Full wwPDB EM Validation Report

Nov 20, 2022 – 03:45 PM EST

PDB ID	:	7MUS
EMDB ID	:	EMD-24020
Title	:	Reconstruction of the Legionella pneumophila Dot/Icm T4SS 3DVA Map 2
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:

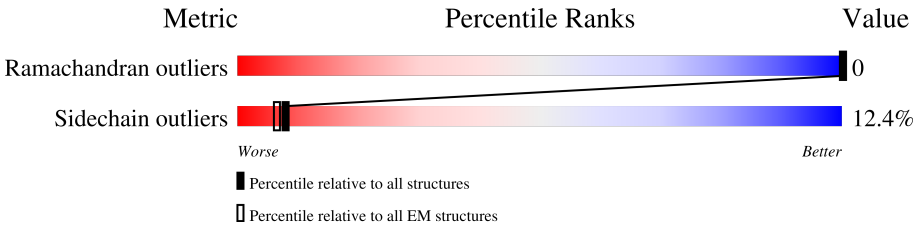
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

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



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

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

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

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Mol	Chain	Length	Quality of chain
1	Eg	1048	97%
1	FG	1048	5% 14% 84%
1	Fg	1048	97%
1	GG	1048	5% 13% 84%
1	Gg	1048	97%
1	HG	1048	5% 14% 84%
1	Hg	1048	97%
1	IG	1048	5% 14% 84%
1	Ig	1048	97%
1	JG	1048	5% 14% 84%
1	Jg	1048	97%
1	KG	1048	5% 14% 84%
1	Kg	1048	97%
1	LG	1048	14% 84%
1	Lg	1048	97%
1	MG	1048	14% 84%
1	Mg	1048	97%
1	NG	1048	14% 84%
1	OG	1048	14% 84%
1	PG	1048	14% 84%
1	VG	1048	97%
1	WG	1048	97%
1	XG	1048	97%
1	YG	1048	97%
1	ZG	1048	97%

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Mol	Chain	Length	Quality of chain
2	AD	163	75% 10% 14%
2	Ad	163	74% 10% 16%
2	BD	163	77% 9% 14%
2	Bd	163	78% 6% 16%
2	CD	163	74% 12% 14%
2	Cd	163	77% 7% 16%
2	DD	163	80% 6% 14%
2	Dd	163	77% 7% 16%
2	ED	163	78% 8% 14%
2	Ed	163	77% 7% 16%
2	FD	163	77% 9% 14%
2	Fd	163	75% 9% 16%
2	GD	163	77% 9% 14%
2	Gd	163	76% 8% 16%
2	HD	163	79% 7% 14%
2	Hd	163	75% 9% 16%
2	ID	163	76% 10% 14%
2	Id	163	74% 10% 16%
2	JD	163	77% 9% 14%
2	Jd	163	74% 10% 16%
2	KD	163	82% 14%
2	Kd	163	76% 8% 16%
2	LD	163	76% 10% 14%
2	Ld	163	76% 8% 16%
2	MD	163	77% 9% 14%

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Mol	Chain	Length	Quality of chain
2	Md	163	77% 7% 16%
3	AF	269	22% 77%
3	Af	269	20% 78%
3	BF	269	21% 77%
3	Bf	269	19% 78%
3	CF	269	22% 77%
3	Cf	269	19% 78%
3	DF	269	22% 77%
3	Df	269	20% 78%
3	EF	269	22% 77%
3	Ef	269	20% 78%
3	FF	269	20% 77%
3	Ff	269	20% 78%
3	GF	269	22% 77%
3	Gf	269	21% 78%
3	HF	269	21% 77%
3	Hf	269	19% 78%
3	IF	269	21% 77%
3	If	269	19% 78%
3	JF	269	23% 77%
3	Jf	269	20% 78%
3	KF	269	20% 77%
3	Kf	269	20% 78%
3	LF	269	21% 77%
3	Lf	269	20% 78%

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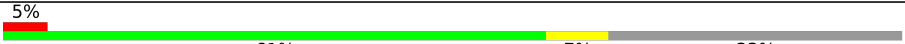
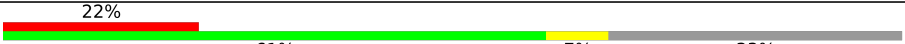
Mol	Chain	Length	Quality of chain
3	MF	269	
3	Mf	269	
3	VF	269	
3	WF	269	
3	XF	269	
3	YF	269	
3	ZF	269	
4	AH	361	
4	BH	361	
4	CH	361	
4	DH	361	
4	EH	361	
4	FH	361	
4	GH	361	
4	HH	361	
4	IH	361	
4	JH	361	
4	KH	361	
4	LH	361	
4	MH	361	
4	VH	361	
4	WH	361	
4	XH	361	
4	YH	361	
4	ZH	361	

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Mol	Chain	Length	Quality of chain
5	AK	189	70% 10% 20%
5	BK	189	70% 10% 20%
5	CK	189	70% 10% 20%
5	DK	189	72% 8% 20%
5	EK	189	73% 7% 20%
5	FK	189	72% 7% 20%
5	GK	189	71% 8% 20%
5	HK	189	71% 9% 20%
5	IK	189	72% 8% 20%
5	JK	189	72% 8% 20%
5	KK	189	72% 8% 20%
5	LK	189	70% 10% 20%
5	MK	189	74% 6% 20%
6	AL	249	65% 5% 31%
6	BL	249	63% 7% 31%
6	CL	249	61% 8% 31%
6	DL	249	63% 6% 31%
6	EL	249	61% 8% 31%
6	FL	249	65% 31%
6	GL	249	63% 6% 31%
6	HL	249	64% 5% 31%
6	IL	249	64% 5% 31%
6	JL	249	63% 6% 31%
6	KL	249	64% 6% 31%
6	LL	249	61% 8% 31%

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Mol	Chain	Length	Quality of chain
6	ML	249	63% 6% 31%
7	AM	320	57% 8% 35%
7	BM	320	58% 7% 35%
7	CM	320	58% 7% 35%
7	DM	320	57% 8% 35%
7	EM	320	58% 7% 35%
7	FM	320	58% 7% 35%
7	GM	320	57% 8% 35%
7	HM	320	58% 7% 35%
7	IM	320	58% 8% 35%
7	JM	320	55% 10% 35%
7	KM	320	58% 7% 35%
7	LM	320	58% 8% 35%
7	MM	320	58% 7% 35%
8	AN	124	56% 6% 37%
8	BN	124	58% 5% 37%
8	CN	124	56% 7% 37%
8	DN	124	60% 37%
8	EN	124	56% 7% 37%
8	FN	124	54% 9% 37%
8	GN	124	57% 6% 37%
8	HN	124	56% 7% 37%
8	IN	124	54% 9% 37%
8	JN	124	57% 6% 37%
8	KN	124	52% 10% 37%

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Mol	Chain	Length	Quality of chain
8	LN	124	52% 10% 37%
8	MN	124	53% 10% 37%
9	AU	9	100%
9	BU	9	100%
9	CU	9	100%
9	DU	9	100%
9	EU	9	100%
9	FU	9	100%
9	GU	9	100%
9	HU	9	100%
9	IU	9	100%
9	JU	9	100%
9	KU	9	100%
9	LU	9	100%
9	MU	9	100%
10	AX	48	15% 100%
10	BX	48	21% 100%
10	CX	48	100%
10	DX	48	19% 100%
10	EX	48	19% 100%
10	FX	48	17% 100%
10	GX	48	23% 100%
10	HX	48	15% 100%
10	IX	48	10% 100%
10	JX	48	17% 100%

