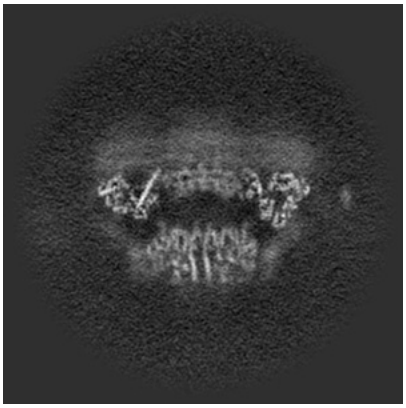
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

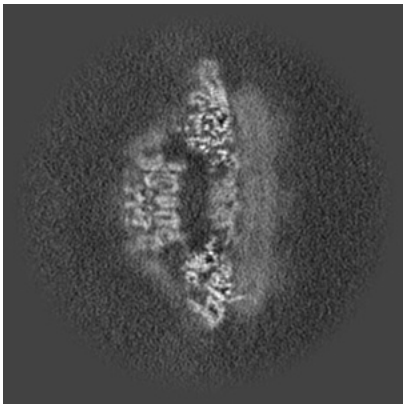
6.3.1 Primary map



X Index: 134



Y Index: 101



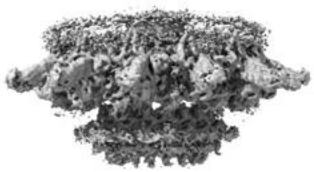
Z Index: 152

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

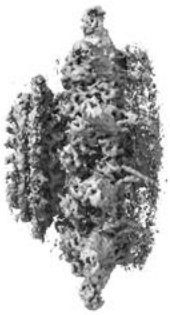
6.4 Orthogonal surface views (i)

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.

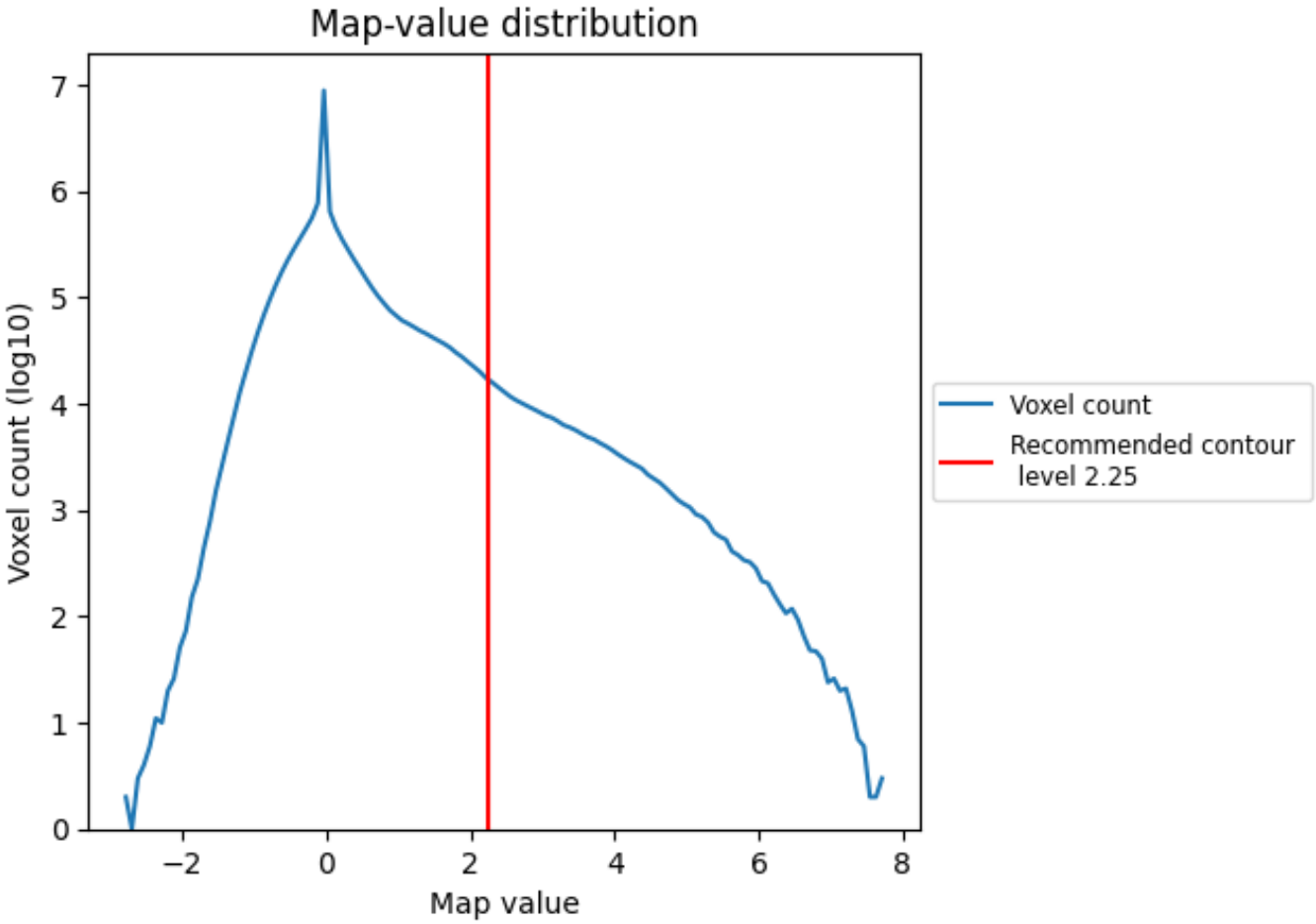
6.5 Mask visualisation (i)

