Full wwPDB EM Validation Report

Nov 10, 2024 – 09:30 PM EST

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

This is a 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 ⓘ 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 ⓘ) were used in the production of this report:

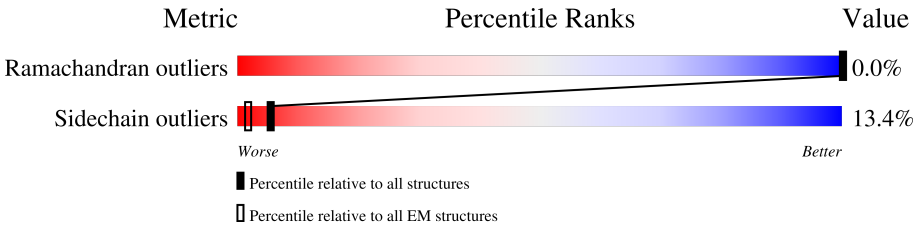
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AG	1048	13% 84%
1	Ag	1048	97%
1	BG	1048	13% 84%
1	Bg	1048	97%
1	CG	1048	13% 84%
1	Cg	1048	97%
1	DG	1048	14% 84%
1	Dg	1048	97%
1	EG	1048	13% 84%

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

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

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

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

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

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

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

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

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 192370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AG	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	BG	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	CG	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	DG	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	Mg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	Ag	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		
1	EG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		

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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	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	FG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	Dg	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	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	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		

- Molecule 2 is a protein called DotC.

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

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

- Molecule 3 is a protein called DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		
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	Df	59	Total	C	N	O	S	0	0
			449	290	77	81	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	CF	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	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	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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		

- Molecule 4 is a protein called DotD.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called Neurogenic locus notch.

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

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

- Molecule 10 is a protein called Unknown protein fragment.

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

- Molecule 11 is a protein called Unknown protein fragment.

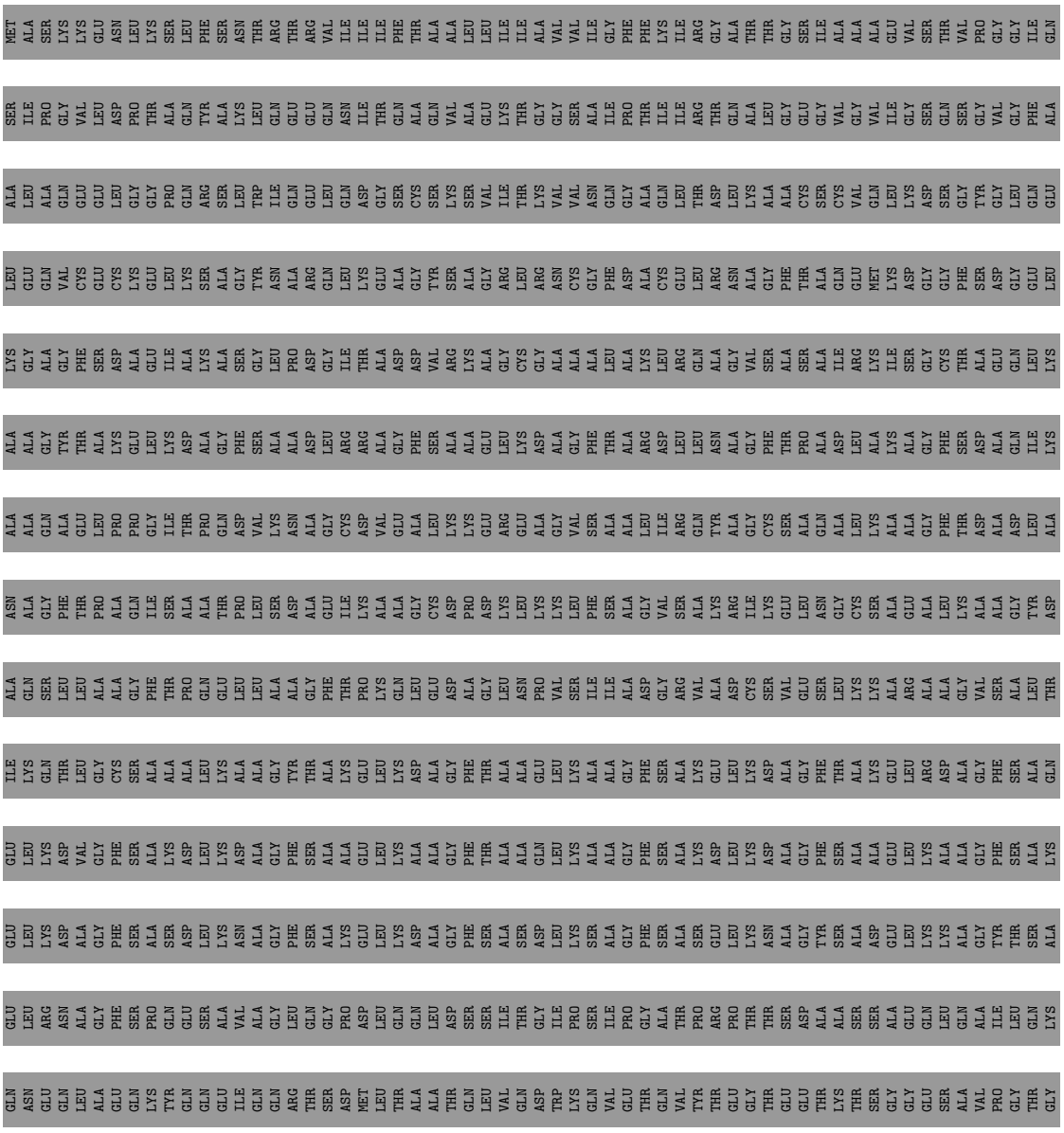
Mol	Chain	Residues	Atoms				AltConf	Trace
11	GX	48	Total	C	N	O	0	0
			240	144	48	48		
11	DX	48	Total	C	N	O	0	0
			240	144	48	48		
11	HX	48	Total	C	N	O	0	0
			240	144	48	48		
11	IX	48	Total	C	N	O	0	0
			240	144	48	48		
11	JX	48	Total	C	N	O	0	0
			240	144	48	48		
11	KX	48	Total	C	N	O	0	0
			240	144	48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

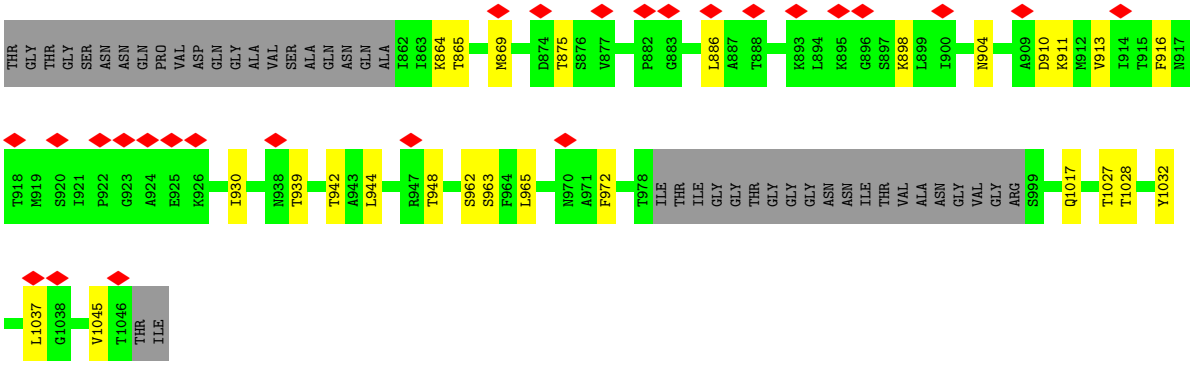
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: IcmE protein

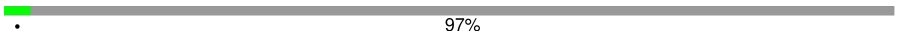
Chain AG:

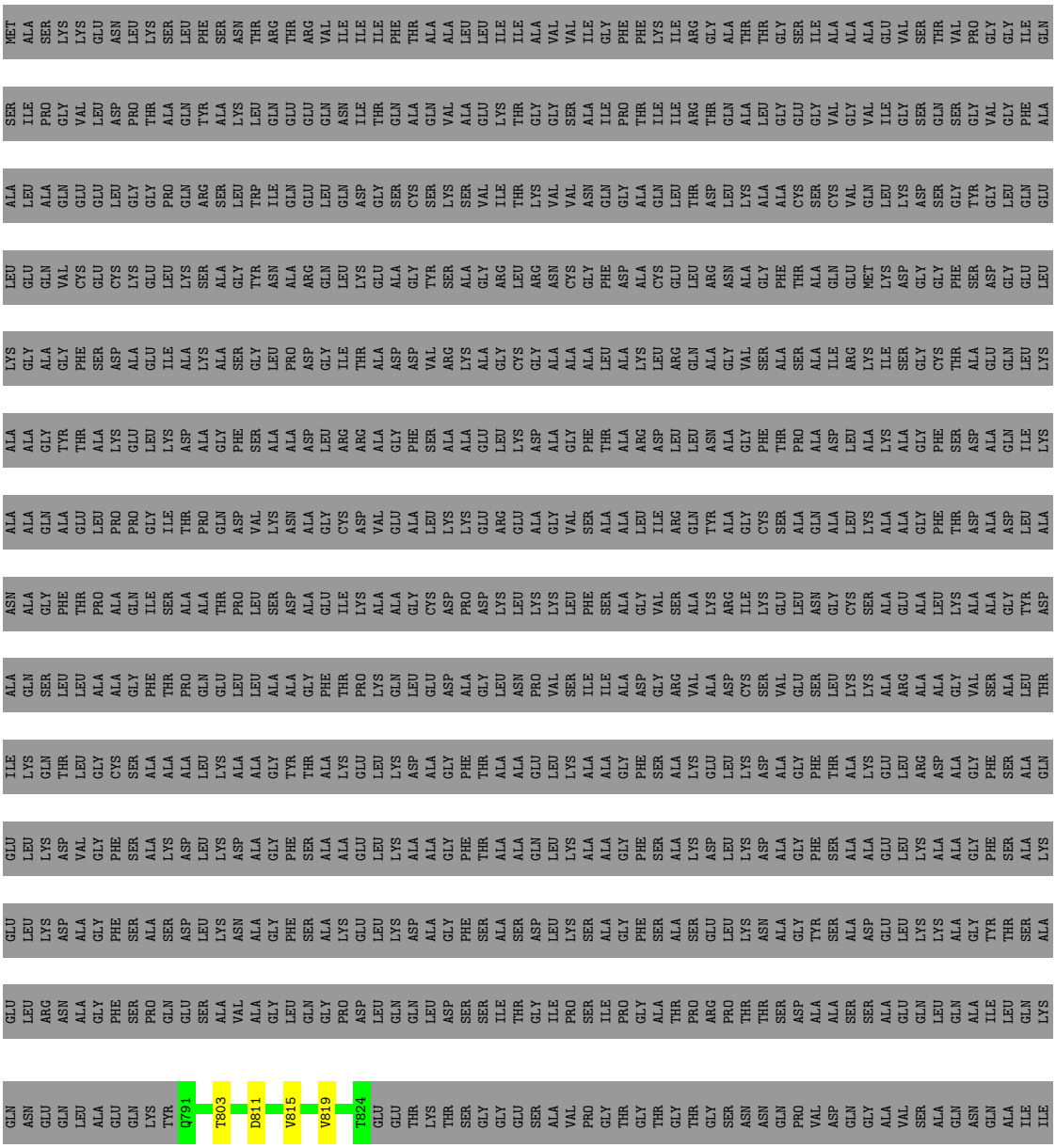


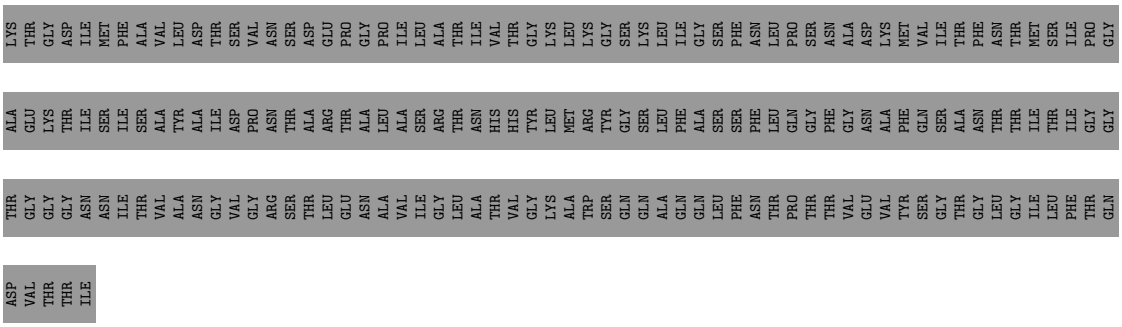


• Molecule 1: IcmE protein

Chain Gg:

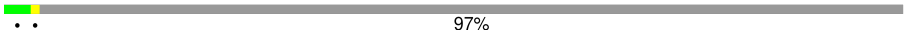


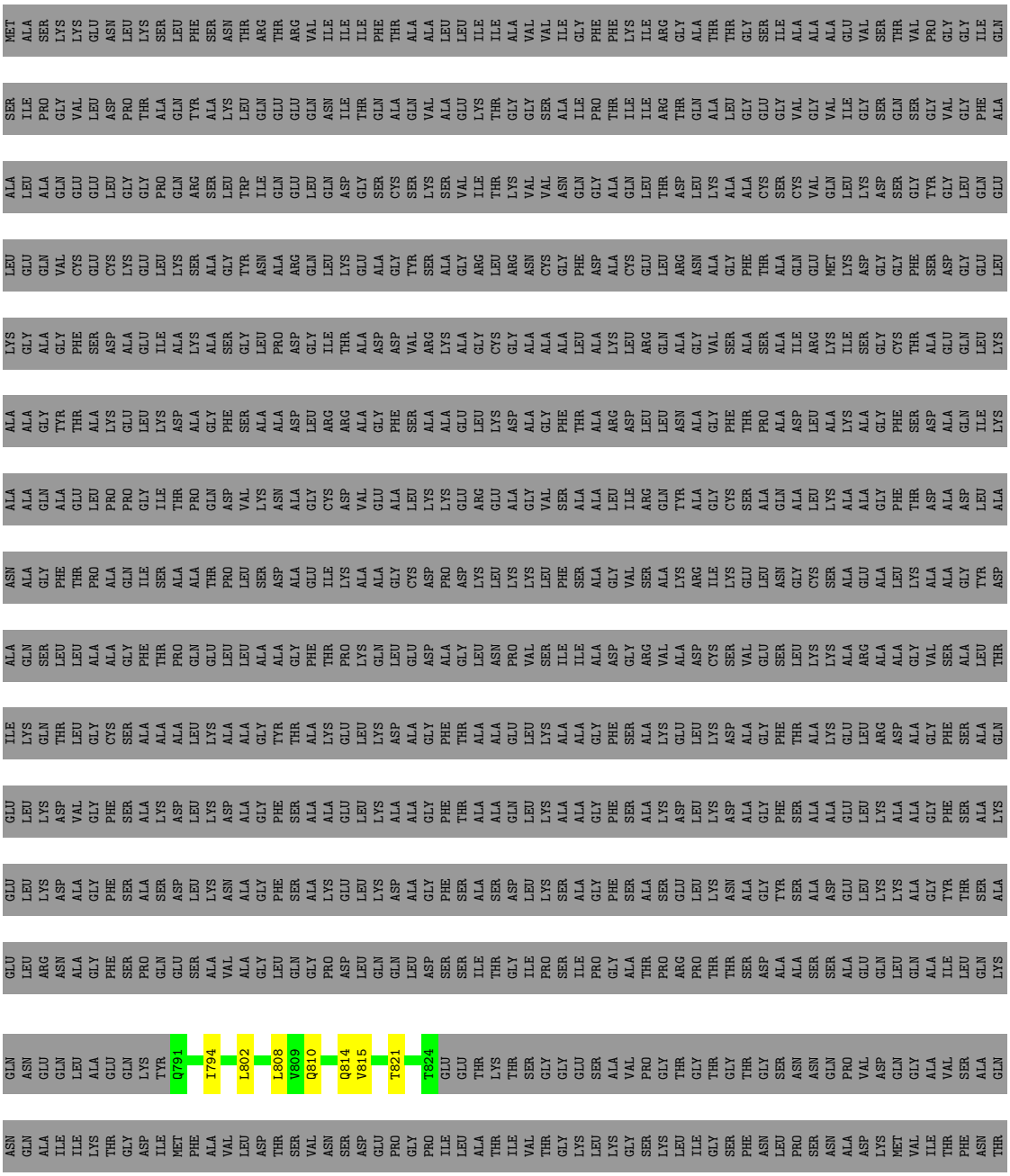


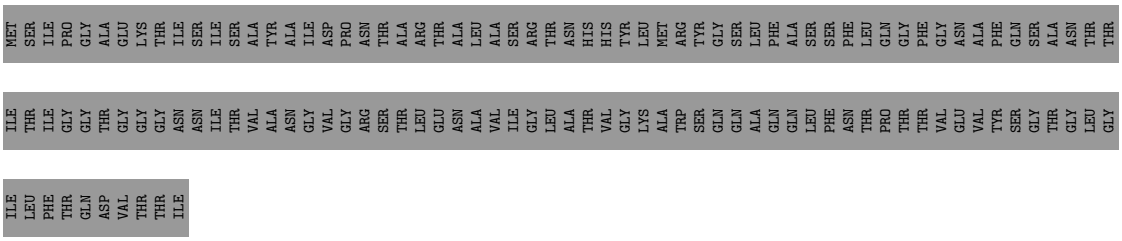


• Molecule 1: IcmE protein

Chain Hg:

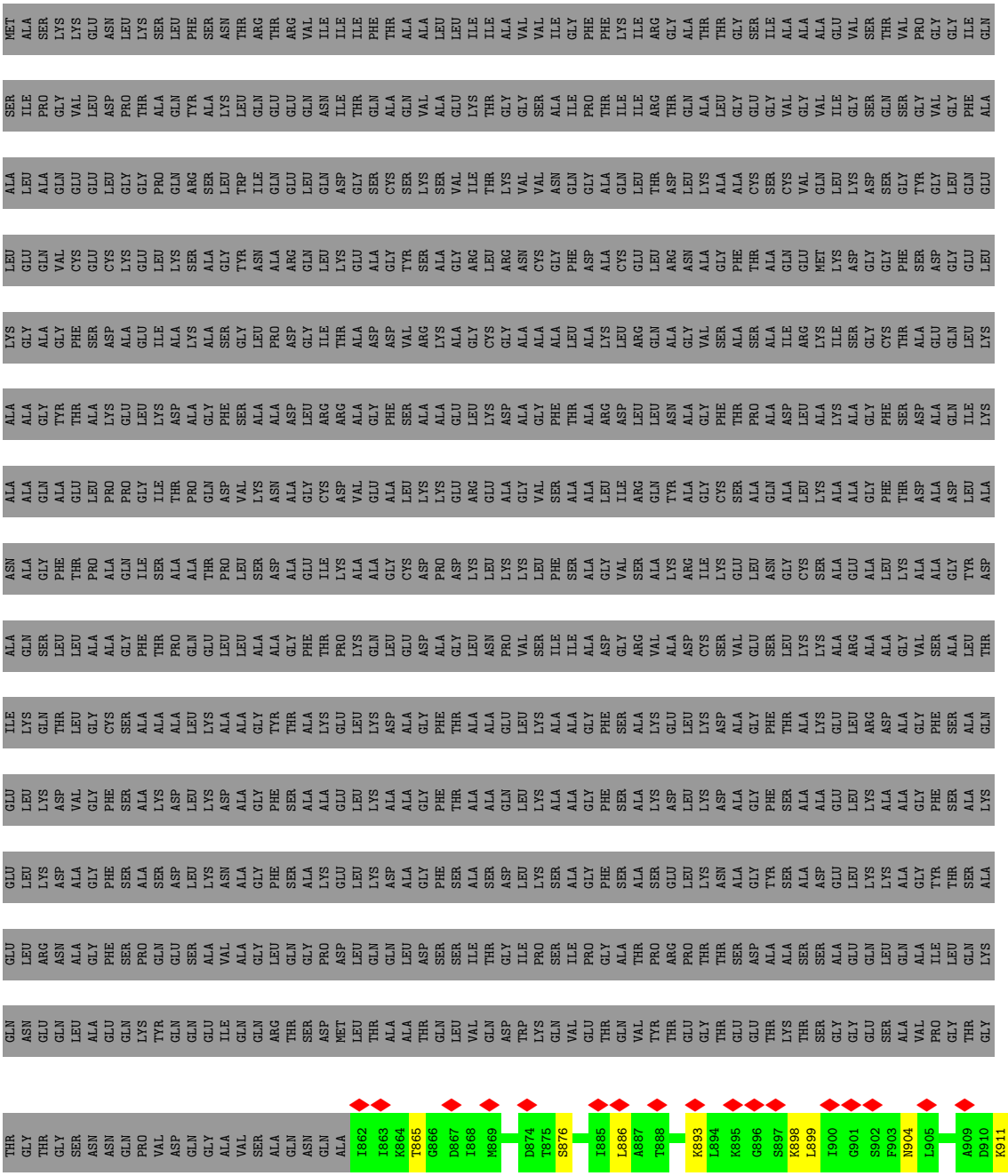


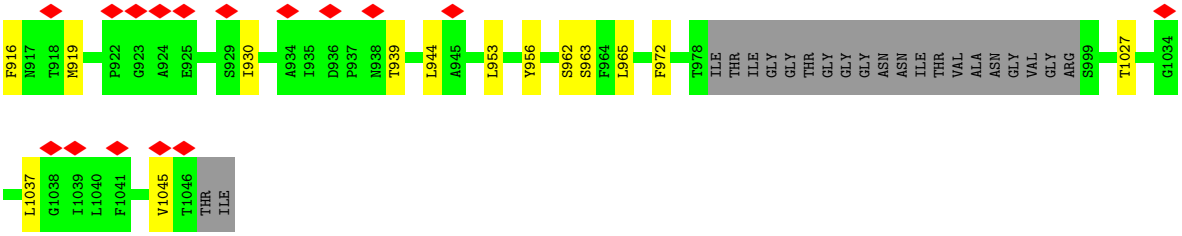




• Molecule 1: IcmE protein

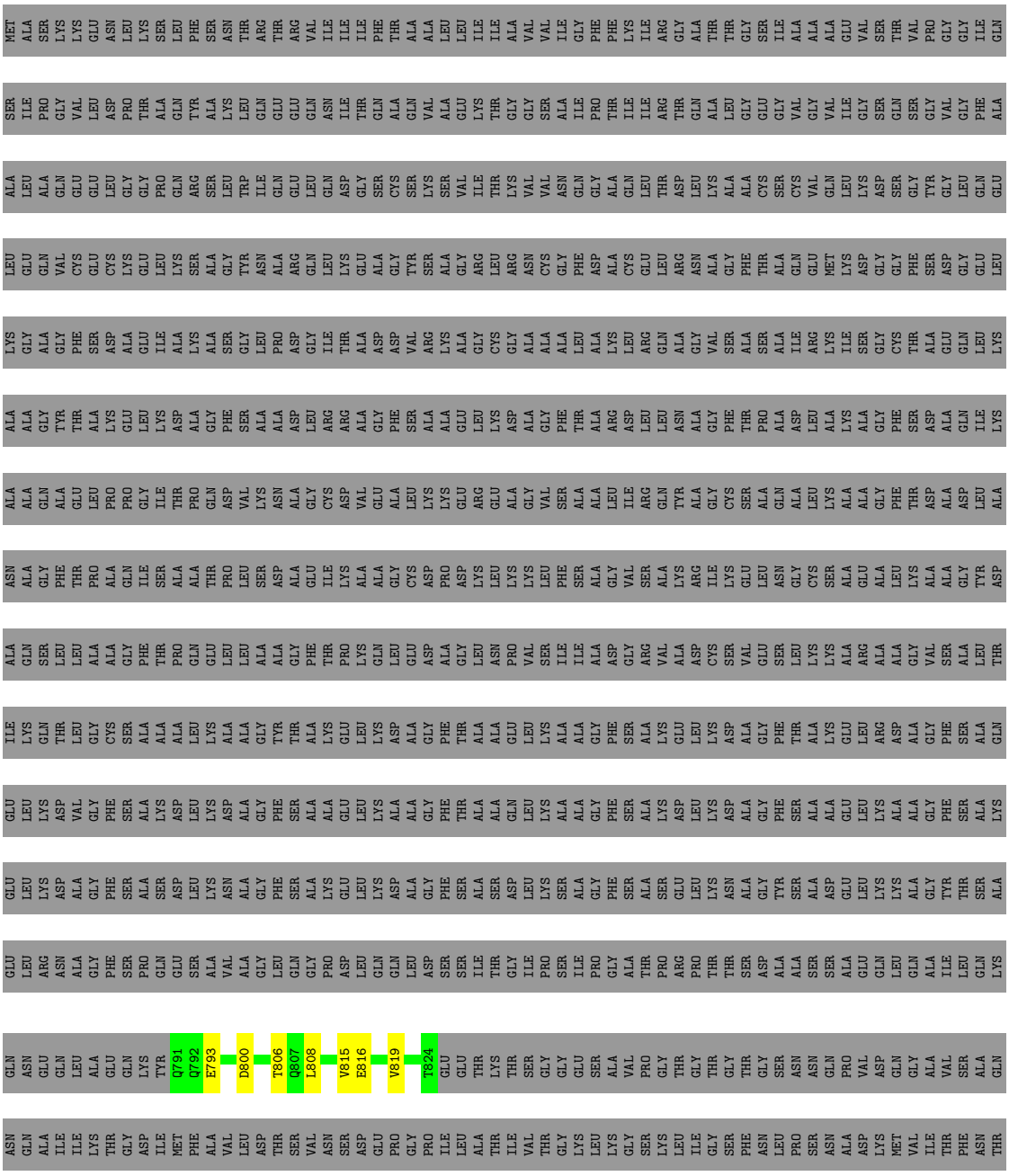
Chain BG:

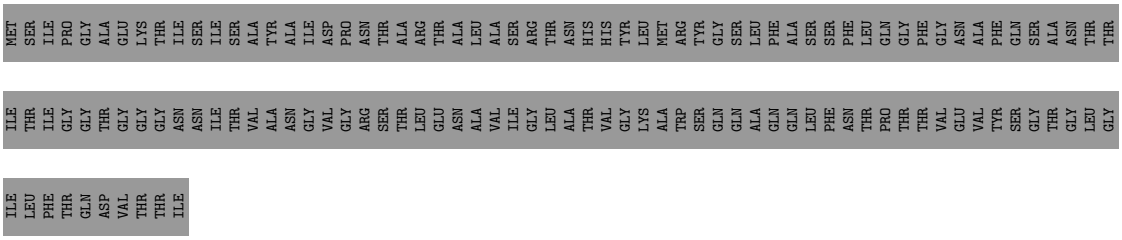




• Molecule 1: IcmE protein

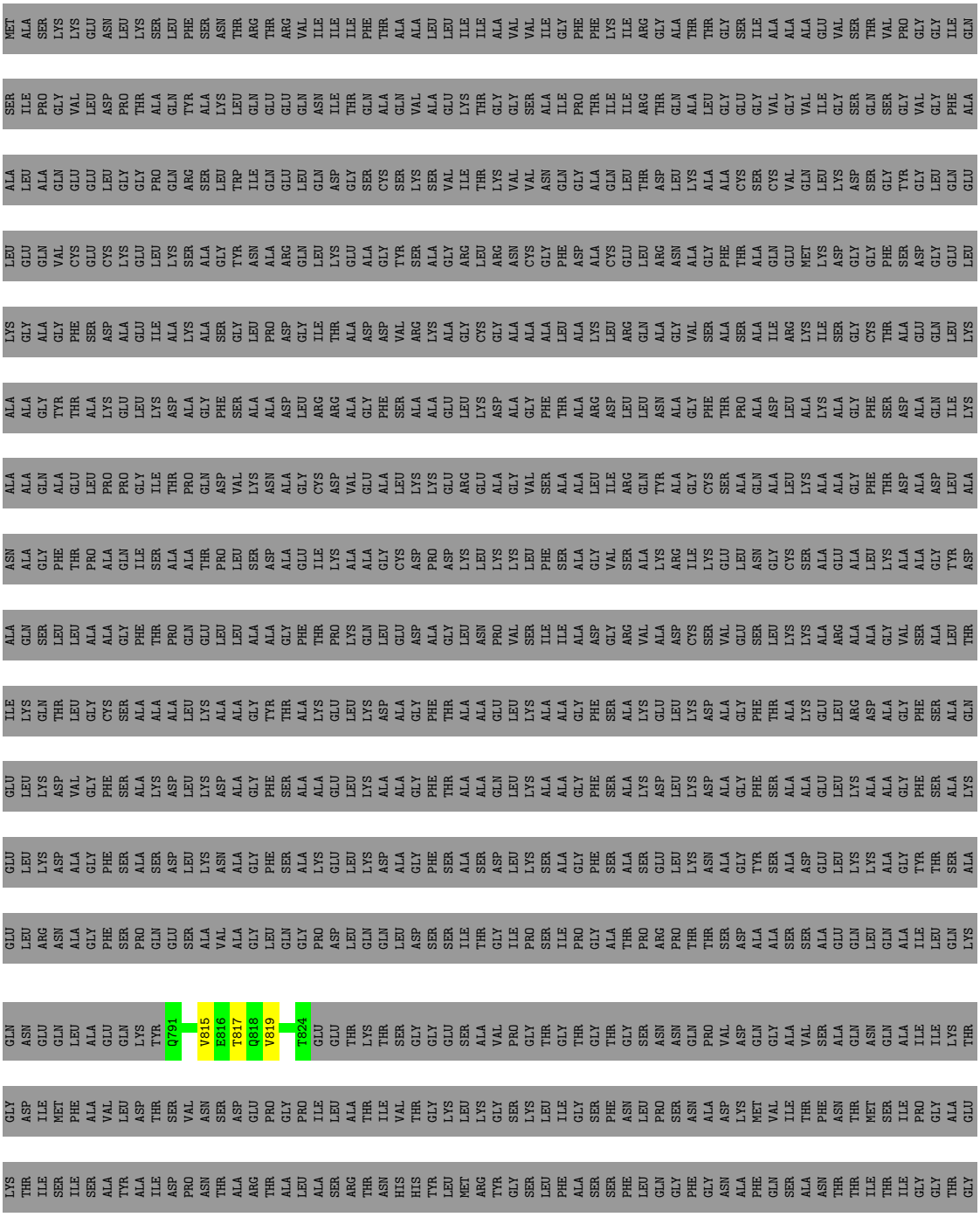
Chain Bg: 97%

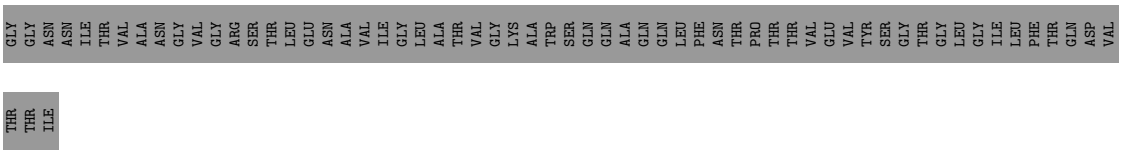




• Molecule 1: IcmE protein

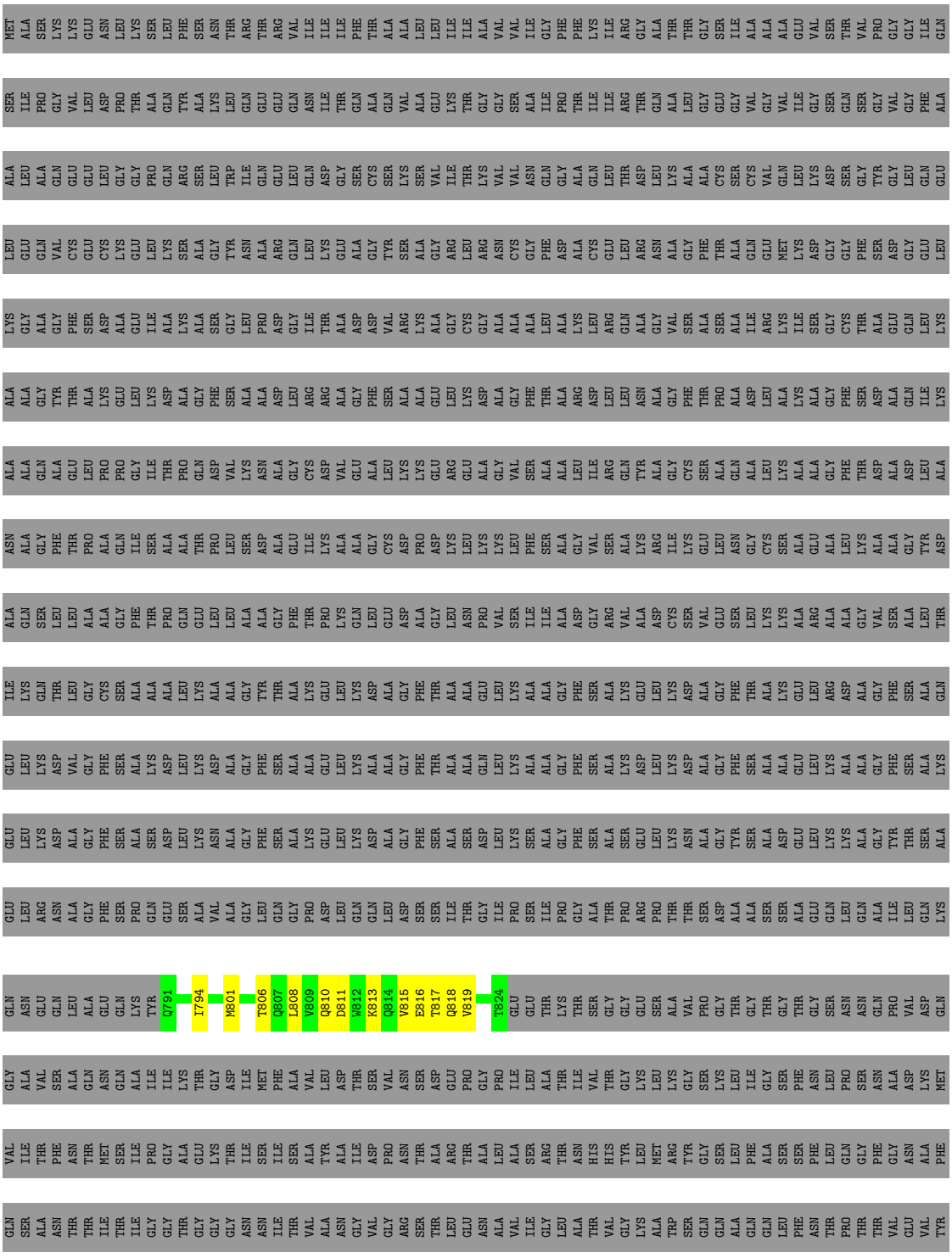
Chain Ig: 97%





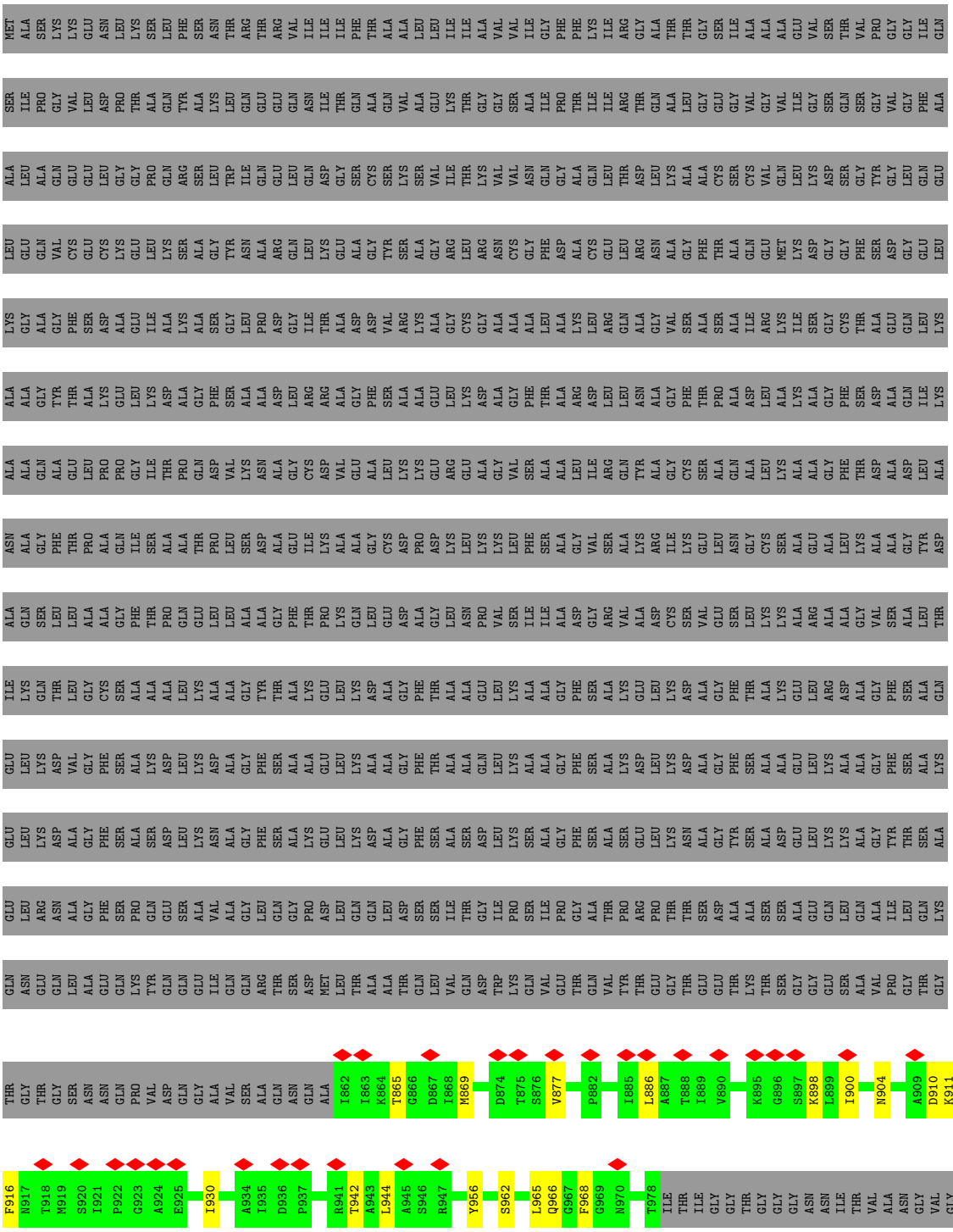
• Molecule 1: IcmE protein

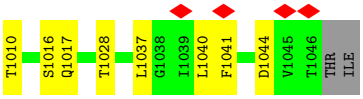
Chain Jg: 97%



• Molecule 1: IcmE protein

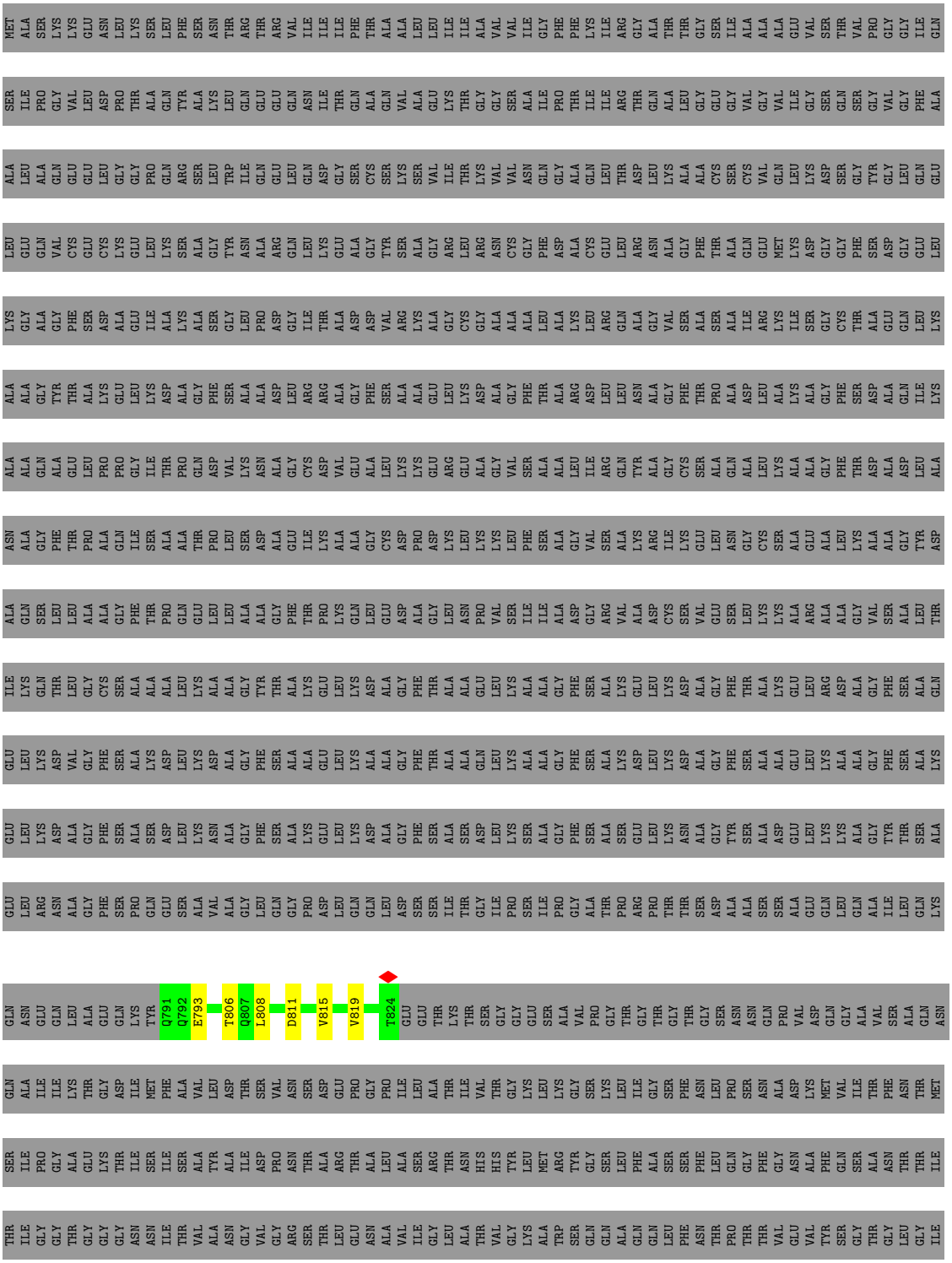
Chain CG:

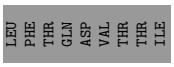




• Molecule 1: IcmE protein

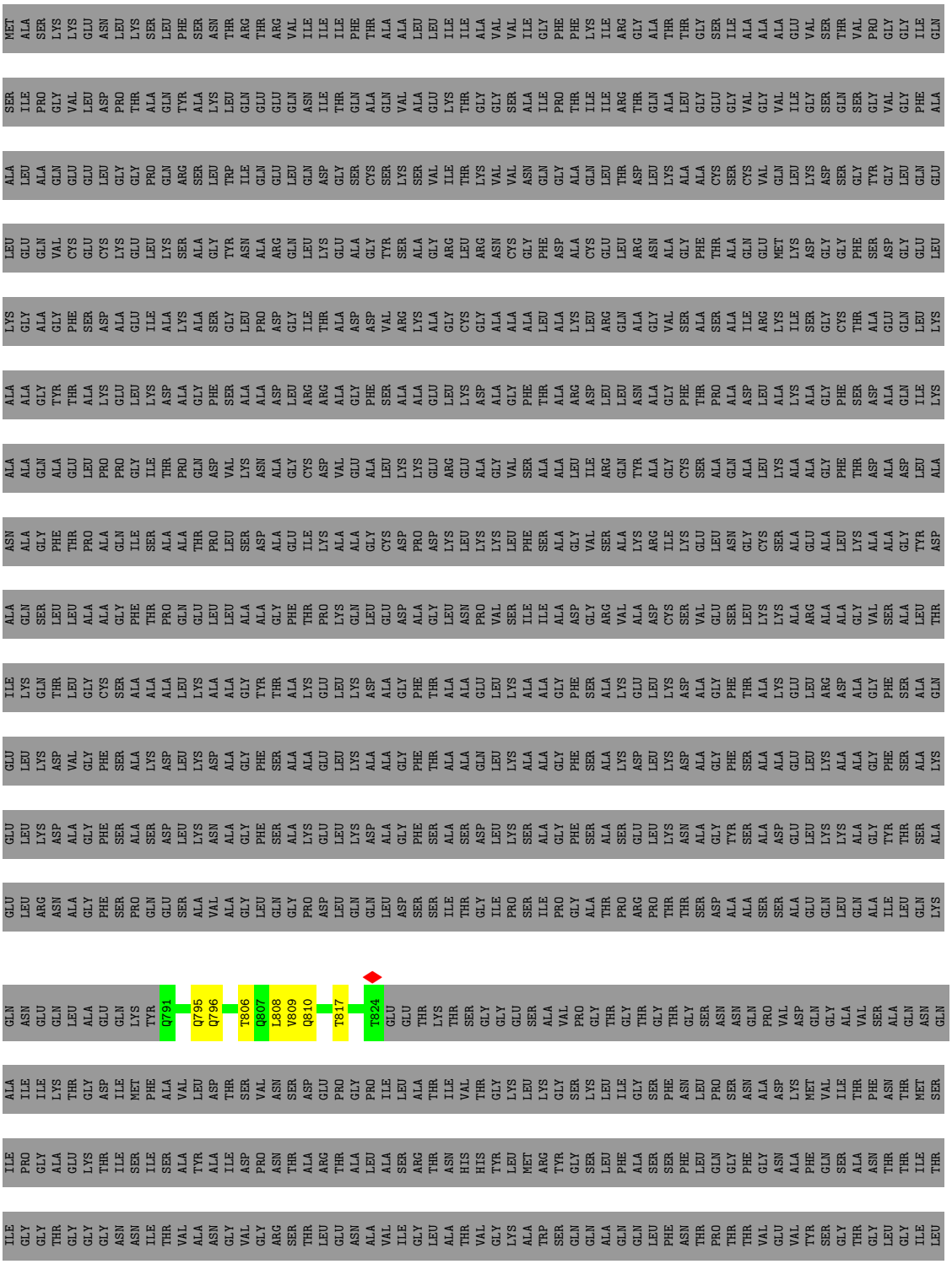
Chain Kg: 97%





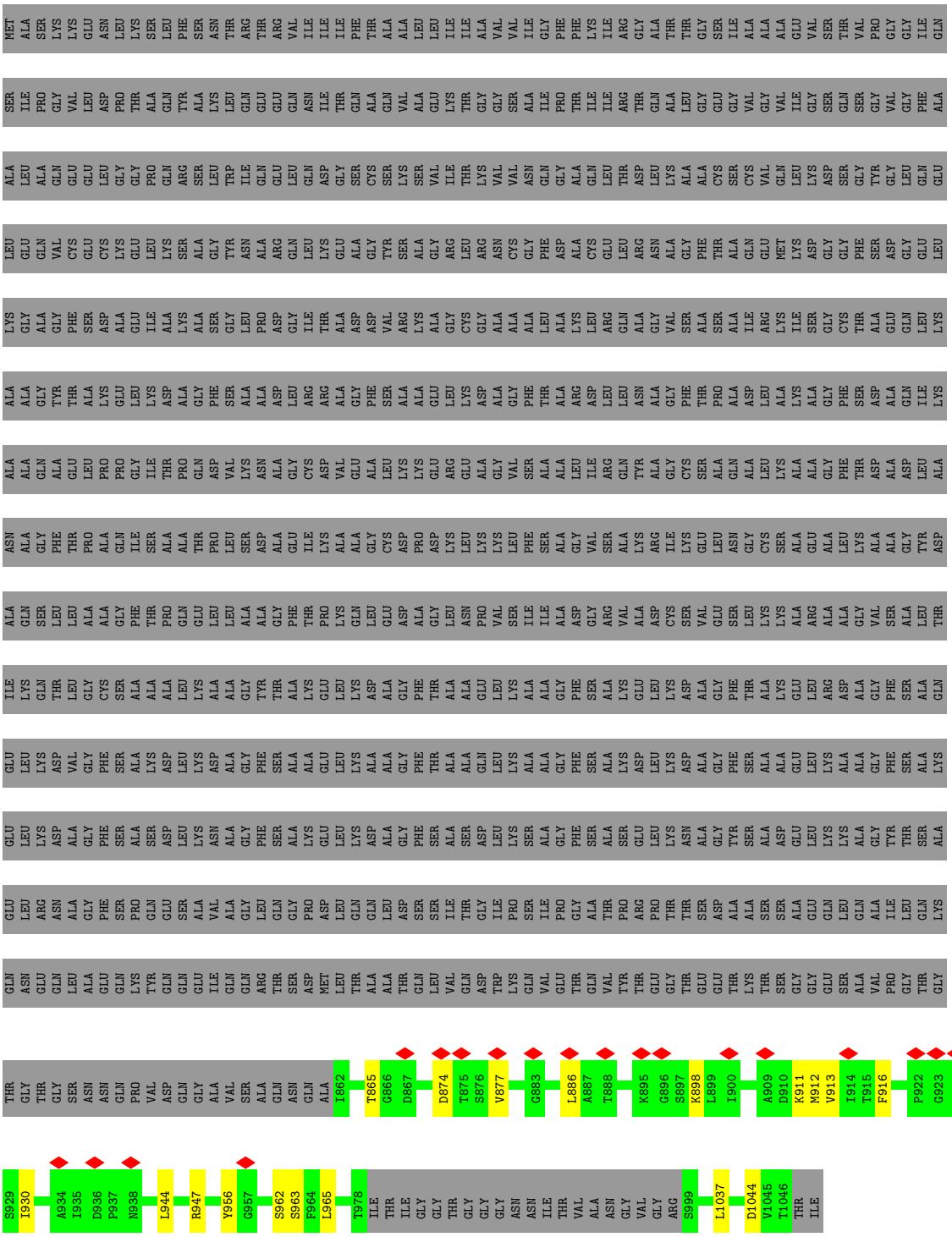
• Molecule 1: IcmE protein

Chain Lg: 97%



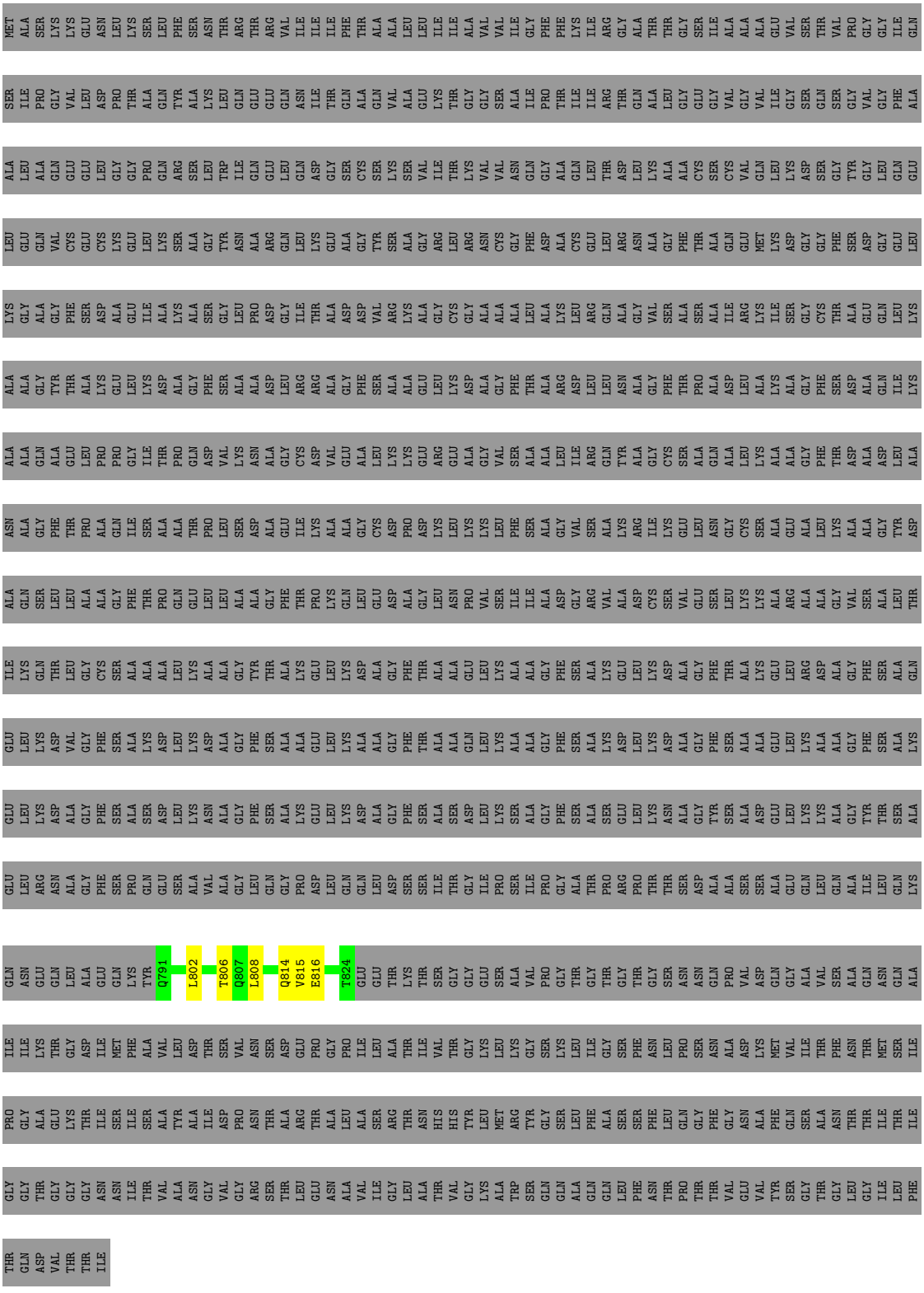
• Molecule 1: IcmE protein

Chain DG:



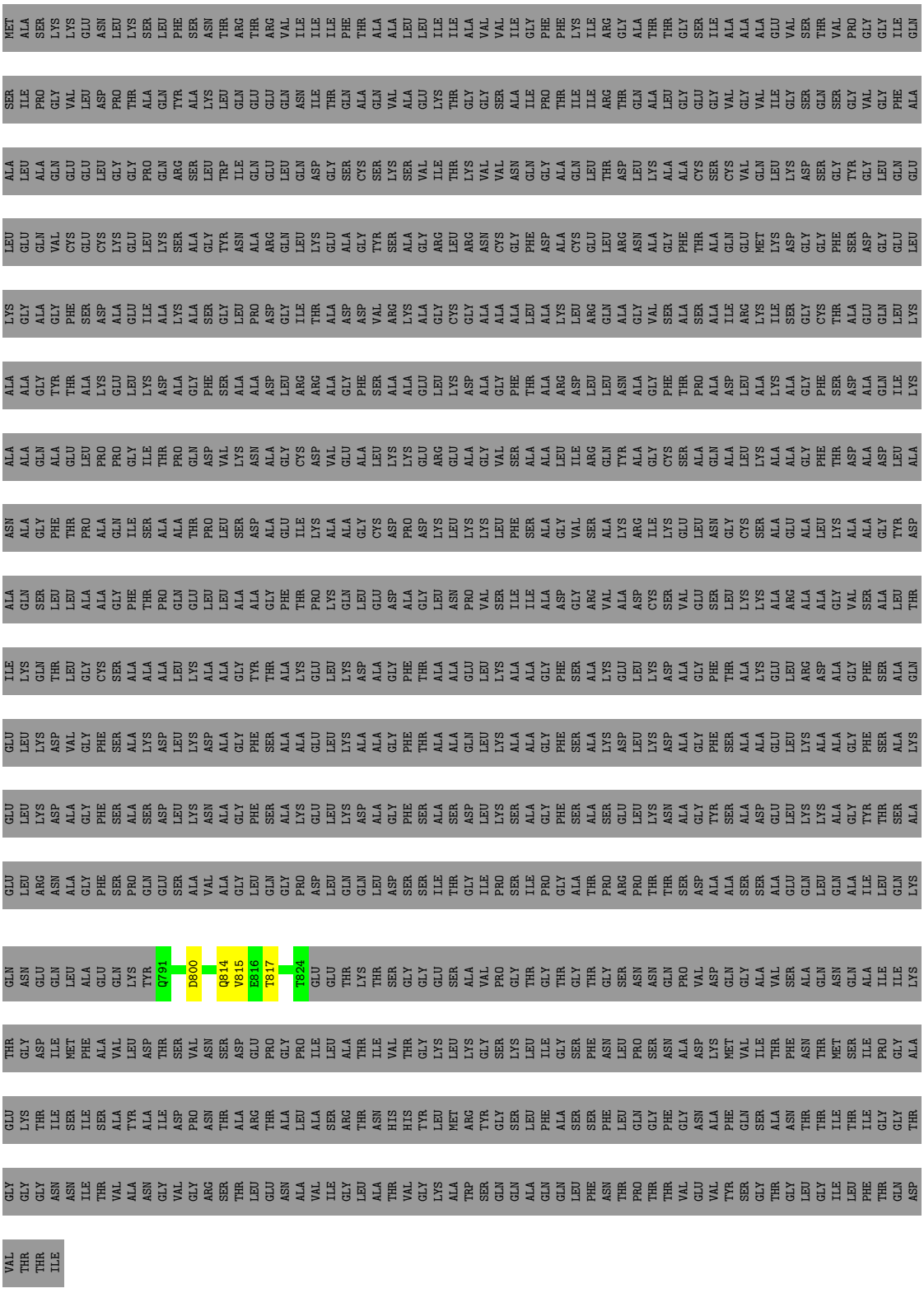
• Molecule 1: IcmE protein

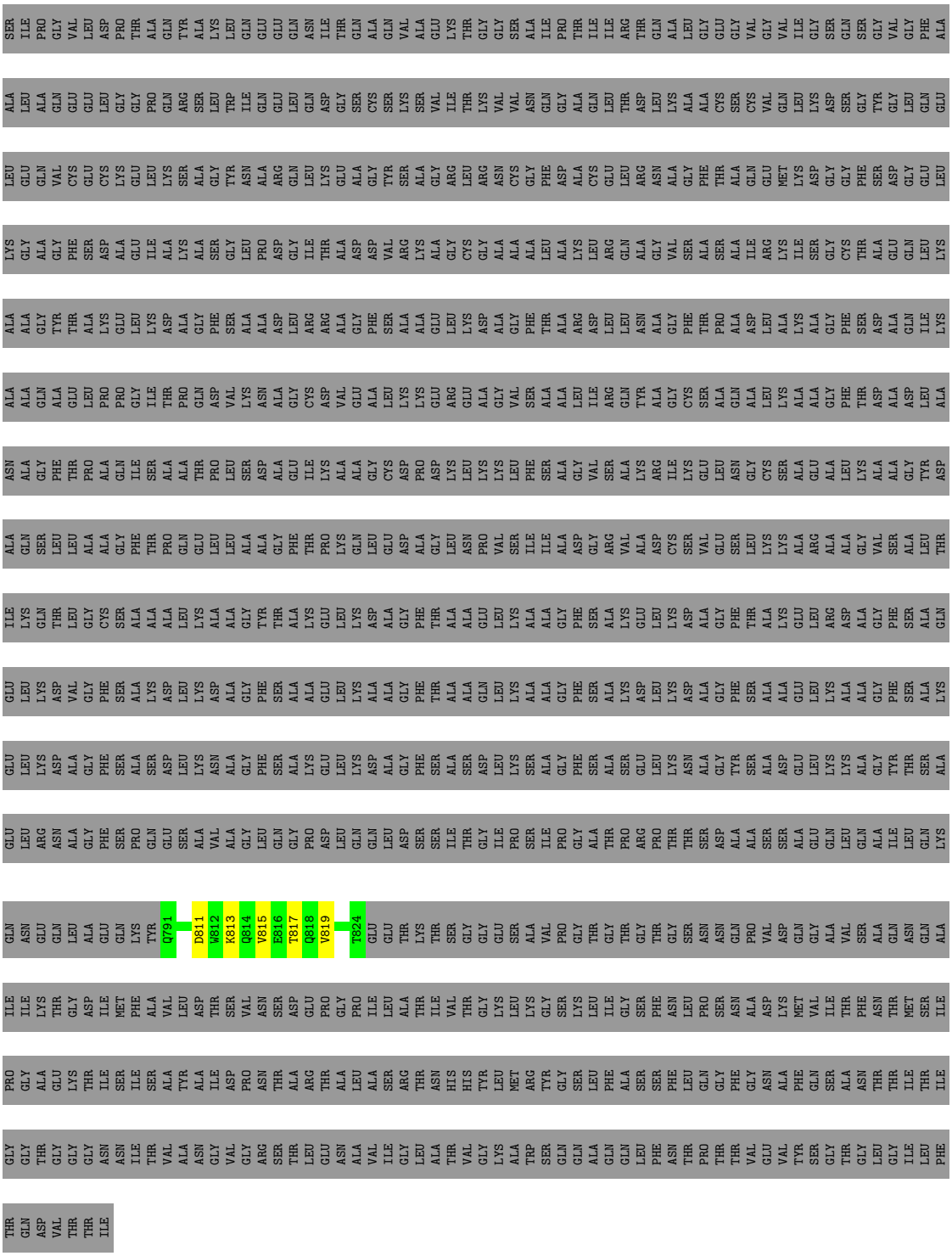
Chain Cg: 97%



• Molecule 1: IcmE protein

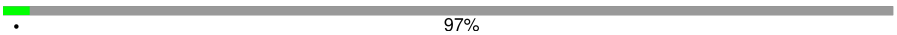
Chain Mg: 97%

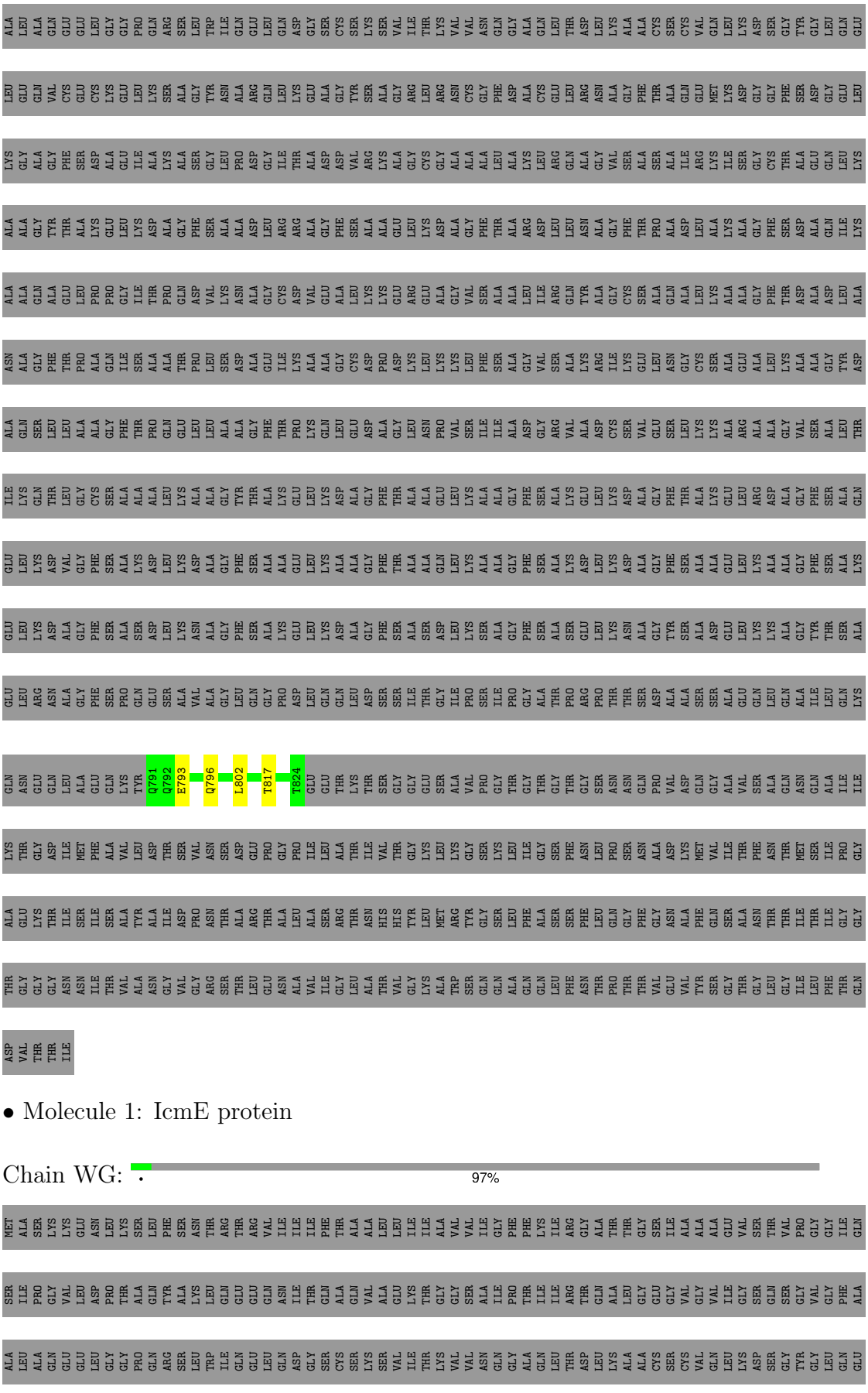

MET ALA SER LYS LYS GLU ASN LEU LYS SER LEU PHE SER ASN THR ARG THR ARG VAL ILE ILE ILE PHE THR ALA ALA LEU LEU ILE ILE ALA VAL VAL ILE GLY PHE PHE LYS ILE ARG GLY ALA THR THR GLY SER ILE ALA ALA GLU VAL SER THR VAL PRO GLY GLY ILE GLN
SER ILE PRO GLY VAL LEU ASP PRO THR ALA GLN TYR ALA LYS LEU GLN GLU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



• Molecule 1: IcmE protein

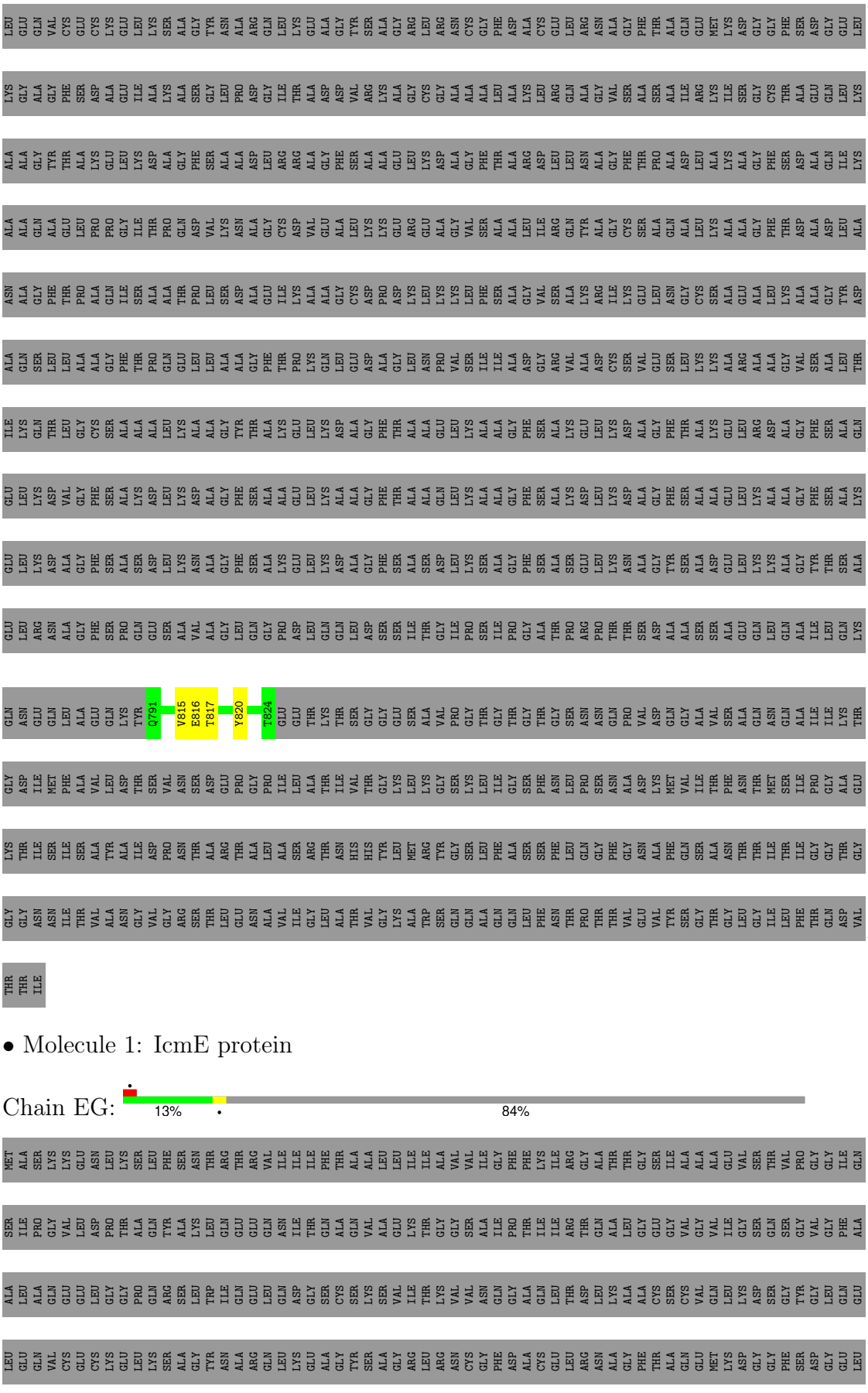
Chain VG:





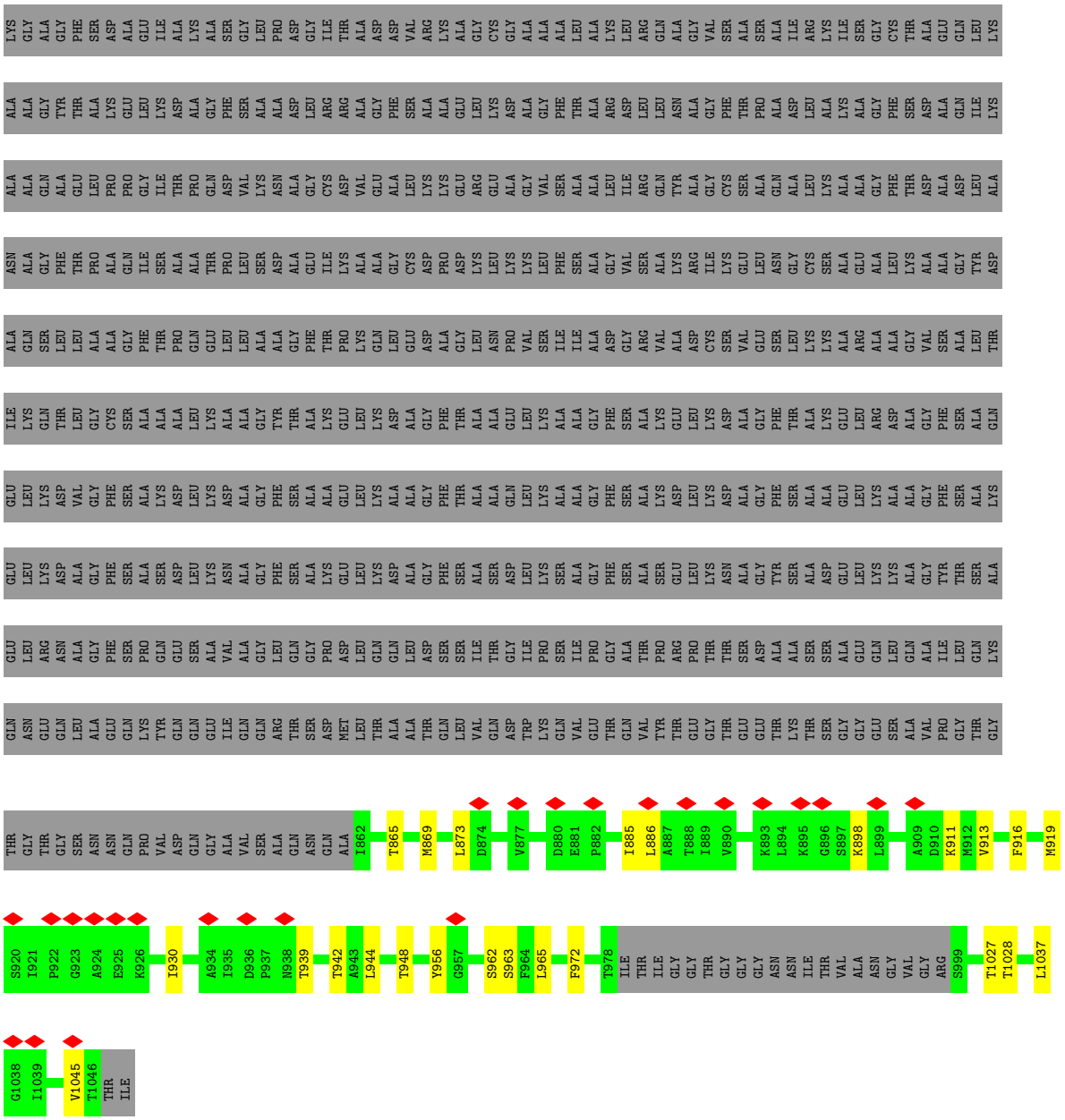
• Molecule 1: IcmE protein

Chain WG:



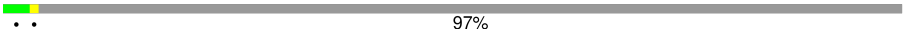
• Molecule 1: IcmE protein

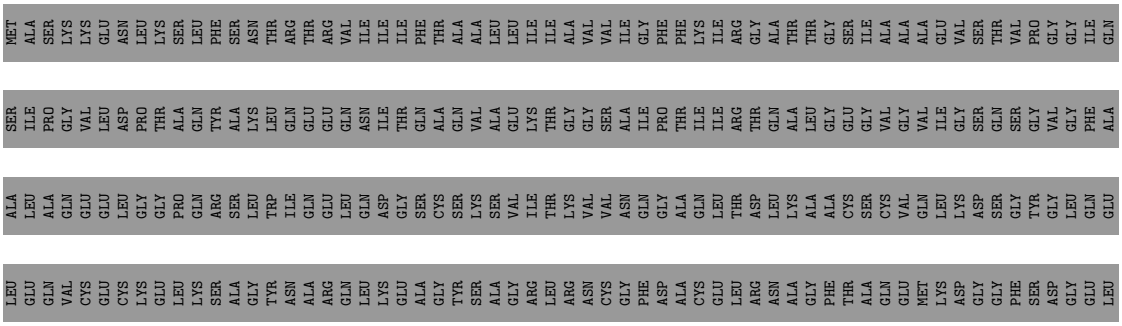
Chain EG:

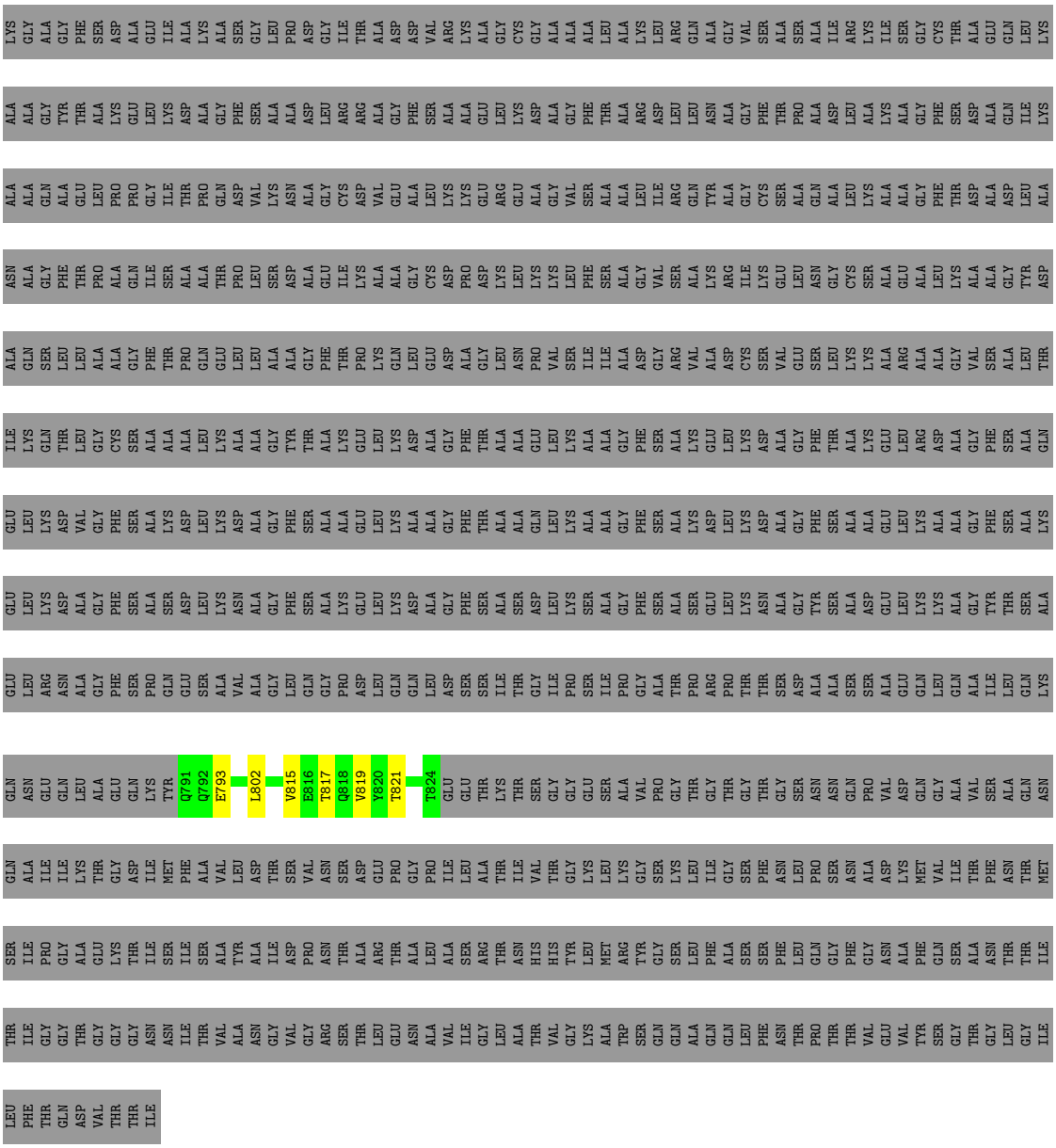


• Molecule 1: IcmE protein

Chain XG:

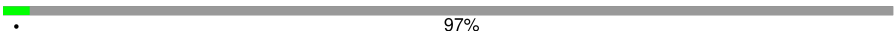


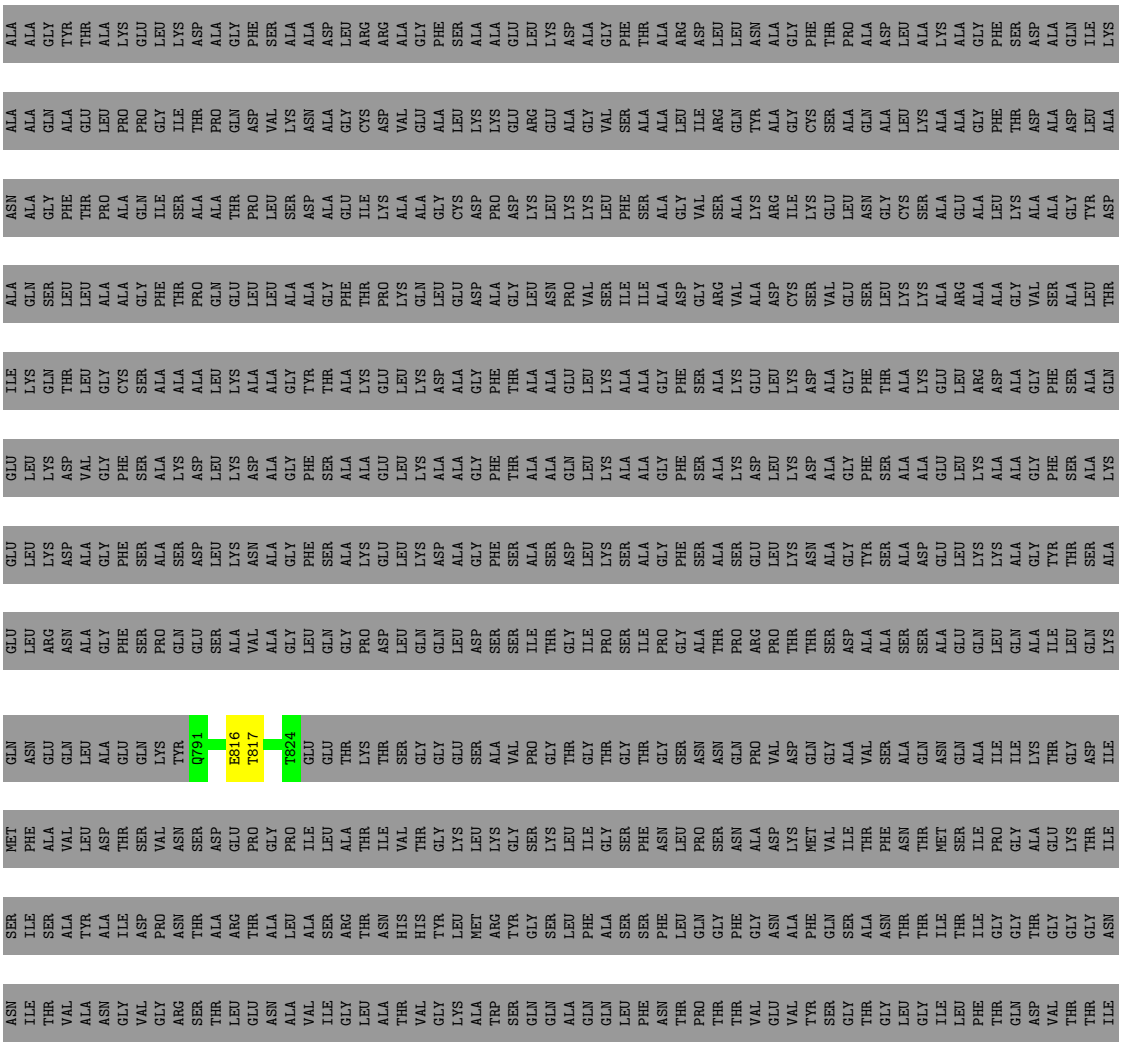




• Molecule 1: IcmE protein

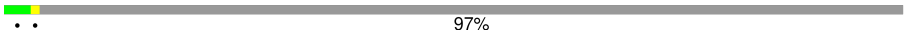
Chain YG:

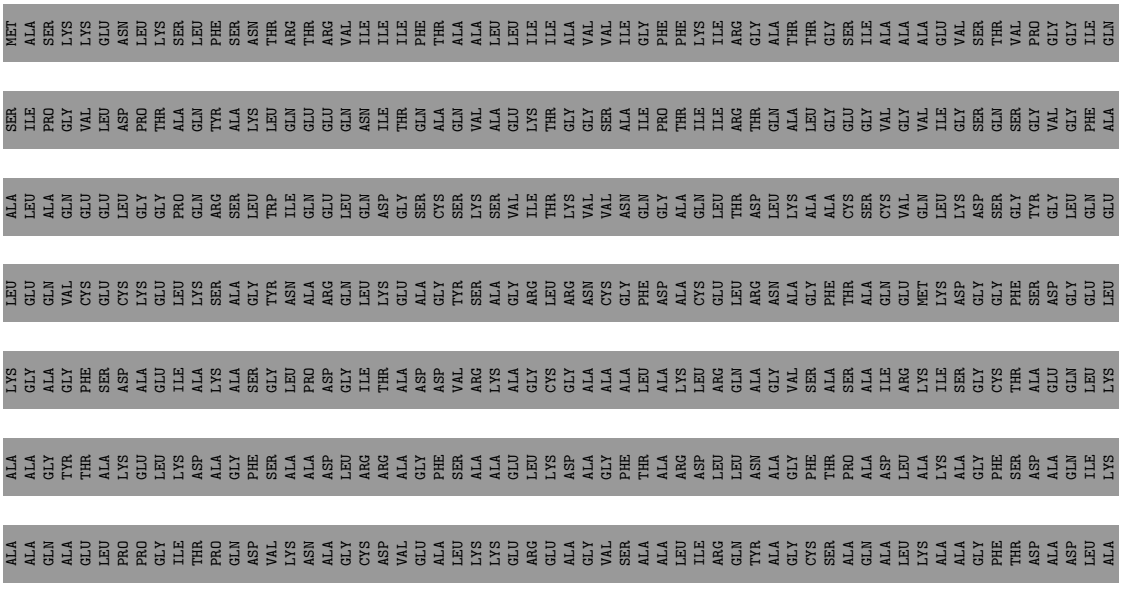


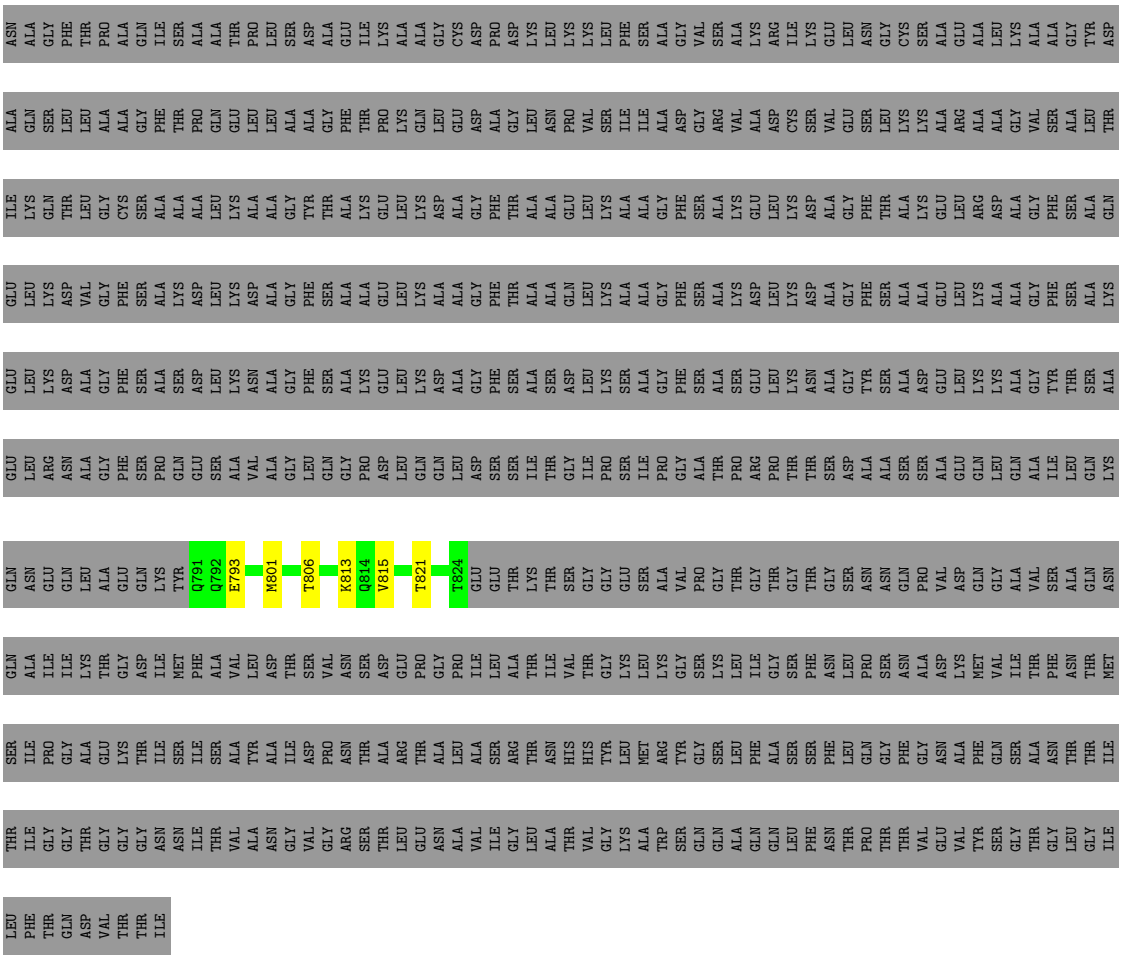


• Molecule 1: IcmE protein

Chain ZG:

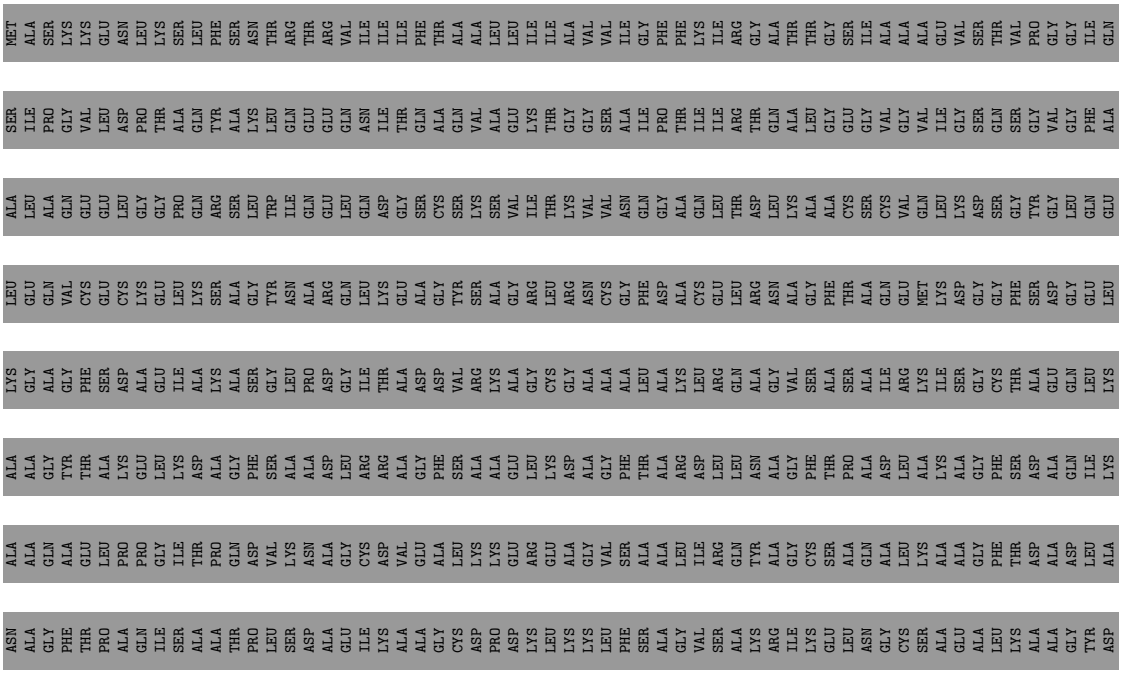


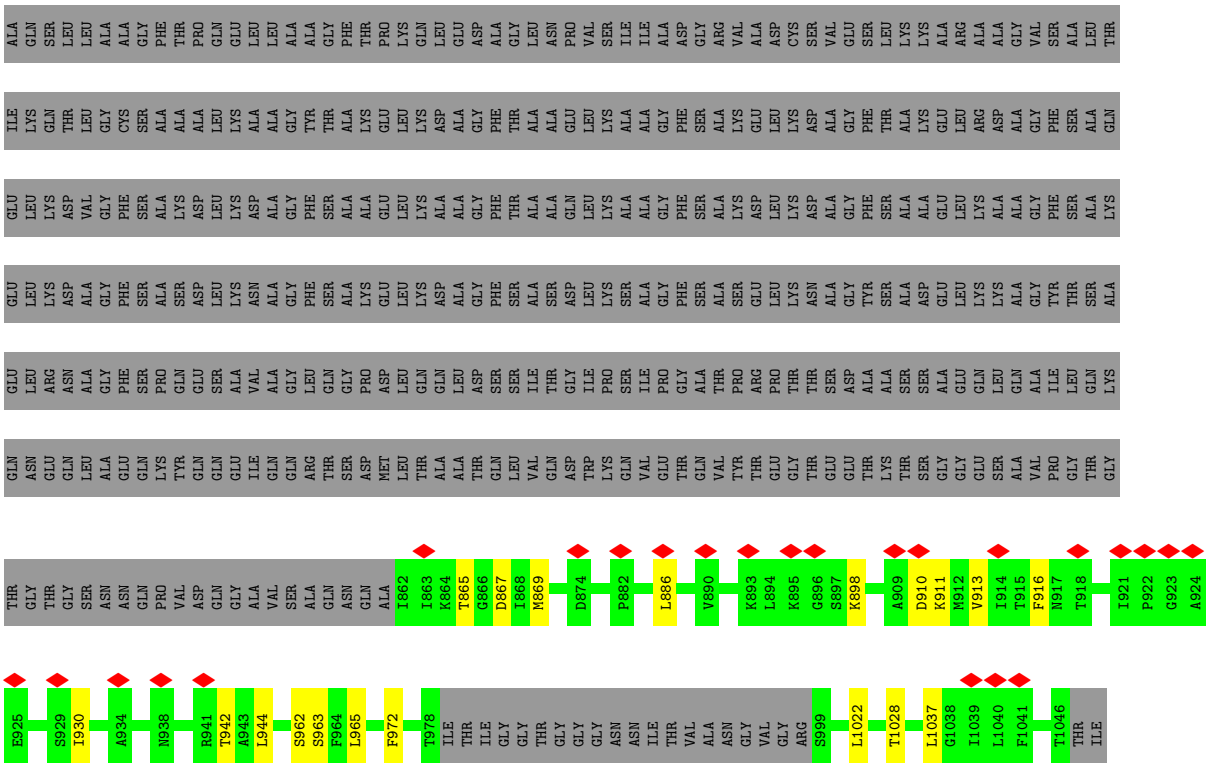




• Molecule 1: IcmE protein

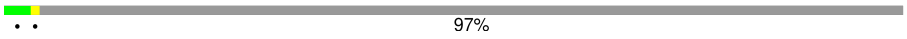
Chain FG:

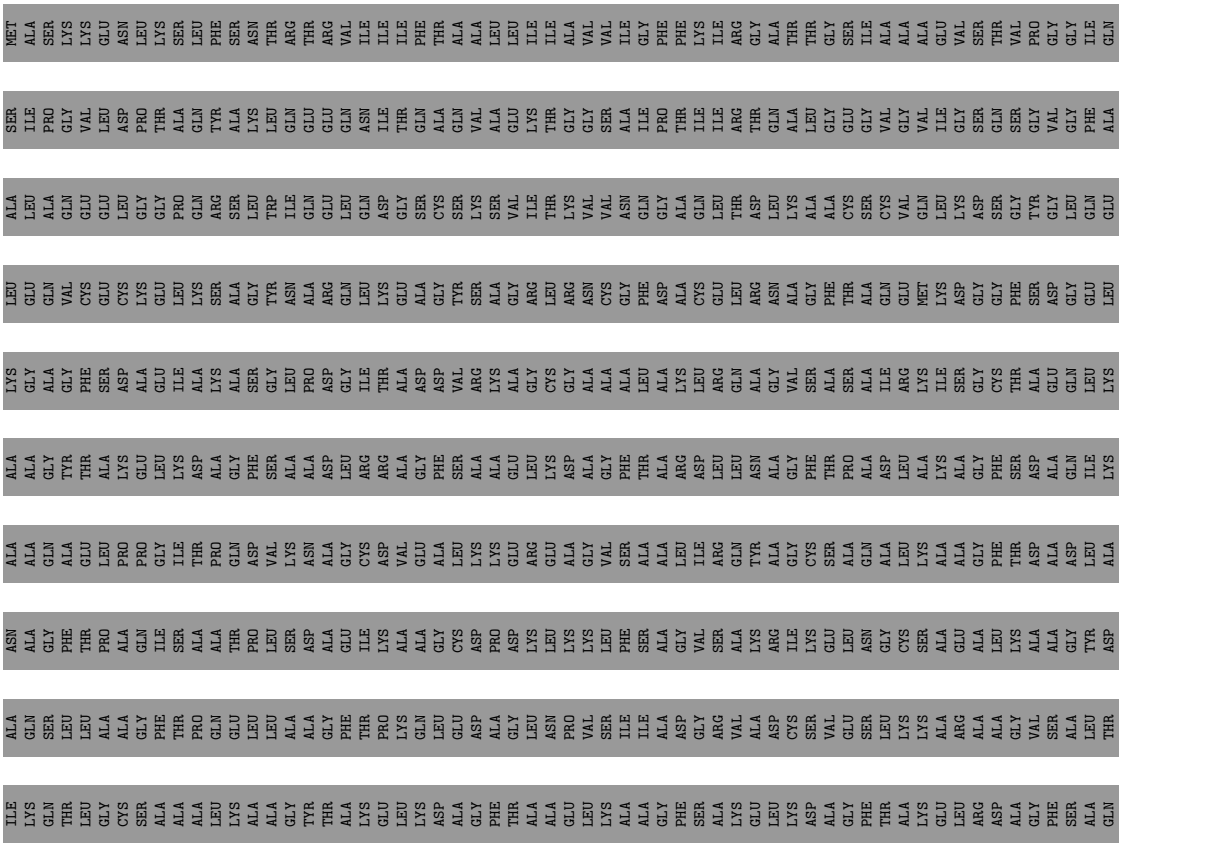




• Molecule 1: IcmE protein

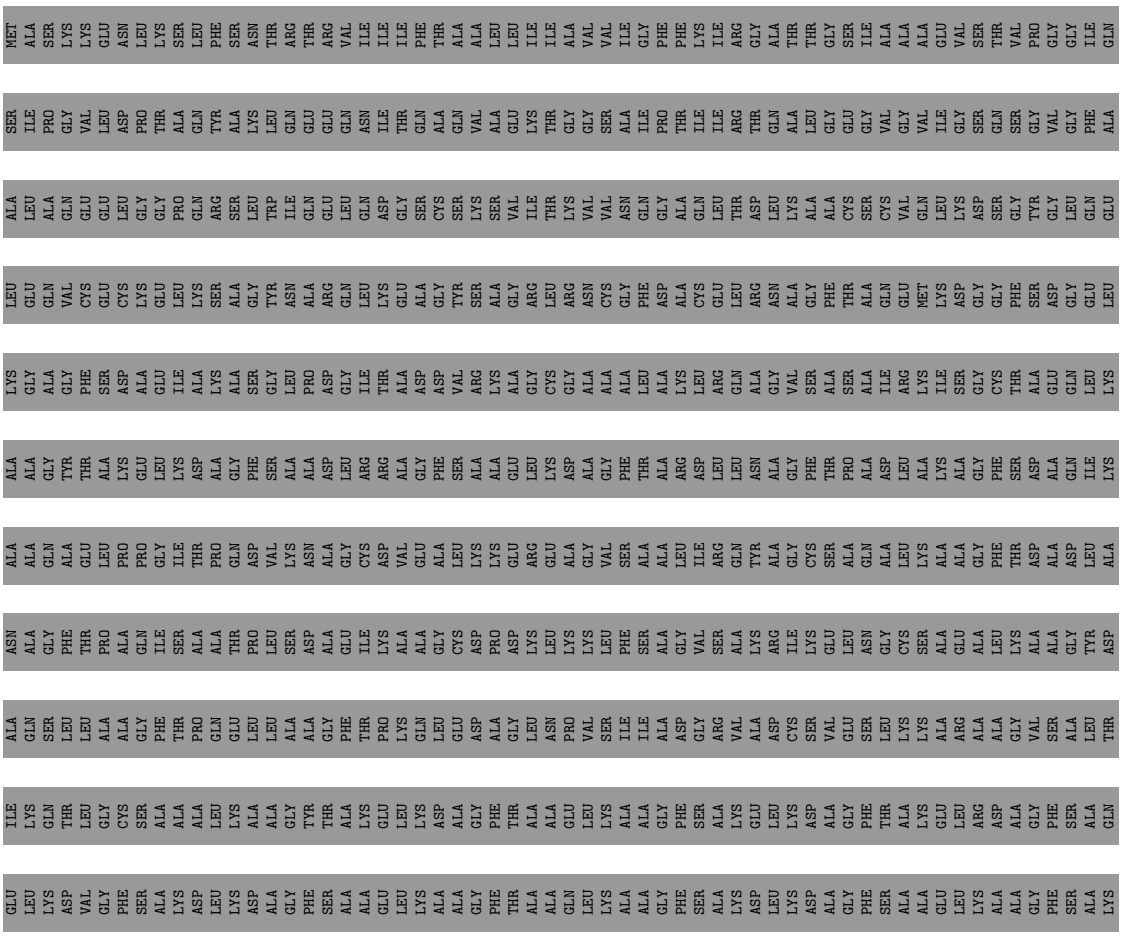
Chain Dg:

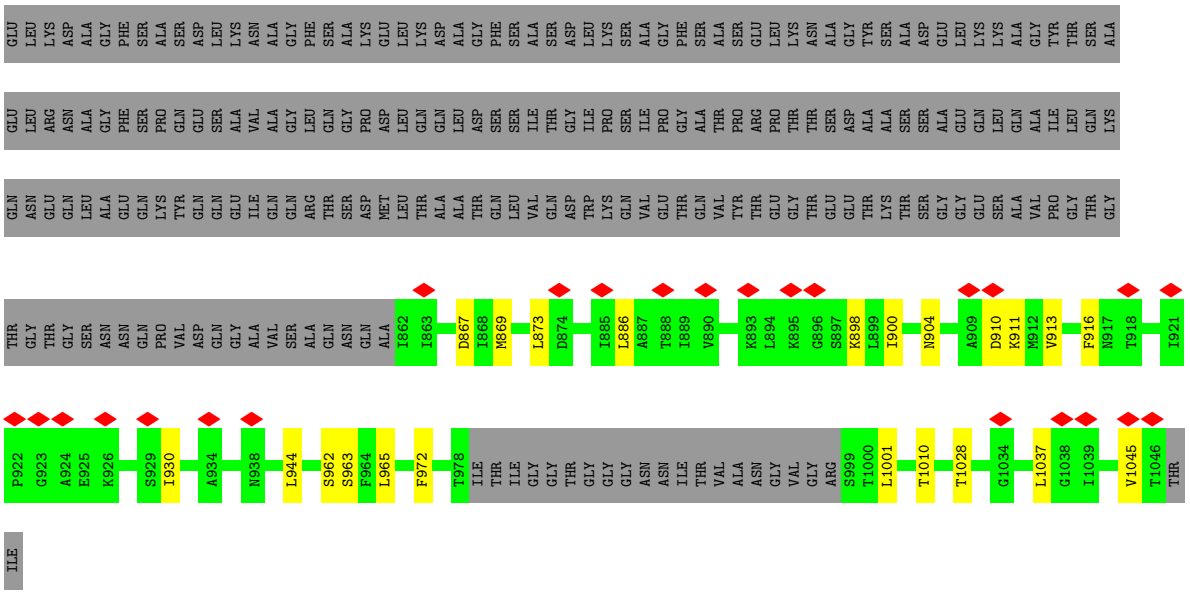




• Molecule 1: IcmE protein

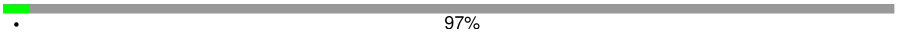
Chain GG:

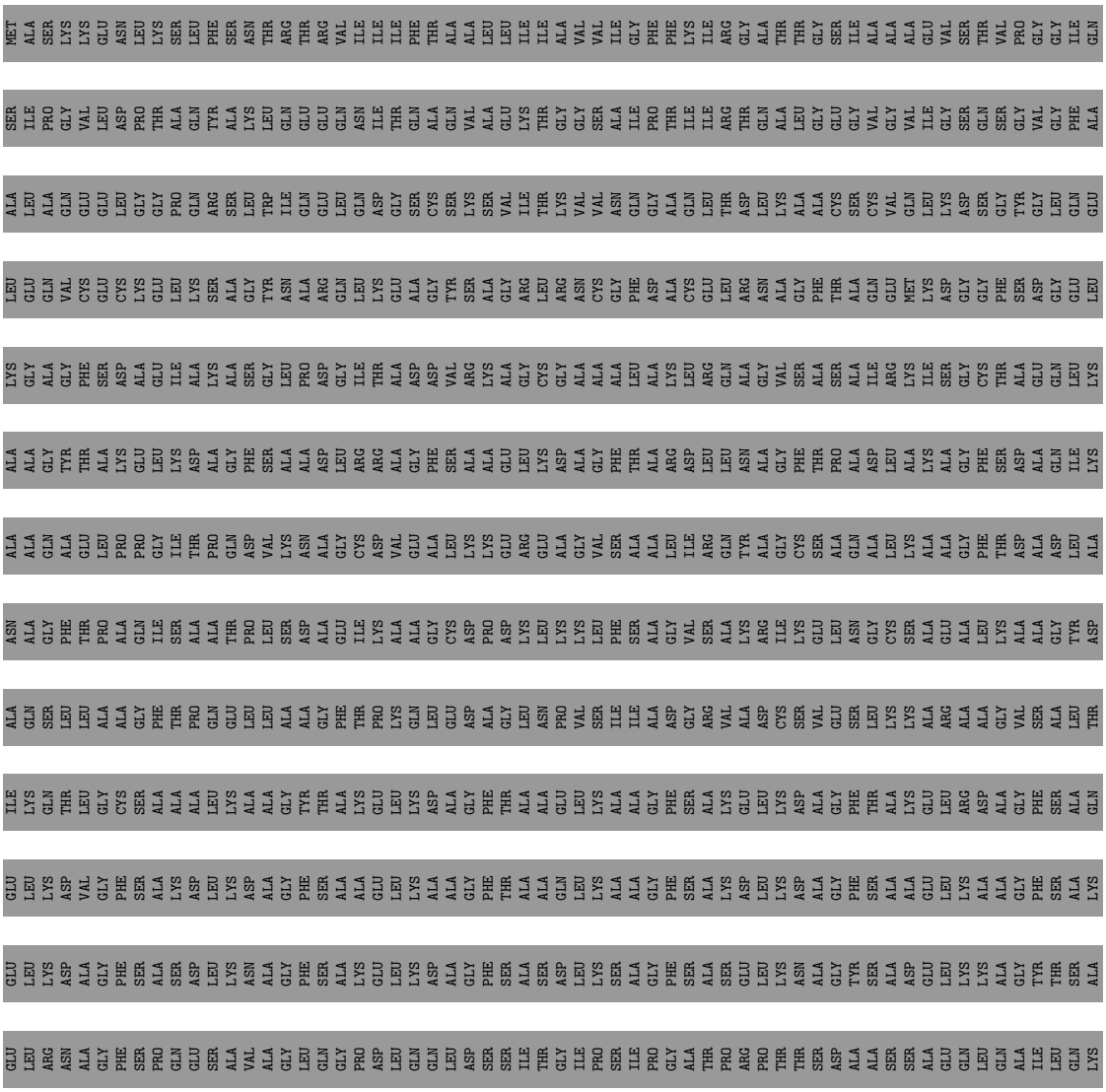


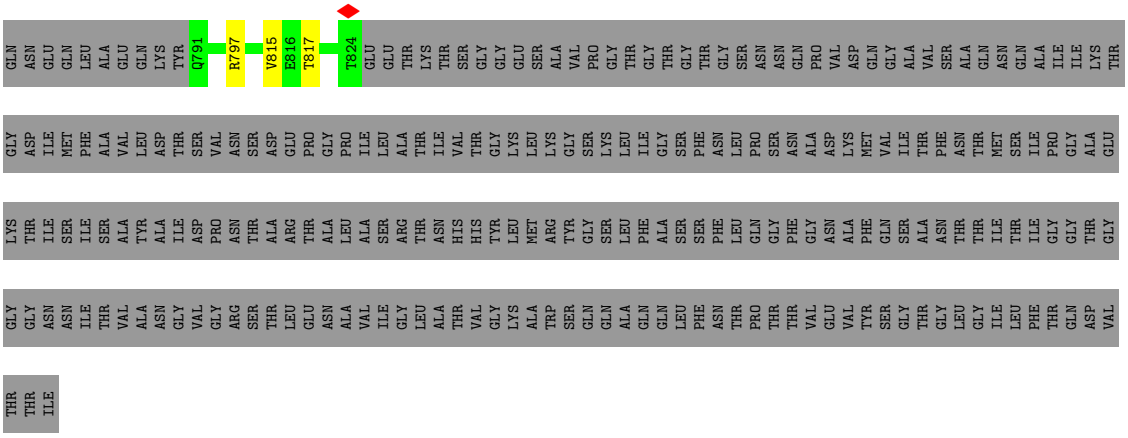


• Molecule 1: IcmE protein

Chain Fg:

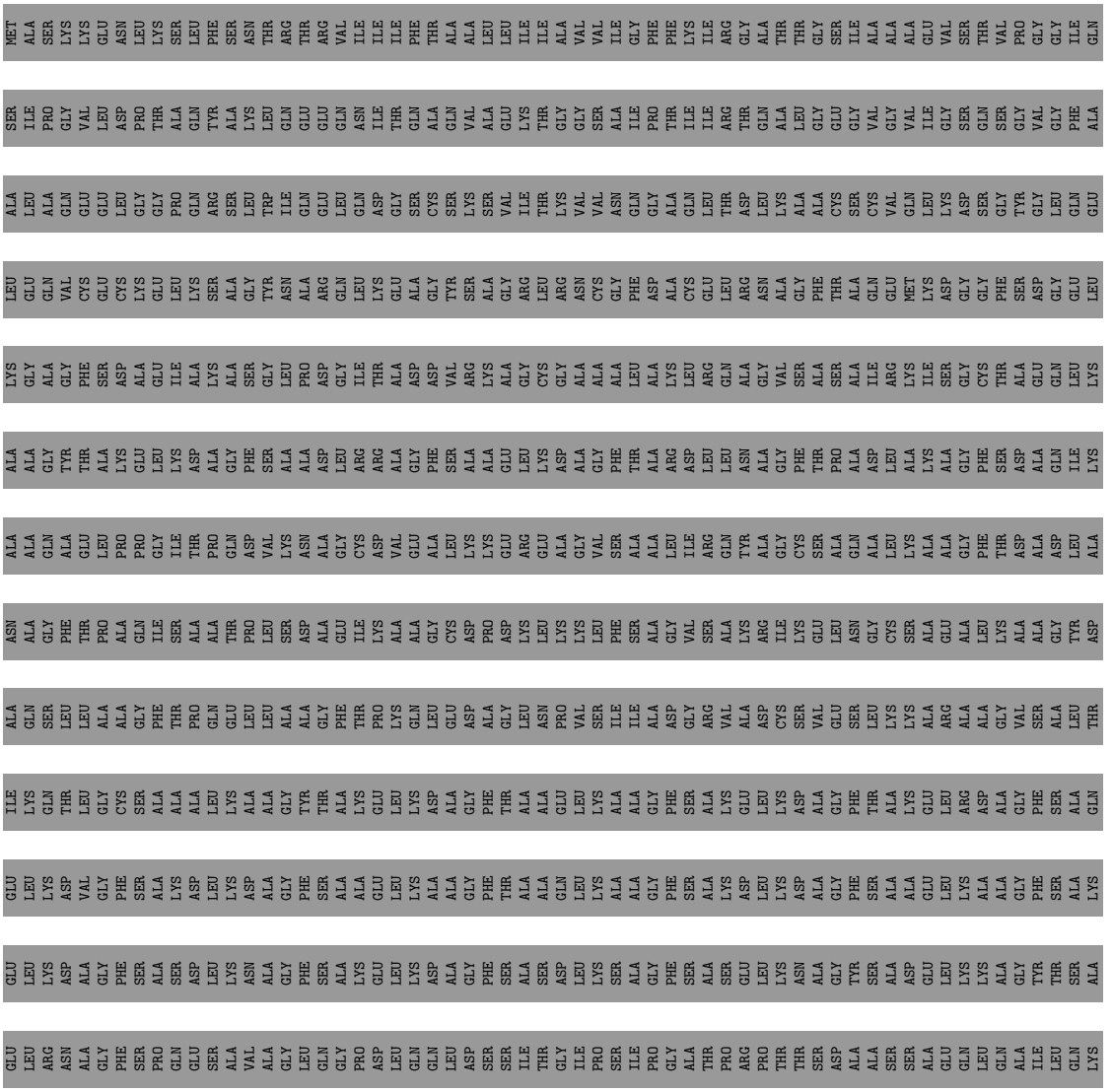


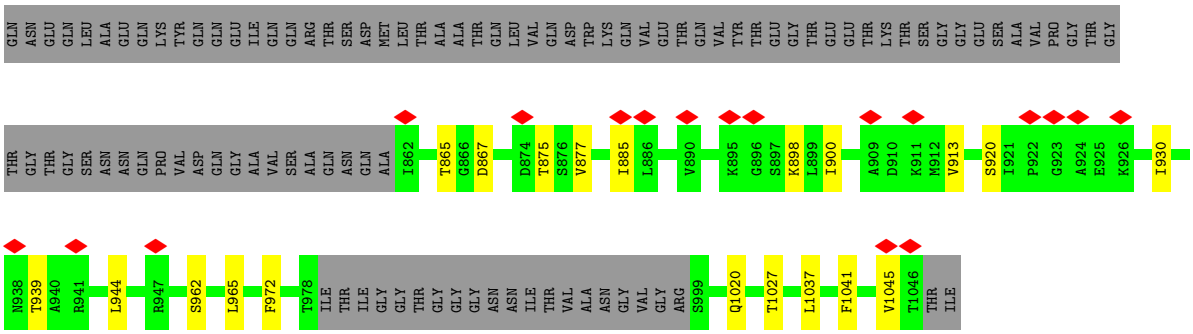




• Molecule 1: IcmE protein

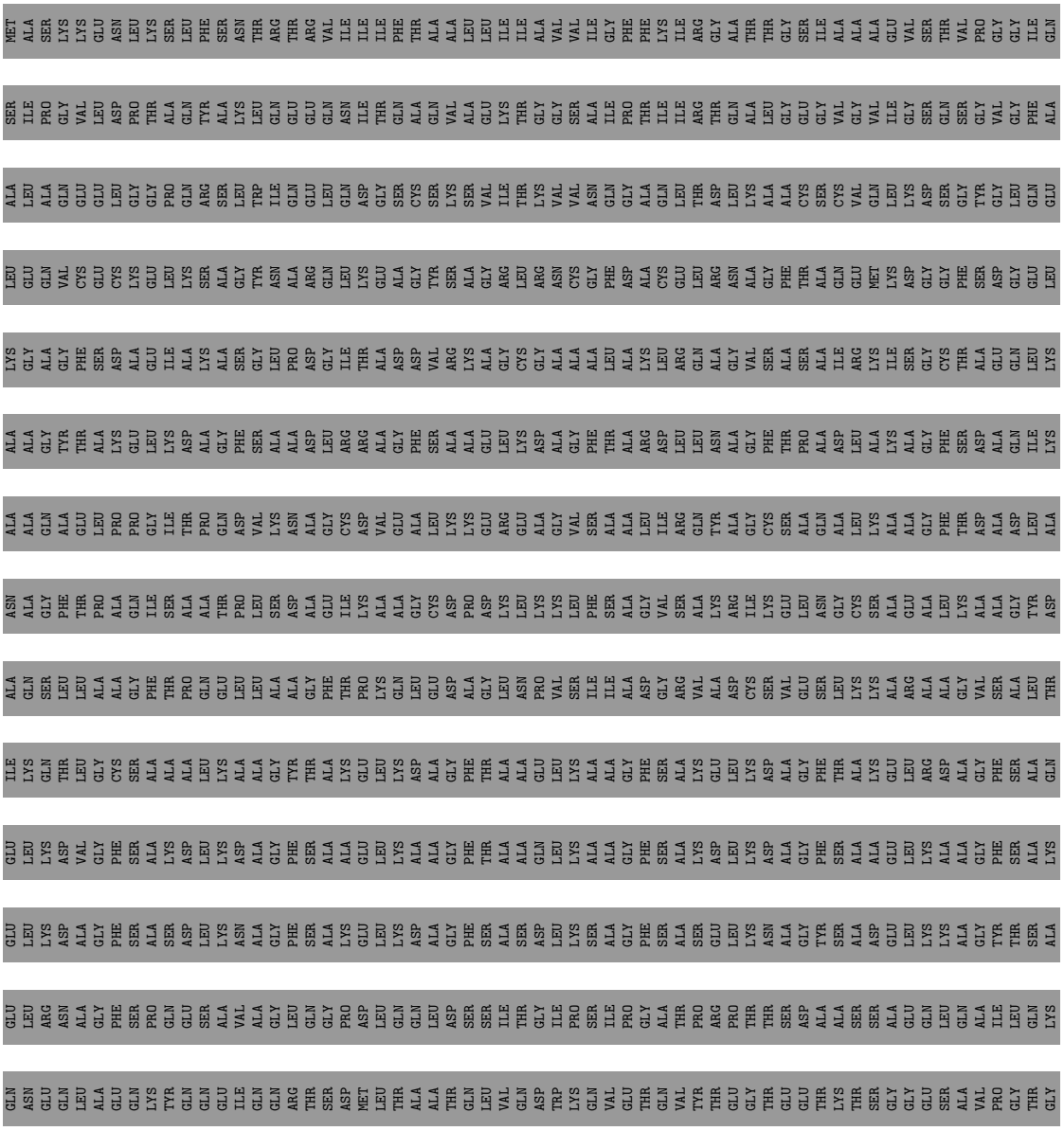
Chain HG:

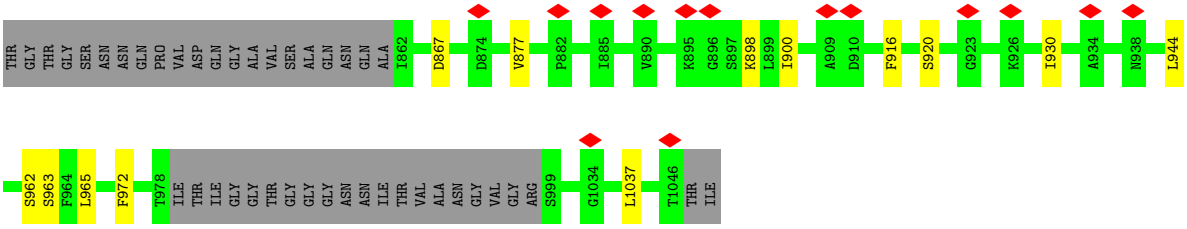




• Molecule 1: IcmE protein

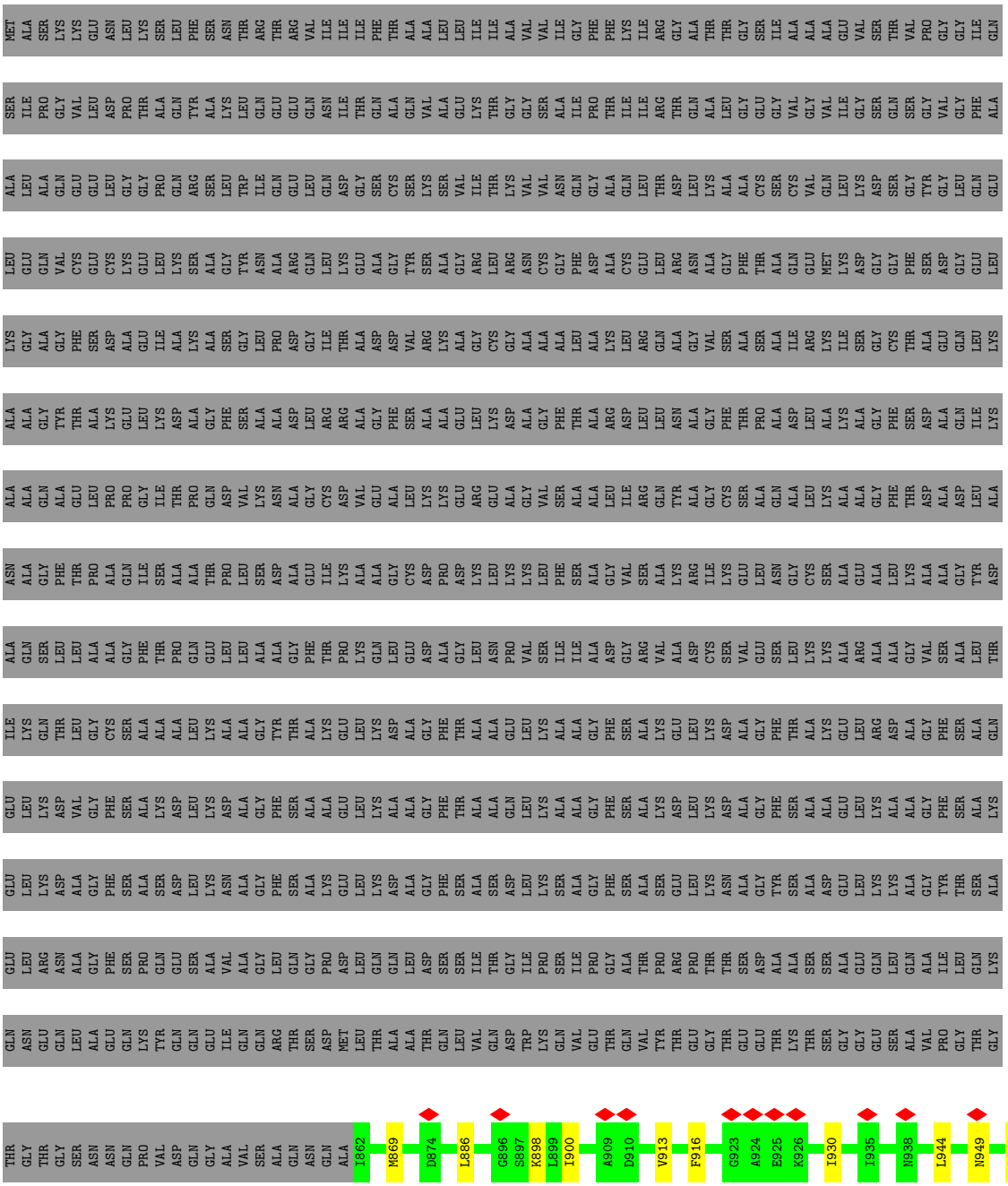
Chain IG:





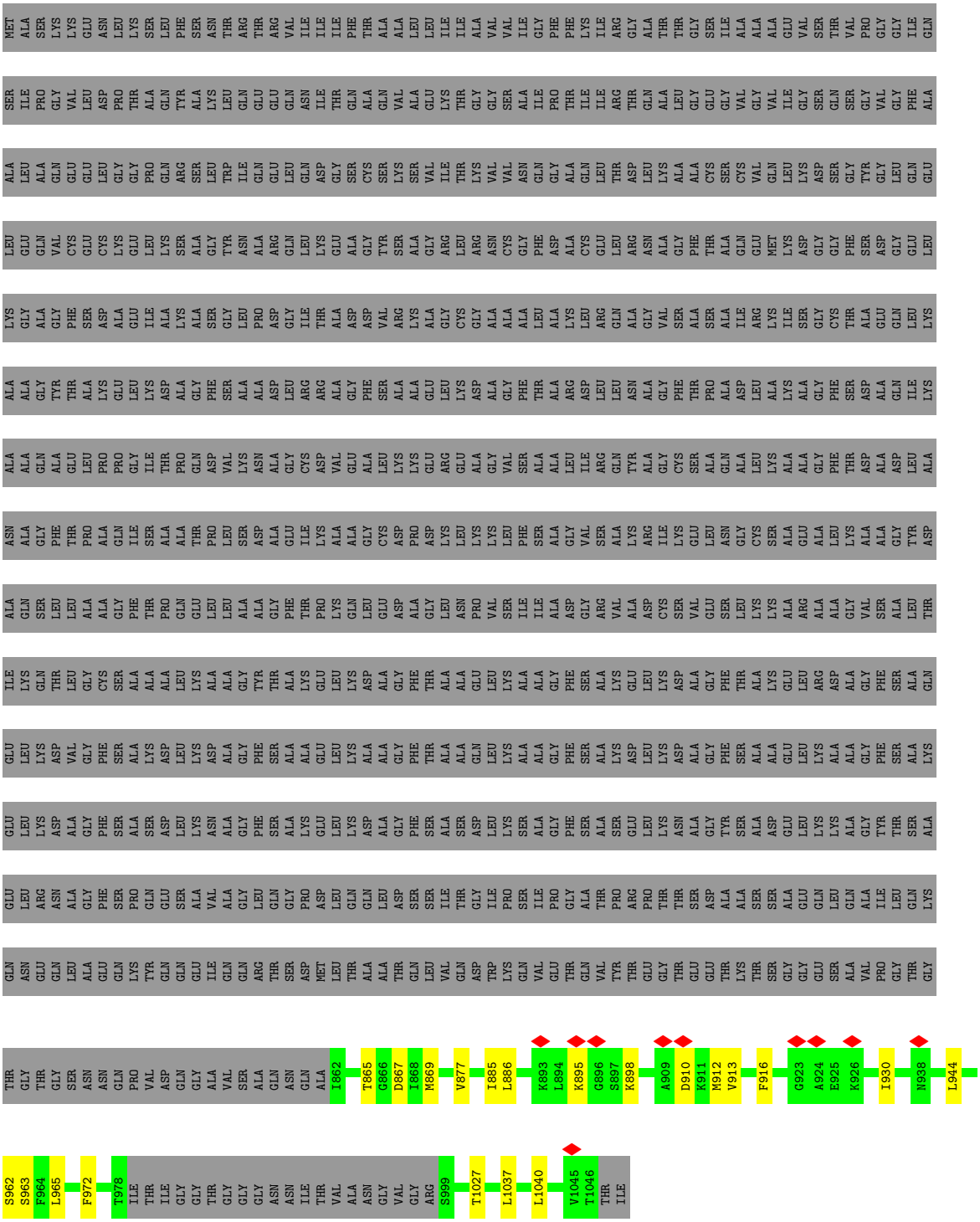
• Molecule 1: IcmE protein

Chain JG:



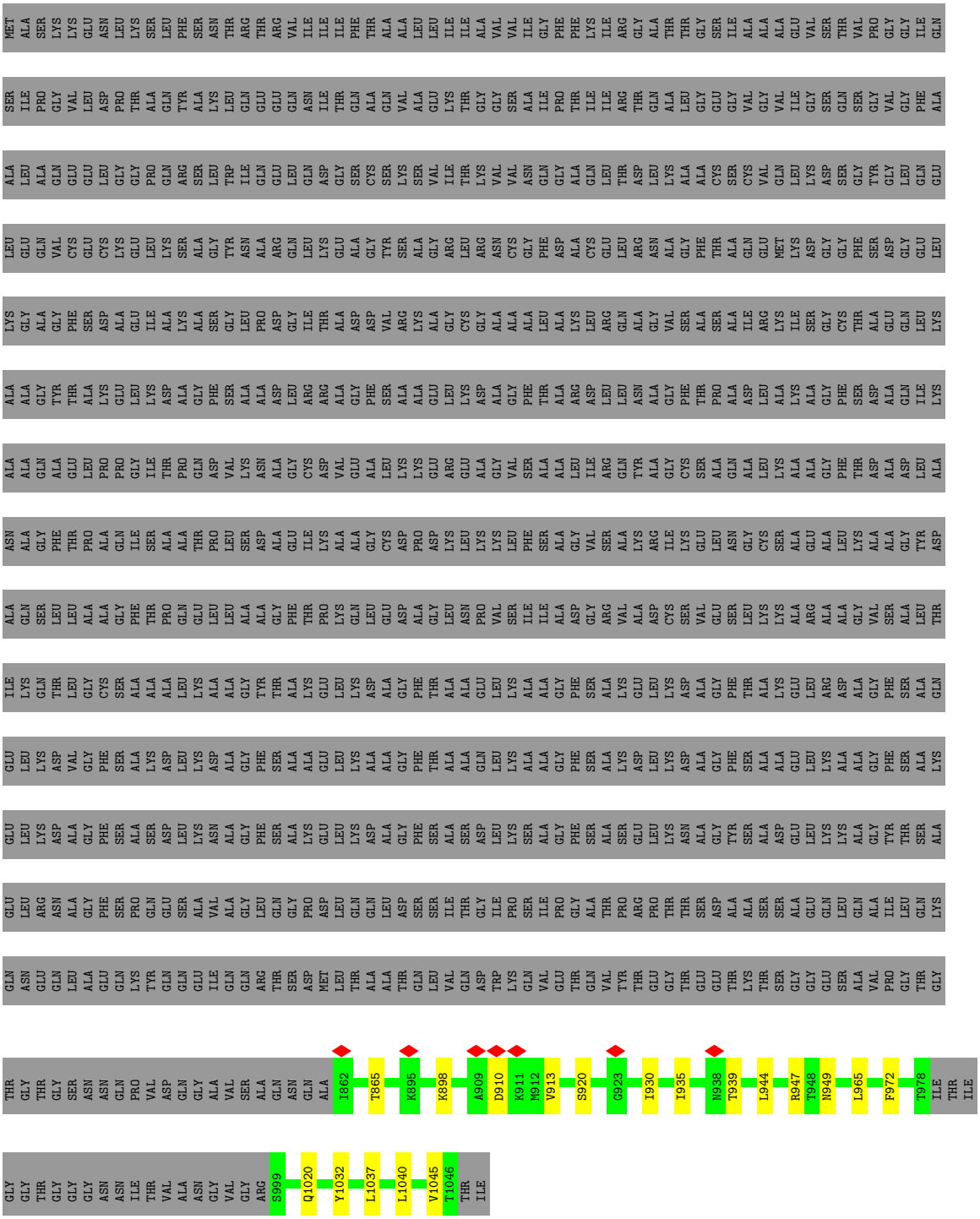
• Molecule 1: IcmE protein

Chain KG:



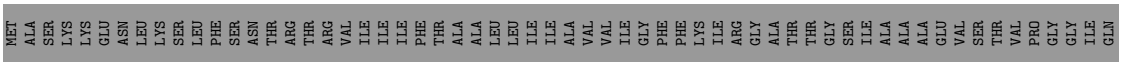
• Molecule 1: IcmE protein

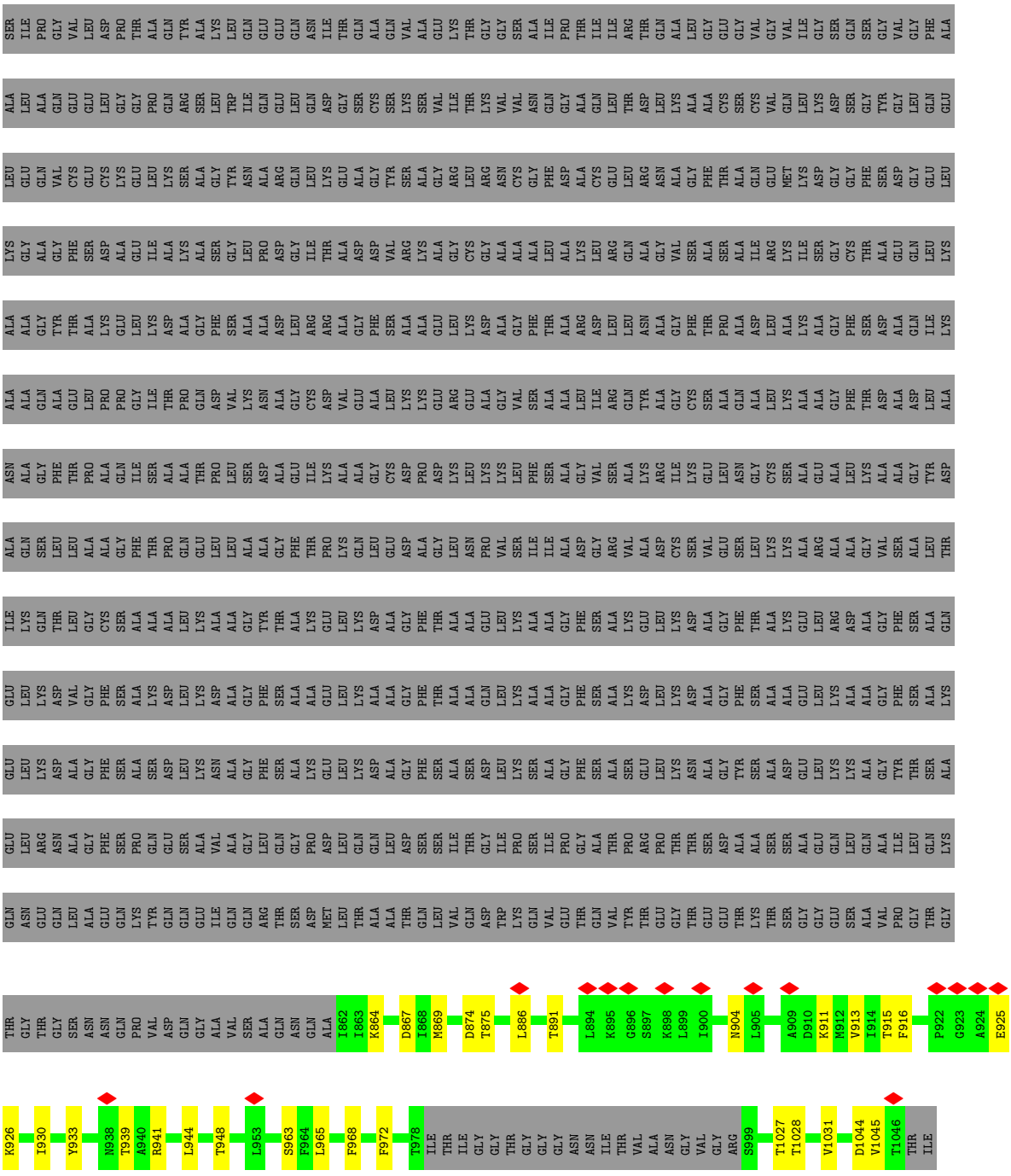
Chain LG:



• Molecule 1: IcmE protein

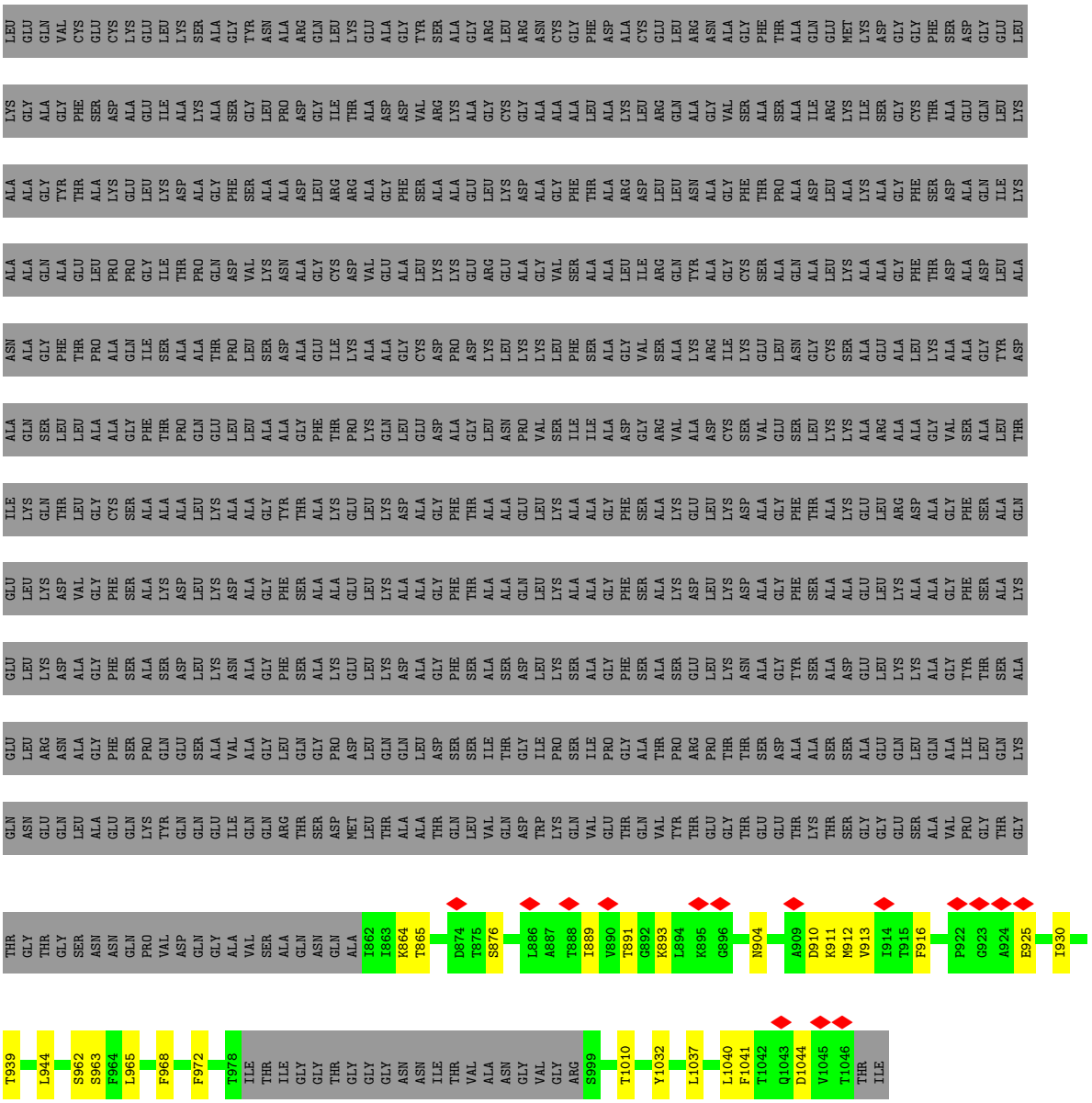
Chain MG:





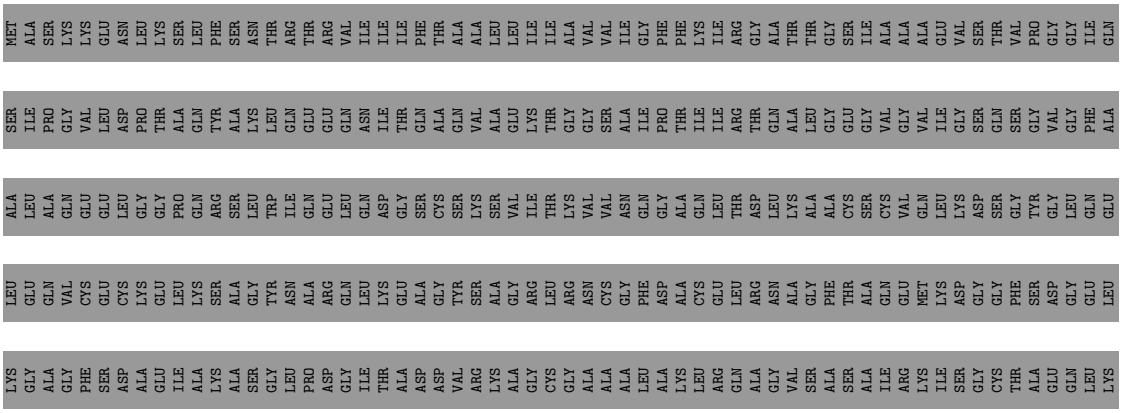
• Molecule 1: IcmE protein

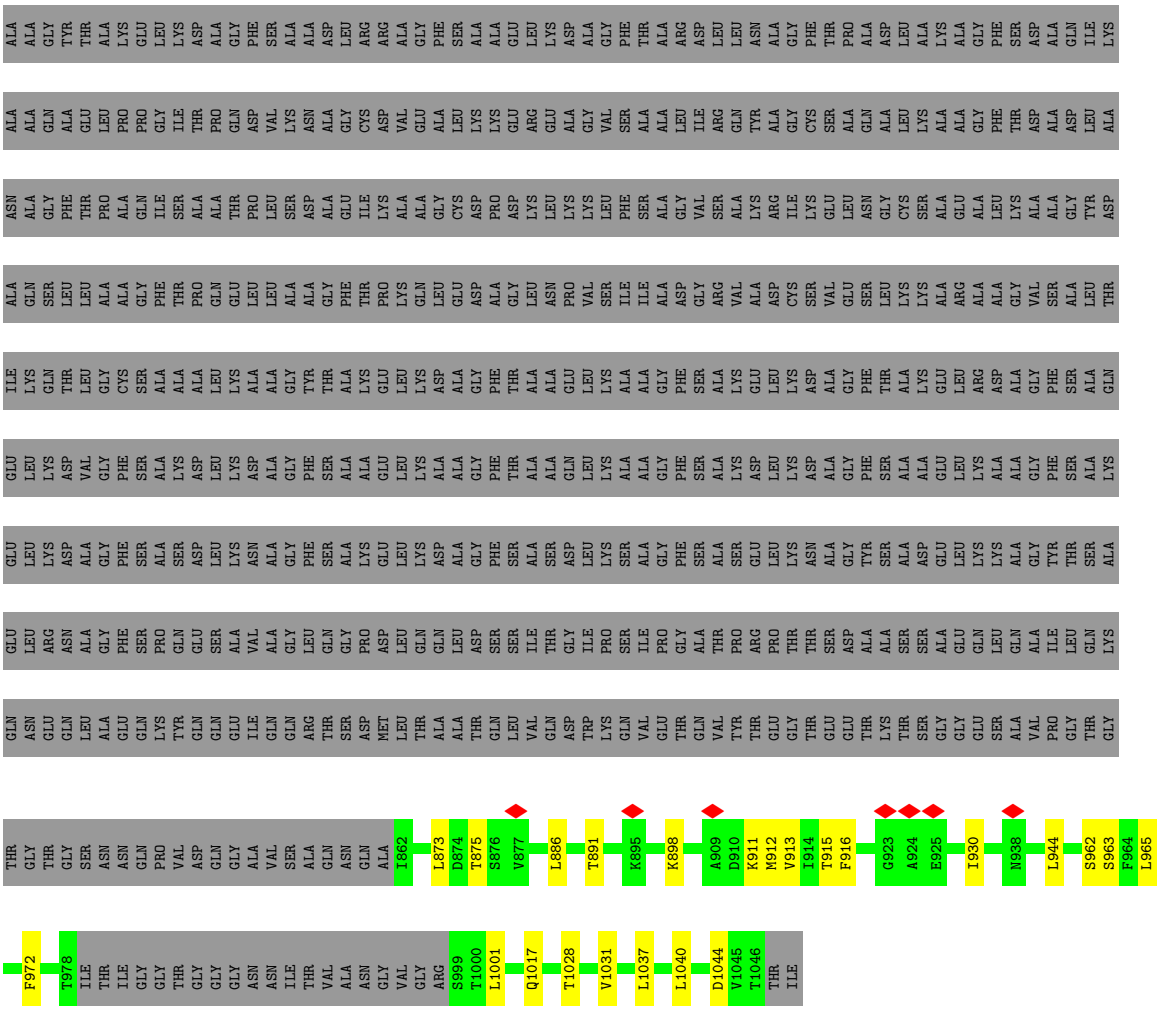
Chain NG:



• Molecule 1: IcmE protein

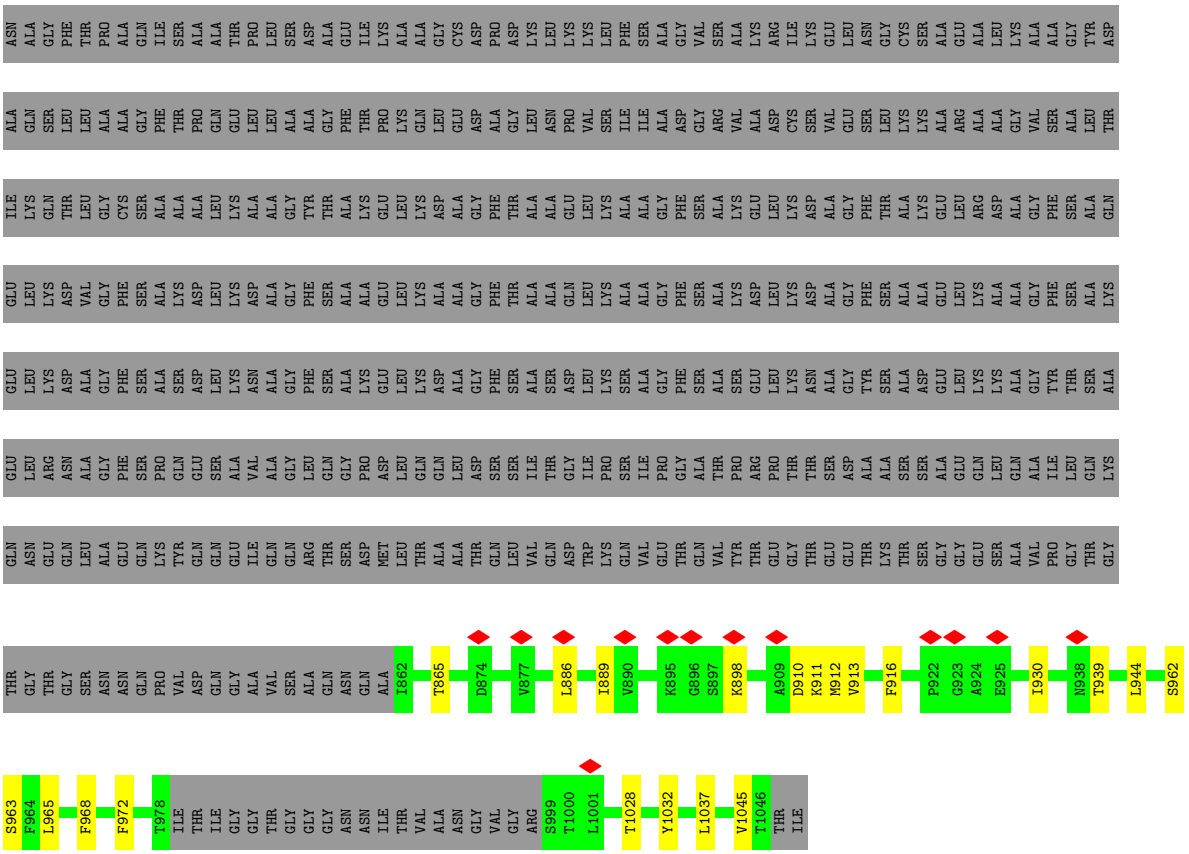
Chain OG:





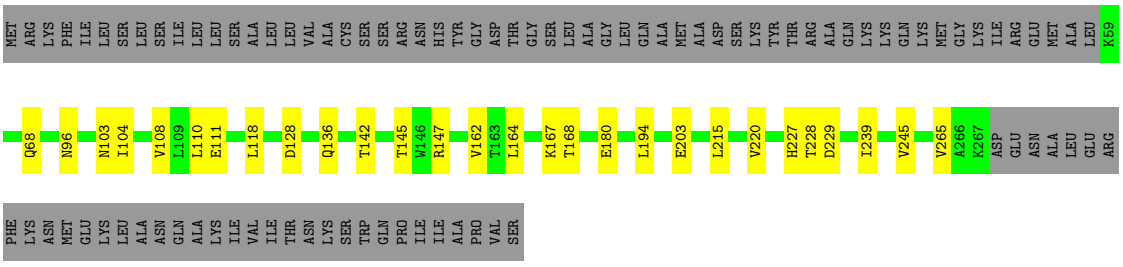
• Molecule 1: IcmE protein

Chain PG:



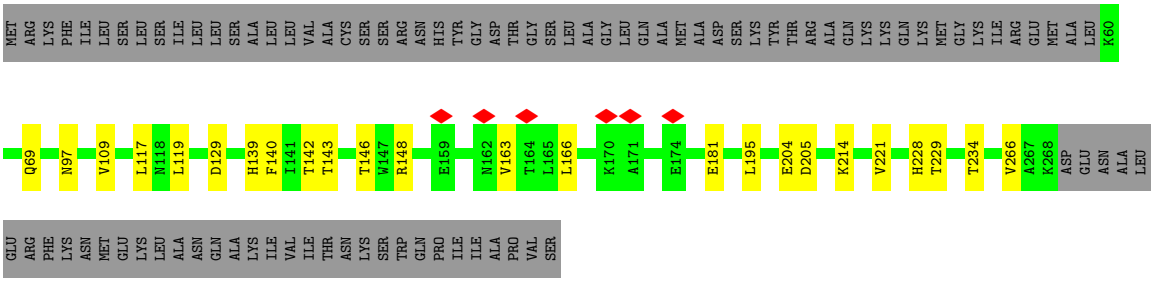
• Molecule 2: DotC

Chain BC:



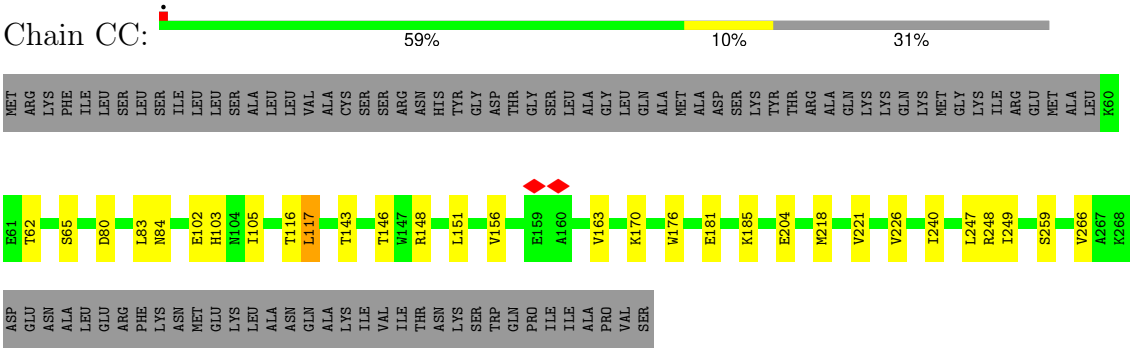
• Molecule 2: DotC

Chain EC:



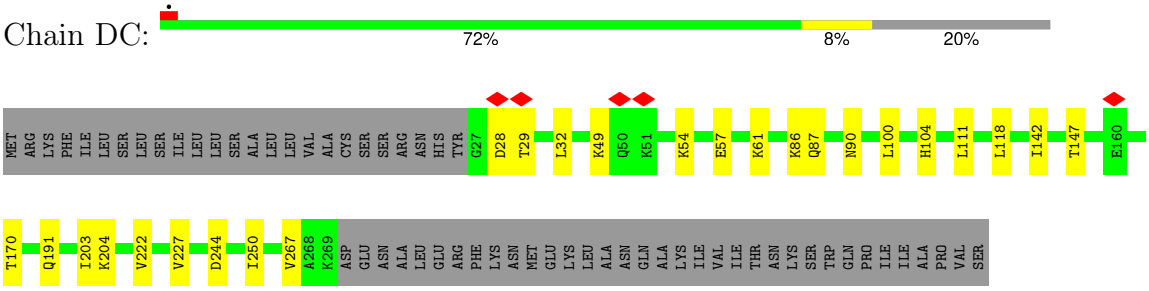
• Molecule 2: DotC

Chain CC:



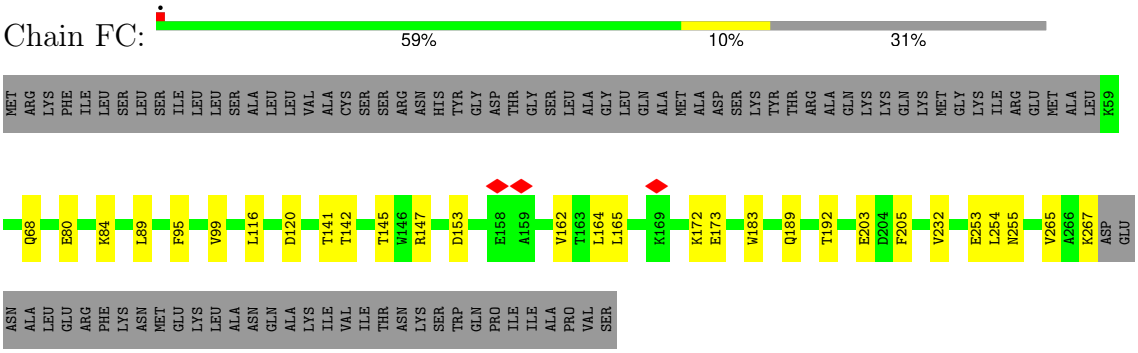
- Molecule 2: DotC

Chain DC:



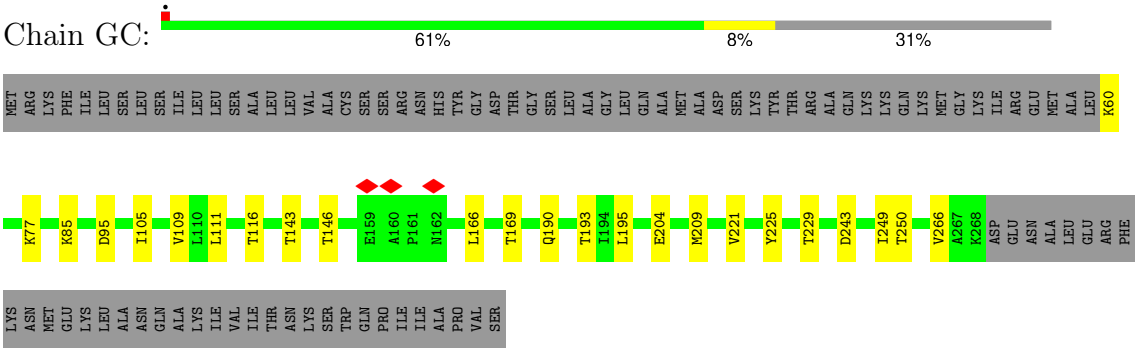
- Molecule 2: DotC

Chain FC:



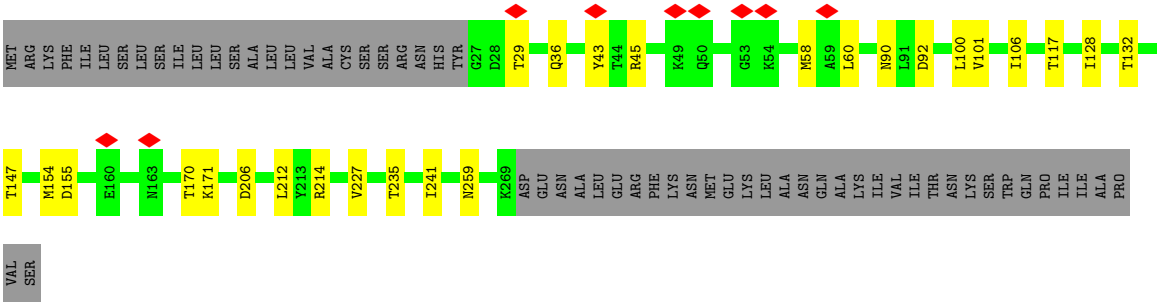
- Molecule 2: DotC

Chain GC:



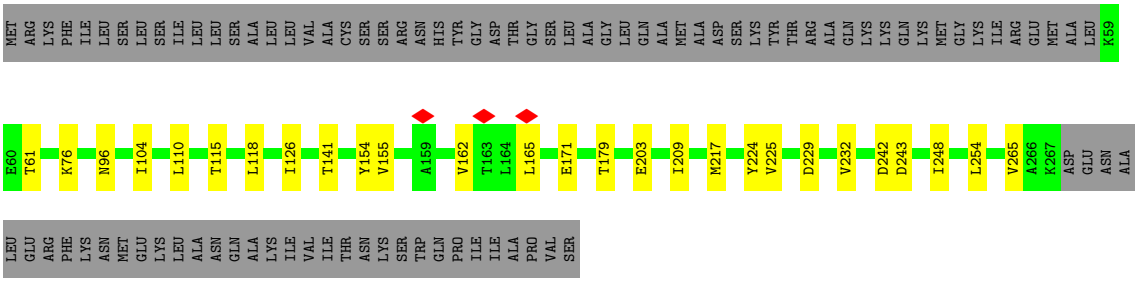
- Molecule 2: DotC

Chain IC:



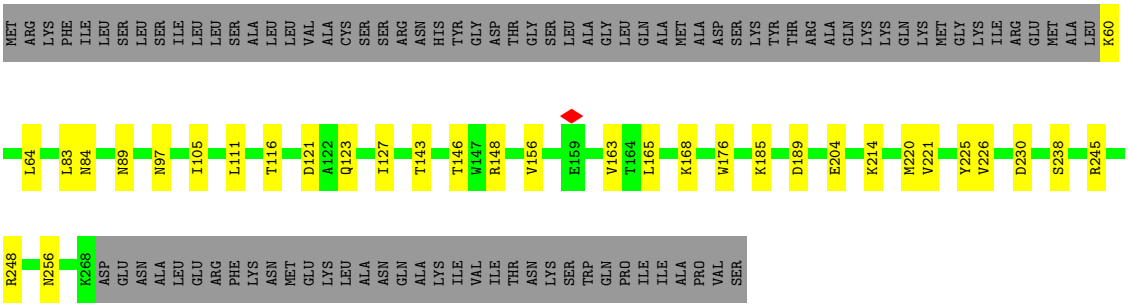
• Molecule 2: DotC

Chain JC:



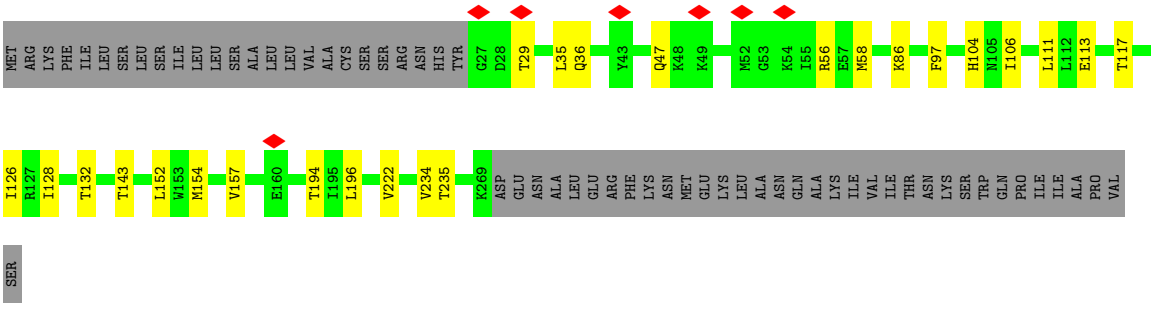
• Molecule 2: DotC

Chain KC:



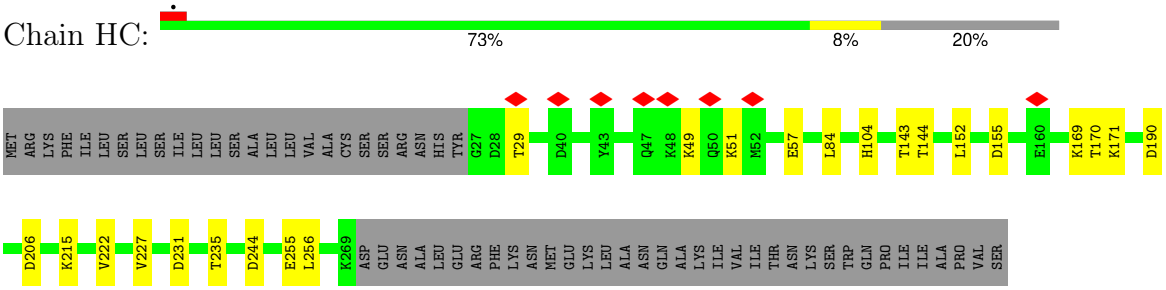
• Molecule 2: DotC

Chain MC:



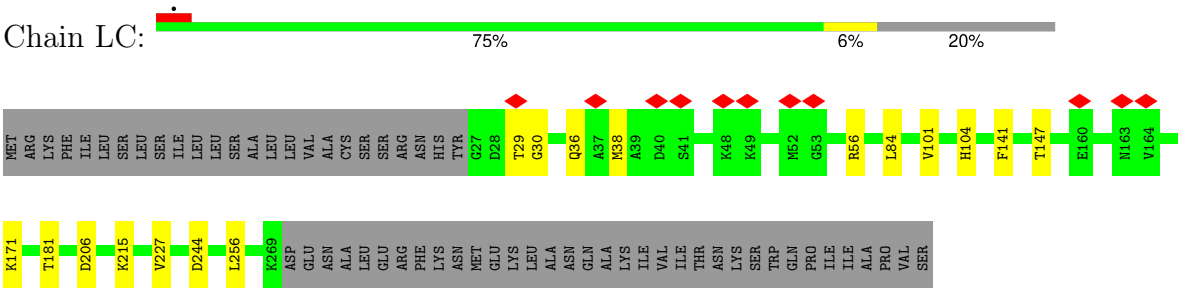
• Molecule 2: DotC

Chain HC:



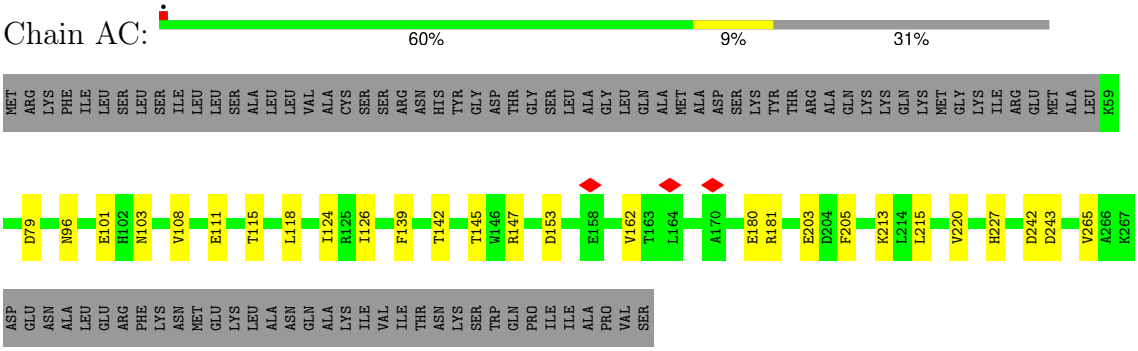
• Molecule 2: DotC

Chain LC:



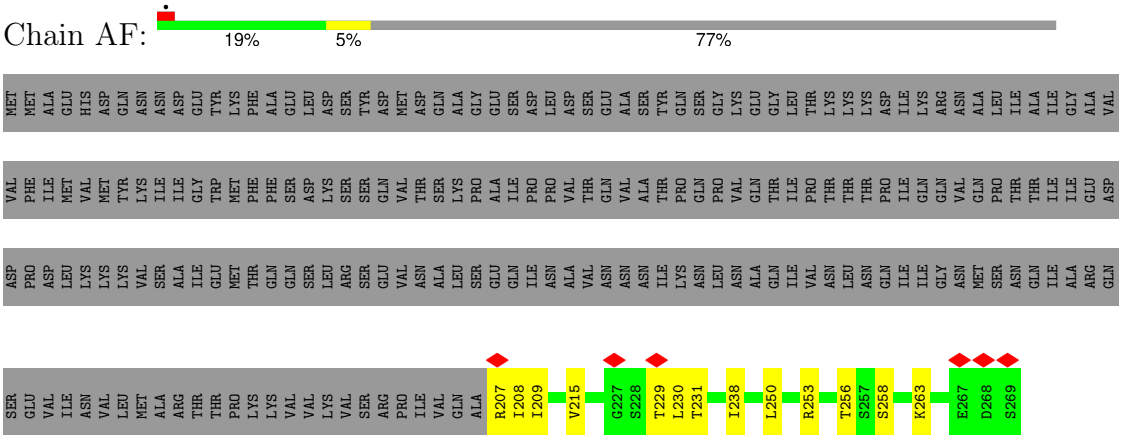
• Molecule 2: DotC

Chain AC:



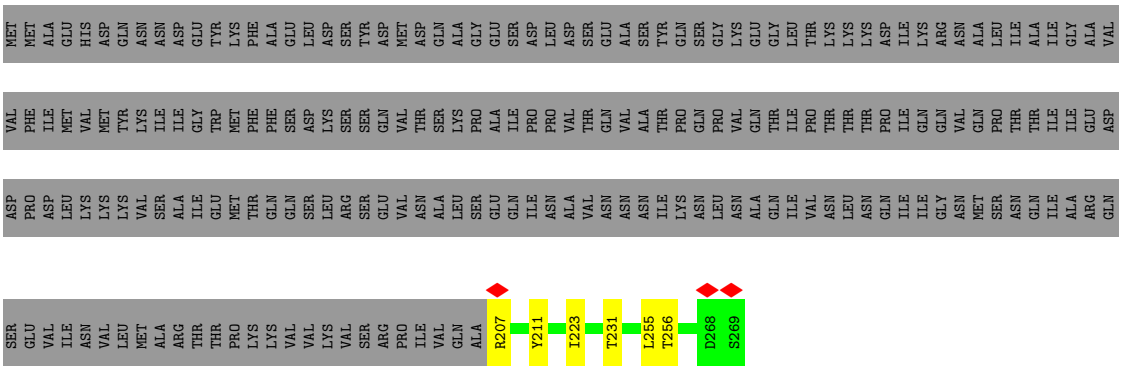
• Molecule 3: DotF

Chain AF:



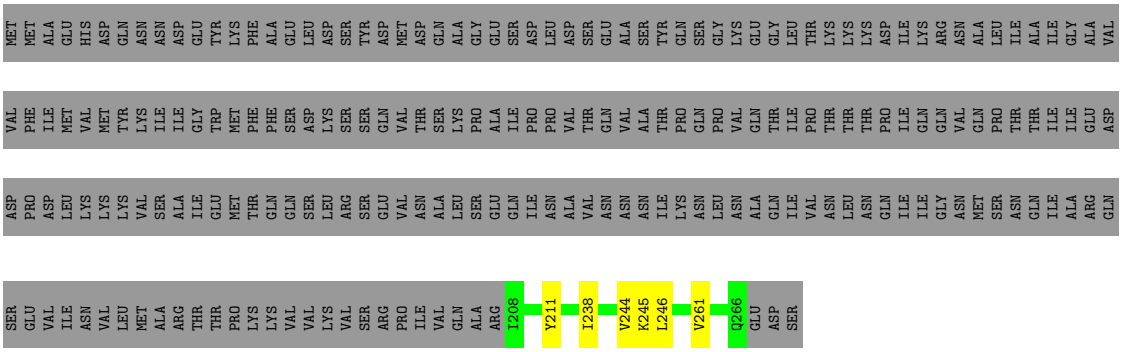
• Molecule 3: DotF

Chain GF:



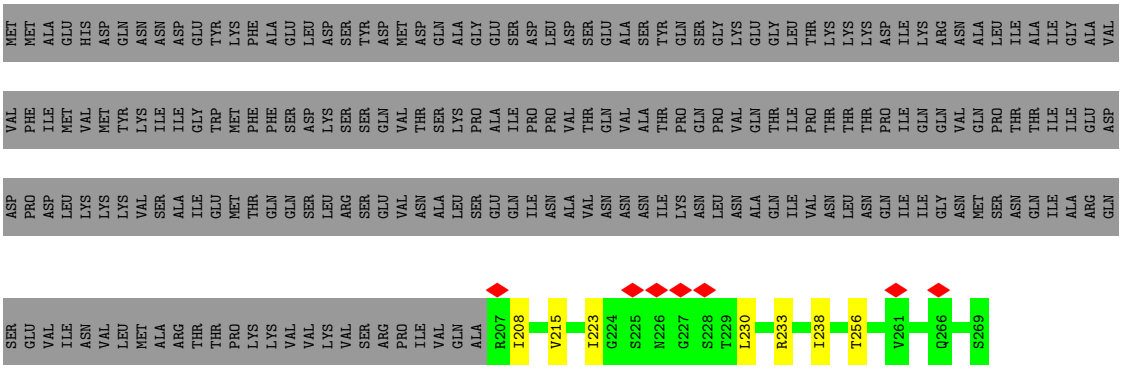
• Molecule 3: DotF

Chain Gf:



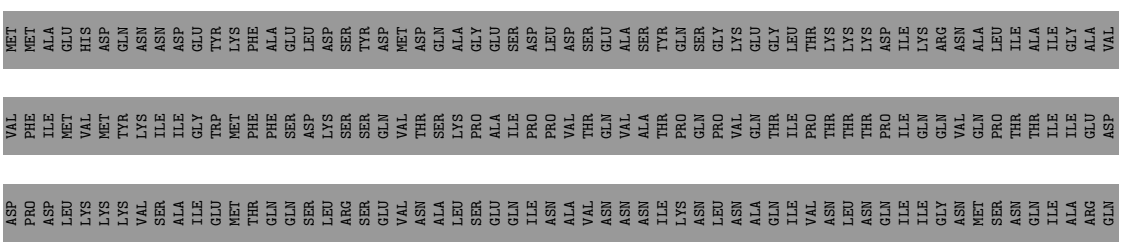
• Molecule 3: DotF

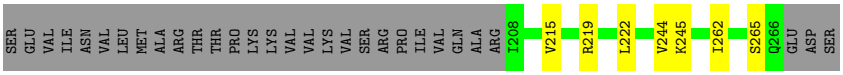
Chain HF:



• Molecule 3: DotF

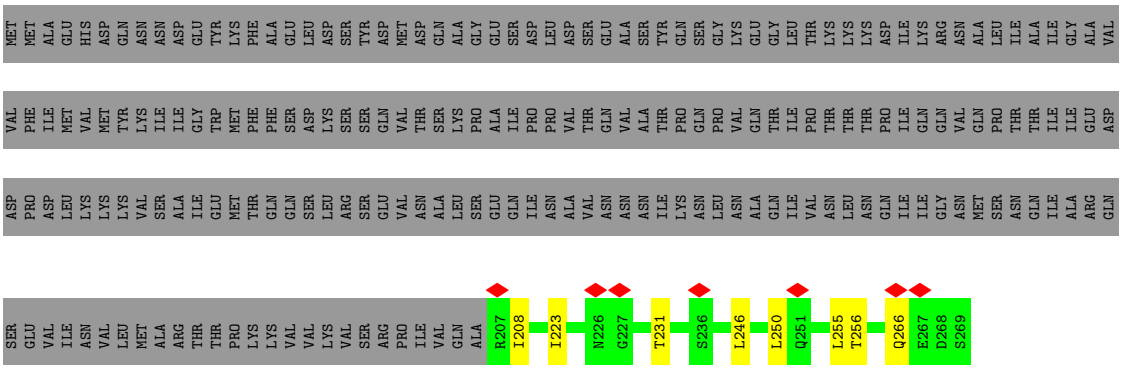
Chain Hf:





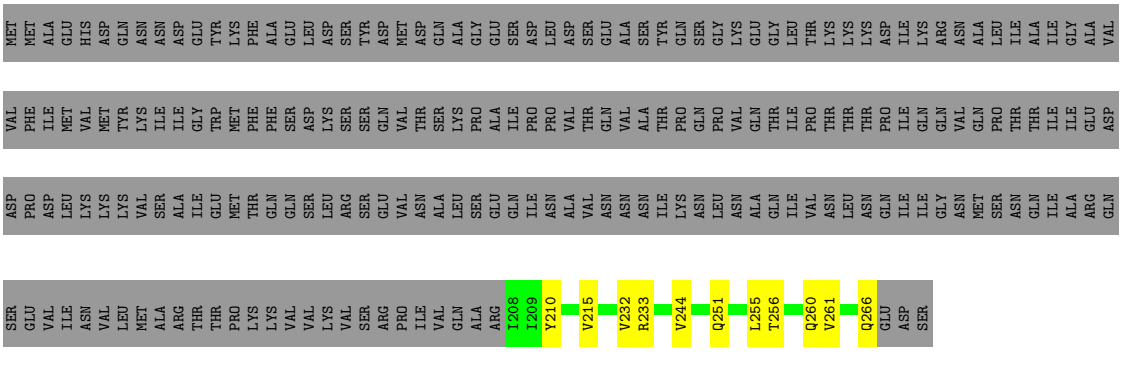
• Molecule 3: DotF

Chain IF:



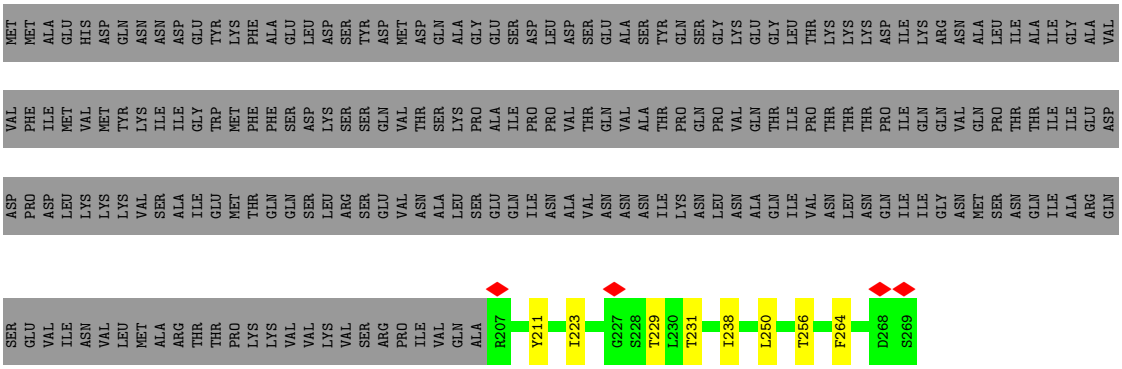
• Molecule 3: DotF

Chain If:



• Molecule 3: DotF

Chain JF:



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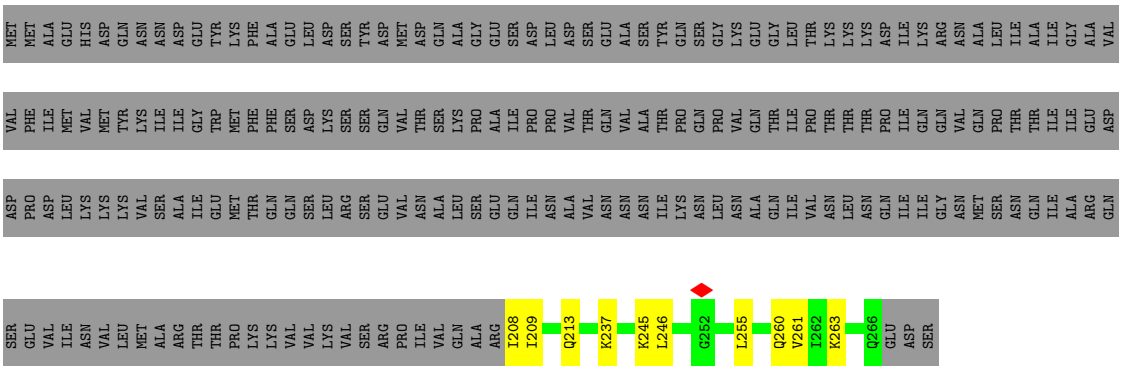
Chain Jf:



• Molecule 3: DotF

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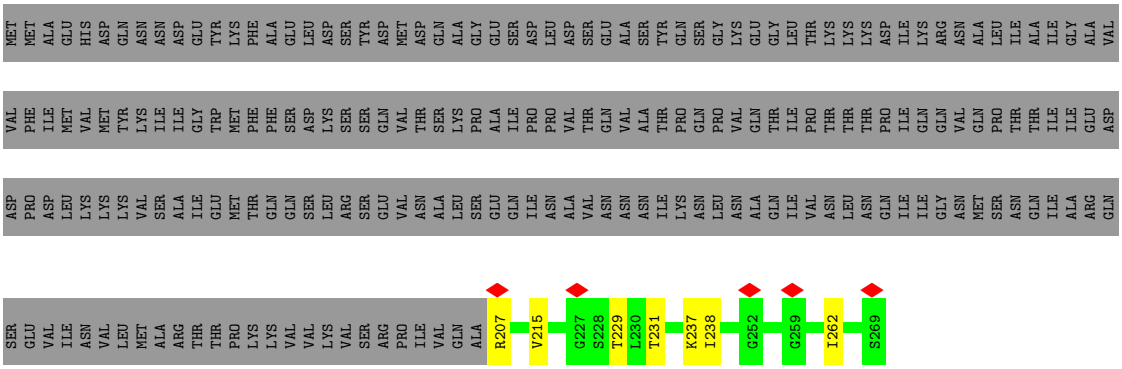

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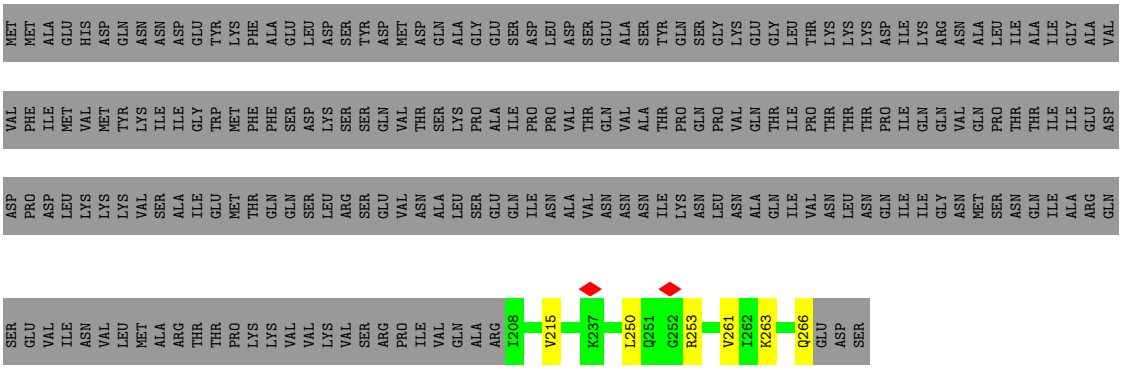
Chain Kf:



• Molecule 3: DotF

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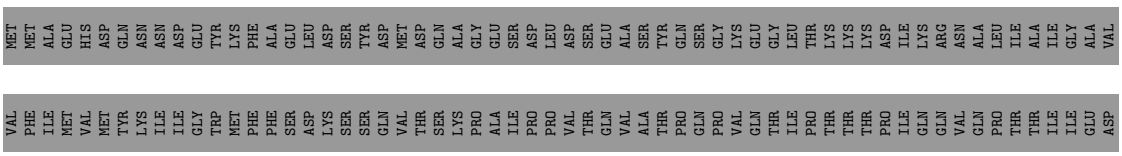
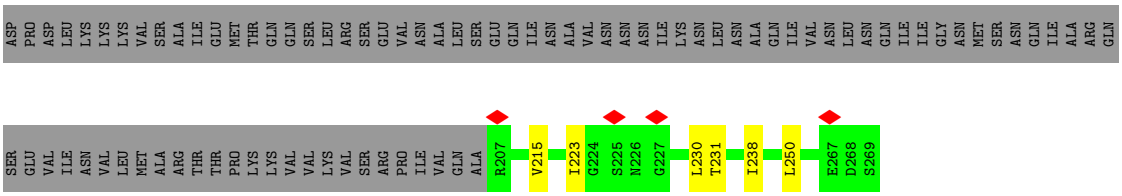
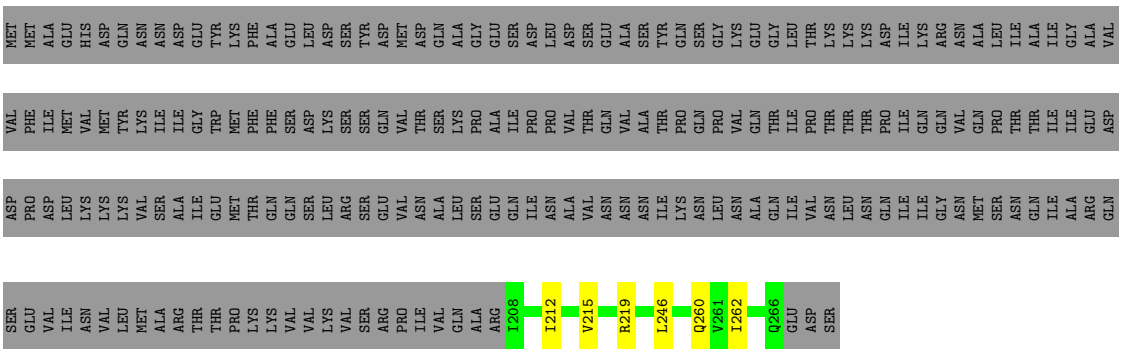




• Molecule 3: DotF

Chain Lf:



• Molecule 3: DotF

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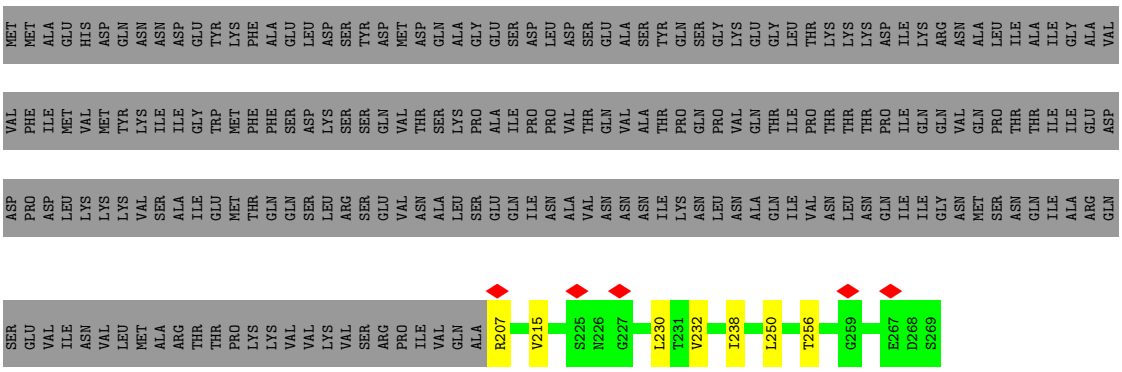

• Molecule 3: DotF

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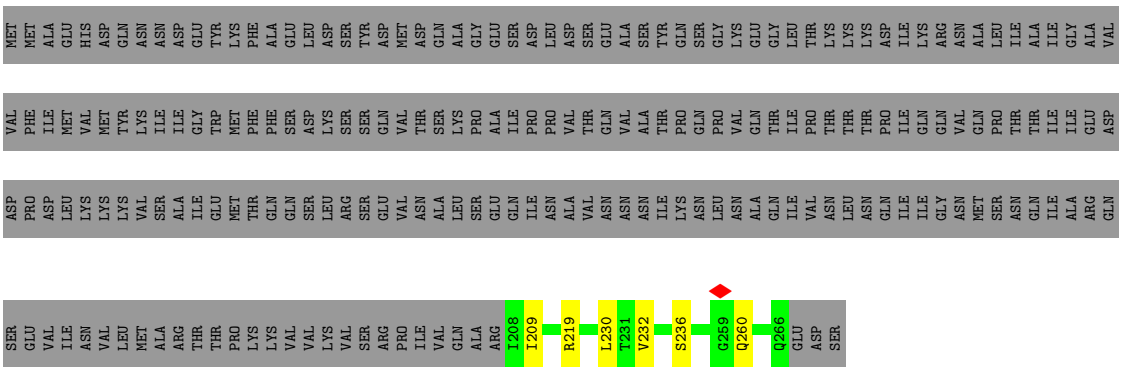
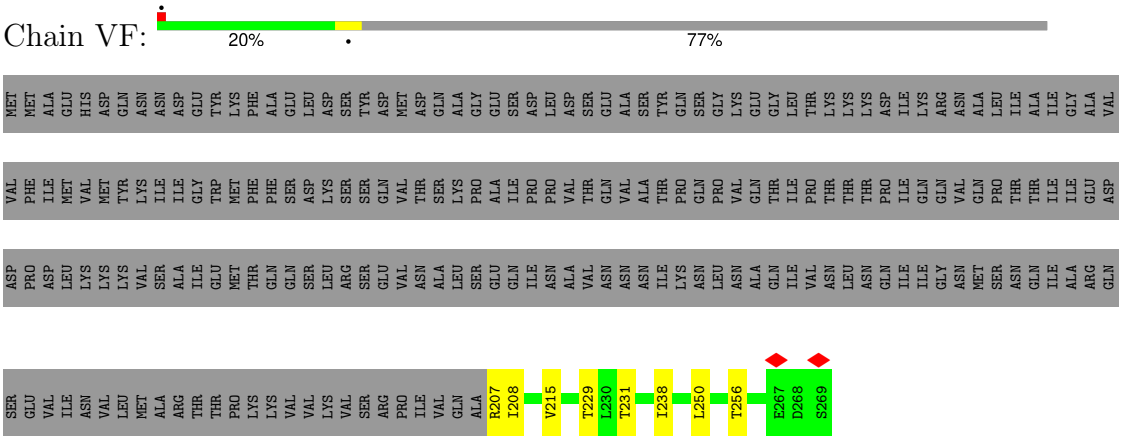


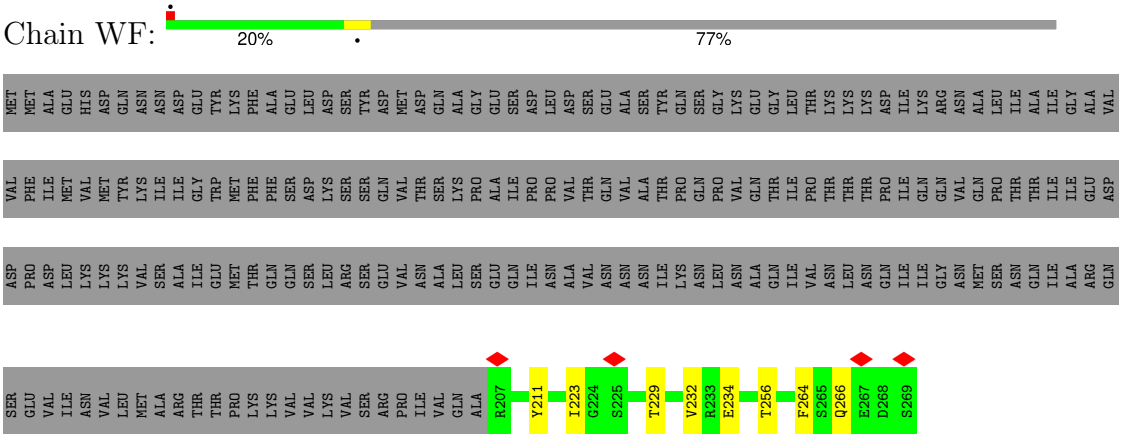
• Molecule 3: DotF

Chain VF:



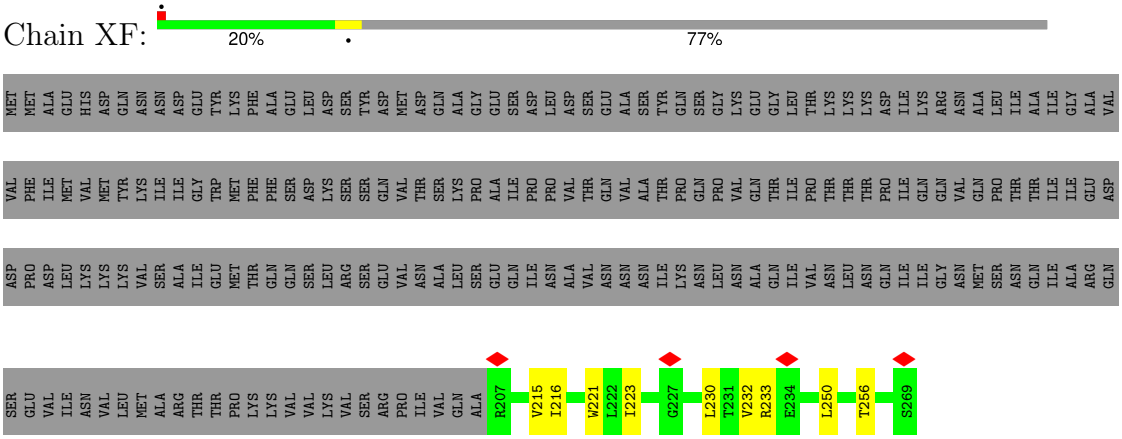
• Molecule 3: DotF

Chain WF:



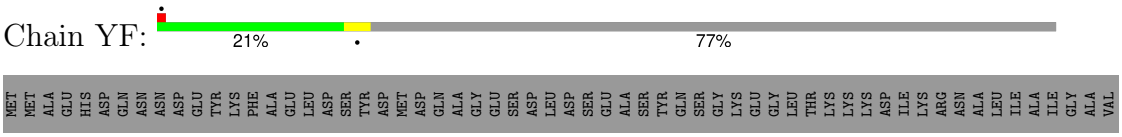
• Molecule 3: DotF

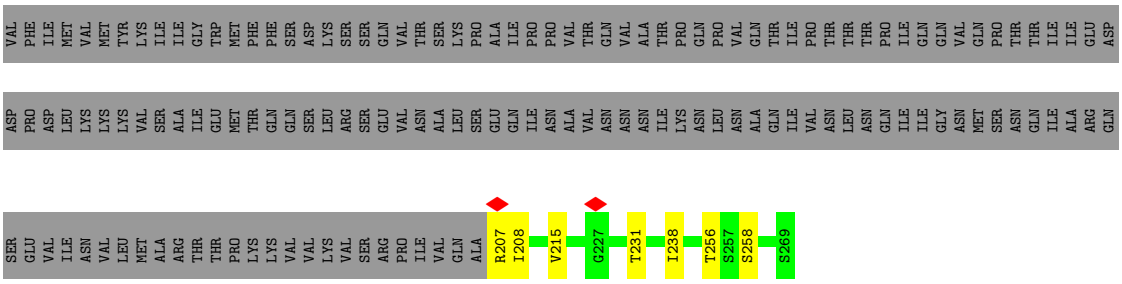
Chain XF:



• Molecule 3: DotF

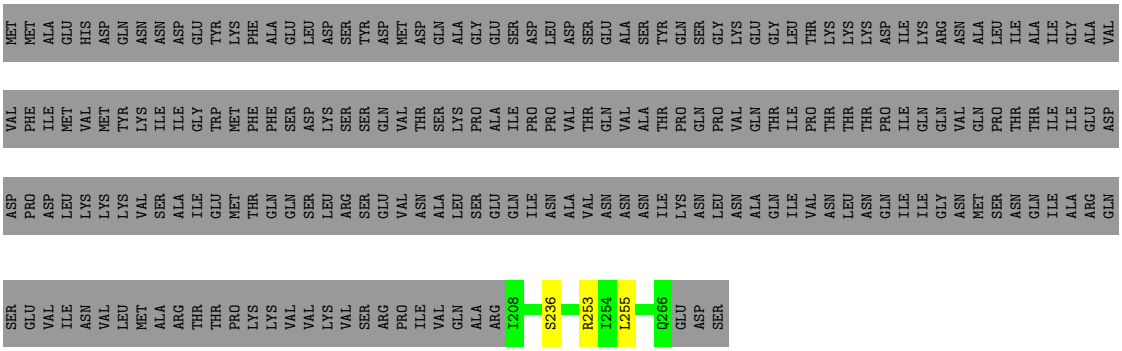
Chain YF:





• Molecule 3: DotF

Chain Df:



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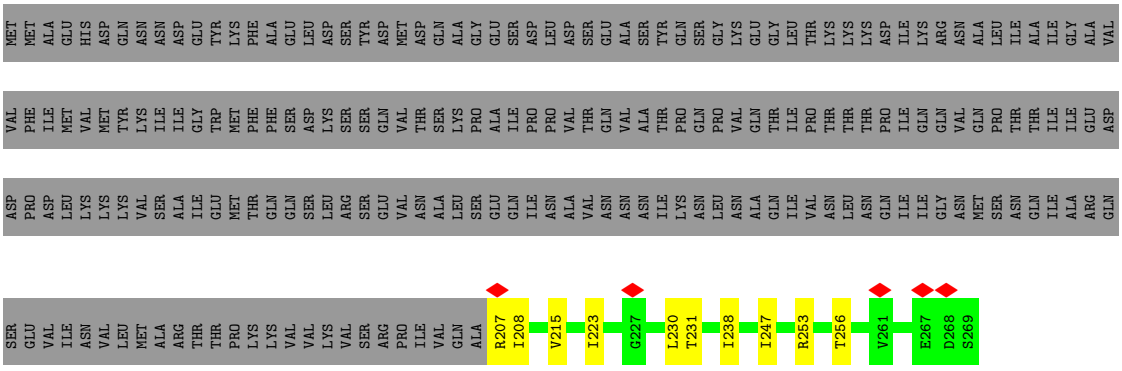

• Molecule 3: DotF

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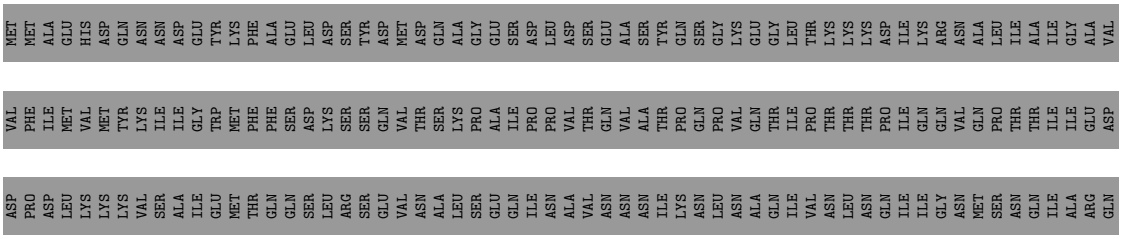
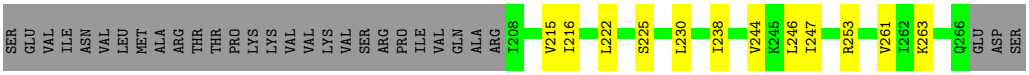
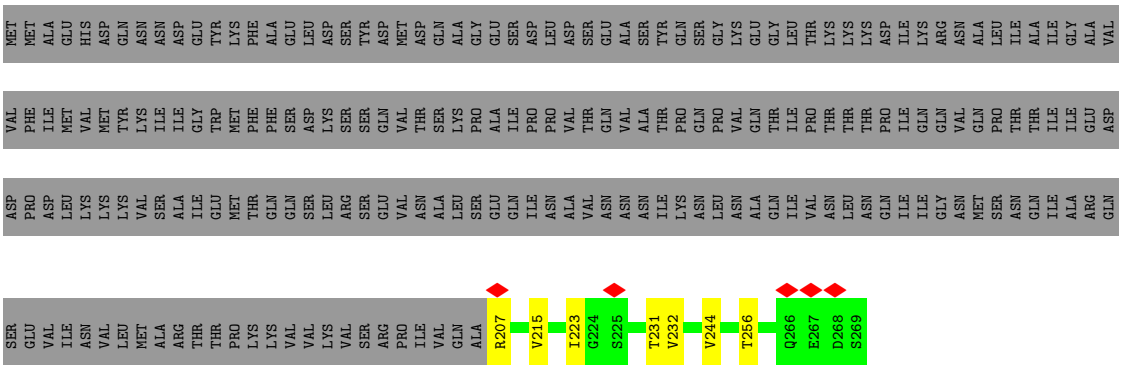




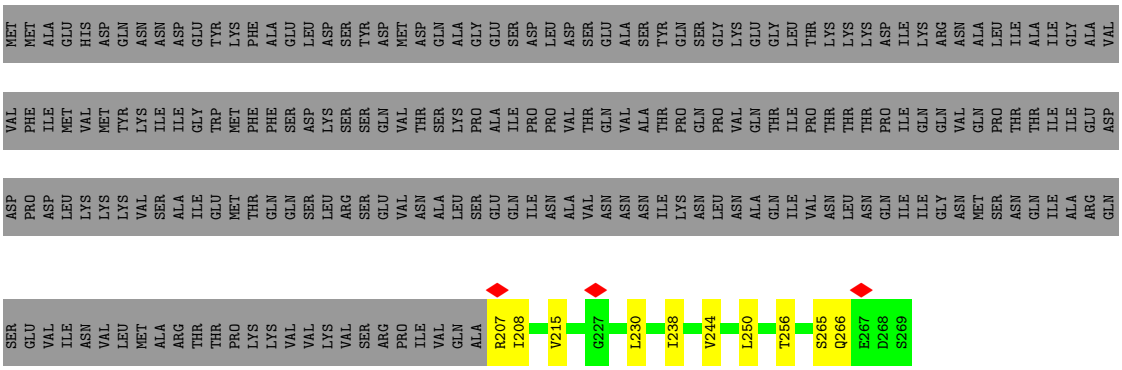
• Molecule 3: DotF

Chain BF:



• Molecule 3: DotF

Chain CF:



• Molecule 3: DotF

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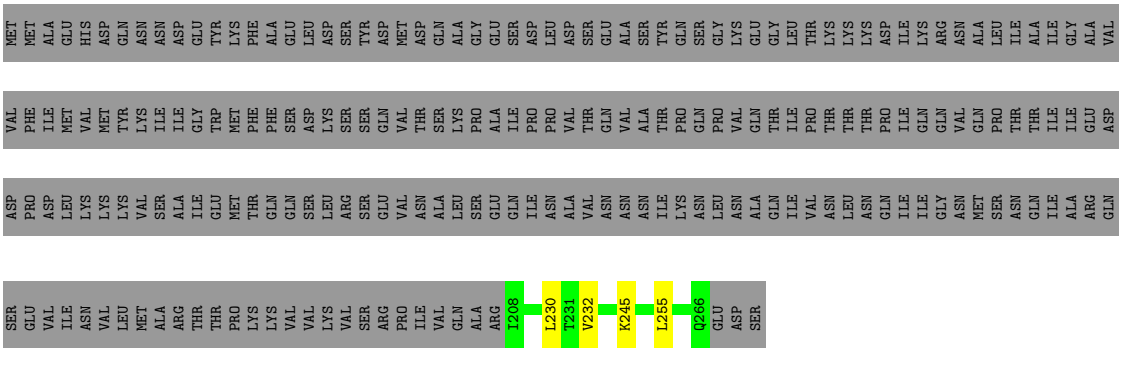

• Molecule 3: DotF

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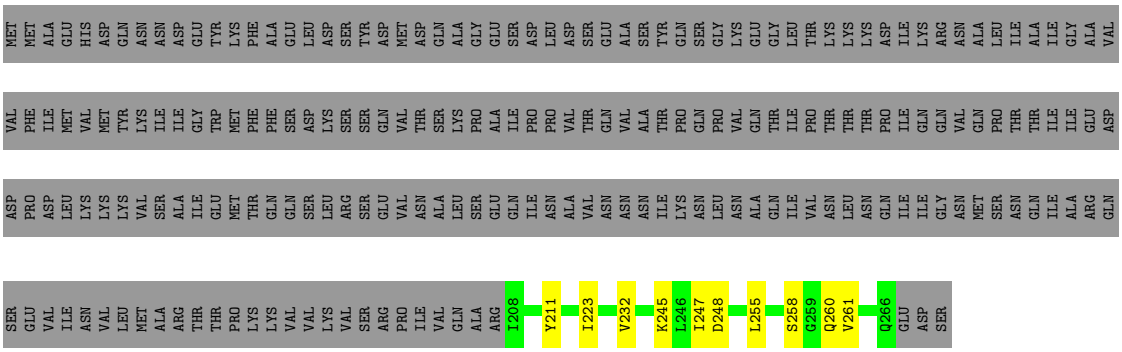

• Molecule 3: DotF

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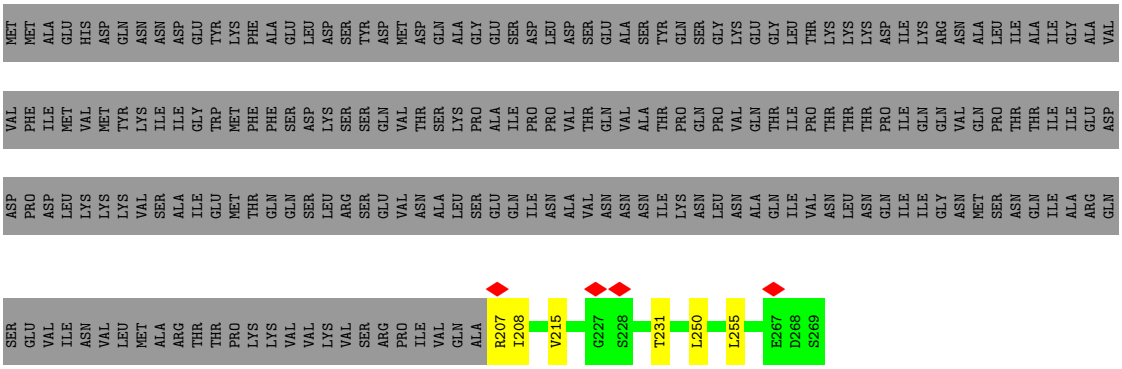

• Molecule 3: DotF

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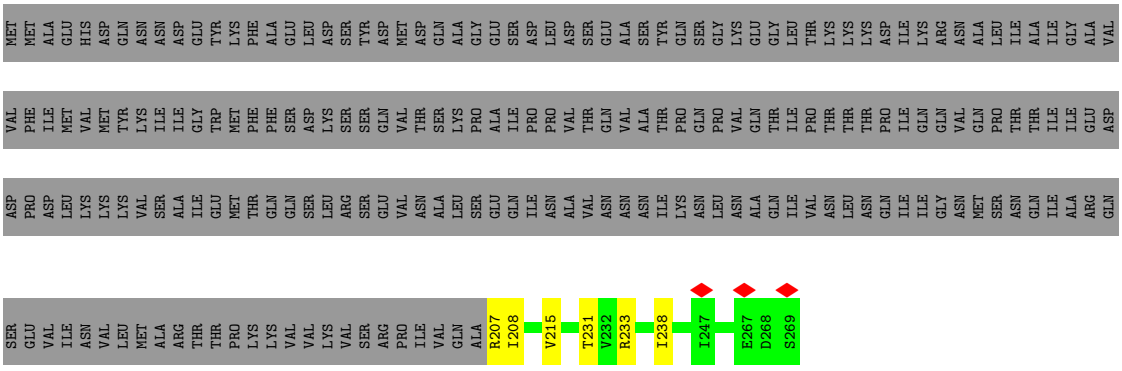

• Molecule 3: DotF

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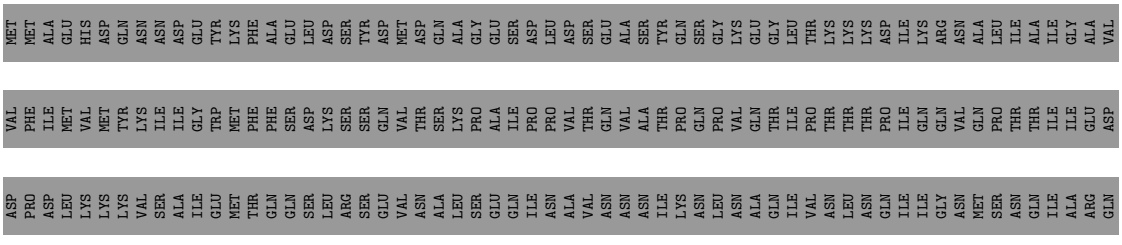
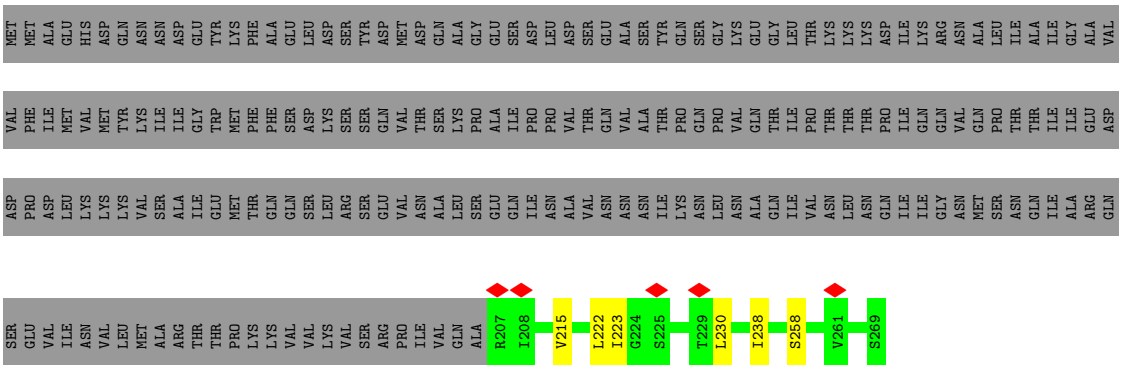


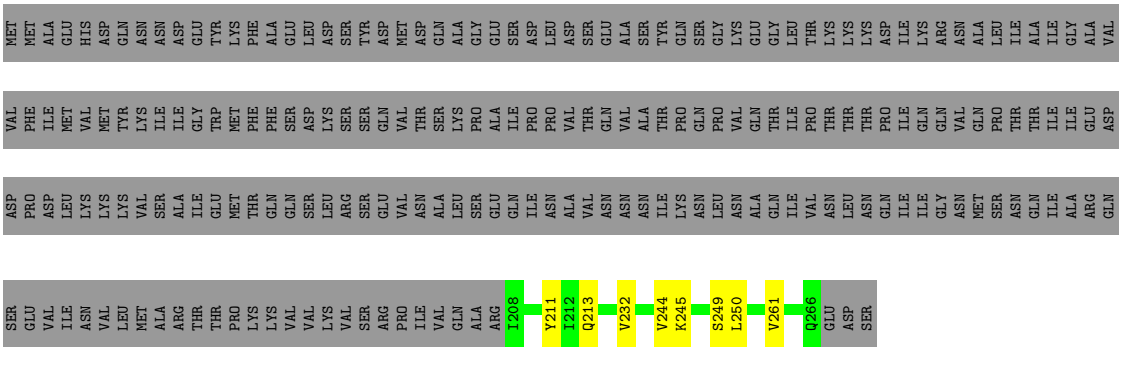
• Molecule 3: DotF

Chain FF:



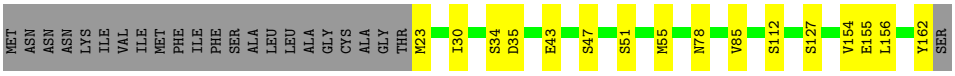
• Molecule 3: DotF

Chain Ff:



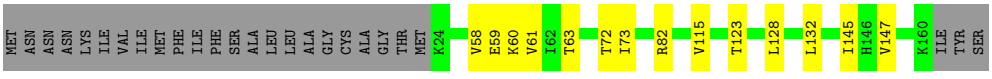
• Molecule 4: DotD

Chain GD:



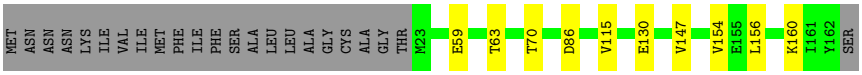
• Molecule 4: DotD

Chain Gd:



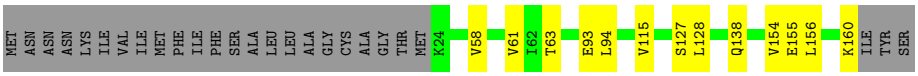
• Molecule 4: DotD

Chain HD:



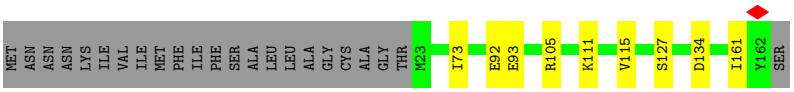
• Molecule 4: DotD

Chain Hd:



• Molecule 4: DotD

Chain ID:



• Molecule 4: DotD

Chain Dd:

• Molecule 4: DotD

Chain Id:

• Molecule 4: DotD

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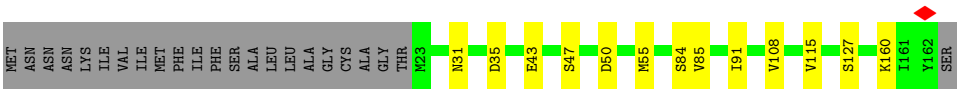

• Molecule 4: DotD

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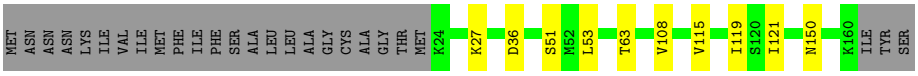
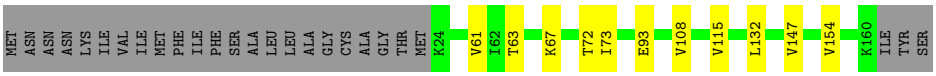


• Molecule 4: DotD

Chain KD:

• Molecule 4: DotD

Chain Kd:



• Molecule 4: DotD

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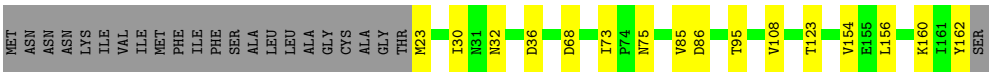

• Molecule 4: DotD

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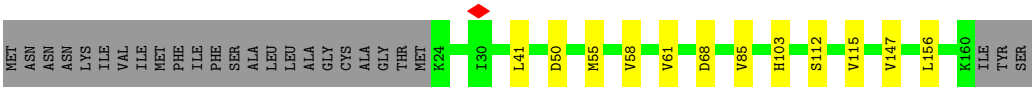

• Molecule 4: DotD

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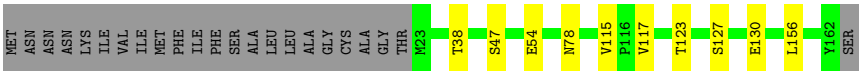
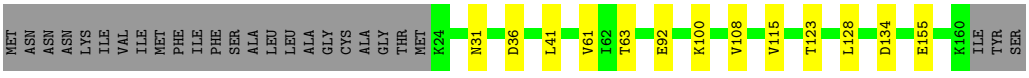


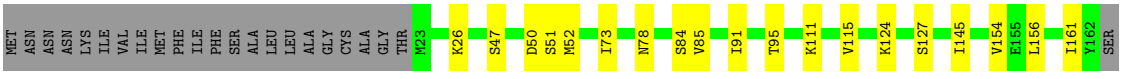
• Molecule 4: DotD

Chain Md:



• Molecule 4: DotD

Chain CD:



• Molecule 4: DotD

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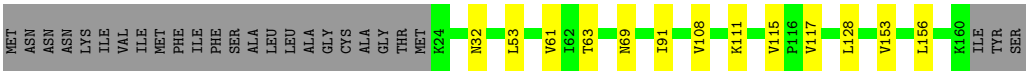
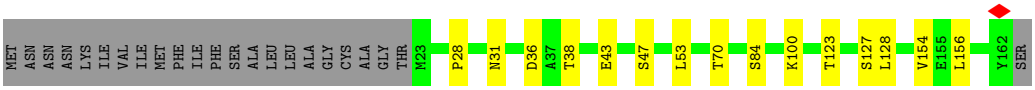


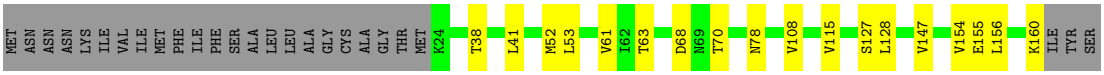
• Molecule 4: DotD

Chain BD:



• Molecule 4: DotD

Chain Bd:

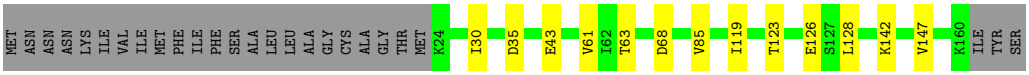


• Molecule 4: DotD

Chain AD:

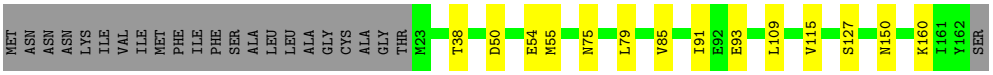
• Molecule 4: DotD

Chain Cd:



• Molecule 4: DotD

Chain DD:



• Molecule 4: DotD

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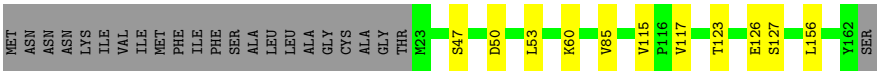
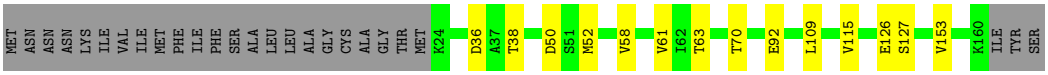


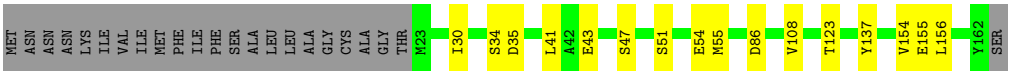
• Molecule 4: DotD

Chain Ed:



• Molecule 4: DotD

Chain FD:

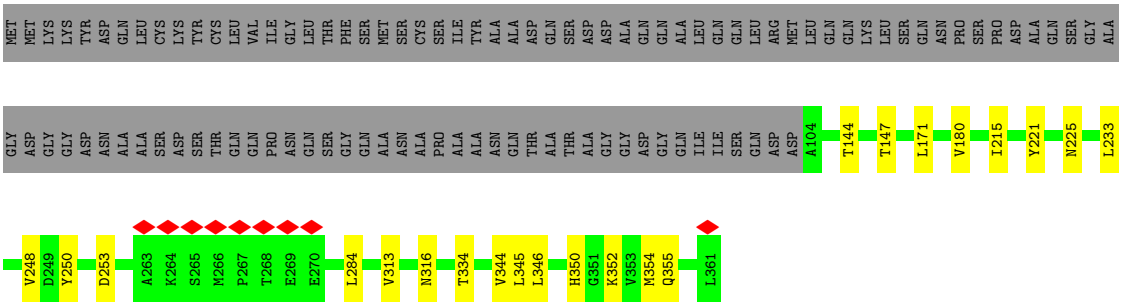


• Molecule 4: DotD

Chain Fd:

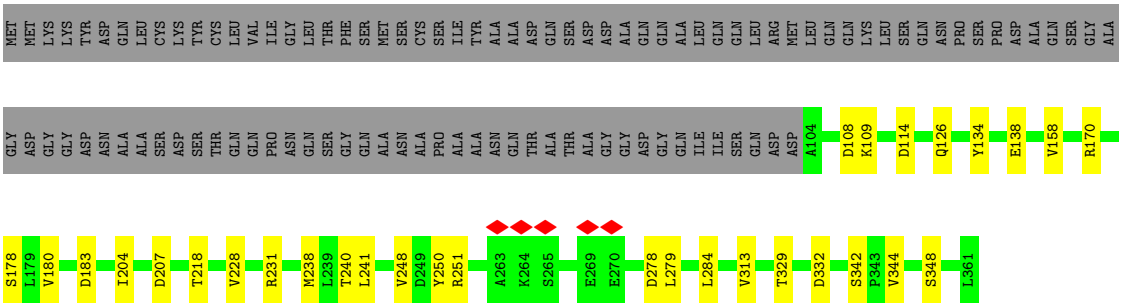
• Molecule 5: Type IV secretion protein IcmK

Chain GH:



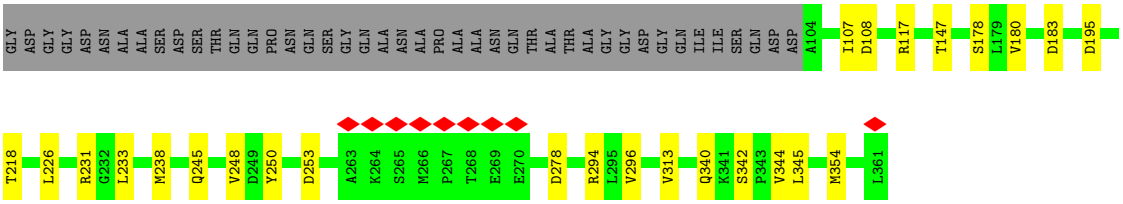
• Molecule 5: Type IV secretion protein IcmK

Chain HH:



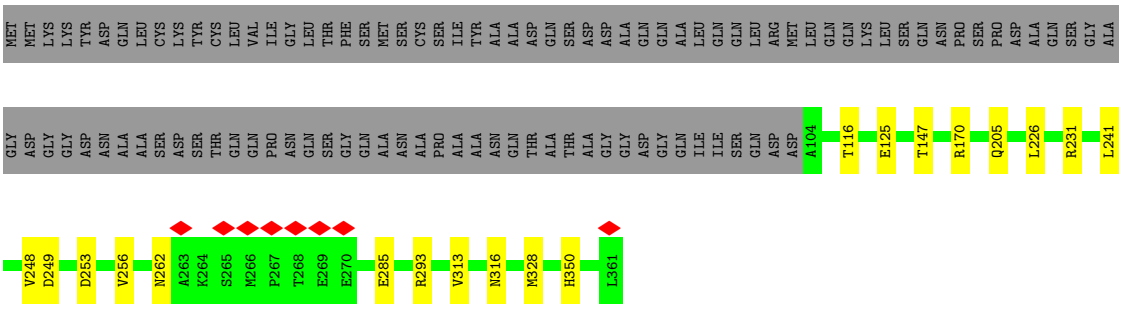
• Molecule 5: Type IV secretion protein IcmK

Chain IH:



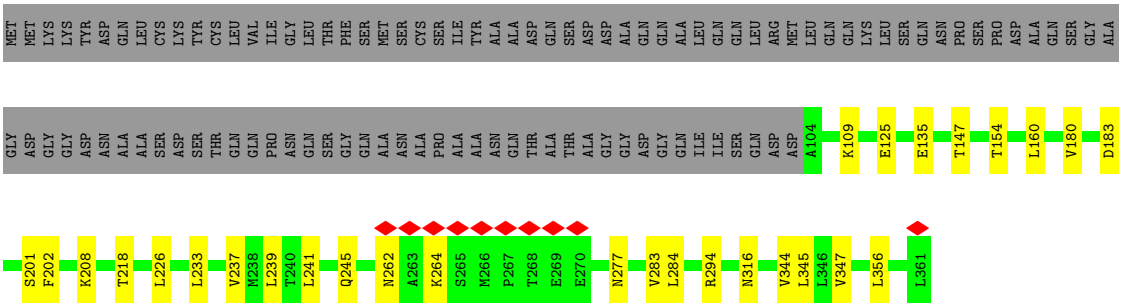
• Molecule 5: Type IV secretion protein IcmK

Chain JH:



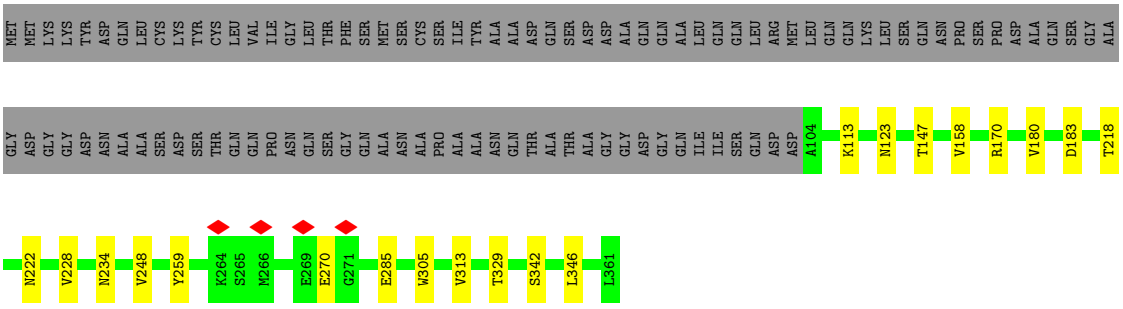
• Molecule 5: Type IV secretion protein IcmK

Chain AH:



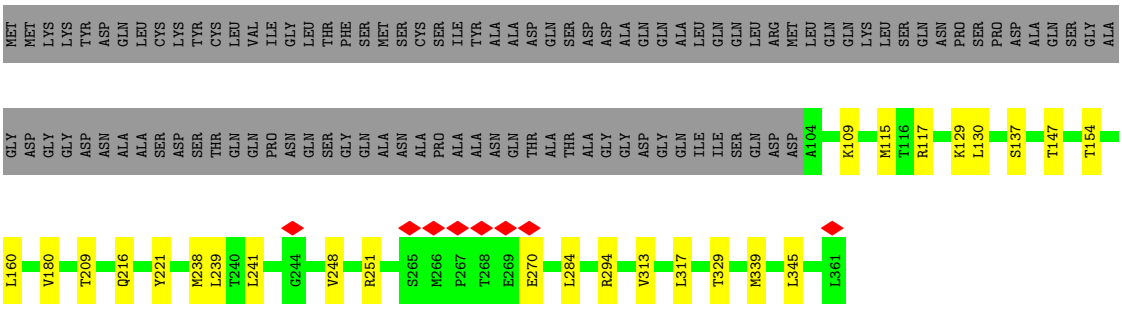
• Molecule 5: Type IV secretion protein IcmK

Chain KH:



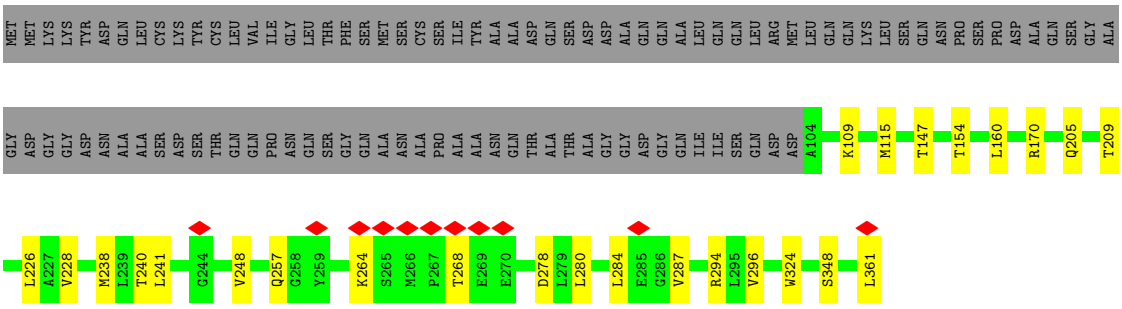
• Molecule 5: Type IV secretion protein IcmK

Chain LH:



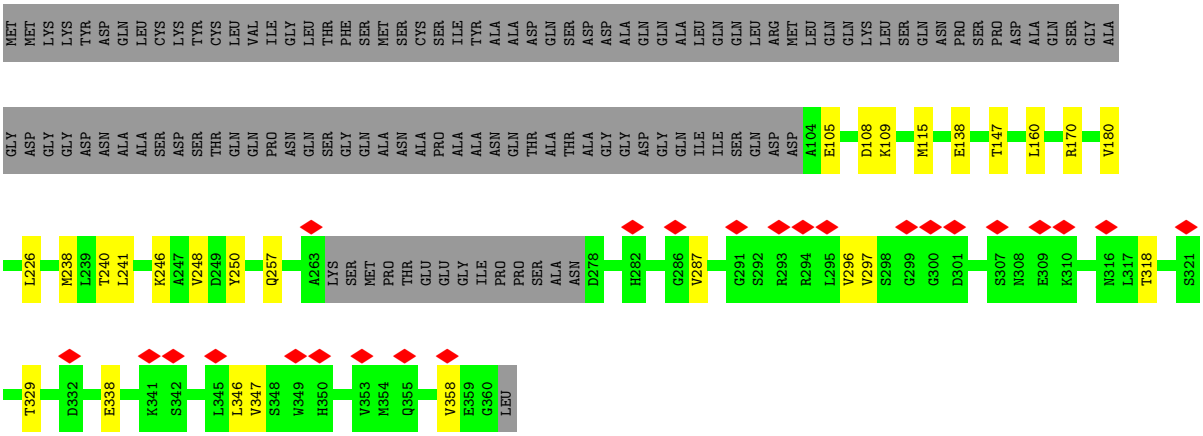
• Molecule 5: Type IV secretion protein IcmK

Chain MH:



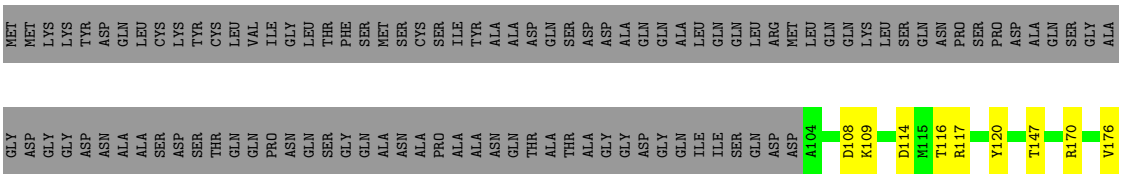
• Molecule 5: Type IV secretion protein IcmK

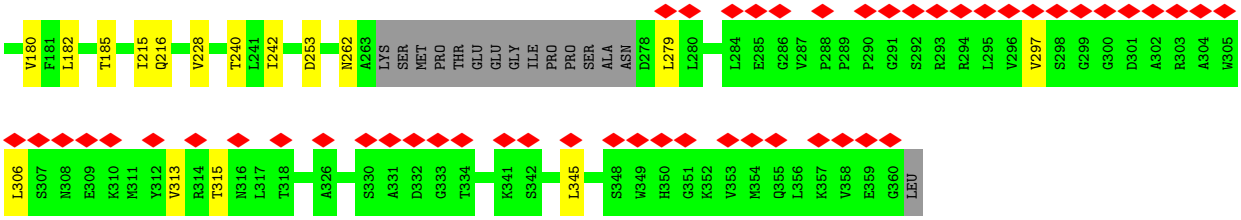
Chain VH:



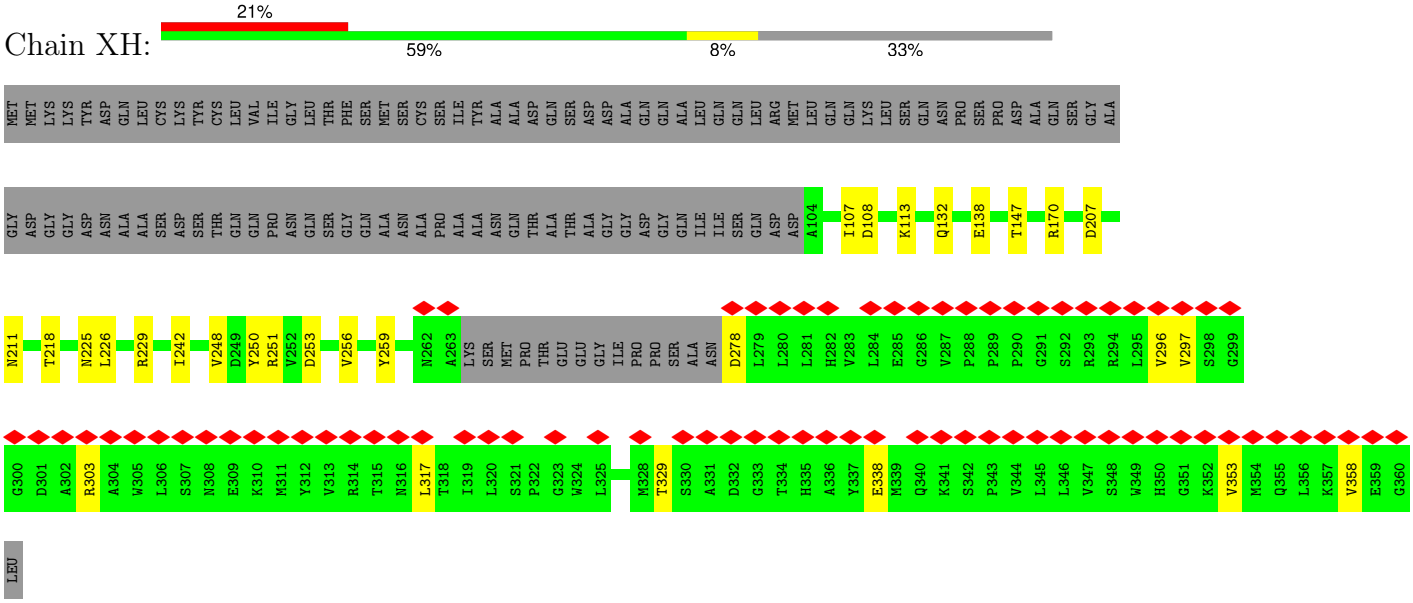
• Molecule 5: Type IV secretion protein IcmK

Chain WH:

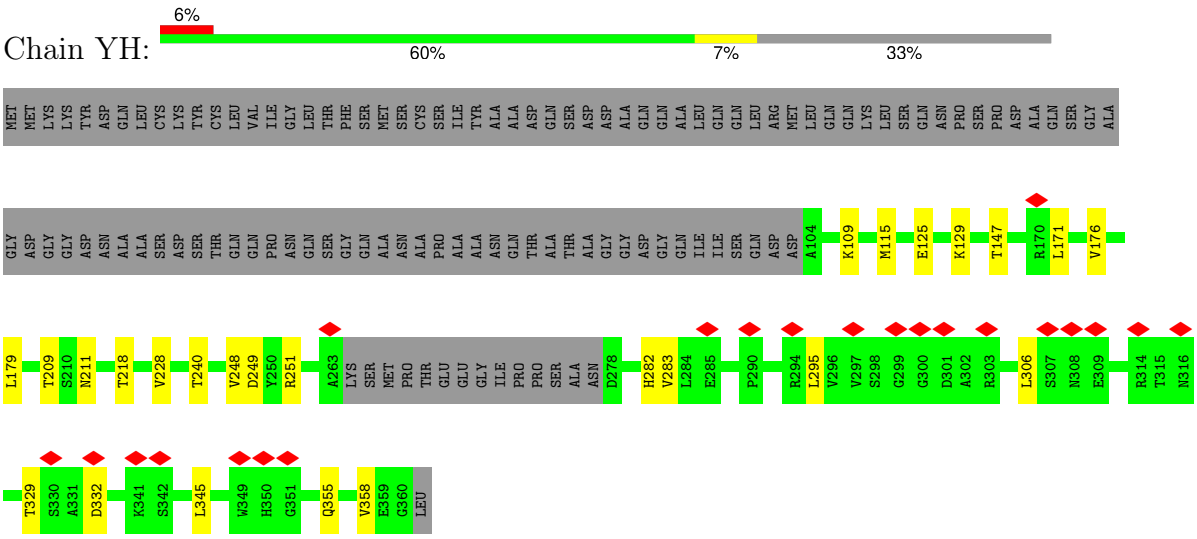




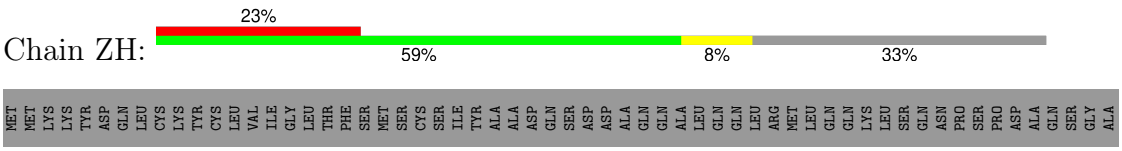
• Molecule 5: Type IV secretion protein IcmK

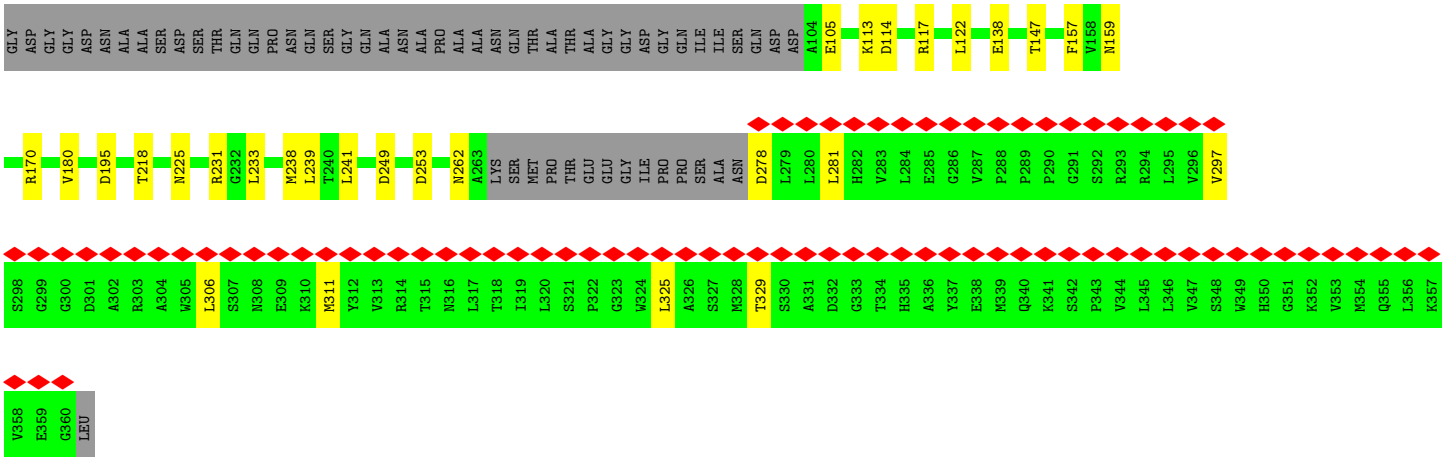


• Molecule 5: Type IV secretion protein IcmK



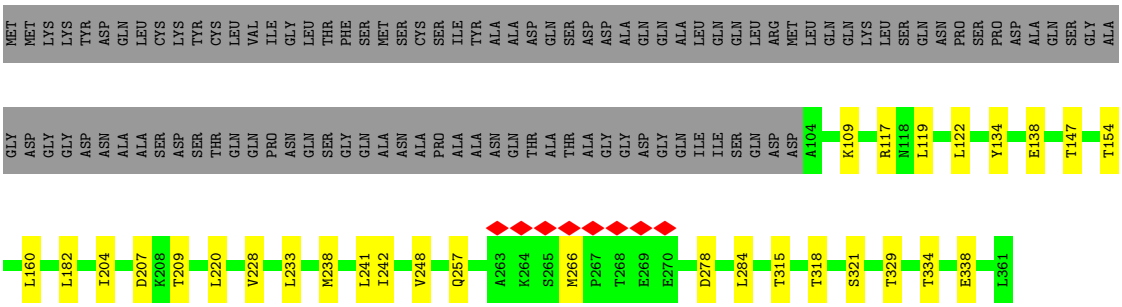
• Molecule 5: Type IV secretion protein IcmK





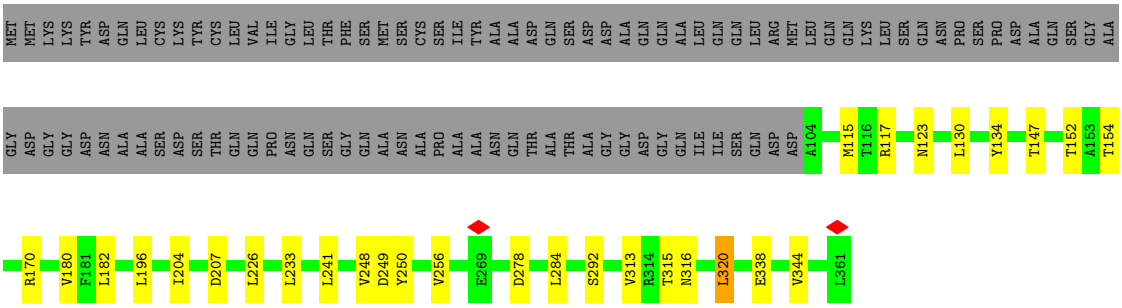
• Molecule 5: Type IV secretion protein IcmK

Chain BH:



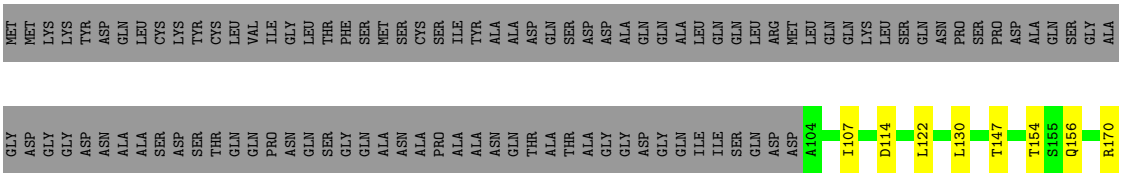
• Molecule 5: Type IV secretion protein IcmK

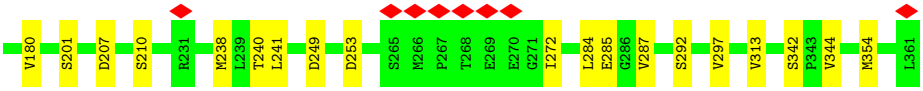
Chain CH:



• Molecule 5: Type IV secretion protein IcmK

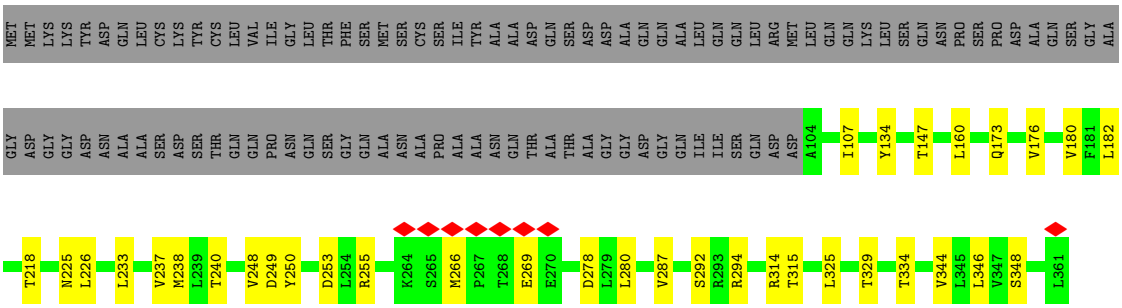
Chain DH:





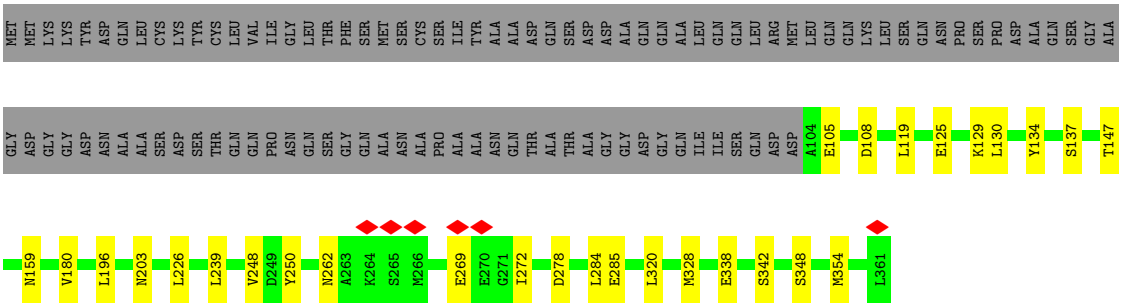
• Molecule 5: Type IV secretion protein IcmK

Chain EH:



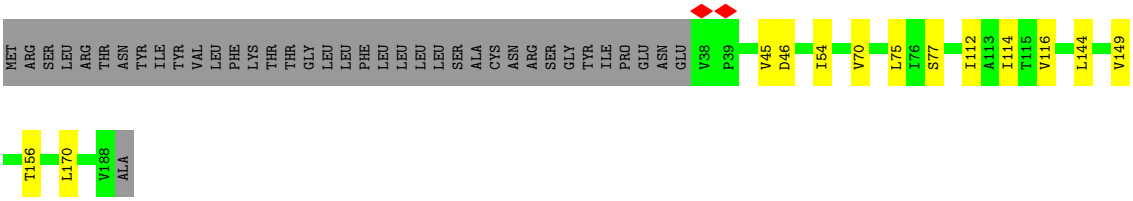
• Molecule 5: Type IV secretion protein IcmK

Chain FH:



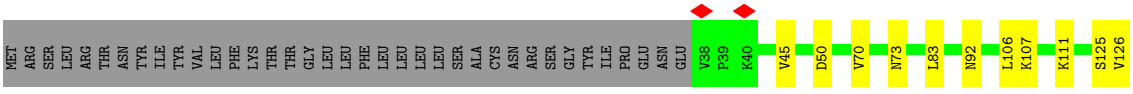
• Molecule 6: Inner membrane lipoprotein YiaD

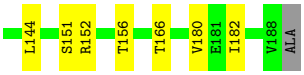
Chain GK:



• Molecule 6: Inner membrane lipoprotein YiaD

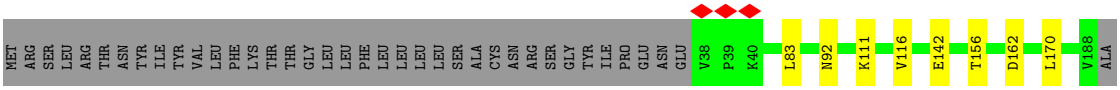
Chain HK:





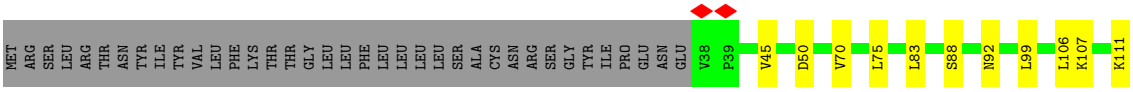
• Molecule 6: Inner membrane lipoprotein YiaD

Chain IK:



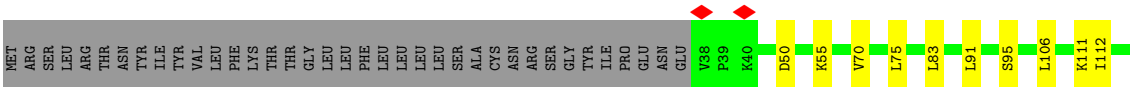
• Molecule 6: Inner membrane lipoprotein YiaD

Chain JK:



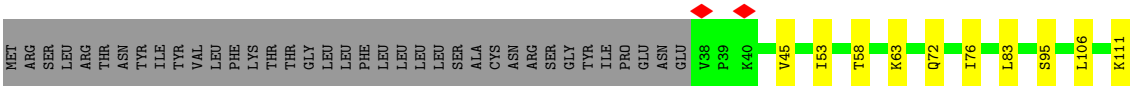
• Molecule 6: Inner membrane lipoprotein YiaD

Chain KK:



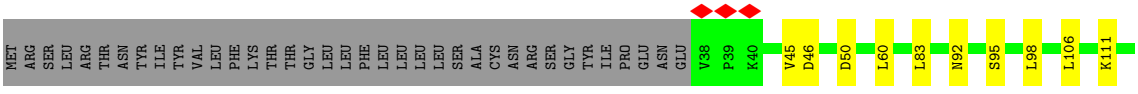
• Molecule 6: Inner membrane lipoprotein YiaD

Chain LK:



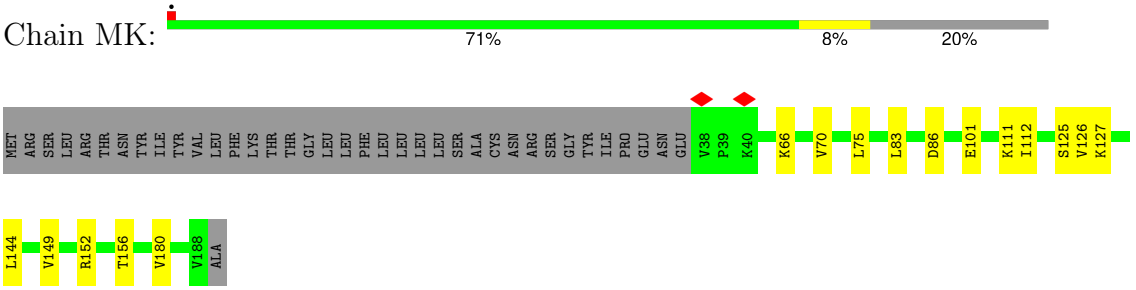
• Molecule 6: Inner membrane lipoprotein YiaD

Chain AK:



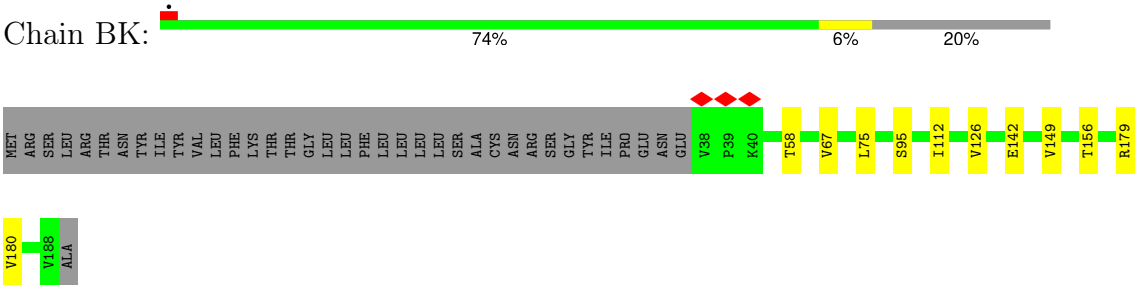
• Molecule 6: Inner membrane lipoprotein YiaD

Chain MK:



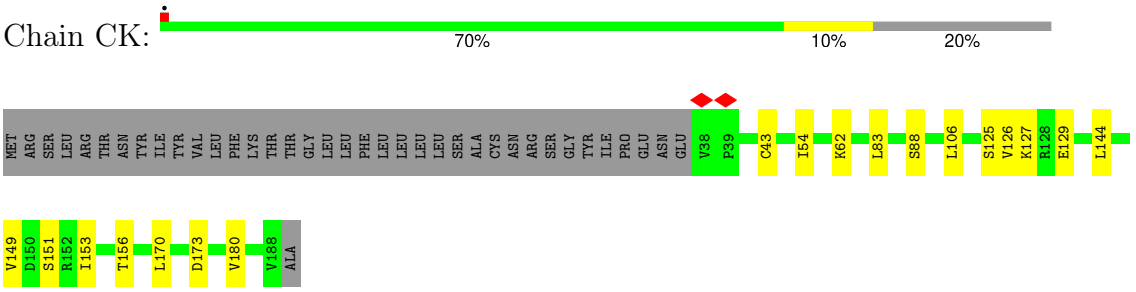
• Molecule 6: Inner membrane lipoprotein YiaD

Chain BK:



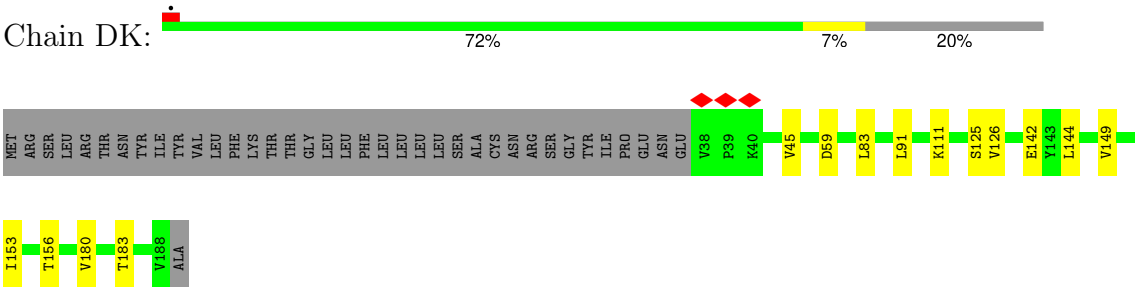
• Molecule 6: Inner membrane lipoprotein YiaD

Chain CK:



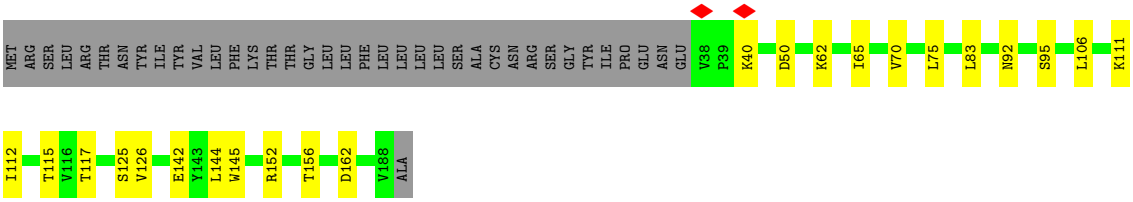
• Molecule 6: Inner membrane lipoprotein YiaD

Chain DK:



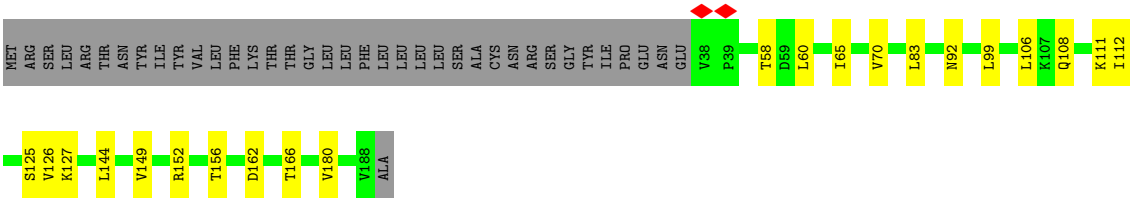
• Molecule 6: Inner membrane lipoprotein YiaD

Chain EK:



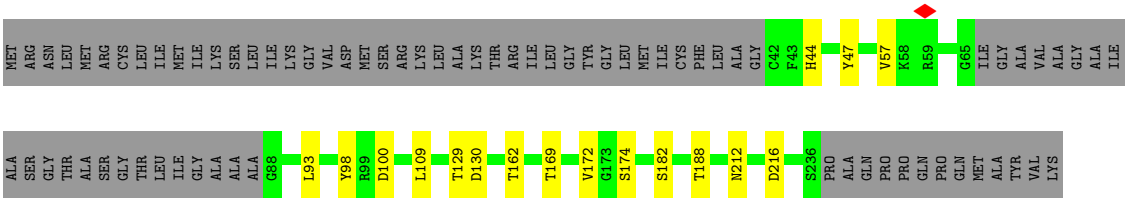
• Molecule 6: Inner membrane lipoprotein YiaD

Chain FK:



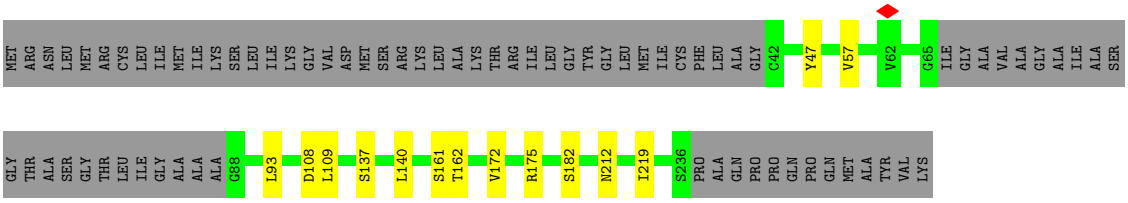
• Molecule 7: Outer membrane protein, OmpA family protein

Chain GL:



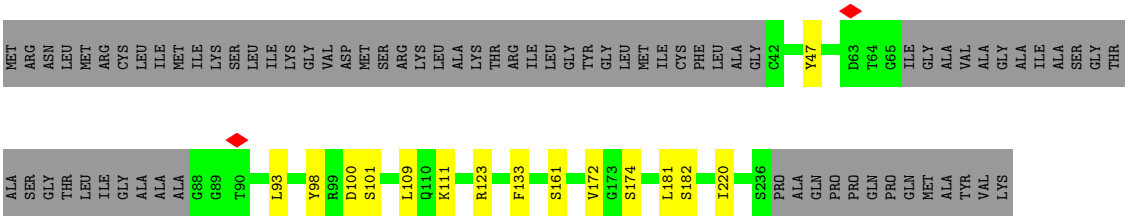
• Molecule 7: Outer membrane protein, OmpA family protein

Chain HL:



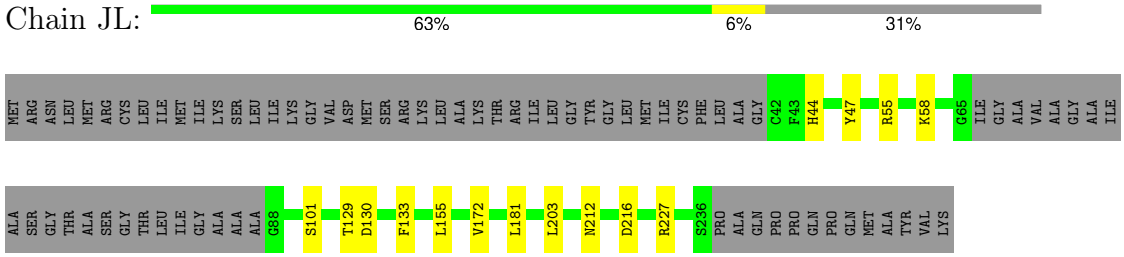
• Molecule 7: Outer membrane protein, OmpA family protein

Chain IL:



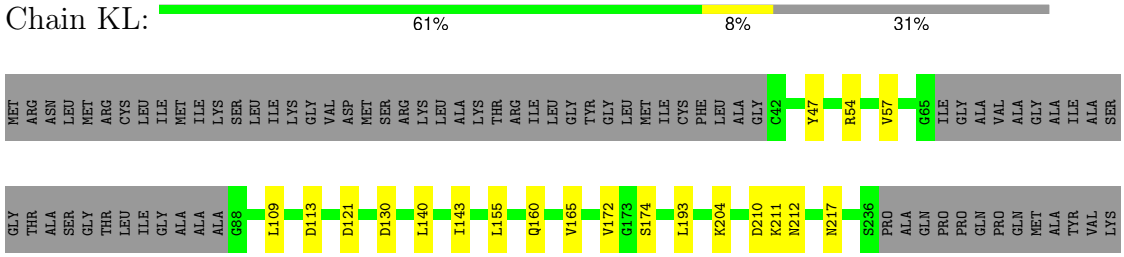
• Molecule 7: Outer membrane protein, OmpA family protein

Chain JL:



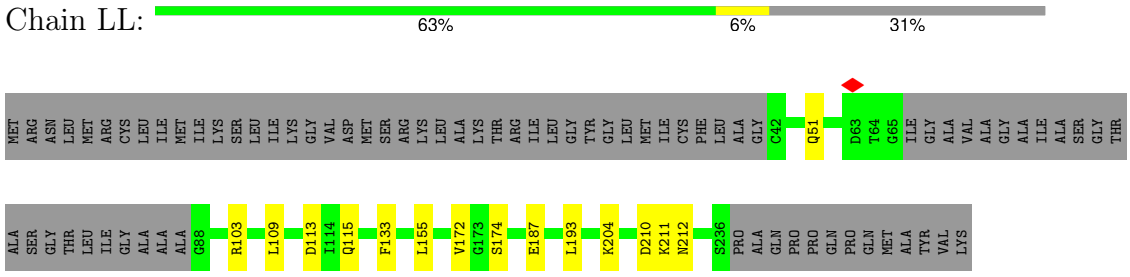
• Molecule 7: Outer membrane protein, OmpA family protein

Chain KL:



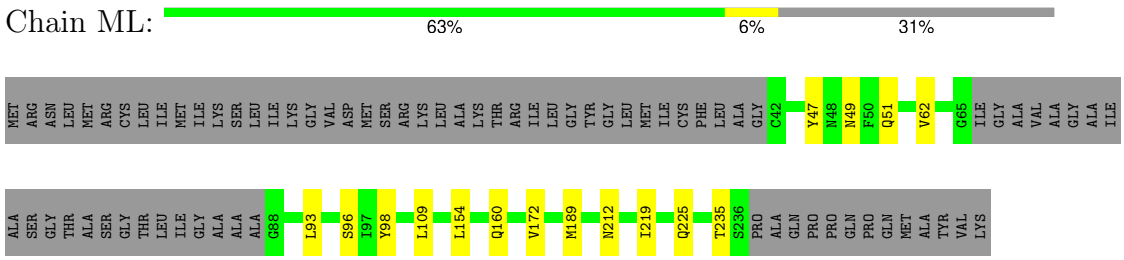
• Molecule 7: Outer membrane protein, OmpA family protein

Chain LL:



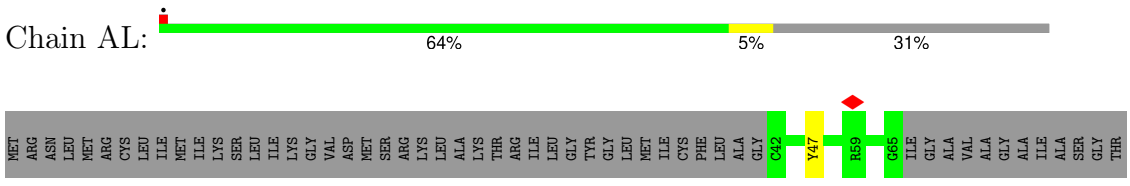
• Molecule 7: Outer membrane protein, OmpA family protein

Chain ML:



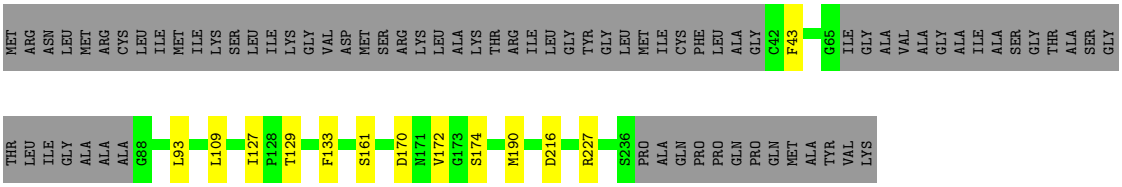
• Molecule 7: Outer membrane protein, OmpA family protein

Chain AL:



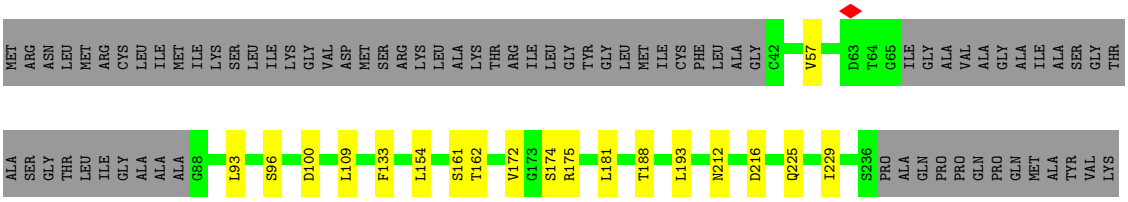
• Molecule 7: Outer membrane protein, OmpA family protein

Chain BL:



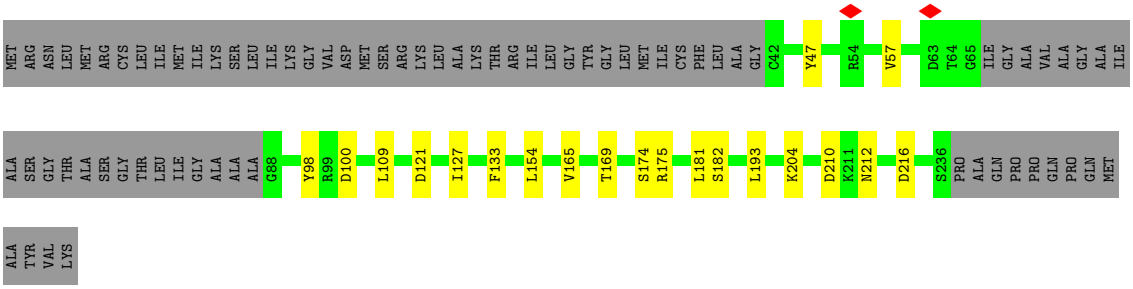
• Molecule 7: Outer membrane protein, OmpA family protein

Chain CL:



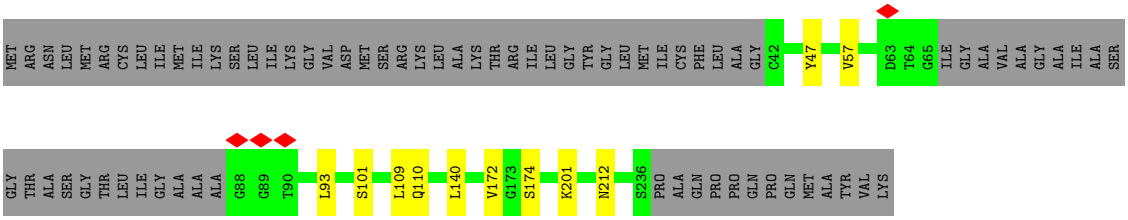
• Molecule 7: Outer membrane protein, OmpA family protein

Chain DL:



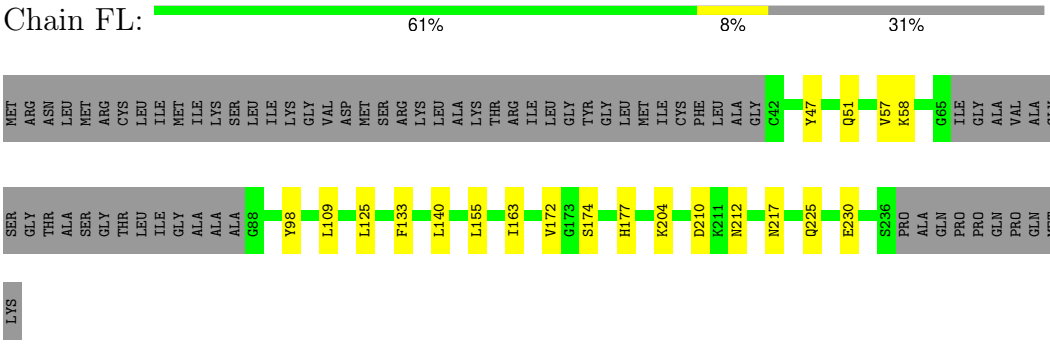
• Molecule 7: Outer membrane protein, OmpA family protein

Chain EL:



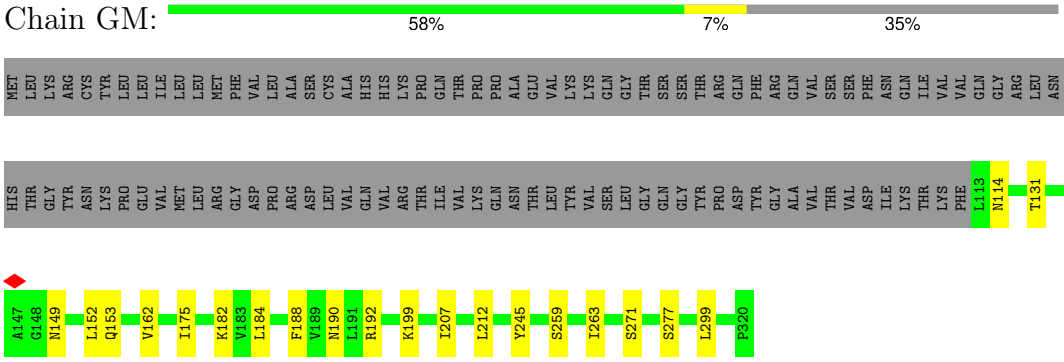
• Molecule 7: Outer membrane protein, OmpA family protein

Chain FL:



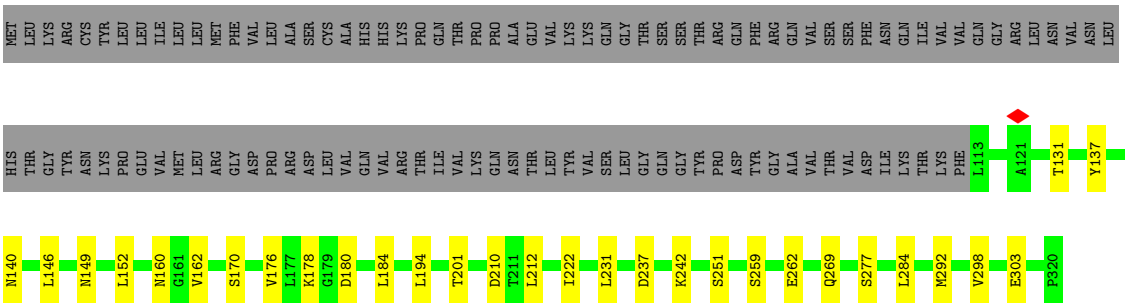
• Molecule 8: DUF2807 domain-containing protein

Chain GM:



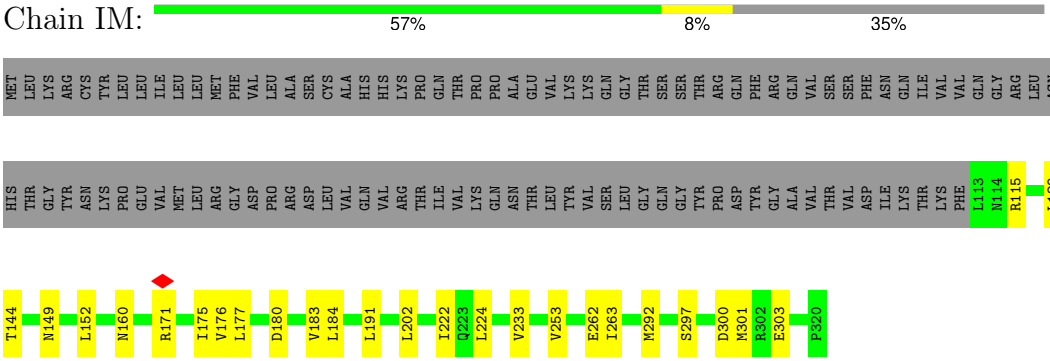
• Molecule 8: DUF2807 domain-containing protein