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Mol	Chain	Length	Quality of chain
10	KX	48	15% 100%
10	LX	48	6% 100%
10	MX	48	15% 100%
10	VX	48	10% 100%
10	WX	48	10% 100%
10	XX	48	10% 100%
10	YX	48	17% 100%
10	ZX	48	6% 100%
11	AC	303	59% 10% 31%
11	BC	303	61% 8% 31%
11	CC	303	60% 9% 31%
11	DC	303	71% 10% 20%
11	EC	303	61% 8% 31%
11	FC	303	63% 6% 31%
11	GC	303	62% 7% 31%
11	HC	303	71% 9% 20%
11	IC	303	70% 10% 20%
11	JC	303	64% 5% 31%
11	KC	303	63% 6% 31%
11	LC	303	72% 8% 20%
11	MC	303	71% 10% 20%

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	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	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	Ag	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	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	XG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EG	165	Total	C	N	O	S	0	0
			1229	780	203	242	4		
1	YG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	ZG	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
1	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 DotD.

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

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

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

- Molecule 3 is a protein called DotF.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
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	CF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	YF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	ZF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Af	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	BF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Bf	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	Cf	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		
3	FF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		
3	Ff	59	Total	C	N	O	S	0	0
			449	290	77	81	1		
3	AF	63	Total	C	N	O	S	0	0
			483	308	84	90	1		

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Neurogenic locus notch.

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

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

- Molecule 9 is a protein called Unknown protein fragment.

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

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

- Molecule 10 is a protein called Unknown protein fragment.

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

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

- Molecule 11 is a protein called DotC.

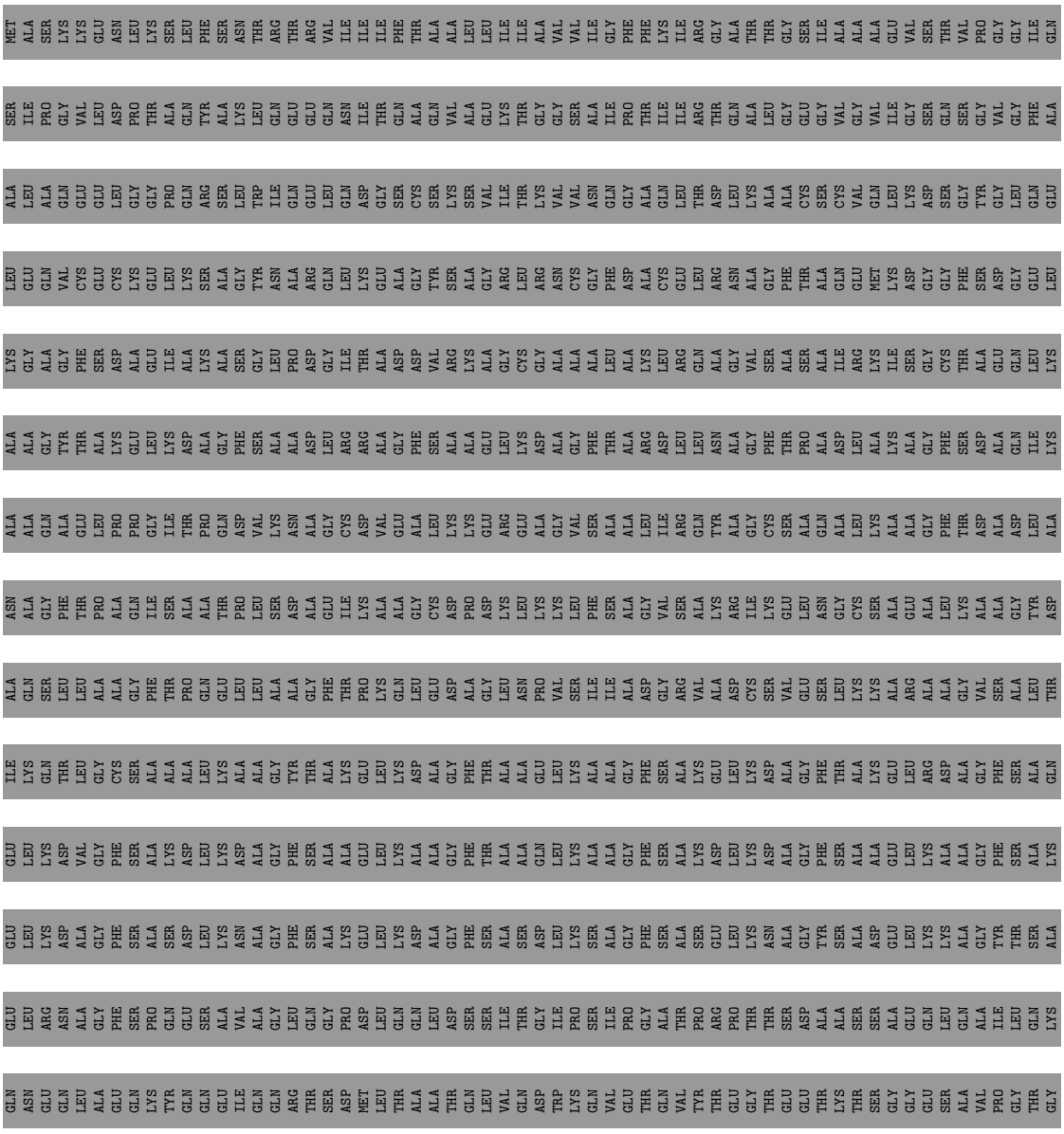
Mol	Chain	Residues	Atoms					AltConf	Trace
11	CC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	EC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	FC	209	Total	C	N	O	S	0	0
			1667	1061	292	309	5		
11	DC	243	Total	C	N	O	S	0	0
			1921	1216	340	357	8		
11	GC	209	Total	C	N	O	S	0	0
			1667	1061	292	309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

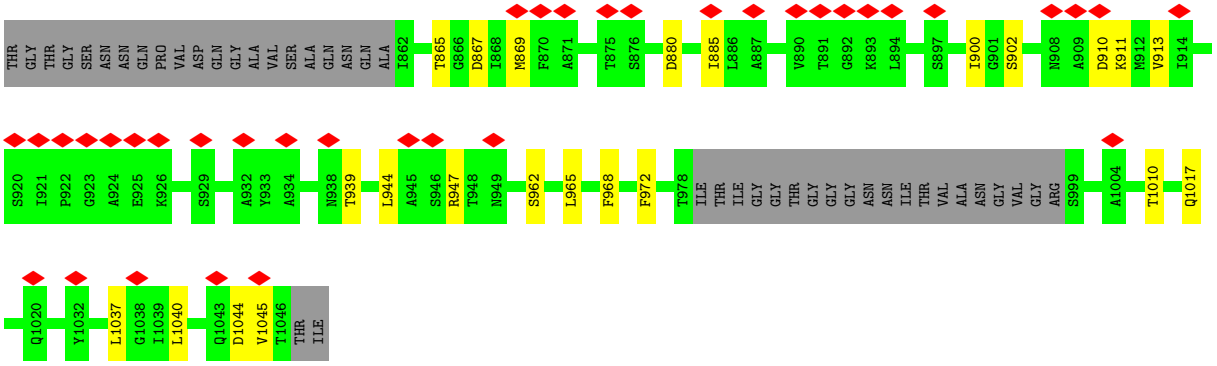
3 Residue-property plots (i)