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

7 Map analysis

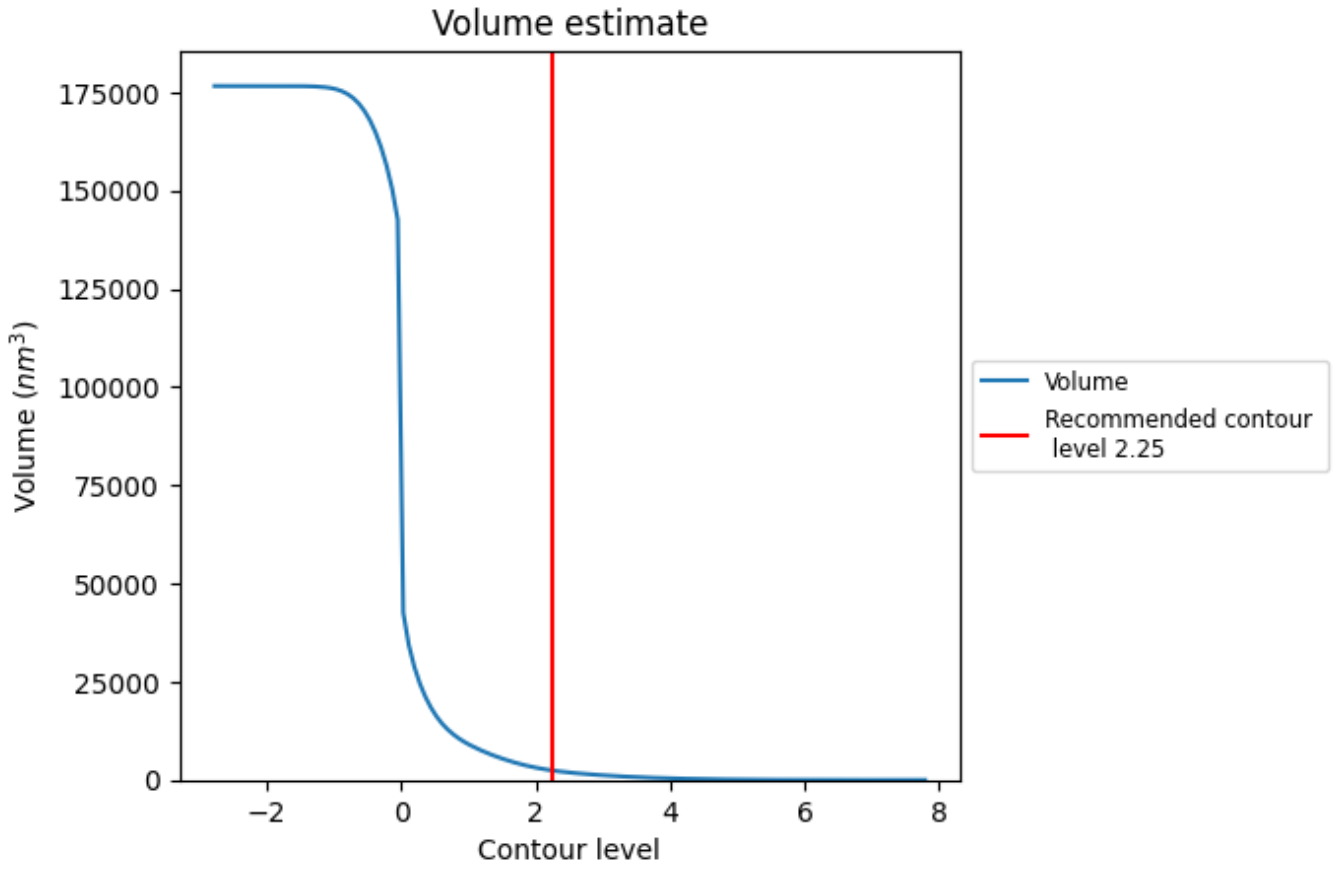
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