Chain HM:



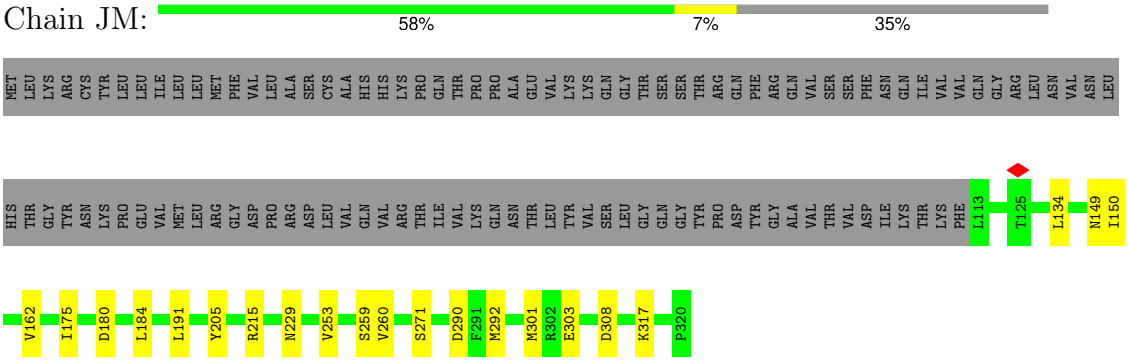
• Molecule 8: DUF2807 domain-containing protein

Chain IM:



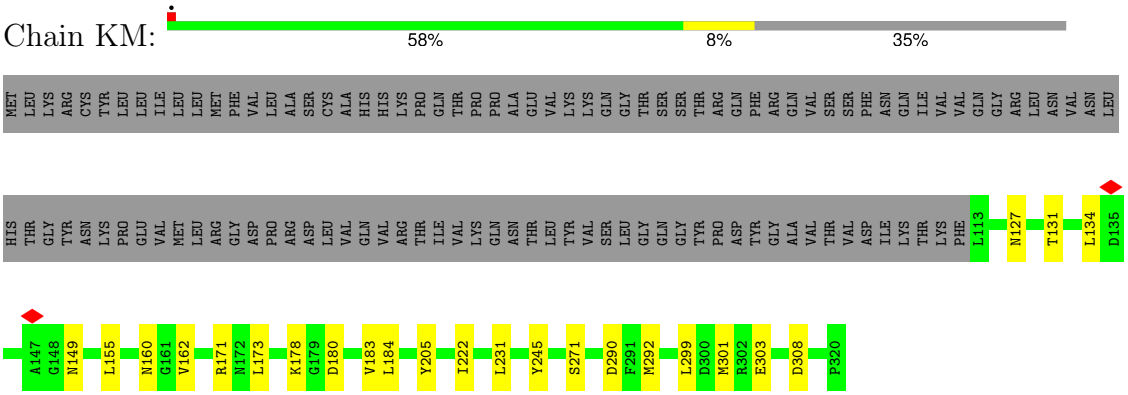
• Molecule 8: DUF2807 domain-containing protein

Chain JM:



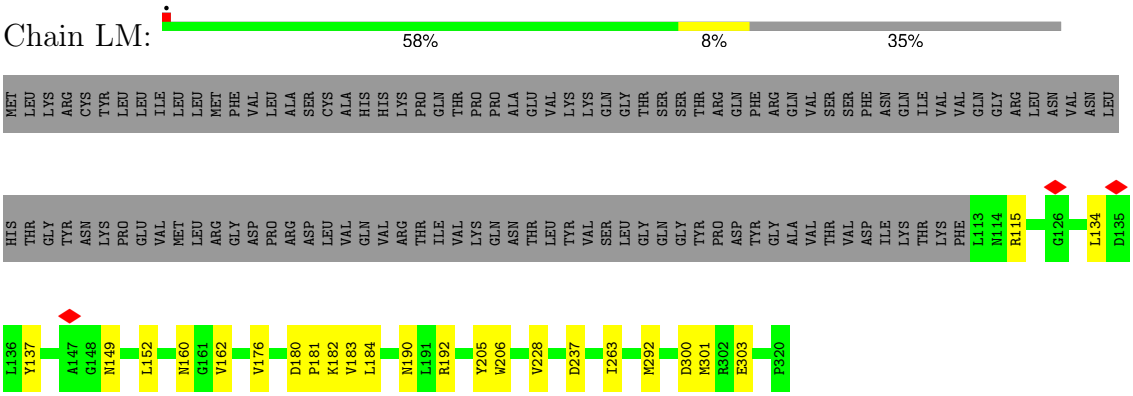
• Molecule 8: DUF2807 domain-containing protein

Chain KM:



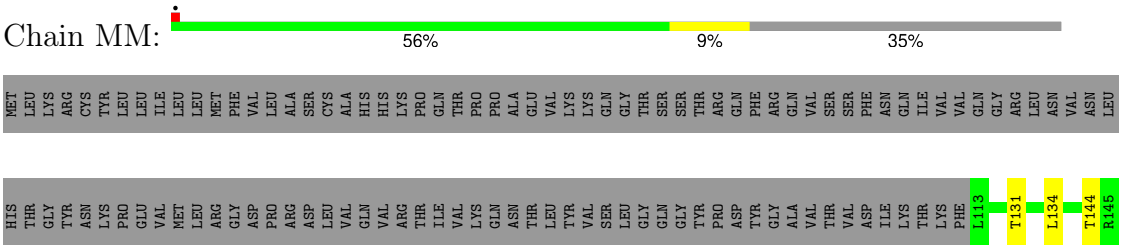
• Molecule 8: DUF2807 domain-containing protein

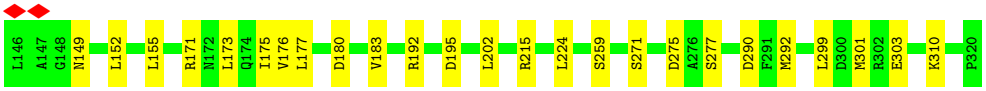
Chain LM:



• Molecule 8: DUF2807 domain-containing protein

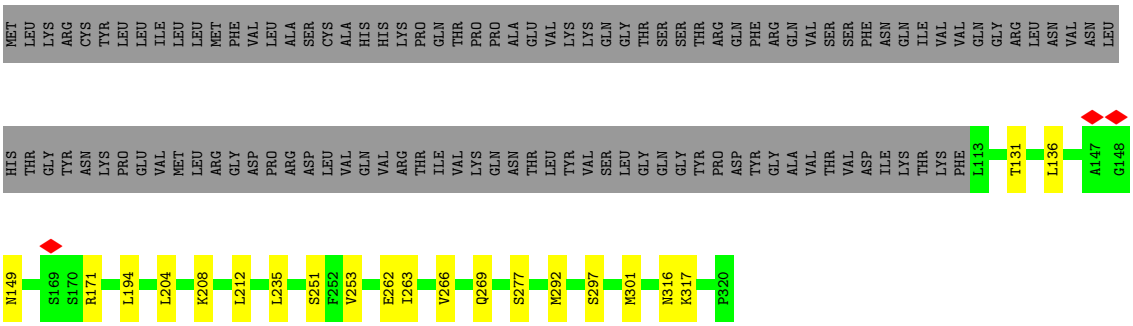
Chain MM:





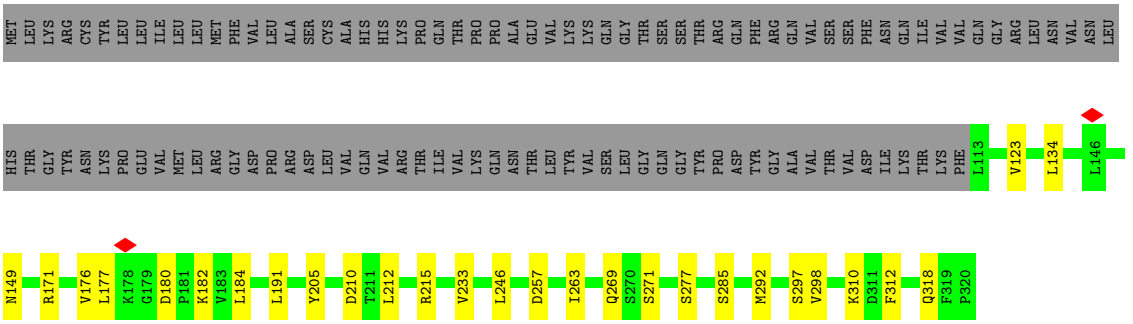
• Molecule 8: DUF2807 domain-containing protein

Chain AM:



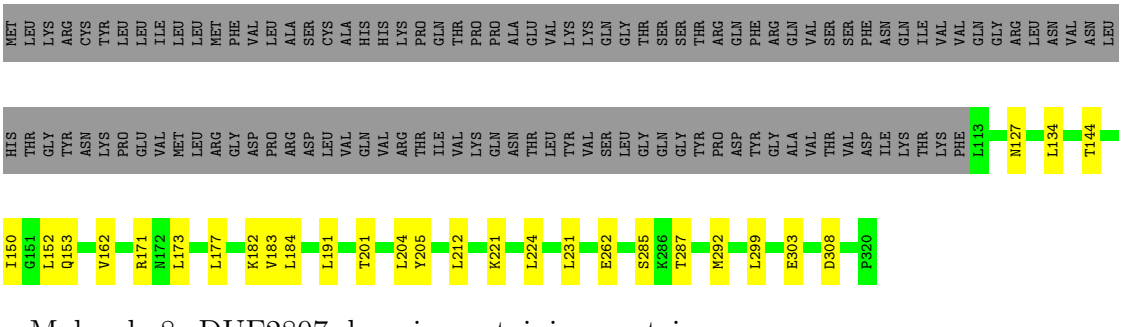
• Molecule 8: DUF2807 domain-containing protein

Chain BM:



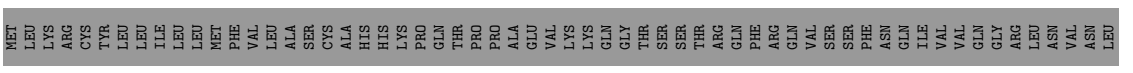
• Molecule 8: DUF2807 domain-containing protein

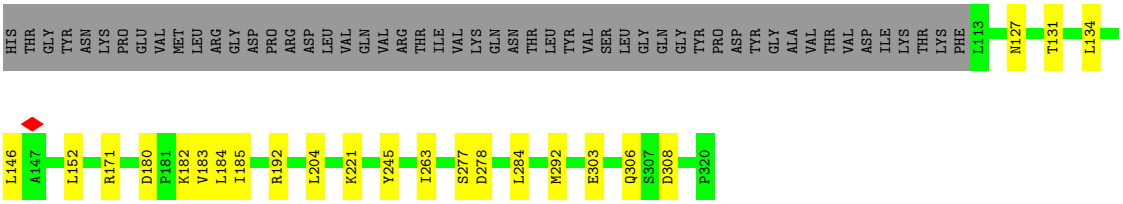
Chain CM:



• Molecule 8: DUF2807 domain-containing protein

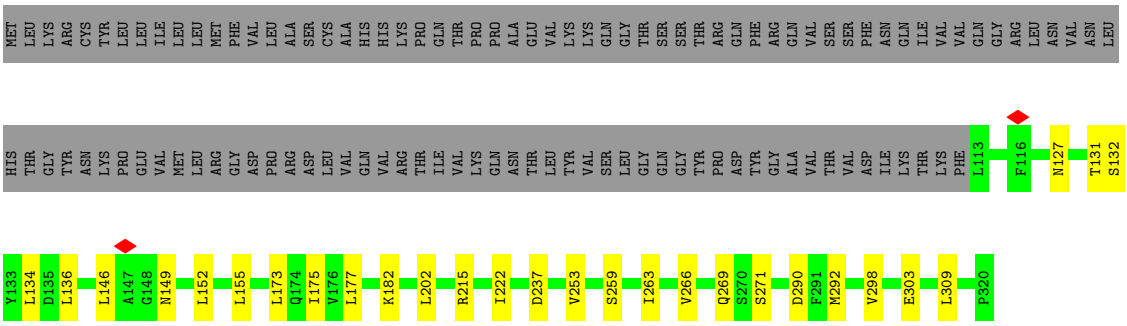
Chain DM:





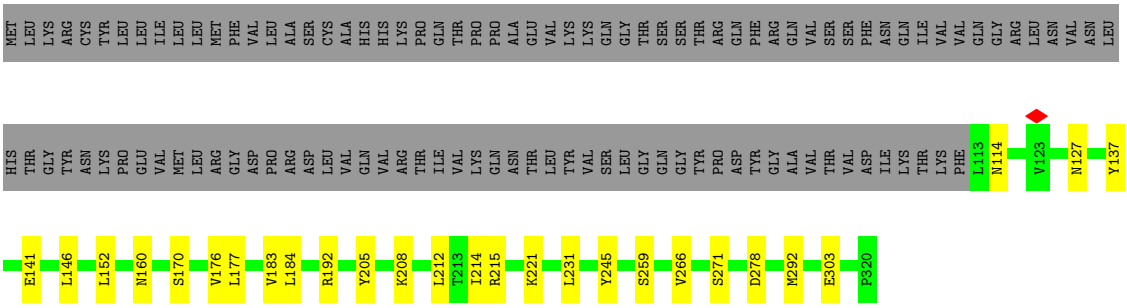
• Molecule 8: DUF2807 domain-containing protein

Chain EM:



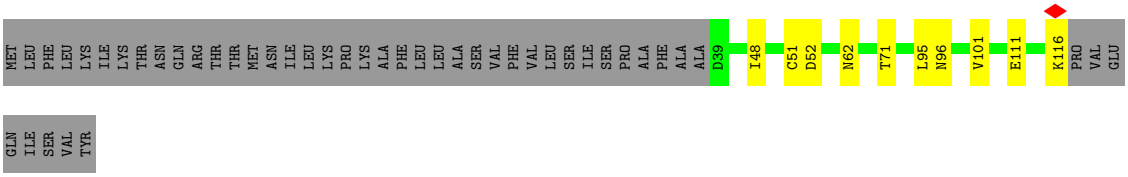
• Molecule 8: DUF2807 domain-containing protein

Chain FM:



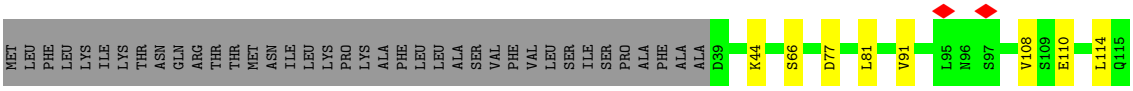
• Molecule 9: Neurogenic locus notch

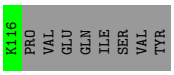
Chain GN:



• Molecule 9: Neurogenic locus notch

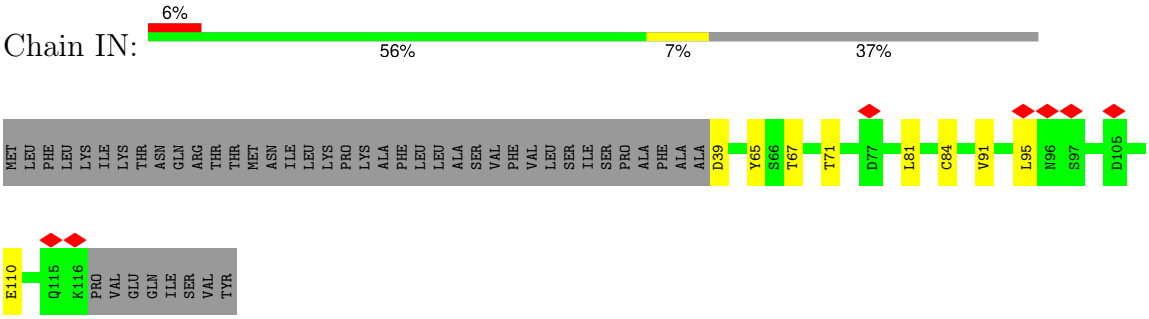
Chain HN:





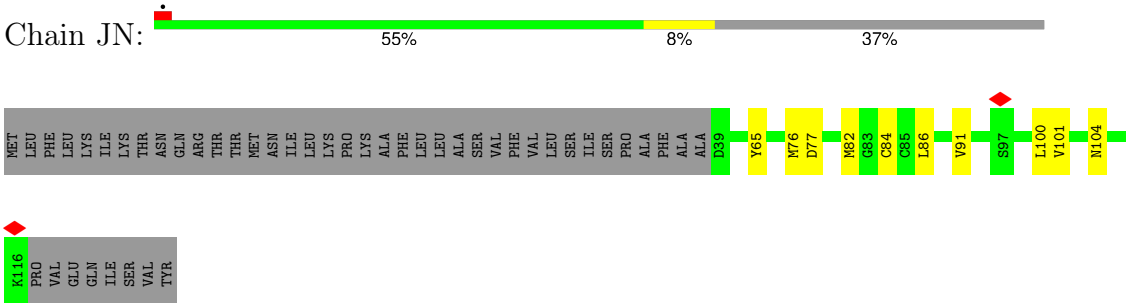
• Molecule 9: Neurogenic locus notch

Chain IN:



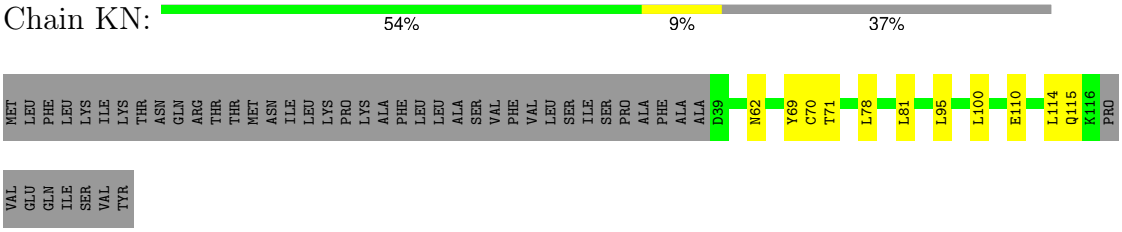
• Molecule 9: Neurogenic locus notch

Chain JN:



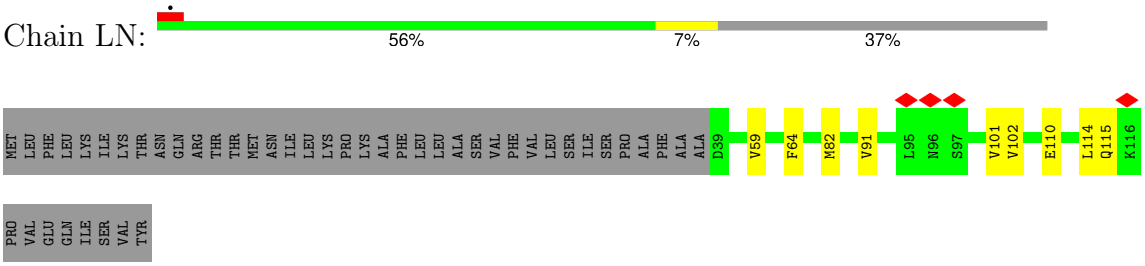
• Molecule 9: Neurogenic locus notch

Chain KN:



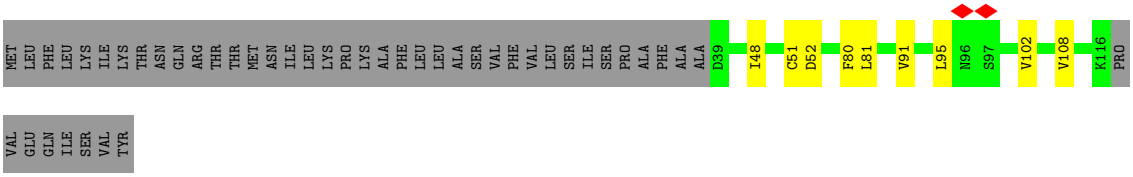
• Molecule 9: Neurogenic locus notch

Chain LN:



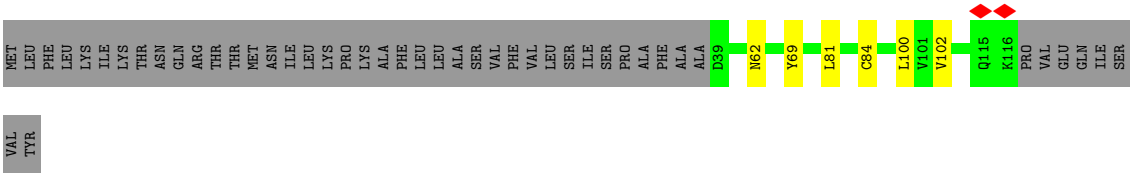
• Molecule 9: Neurogenic locus notch

Chain MN:



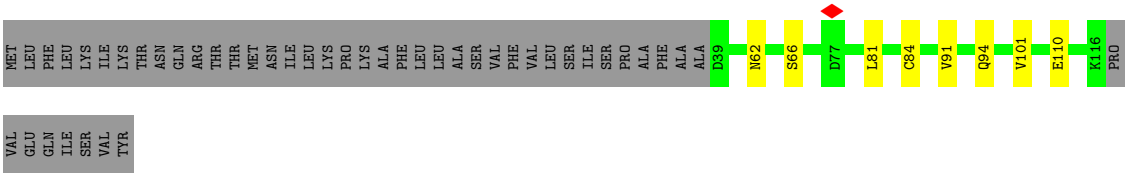
• Molecule 9: Neurogenic locus notch

Chain AN:



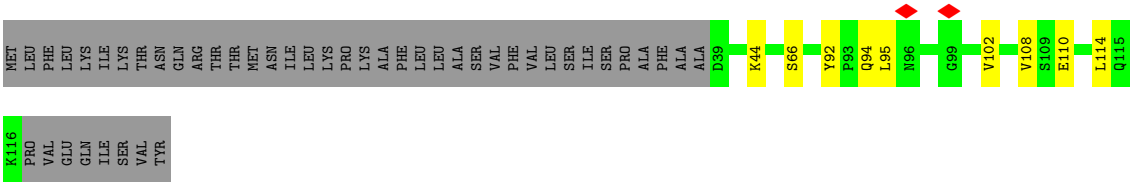
• Molecule 9: Neurogenic locus notch

Chain BN:



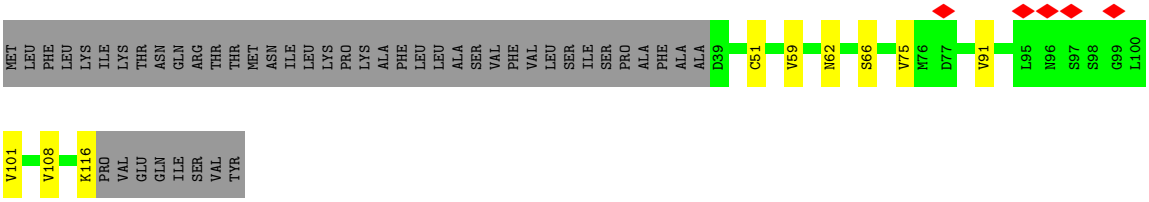
• Molecule 9: Neurogenic locus notch

Chain CN:



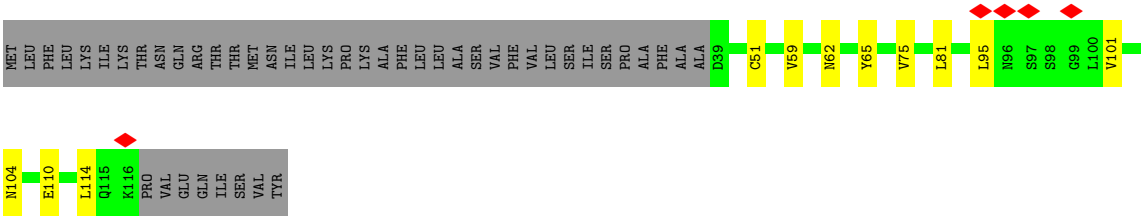
• Molecule 9: Neurogenic locus notch

Chain DN:

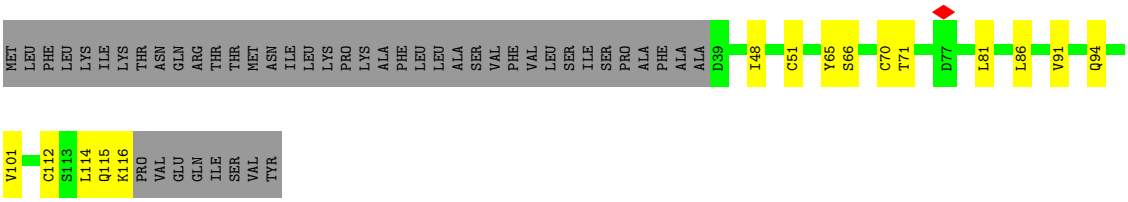


• Molecule 9: Neurogenic locus notch

Chain EN:



• Molecule 9: Neurogenic locus notch



• Molecule 10: Unknown protein fragment

There are no outlier residues recorded for this chain.

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• Molecule 10: Unknown protein fragment

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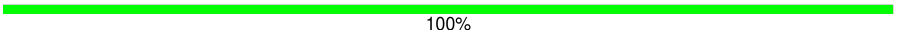
• Molecule 10: Unknown protein fragment

Chain MU: 

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain AU:

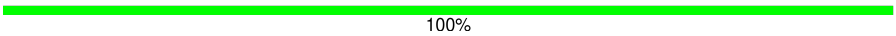
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain BU:

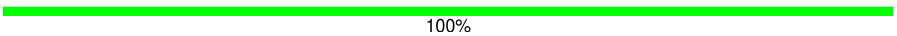
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain CU: 

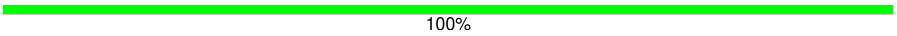
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain DU: 

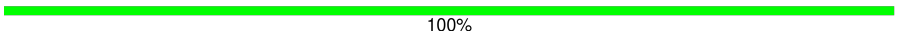
There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain EU: 

There are no outlier residues recorded for this chain.

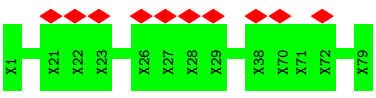
• Molecule 10: Unknown protein fragment

Chain FU: 

There are no outlier residues recorded for this chain.

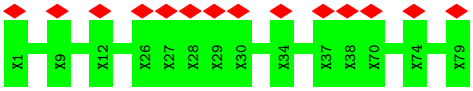
• Molecule 11: Unknown protein fragment

Chain GX:



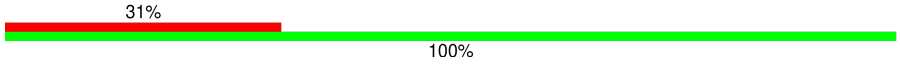
• Molecule 11: Unknown protein fragment

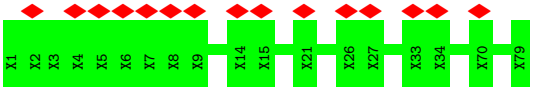
Chain DX:



• Molecule 11: Unknown protein fragment

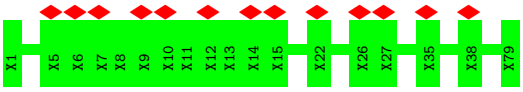
Chain HX:





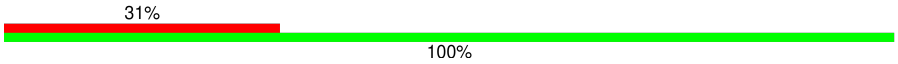
• Molecule 11: Unknown protein fragment

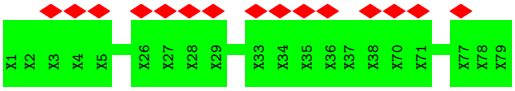
Chain IX:



• Molecule 11: Unknown protein fragment

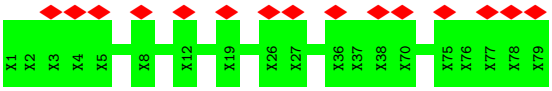
Chain JX:





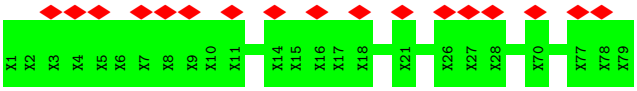
• Molecule 11: Unknown protein fragment

Chain KX:



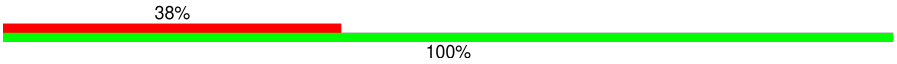
• Molecule 11: Unknown protein fragment

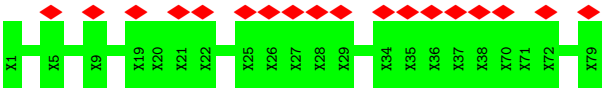
Chain LX:



• Molecule 11: Unknown protein fragment

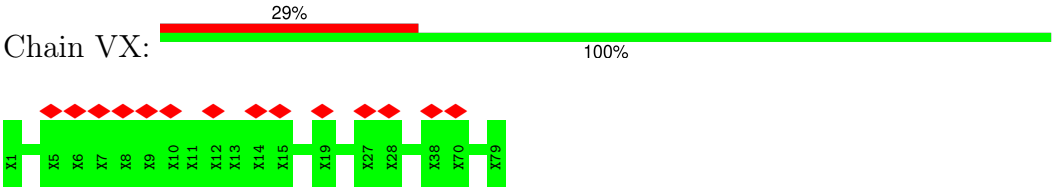
Chain MX:





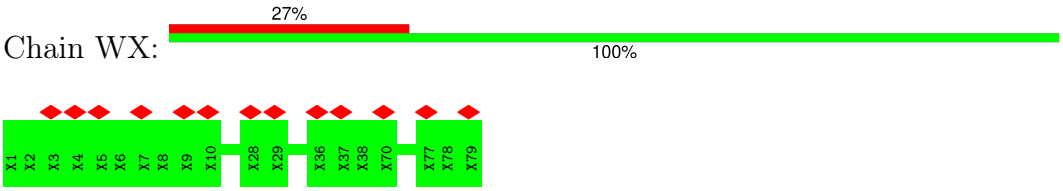
• Molecule 11: Unknown protein fragment

Chain VX:



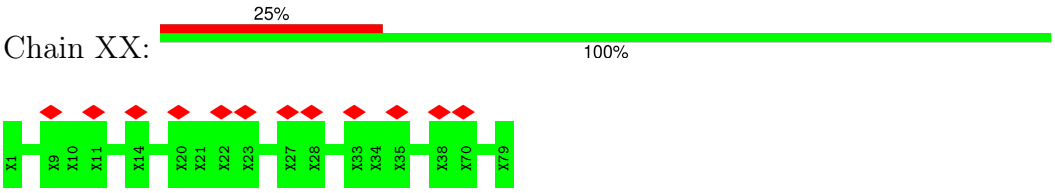
• Molecule 11: Unknown protein fragment

Chain WX:



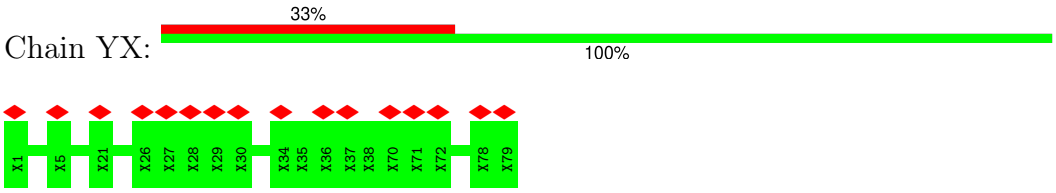
• Molecule 11: Unknown protein fragment

Chain XX:



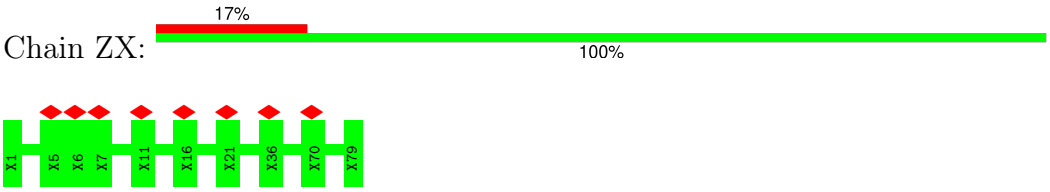
• Molecule 11: Unknown protein fragment

Chain YX:



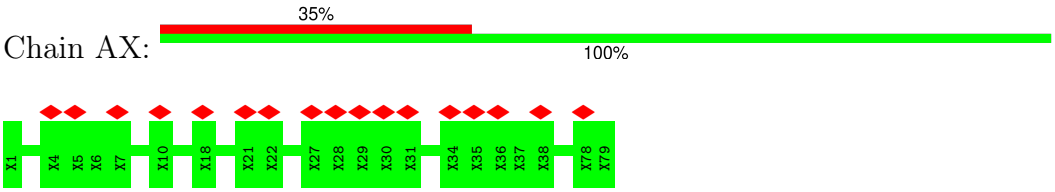
• Molecule 11: Unknown protein fragment

Chain ZX:



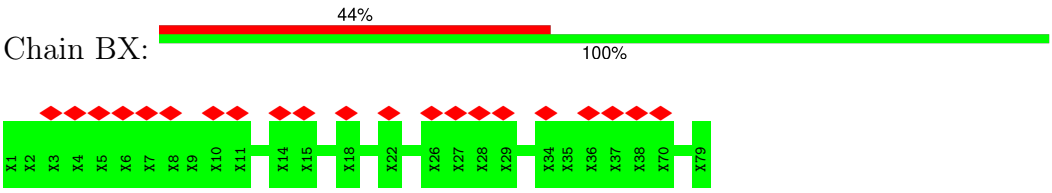
• Molecule 11: Unknown protein fragment

Chain AX:



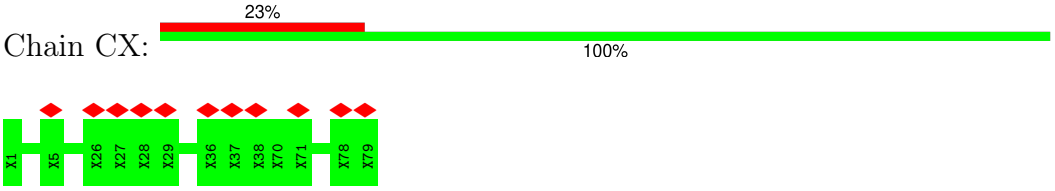
• Molecule 11: Unknown protein fragment

Chain BX:



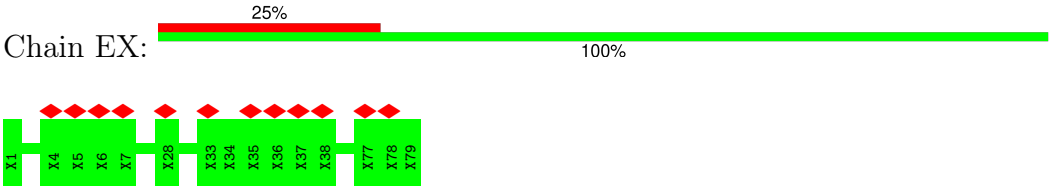
• Molecule 11: Unknown protein fragment

Chain CX:



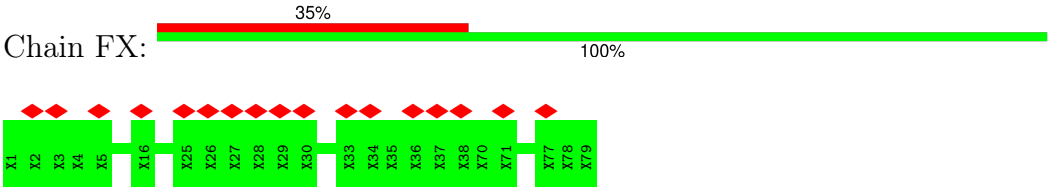
• Molecule 11: Unknown protein fragment

Chain EX:



• Molecule 11: Unknown protein fragment

Chain FX:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79720	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.547	Depositor
Minimum map value	-4.150	Depositor
Average map value	0.089	Depositor
Map value standard deviation	0.575	Depositor
Recommended contour level	2.25	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.244, 2.244, 2.244	Depositor

5 Model quality

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

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

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

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

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

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

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

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ef	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	FF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	Ff	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	GF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Gf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	HF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Hf	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	IF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	JF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Jf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	KF	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
3	Kf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	LF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Lf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	MF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Mf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	VF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	WF	61/269 (23%)	54 (88%)	7 (12%)	0	100	100
3	XF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	YF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	ZF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
4	AD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
4	Ad	135/163 (83%)	133 (98%)	2 (2%)	0	100	100
4	BD	138/163 (85%)	127 (92%)	10 (7%)	1 (1%)	19	56
4	Bd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
4	CD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
4	Cd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
4	DD	138/163 (85%)	127 (92%)	11 (8%)	0	100	100
4	Dd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
4	ED	138/163 (85%)	132 (96%)	6 (4%)	0	100	100

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

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

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	28	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AG	135/765 (18%)	109 (81%)	26 (19%)	1 7
1	Ag	31/765 (4%)	26 (84%)	5 (16%)	2 11
1	BG	135/765 (18%)	110 (82%)	25 (18%)	1 8
1	Bg	31/765 (4%)	24 (77%)	7 (23%)	1 5
1	CG	135/765 (18%)	108 (80%)	27 (20%)	1 6
1	Cg	31/765 (4%)	25 (81%)	6 (19%)	1 7
1	DG	135/765 (18%)	115 (85%)	20 (15%)	2 13
1	Dg	31/765 (4%)	24 (77%)	7 (23%)	1 5
1	EG	135/765 (18%)	111 (82%)	24 (18%)	1 9
1	Eg	31/765 (4%)	27 (87%)	4 (13%)	3 15
1	FG	135/765 (18%)	116 (86%)	19 (14%)	3 14
1	Fg	31/765 (4%)	28 (90%)	3 (10%)	6 22
1	GG	135/765 (18%)	113 (84%)	22 (16%)	2 11
1	Gg	31/765 (4%)	27 (87%)	4 (13%)	3 15
1	HG	135/765 (18%)	115 (85%)	20 (15%)	2 13
1	Hg	31/765 (4%)	24 (77%)	7 (23%)	1 5
1	IG	135/765 (18%)	122 (90%)	13 (10%)	7 22
1	Ig	31/765 (4%)	28 (90%)	3 (10%)	6 22
1	JG	135/765 (18%)	117 (87%)	18 (13%)	3 15
1	Jg	31/765 (4%)	19 (61%)	12 (39%)	0 0
1	KG	135/765 (18%)	114 (84%)	21 (16%)	2 12
1	Kg	31/765 (4%)	25 (81%)	6 (19%)	1 7
1	LG	135/765 (18%)	117 (87%)	18 (13%)	3 15
1	Lg	31/765 (4%)	24 (77%)	7 (23%)	1 5
1	MG	135/765 (18%)	106 (78%)	29 (22%)	1 5
1	Mg	31/765 (4%)	27 (87%)	4 (13%)	3 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	NG	135/765 (18%)	108 (80%)	27 (20%)	1 6
1	OG	135/765 (18%)	112 (83%)	23 (17%)	1 10
1	PG	135/765 (18%)	114 (84%)	21 (16%)	2 12
1	VG	31/765 (4%)	27 (87%)	4 (13%)	3 15
1	WG	31/765 (4%)	27 (87%)	4 (13%)	3 15
1	XG	31/765 (4%)	25 (81%)	6 (19%)	1 7
1	YG	31/765 (4%)	29 (94%)	2 (6%)	14 35
1	ZG	31/765 (4%)	25 (81%)	6 (19%)	1 7
2	AC	178/257 (69%)	151 (85%)	27 (15%)	2 12
2	BC	178/257 (69%)	150 (84%)	28 (16%)	2 12
2	CC	178/257 (69%)	148 (83%)	30 (17%)	1 10
2	DC	203/257 (79%)	178 (88%)	25 (12%)	4 16
2	EC	178/257 (69%)	154 (86%)	24 (14%)	3 15
2	FC	178/257 (69%)	149 (84%)	29 (16%)	2 11
2	GC	178/257 (69%)	154 (86%)	24 (14%)	3 15
2	HC	203/257 (79%)	180 (89%)	23 (11%)	4 18
2	IC	203/257 (79%)	177 (87%)	26 (13%)	3 15
2	JC	178/257 (69%)	151 (85%)	27 (15%)	2 12
2	KC	178/257 (69%)	145 (82%)	33 (18%)	1 8
2	LC	203/257 (79%)	187 (92%)	16 (8%)	10 29
2	MC	203/257 (79%)	178 (88%)	25 (12%)	4 16
3	AF	53/237 (22%)	40 (76%)	13 (24%)	0 3
3	Af	49/237 (21%)	37 (76%)	12 (24%)	0 3
3	BF	53/237 (22%)	46 (87%)	7 (13%)	3 15
3	Bf	49/237 (21%)	45 (92%)	4 (8%)	9 28
3	CF	53/237 (22%)	43 (81%)	10 (19%)	1 7
3	Cf	49/237 (21%)	39 (80%)	10 (20%)	1 6
3	DF	53/237 (22%)	47 (89%)	6 (11%)	4 18
3	Df	49/237 (21%)	46 (94%)	3 (6%)	15 37
3	EF	53/237 (22%)	47 (89%)	6 (11%)	4 18
3	Ef	49/237 (21%)	42 (86%)	7 (14%)	2 13

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	FD	121/139 (87%)	105 (87%)	16 (13%)	3	15
4	Fd	118/139 (85%)	103 (87%)	15 (13%)	3	15
4	GD	121/139 (87%)	105 (87%)	16 (13%)	3	15
4	Gd	118/139 (85%)	104 (88%)	14 (12%)	4	17
4	HD	121/139 (87%)	111 (92%)	10 (8%)	9	28
4	Hd	118/139 (85%)	105 (89%)	13 (11%)	5	19
4	ID	121/139 (87%)	112 (93%)	9 (7%)	11	31
4	Id	118/139 (85%)	103 (87%)	15 (13%)	3	15
4	JD	121/139 (87%)	108 (89%)	13 (11%)	5	19
4	Jd	118/139 (85%)	108 (92%)	10 (8%)	8	27
4	KD	121/139 (87%)	113 (93%)	8 (7%)	14	34
4	Kd	118/139 (85%)	107 (91%)	11 (9%)	7	23
4	LD	121/139 (87%)	105 (87%)	16 (13%)	3	15
4	Ld	118/139 (85%)	106 (90%)	12 (10%)	6	21
4	MD	121/139 (87%)	111 (92%)	10 (8%)	9	28
4	Md	118/139 (85%)	105 (89%)	13 (11%)	5	19
5	AH	220/300 (73%)	191 (87%)	29 (13%)	3	15
5	BH	220/300 (73%)	190 (86%)	30 (14%)	3	14
5	CH	220/300 (73%)	190 (86%)	30 (14%)	3	14
5	DH	220/300 (73%)	193 (88%)	27 (12%)	4	16
5	EH	220/300 (73%)	185 (84%)	35 (16%)	2	11
5	FH	220/300 (73%)	191 (87%)	29 (13%)	3	15
5	GH	220/300 (73%)	198 (90%)	22 (10%)	6	21
5	HH	220/300 (73%)	189 (86%)	31 (14%)	3	14
5	IH	220/300 (73%)	194 (88%)	26 (12%)	4	17
5	JH	220/300 (73%)	201 (91%)	19 (9%)	8	27
5	KH	220/300 (73%)	200 (91%)	20 (9%)	7	24
5	LH	220/300 (73%)	194 (88%)	26 (12%)	4	17
5	MH	220/300 (73%)	194 (88%)	26 (12%)	4	17
5	VH	207/300 (69%)	181 (87%)	26 (13%)	3	16
5	WH	207/300 (69%)	182 (88%)	25 (12%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	XH	207/300 (69%)	178 (86%)	29 (14%)	3	14
5	YH	207/300 (69%)	182 (88%)	25 (12%)	4	16
5	ZH	207/300 (69%)	178 (86%)	29 (14%)	3	14
6	AK	129/163 (79%)	109 (84%)	20 (16%)	2	12
6	BK	129/163 (79%)	118 (92%)	11 (8%)	8	27
6	CK	129/163 (79%)	111 (86%)	18 (14%)	3	14
6	DK	129/163 (79%)	115 (89%)	14 (11%)	5	19
6	EK	129/163 (79%)	107 (83%)	22 (17%)	1	10
6	FK	129/163 (79%)	108 (84%)	21 (16%)	2	11
6	GK	129/163 (79%)	116 (90%)	13 (10%)	6	21
6	HK	129/163 (79%)	111 (86%)	18 (14%)	3	14
6	IK	129/163 (79%)	121 (94%)	8 (6%)	15	37
6	JK	129/163 (79%)	109 (84%)	20 (16%)	2	12
6	KK	129/163 (79%)	109 (84%)	20 (16%)	2	12
6	LK	129/163 (79%)	110 (85%)	19 (15%)	2	13
6	MK	129/163 (79%)	113 (88%)	16 (12%)	4	16
7	AL	148/203 (73%)	135 (91%)	13 (9%)	8	25
7	BL	148/203 (73%)	135 (91%)	13 (9%)	8	25
7	CL	148/203 (73%)	129 (87%)	19 (13%)	3	15
7	DL	148/203 (73%)	128 (86%)	20 (14%)	3	15
7	EL	148/203 (73%)	137 (93%)	11 (7%)	11	31
7	FL	148/203 (73%)	128 (86%)	20 (14%)	3	15
7	GL	148/203 (73%)	131 (88%)	17 (12%)	4	17
7	HL	148/203 (73%)	134 (90%)	14 (10%)	7	22
7	IL	148/203 (73%)	133 (90%)	15 (10%)	6	21
7	JL	148/203 (73%)	133 (90%)	15 (10%)	6	21
7	KL	148/203 (73%)	128 (86%)	20 (14%)	3	15
7	LL	148/203 (73%)	133 (90%)	15 (10%)	6	21
7	ML	148/203 (73%)	132 (89%)	16 (11%)	5	19
8	AM	175/276 (63%)	154 (88%)	21 (12%)	4	17
8	BM	175/276 (63%)	147 (84%)	28 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	CM	175/276 (63%)	147 (84%)	28 (16%)	2 11
8	DM	175/276 (63%)	152 (87%)	23 (13%)	3 15
8	EM	175/276 (63%)	147 (84%)	28 (16%)	2 11
8	FM	175/276 (63%)	148 (85%)	27 (15%)	2 12
8	GM	175/276 (63%)	152 (87%)	23 (13%)	3 15
8	HM	175/276 (63%)	145 (83%)	30 (17%)	1 10
8	IM	175/276 (63%)	148 (85%)	27 (15%)	2 12
8	JM	175/276 (63%)	155 (89%)	20 (11%)	4 17
8	KM	175/276 (63%)	151 (86%)	24 (14%)	3 14
8	LM	175/276 (63%)	151 (86%)	24 (14%)	3 14
8	MM	175/276 (63%)	147 (84%)	28 (16%)	2 11
9	AN	66/107 (62%)	60 (91%)	6 (9%)	7 24
9	BN	66/107 (62%)	58 (88%)	8 (12%)	4 16
9	CN	66/107 (62%)	57 (86%)	9 (14%)	3 14
9	DN	66/107 (62%)	57 (86%)	9 (14%)	3 14
9	EN	66/107 (62%)	55 (83%)	11 (17%)	2 10
9	FN	66/107 (62%)	51 (77%)	15 (23%)	0 5
9	GN	66/107 (62%)	56 (85%)	10 (15%)	2 12
9	HN	66/107 (62%)	58 (88%)	8 (12%)	4 16
9	IN	66/107 (62%)	57 (86%)	9 (14%)	3 14
9	JN	66/107 (62%)	56 (85%)	10 (15%)	2 12
9	KN	66/107 (62%)	55 (83%)	11 (17%)	2 10
9	LN	66/107 (62%)	57 (86%)	9 (14%)	3 14
9	MN	66/107 (62%)	57 (86%)	9 (14%)	3 14
All	All	20484/55449 (37%)	17744 (87%)	2740 (13%)	5 14

All (2740) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AG	864	LYS
1	AG	865	THR
1	AG	869	MET
1	AG	875	THR
1	AG	886	LEU

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Mol	Chain	Res	Type
1	AG	898	LYS
1	AG	904	ASN
1	AG	910	ASP
1	AG	911	LYS
1	AG	913	VAL
1	AG	916	PHE
1	AG	930	ILE
1	AG	939	THR
1	AG	942	THR
1	AG	944	LEU
1	AG	948	THR
1	AG	962	SER
1	AG	963	SER
1	AG	965	LEU
1	AG	972	PHE
1	AG	1017	GLN
1	AG	1027	THR
1	AG	1028	THR
1	AG	1032	TYR
1	AG	1037	LEU
1	AG	1045	VAL
2	BC	68	GLN
2	BC	96	ASN
2	BC	103	ASN
2	BC	104	ILE
2	BC	108	VAL
2	BC	110	LEU
2	BC	111	GLU
2	BC	118	LEU
2	BC	128	ASP
2	BC	136	GLN
2	BC	142	THR
2	BC	145	THR
2	BC	147	ARG
2	BC	162	VAL
2	BC	164	LEU
2	BC	167	LYS
2	BC	168	THR
2	BC	180	GLU
2	BC	194	LEU
2	BC	203	GLU
2	BC	215	LEU

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Mol	Chain	Res	Type
2	BC	220	VAL
2	BC	227	HIS
2	BC	228	THR
2	BC	229	ASP
2	BC	239	ILE
2	BC	245	VAL
2	BC	265	VAL
2	EC	69	GLN
2	EC	97	ASN
2	EC	109	VAL
2	EC	117	LEU
2	EC	119	LEU
2	EC	129	ASP
2	EC	139	HIS
2	EC	140	PHE
2	EC	142	THR
2	EC	143	THR
2	EC	146	THR
2	EC	148	ARG
2	EC	163	VAL
2	EC	166	LEU
2	EC	181	GLU
2	EC	195	LEU
2	EC	204	GLU
2	EC	205	ASP
2	EC	214	LYS
2	EC	221	VAL
2	EC	228	HIS
2	EC	229	THR
2	EC	234	THR
2	EC	266	VAL
3	AF	207	ARG
3	AF	208	ILE
3	AF	209	ILE
3	AF	215	VAL
3	AF	229	THR
3	AF	230	LEU
3	AF	231	THR
3	AF	238	ILE
3	AF	250	LEU
3	AF	253	ARG
3	AF	256	THR

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Mol	Chain	Res	Type
3	AF	258	SER
3	AF	263	LYS
4	GD	23	MET
4	GD	30	ILE
4	GD	34	SER
4	GD	35	ASP
4	GD	43	GLU
4	GD	47	SER
4	GD	51	SER
4	GD	55	MET
4	GD	78	ASN
4	GD	85	VAL
4	GD	112	SER
4	GD	127	SER
4	GD	154	VAL
4	GD	155	GLU
4	GD	156	LEU
4	GD	162	TYR
3	GF	207	ARG
3	GF	211	TYR
3	GF	223	ILE
3	GF	231	THR
3	GF	255	LEU
3	GF	256	THR
1	Gg	803	THR
1	Gg	811	ASP
1	Gg	815	VAL
1	Gg	819	VAL
5	GH	144	THR
5	GH	147	THR
5	GH	171	LEU
5	GH	180	VAL
5	GH	215	ILE
5	GH	221	TYR
5	GH	225	ASN
5	GH	233	LEU
5	GH	248	VAL
5	GH	250	TYR
5	GH	253	ASP
5	GH	284	LEU
5	GH	313	VAL
5	GH	316	ASN

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Mol	Chain	Res	Type
5	GH	334	THR
5	GH	344	VAL
5	GH	345	LEU
5	GH	346	LEU
5	GH	350	HIS
5	GH	352	LYS
5	GH	354	MET
5	GH	355	GLN
6	GK	45	VAL
6	GK	46	ASP
6	GK	54	ILE
6	GK	70	VAL
6	GK	75	LEU
6	GK	77	SER
6	GK	112	ILE
6	GK	114	ILE
6	GK	116	VAL
6	GK	144	LEU
6	GK	149	VAL
6	GK	156	THR
6	GK	170	LEU
7	GL	44	HIS
7	GL	47	TYR
7	GL	57	VAL
7	GL	93	LEU
7	GL	98	TYR
7	GL	100	ASP
7	GL	109	LEU
7	GL	129	THR
7	GL	130	ASP
7	GL	162	THR
7	GL	169	THR
7	GL	172	VAL
7	GL	174	SER
7	GL	182	SER
7	GL	188	THR
7	GL	212	ASN
7	GL	216	ASP
8	GM	114	ASN
8	GM	131	THR
8	GM	134	LEU
8	GM	146	LEU

