Full wwPDB EM Validation Report

Nov 20, 2022 – 01:15 AM EST

PDB ID	:	7MUE
EMDB ID	:	EMD-24006
Title	:	Legionella pneumophila Dot/Icm T4SS PR
Authors	:	Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.
Deposited on	:	2021-05-14
Resolution	:	2.80 Å(reported)

This is a Full wwPDB EM Validation 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:

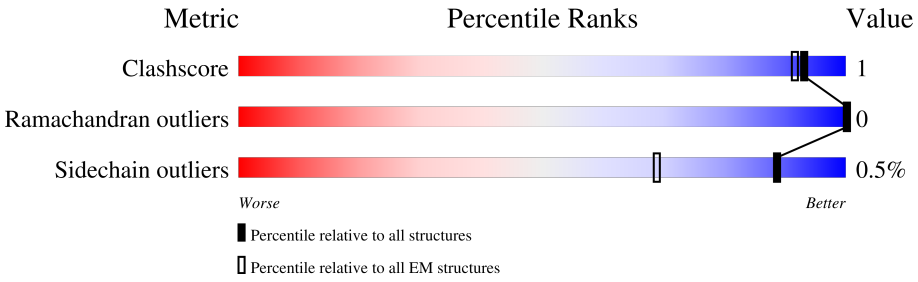
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	AF	269	22% · 77%
1	BF	269	21% · 77%
1	CF	269	22% · 77%
1	DF	269	22% · 77%
1	EF	269	22% · 77%
1	FF	269	22% · 77%
1	GF	269	22% · 77%
1	HF	269	21% · 77%
1	IF	269	22% · 77%

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Mol	Chain	Length	Quality of chain
1	JF	269	22% 77%
1	KF	269	23% 77%
1	LF	269	22% 77%
1	MF	269	22% 77%
1	VF	269	23% 77%
1	WF	269	22% 77%
1	XF	269	21% 77%
1	YF	269	22% 77%
1	ZF	269	23% 77%
2	AH	361	41% 56%
2	BH	361	42% 56%
2	CH	361	42% 56%
2	DH	361	42% 56%
2	EH	361	42% 56%
2	FH	361	42% 56%
2	GH	361	43% 56%
2	HH	361	42% 56%
2	IH	361	42% 56%
2	JH	361	43% 56%
2	KH	361	43% 56%
2	LH	361	42% 56%
2	MH	361	42% 56%
2	VH	361	43% 56%
2	WH	361	42% 56%
2	XH	361	43% 56%

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Mol	Chain	Length	Quality of chain
2	YH	361	42% 56%
2	ZH	361	42% 56%
3	AX	48	100%
3	BX	48	100%
3	CX	48	100%
3	DX	48	100%
3	EX	48	100%
3	FX	48	100%
3	GX	48	100%
3	HX	48	100%
3	IX	48	100%
3	JX	48	100%
3	KX	48	100%
3	LX	48	100%
3	MX	48	100%
3	VX	48	100%
3	WX	48	100%
3	XX	48	100%
3	YX	48	100%
3	ZX	48	100%
4	AG	1048	97%
4	BG	1048	97%
4	CG	1048	97%
4	DG	1048	97%
4	EG	1048	97%

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Mol	Chain	Length	Quality of chain
4	FG	1048	97%
4	GG	1048	97%
4	HG	1048	97%
4	IG	1048	97%
4	JG	1048	97%
4	KG	1048	97%
4	LG	1048	97%
4	MG	1048	97%
4	VG	1048	97%
4	WG	1048	97%
4	XG	1048	97%
4	YG	1048	97%
4	ZG	1048	97%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 40266 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 DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	BF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	CF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	DF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	EF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	FF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	GF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	HF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	IF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	JF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	KF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	LF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	MF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	VF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	WF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	XF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
1	YF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		

- Molecule 2 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	XH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	YH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	ZH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	AH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	BH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	CH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	DH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	EH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	FH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	GH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	HH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	IH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	JH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	KH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	LH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	MH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	VH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
2	WH	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		

- Molecule 3 is a protein called Unknown protein fragment.

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

- Molecule 4 is a protein called IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	IG	34	Total 276	C 168	N 47	O 60	S 1	0	0

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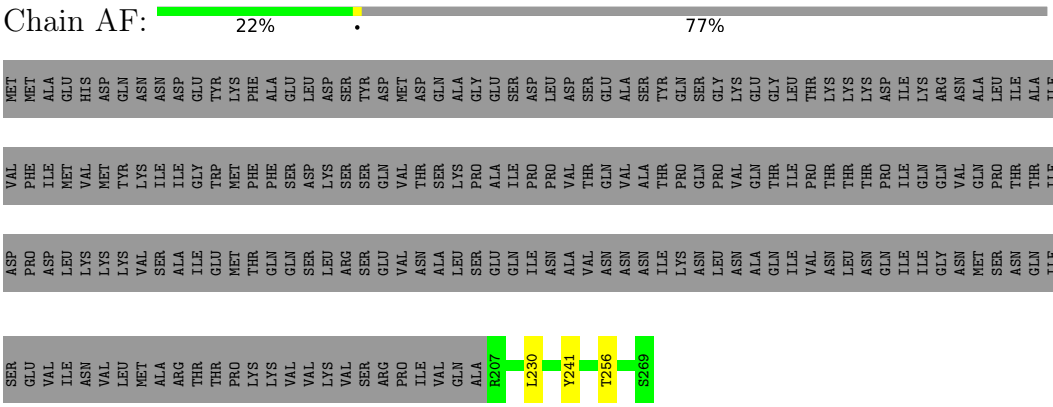
Mol	Chain	Residues	Atoms					AltConf	Trace
4	AG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	BG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	CG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	DG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	EG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	FG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	GG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	HG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	JG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	KG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	LG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	MG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	VG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	WG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	XG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	YG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
4	ZG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

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. 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. 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.

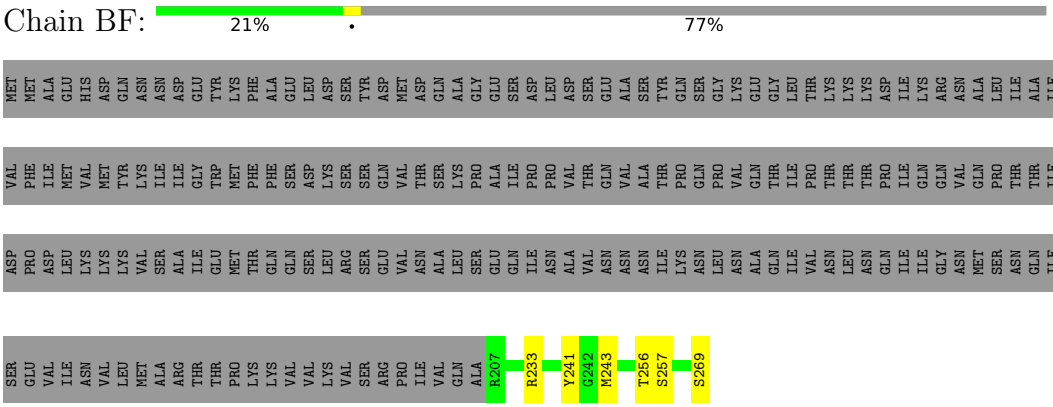
- Molecule 1: DotF

Chain AF:



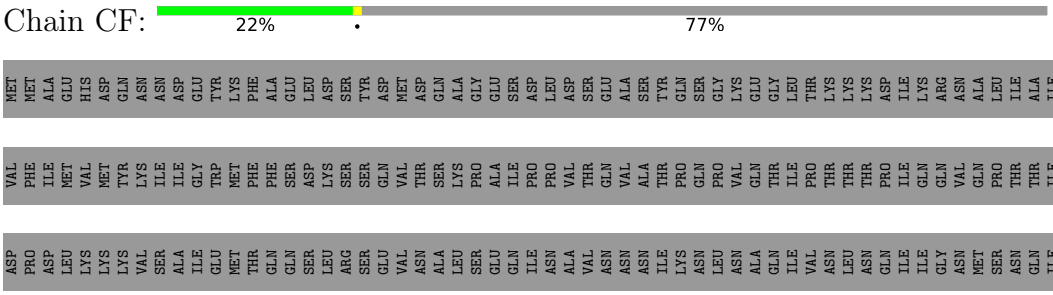
- Molecule 1: DotF

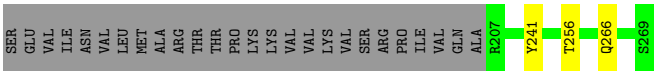
Chain BF:



- Molecule 1: DotF

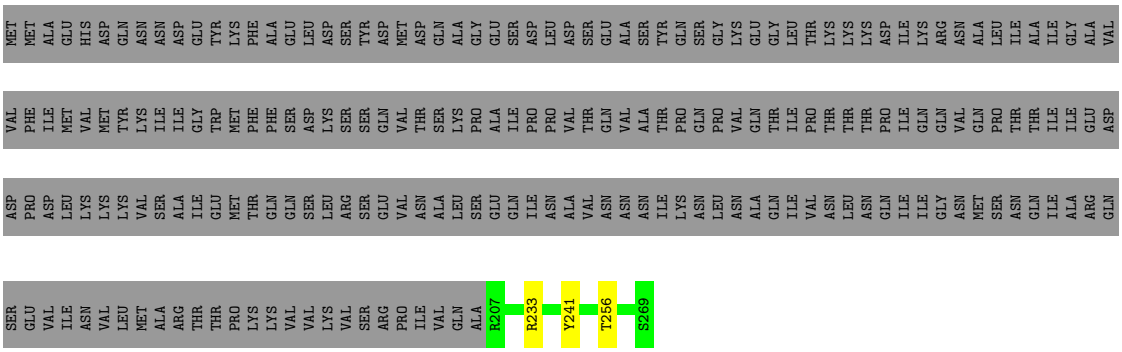
Chain CF:





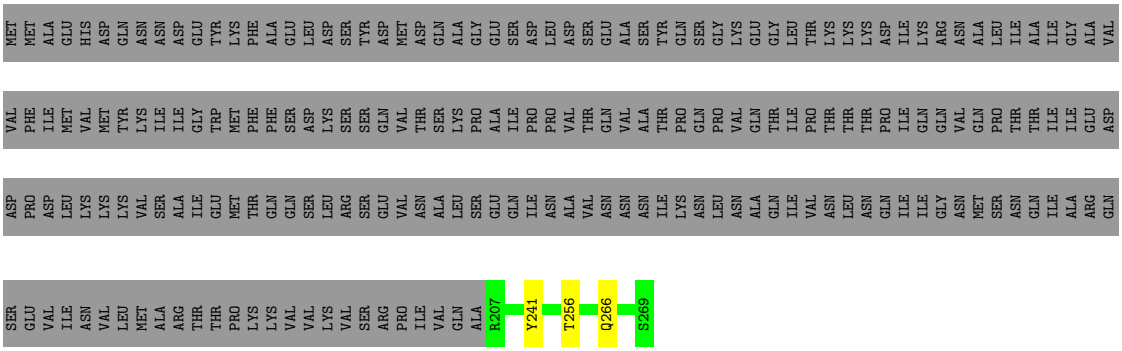
• Molecule 1: DotF

Chain DF:



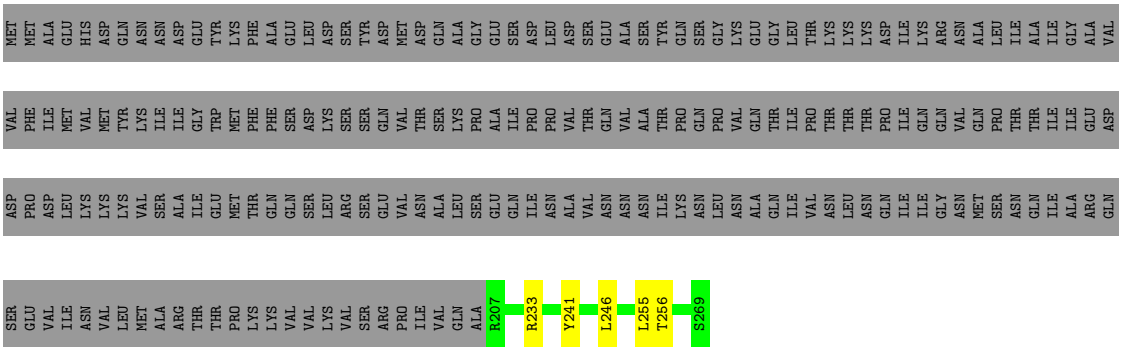
• Molecule 1: DotF

Chain EF:



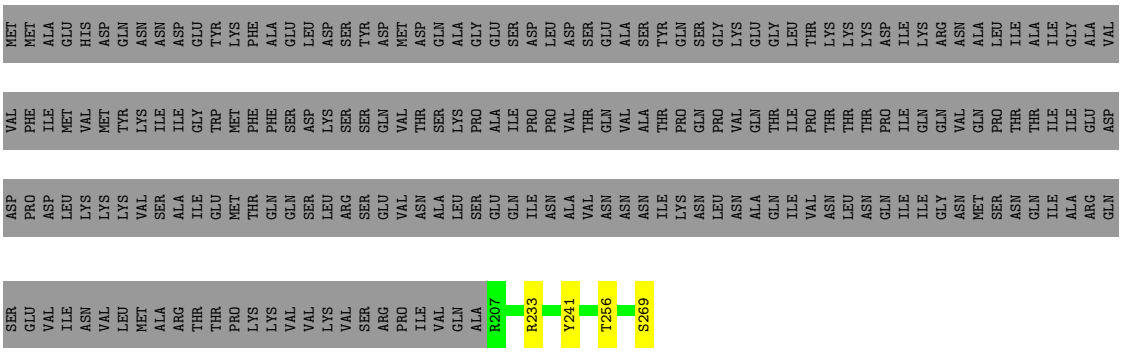
• Molecule 1: DotF

Chain FF:



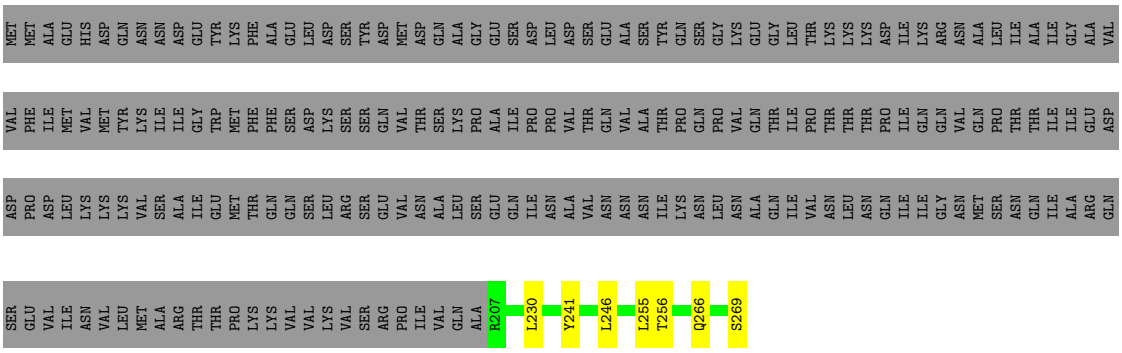
• Molecule 1: DotF

Chain GF:



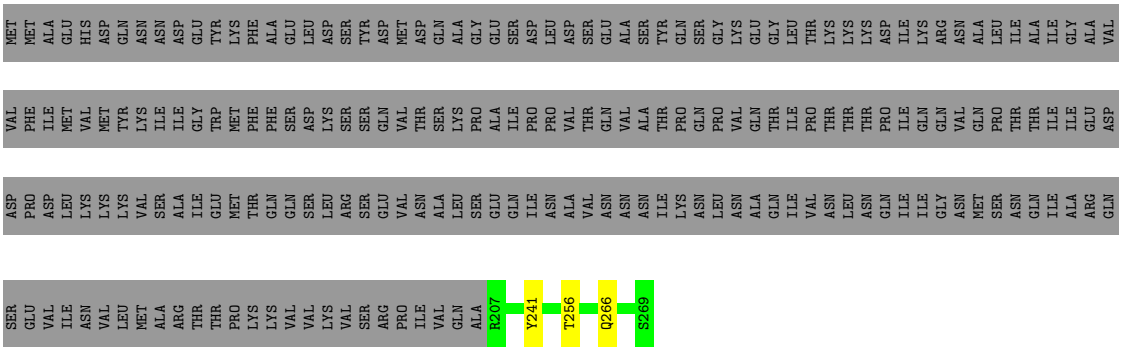
• Molecule 1: DotF

Chain HF: 21% 77%



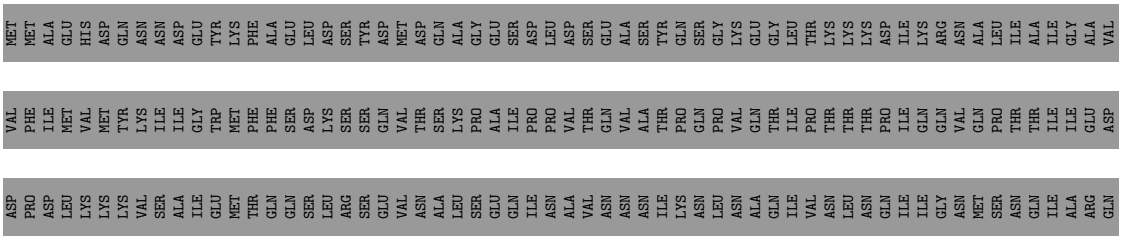
• Molecule 1: DotF

Chain IF: 22% 77%



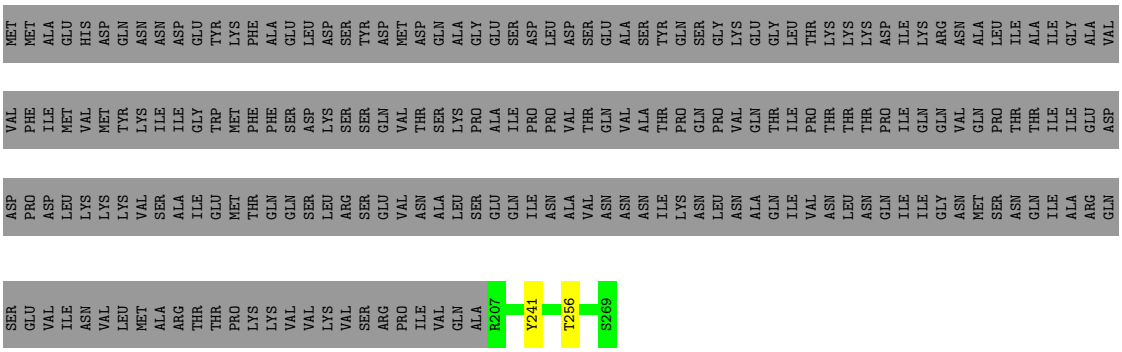
• Molecule 1: DotF

Chain JF: 22% 77%



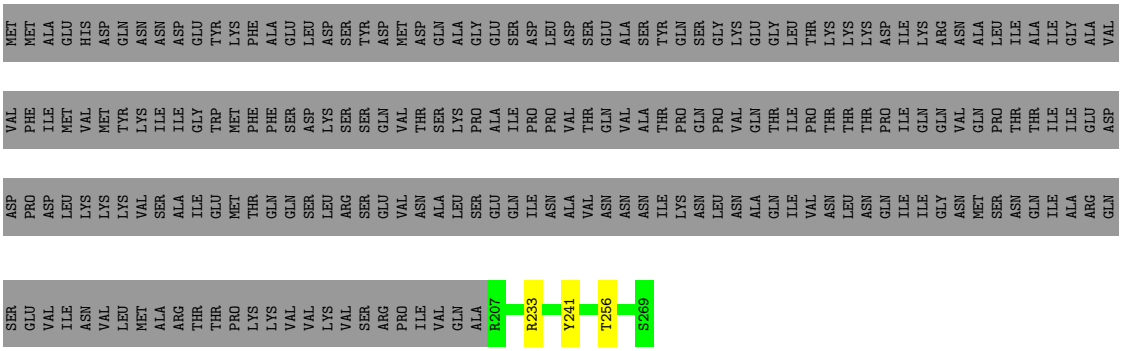
• Molecule 1: DotF

Chain KF:



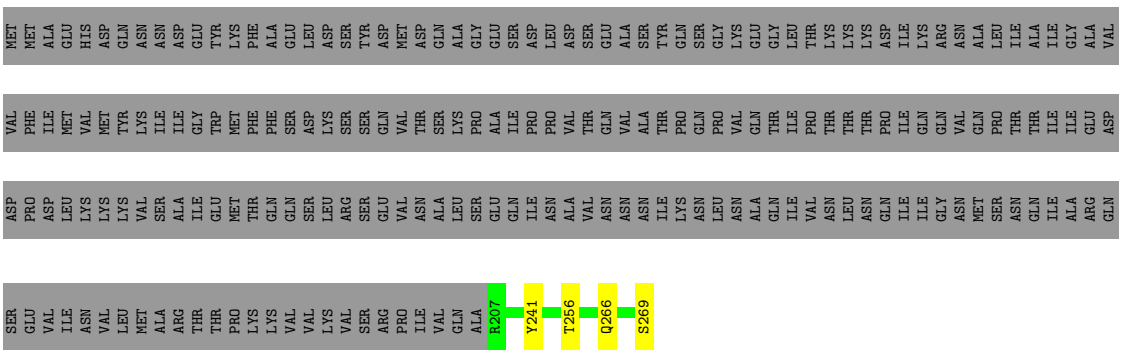
• Molecule 1: DotF

Chain LF:



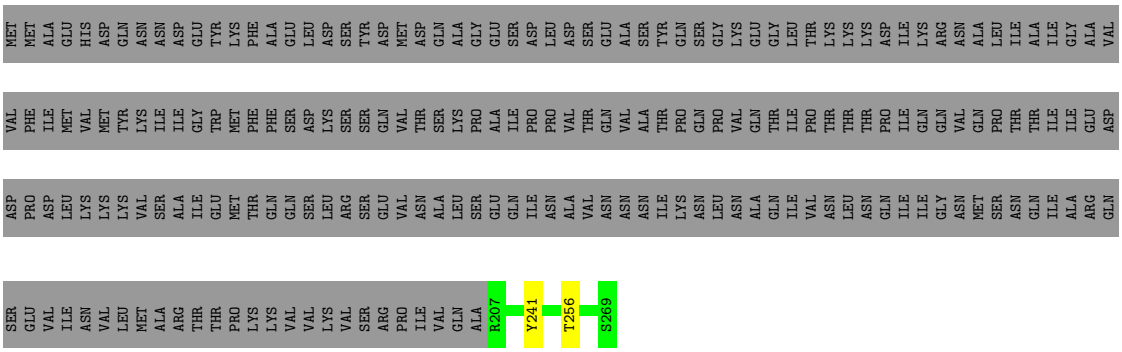
• Molecule 1: DotF

Chain MF:



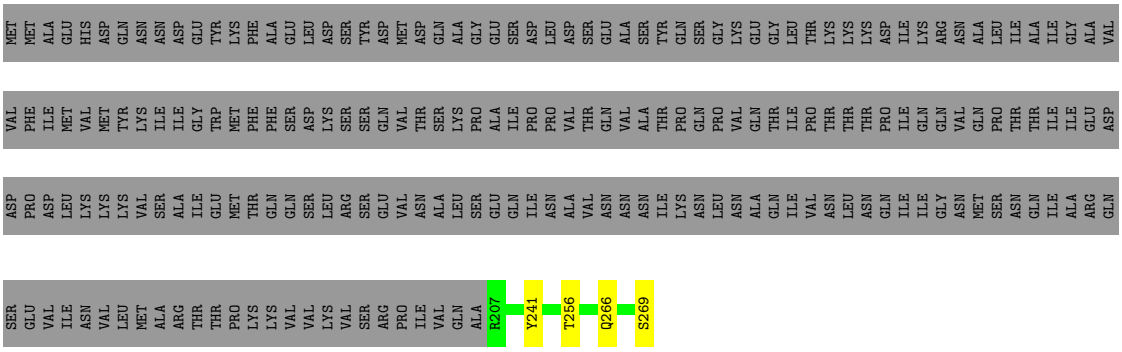
• Molecule 1: DotF

Chain VF:



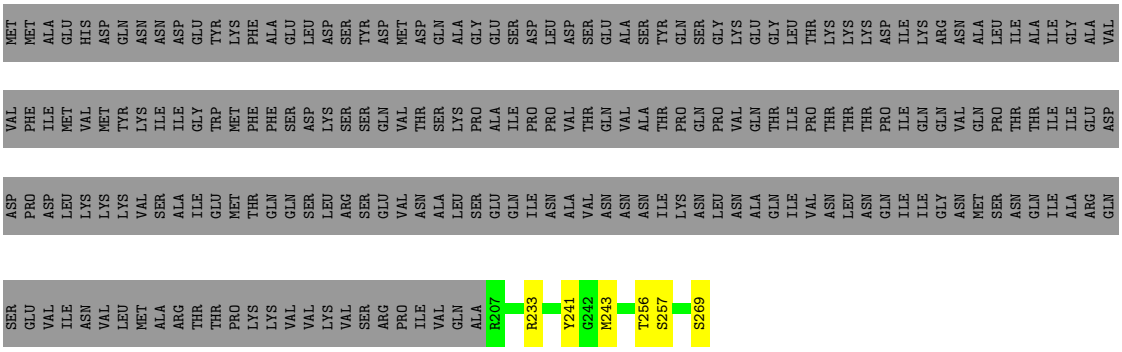
• Molecule 1: DotF

Chain WF:



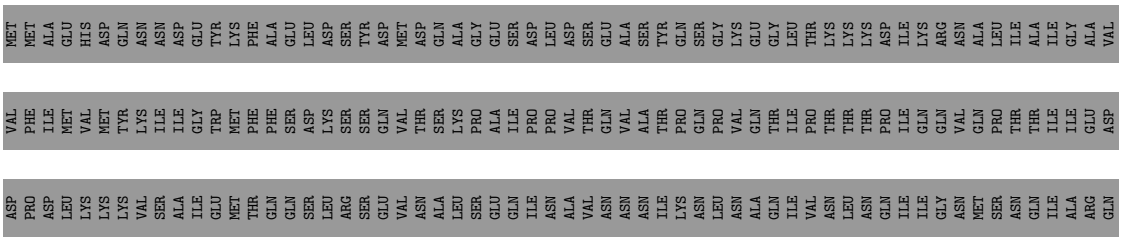
• Molecule 1: DotF

Chain XF:



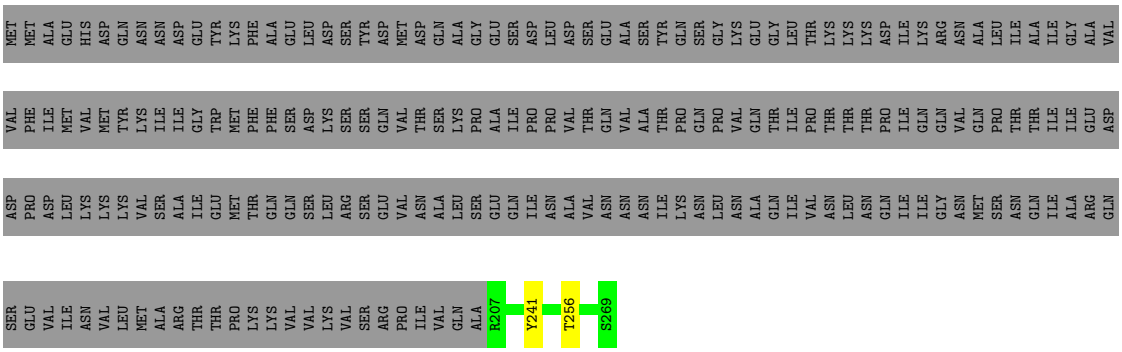
• Molecule 1: DotF

Chain YF:



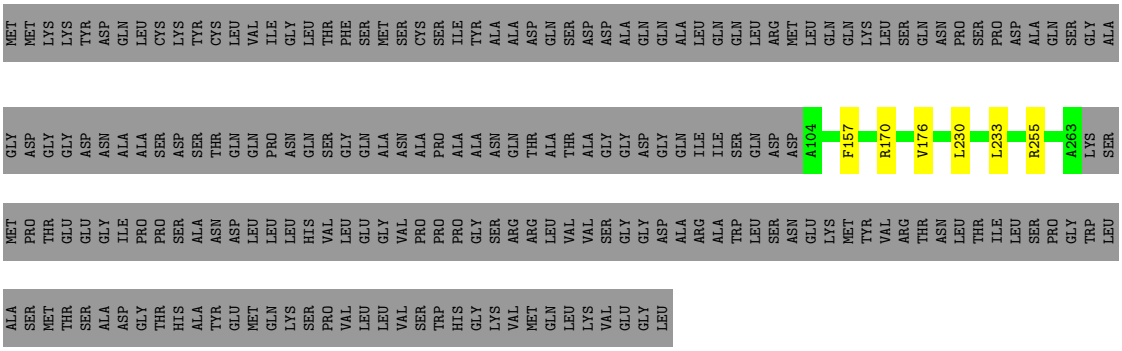
• Molecule 1: DotF

Chain ZF:



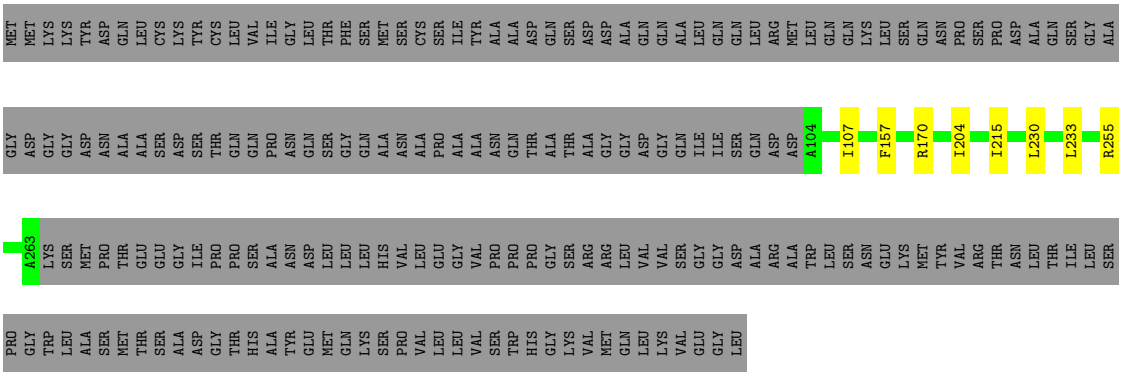
• Molecule 2: Type IV secretion protein IcmK

Chain XH:



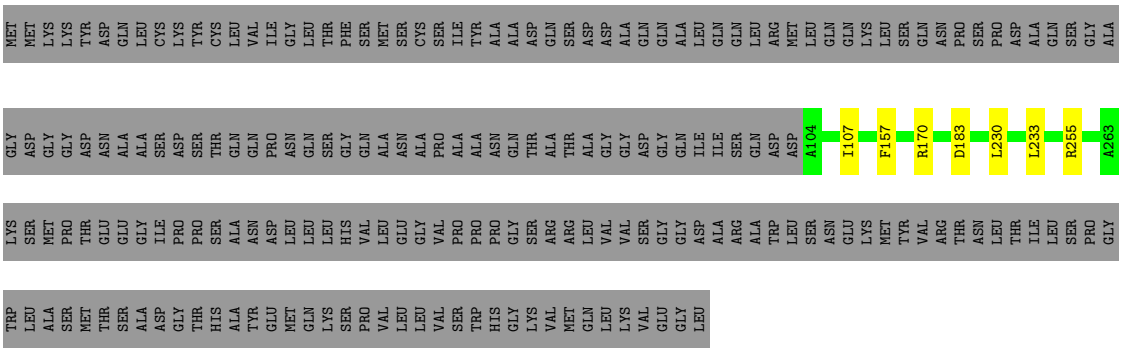
• Molecule 2: Type IV secretion protein IcmK

Chain YH:



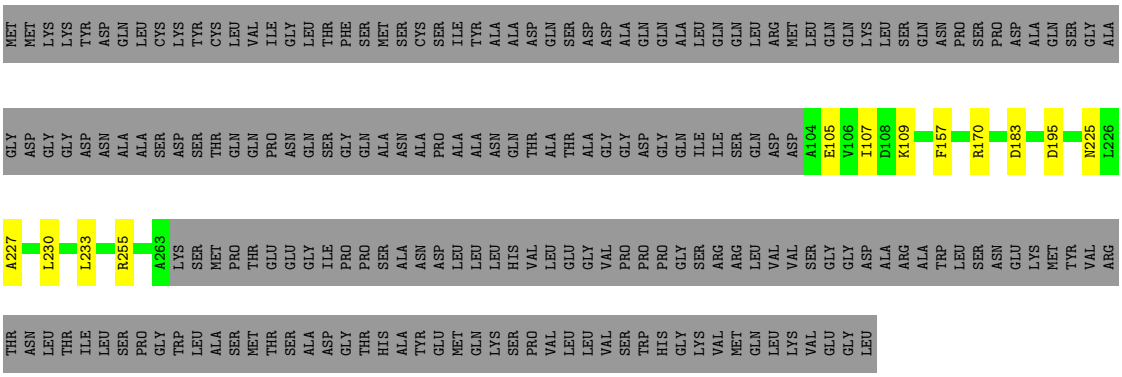
• Molecule 2: Type IV secretion protein IcmK

Chain ZH:



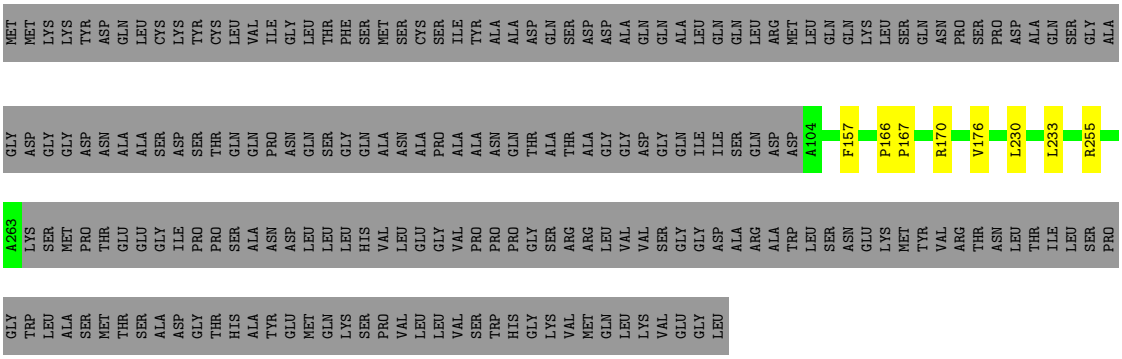
• Molecule 2: Type IV secretion protein IcmK

Chain AH:



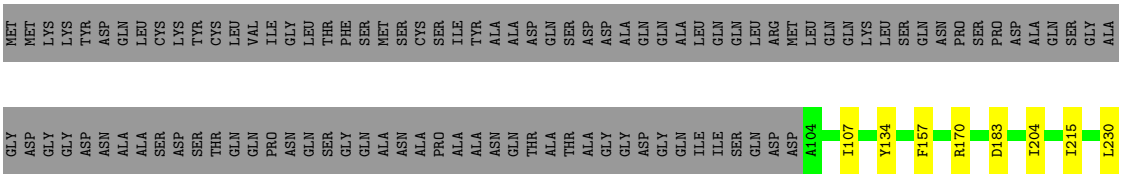
• Molecule 2: Type IV secretion protein IcmK

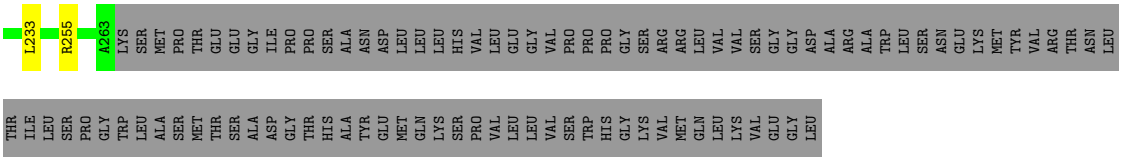
Chain BH:



• Molecule 2: Type IV secretion protein IcmK

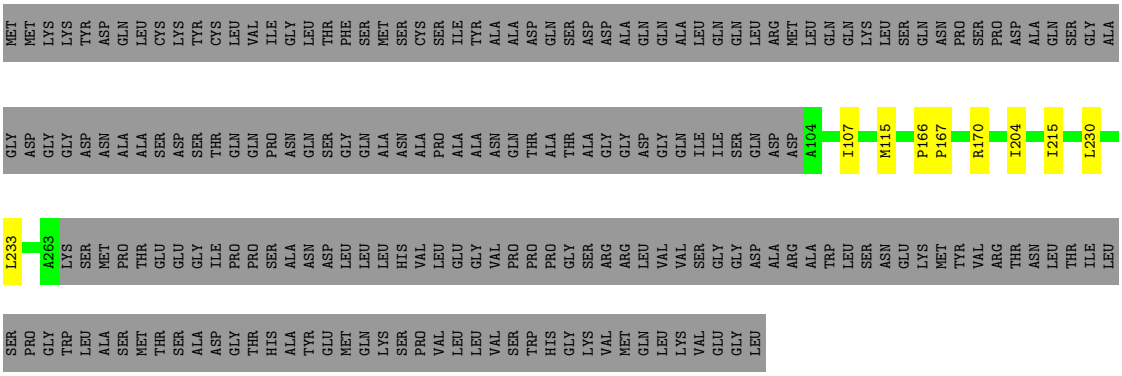
Chain CH:





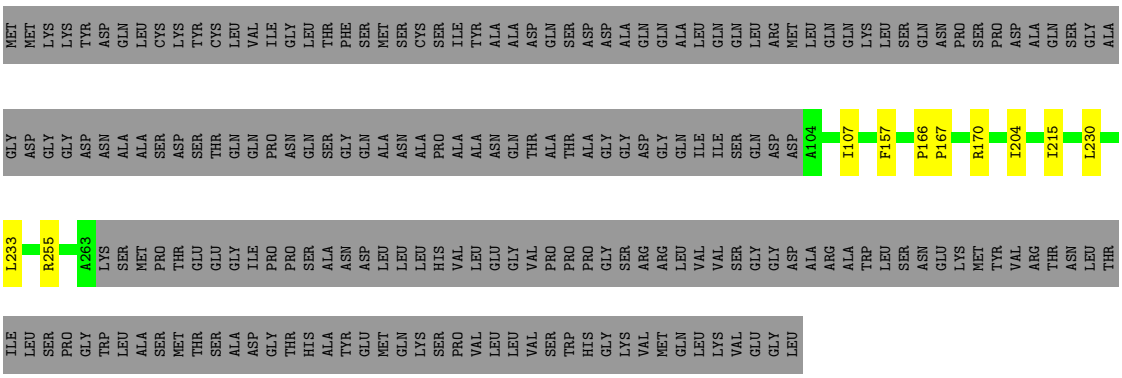
• Molecule 2: Type IV secretion protein IcmK

Chain DH:



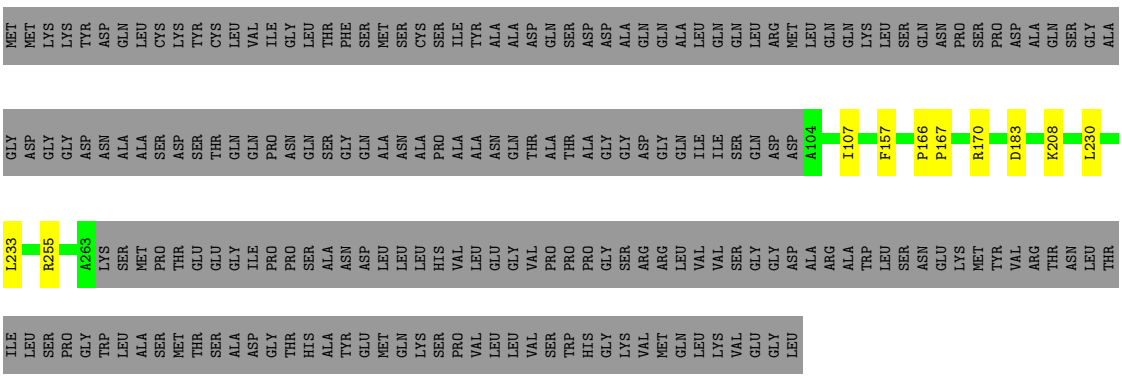
• Molecule 2: Type IV secretion protein IcmK

Chain EH:



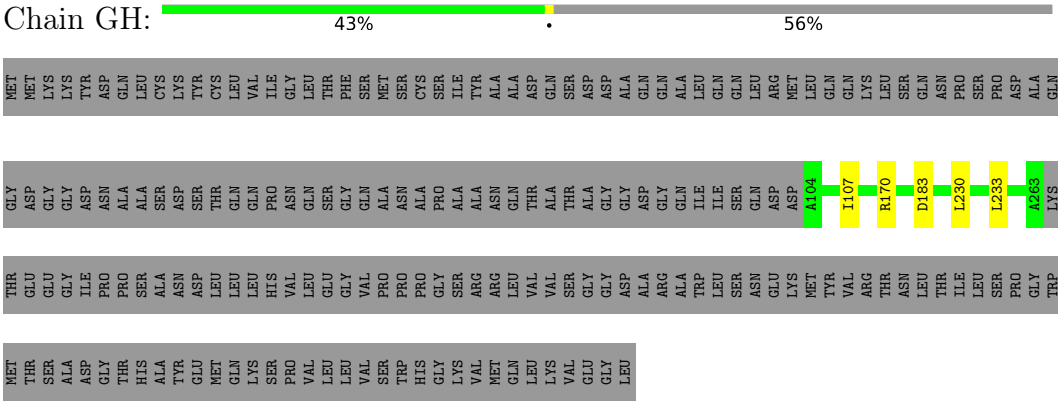
• Molecule 2: Type IV secretion protein IcmK

Chain FH:



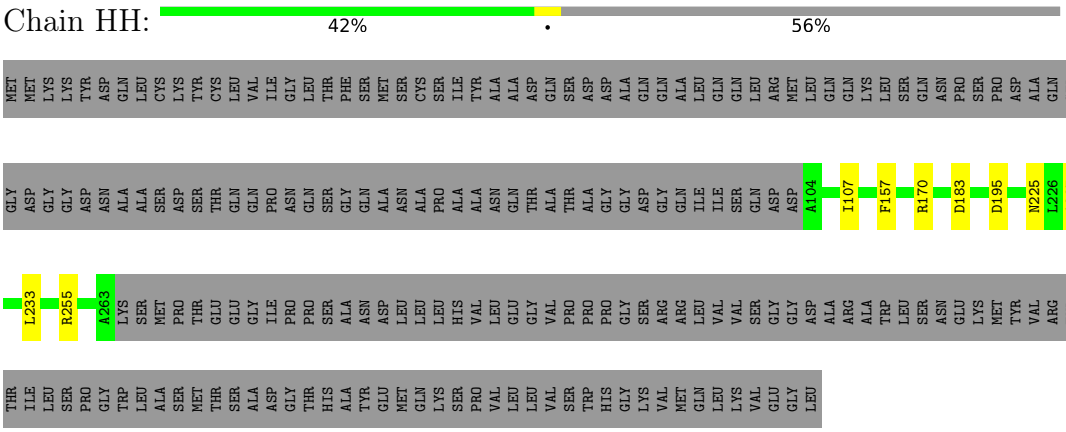
• Molecule 2: Type IV secretion protein IcmK

Chain GH:



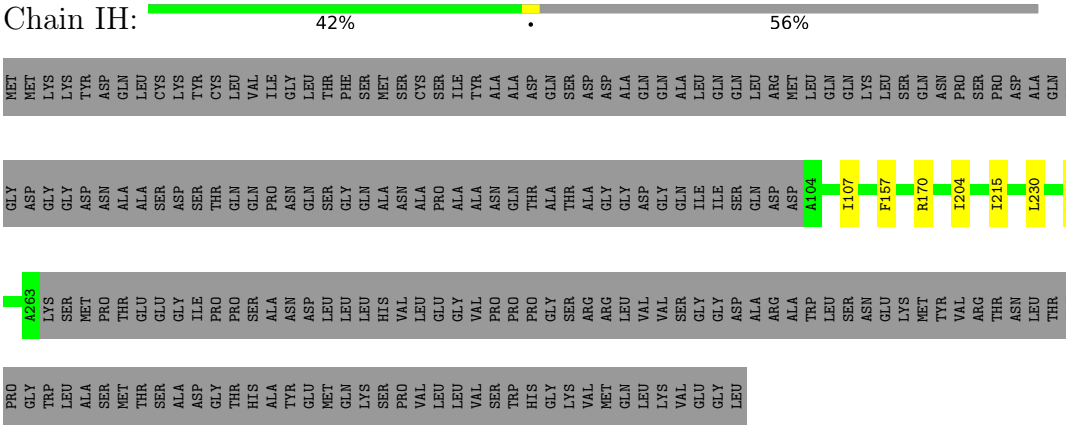
• Molecule 2: Type IV secretion protein IcmK

Chain HH:



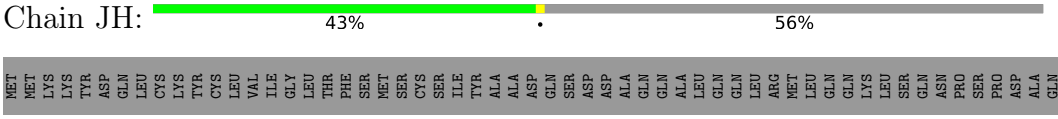
• Molecule 2: Type IV secretion protein IcmK

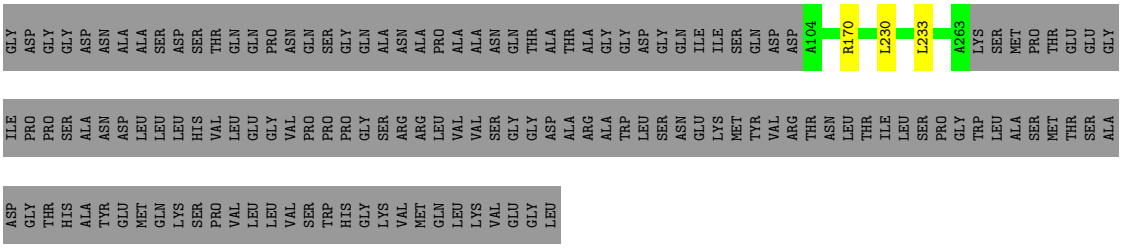
Chain IH:



• Molecule 2: Type IV secretion protein IcmK

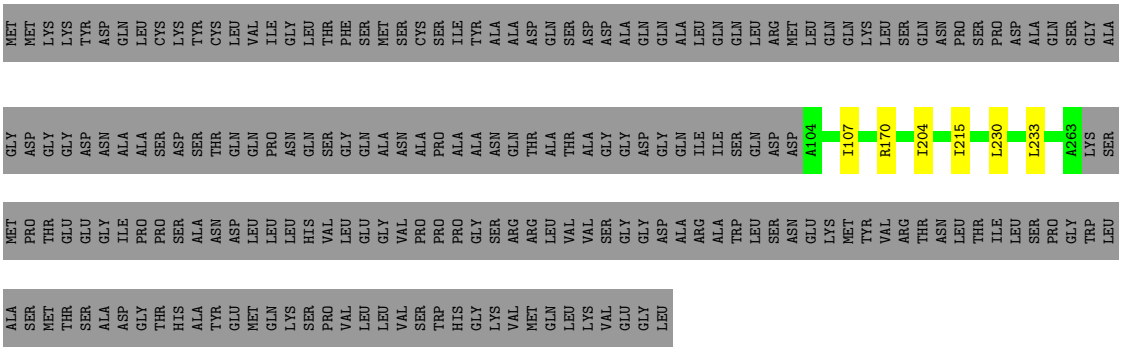
Chain JH:





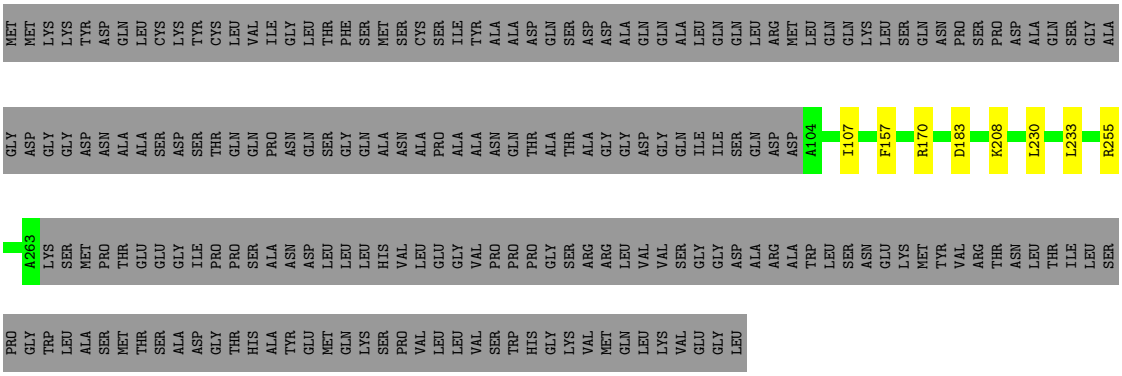
• Molecule 2: Type IV secretion protein IcmK

Chain KH:



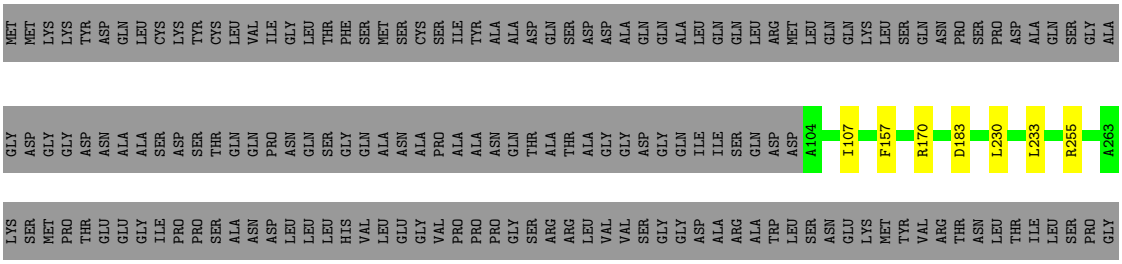
• Molecule 2: Type IV secretion protein IcmK

Chain LH:



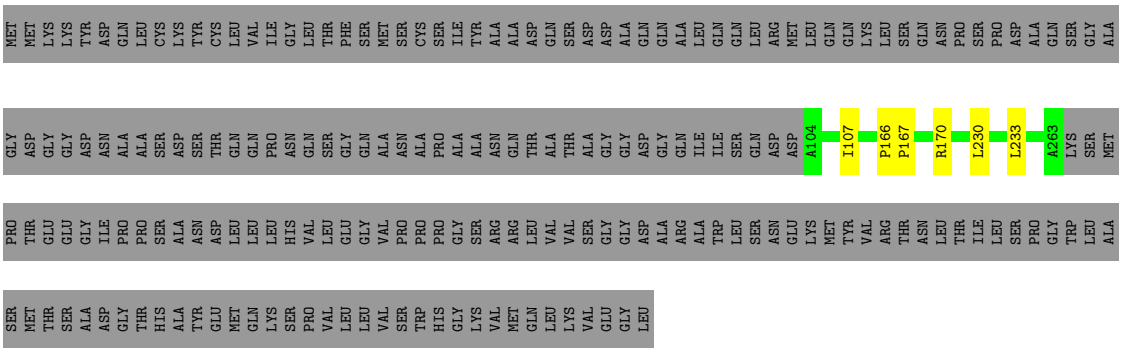
• Molecule 2: Type IV secretion protein IcmK

Chain MH:



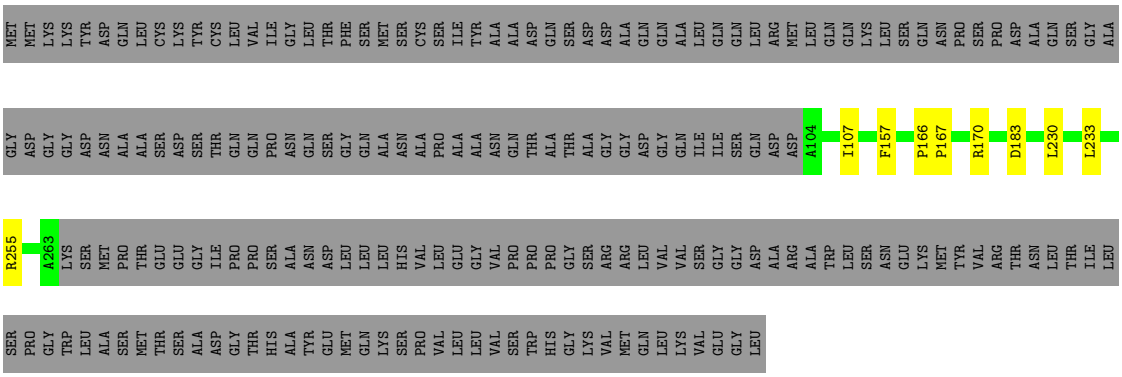
• Molecule 2: Type IV secretion protein IcmK

Chain VH:



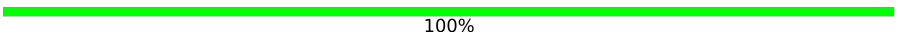
• Molecule 2: Type IV secretion protein IcmK

Chain WH:



• Molecule 3: Unknown protein fragment

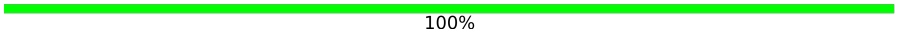
Chain AX:



There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

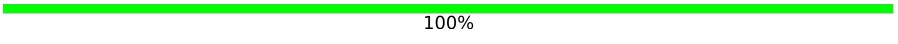
Chain BX:



There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain CX:



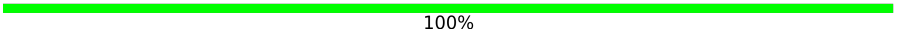
There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain DX: 

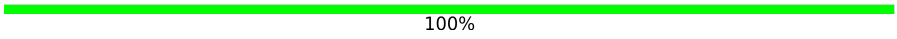
There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain EX: 

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain FX: 

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain GX: 

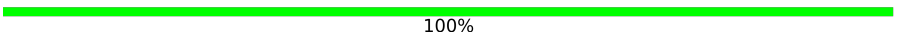
There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain HX: 

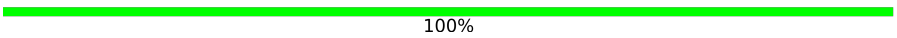
There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain IX: 

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain JX: 

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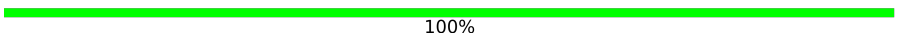
• Molecule 3: Unknown protein fragment

Chain KX: 

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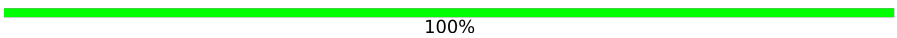
• Molecule 3: Unknown protein fragment

Chain LX: 

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain MX: 100%

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain VX: 100%

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain WX: 100%

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain XX: 100%

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain YX: 100%

There are no outlier residues recorded for this chain.

• Molecule 3: Unknown protein fragment

Chain ZX: 100%

There are no outlier residues recorded for this chain.

• Molecule 4: IcmE protein

Chain IG: 97%

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

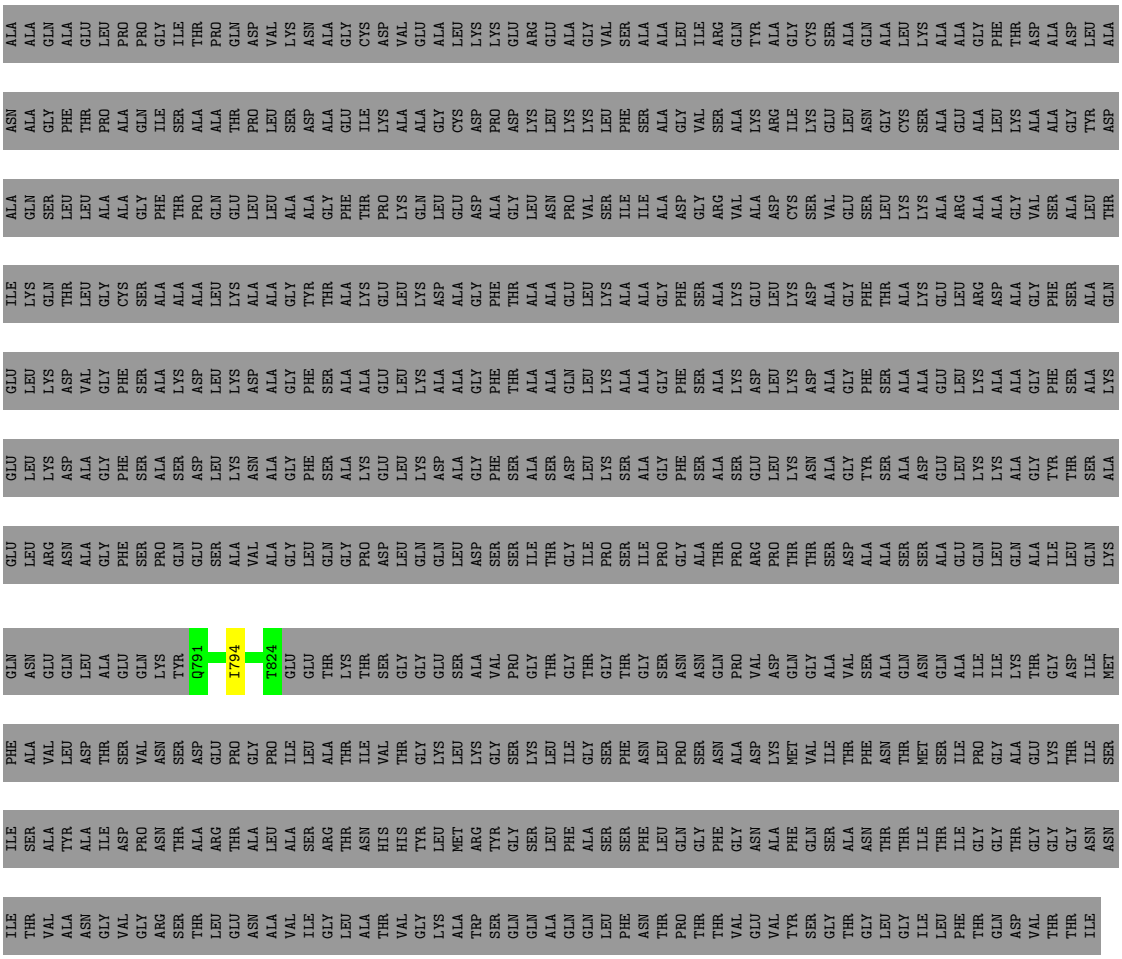
SER ILE PRO GLY VAL LEU ASP PRO THR ALA GLN TYR ALA LYS LEU GLN GLU GLU GLN ASN ILE THR GLN ALA GLN VAL ALA GLU LYS THR GLY GLY SER ALA ILE PRO THR ILE ILE ARG THR GLN ALA LEU GLY GLU GLY VAL GLY VAL ILE GLY SER GLN SER GLY VAL GLY PHE ALA