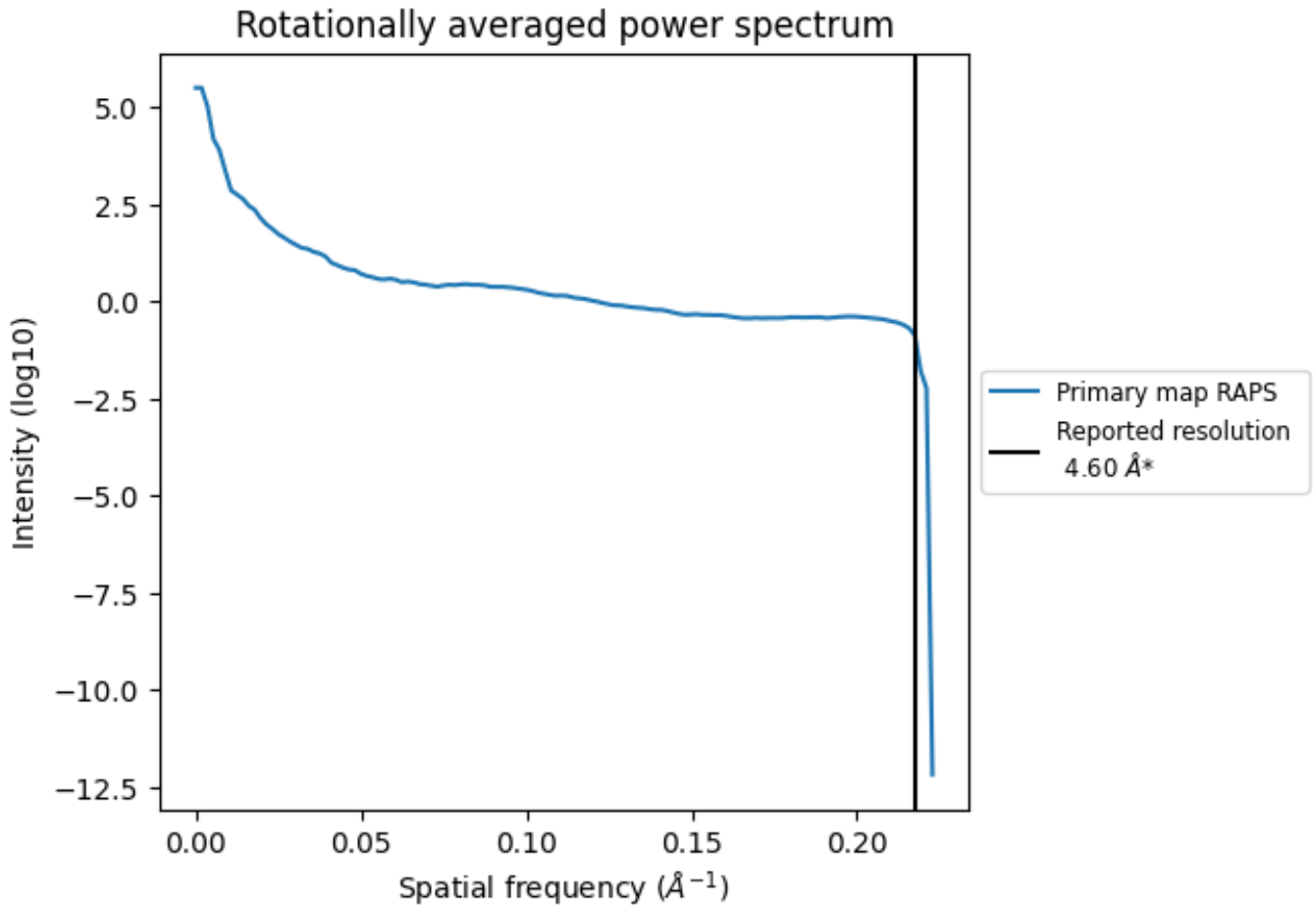
7.2 Volume estimate (i)