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Mol	Chain	Res	Type
8	GM	149	ASN
8	GM	152	LEU
8	GM	153	GLN
8	GM	162	VAL
8	GM	175	ILE
8	GM	182	LYS
8	GM	184	LEU
8	GM	188	PHE
8	GM	190	ASN
8	GM	192	ARG
8	GM	199	LYS
8	GM	207	ILE
8	GM	212	LEU
8	GM	245	TYR
8	GM	259	SER
8	GM	263	ILE
8	GM	271	SER
8	GM	277	SER
8	GM	299	LEU
9	GN	48	ILE
9	GN	51	CYS
9	GN	52	ASP
9	GN	62	ASN
9	GN	71	THR
9	GN	95	LEU
9	GN	96	ASN
9	GN	101	VAL
9	GN	111	GLU
9	GN	116	LYS
4	Gd	58	VAL
4	Gd	59	GLU
4	Gd	60	LYS
4	Gd	61	VAL
4	Gd	63	THR
4	Gd	72	THR
4	Gd	73	ILE
4	Gd	82	ARG
4	Gd	115	VAL
4	Gd	123	THR
4	Gd	128	LEU
4	Gd	132	LEU
4	Gd	145	ILE

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Mol	Chain	Res	Type
4	Gd	147	VAL
3	Gf	211	TYR
3	Gf	238	ILE
3	Gf	244	VAL
3	Gf	245	LYS
3	Gf	246	LEU
3	Gf	261	VAL
4	HD	59	GLU
4	HD	63	THR
4	HD	70	THR
4	HD	86	ASP
4	HD	115	VAL
4	HD	130	GLU
4	HD	147	VAL
4	HD	154	VAL
4	HD	156	LEU
4	HD	160	LYS
3	HF	208	ILE
3	HF	215	VAL
3	HF	223	ILE
3	HF	230	LEU
3	HF	233	ARG
3	HF	238	ILE
3	HF	256	THR
1	Hg	794	ILE
1	Hg	802	LEU
1	Hg	808	LEU
1	Hg	810	GLN
1	Hg	814	GLN
1	Hg	815	VAL
1	Hg	821	THR
5	HH	108	ASP
5	HH	109	LYS
5	HH	114	ASP
5	HH	126	GLN
5	HH	134	TYR
5	HH	138	GLU
5	HH	158	VAL
5	HH	170	ARG
5	HH	178	SER
5	HH	180	VAL
5	HH	183	ASP

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Mol	Chain	Res	Type
5	HH	204	ILE
5	HH	207	ASP
5	HH	218	THR
5	HH	228	VAL
5	HH	231	ARG
5	HH	238	MET
5	HH	240	THR
5	HH	241	LEU
5	HH	248	VAL
5	HH	250	TYR
5	HH	251	ARG
5	HH	278	ASP
5	HH	279	LEU
5	HH	284	LEU
5	HH	313	VAL
5	HH	329	THR
5	HH	332	ASP
5	HH	342	SER
5	HH	344	VAL
5	HH	348	SER
6	HK	45	VAL
6	HK	50	ASP
6	HK	70	VAL
6	HK	73	ASN
6	HK	83	LEU
6	HK	92	ASN
6	HK	106	LEU
6	HK	107	LYS
6	HK	111	LYS
6	HK	125	SER
6	HK	126	VAL
6	HK	144	LEU
6	HK	151	SER
6	HK	152	ARG
6	HK	156	THR
6	HK	166	THR
6	HK	180	VAL
6	HK	182	ILE
7	HL	47	TYR
7	HL	57	VAL
7	HL	93	LEU
7	HL	108	ASP

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Mol	Chain	Res	Type
7	HL	109	LEU
7	HL	137	SER
7	HL	140	LEU
7	HL	161	SER
7	HL	162	THR
7	HL	172	VAL
7	HL	175	ARG
7	HL	182	SER
7	HL	212	ASN
7	HL	219	ILE
8	HM	131	THR
8	HM	137	TYR
8	HM	140	ASN
8	HM	146	LEU
8	HM	149	ASN
8	HM	152	LEU
8	HM	160	ASN
8	HM	162	VAL
8	HM	170	SER
8	HM	176	VAL
8	HM	178	LYS
8	HM	180	ASP
8	HM	184	LEU
8	HM	194	LEU
8	HM	201	THR
8	HM	210	ASP
8	HM	212	LEU
8	HM	222	ILE
8	HM	231	LEU
8	HM	237	ASP
8	HM	242	LYS
8	HM	251	SER
8	HM	259	SER
8	HM	262	GLU
8	HM	269	GLN
8	HM	277	SER
8	HM	284	LEU
8	HM	292	MET
8	HM	298	VAL
8	HM	303	GLU
9	HN	44	LYS
9	HN	66	SER

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Mol	Chain	Res	Type
9	HN	77	ASP
9	HN	81	LEU
9	HN	91	VAL
9	HN	108	VAL
9	HN	110	GLU
9	HN	114	LEU
1	BG	865	THR
1	BG	876	SER
1	BG	886	LEU
1	BG	893	LYS
1	BG	898	LYS
1	BG	899	LEU
1	BG	904	ASN
1	BG	911	LYS
1	BG	912	MET
1	BG	913	VAL
1	BG	915	THR
1	BG	916	PHE
1	BG	919	MET
1	BG	930	ILE
1	BG	939	THR
1	BG	944	LEU
1	BG	953	LEU
1	BG	956	TYR
1	BG	962	SER
1	BG	963	SER
1	BG	965	LEU
1	BG	972	PHE
1	BG	1027	THR
1	BG	1037	LEU
1	BG	1045	VAL
4	Hd	58	VAL
4	Hd	61	VAL
4	Hd	63	THR
4	Hd	93	GLU
4	Hd	94	LEU
4	Hd	115	VAL
4	Hd	127	SER
4	Hd	128	LEU
4	Hd	138	GLN
4	Hd	154	VAL
4	Hd	155	GLU

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Mol	Chain	Res	Type
4	Hd	156	LEU
4	Hd	160	LYS
3	Hf	215	VAL
3	Hf	219	ARG
3	Hf	222	LEU
3	Hf	244	VAL
3	Hf	245	LYS
3	Hf	262	ILE
3	Hf	265	SER
1	Bg	793	GLU
1	Bg	800	ASP
1	Bg	806	THR
1	Bg	808	LEU
1	Bg	815	VAL
1	Bg	816	GLU
1	Bg	819	VAL
4	ID	73	ILE
4	ID	92	GLU
4	ID	93	GLU
4	ID	105	ARG
4	ID	111	LYS
4	ID	115	VAL
4	ID	127	SER
4	ID	134	ASP
4	ID	161	ILE
3	IF	208	ILE
3	IF	223	ILE
3	IF	231	THR
3	IF	246	LEU
3	IF	250	LEU
3	IF	255	LEU
3	IF	256	THR
3	IF	266	GLN
1	Ig	815	VAL
1	Ig	817	THR
1	Ig	819	VAL
5	IH	107	ILE
5	IH	108	ASP
5	IH	117	ARG
5	IH	147	THR
5	IH	178	SER
5	IH	180	VAL

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Mol	Chain	Res	Type
5	IH	183	ASP
5	IH	195	ASP
5	IH	218	THR
5	IH	226	LEU
5	IH	231	ARG
5	IH	233	LEU
5	IH	238	MET
5	IH	245	GLN
5	IH	248	VAL
5	IH	250	TYR
5	IH	253	ASP
5	IH	278	ASP
5	IH	294	ARG
5	IH	296	VAL
5	IH	313	VAL
5	IH	340	GLN
5	IH	342	SER
5	IH	344	VAL
5	IH	345	LEU
5	IH	354	MET
6	IK	83	LEU
6	IK	92	ASN
6	IK	111	LYS
6	IK	116	VAL
6	IK	142	GLU
6	IK	156	THR
6	IK	162	ASP
6	IK	170	LEU
7	IL	47	TYR
7	IL	93	LEU
7	IL	98	TYR
7	IL	100	ASP
7	IL	101	SER
7	IL	109	LEU
7	IL	111	LYS
7	IL	123	ARG
7	IL	133	PHE
7	IL	161	SER
7	IL	172	VAL
7	IL	174	SER
7	IL	181	LEU
7	IL	182	SER

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Mol	Chain	Res	Type
7	IL	220	ILE
8	IM	115	ARG
8	IM	129	LEU
8	IM	134	LEU
8	IM	144	THR
8	IM	149	ASN
8	IM	152	LEU
8	IM	160	ASN
8	IM	171	ARG
8	IM	175	ILE
8	IM	176	VAL
8	IM	177	LEU
8	IM	180	ASP
8	IM	183	VAL
8	IM	184	LEU
8	IM	191	LEU
8	IM	202	LEU
8	IM	222	ILE
8	IM	224	LEU
8	IM	233	VAL
8	IM	253	VAL
8	IM	262	GLU
8	IM	263	ILE
8	IM	292	MET
8	IM	297	SER
8	IM	300	ASP
8	IM	301	MET
8	IM	303	GLU
9	IN	39	ASP
9	IN	65	TYR
9	IN	67	THR
9	IN	71	THR
9	IN	81	LEU
9	IN	84	CYS
9	IN	91	VAL
9	IN	95	LEU
9	IN	110	GLU
4	Dd	26	LYS
4	Dd	53	LEU
4	Dd	57	LYS
4	Dd	58	VAL
4	Dd	62	ILE

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Mol	Chain	Res	Type
4	Dd	63	THR
4	Dd	85	VAL
4	Dd	88	SER
4	Dd	91	ILE
4	Dd	92	GLU
4	Dd	93	GLU
4	Dd	115	VAL
4	Dd	138	GLN
4	Dd	146	HIS
4	Dd	154	VAL
4	Dd	160	LYS
4	Id	30	ILE
4	Id	36	ASP
4	Id	52	MET
4	Id	60	LYS
4	Id	61	VAL
4	Id	63	THR
4	Id	72	THR
4	Id	78	ASN
4	Id	85	VAL
4	Id	92	GLU
4	Id	108	VAL
4	Id	115	VAL
4	Id	119	ILE
4	Id	142	LYS
4	Id	154	VAL
3	If	210	TYR
3	If	215	VAL
3	If	232	VAL
3	If	233	ARG
3	If	244	VAL
3	If	251	GLN
3	If	255	LEU
3	If	256	THR
3	If	260	GLN
3	If	261	VAL
3	If	266	GLN
4	JD	31	ASN
4	JD	35	ASP
4	JD	43	GLU
4	JD	47	SER
4	JD	50	ASP

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Mol	Chain	Res	Type
4	JD	55	MET
4	JD	84	SER
4	JD	85	VAL
4	JD	91	ILE
4	JD	108	VAL
4	JD	115	VAL
4	JD	127	SER
4	JD	160	LYS
3	JF	211	TYR
3	JF	223	ILE
3	JF	229	THR
3	JF	231	THR
3	JF	238	ILE
3	JF	250	LEU
3	JF	256	THR
3	JF	264	PHE
1	Jg	794	ILE
1	Jg	801	MET
1	Jg	806	THR
1	Jg	808	LEU
1	Jg	810	GLN
1	Jg	811	ASP
1	Jg	813	LYS
1	Jg	815	VAL
1	Jg	816	GLU
1	Jg	817	THR
1	Jg	818	GLN
1	Jg	819	VAL
5	JH	116	THR
5	JH	125	GLU
5	JH	147	THR
5	JH	170	ARG
5	JH	205	GLN
5	JH	226	LEU
5	JH	231	ARG
5	JH	241	LEU
5	JH	248	VAL
5	JH	249	ASP
5	JH	253	ASP
5	JH	256	VAL
5	JH	262	ASN
5	JH	285	GLU

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Mol	Chain	Res	Type
5	JH	293	ARG
5	JH	313	VAL
5	JH	316	ASN
5	JH	328	MET
5	JH	350	HIS
6	JK	45	VAL
6	JK	50	ASP
6	JK	70	VAL
6	JK	75	LEU
6	JK	83	LEU
6	JK	88	SER
6	JK	92	ASN
6	JK	99	LEU
6	JK	106	LEU
6	JK	107	LYS
6	JK	111	LYS
6	JK	117	THR
6	JK	126	VAL
6	JK	144	LEU
6	JK	152	ARG
6	JK	156	THR
6	JK	157	GLN
6	JK	159	LEU
6	JK	180	VAL
6	JK	183	THR
7	JL	44	HIS
7	JL	47	TYR
7	JL	55	ARG
7	JL	58	LYS
7	JL	101	SER
7	JL	129	THR
7	JL	130	ASP
7	JL	133	PHE
7	JL	155	LEU
7	JL	172	VAL
7	JL	181	LEU
7	JL	203	LEU
7	JL	212	ASN
7	JL	216	ASP
7	JL	227	ARG
8	JM	149	ASN
8	JM	150	ILE

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Mol	Chain	Res	Type
8	JM	162	VAL
8	JM	175	ILE
8	JM	180	ASP
8	JM	184	LEU
8	JM	191	LEU
8	JM	205	TYR
8	JM	215	ARG
8	JM	229	ASN
8	JM	253	VAL
8	JM	259	SER
8	JM	260	VAL
8	JM	271	SER
8	JM	290	ASP
8	JM	292	MET
8	JM	301	MET
8	JM	303	GLU
8	JM	308	ASP
8	JM	317	LYS
9	JN	65	TYR
9	JN	76	MET
9	JN	77	ASP
9	JN	82	MET
9	JN	84	CYS
9	JN	86	LEU
9	JN	91	VAL
9	JN	100	LEU
9	JN	101	VAL
9	JN	104	ASN
1	CG	865	THR
1	CG	869	MET
1	CG	877	VAL
1	CG	886	LEU
1	CG	898	LYS
1	CG	900	ILE
1	CG	904	ASN
1	CG	910	ASP
1	CG	911	LYS
1	CG	913	VAL
1	CG	916	PHE
1	CG	930	ILE
1	CG	942	THR
1	CG	944	LEU

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Mol	Chain	Res	Type
1	CG	956	TYR
1	CG	962	SER
1	CG	965	LEU
1	CG	966	GLN
1	CG	968	PHE
1	CG	1010	THR
1	CG	1016	SER
1	CG	1017	GLN
1	CG	1028	THR
1	CG	1037	LEU
1	CG	1040	LEU
1	CG	1041	PHE
1	CG	1044	ASP
4	Jd	27	LYS
4	Jd	36	ASP
4	Jd	51	SER
4	Jd	53	LEU
4	Jd	63	THR
4	Jd	108	VAL
4	Jd	115	VAL
4	Jd	119	ILE
4	Jd	121	ILE
4	Jd	150	ASN
3	Jf	208	ILE
3	Jf	209	ILE
3	Jf	213	GLN
3	Jf	237	LYS
3	Jf	245	LYS
3	Jf	246	LEU
3	Jf	255	LEU
3	Jf	260	GLN
3	Jf	261	VAL
3	Jf	263	LYS
5	AH	109	LYS
5	AH	125	GLU
5	AH	135	GLU
5	AH	147	THR
5	AH	154	THR
5	AH	160	LEU
5	AH	180	VAL
5	AH	183	ASP
5	AH	201	SER

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Mol	Chain	Res	Type
5	AH	202	PHE
5	AH	208	LYS
5	AH	218	THR
5	AH	226	LEU
5	AH	233	LEU
5	AH	237	VAL
5	AH	239	LEU
5	AH	241	LEU
5	AH	245	GLN
5	AH	262	ASN
5	AH	264	LYS
5	AH	277	ASN
5	AH	283	VAL
5	AH	284	LEU
5	AH	294	ARG
5	AH	316	ASN
5	AH	344	VAL
5	AH	345	LEU
5	AH	347	VAL
5	AH	356	LEU
4	KD	38	THR
4	KD	63	THR
4	KD	79	LEU
4	KD	85	VAL
4	KD	105	ARG
4	KD	108	VAL
4	KD	156	LEU
4	KD	160	LYS
2	CC	62	THR
2	CC	65	SER
2	CC	80	ASP
2	CC	83	LEU
2	CC	84	ASN
2	CC	102	GLU
2	CC	103	HIS
2	CC	105	ILE
2	CC	116	THR
2	CC	117	LEU
2	CC	143	THR
2	CC	146	THR
2	CC	148	ARG
2	CC	151	LEU

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Mol	Chain	Res	Type
2	CC	156	VAL
2	CC	163	VAL
2	CC	170	LYS
2	CC	176	TRP
2	CC	181	GLU
2	CC	185	LYS
2	CC	204	GLU
2	CC	218	MET
2	CC	221	VAL
2	CC	226	VAL
2	CC	240	ILE
2	CC	247	LEU
2	CC	248	ARG
2	CC	249	ILE
2	CC	259	SER
2	CC	266	VAL
3	KF	207	ARG
3	KF	215	VAL
3	KF	229	THR
3	KF	231	THR
3	KF	237	LYS
3	KF	238	ILE
3	KF	262	ILE
1	Kg	793	GLU
1	Kg	806	THR
1	Kg	808	LEU
1	Kg	811	ASP
1	Kg	815	VAL
1	Kg	819	VAL
5	KH	113	LYS
5	KH	123	ASN
5	KH	147	THR
5	KH	158	VAL
5	KH	170	ARG
5	KH	180	VAL
5	KH	183	ASP
5	KH	218	THR
5	KH	222	ASN
5	KH	228	VAL
5	KH	234	ASN
5	KH	248	VAL
5	KH	259	TYR

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Mol	Chain	Res	Type
5	KH	270	GLU
5	KH	285	GLU
5	KH	305	TRP
5	KH	313	VAL
5	KH	329	THR
5	KH	342	SER
5	KH	346	LEU
6	KK	50	ASP
6	KK	55	LYS
6	KK	70	VAL
6	KK	75	LEU
6	KK	83	LEU
6	KK	91	LEU
6	KK	95	SER
6	KK	106	LEU
6	KK	111	LYS
6	KK	112	ILE
6	KK	125	SER
6	KK	133	THR
6	KK	134	LEU
6	KK	144	LEU
6	KK	149	VAL
6	KK	152	ARG
6	KK	156	THR
6	KK	166	THR
6	KK	180	VAL
6	KK	183	THR
7	KL	47	TYR
7	KL	54	ARG
7	KL	57	VAL
7	KL	109	LEU
7	KL	113	ASP
7	KL	121	ASP
7	KL	130	ASP
7	KL	140	LEU
7	KL	143	ILE
7	KL	155	LEU
7	KL	160	GLN
7	KL	165	VAL
7	KL	172	VAL
7	KL	174	SER
7	KL	193	LEU

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Mol	Chain	Res	Type
7	KL	204	LYS
7	KL	210	ASP
7	KL	211	LYS
7	KL	212	ASN
7	KL	217	ASN
8	KM	127	ASN
8	KM	131	THR
8	KM	134	LEU
8	KM	149	ASN
8	KM	155	LEU
8	KM	160	ASN
8	KM	162	VAL
8	KM	171	ARG
8	KM	173	LEU
8	KM	178	LYS
8	KM	180	ASP
8	KM	183	VAL
8	KM	184	LEU
8	KM	205	TYR
8	KM	222	ILE
8	KM	231	LEU
8	KM	245	TYR
8	KM	271	SER
8	KM	290	ASP
8	KM	292	MET
8	KM	299	LEU
8	KM	301	MET
8	KM	303	GLU
8	KM	308	ASP
9	KN	62	ASN
9	KN	69	TYR
9	KN	70	CYS
9	KN	71	THR
9	KN	78	LEU
9	KN	81	LEU
9	KN	95	LEU
9	KN	100	LEU
9	KN	110	GLU
9	KN	114	LEU
9	KN	115	GLN
4	Kd	61	VAL
4	Kd	63	THR

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Mol	Chain	Res	Type
4	Kd	67	LYS
4	Kd	72	THR
4	Kd	73	ILE
4	Kd	93	GLU
4	Kd	108	VAL
4	Kd	115	VAL
4	Kd	132	LEU
4	Kd	147	VAL
4	Kd	154	VAL
3	Kf	215	VAL
3	Kf	250	LEU
3	Kf	253	ARG
3	Kf	261	VAL
3	Kf	263	LYS
3	Kf	266	GLN
4	LD	23	MET
4	LD	30	ILE
4	LD	32	ASN
4	LD	36	ASP
4	LD	68	ASP
4	LD	73	ILE
4	LD	75	ASN
4	LD	85	VAL
4	LD	86	ASP
4	LD	95	THR
4	LD	108	VAL
4	LD	123	THR
4	LD	154	VAL
4	LD	156	LEU
4	LD	160	LYS
4	LD	162	TYR
3	LF	215	VAL
3	LF	223	ILE
3	LF	230	LEU
3	LF	231	THR
3	LF	238	ILE
3	LF	250	LEU
1	Lg	795	GLN
1	Lg	796	GLN
1	Lg	806	THR
1	Lg	808	LEU
1	Lg	809	VAL

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Mol	Chain	Res	Type
1	Lg	810	GLN
1	Lg	817	THR
5	LH	109	LYS
5	LH	115	MET
5	LH	117	ARG
5	LH	129	LYS
5	LH	130	LEU
5	LH	137	SER
5	LH	147	THR
5	LH	154	THR
5	LH	160	LEU
5	LH	180	VAL
5	LH	209	THR
5	LH	216	GLN
5	LH	221	TYR
5	LH	238	MET
5	LH	239	LEU
5	LH	241	LEU
5	LH	248	VAL
5	LH	251	ARG
5	LH	270	GLU
5	LH	284	LEU
5	LH	294	ARG
5	LH	313	VAL
5	LH	317	LEU
5	LH	329	THR
5	LH	339	MET
5	LH	345	LEU
6	LK	45	VAL
6	LK	53	ILE
6	LK	58	THR
6	LK	63	LYS
6	LK	72	GLN
6	LK	76	ILE
6	LK	83	LEU
6	LK	95	SER
6	LK	106	LEU
6	LK	111	LYS
6	LK	116	VAL
6	LK	125	SER
6	LK	126	VAL
6	LK	144	LEU

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Mol	Chain	Res	Type
6	LK	149	VAL
6	LK	156	THR
6	LK	162	ASP
6	LK	177	ASN
6	LK	183	THR
7	LL	51	GLN
7	LL	103	ARG
7	LL	109	LEU
7	LL	113	ASP
7	LL	115	GLN
7	LL	133	PHE
7	LL	155	LEU
7	LL	172	VAL
7	LL	174	SER
7	LL	187	GLU
7	LL	193	LEU
7	LL	204	LYS
7	LL	210	ASP
7	LL	211	LYS
7	LL	212	ASN
8	LM	115	ARG
8	LM	134	LEU
8	LM	137	TYR
8	LM	149	ASN
8	LM	152	LEU
8	LM	160	ASN
8	LM	162	VAL
8	LM	176	VAL
8	LM	180	ASP
8	LM	181	PRO
8	LM	182	LYS
8	LM	183	VAL
8	LM	184	LEU
8	LM	190	ASN
8	LM	192	ARG
8	LM	205	TYR
8	LM	206	TRP
8	LM	228	VAL
8	LM	237	ASP
8	LM	263	ILE
8	LM	292	MET
8	LM	300	ASP

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Mol	Chain	Res	Type
8	LM	301	MET
8	LM	303	GLU
9	LN	59	VAL
9	LN	64	PHE
9	LN	82	MET
9	LN	91	VAL
9	LN	101	VAL
9	LN	102	VAL
9	LN	110	GLU
9	LN	114	LEU
9	LN	115	GLN
1	DG	865	THR
1	DG	874	ASP
1	DG	877	VAL
1	DG	886	LEU
1	DG	898	LYS
1	DG	911	LYS
1	DG	912	MET
1	DG	913	VAL
1	DG	916	PHE
1	DG	925	GLU
1	DG	928	ILE
1	DG	930	ILE
1	DG	944	LEU
1	DG	947	ARG
1	DG	956	TYR
1	DG	962	SER
1	DG	963	SER
1	DG	965	LEU
1	DG	1037	LEU
1	DG	1044	ASP
4	Ld	41	LEU
4	Ld	50	ASP
4	Ld	55	MET
4	Ld	58	VAL
4	Ld	61	VAL
4	Ld	68	ASP
4	Ld	85	VAL
4	Ld	103	HIS
4	Ld	112	SER
4	Ld	115	VAL
4	Ld	147	VAL

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Mol	Chain	Res	Type
4	Ld	156	LEU
3	Lf	212	ILE
3	Lf	215	VAL
3	Lf	219	ARG
3	Lf	246	LEU
3	Lf	260	GLN
3	Lf	262	ILE
6	AK	45	VAL
6	AK	46	ASP
6	AK	50	ASP
6	AK	60	LEU
6	AK	83	LEU
6	AK	92	ASN
6	AK	95	SER
6	AK	98	LEU
6	AK	106	LEU
6	AK	111	LYS
6	AK	125	SER
6	AK	126	VAL
6	AK	129	GLU
6	AK	134	LEU
6	AK	144	LEU
6	AK	149	VAL
6	AK	156	THR
6	AK	162	ASP
6	AK	170	LEU
6	AK	180	VAL
4	MD	38	THR
4	MD	47	SER
4	MD	54	GLU
4	MD	78	ASN
4	MD	115	VAL
4	MD	117	VAL
4	MD	123	THR
4	MD	127	SER
4	MD	130	GLU
4	MD	156	LEU
3	MF	207	ARG
3	MF	215	VAL
3	MF	230	LEU
3	MF	232	VAL
3	MF	238	ILE

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Mol	Chain	Res	Type
3	MF	250	LEU
3	MF	256	THR
1	Cg	802	LEU
1	Cg	806	THR
1	Cg	808	LEU
1	Cg	814	GLN
1	Cg	815	VAL
1	Cg	816	GLU
1	Mg	800	ASP
1	Mg	814	GLN
1	Mg	815	VAL
1	Mg	817	THR
1	Ag	811	ASP
1	Ag	813	LYS
1	Ag	815	VAL
1	Ag	817	THR
1	Ag	819	VAL
5	MH	109	LYS
5	MH	115	MET
5	MH	147	THR
5	MH	154	THR
5	MH	160	LEU
5	MH	170	ARG
5	MH	205	GLN
5	MH	209	THR
5	MH	226	LEU
5	MH	228	VAL
5	MH	238	MET
5	MH	240	THR
5	MH	241	LEU
5	MH	248	VAL
5	MH	257	GLN
5	MH	264	LYS
5	MH	268	THR
5	MH	278	ASP
5	MH	280	LEU
5	MH	284	LEU
5	MH	287	VAL
5	MH	294	ARG
5	MH	296	VAL
5	MH	324	TRP
5	MH	348	SER

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Mol	Chain	Res	Type
5	MH	361	LEU
6	MK	66	LYS
6	MK	70	VAL
6	MK	75	LEU
6	MK	83	LEU
6	MK	86	ASP
6	MK	101	GLU
6	MK	111	LYS
6	MK	112	ILE
6	MK	125	SER
6	MK	126	VAL
6	MK	127	LYS
6	MK	144	LEU
6	MK	149	VAL
6	MK	152	ARG
6	MK	156	THR
6	MK	180	VAL
7	ML	47	TYR
7	ML	49	ASN
7	ML	51	GLN
7	ML	62	VAL
7	ML	93	LEU
7	ML	96	SER
7	ML	98	TYR
7	ML	109	LEU
7	ML	154	LEU
7	ML	160	GLN
7	ML	172	VAL
7	ML	189	MET
7	ML	212	ASN
7	ML	219	ILE
7	ML	225	GLN
7	ML	235	THR
8	MM	131	THR
8	MM	134	LEU
8	MM	144	THR
8	MM	149	ASN
8	MM	152	LEU
8	MM	155	LEU
8	MM	171	ARG
8	MM	173	LEU
8	MM	175	ILE

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Mol	Chain	Res	Type
8	MM	176	VAL
8	MM	177	LEU
8	MM	180	ASP
8	MM	183	VAL
8	MM	192	ARG
8	MM	195	ASP
8	MM	202	LEU
8	MM	215	ARG
8	MM	224	LEU
8	MM	259	SER
8	MM	271	SER
8	MM	275	ASP
8	MM	277	SER
8	MM	290	ASP
8	MM	292	MET
8	MM	299	LEU
8	MM	301	MET
8	MM	303	GLU
8	MM	310	LYS
9	MN	48	ILE
9	MN	51	CYS
9	MN	52	ASP
9	MN	80	PHE
9	MN	81	LEU
9	MN	91	VAL
9	MN	95	LEU
9	MN	102	VAL
9	MN	108	VAL
4	Md	31	ASN
4	Md	36	ASP
4	Md	41	LEU
4	Md	61	VAL
4	Md	63	THR
4	Md	92	GLU
4	Md	100	LYS
4	Md	108	VAL
4	Md	115	VAL
4	Md	123	THR
4	Md	128	LEU
4	Md	134	ASP
4	Md	155	GLU
3	Mf	209	ILE

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Mol	Chain	Res	Type
3	Mf	219	ARG
3	Mf	230	LEU
3	Mf	232	VAL
3	Mf	236	SER
3	Mf	260	GLN
3	VF	207	ARG
3	VF	208	ILE
3	VF	215	VAL
3	VF	229	THR
3	VF	231	THR
3	VF	238	ILE
3	VF	250	LEU
3	VF	256	THR
1	VG	793	GLU
1	VG	796	GLN
1	VG	802	LEU
1	VG	817	THR
5	VH	105	GLU
5	VH	108	ASP
5	VH	109	LYS
5	VH	115	MET
5	VH	138	GLU
5	VH	147	THR
5	VH	160	LEU
5	VH	170	ARG
5	VH	180	VAL
5	VH	226	LEU
5	VH	238	MET
5	VH	240	THR
5	VH	241	LEU
5	VH	246	LYS
5	VH	248	VAL
5	VH	250	TYR
5	VH	257	GLN
5	VH	287	VAL
5	VH	296	VAL
5	VH	297	VAL
5	VH	318	THR
5	VH	329	THR
5	VH	338	GLU
5	VH	346	LEU
5	VH	347	VAL

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Mol	Chain	Res	Type
5	VH	358	VAL
3	WF	211	TYR
3	WF	223	ILE
3	WF	229	THR
3	WF	232	VAL
3	WF	234	GLU
3	WF	256	THR
3	WF	264	PHE
3	WF	266	GLN
1	WG	815	VAL
1	WG	816	GLU
1	WG	817	THR
1	WG	820	TYR
5	WH	108	ASP
5	WH	109	LYS
5	WH	114	ASP
5	WH	116	THR
5	WH	117	ARG
5	WH	120	TYR
5	WH	147	THR
5	WH	170	ARG
5	WH	176	VAL
5	WH	180	VAL
5	WH	182	LEU
5	WH	185	THR
5	WH	215	ILE
5	WH	216	GLN
5	WH	228	VAL
5	WH	240	THR
5	WH	242	ILE
5	WH	253	ASP
5	WH	262	ASN
5	WH	279	LEU
5	WH	297	VAL
5	WH	306	LEU
5	WH	313	VAL
5	WH	315	THR
5	WH	345	LEU
4	CD	26	LYS
4	CD	47	SER
4	CD	50	ASP
4	CD	51	SER

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Mol	Chain	Res	Type
4	CD	52	MET
4	CD	73	ILE
4	CD	78	ASN
4	CD	84	SER
4	CD	85	VAL
4	CD	91	ILE
4	CD	95	THR
4	CD	111	LYS
4	CD	115	VAL
4	CD	124	LYS
4	CD	127	SER
4	CD	145	ILE
4	CD	154	VAL
4	CD	156	LEU
4	CD	161	ILE
1	EG	865	THR
1	EG	869	MET
1	EG	873	LEU
1	EG	885	ILE
1	EG	886	LEU
1	EG	898	LYS
1	EG	911	LYS
1	EG	913	VAL
1	EG	916	PHE
1	EG	919	MET
1	EG	930	ILE
1	EG	939	THR
1	EG	942	THR
1	EG	944	LEU
1	EG	948	THR
1	EG	956	TYR
1	EG	962	SER
1	EG	963	SER
1	EG	965	LEU
1	EG	972	PHE
1	EG	1027	THR
1	EG	1028	THR
1	EG	1037	LEU
1	EG	1045	VAL
3	XF	215	VAL
3	XF	216	ILE
3	XF	221	TRP

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Mol	Chain	Res	Type
3	XF	223	ILE
3	XF	230	LEU
3	XF	232	VAL
3	XF	233	ARG
3	XF	250	LEU
3	XF	256	THR
1	XG	793	GLU
1	XG	802	LEU
1	XG	815	VAL
1	XG	817	THR
1	XG	819	VAL
1	XG	821	THR
5	XH	107	ILE
5	XH	108	ASP
5	XH	113	LYS
5	XH	132	GLN
5	XH	138	GLU
5	XH	147	THR
5	XH	170	ARG
5	XH	207	ASP
5	XH	211	ASN
5	XH	218	THR
5	XH	225	ASN
5	XH	226	LEU
5	XH	229	ARG
5	XH	242	ILE
5	XH	248	VAL
5	XH	250	TYR
5	XH	251	ARG
5	XH	253	ASP
5	XH	256	VAL
5	XH	259	TYR
5	XH	278	ASP
5	XH	296	VAL
5	XH	297	VAL
5	XH	303	ARG
5	XH	317	LEU
5	XH	329	THR
5	XH	338	GLU
5	XH	353	VAL
5	XH	358	VAL
3	YF	207	ARG

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Mol	Chain	Res	Type
3	YF	208	ILE
3	YF	215	VAL
3	YF	231	THR
3	YF	238	ILE
3	YF	256	THR
3	YF	258	SER
7	AL	47	TYR
7	AL	102	LYS
7	AL	109	LEU
7	AL	110	GLN
7	AL	154	LEU
7	AL	155	LEU
7	AL	162	THR
7	AL	165	VAL
7	AL	172	VAL
7	AL	177	HIS
7	AL	210	ASP
7	AL	211	LYS
7	AL	227	ARG
1	YG	816	GLU
1	YG	817	THR
5	YH	109	LYS
5	YH	115	MET
5	YH	125	GLU
5	YH	129	LYS
5	YH	147	THR
5	YH	171	LEU
5	YH	176	VAL
5	YH	179	LEU
5	YH	209	THR
5	YH	211	ASN
5	YH	218	THR
5	YH	228	VAL
5	YH	240	THR
5	YH	248	VAL
5	YH	249	ASP
5	YH	251	ARG
5	YH	282	HIS
5	YH	283	VAL
5	YH	295	LEU
5	YH	306	LEU
5	YH	329	THR

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Mol	Chain	Res	Type
5	YH	332	ASP
5	YH	345	LEU
5	YH	355	GLN
5	YH	358	VAL
3	Df	236	SER
3	Df	253	ARG
3	Df	255	LEU
2	DC	28	ASP
2	DC	29	THR
2	DC	32	LEU
2	DC	49	LYS
2	DC	54	LYS
2	DC	57	GLU
2	DC	61	LYS
2	DC	86	LYS
2	DC	87	GLN
2	DC	90	ASN
2	DC	100	LEU
2	DC	104	HIS
2	DC	111	LEU
2	DC	118	LEU
2	DC	142	ILE
2	DC	147	THR
2	DC	170	THR
2	DC	191	GLN
2	DC	203	ILE
2	DC	204	LYS
2	DC	222	VAL
2	DC	227	VAL
2	DC	244	ASP
2	DC	250	ILE
2	DC	267	VAL
3	ZF	207	ARG
3	ZF	208	ILE
3	ZF	215	VAL
3	ZF	223	ILE
3	ZF	230	LEU
3	ZF	231	THR
3	ZF	238	ILE
3	ZF	247	ILE
3	ZF	253	ARG
3	ZF	256	THR

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Mol	Chain	Res	Type
1	ZG	793	GLU
1	ZG	801	MET
1	ZG	806	THR
1	ZG	813	LYS
1	ZG	815	VAL
1	ZG	821	THR
5	ZH	105	GLU
5	ZH	113	LYS
5	ZH	114	ASP
5	ZH	117	ARG
5	ZH	122	LEU
5	ZH	138	GLU
5	ZH	147	THR
5	ZH	157	PHE
5	ZH	159	ASN
5	ZH	170	ARG
5	ZH	180	VAL
5	ZH	195	ASP
5	ZH	218	THR
5	ZH	225	ASN
5	ZH	231	ARG
5	ZH	233	LEU
5	ZH	238	MET
5	ZH	239	LEU
5	ZH	241	LEU
5	ZH	249	ASP
5	ZH	253	ASP
5	ZH	262	ASN
5	ZH	278	ASP
5	ZH	281	LEU
5	ZH	297	VAL
5	ZH	306	LEU
5	ZH	311	MET
5	ZH	325	LEU
5	ZH	329	THR
8	AM	131	THR
8	AM	136	LEU
8	AM	149	ASN
8	AM	171	ARG
8	AM	194	LEU
8	AM	204	LEU
8	AM	208	LYS

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Mol	Chain	Res	Type
8	AM	212	LEU
8	AM	235	LEU
8	AM	251	SER
8	AM	253	VAL
8	AM	262	GLU
8	AM	263	ILE
8	AM	266	VAL
8	AM	269	GLN
8	AM	277	SER
8	AM	292	MET
8	AM	297	SER
8	AM	301	MET
8	AM	316	ASN
8	AM	317	LYS
9	AN	62	ASN
9	AN	69	TYR
9	AN	81	LEU
9	AN	84	CYS
9	AN	100	LEU
9	AN	102	VAL
4	Ad	32	ASN
4	Ad	53	LEU
4	Ad	61	VAL
4	Ad	63	THR
4	Ad	69	ASN
4	Ad	91	ILE
4	Ad	108	VAL
4	Ad	111	LYS
4	Ad	115	VAL
4	Ad	117	VAL
4	Ad	128	LEU
4	Ad	153	VAL
4	Ad	156	LEU
3	Af	215	VAL
3	Af	216	ILE
3	Af	222	LEU
3	Af	225	SER
3	Af	230	LEU
3	Af	238	ILE
3	Af	244	VAL
3	Af	246	LEU
3	Af	247	ILE

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Mol	Chain	Res	Type
3	Af	253	ARG
3	Af	261	VAL
3	Af	263	LYS
4	BD	31	ASN
4	BD	36	ASP
4	BD	38	THR
4	BD	43	GLU
4	BD	47	SER
4	BD	53	LEU
4	BD	70	THR
4	BD	84	SER
4	BD	100	LYS
4	BD	123	THR
4	BD	127	SER
4	BD	128	LEU
4	BD	154	VAL
4	BD	156	LEU
3	BF	207	ARG
3	BF	215	VAL
3	BF	223	ILE
3	BF	231	THR
3	BF	232	VAL
3	BF	244	VAL
3	BF	256	THR
5	BH	109	LYS
5	BH	117	ARG
5	BH	119	LEU
5	BH	122	LEU
5	BH	134	TYR
5	BH	138	GLU
5	BH	147	THR
5	BH	154	THR
5	BH	160	LEU
5	BH	182	LEU
5	BH	204	ILE
5	BH	207	ASP
5	BH	209	THR
5	BH	220	LEU
5	BH	228	VAL
5	BH	233	LEU
5	BH	238	MET
5	BH	241	LEU

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Mol	Chain	Res	Type
5	BH	242	ILE
5	BH	248	VAL
5	BH	257	GLN
5	BH	266	MET
5	BH	278	ASP
5	BH	284	LEU
5	BH	315	THR
5	BH	318	THR
5	BH	321	SER
5	BH	329	THR
5	BH	334	THR
5	BH	338	GLU
6	BK	58	THR
6	BK	67	VAL
6	BK	75	LEU
6	BK	95	SER
6	BK	112	ILE
6	BK	126	VAL
6	BK	142	GLU
6	BK	149	VAL
6	BK	156	THR
6	BK	179	ARG
6	BK	180	VAL
3	CF	207	ARG
3	CF	208	ILE
3	CF	215	VAL
3	CF	230	LEU
3	CF	238	ILE
3	CF	244	VAL
3	CF	250	LEU
3	CF	256	THR
3	CF	265	SER
3	CF	266	GLN
1	FG	865	THR
1	FG	867	ASP
1	FG	869	MET
1	FG	886	LEU
1	FG	898	LYS
1	FG	910	ASP
1	FG	911	LYS
1	FG	913	VAL
1	FG	916	PHE

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Mol	Chain	Res	Type
1	FG	930	ILE
1	FG	942	THR
1	FG	944	LEU
1	FG	962	SER
1	FG	963	SER
1	FG	965	LEU
1	FG	972	PHE
1	FG	1022	LEU
1	FG	1028	THR
1	FG	1037	LEU
7	BL	43	PHE
7	BL	93	LEU
7	BL	109	LEU
7	BL	127	ILE
7	BL	129	THR
7	BL	133	PHE
7	BL	161	SER
7	BL	170	ASP
7	BL	172	VAL
7	BL	174	SER
7	BL	190	MET
7	BL	216	ASP
7	BL	227	ARG
8	BM	123	VAL
8	BM	134	LEU
8	BM	149	ASN
8	BM	171	ARG
8	BM	176	VAL
8	BM	177	LEU
8	BM	180	ASP
8	BM	182	LYS
8	BM	184	LEU
8	BM	191	LEU
8	BM	205	TYR
8	BM	210	ASP
8	BM	212	LEU
8	BM	215	ARG
8	BM	233	VAL
8	BM	246	LEU
8	BM	257	ASP
8	BM	263	ILE
8	BM	269	GLN

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Mol	Chain	Res	Type
8	BM	271	SER
8	BM	277	SER
8	BM	285	SER
8	BM	292	MET
8	BM	297	SER
8	BM	298	VAL
8	BM	310	LYS
8	BM	312	PHE
8	BM	318	GLN
9	BN	62	ASN
9	BN	66	SER
9	BN	81	LEU
9	BN	84	CYS
9	BN	91	VAL
9	BN	94	GLN
9	BN	101	VAL
9	BN	110	GLU
4	Bd	38	THR
4	Bd	41	LEU
4	Bd	52	MET
4	Bd	53	LEU
4	Bd	61	VAL
4	Bd	63	THR
4	Bd	68	ASP
4	Bd	70	THR
4	Bd	78	ASN
4	Bd	108	VAL
4	Bd	115	VAL
4	Bd	127	SER
4	Bd	128	LEU
4	Bd	147	VAL
4	Bd	154	VAL
4	Bd	155	GLU
4	Bd	156	LEU
4	Bd	160	LYS
3	Bf	230	LEU
3	Bf	232	VAL
3	Bf	245	LYS
3	Bf	255	LEU
1	Dg	792	GLN
1	Dg	808	LEU
1	Dg	811	ASP

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Mol	Chain	Res	Type
1	Dg	814	GLN
1	Dg	815	VAL
1	Dg	816	GLU
1	Dg	817	THR
4	AD	24	LYS
4	AD	35	ASP
4	AD	41	LEU
4	AD	47	SER
4	AD	50	ASP
4	AD	51	SER
4	AD	53	LEU
4	AD	85	VAL
4	AD	86	ASP
4	AD	91	ILE
4	AD	92	GLU
4	AD	93	GLU
4	AD	115	VAL
4	AD	117	VAL
4	AD	127	SER
4	AD	137	TYR
4	AD	154	VAL
4	AD	160	LYS
2	FC	68	GLN
2	FC	80	GLU
2	FC	84	LYS
2	FC	89	LEU
2	FC	95	PHE
2	FC	99	VAL
2	FC	116	LEU
2	FC	120	ASP
2	FC	141	THR
2	FC	142	THR
2	FC	145	THR
2	FC	147	ARG
2	FC	153	ASP
2	FC	162	VAL
2	FC	164	LEU
2	FC	165	LEU
2	FC	172	LYS
2	FC	173	GLU
2	FC	183	TRP
2	FC	189	GLN

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Mol	Chain	Res	Type
2	FC	192	THR
2	FC	203	GLU
2	FC	205	PHE
2	FC	232	VAL
2	FC	253	GLU
2	FC	254	LEU
2	FC	255	ASN
2	FC	265	VAL
2	FC	267	LYS
2	GC	60	LYS
2	GC	77	LYS
2	GC	85	LYS
2	GC	95	ASP
2	GC	105	ILE
2	GC	109	VAL
2	GC	111	LEU
2	GC	116	THR
2	GC	143	THR
2	GC	146	THR
2	GC	166	LEU
2	GC	169	THR
2	GC	190	GLN
2	GC	193	THR
2	GC	195	LEU
2	GC	204	GLU
2	GC	209	MET
2	GC	221	VAL
2	GC	225	TYR
2	GC	229	THR
2	GC	243	ASP
2	GC	249	ILE
2	GC	250	THR
2	GC	266	VAL
2	IC	29	THR
2	IC	36	GLN
2	IC	43	TYR
2	IC	45	ARG
2	IC	58	MET
2	IC	60	LEU
2	IC	90	ASN
2	IC	92	ASP
2	IC	100	LEU

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Mol	Chain	Res	Type
2	IC	101	VAL
2	IC	106	ILE
2	IC	117	THR
2	IC	128	ILE
2	IC	132	THR
2	IC	147	THR
2	IC	154	MET
2	IC	155	ASP
2	IC	170	THR
2	IC	171	LYS
2	IC	206	ASP
2	IC	212	LEU
2	IC	214	ARG
2	IC	227	VAL
2	IC	235	THR
2	IC	241	ILE
2	IC	259	ASN
2	JC	61	THR
2	JC	76	LYS
2	JC	96	ASN
2	JC	104	ILE
2	JC	110	LEU
2	JC	115	THR
2	JC	118	LEU
2	JC	126	ILE
2	JC	141	THR
2	JC	154	TYR
2	JC	155	VAL
2	JC	162	VAL
2	JC	165	LEU
2	JC	171	GLU
2	JC	179	THR
2	JC	203	GLU
2	JC	209	ILE
2	JC	217	MET
2	JC	224	TYR
2	JC	225	VAL
2	JC	229	ASP
2	JC	232	VAL
2	JC	242	ASP
2	JC	243	ASP
2	JC	248	ILE

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Mol	Chain	Res	Type
2	JC	254	LEU
2	JC	265	VAL
2	KC	60	LYS
2	KC	64	LEU
2	KC	83	LEU
2	KC	84	ASN
2	KC	89	ASN
2	KC	97	ASN
2	KC	105	ILE
2	KC	111	LEU
2	KC	116	THR
2	KC	121	ASP
2	KC	123	GLN
2	KC	127	ILE
2	KC	143	THR
2	KC	146	THR
2	KC	148	ARG
2	KC	156	VAL
2	KC	163	VAL
2	KC	165	LEU
2	KC	168	LYS
2	KC	176	TRP
2	KC	185	LYS
2	KC	189	ASP
2	KC	204	GLU
2	KC	214	LYS
2	KC	220	MET
2	KC	221	VAL
2	KC	225	TYR
2	KC	226	VAL
2	KC	230	ASP
2	KC	238	SER
2	KC	245	ARG
2	KC	248	ARG
2	KC	256	ASN
2	MC	29	THR
2	MC	35	LEU
2	MC	36	GLN
2	MC	47	GLN
2	MC	56	ARG
2	MC	58	MET
2	MC	86	LYS

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Mol	Chain	Res	Type
2	MC	97	PHE
2	MC	104	HIS
2	MC	106	ILE
2	MC	111	LEU
2	MC	113	GLU
2	MC	117	THR
2	MC	126	ILE
2	MC	128	ILE
2	MC	132	THR
2	MC	143	THR
2	MC	152	LEU
2	MC	154	MET
2	MC	157	VAL
2	MC	194	THR
2	MC	196	LEU
2	MC	222	VAL
2	MC	234	VAL
2	MC	235	THR
5	CH	115	MET
5	CH	117	ARG
5	CH	123	ASN
5	CH	130	LEU
5	CH	134	TYR
5	CH	147	THR
5	CH	152	THR
5	CH	154	THR
5	CH	170	ARG
5	CH	180	VAL
5	CH	182	LEU
5	CH	196	LEU
5	CH	204	ILE
5	CH	207	ASP
5	CH	226	LEU
5	CH	233	LEU
5	CH	241	LEU
5	CH	248	VAL
5	CH	249	ASP
5	CH	250	TYR
5	CH	256	VAL
5	CH	278	ASP
5	CH	284	LEU
5	CH	292	SER

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Mol	Chain	Res	Type
5	CH	313	VAL
5	CH	315	THR
5	CH	316	ASN
5	CH	320	LEU
5	CH	338	GLU
5	CH	344	VAL
6	CK	43	CYS
6	CK	54	ILE
6	CK	62	LYS
6	CK	83	LEU
6	CK	88	SER
6	CK	106	LEU
6	CK	125	SER
6	CK	126	VAL
6	CK	127	LYS
6	CK	129	GLU
6	CK	144	LEU
6	CK	149	VAL
6	CK	151	SER
6	CK	153	ILE
6	CK	156	THR
6	CK	170	LEU
6	CK	173	ASP
6	CK	180	VAL
7	CL	57	VAL
7	CL	93	LEU
7	CL	96	SER
7	CL	100	ASP
7	CL	109	LEU
7	CL	133	PHE
7	CL	154	LEU
7	CL	161	SER
7	CL	162	THR
7	CL	172	VAL
7	CL	174	SER
7	CL	175	ARG
7	CL	181	LEU
7	CL	188	THR
7	CL	193	LEU
7	CL	212	ASN
7	CL	216	ASP
7	CL	225	GLN

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Mol	Chain	Res	Type
7	CL	229	ILE
8	CM	127	ASN
8	CM	134	LEU
8	CM	144	THR
8	CM	150	ILE
8	CM	152	LEU
8	CM	153	GLN
8	CM	162	VAL
8	CM	171	ARG
8	CM	173	LEU
8	CM	177	LEU
8	CM	182	LYS
8	CM	183	VAL
8	CM	184	LEU
8	CM	191	LEU
8	CM	201	THR
8	CM	204	LEU
8	CM	205	TYR
8	CM	212	LEU
8	CM	221	LYS
8	CM	224	LEU
8	CM	231	LEU
8	CM	262	GLU
8	CM	285	SER
8	CM	287	THR
8	CM	292	MET
8	CM	299	LEU
8	CM	303	GLU
8	CM	308	ASP
9	CN	44	LYS
9	CN	66	SER
9	CN	92	TYR
9	CN	94	GLN
9	CN	95	LEU
9	CN	102	VAL
9	CN	108	VAL
9	CN	110	GLU
9	CN	114	LEU
4	Cd	30	ILE
4	Cd	35	ASP
4	Cd	43	GLU
4	Cd	61	VAL

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Mol	Chain	Res	Type
4	Cd	63	THR
4	Cd	68	ASP
4	Cd	85	VAL
4	Cd	119	ILE
4	Cd	123	THR
4	Cd	126	GLU
4	Cd	128	LEU
4	Cd	142	LYS
4	Cd	147	VAL
3	Cf	211	TYR
3	Cf	223	ILE
3	Cf	232	VAL
3	Cf	245	LYS
3	Cf	247	ILE
3	Cf	248	ASP
3	Cf	255	LEU
3	Cf	258	SER
3	Cf	260	GLN
3	Cf	261	VAL
4	DD	38	THR
4	DD	50	ASP
4	DD	54	GLU
4	DD	55	MET
4	DD	75	ASN
4	DD	79	LEU
4	DD	85	VAL
4	DD	91	ILE
4	DD	93	GLU
4	DD	109	LEU
4	DD	115	VAL
4	DD	127	SER
4	DD	150	ASN
4	DD	160	LYS
3	DF	207	ARG
3	DF	208	ILE
3	DF	215	VAL
3	DF	231	THR
3	DF	250	LEU
3	DF	255	LEU
1	GG	867	ASP
1	GG	869	MET
1	GG	873	LEU

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Mol	Chain	Res	Type
1	GG	886	LEU
1	GG	898	LYS
1	GG	900	ILE
1	GG	904	ASN
1	GG	910	ASP
1	GG	911	LYS
1	GG	913	VAL
1	GG	916	PHE
1	GG	930	ILE
1	GG	944	LEU
1	GG	962	SER
1	GG	963	SER
1	GG	965	LEU
1	GG	972	PHE
1	GG	1001	LEU
1	GG	1010	THR
1	GG	1028	THR
1	GG	1037	LEU
1	GG	1045	VAL
5	DH	107	ILE
5	DH	114	ASP
5	DH	122	LEU
5	DH	130	LEU
5	DH	147	THR
5	DH	154	THR
5	DH	156	GLN
5	DH	170	ARG
5	DH	180	VAL
5	DH	201	SER
5	DH	207	ASP
5	DH	210	SER
5	DH	238	MET
5	DH	240	THR
5	DH	241	LEU
5	DH	249	ASP
5	DH	253	ASP
5	DH	272	ILE
5	DH	284	LEU
5	DH	285	GLU
5	DH	287	VAL
5	DH	292	SER
5	DH	297	VAL

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Mol	Chain	Res	Type
5	DH	313	VAL
5	DH	342	SER
5	DH	344	VAL
5	DH	354	MET
6	DK	45	VAL
6	DK	59	ASP
6	DK	83	LEU
6	DK	91	LEU
6	DK	111	LYS
6	DK	125	SER
6	DK	126	VAL
6	DK	142	GLU
6	DK	144	LEU
6	DK	149	VAL
6	DK	153	ILE
6	DK	156	THR
6	DK	180	VAL
6	DK	183	THR
7	DL	47	TYR
7	DL	57	VAL
7	DL	98	TYR
7	DL	100	ASP
7	DL	109	LEU
7	DL	121	ASP
7	DL	127	ILE
7	DL	133	PHE
7	DL	154	LEU
7	DL	165	VAL
7	DL	169	THR
7	DL	174	SER
7	DL	175	ARG
7	DL	181	LEU
7	DL	182	SER
7	DL	193	LEU
7	DL	204	LYS
7	DL	210	ASP
7	DL	212	ASN
7	DL	216	ASP
8	DM	127	ASN
8	DM	131	THR
8	DM	134	LEU
8	DM	146	LEU