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

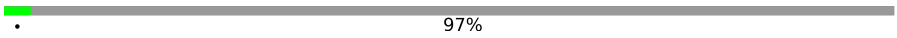
Chain AG:

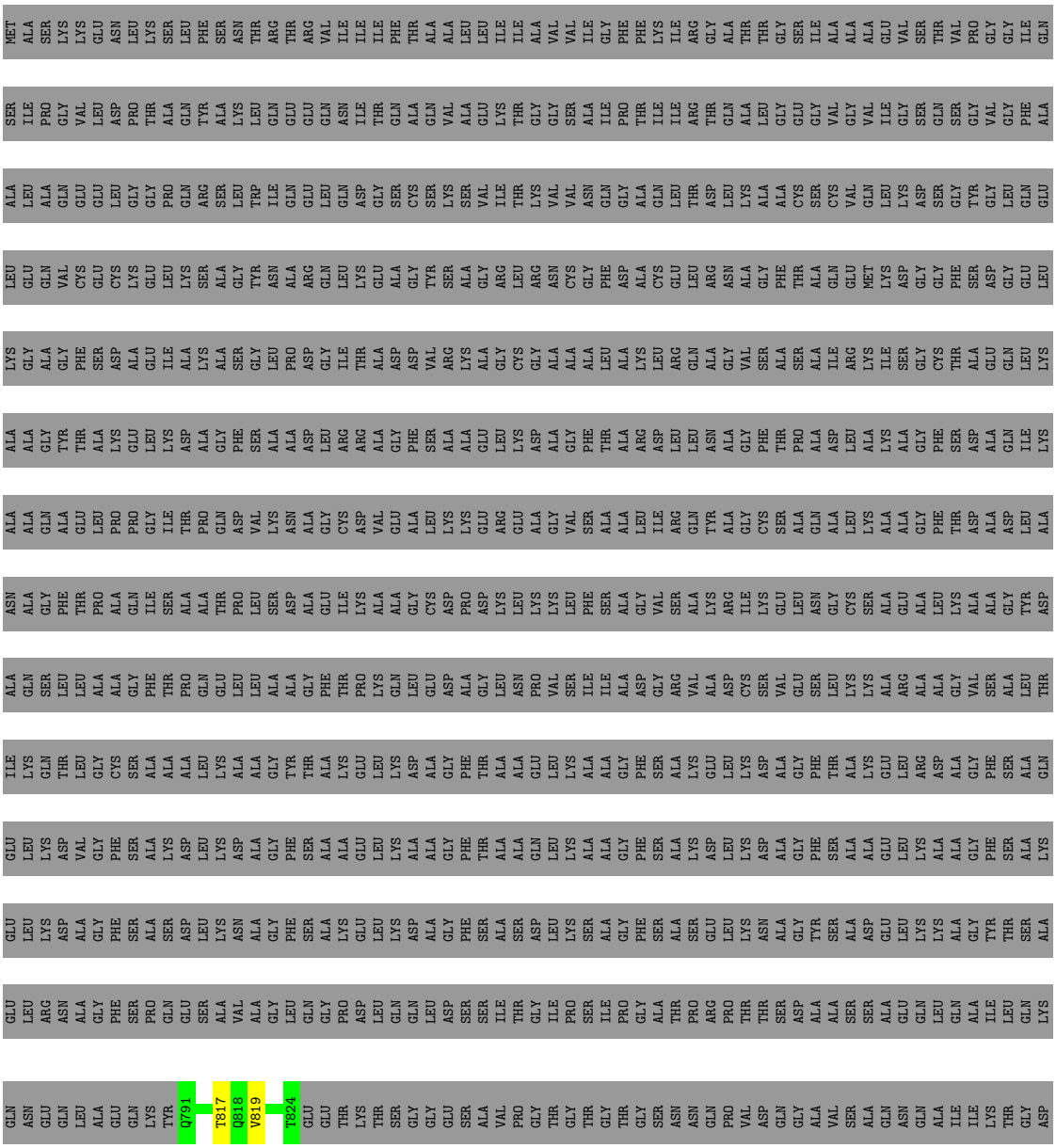


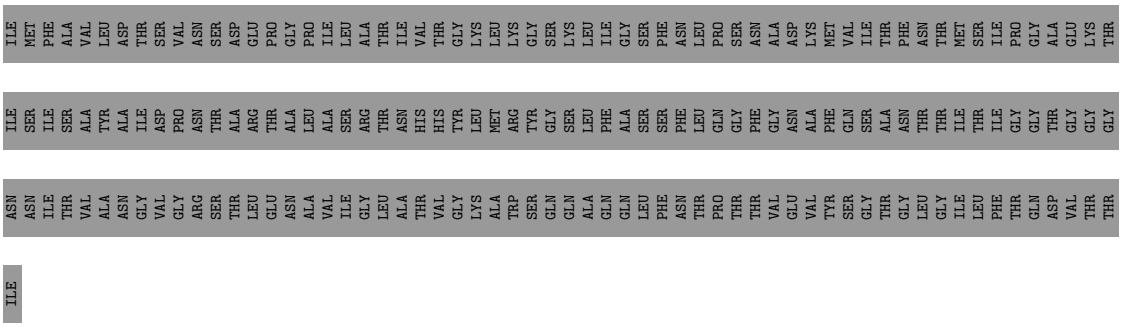


• Molecule 1: IcmE protein

Chain Gg:

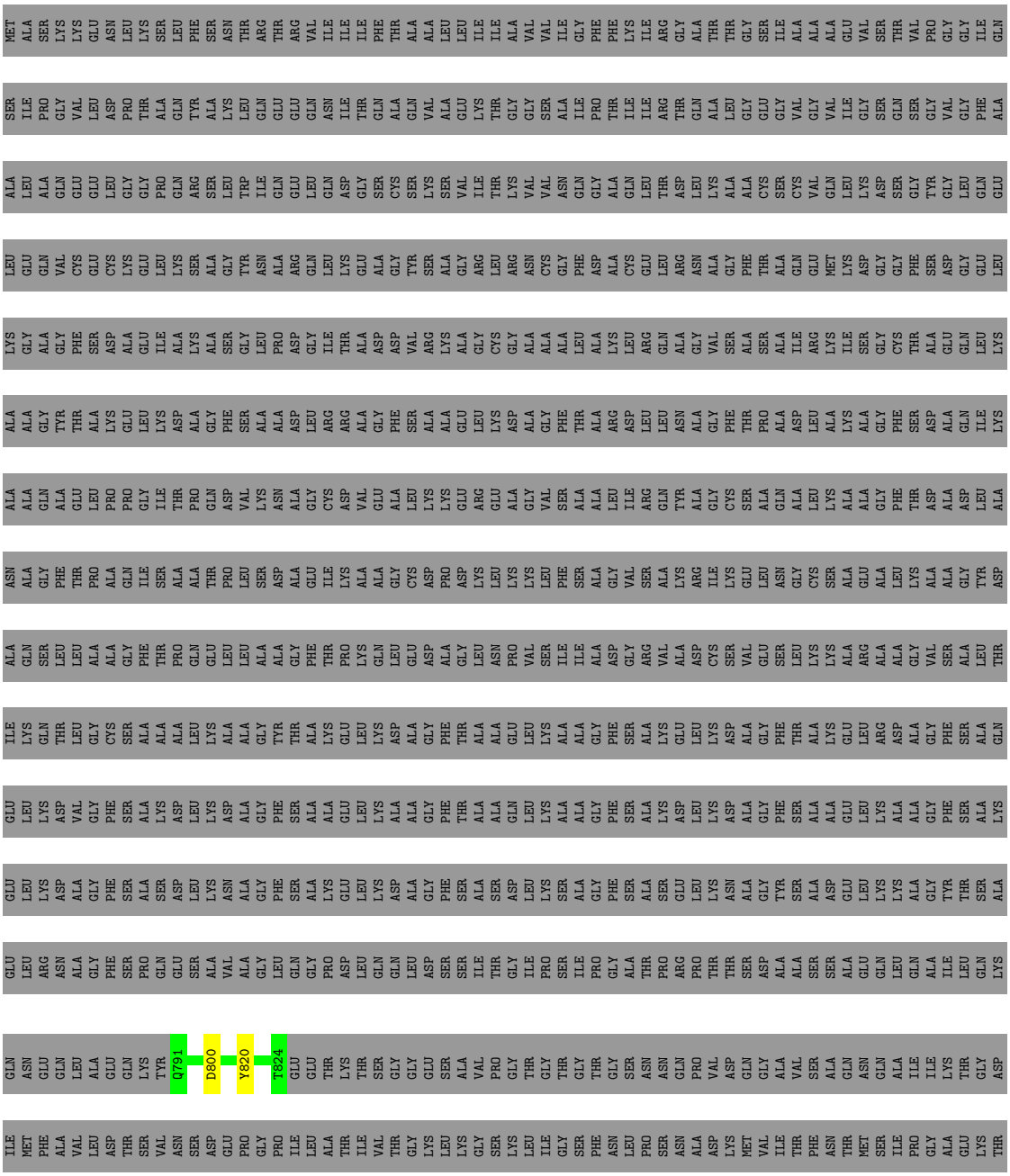


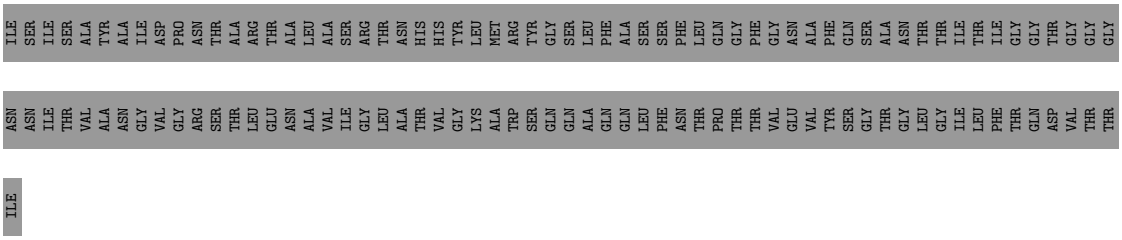




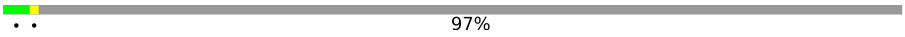
• Molecule 1: IcmE protein

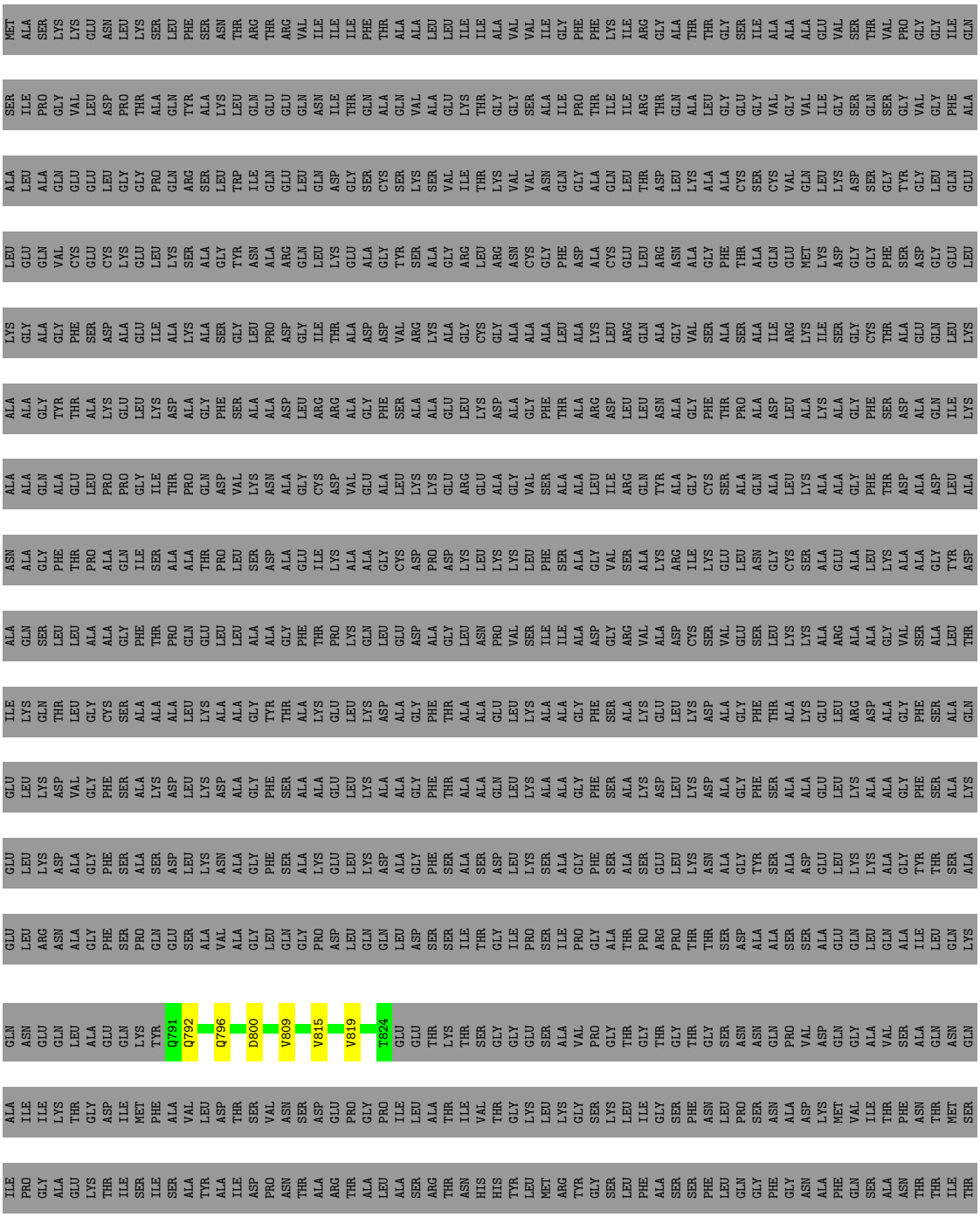
Chain Hg: 97%