The volume at the recommended contour level is 2412 nm^3; this corresponds to an approximate mass of 2179 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 $Å^{-1}$

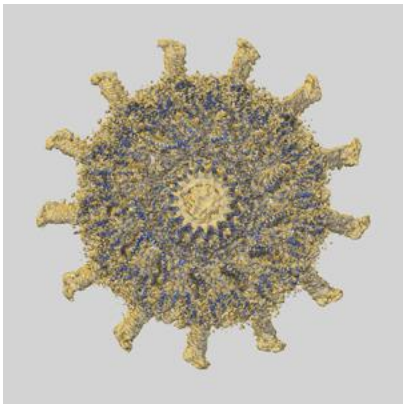
8 Fourier-Shell correlation

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

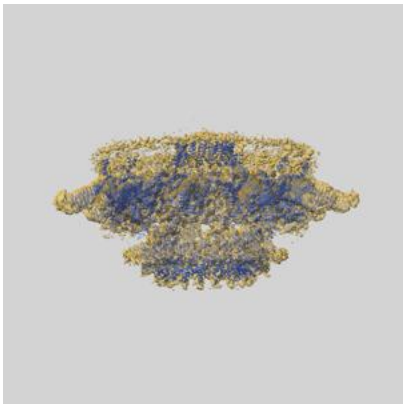
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24026 and PDB model 7MUY. Per-residue inclusion information can be found in section 3 on page 22.

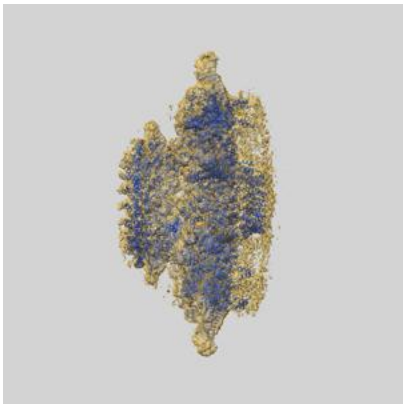
9.1 Map-model overlay



X



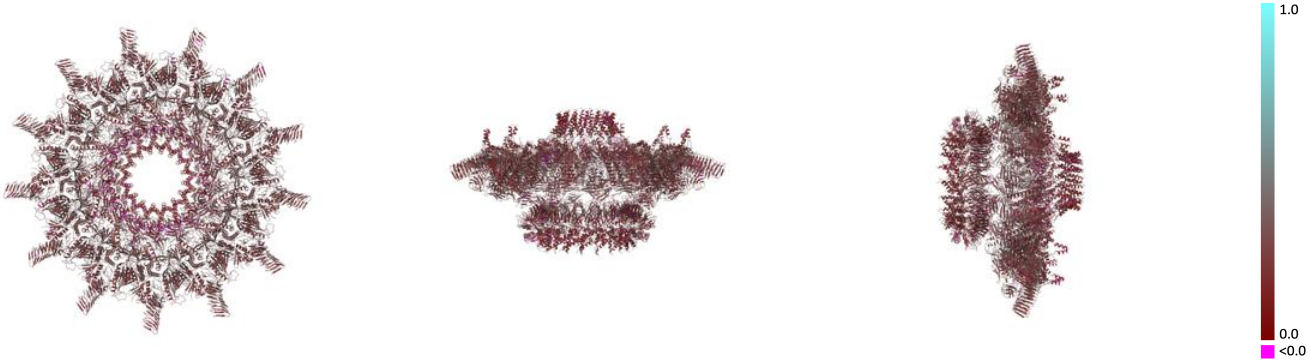
Y



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.