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Mol	Chain	Res	Type
8	DM	152	LEU
8	DM	171	ARG
8	DM	180	ASP
8	DM	182	LYS
8	DM	183	VAL
8	DM	184	LEU
8	DM	185	ILE
8	DM	192	ARG
8	DM	204	LEU
8	DM	221	LYS
8	DM	245	TYR
8	DM	263	ILE
8	DM	277	SER
8	DM	278	ASP
8	DM	284	LEU
8	DM	292	MET
8	DM	303	GLU
8	DM	306	GLN
8	DM	308	ASP
9	DN	51	CYS
9	DN	59	VAL
9	DN	62	ASN
9	DN	66	SER
9	DN	75	VAL
9	DN	91	VAL
9	DN	101	VAL
9	DN	108	VAL
9	DN	116	LYS
4	ED	47	SER
4	ED	50	ASP
4	ED	53	LEU
4	ED	60	LYS
4	ED	85	VAL
4	ED	115	VAL
4	ED	117	VAL
4	ED	123	THR
4	ED	126	GLU
4	ED	127	SER
4	ED	156	LEU
3	EF	207	ARG
3	EF	208	ILE
3	EF	215	VAL

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Mol	Chain	Res	Type
3	EF	231	THR
3	EF	233	ARG
3	EF	238	ILE
1	Eg	808	LEU
1	Eg	811	ASP
1	Eg	815	VAL
1	Eg	819	VAL
5	EH	107	ILE
5	EH	134	TYR
5	EH	147	THR
5	EH	160	LEU
5	EH	173	GLN
5	EH	176	VAL
5	EH	180	VAL
5	EH	182	LEU
5	EH	218	THR
5	EH	225	ASN
5	EH	226	LEU
5	EH	233	LEU
5	EH	237	VAL
5	EH	238	MET
5	EH	240	THR
5	EH	248	VAL
5	EH	249	ASP
5	EH	250	TYR
5	EH	253	ASP
5	EH	255	ARG
5	EH	266	MET
5	EH	269	GLU
5	EH	278	ASP
5	EH	280	LEU
5	EH	287	VAL
5	EH	292	SER
5	EH	294	ARG
5	EH	314	ARG
5	EH	315	THR
5	EH	325	LEU
5	EH	329	THR
5	EH	334	THR
5	EH	344	VAL
5	EH	346	LEU
5	EH	348	SER

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Mol	Chain	Res	Type
6	EK	40	LYS
6	EK	50	ASP
6	EK	62	LYS
6	EK	65	ILE
6	EK	70	VAL
6	EK	75	LEU
6	EK	83	LEU
6	EK	92	ASN
6	EK	95	SER
6	EK	106	LEU
6	EK	111	LYS
6	EK	112	ILE
6	EK	115	THR
6	EK	117	THR
6	EK	125	SER
6	EK	126	VAL
6	EK	142	GLU
6	EK	144	LEU
6	EK	145	TRP
6	EK	152	ARG
6	EK	156	THR
6	EK	162	ASP
7	EL	47	TYR
7	EL	57	VAL
7	EL	93	LEU
7	EL	101	SER
7	EL	109	LEU
7	EL	110	GLN
7	EL	140	LEU
7	EL	172	VAL
7	EL	174	SER
7	EL	201	LYS
7	EL	212	ASN
8	EM	127	ASN
8	EM	131	THR
8	EM	132	SER
8	EM	134	LEU
8	EM	136	LEU
8	EM	146	LEU
8	EM	149	ASN
8	EM	152	LEU
8	EM	155	LEU

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Mol	Chain	Res	Type
8	EM	173	LEU
8	EM	175	ILE
8	EM	177	LEU
8	EM	182	LYS
8	EM	202	LEU
8	EM	215	ARG
8	EM	222	ILE
8	EM	237	ASP
8	EM	253	VAL
8	EM	259	SER
8	EM	263	ILE
8	EM	266	VAL
8	EM	269	GLN
8	EM	271	SER
8	EM	290	ASP
8	EM	292	MET
8	EM	298	VAL
8	EM	303	GLU
8	EM	309	LEU
9	EN	51	CYS
9	EN	59	VAL
9	EN	62	ASN
9	EN	65	TYR
9	EN	75	VAL
9	EN	81	LEU
9	EN	95	LEU
9	EN	101	VAL
9	EN	104	ASN
9	EN	110	GLU
9	EN	114	LEU
4	Ed	36	ASP
4	Ed	38	THR
4	Ed	50	ASP
4	Ed	52	MET
4	Ed	58	VAL
4	Ed	61	VAL
4	Ed	63	THR
4	Ed	70	THR
4	Ed	92	GLU
4	Ed	109	LEU
4	Ed	115	VAL
4	Ed	126	GLU

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Mol	Chain	Res	Type
4	Ed	127	SER
4	Ed	153	VAL
3	Ef	209	ILE
3	Ef	222	LEU
3	Ef	232	VAL
3	Ef	233	ARG
3	Ef	244	VAL
3	Ef	253	ARG
3	Ef	265	SER
4	FD	30	ILE
4	FD	34	SER
4	FD	35	ASP
4	FD	41	LEU
4	FD	43	GLU
4	FD	47	SER
4	FD	51	SER
4	FD	54	GLU
4	FD	55	MET
4	FD	86	ASP
4	FD	108	VAL
4	FD	123	THR
4	FD	137	TYR
4	FD	154	VAL
4	FD	155	GLU
4	FD	156	LEU
3	FF	215	VAL
3	FF	222	LEU
3	FF	223	ILE
3	FF	230	LEU
3	FF	238	ILE
3	FF	258	SER
1	Fg	797	ARG
1	Fg	815	VAL
1	Fg	817	THR
5	FH	105	GLU
5	FH	108	ASP
5	FH	119	LEU
5	FH	125	GLU
5	FH	129	LYS
5	FH	130	LEU
5	FH	134	TYR
5	FH	137	SER

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Mol	Chain	Res	Type
5	FH	147	THR
5	FH	159	ASN
5	FH	180	VAL
5	FH	196	LEU
5	FH	203	ASN
5	FH	226	LEU
5	FH	239	LEU
5	FH	248	VAL
5	FH	250	TYR
5	FH	262	ASN
5	FH	269	GLU
5	FH	272	ILE
5	FH	278	ASP
5	FH	284	LEU
5	FH	285	GLU
5	FH	320	LEU
5	FH	328	MET
5	FH	338	GLU
5	FH	342	SER
5	FH	348	SER
5	FH	354	MET
6	FK	58	THR
6	FK	60	LEU
6	FK	65	ILE
6	FK	70	VAL
6	FK	83	LEU
6	FK	92	ASN
6	FK	99	LEU
6	FK	106	LEU
6	FK	108	GLN
6	FK	111	LYS
6	FK	112	ILE
6	FK	125	SER
6	FK	126	VAL
6	FK	127	LYS
6	FK	144	LEU
6	FK	149	VAL
6	FK	152	ARG
6	FK	156	THR
6	FK	162	ASP
6	FK	166	THR
6	FK	180	VAL

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Mol	Chain	Res	Type
1	HG	865	THR
1	HG	867	ASP
1	HG	875	THR
1	HG	877	VAL
1	HG	885	ILE
1	HG	898	LYS
1	HG	900	ILE
1	HG	913	VAL
1	HG	920	SER
1	HG	930	ILE
1	HG	939	THR
1	HG	944	LEU
1	HG	962	SER
1	HG	965	LEU
1	HG	972	PHE
1	HG	1020	GLN
1	HG	1027	THR
1	HG	1037	LEU
1	HG	1041	PHE
1	HG	1045	VAL
1	IG	867	ASP
1	IG	877	VAL
1	IG	898	LYS
1	IG	900	ILE
1	IG	916	PHE
1	IG	920	SER
1	IG	930	ILE
1	IG	944	LEU
1	IG	962	SER
1	IG	963	SER
1	IG	965	LEU
1	IG	972	PHE
1	IG	1037	LEU
1	JG	869	MET
1	JG	886	LEU
1	JG	898	LYS
1	JG	900	ILE
1	JG	913	VAL
1	JG	916	PHE
1	JG	930	ILE
1	JG	944	LEU
1	JG	949	ASN

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Mol	Chain	Res	Type
1	JG	962	SER
1	JG	965	LEU
1	JG	972	PHE
1	JG	999	SER
1	JG	1020	GLN
1	JG	1027	THR
1	JG	1028	THR
1	JG	1037	LEU
1	JG	1040	LEU
1	KG	865	THR
1	KG	867	ASP
1	KG	869	MET
1	KG	877	VAL
1	KG	885	ILE
1	KG	886	LEU
1	KG	895	LYS
1	KG	898	LYS
1	KG	910	ASP
1	KG	912	MET
1	KG	913	VAL
1	KG	916	PHE
1	KG	930	ILE
1	KG	944	LEU
1	KG	962	SER
1	KG	963	SER
1	KG	965	LEU
1	KG	972	PHE
1	KG	1027	THR
1	KG	1037	LEU
1	KG	1040	LEU
1	LG	865	THR
1	LG	898	LYS
1	LG	910	ASP
1	LG	913	VAL
1	LG	920	SER
1	LG	930	ILE
1	LG	935	ILE
1	LG	939	THR
1	LG	944	LEU
1	LG	947	ARG
1	LG	949	ASN
1	LG	965	LEU

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Mol	Chain	Res	Type
1	LG	972	PHE
1	LG	1020	GLN
1	LG	1032	TYR
1	LG	1037	LEU
1	LG	1040	LEU
1	LG	1045	VAL
1	MG	864	LYS
1	MG	867	ASP
1	MG	869	MET
1	MG	874	ASP
1	MG	875	THR
1	MG	886	LEU
1	MG	891	THR
1	MG	904	ASN
1	MG	911	LYS
1	MG	913	VAL
1	MG	915	THR
1	MG	916	PHE
1	MG	925	GLU
1	MG	926	LYS
1	MG	930	ILE
1	MG	933	TYR
1	MG	939	THR
1	MG	941	ARG
1	MG	944	LEU
1	MG	948	THR
1	MG	963	SER
1	MG	965	LEU
1	MG	968	PHE
1	MG	972	PHE
1	MG	1027	THR
1	MG	1028	THR
1	MG	1031	VAL
1	MG	1044	ASP
1	MG	1045	VAL
1	NG	864	LYS
1	NG	865	THR
1	NG	876	SER
1	NG	889	ILE
1	NG	891	THR
1	NG	893	LYS
1	NG	904	ASN

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Mol	Chain	Res	Type
1	NG	910	ASP
1	NG	911	LYS
1	NG	912	MET
1	NG	913	VAL
1	NG	916	PHE
1	NG	925	GLU
1	NG	930	ILE
1	NG	939	THR
1	NG	944	LEU
1	NG	962	SER
1	NG	963	SER
1	NG	965	LEU
1	NG	968	PHE
1	NG	972	PHE
1	NG	1010	THR
1	NG	1032	TYR
1	NG	1037	LEU
1	NG	1040	LEU
1	NG	1041	PHE
1	NG	1044	ASP
1	OG	873	LEU
1	OG	875	THR
1	OG	886	LEU
1	OG	891	THR
1	OG	898	LYS
1	OG	911	LYS
1	OG	912	MET
1	OG	913	VAL
1	OG	915	THR
1	OG	916	PHE
1	OG	930	ILE
1	OG	944	LEU
1	OG	962	SER
1	OG	963	SER
1	OG	965	LEU
1	OG	972	PHE
1	OG	1001	LEU
1	OG	1017	GLN
1	OG	1028	THR
1	OG	1031	VAL
1	OG	1037	LEU
1	OG	1040	LEU

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Mol	Chain	Res	Type
1	OG	1044	ASP
1	PG	865	THR
1	PG	886	LEU
1	PG	889	ILE
1	PG	898	LYS
1	PG	910	ASP
1	PG	911	LYS
1	PG	912	MET
1	PG	913	VAL
1	PG	916	PHE
1	PG	930	ILE
1	PG	939	THR
1	PG	944	LEU
1	PG	962	SER
1	PG	963	SER
1	PG	965	LEU
1	PG	968	PHE
1	PG	972	PHE
1	PG	1028	THR
1	PG	1032	TYR
1	PG	1037	LEU
1	PG	1045	VAL
2	HC	29	THR
2	HC	49	LYS
2	HC	51	LYS
2	HC	57	GLU
2	HC	84	LEU
2	HC	104	HIS
2	HC	143	THR
2	HC	144	THR
2	HC	152	LEU
2	HC	155	ASP
2	HC	169	LYS
2	HC	170	THR
2	HC	171	LYS
2	HC	190	ASP
2	HC	206	ASP
2	HC	215	LYS
2	HC	222	VAL
2	HC	227	VAL
2	HC	231	ASP
2	HC	235	THR

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Mol	Chain	Res	Type
2	HC	244	ASP
2	HC	255	GLU
2	HC	256	LEU
7	FL	47	TYR
7	FL	51	GLN
7	FL	57	VAL
7	FL	58	LYS
7	FL	98	TYR
7	FL	109	LEU
7	FL	125	LEU
7	FL	133	PHE
7	FL	140	LEU
7	FL	155	LEU
7	FL	163	ILE
7	FL	172	VAL
7	FL	174	SER
7	FL	177	HIS
7	FL	204	LYS
7	FL	210	ASP
7	FL	212	ASN
7	FL	217	ASN
7	FL	225	GLN
7	FL	230	GLU
8	FM	114	ASN
8	FM	127	ASN
8	FM	137	TYR
8	FM	141	GLU
8	FM	146	LEU
8	FM	152	LEU
8	FM	160	ASN
8	FM	170	SER
8	FM	176	VAL
8	FM	177	LEU
8	FM	183	VAL
8	FM	184	LEU
8	FM	192	ARG
8	FM	205	TYR
8	FM	208	LYS
8	FM	212	LEU
8	FM	214	ILE
8	FM	215	ARG
8	FM	221	LYS

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Mol	Chain	Res	Type
8	FM	231	LEU
8	FM	245	TYR
8	FM	259	SER
8	FM	266	VAL
8	FM	271	SER
8	FM	278	ASP
8	FM	292	MET
8	FM	303	GLU
9	FN	48	ILE
9	FN	51	CYS
9	FN	65	TYR
9	FN	66	SER
9	FN	70	CYS
9	FN	71	THR
9	FN	81	LEU
9	FN	86	LEU
9	FN	91	VAL
9	FN	94	GLN
9	FN	101	VAL
9	FN	112	CYS
9	FN	114	LEU
9	FN	115	GLN
9	FN	116	LYS
2	LC	29	THR
2	LC	36	GLN
2	LC	38	MET
2	LC	56	ARG
2	LC	84	LEU
2	LC	101	VAL
2	LC	104	HIS
2	LC	141	PHE
2	LC	147	THR
2	LC	171	LYS
2	LC	181	THR
2	LC	206	ASP
2	LC	215	LYS
2	LC	227	VAL
2	LC	244	ASP
2	LC	256	LEU
4	Fd	41	LEU
4	Fd	43	GLU
4	Fd	63	THR

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Mol	Chain	Res	Type
4	Fd	82	ARG
4	Fd	85	VAL
4	Fd	93	GLU
4	Fd	115	VAL
4	Fd	119	ILE
4	Fd	123	THR
4	Fd	124	LYS
4	Fd	126	GLU
4	Fd	134	ASP
4	Fd	142	LYS
4	Fd	145	ILE
4	Fd	156	LEU
3	Ff	211	TYR
3	Ff	213	GLN
3	Ff	232	VAL
3	Ff	244	VAL
3	Ff	245	LYS
3	Ff	249	SER
3	Ff	250	LEU
3	Ff	261	VAL
2	AC	79	ASP
2	AC	96	ASN
2	AC	101	GLU
2	AC	103	ASN
2	AC	108	VAL
2	AC	111	GLU
2	AC	115	THR
2	AC	118	LEU
2	AC	124	ILE
2	AC	126	ILE
2	AC	139	PHE
2	AC	142	THR
2	AC	145	THR
2	AC	147	ARG
2	AC	153	ASP
2	AC	162	VAL
2	AC	180	GLU
2	AC	181	ARG
2	AC	203	GLU
2	AC	205	PHE
2	AC	213	LYS
2	AC	215	LEU

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Mol	Chain	Res	Type
2	AC	220	VAL
2	AC	227	HIS
2	AC	242	ASP
2	AC	243	ASP
2	AC	265	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	Gg	818	GLN
9	GN	79	GLN
4	Gd	32	ASN
4	HD	152	GLN
7	IL	112	GLN
7	IL	150	ASN
3	JF	251	GLN
7	JL	150	ASN
4	Jd	78	ASN
7	KL	150	ASN
1	Lg	807	GLN
7	LL	221	HIS
1	Cg	818	GLN
5	MH	156	GLN
5	YH	159	ASN
2	JC	148	GLN
2	JC	218	ASN
5	CH	205	GLN
4	DD	75	ASN
1	GG	1017	GLN
7	DL	110	GLN
1	IG	1017	GLN
1	LG	1017	GLN
1	MG	1017	GLN
1	NG	1020	GLN
1	OG	1017	GLN
7	FL	225	GLN
9	FN	115	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 oligosaccharides 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
11	JX	1
11	BX	1
11	VX	1
11	KX	1
11	DX	1
11	YX	1
11	XX	1
11	ZX	1
11	LX	1
11	GX	1
11	EX	1
11	MX	1
11	WX	1
11	HX	1
11	CX	1
11	IX	1
11	FX	1
11	AX	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	JX	38:UNK	C	70:UNK	N	26.33
1	BX	38:UNK	C	70:UNK	N	25.95
1	VX	38:UNK	C	70:UNK	N	25.89
1	KX	38:UNK	C	70:UNK	N	25.61
1	DX	38:UNK	C	70:UNK	N	25.45
1	YX	38:UNK	C	70:UNK	N	25.38
1	XX	38:UNK	C	70:UNK	N	25.33
1	ZX	38:UNK	C	70:UNK	N	25.15
1	LX	38:UNK	C	70:UNK	N	25.12
1	GX	38:UNK	C	70:UNK	N	24.88
1	EX	38:UNK	C	70:UNK	N	24.75
1	MX	38:UNK	C	70:UNK	N	24.71
1	WX	38:UNK	C	70:UNK	N	24.65
1	HX	38:UNK	C	70:UNK	N	23.96
1	CX	38:UNK	C	70:UNK	N	23.84
1	IX	38:UNK	C	70:UNK	N	23.62
1	FX	38:UNK	C	70:UNK	N	23.09
1	AX	38:UNK	C	70:UNK	N	22.49

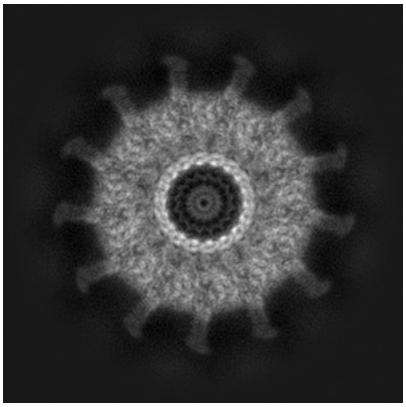
6 Map visualisation

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

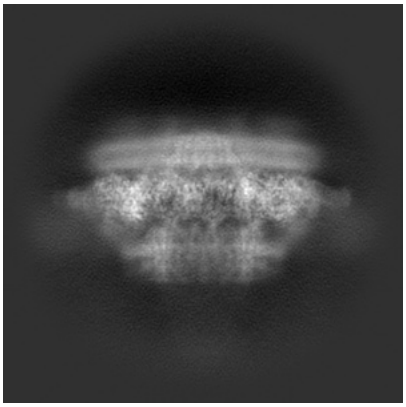
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

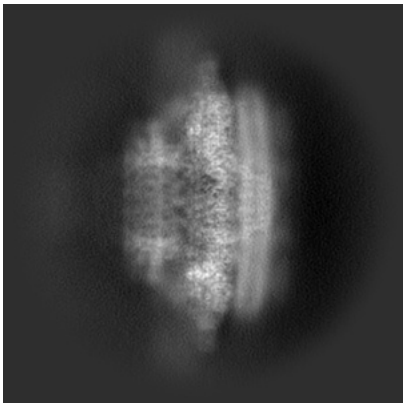
6.1.1 Primary map



X



Y

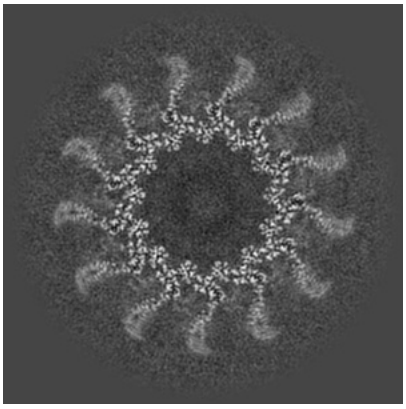


Z

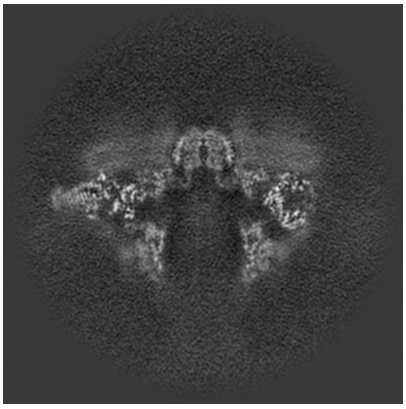
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 125



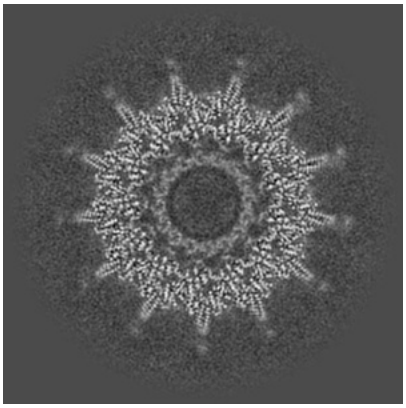
Y Index: 125

Z Index: 125

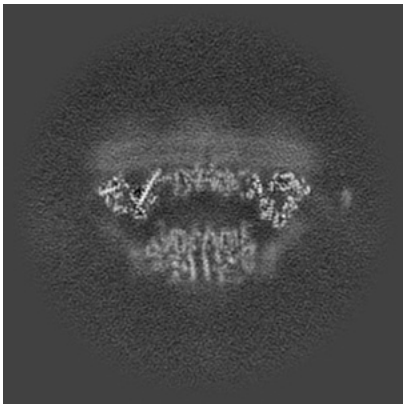
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

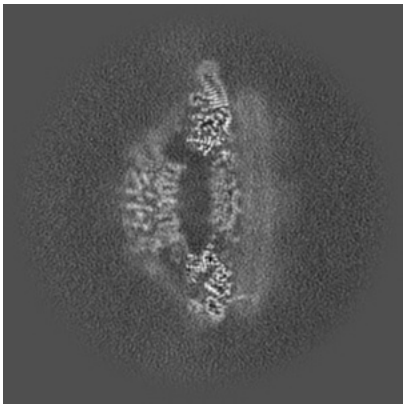
6.3.1 Primary map



X Index: 134



Y Index: 101

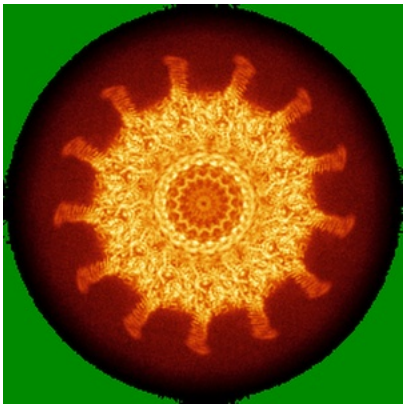


Z Index: 151

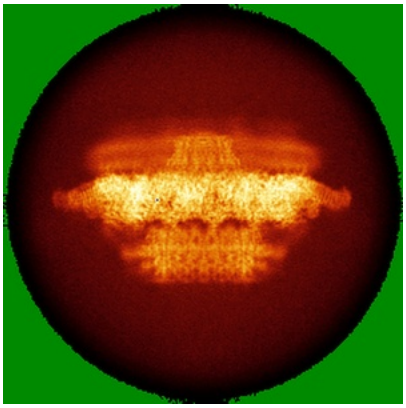
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

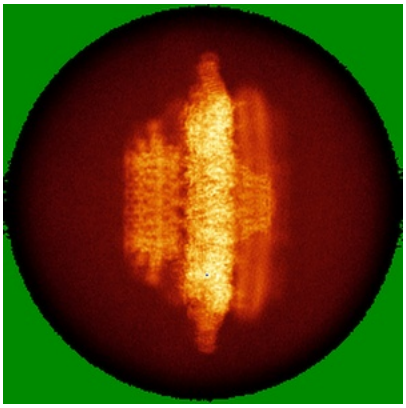
6.4.1 Primary map



X



Y

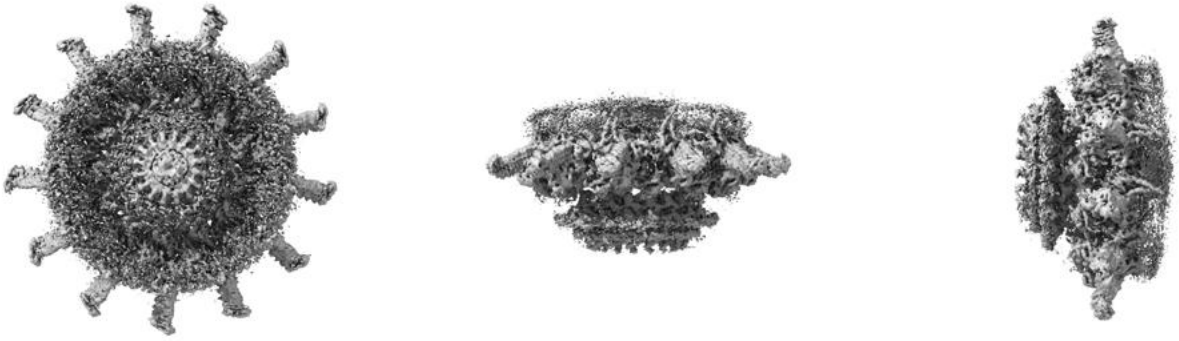


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 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.

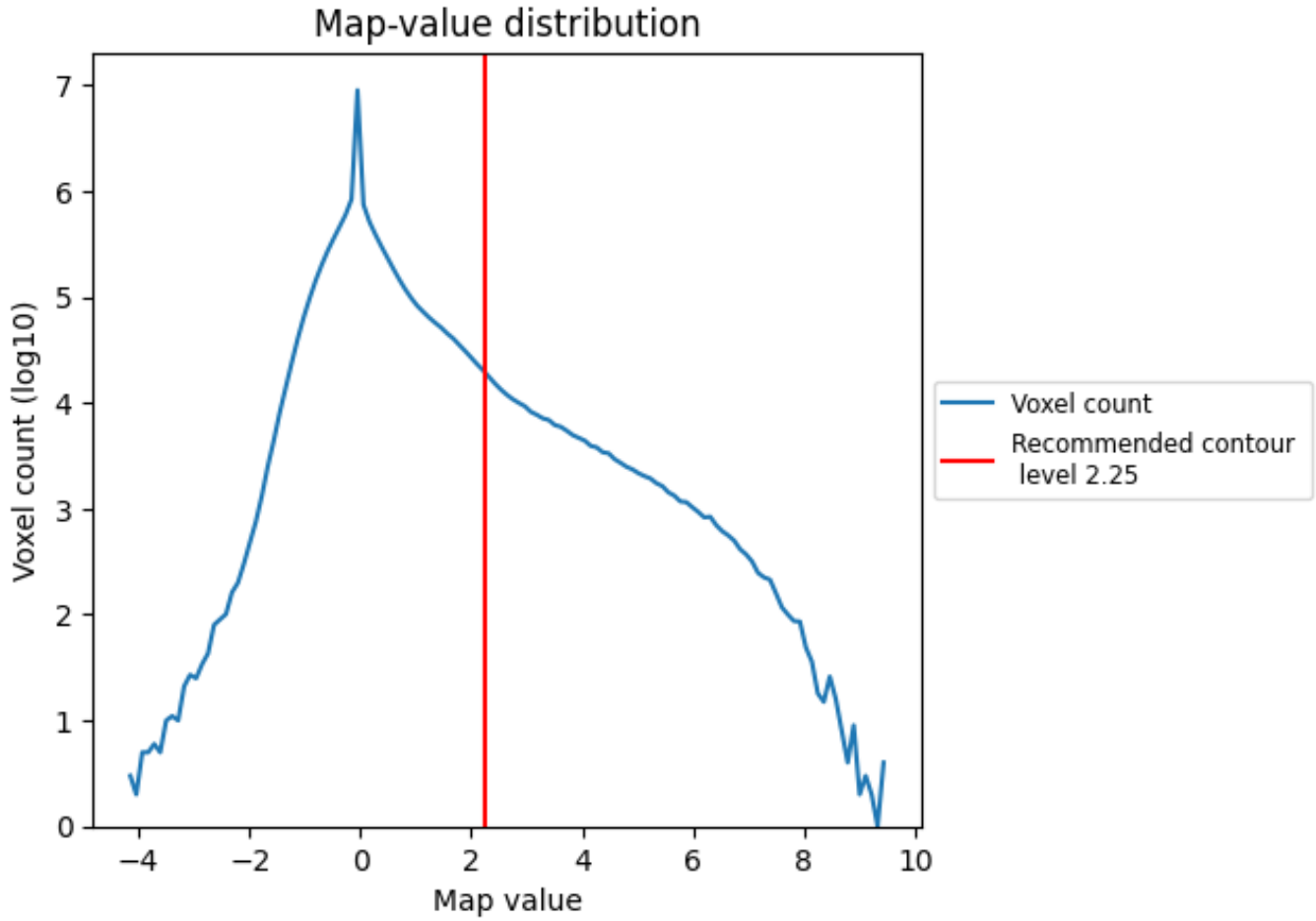
6.6 Mask visualisation (i)

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

7 Map analysis

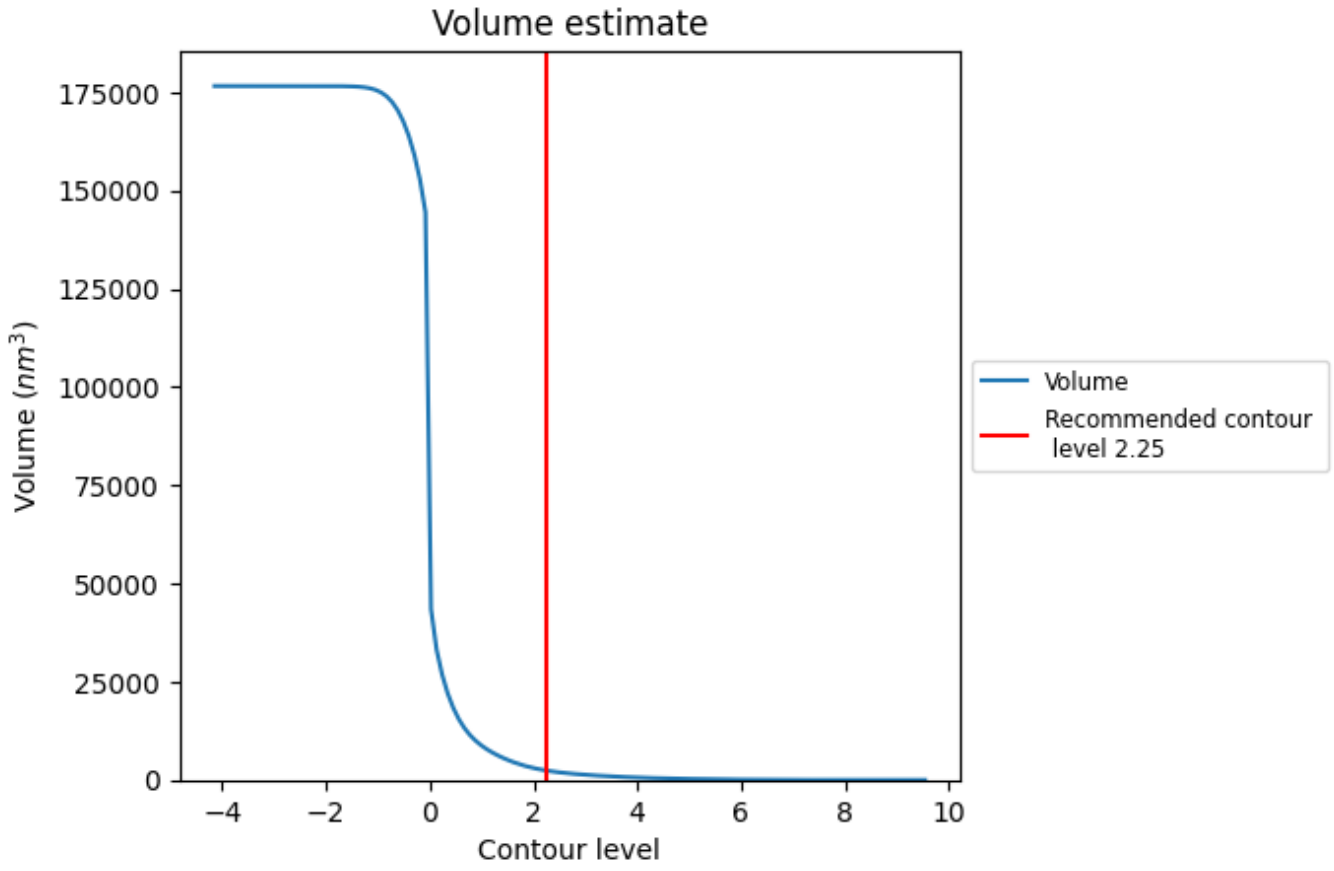
This section contains the results of statistical analysis of the map.

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.

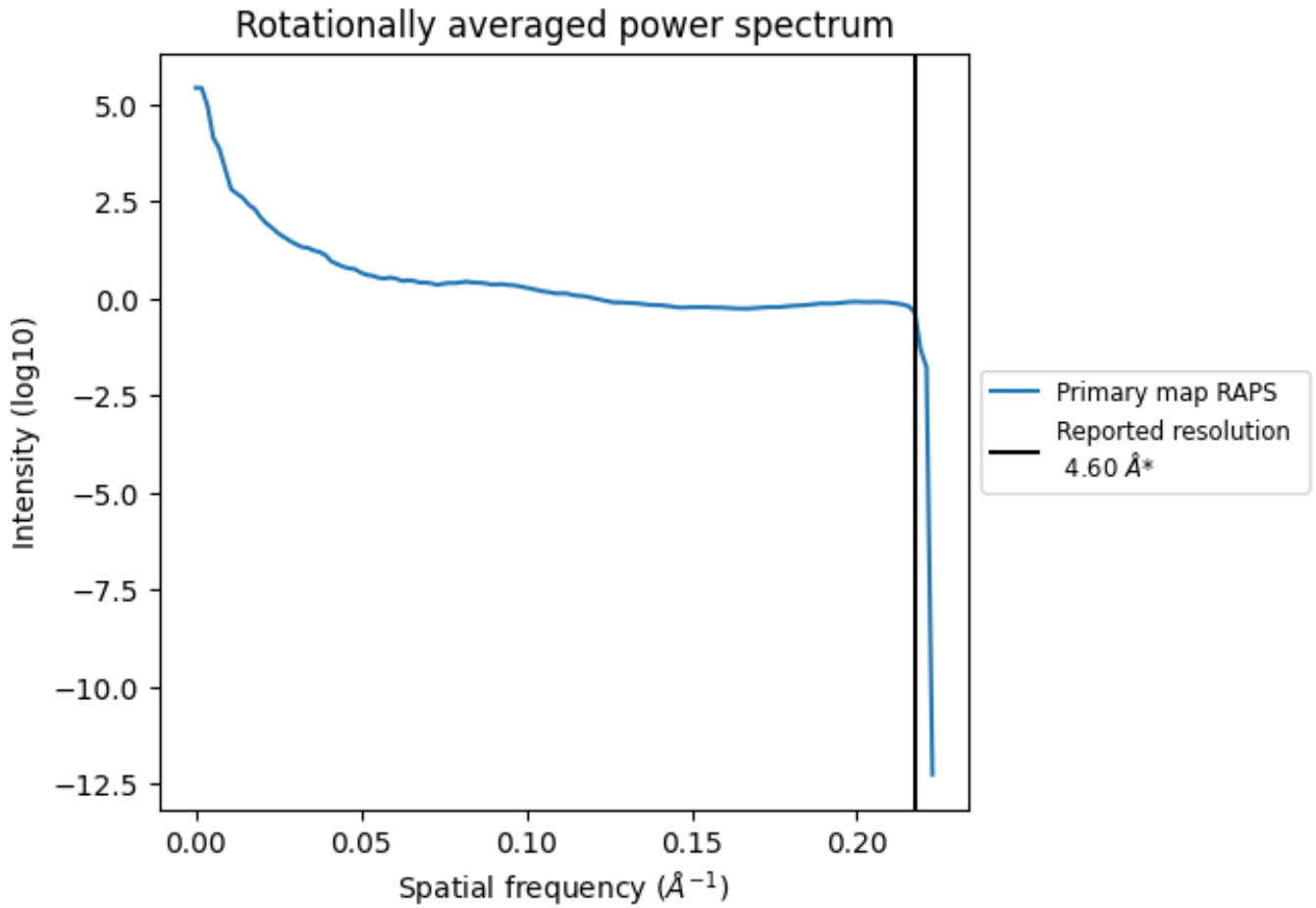
7.2 Volume estimate



The volume at the recommended contour level is 2389 nm^3; this corresponds to an approximate mass of 2158 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.217 $Å^{-1}$

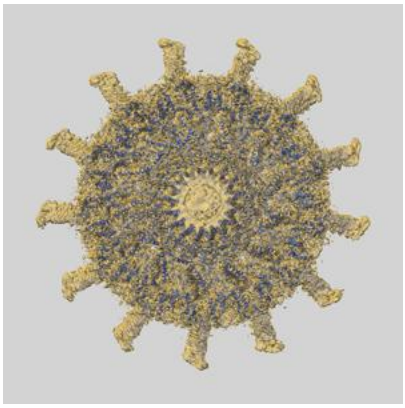
8 Fourier-Shell correlation

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

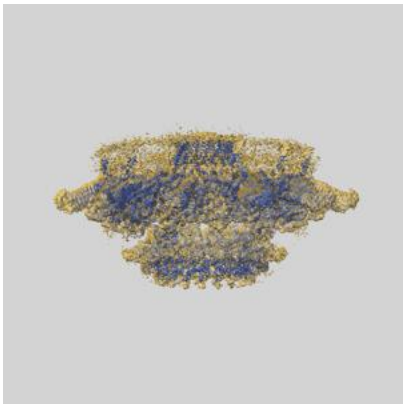
9 Map-model fit

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

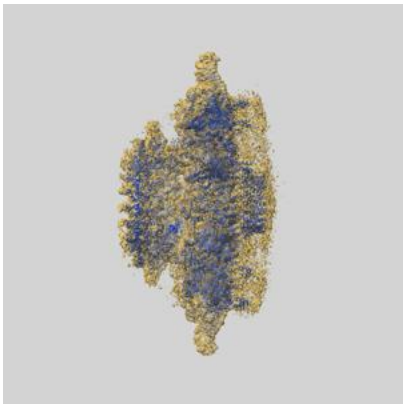
9.1 Map-model overlay



X



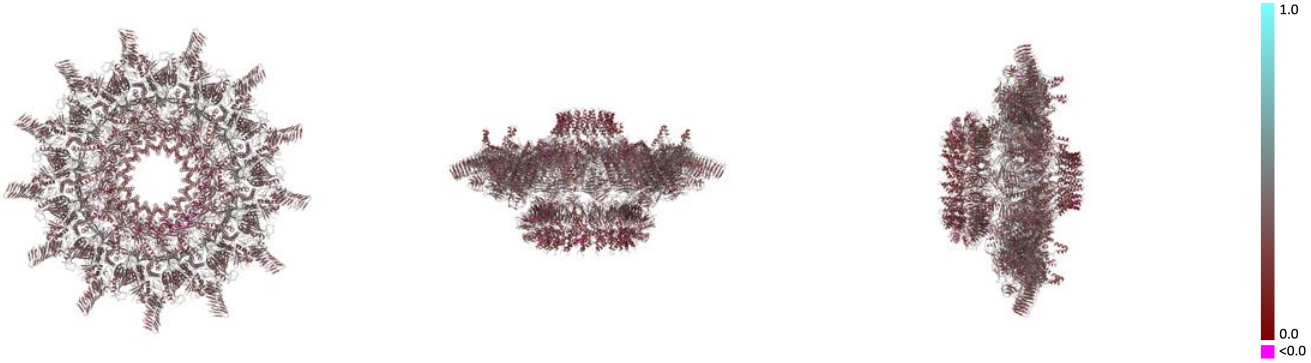
Y



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.

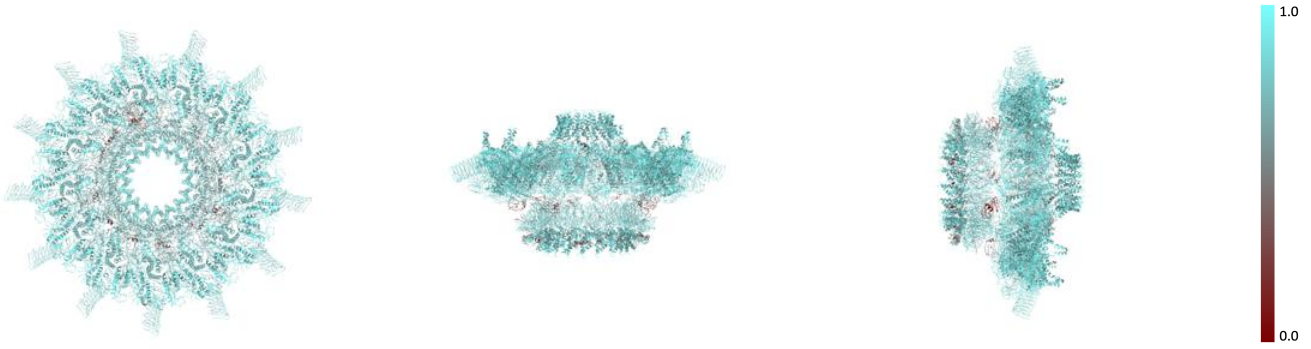
9.2 Q-score mapped to coordinate model



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.

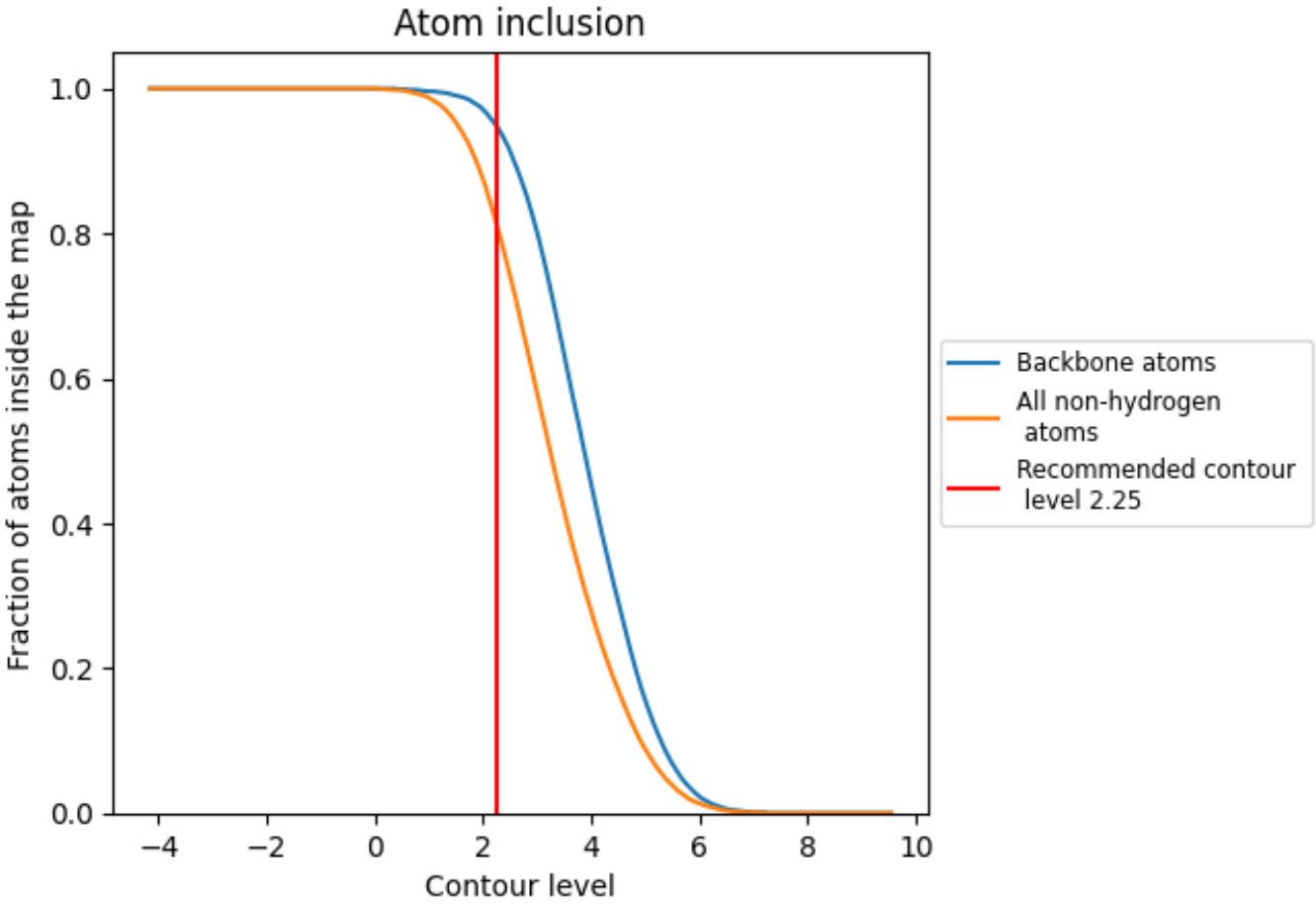
9.3 Atom inclusion mapped to coordinate model



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, 95% of all backbone atoms, 82% 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	0.8150	0.3350
AC	0.8600	0.3620
AD	0.8420	0.3710
AF	0.7790	0.2470
AG	0.7070	0.2330
AH	0.8130	0.3320
AK	0.8490	0.3780
AL	0.8630	0.3550
AM	0.8350	0.3520
AN	0.8020	0.3790
AU	1.0000	0.4870
AX	0.5670	0.2380
Ad	0.8570	0.3580
Af	0.8040	0.3300
Ag	0.8490	0.3040
BC	0.8730	0.3660
BD	0.8460	0.3790
BF	0.7790	0.2670
BG	0.6860	0.2220
BH	0.8100	0.3300
BK	0.8510	0.3730
BL	0.8640	0.3530
BM	0.8420	0.3600
BN	0.8550	0.3800
BU	1.0000	0.5100
BX	0.5580	0.2280
Bd	0.8450	0.3640
Bf	0.8410	0.3260
Bg	0.8240	0.3030
CC	0.8620	0.3660
CD	0.8650	0.3770
CF	0.7920	0.2800
CG	0.6740	0.2220
CH	0.8380	0.3380
CK	0.8610	0.3650

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Chain	Atom inclusion	Q-score
CL	0.8660	0.3510
CM	0.8540	0.3480
CN	0.8440	0.3790
CU	1.0000	0.4610
CX	0.7250	0.3180
Cd	0.8520	0.3640
Cf	0.8200	0.3220
Cg	0.8490	0.2960
DC	0.8100	0.3530
DD	0.8560	0.3670
DF	0.7640	0.2450
DG	0.7190	0.2400
DH	0.8280	0.3300
DK	0.8480	0.3720
DL	0.8540	0.3500
DM	0.8500	0.3510
DN	0.8180	0.3700
DU	1.0000	0.4710
DX	0.6170	0.2590
Dd	0.8660	0.3620
Df	0.8360	0.3250
Dg	0.8270	0.2810
EC	0.8380	0.3520
ED	0.8440	0.3740
EF	0.8130	0.2610
EG	0.7070	0.2470
EH	0.8310	0.3220
EK	0.8510	0.3730
EL	0.8470	0.3520
EM	0.8470	0.3520
EN	0.8110	0.3730
EU	1.0000	0.4780
EX	0.7210	0.2470
Ed	0.8440	0.3490
Ef	0.8250	0.3470
Eg	0.8050	0.2740
FC	0.8620	0.3580
FD	0.8440	0.3680
FF	0.7660	0.2560
FG	0.7180	0.2540
FH	0.8420	0.3240
FK	0.8580	0.3710

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Chain	Atom inclusion	Q-score
FL	0.8600	0.3500
FM	0.8550	0.3540
FN	0.8550	0.3970
FU	1.0000	0.5090
FX	0.5960	0.2440
Fd	0.8460	0.3530
Ff	0.8570	0.3430
Fg	0.7980	0.2630
GC	0.8550	0.3660
GD	0.8480	0.3710
GF	0.7960	0.2650
GG	0.7270	0.2700
GH	0.8210	0.3260
GK	0.8700	0.3790
GL	0.8750	0.3560
GM	0.8420	0.3520
GN	0.8530	0.3860
GU	0.9780	0.4780
GX	0.7330	0.2880
Gd	0.8560	0.3620
Gf	0.7990	0.3160
Gg	0.8570	0.2720
HC	0.8190	0.3550
HD	0.8400	0.3820
HF	0.7500	0.2500
HG	0.7410	0.2810
HH	0.8390	0.3350
HK	0.8570	0.3750
HL	0.8760	0.3540
HM	0.8520	0.3550
HN	0.8360	0.3850
HU	0.9780	0.5230
HX	0.6370	0.2570
Hd	0.8520	0.3510
Hf	0.8200	0.3240
Hg	0.8750	0.3090
IC	0.8060	0.3470
ID	0.8360	0.3690
IF	0.7600	0.2630
IG	0.7360	0.2920
IH	0.8210	0.3290
IK	0.8550	0.3760

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Chain	Atom inclusion	Q-score
IL	0.8550	0.3550
IM	0.8490	0.3540
IN	0.8110	0.3860
IU	1.0000	0.5190
IX	0.6790	0.2750
Id	0.8540	0.3610
If	0.8470	0.3300
Ig	0.8380	0.2770
JC	0.8470	0.3620
JD	0.8380	0.3750
JF	0.8020	0.2510
JG	0.7540	0.2950
JH	0.8260	0.3320
JK	0.8540	0.3750
JL	0.8610	0.3600
JM	0.8590	0.3540
JN	0.8250	0.3750
JU	0.9780	0.5050
JX	0.6250	0.2110
Jd	0.8500	0.3660
Jf	0.8180	0.3440
Jg	0.8380	0.2980
KC	0.8540	0.3650
KD	0.8420	0.3680
KF	0.7880	0.2610
KG	0.7540	0.3050
KH	0.8320	0.3340
KK	0.8690	0.3770
KL	0.8640	0.3520
KM	0.8320	0.3570
KN	0.8580	0.3910
KU	0.9780	0.4860
KX	0.6620	0.2820
Kd	0.8630	0.3620
Kf	0.7930	0.3310
Kg	0.8380	0.3100
LC	0.8150	0.3410
LD	0.8500	0.3630
LF	0.7920	0.2840
LG	0.7540	0.3100
LH	0.8150	0.3330
LK	0.8600	0.3690

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Chain	Atom inclusion	Q-score
LL	0.8750	0.3590
LM	0.8280	0.3450
LN	0.8370	0.3890
LU	1.0000	0.4790
LX	0.6370	0.2470
Ld	0.8640	0.3640
Lf	0.8500	0.3280
Lg	0.8460	0.2740
MC	0.8210	0.3530
MD	0.8460	0.3630
MF	0.7370	0.2480
MG	0.7350	0.2550
MH	0.8040	0.3280
MK	0.8590	0.3770
ML	0.8640	0.3650
MM	0.8430	0.3620
MN	0.8230	0.3820
MU	1.0000	0.4830
MX	0.5670	0.2530
Md	0.8520	0.3590
Mf	0.8270	0.3410
Mg	0.8380	0.2750
NG	0.7270	0.2380
OG	0.7790	0.2970
PG	0.7340	0.2450
VF	0.7980	0.2570
VG	0.7680	0.2800
VH	0.7210	0.3100
VX	0.6370	0.2660
WF	0.8050	0.2480
WG	0.7720	0.2560
WH	0.6650	0.3050
WX	0.6620	0.2720
XF	0.8130	0.2470
XG	0.7980	0.2560
XH	0.6070	0.2980
XX	0.6620	0.2760
YF	0.8090	0.2640
YG	0.8120	0.2890
YH	0.7270	0.3090
YX	0.6170	0.2650
ZF	0.7450	0.2580

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Chain	Atom inclusion	Q-score
ZG	0.7980	0.2780
ZH	0.5240	0.2790
ZX	0.7460	0.3150