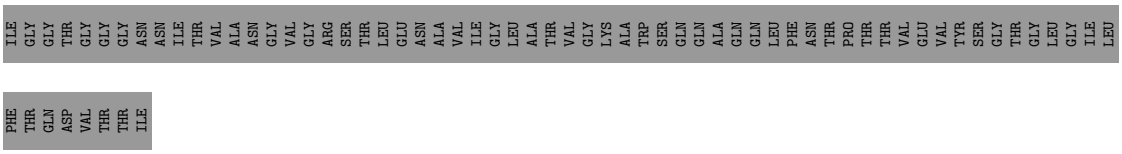




• Molecule 1: IcmE protein

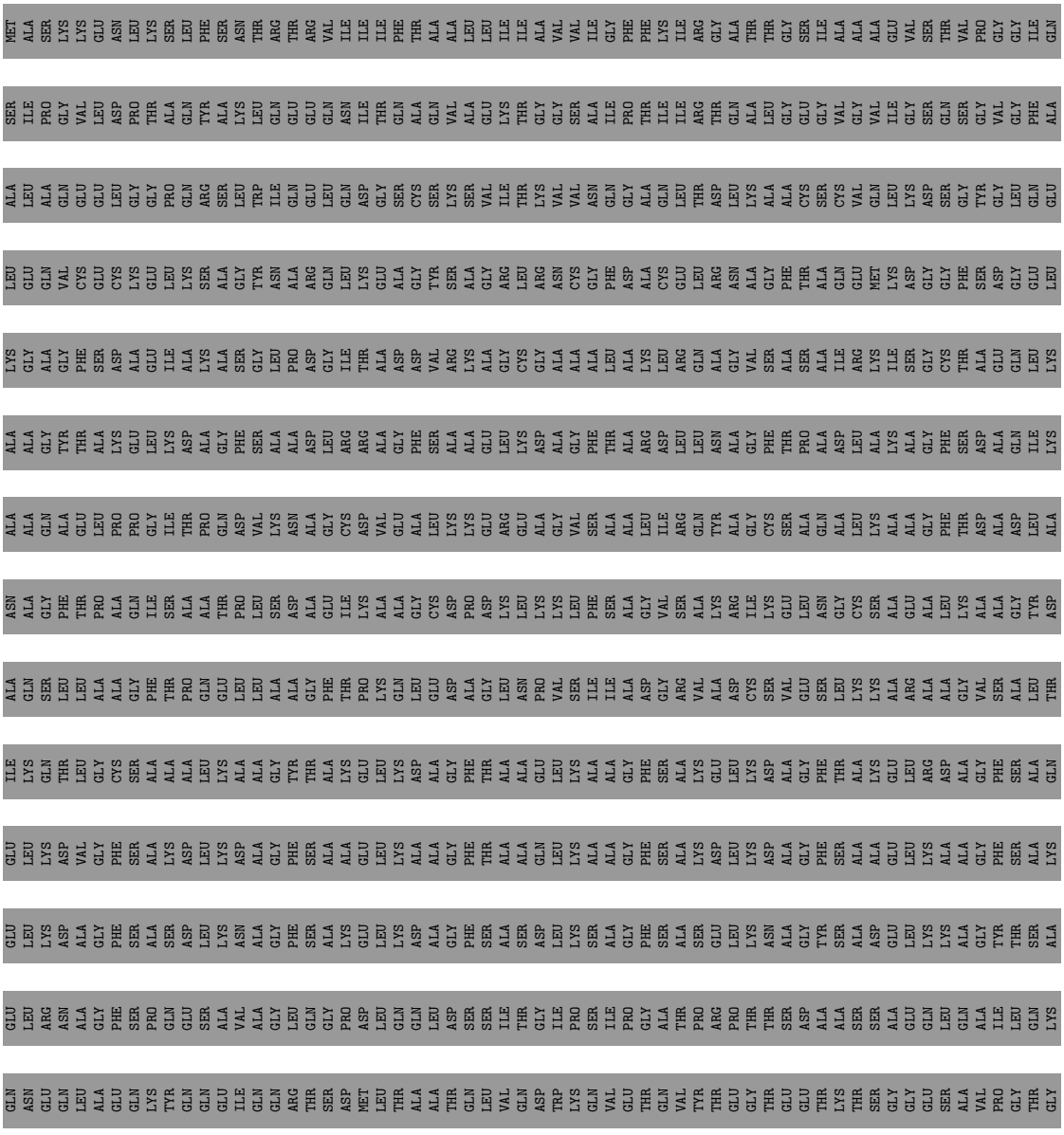
Chain Bg: 

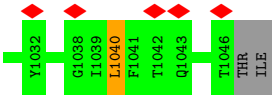




• Molecule 1: IcmE protein

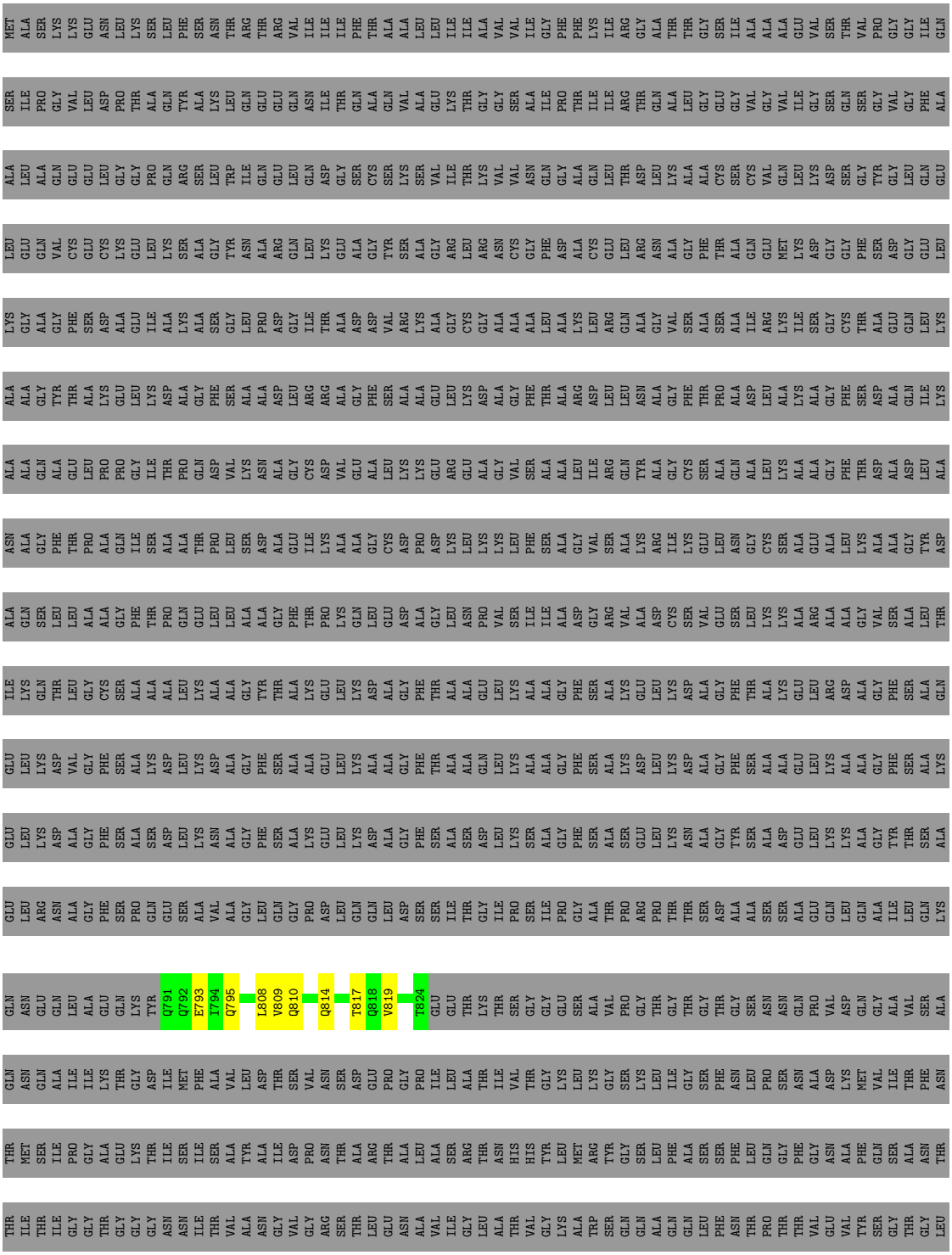
Chain BG:





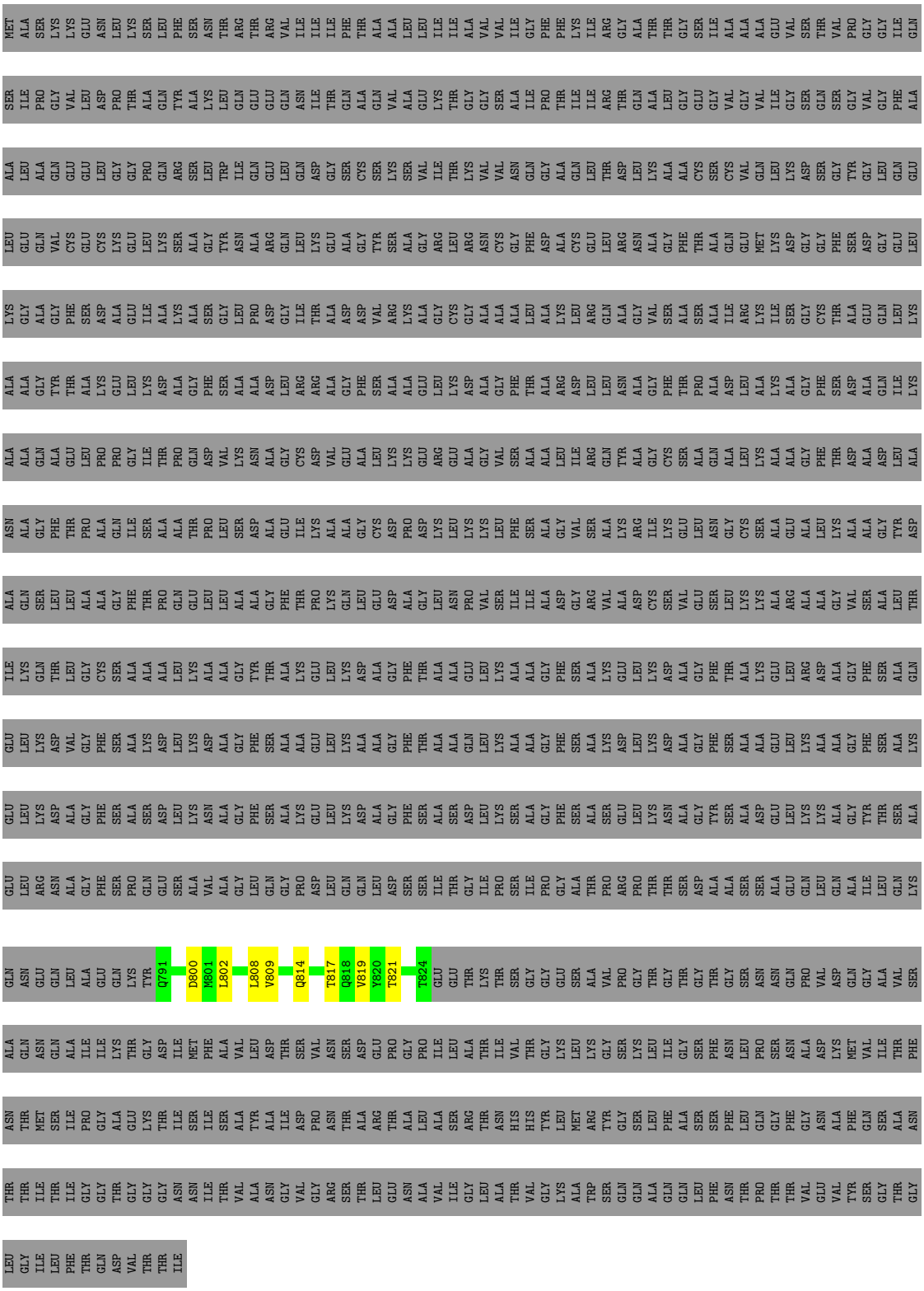
• Molecule 1: IcmE protein

Chain Ig: 97%



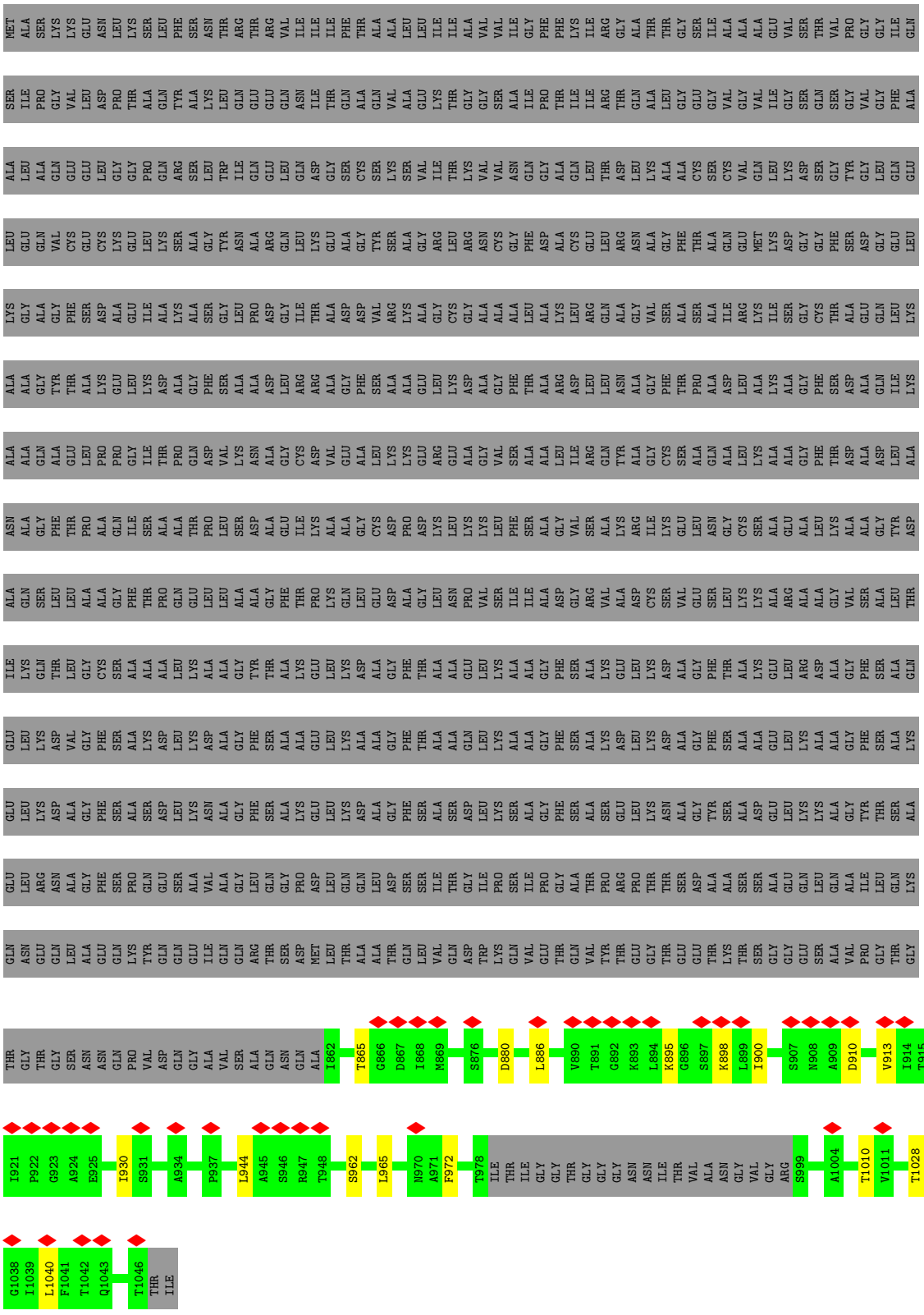