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

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

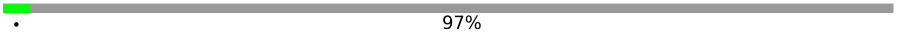
LYS GLY ALA GLY PHE SER ASP ALA GLU ILE ALA LYS ALA SER GLY LEU PRO ASP GLY ILE THR ALA ASP ASP VAL ARG LYS ALA GLY CYS GLY ALA ALA ALA LEU ALA LYS LEU ARG GLN ALA GLY VAL SER ALA SER ALA ILE ARG LYS ILE SER GLY CYS THR ALA GLU GLN LEU LYS

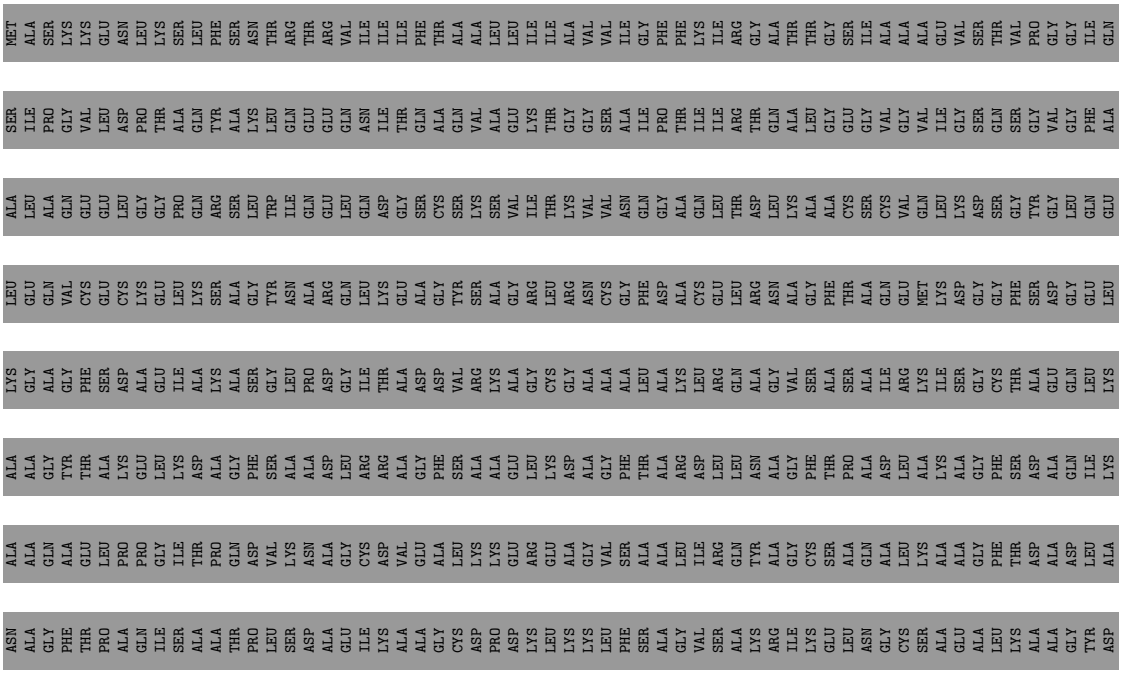
ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA ASP LEU ARG ARG ALA GLY PHE SER ALA GLU LEU LYS ASP ALA GLY PHE THR ALA ARG ASP LEU LEU ASN ALA GLY PHE THR PRO ALA ASP LEU ALA LYS ALA GLY PHE SER ASP ALA GLN ILE LYS

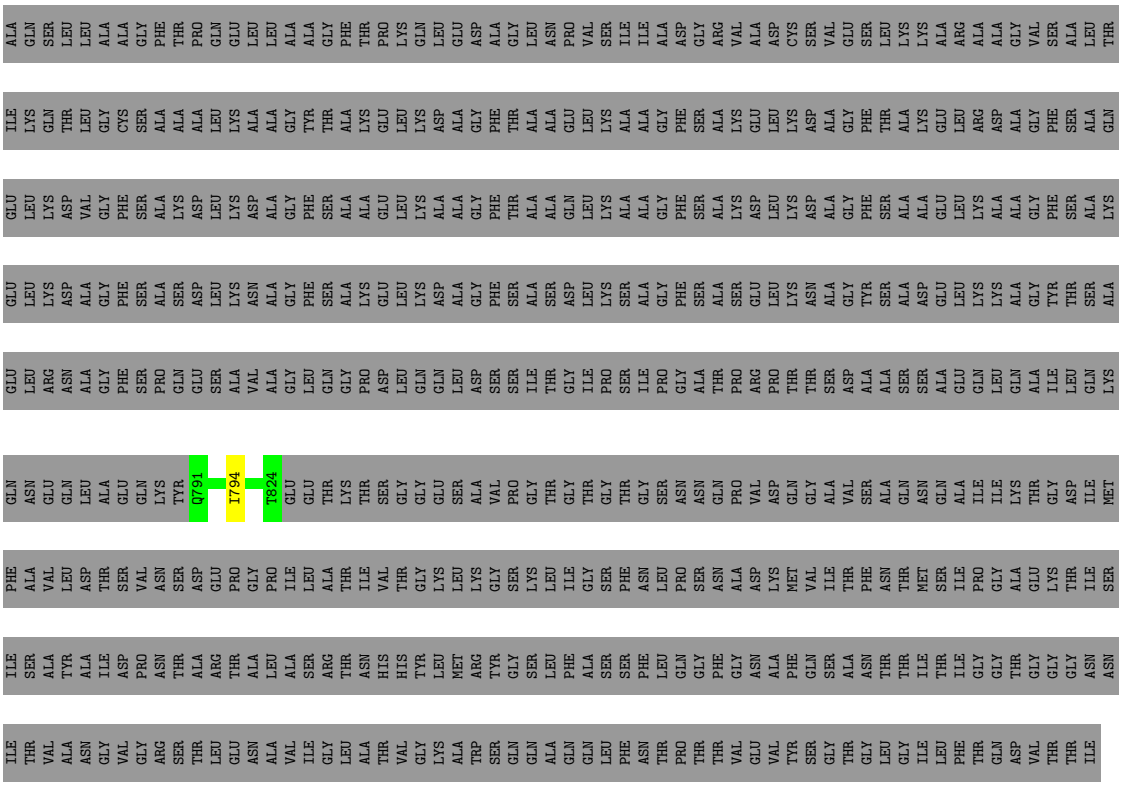


• Molecule 4: IcmE protein

Chain AG:

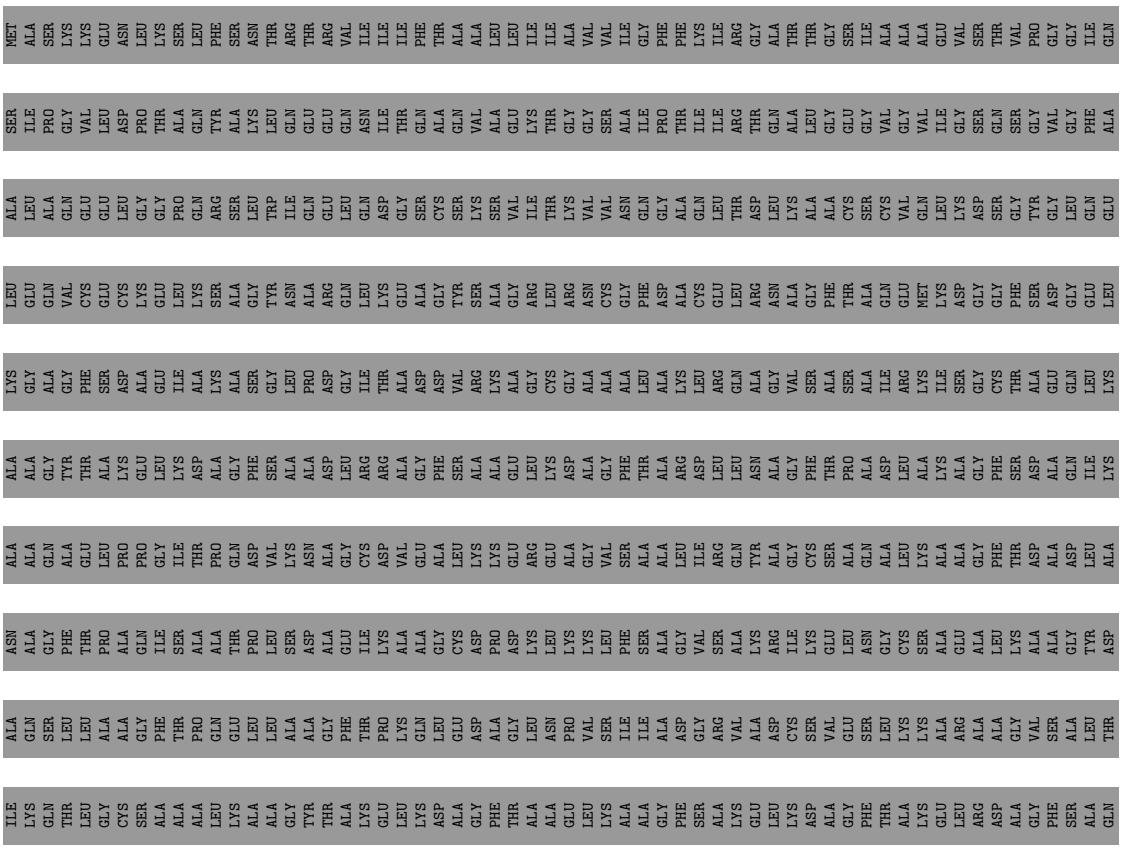






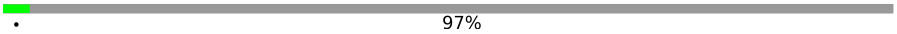
• Molecule 4: IcmE protein

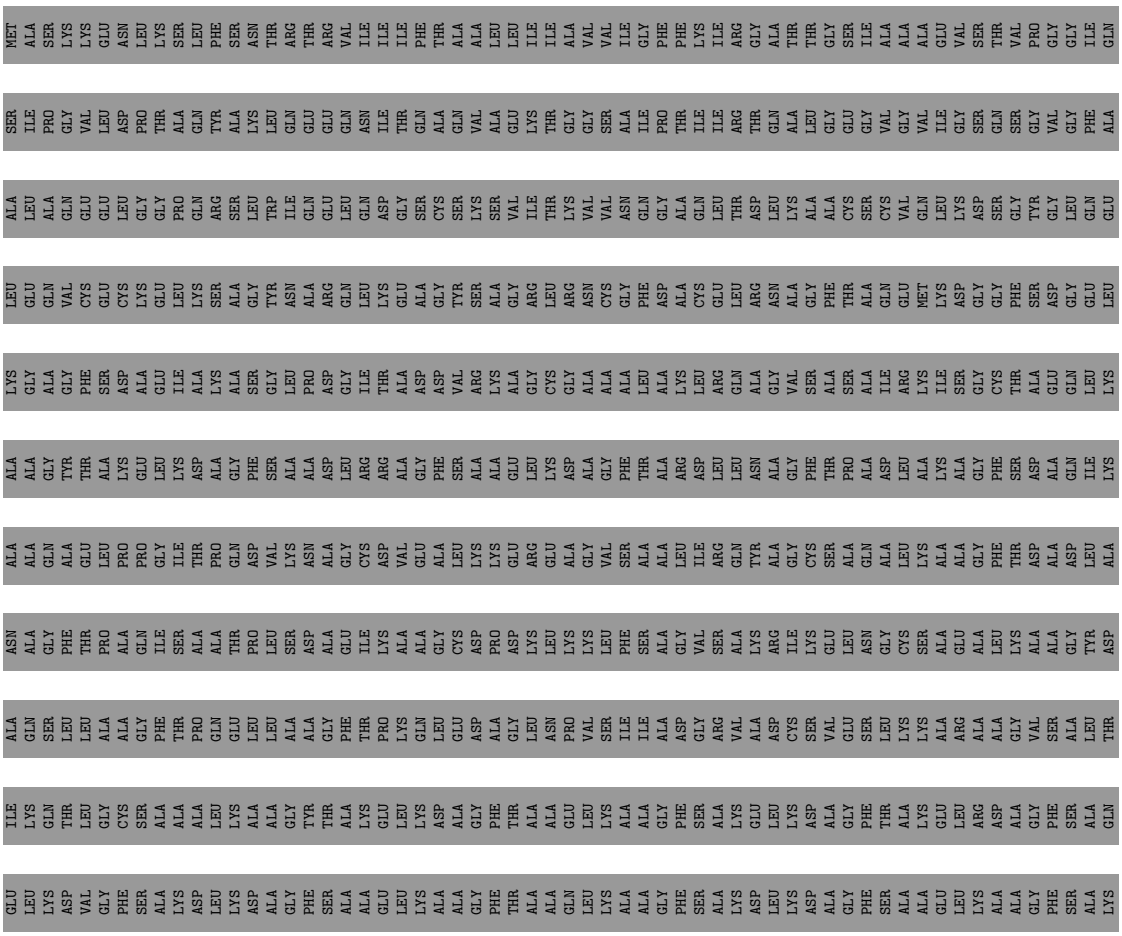
Chain BG:

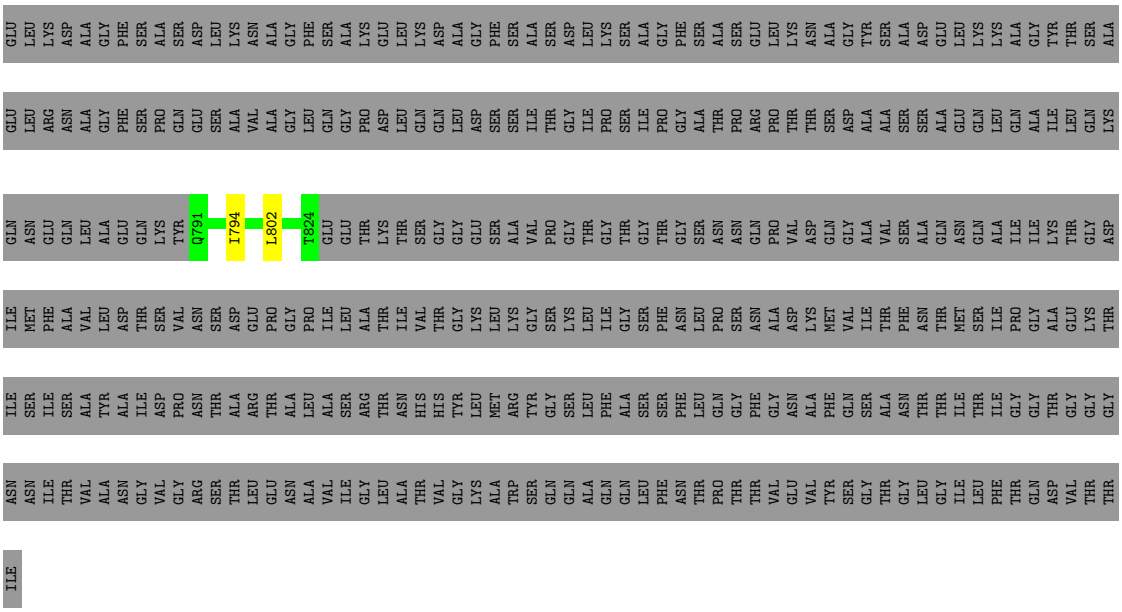


• Molecule 4: IcmE protein

Chain CG:

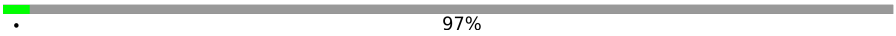


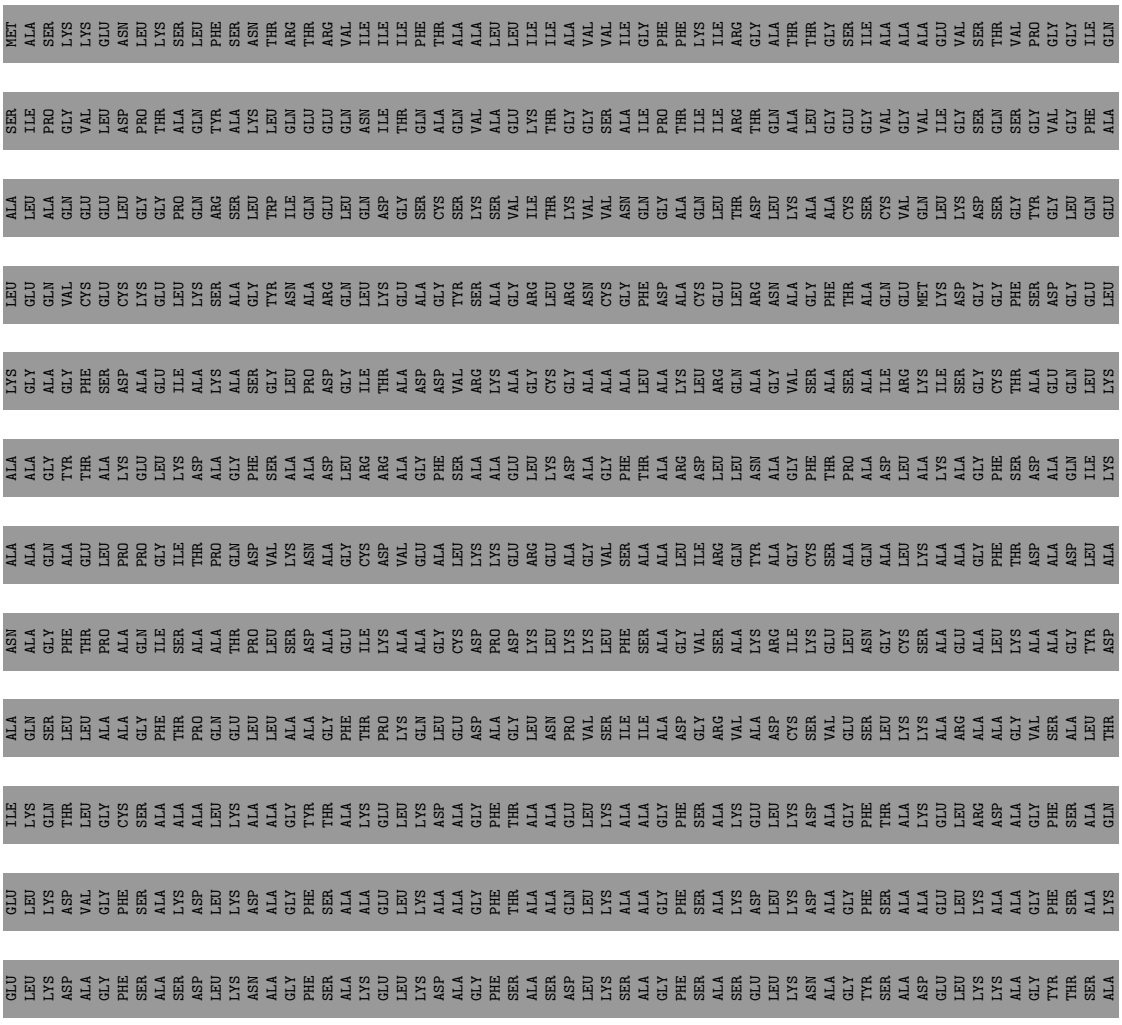


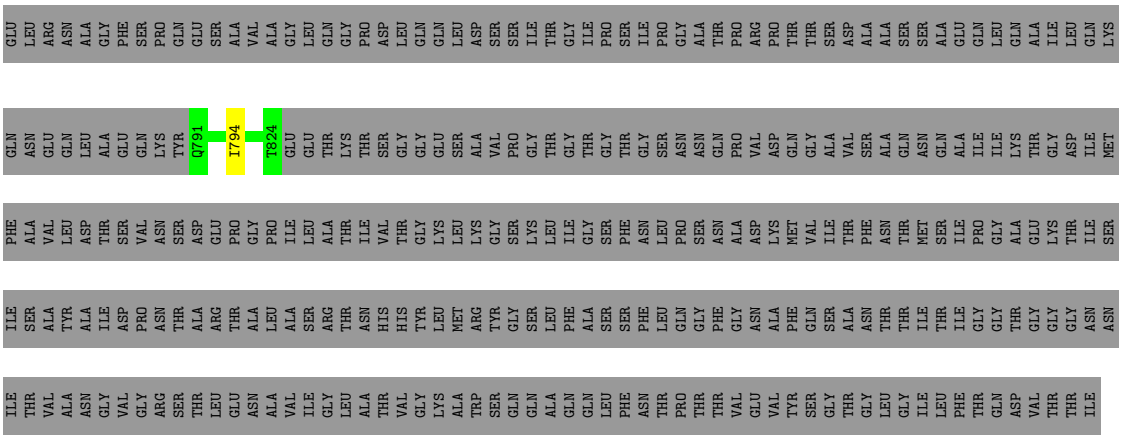


• Molecule 4: IcmE protein

Chain DG:

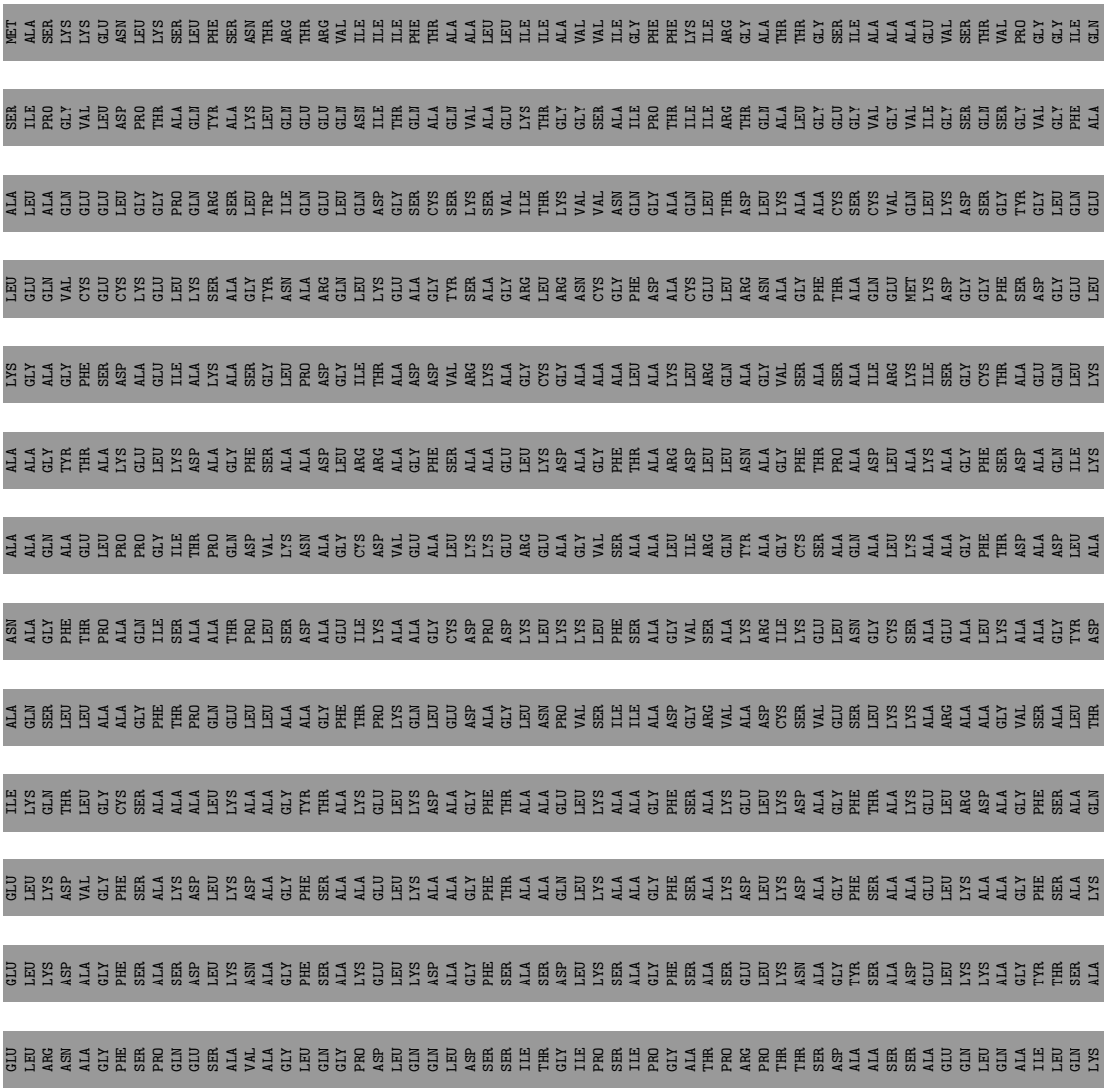


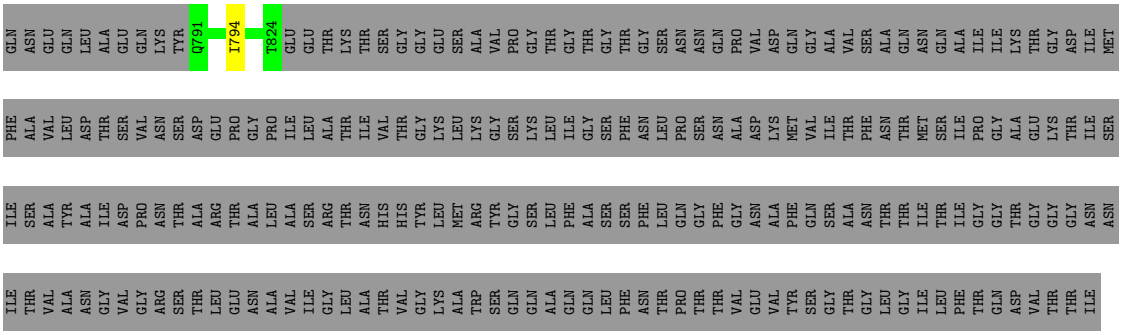




• Molecule 4: IcmE protein

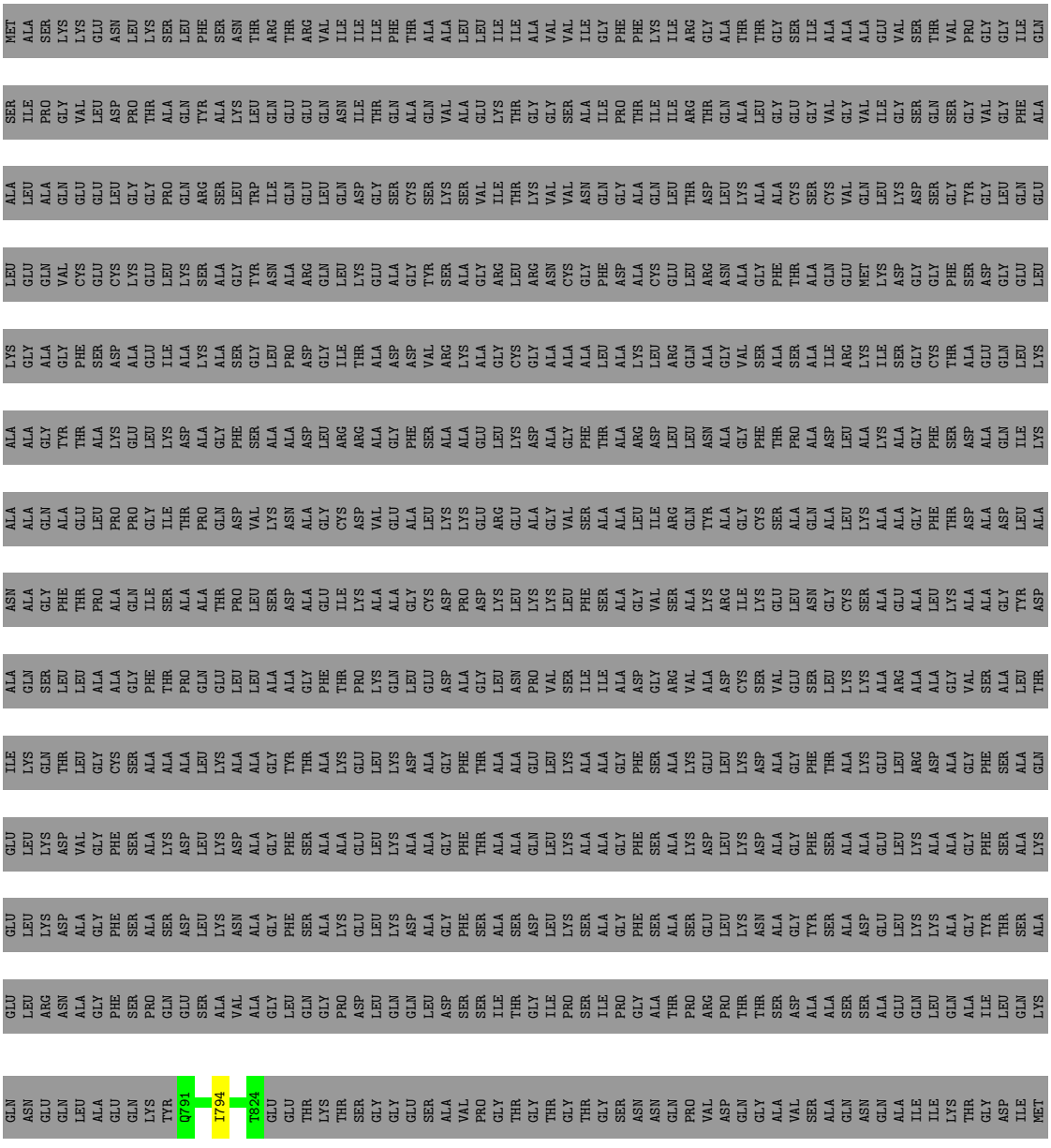
Chain EG: 97%

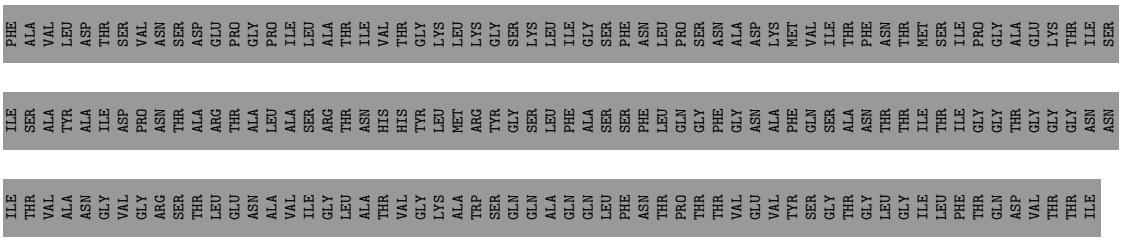




• Molecule 4: IcmE protein

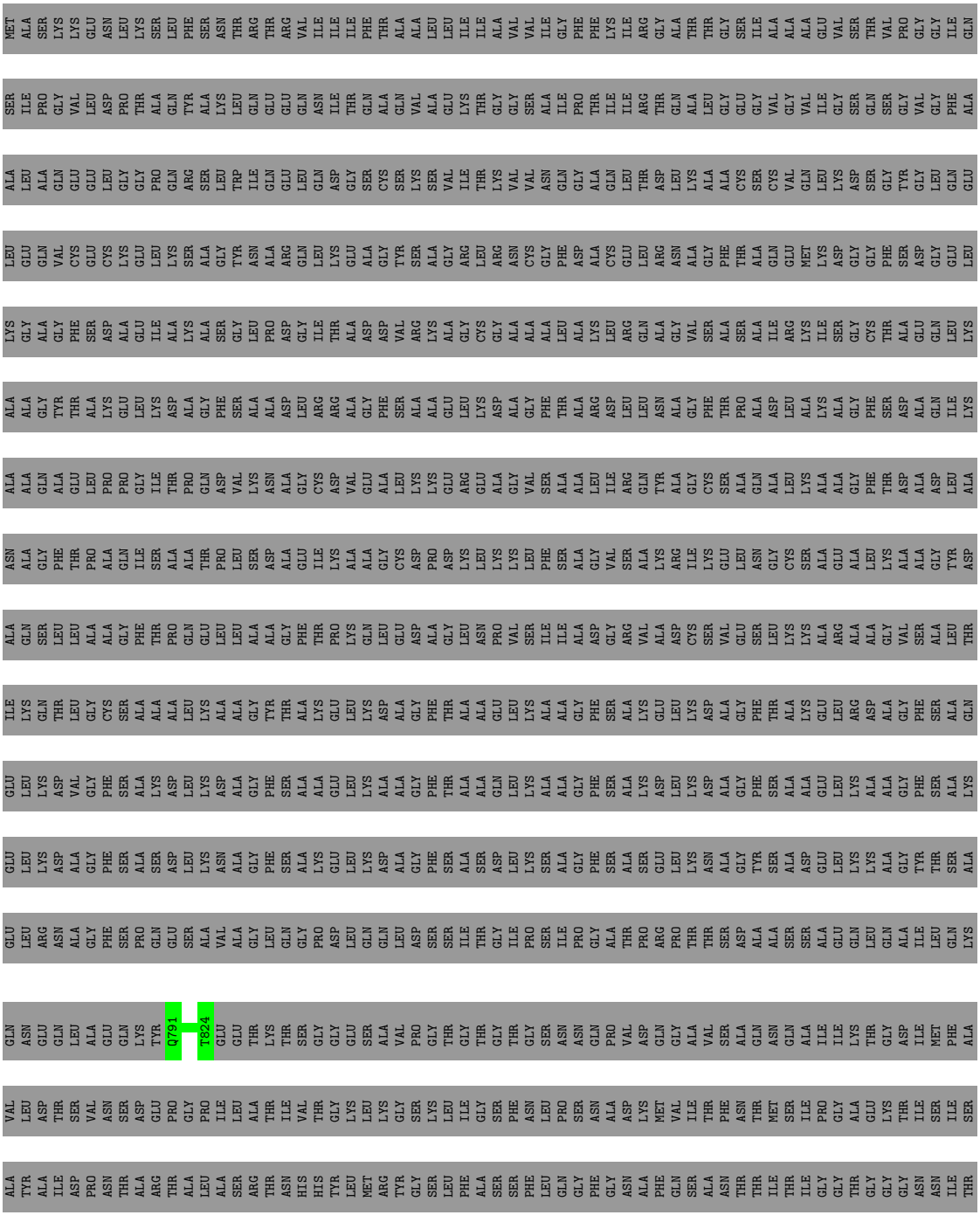
Chain FG: 97%





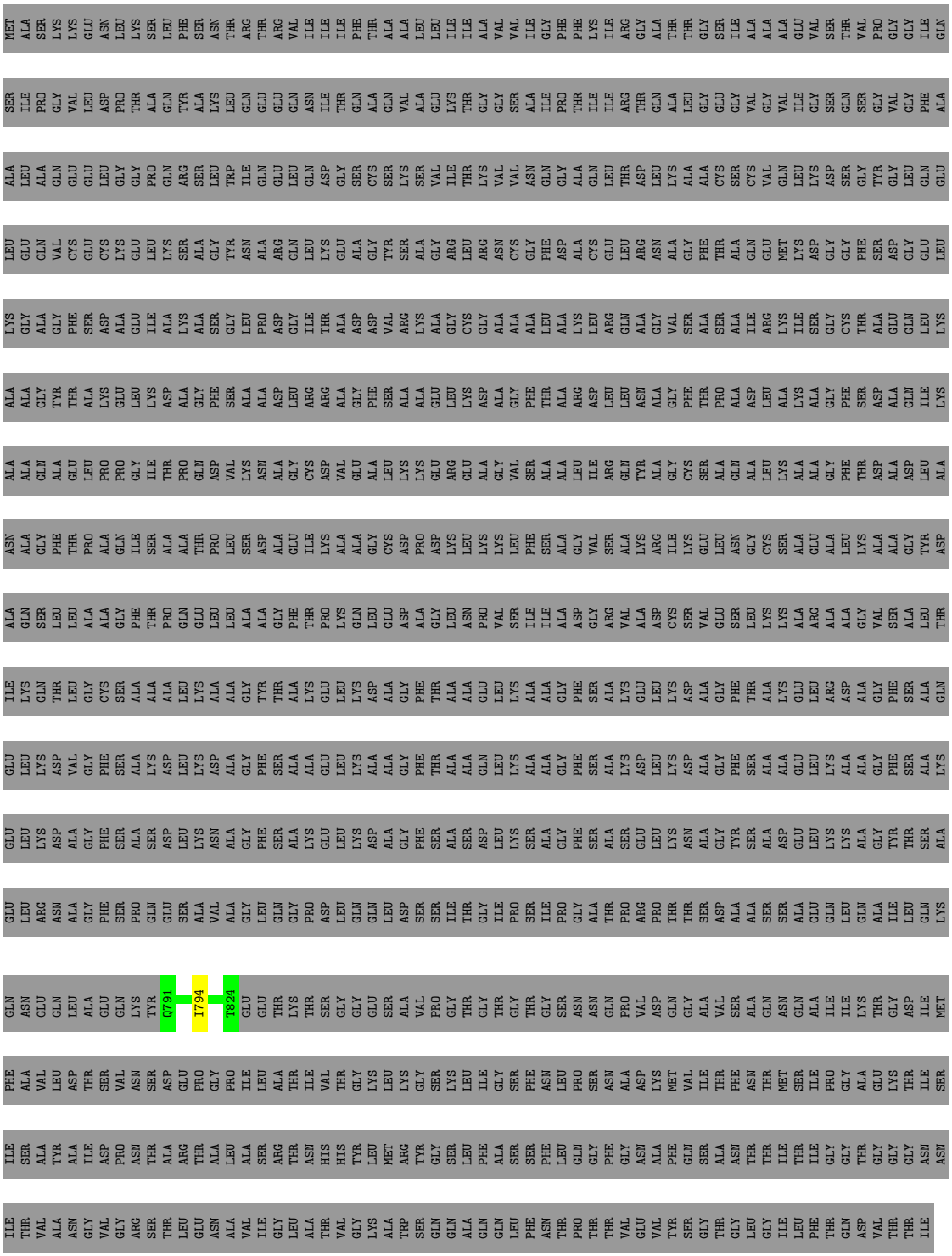
• Molecule 4: IcmE protein

Chain GG: 97%



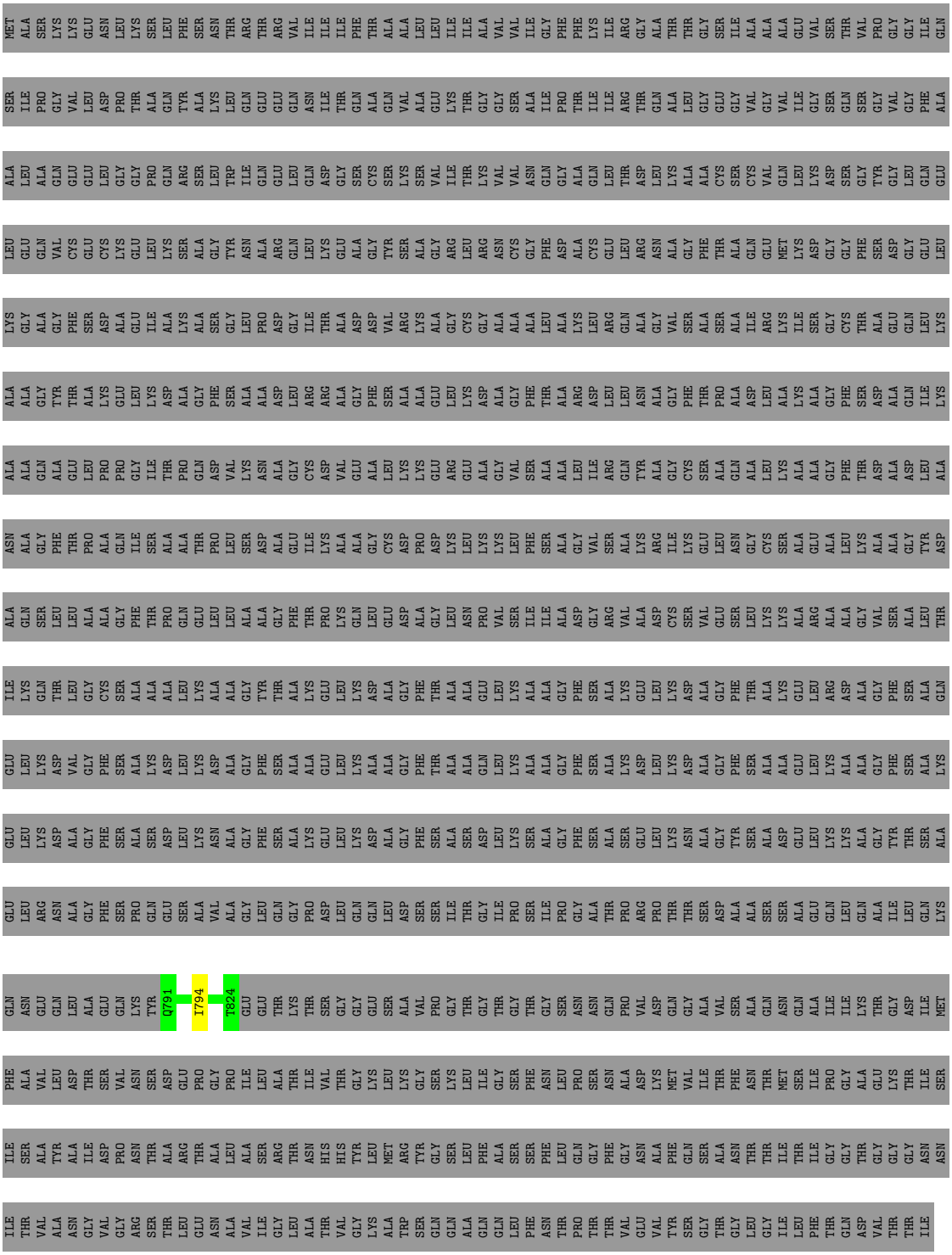
• Molecule 4: IcmE protein

Chain HG: 97%