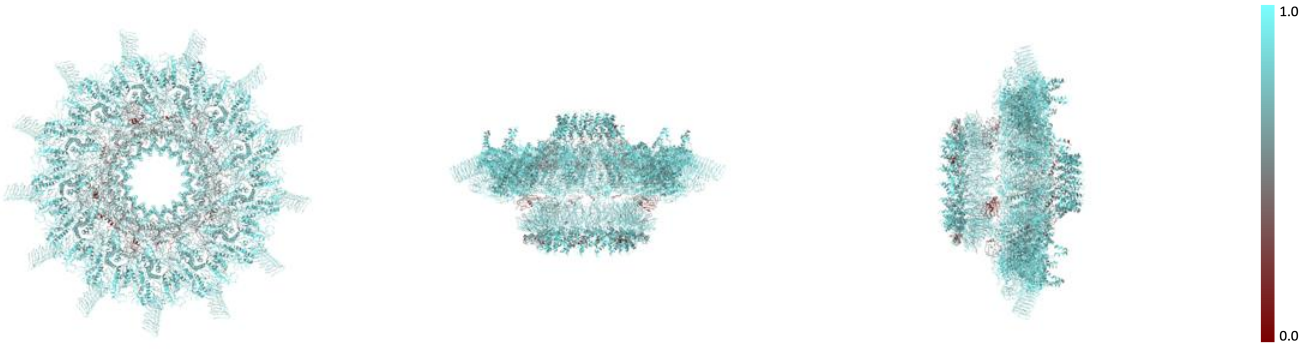
9.2 Q-score mapped to coordinate model



X Y Z

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

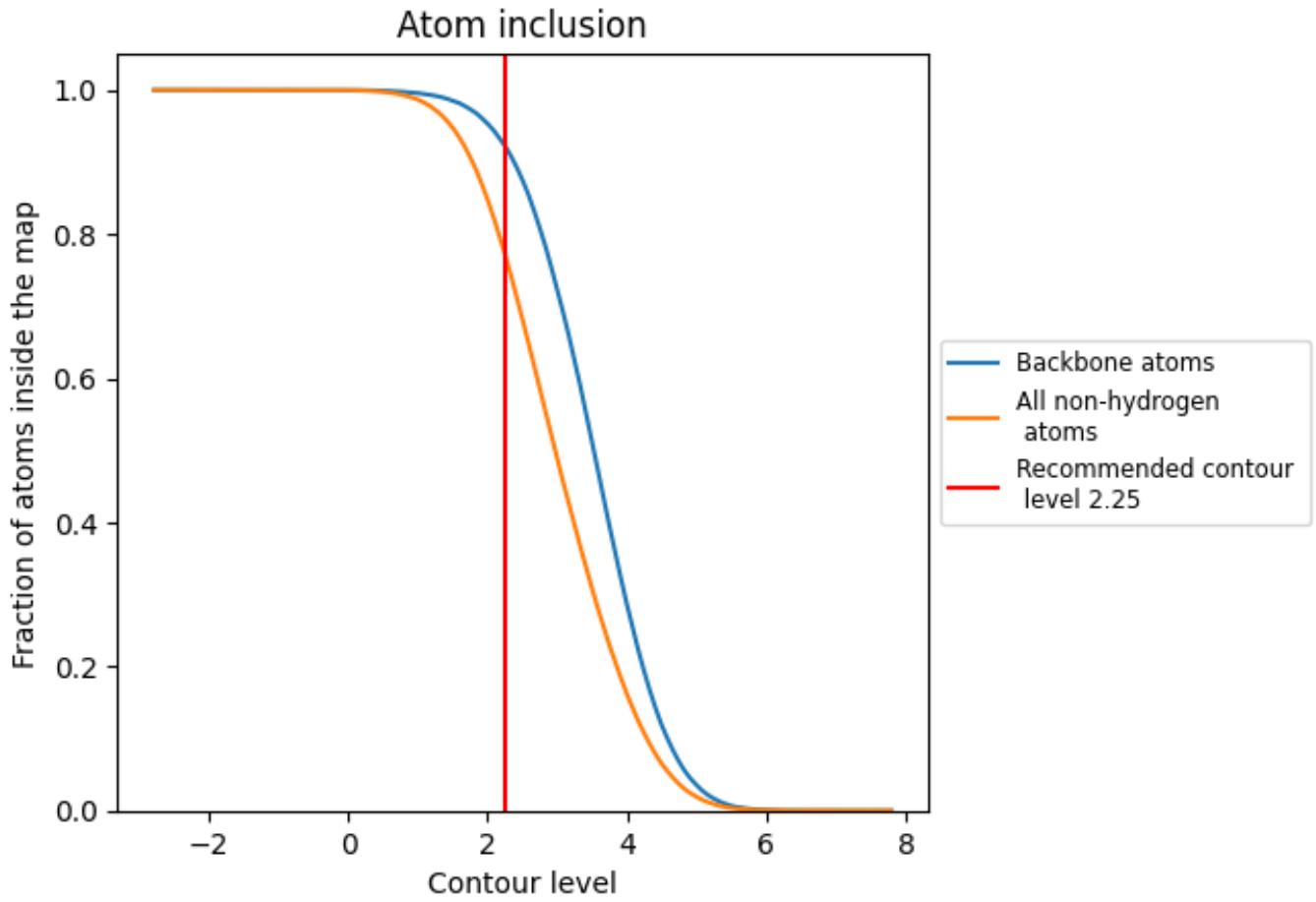
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.25).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.7728	0.2760
AC	0.8092	0.3010
AD	0.8296	0.3070
AF	0.8068	0.2390
AG	0.6782	0.1990
AH	0.7931	0.2780
AK	0.8241	0.3060
AL	0.8317	0.2870
AM	0.8113	0.2930
AN	0.8059	0.3290
AU	0.9778	0.4800
AX	0.5625	0.1910
Ad	0.8357	0.3050
Af	0.8405	0.2840
Ag	0.8676	0.2400
BC	0.7685	0.3000
BD	0.8109	0.3100
BF	0.8004	0.2210
BG	0.5764	0.1780
BH	0.8039	0.2840
BK	0.8443	0.3160
BL	0.8480	0.2920
BM	0.8367	0.2960
BN	0.7727	0.3370
BU	1.0000	0.4440
BX	0.5167	0.1940
Bd	0.8271	0.3040
Bf	0.7950	0.2670
Bg	0.8419	0.2520
CC	0.7445	0.2840
CD	0.8221	0.3190
CF	0.7367	0.2400