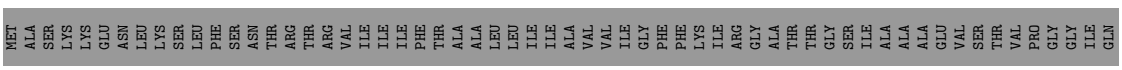
• Molecule 4: IcmE protein

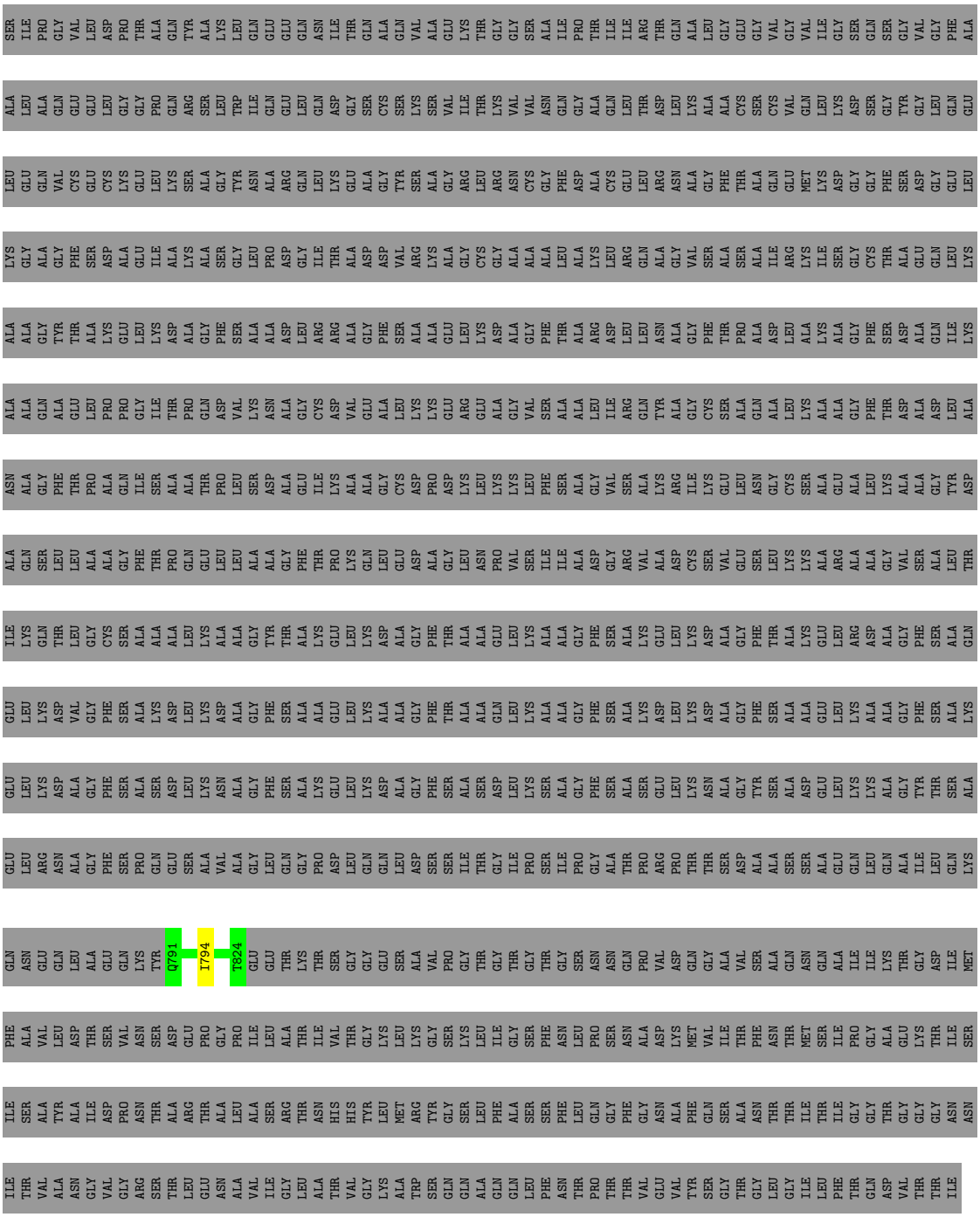
Chain JG: 97%



• Molecule 4: IcmE protein

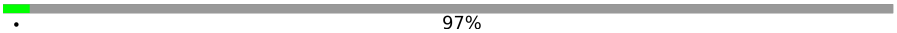
Chain KG: 97%

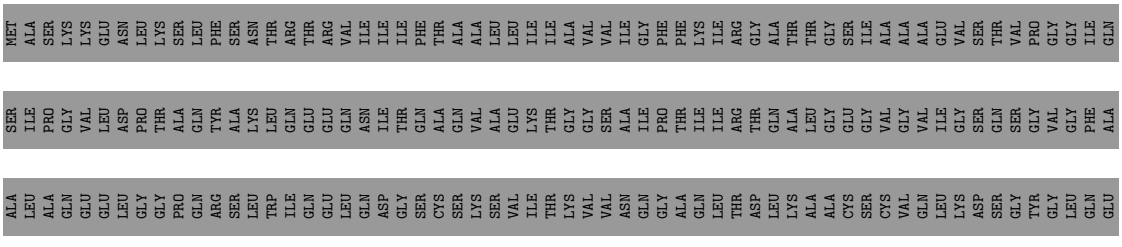


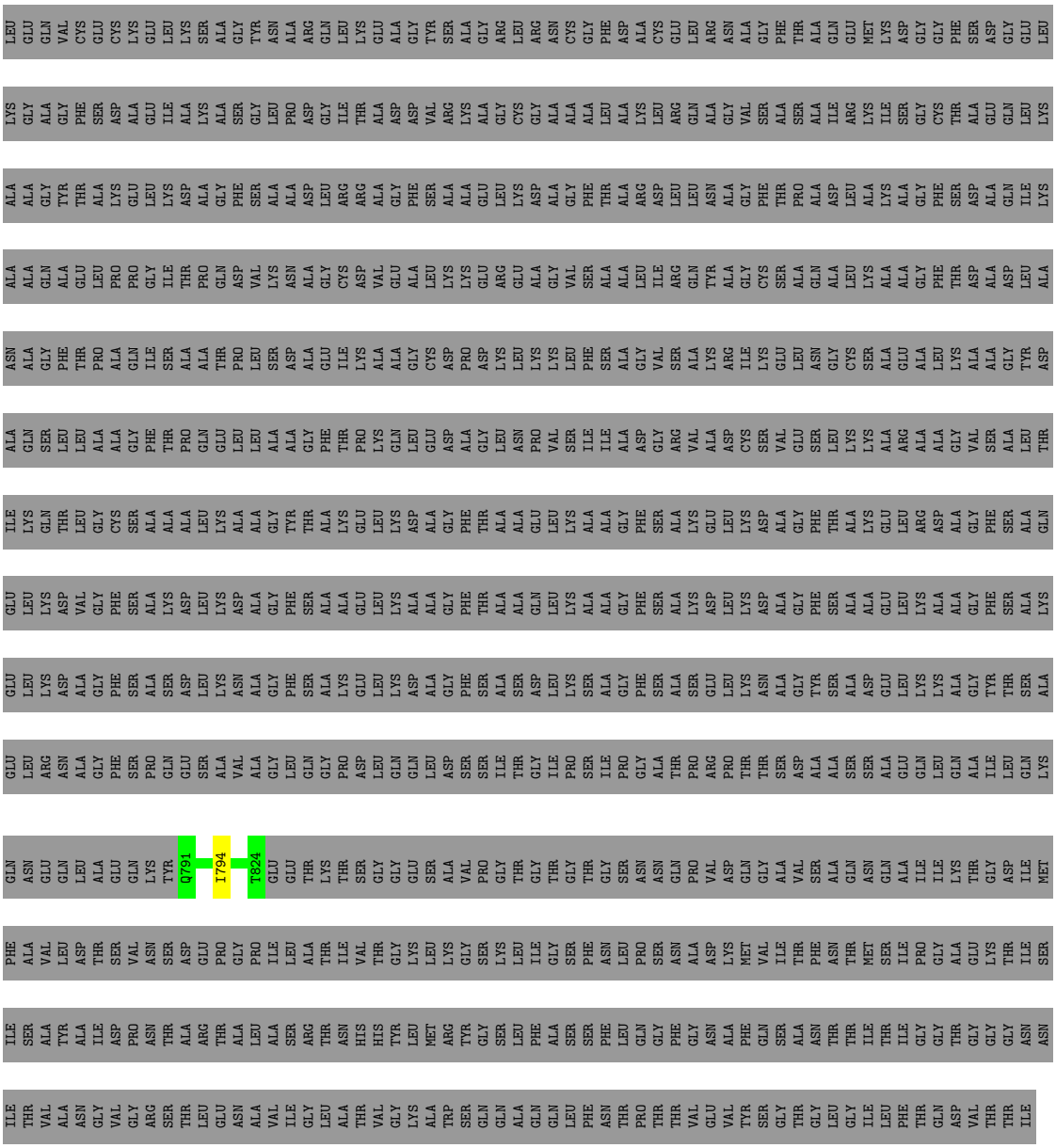


• Molecule 4: IcmE protein

Chain LG:

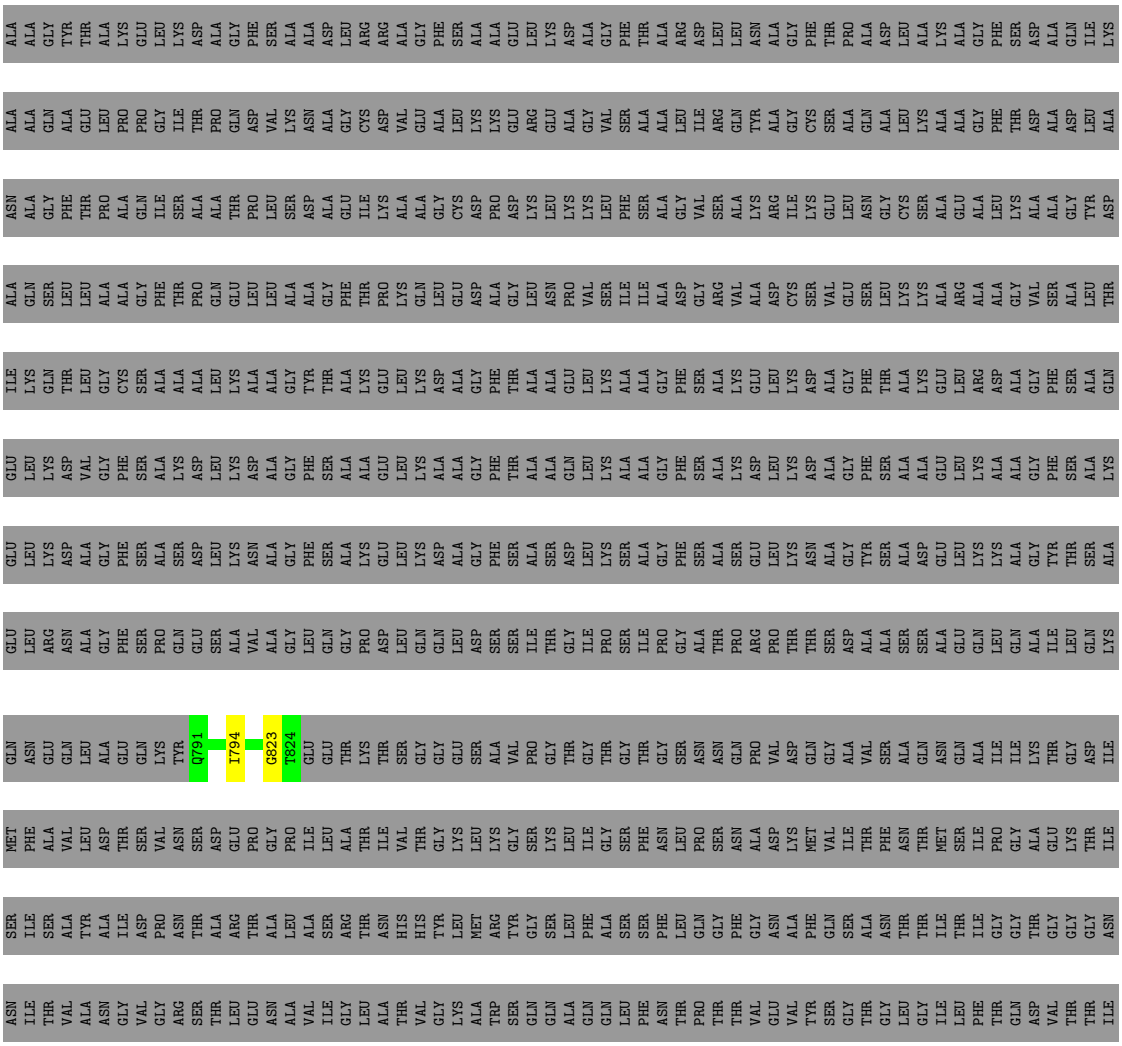






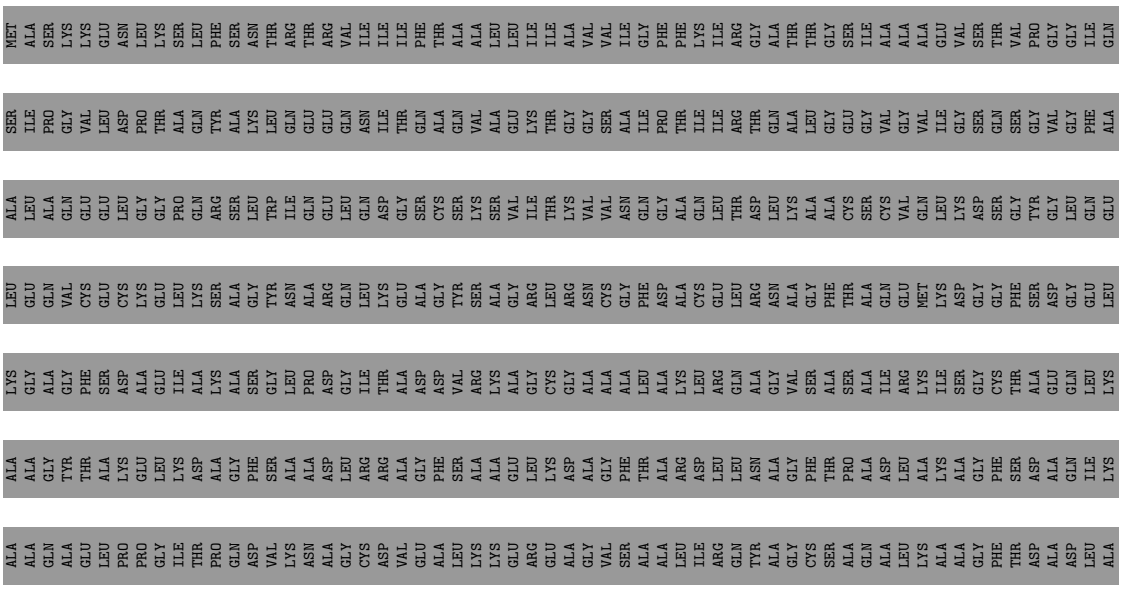
• Molecule 4: IcmE protein

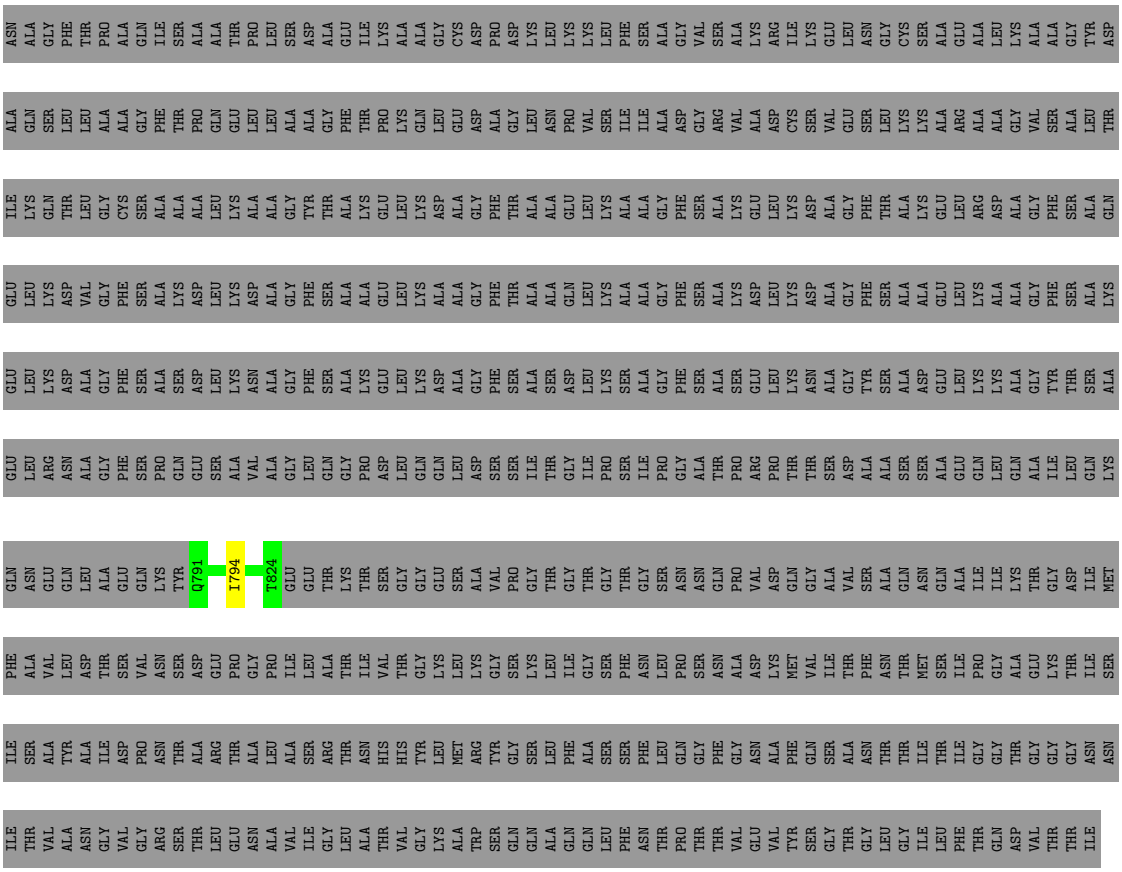
Chain MG:



• Molecule 4: IcmE protein

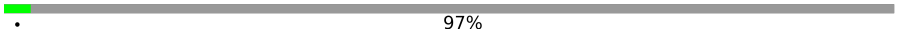
Chain VG: 97%

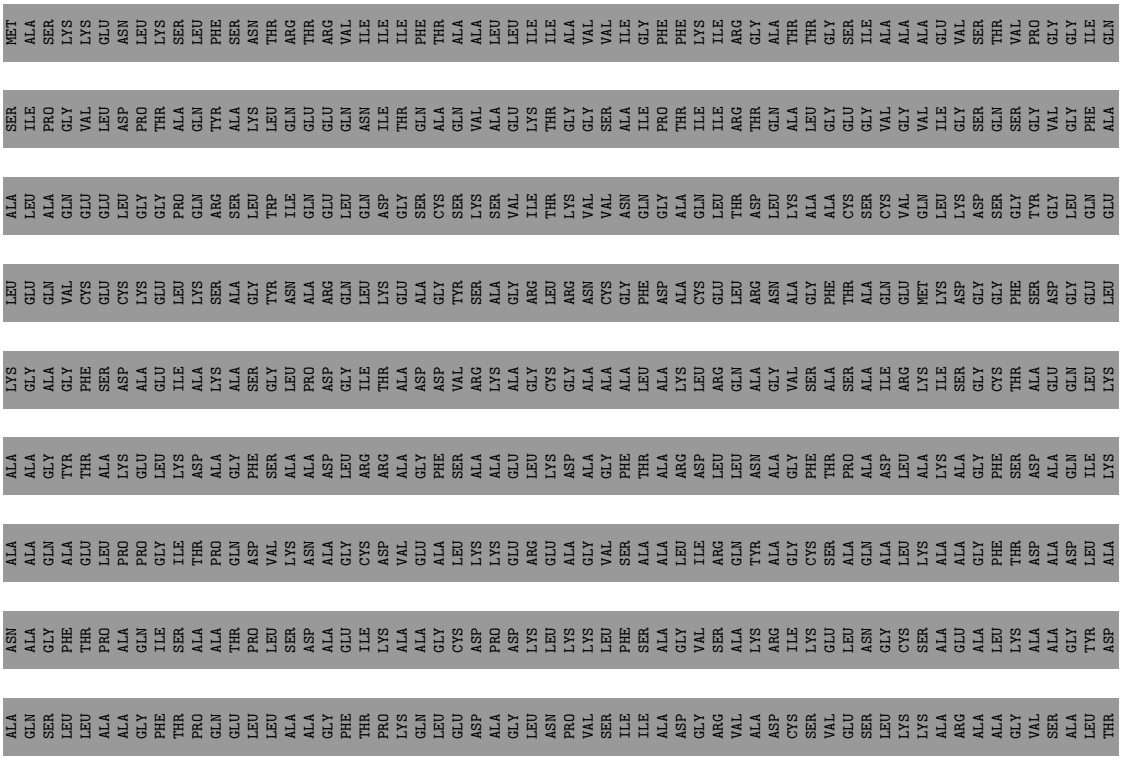




• Molecule 4: IcmE protein

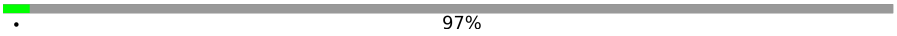
Chain WG:

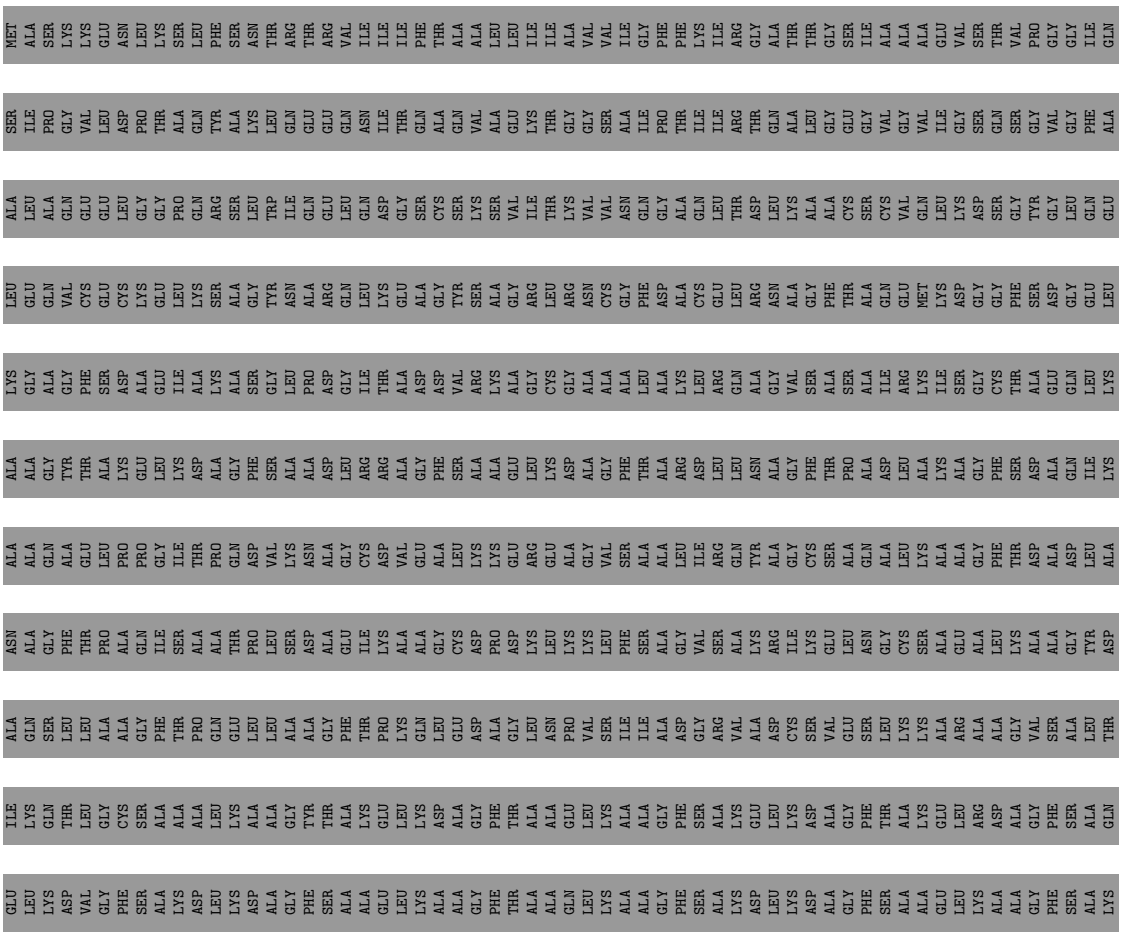




• Molecule 4: IcmE protein

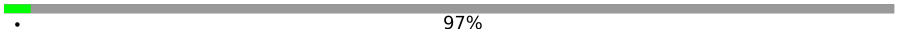
Chain XG:

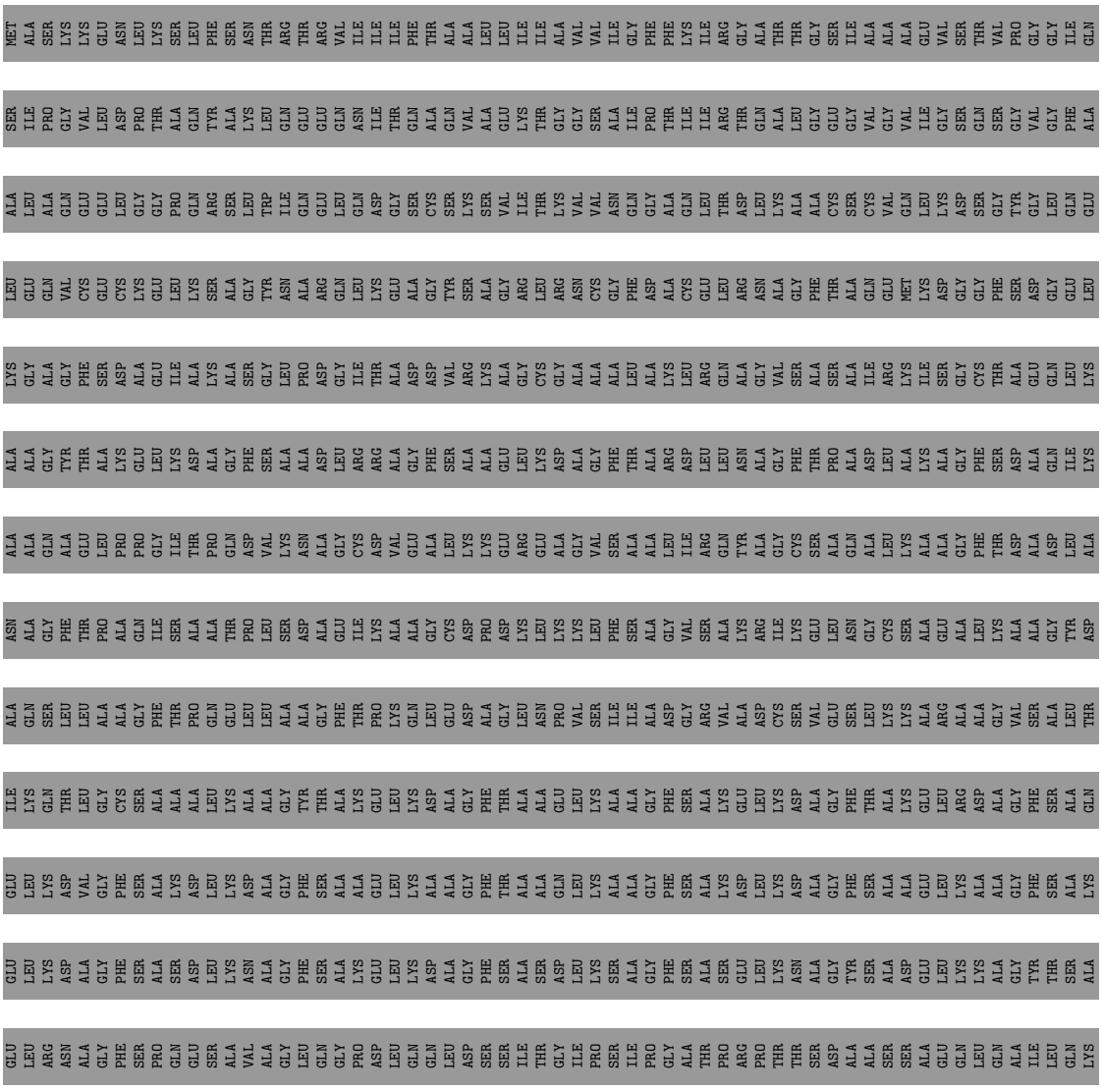


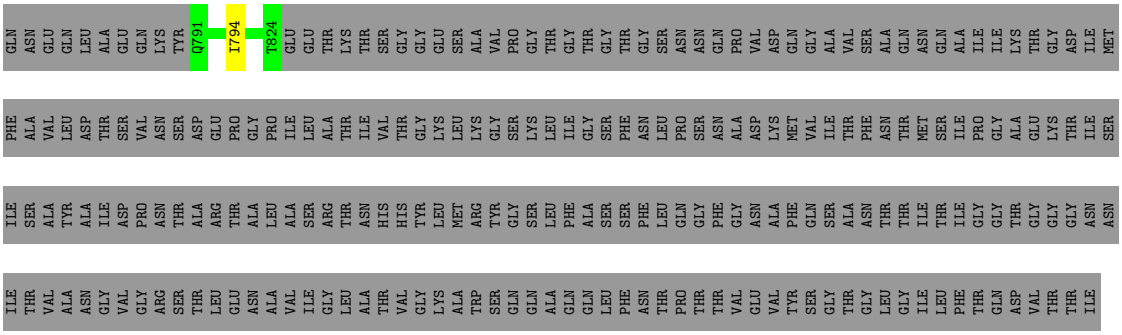


• Molecule 4: IcmE protein

Chain YG:

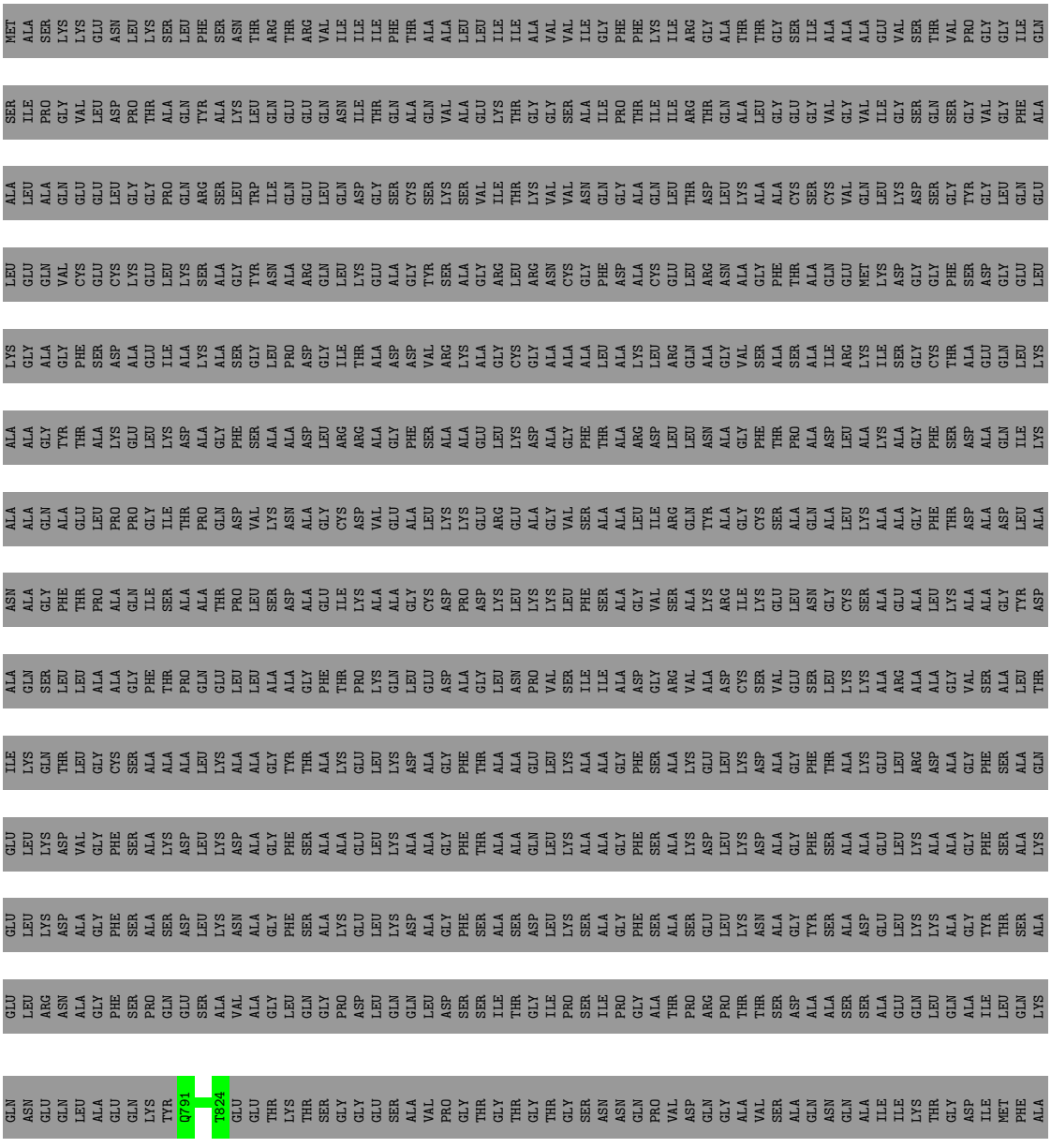


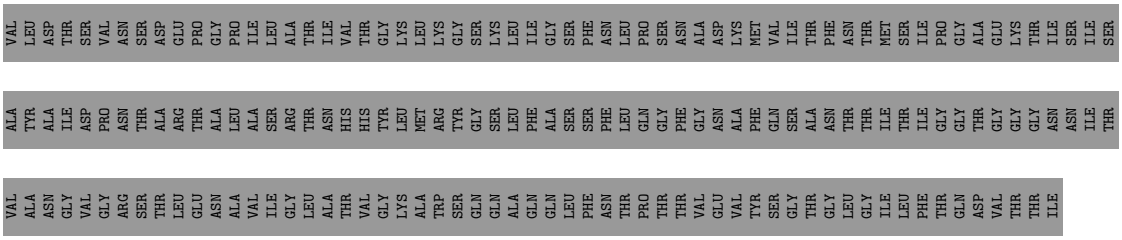




• Molecule 4: IcmE protein

Chain ZG: 97%




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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43907	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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AF	0.26	0/490	0.63	1/660 (0.2%)
1	BF	0.25	0/490	0.62	0/660
1	CF	0.26	0/490	0.63	0/660
1	DF	0.25	0/490	0.59	0/660
1	EF	0.26	0/490	0.61	0/660
1	FF	0.26	0/490	0.60	0/660
1	GF	0.26	0/490	0.58	0/660
1	HF	0.26	0/490	0.63	1/660 (0.2%)
1	IF	0.25	0/490	0.59	0/660
1	JF	0.26	0/490	0.60	0/660
1	KF	0.26	0/490	0.59	0/660
1	LF	0.26	0/490	0.62	0/660
1	MF	0.26	0/490	0.60	0/660
1	VF	0.26	0/490	0.61	0/660
1	WF	0.26	0/490	0.60	0/660
1	XF	0.26	0/490	0.63	0/660
1	YF	0.26	0/490	0.60	0/660
1	ZF	0.25	0/490	0.59	0/660
2	AH	0.26	0/1269	0.58	1/1734 (0.1%)
2	BH	0.26	0/1269	0.53	0/1734
2	CH	0.26	0/1269	0.58	1/1734 (0.1%)
2	DH	0.26	0/1269	0.52	0/1734
2	EH	0.26	0/1269	0.55	0/1734
2	FH	0.26	0/1269	0.55	1/1734 (0.1%)
2	GH	0.26	0/1269	0.57	1/1734 (0.1%)
2	HH	0.26	0/1269	0.57	1/1734 (0.1%)
2	IH	0.26	0/1269	0.54	0/1734
2	JH	0.25	0/1269	0.52	0/1734
2	KH	0.26	0/1269	0.52	0/1734
2	LH	0.26	0/1269	0.56	1/1734 (0.1%)
2	MH	0.26	0/1269	0.56	1/1734 (0.1%)
2	VH	0.25	0/1269	0.53	0/1734
2	WH	0.26	0/1269	0.56	1/1734 (0.1%)
2	XH	0.26	0/1269	0.53	0/1734