CG	0.5846	0.1750
CH	0.8054	0.2760
CK	0.8268	0.3190

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Chain	Atom inclusion	Q-score
CL	0.8288	0.2950
CM	0.8101	0.2900
CN	0.7413	0.3380
CU	0.9778	0.4570
CX	0.6042	0.2160
Cd	0.8280	0.2950
Cf	0.8018	0.2600
Cg	0.8603	0.2560
DC	0.8215	0.2960
DD	0.8006	0.3120
DF	0.8004	0.2370
DG	0.5665	0.1720
DH	0.7900	0.2790
DK	0.8101	0.3170
DL	0.8221	0.2850
DM	0.8225	0.2840
DN	0.8112	0.3340
DU	0.8667	0.4170
DX	0.6917	0.2460
Dd	0.8108	0.3070
Df	0.7677	0.2910
Dg	0.8419	0.2580
EC	0.8135	0.3010
ED	0.8034	0.3060
EF	0.7665	0.2310
EG	0.5673	0.1690
EH	0.7834	0.2780
EK	0.8364	0.3140
EL	0.8288	0.2990
EM	0.8355	0.2900
EN	0.8077	0.3250
EU	1.0000	0.4630
EX	0.5000	0.2210
Ed	0.8309	0.3090
Ef	0.8064	0.2840
Eg	0.8088	0.2370
FC	0.7653	0.2860
FD	0.8062	0.3090
FF	0.7792	0.2250
FG	0.5722	0.1640
FH	0.7885	0.2810
FK	0.8233	0.3110