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	YH	0.26	0/1269	0.54	0/1734
2	ZH	0.26	0/1269	0.58	1/1734 (0.1%)
4	AG	0.24	0/278	0.44	0/377
4	BG	0.23	0/278	0.45	0/377
4	CG	0.24	0/278	0.49	0/377
4	DG	0.23	0/278	0.43	0/377
4	EG	0.23	0/278	0.43	0/377
4	FG	0.23	0/278	0.43	0/377
4	GG	0.23	0/278	0.44	0/377
4	HG	0.29	0/278	0.49	0/377
4	IG	0.25	0/278	0.47	0/377
4	JG	0.24	0/278	0.45	0/377
4	KG	0.23	0/278	0.43	0/377
4	LG	0.23	0/278	0.43	0/377
4	MG	0.26	0/278	0.46	0/377
4	VG	0.25	0/278	0.45	0/377
4	WG	0.23	0/278	0.44	0/377
4	XG	0.27	0/278	0.48	0/377
4	YG	0.24	0/278	0.43	0/377
4	ZG	0.23	0/278	0.44	0/377
All	All	0.26	0/36666	0.55	11/49878 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	WH	183	ASP	CB-CG-OD1	7.75	125.28	118.30
2	CH	183	ASP	CB-CG-OD1	7.73	125.26	118.30
2	MH	183	ASP	CB-CG-OD1	7.72	125.25	118.30
2	ZH	183	ASP	CB-CG-OD1	7.70	125.23	118.30
2	GH	183	ASP	CB-CG-OD1	7.62	125.15	118.30
2	AH	183	ASP	CB-CG-OD1	7.35	124.92	118.30
2	HH	183	ASP	CB-CG-OD1	7.32	124.89	118.30
2	LH	183	ASP	CB-CG-OD1	7.22	124.80	118.30
2	FH	183	ASP	CB-CG-OD1	7.18	124.76	118.30
1	AF	230	LEU	CA-CB-CG	5.14	127.13	115.30
1	HF	230	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AF	483	0	502	1	0
1	BF	483	0	502	4	0
1	CF	483	0	502	2	0
1	DF	483	0	502	2	0
1	EF	483	0	502	2	0
1	FF	483	0	502	3	0
1	GF	483	0	502	3	0
1	HF	483	0	502	4	0
1	IF	483	0	502	2	0
1	JF	483	0	502	2	0
1	KF	483	0	502	1	0
1	LF	483	0	502	2	0
1	MF	483	0	502	3	0
1	VF	483	0	502	1	0
1	WF	483	0	502	3	0
1	XF	483	0	502	4	0
1	YF	483	0	502	2	0
1	ZF	483	0	502	1	0
2	AH	1238	0	1252	6	0
2	BH	1238	0	1252	4	0
2	CH	1238	0	1252	5	0
2	DH	1238	0	1252	5	0
2	EH	1238	0	1252	5	0
2	FH	1238	0	1252	5	0
2	GH	1238	0	1252	2	0
2	HH	1238	0	1252	5	0
2	IH	1238	0	1252	4	0
2	JH	1238	0	1252	1	0
2	KH	1238	0	1252	3	0
2	LH	1238	0	1252	4	0
2	MH	1238	0	1252	3	0
2	VH	1238	0	1252	3	0
2	WH	1238	0	1252	4	0
2	XH	1238	0	1252	3	0
2	YH	1238	0	1252	4	0
2	ZH	1238	0	1252	3	0
3	AX	240	0	55	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BX	240	0	55	0	0
3	CX	240	0	55	0	0
3	DX	240	0	54	0	0
3	EX	240	0	54	0	0
3	FX	240	0	55	0	0
3	GX	240	0	55	0	0
3	HX	240	0	54	0	0
3	IX	240	0	54	0	0
3	JX	240	0	55	0	0
3	KX	240	0	55	0	0
3	LX	240	0	55	0	0
3	MX	240	0	55	0	0
3	VX	240	0	55	0	0
3	WX	240	0	54	0	0
3	XX	240	0	55	0	0
3	YX	240	0	54	0	0
3	ZX	240	0	55	0	0
4	AG	276	0	263	1	0
4	BG	276	0	263	2	0
4	CG	276	0	263	2	0
4	DG	276	0	263	1	0
4	EG	276	0	263	1	0
4	FG	276	0	263	1	0
4	GG	276	0	263	0	0
4	HG	276	0	263	1	0
4	IG	276	0	263	1	0
4	JG	276	0	263	1	0
4	KG	276	0	263	1	0
4	LG	276	0	263	1	0
4	MG	276	0	263	2	0
4	VG	276	0	263	1	0
4	WG	276	0	263	2	0
4	XG	276	0	263	0	0
4	YG	276	0	263	1	0
4	ZG	276	0	263	0	0
All	All	40266	0	37290	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DH:204:ILE:HG12	2:DH:215:ILE:HG12	1.81	0.63
2:KH:204:ILE:HG12	2:KH:215:ILE:HG12	1.81	0.62
2:CH:204:ILE:HG12	2:CH:215:ILE:HG12	1.83	0.61
2:IH:204:ILE:HG12	2:IH:215:ILE:HG12	1.83	0.60
2:YH:204:ILE:HG12	2:YH:215:ILE:HG12	1.84	0.60
2:EH:204:ILE:HG12	2:EH:215:ILE:HG12	1.84	0.59
1:LF:241:TYR:HB3	1:LF:256:THR:HG21	1.86	0.58
1:IF:241:TYR:HB3	1:IF:256:THR:HG21	1.85	0.58
1:WF:241:TYR:HB3	1:WF:256:THR:HG21	1.86	0.57
1:MF:241:TYR:HB3	1:MF:256:THR:HG21	1.86	0.57
1:FF:241:TYR:HB3	1:FF:256:THR:HG21	1.87	0.56
1:JF:241:TYR:HB3	1:JF:256:THR:HG21	1.89	0.55
1:HF:241:TYR:HB3	1:HF:256:THR:HG21	1.88	0.55
2:WH:230:LEU:HD12	2:WH:233:LEU:HD12	1.89	0.55
1:AF:241:TYR:HB3	1:AF:256:THR:HG21	1.89	0.55
1:CF:241:TYR:HB3	1:CF:256:THR:HG21	1.87	0.55
1:DF:241:TYR:HB3	1:DF:256:THR:HG21	1.89	0.55
1:GF:241:TYR:HB3	1:GF:256:THR:HG21	1.89	0.55
1:VF:241:TYR:HB3	1:VF:256:THR:HG21	1.89	0.55
1:ZF:241:TYR:HB3	1:ZF:256:THR:HG21	1.89	0.55
2:HH:157:PHE:HA	2:HH:255:ARG:HB2	1.89	0.55
2:AH:157:PHE:HA	2:AH:255:ARG:HB2	1.89	0.55
1:KF:241:TYR:HB3	1:KF:256:THR:HG21	1.89	0.54
1:XF:241:TYR:HB3	1:XF:256:THR:HG21	1.90	0.54
2:VH:230:LEU:HD12	2:VH:233:LEU:HD12	1.90	0.54
1:EF:241:TYR:HB3	1:EF:256:THR:HG21	1.88	0.54
2:JH:230:LEU:HD12	2:JH:233:LEU:HD12	1.89	0.54
2:FH:230:LEU:HD12	2:FH:233:LEU:HD12	1.90	0.54
2:EH:230:LEU:HD12	2:EH:233:LEU:HD12	1.91	0.53
1:BF:241:TYR:HB3	1:BF:256:THR:HG21	1.90	0.53
1:YF:241:TYR:HB3	1:YF:256:THR:HG21	1.90	0.53
2:XH:230:LEU:HD12	2:XH:233:LEU:HD12	1.91	0.53
2:MH:230:LEU:HD12	2:MH:233:LEU:HD12	1.91	0.52
2:LH:230:LEU:HD12	2:LH:233:LEU:HD12	1.90	0.52
2:BH:230:LEU:HD12	2:BH:233:LEU:HD12	1.91	0.52
2:YH:230:LEU:HD12	2:YH:233:LEU:HD12	1.91	0.52
4:VG:794:ILE:HG12	2:EH:107:ILE:HG23	1.91	0.52
2:AH:230:LEU:HD12	2:AH:233:LEU:HD12	1.92	0.51
2:GH:230:LEU:HD12	2:GH:233:LEU:HD12	1.93	0.50
2:CH:230:LEU:HD12	2:CH:233:LEU:HD12	1.92	0.50
2:WH:157:PHE:HA	2:WH:255:ARG:HB2	1.94	0.50
2:ZH:230:LEU:HD12	2:ZH:233:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IH:230:LEU:HD12	2:IH:233:LEU:HD12	1.92	0.50
4:CG:794:ILE:HG12	2:DH:107:ILE:HG23	1.93	0.49
4:CG:802:LEU:HD22	2:DH:115:MET:HG2	1.94	0.49
4:WG:823:GLY:HA2	2:FH:208:LYS:HG3	1.94	0.49
2:HH:230:LEU:HD12	2:HH:233:LEU:HD12	1.93	0.49
2:MH:157:PHE:HA	2:MH:255:ARG:HB2	1.94	0.49
2:EH:157:PHE:HA	2:EH:255:ARG:HB2	1.96	0.48
2:FH:157:PHE:HA	2:FH:255:ARG:HB2	1.94	0.48
4:FG:794:ILE:HG12	2:GH:107:ILE:HG23	1.95	0.48
2:YH:107:ILE:HG23	4:JG:794:ILE:HG12	1.95	0.47
4:AG:794:ILE:HG12	2:CH:107:ILE:HG23	1.96	0.47
4:BG:813:LYS:HE3	2:CH:134:TYR:HE1	1.79	0.47
4:EG:794:ILE:HG12	2:WH:107:ILE:HG23	1.96	0.47
4:HG:794:ILE:HG12	2:IH:107:ILE:HG23	1.96	0.47
2:YH:157:PHE:HA	2:YH:255:ARG:HB2	1.95	0.47
2:DH:230:LEU:HD12	2:DH:233:LEU:HD12	1.96	0.47
2:ZH:157:PHE:HA	2:ZH:255:ARG:HB2	1.97	0.47
2:KH:230:LEU:HD12	2:KH:233:LEU:HD12	1.95	0.47
4:MG:823:GLY:HA2	2:LH:208:LYS:HG3	1.96	0.46
4:YG:794:ILE:HG12	2:MH:107:ILE:HG23	1.97	0.46
2:ZH:107:ILE:HG23	4:LG:794:ILE:HG12	1.96	0.46
4:IG:794:ILE:HG12	2:KH:107:ILE:HG23	1.96	0.46
2:LH:157:PHE:HA	2:LH:255:ARG:HB2	1.95	0.46
1:FF:233:ARG:NH2	1:WF:266:GLN:OE1	2.49	0.46
1:LF:233:ARG:NH2	1:MF:266:GLN:OE1	2.47	0.46
2:CH:157:PHE:HA	2:CH:255:ARG:HB2	1.97	0.46
1:BF:269:SER:O	1:BF:269:SER:OG	2.35	0.45
4:KG:794:ILE:HG12	2:LH:107:ILE:HG23	1.97	0.45
4:DG:794:ILE:HG12	2:FH:107:ILE:HG23	1.99	0.45
4:MG:794:ILE:HG12	2:AH:107:ILE:HG23	1.98	0.45
2:IH:157:PHE:HA	2:IH:255:ARG:HB2	1.98	0.45
4:WG:794:ILE:HG12	2:HH:107:ILE:HG23	2.00	0.44
1:BF:233:ARG:NH2	1:CF:266:GLN:OE1	2.48	0.44
1:MF:269:SER:O	1:MF:269:SER:OG	2.35	0.43
1:BF:243:MET:HB2	1:BF:257:SER:HB3	2.01	0.43
2:BH:157:PHE:HA	2:BH:255:ARG:HB2	2.00	0.42
1:FF:246:LEU:HD23	1:FF:255:LEU:HD23	2.01	0.42
4:BG:794:ILE:HG12	2:VH:107:ILE:HG23	2.01	0.42
2:DH:166:PRO:HA	2:DH:167:PRO:HD3	1.93	0.42
1:DF:233:ARG:NH2	1:EF:266:GLN:OE1	2.49	0.42
1:GF:233:ARG:NH2	1:HF:266:GLN:OE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XH:157:PHE:HA	2:XH:255:ARG:HB2	2.00	0.42
1:JF:246:LEU:HD23	1:JF:255:LEU:HD23	2.01	0.42
2:FH:166:PRO:HA	2:FH:167:PRO:HD3	1.92	0.42
2:XH:176:VAL:H	2:HH:225:ASN:HD21	1.67	0.42
2:AH:195:ASP:HB3	2:AH:227:ALA:HB3	2.02	0.42
1:XF:269:SER:O	1:XF:269:SER:OG	2.35	0.42
2:EH:166:PRO:HA	2:EH:167:PRO:HD3	1.94	0.41
1:XF:243:MET:HB2	1:XF:257:SER:HB3	2.01	0.41
1:HF:246:LEU:HD23	1:HF:255:LEU:HD23	2.03	0.41
2:WH:166:PRO:HA	2:WH:167:PRO:HD3	1.93	0.41
2:AH:225:ASN:HD21	2:BH:176:VAL:H	1.68	0.41
2:HH:195:ASP:HB3	2:HH:227:ALA:HB3	2.02	0.41
2:AH:105:GLU:O	2:AH:109:LYS:NZ	2.41	0.41
2:VH:166:PRO:HA	2:VH:167:PRO:HD3	1.93	0.41
1:GF:269:SER:O	1:GF:269:SER:OG	2.36	0.41
1:HF:269:SER:O	1:HF:269:SER:OG	2.36	0.41
2:BH:166:PRO:HA	2:BH:167:PRO:HD3	1.92	0.40
1:IF:266:GLN:OE1	1:XF:233:ARG:NH2	2.49	0.40
1:WF:269:SER:O	1:WF:269:SER:OG	2.35	0.40
1:YF:243:MET:HB3	1:YF:257:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	BF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	CF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	DF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	FF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	GF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	HF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	IF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	JF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
1	KF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	LF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	MF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	VF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
1	WF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	XF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	YF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
1	ZF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
2	AH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	BH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	CH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	DH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	EH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	FH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	GH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	HH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	IH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	JH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	KH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	LH	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
2	MH	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
2	VH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	WH	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
2	XH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
2	YH	158/361 (44%)	153 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	ZH	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
4	AG	32/1048 (3%)	32 (100%)	0	0	100	100
4	BG	32/1048 (3%)	32 (100%)	0	0	100	100
4	CG	32/1048 (3%)	32 (100%)	0	0	100	100
4	DG	32/1048 (3%)	32 (100%)	0	0	100	100
4	EG	32/1048 (3%)	32 (100%)	0	0	100	100
4	FG	32/1048 (3%)	32 (100%)	0	0	100	100
4	GG	32/1048 (3%)	32 (100%)	0	0	100	100
4	HG	32/1048 (3%)	32 (100%)	0	0	100	100
4	IG	32/1048 (3%)	32 (100%)	0	0	100	100
4	JG	32/1048 (3%)	32 (100%)	0	0	100	100
4	KG	32/1048 (3%)	32 (100%)	0	0	100	100
4	LG	32/1048 (3%)	32 (100%)	0	0	100	100
4	MG	32/1048 (3%)	32 (100%)	0	0	100	100
4	VG	32/1048 (3%)	32 (100%)	0	0	100	100
4	WG	32/1048 (3%)	32 (100%)	0	0	100	100
4	XG	32/1048 (3%)	32 (100%)	0	0	100	100
4	YG	32/1048 (3%)	32 (100%)	0	0	100	100
4	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
All	All	4518/30204 (15%)	4378 (97%)	140 (3%)	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	AF	53/237 (22%)	53 (100%)	0	100	100
1	BF	53/237 (22%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CF	53/237 (22%)	53 (100%)	0	100	100
1	DF	53/237 (22%)	53 (100%)	0	100	100
1	EF	53/237 (22%)	53 (100%)	0	100	100
1	FF	53/237 (22%)	53 (100%)	0	100	100
1	GF	53/237 (22%)	53 (100%)	0	100	100
1	HF	53/237 (22%)	53 (100%)	0	100	100
1	IF	53/237 (22%)	53 (100%)	0	100	100
1	JF	53/237 (22%)	53 (100%)	0	100	100
1	KF	53/237 (22%)	53 (100%)	0	100	100
1	LF	53/237 (22%)	53 (100%)	0	100	100
1	MF	53/237 (22%)	53 (100%)	0	100	100
1	VF	53/237 (22%)	53 (100%)	0	100	100
1	WF	53/237 (22%)	53 (100%)	0	100	100
1	XF	53/237 (22%)	53 (100%)	0	100	100
1	YF	53/237 (22%)	53 (100%)	0	100	100
1	ZF	53/237 (22%)	53 (100%)	0	100	100
2	AH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	BH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	CH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	DH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	EH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	FH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	GH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	HH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	IH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	JH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	KH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	LH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	MH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	VH	137/300 (46%)	136 (99%)	1 (1%)	84	95
2	WH	137/300 (46%)	136 (99%)	1 (1%)	84	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	XH	137/300 (46%)	136 (99%)	1 (1%)	84 95
2	YH	137/300 (46%)	136 (99%)	1 (1%)	84 95
2	ZH	137/300 (46%)	136 (99%)	1 (1%)	84 95
4	AG	31/765 (4%)	31 (100%)	0	100 100
4	BG	31/765 (4%)	31 (100%)	0	100 100
4	CG	31/765 (4%)	31 (100%)	0	100 100
4	DG	31/765 (4%)	31 (100%)	0	100 100
4	EG	31/765 (4%)	31 (100%)	0	100 100
4	FG	31/765 (4%)	31 (100%)	0	100 100
4	GG	31/765 (4%)	31 (100%)	0	100 100
4	HG	31/765 (4%)	31 (100%)	0	100 100
4	IG	31/765 (4%)	31 (100%)	0	100 100
4	JG	31/765 (4%)	31 (100%)	0	100 100
4	KG	31/765 (4%)	31 (100%)	0	100 100
4	LG	31/765 (4%)	31 (100%)	0	100 100
4	MG	31/765 (4%)	31 (100%)	0	100 100
4	VG	31/765 (4%)	31 (100%)	0	100 100
4	WG	31/765 (4%)	31 (100%)	0	100 100
4	XG	31/765 (4%)	31 (100%)	0	100 100
4	YG	31/765 (4%)	31 (100%)	0	100 100
4	ZG	31/765 (4%)	31 (100%)	0	100 100
All	All	3978/23436 (17%)	3960 (100%)	18 (0%)	89 96

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	XH	170	ARG
2	YH	170	ARG
2	ZH	170	ARG
2	AH	170	ARG
2	BH	170	ARG
2	CH	170	ARG
2	DH	170	ARG
2	EH	170	ARG
2	FH	170	ARG

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Mol	Chain	Res	Type
2	GH	170	ARG
2	HH	170	ARG
2	IH	170	ARG
2	JH	170	ARG
2	KH	170	ARG
2	LH	170	ARG
2	MH	170	ARG
2	VH	170	ARG
2	WH	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	ZX	38:UNK	C	70:UNK	N	24.53
1	GX	38:UNK	C	70:UNK	N	24.52
1	CX	38:UNK	C	70:UNK	N	24.51
1	KX	38:UNK	C	70:UNK	N	24.51
1	BX	38:UNK	C	70:UNK	N	24.49
1	HX	38:UNK	C	70:UNK	N	24.49
1	YX	38:UNK	C	70:UNK	N	24.49
1	MX	38:UNK	C	70:UNK	N	24.48
1	XX	38:UNK	C	70:UNK	N	24.47
1	IX	38:UNK	C	70:UNK	N	24.46
1	LX	38:UNK	C	70:UNK	N	24.46
1	WX	38:UNK	C	70:UNK	N	24.46
1	FX	38:UNK	C	70:UNK	N	24.45
1	AX	38:UNK	C	70:UNK	N	24.43
1	EX	38:UNK	C	70:UNK	N	24.42
1	DX	38:UNK	C	70:UNK	N	24.41
1	JX	38:UNK	C	70:UNK	N	24.41
1	VX	38:UNK	C	70:UNK	N	24.40

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24006. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.