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Chain	Atom inclusion	Q-score
FL	0.8184	0.2830
FM	0.8107	0.2900
FN	0.7920	0.3320
FU	0.8889	0.4460
FX	0.6833	0.2640
Fd	0.8223	0.3010
Ff	0.7631	0.2770
Fg	0.8199	0.2510
GC	0.7541	0.2760
GD	0.8071	0.3110
GF	0.7941	0.2330
GG	0.5493	0.1540
GH	0.7895	0.2720
GK	0.8285	0.3170
GL	0.8458	0.2970
GM	0.8063	0.2900
GN	0.7605	0.3230
GU	0.9778	0.4930
GX	0.7542	0.2280
Gd	0.8156	0.3040
Gf	0.7813	0.2770
Gg	0.8125	0.2400
HC	0.8190	0.2860
HD	0.7987	0.3110
HF	0.7558	0.2290
HG	0.5739	0.1470
HH	0.7900	0.2830
HK	0.8128	0.3070
HL	0.8354	0.2900
HM	0.8268	0.2810
HN	0.7430	0.3150
HU	0.9778	0.4660
HX	0.6333	0.2130
Hd	0.8338	0.3130
Hf	0.8087	0.2770
Hg	0.8235	0.2530
IC	0.8117	0.3000
ID	0.8127	0.3190
IF	0.7919	0.2090
IG	0.5887	0.1470
IH	0.7772	0.2780
IK	0.8198	0.3100

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Chain	Atom inclusion	Q-score
IL	0.8191	0.2860
IM	0.8038	0.2980
IN	0.8199	0.3340
IU	0.9333	0.4130
IX	0.5333	0.2020
Id	0.8357	0.3110
If	0.7768	0.2870
Ig	0.8382	0.2560
JC	0.8135	0.3040
JD	0.8006	0.3240
JF	0.7919	0.2260
JG	0.5468	0.1340
JH	0.7972	0.2810
JK	0.8023	0.3110
JL	0.8258	0.2990
JM	0.8156	0.2980
JN	0.7762	0.3380
JU	0.9556	0.4960
JX	0.5917	0.1790
Jd	0.8252	0.3120
Jf	0.7859	0.2530
Jg	0.8382	0.2630
KC	0.7722	0.2850
KD	0.8221	0.3120
KF	0.7558	0.2180
KG	0.5583	0.1490
KH	0.8070	0.2800
KK	0.8136	0.3140
KL	0.8073	0.2920
KM	0.8057	0.2860
KN	0.7500	0.3350
KU	0.9556	0.4320
KX	0.6000	0.2380
Kd	0.8396	0.3020
Kf	0.8223	0.2720
Kg	0.8419	0.2560
LC	0.8153	0.2930
LD	0.8184	0.3060
LF	0.8089	0.2360
LG	0.6232	0.1850
LH	0.7906	0.2780
LK	0.8285	0.3050

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Chain	Atom inclusion	Q-score
LL	0.8362	0.2980
LM	0.8293	0.2920
LN	0.7920	0.3200
LU	0.9778	0.4390
LX	0.5708	0.2220
Ld	0.8136	0.2990
Lf	0.8178	0.2670
Lg	0.8382	0.2540
MC	0.8258	0.3020
MD	0.8240	0.3130
MF	0.7622	0.2100
MG	0.6429	0.2100
MH	0.7803	0.2660
MK	0.8154	0.3140
ML	0.8480	0.2960
MM	0.8181	0.2790
MN	0.8042	0.3250
MU	0.9556	0.4300
MX	0.7208	0.2410
Md	0.8453	0.3040
Mf	0.7517	0.2790
Mg	0.8088	0.2370
NG	0.6149	0.1880
OG	0.6429	0.2060
PG	0.6461	0.1920
VF	0.7877	0.2260
VG	0.8272	0.2320
VH	0.6908	0.2720
VX	0.5583	0.2250
WF	0.7580	0.2210
WG	0.7941	0.2310
WH	0.6337	0.2520
WX	0.6042	0.2630
XF	0.7325	0.2210
XG	0.8382	0.2520
XH	0.5364	0.2570
XX	0.7583	0.2450
YF	0.7877	0.2220
YG	0.8125	0.2310
YH	0.6783	0.2530
YX	0.6875	0.2570
ZF	0.7452	0.2220

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Chain	Atom inclusion	Q-score
ZG	0.8309	0.2490
ZH	0.5511	0.2250
ZX	0.6000	0.2180