• Molecule 1: IcmE protein

Chain Jg: 97%



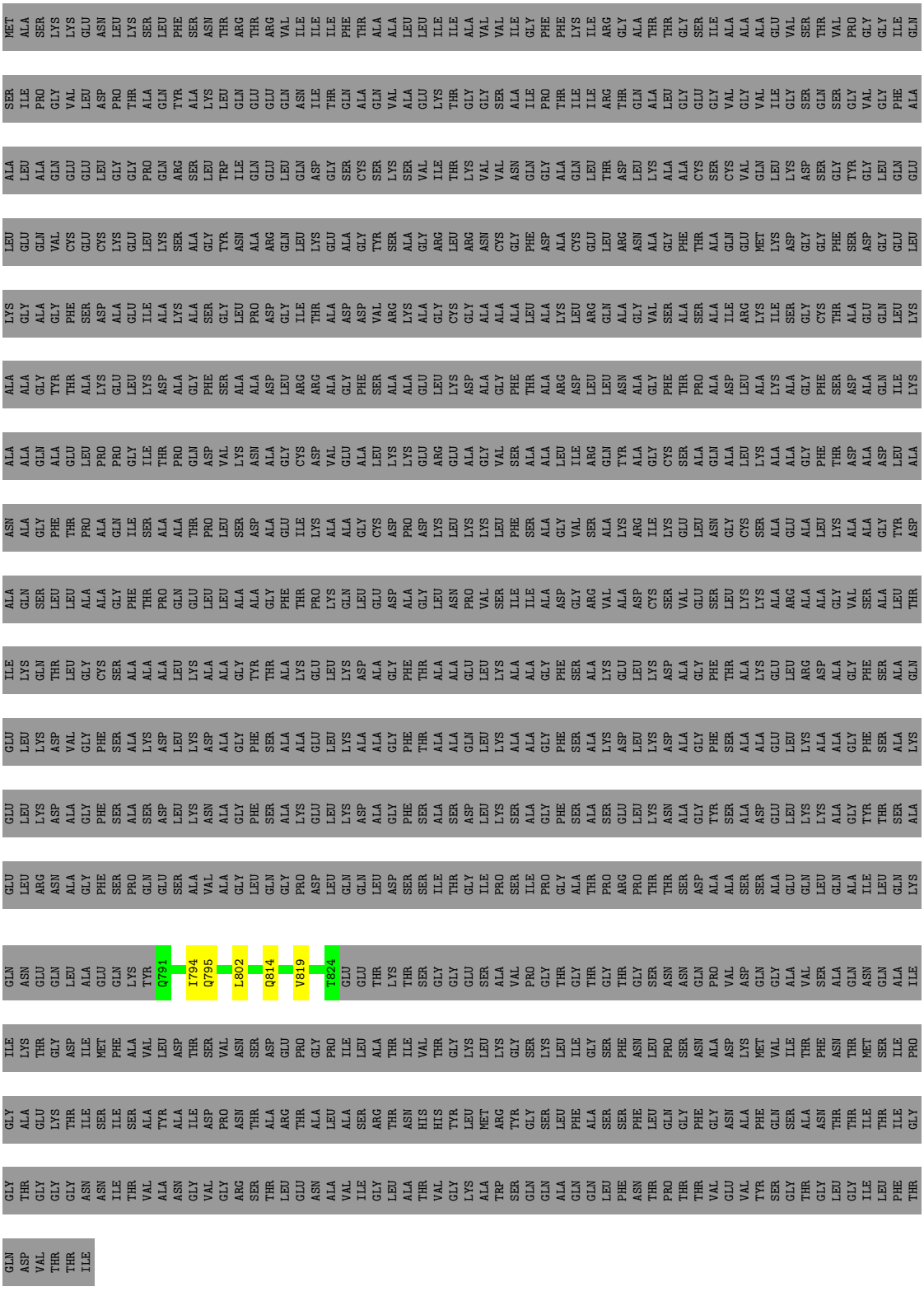
• Molecule 1: IcmE protein

Chain CG:



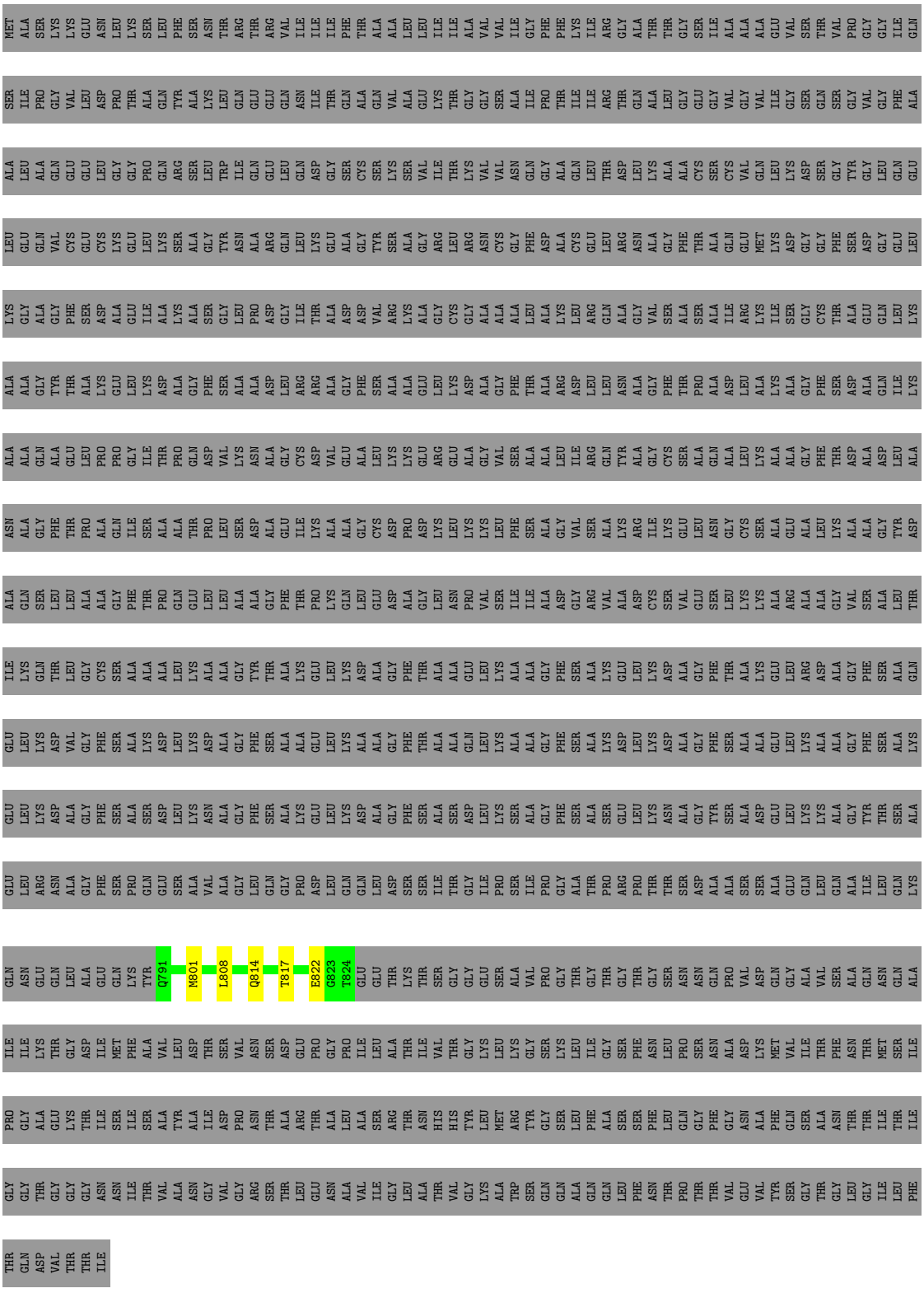
• Molecule 1: IcmE protein

Chain Kg: 97%



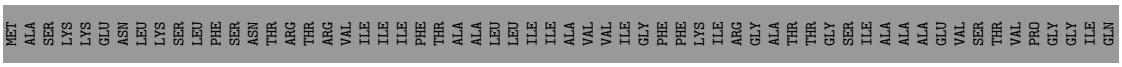
• Molecule 1: IcmE protein

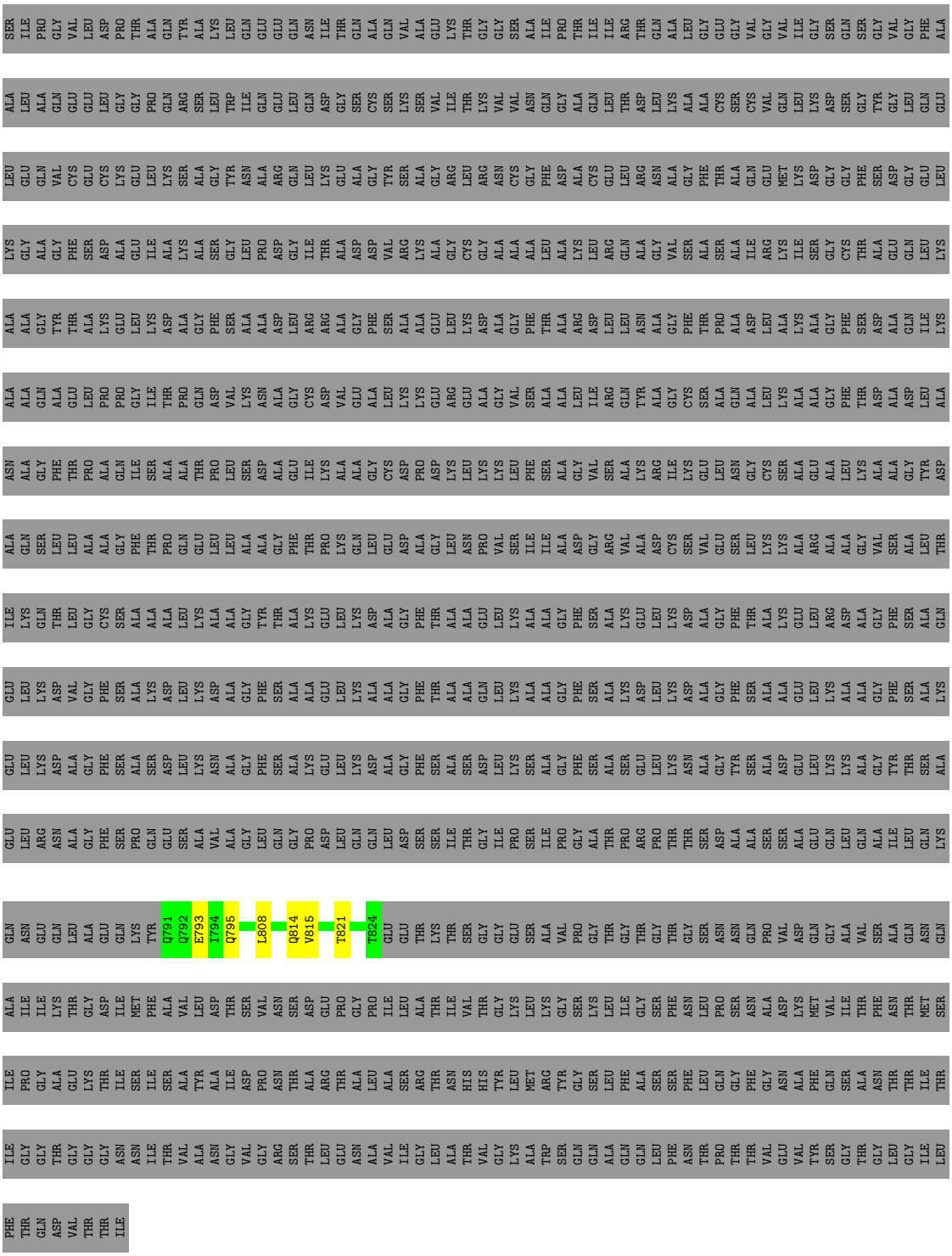
Chain Ag: 97%



• Molecule 1: IcmE protein

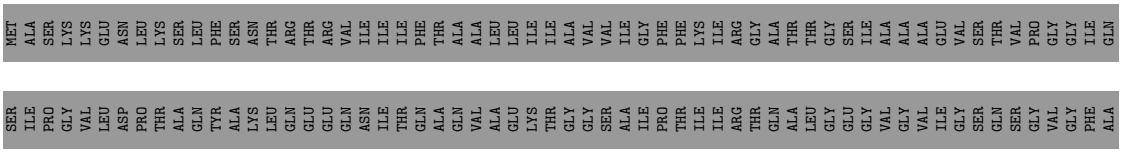
Chain Lg: 97%

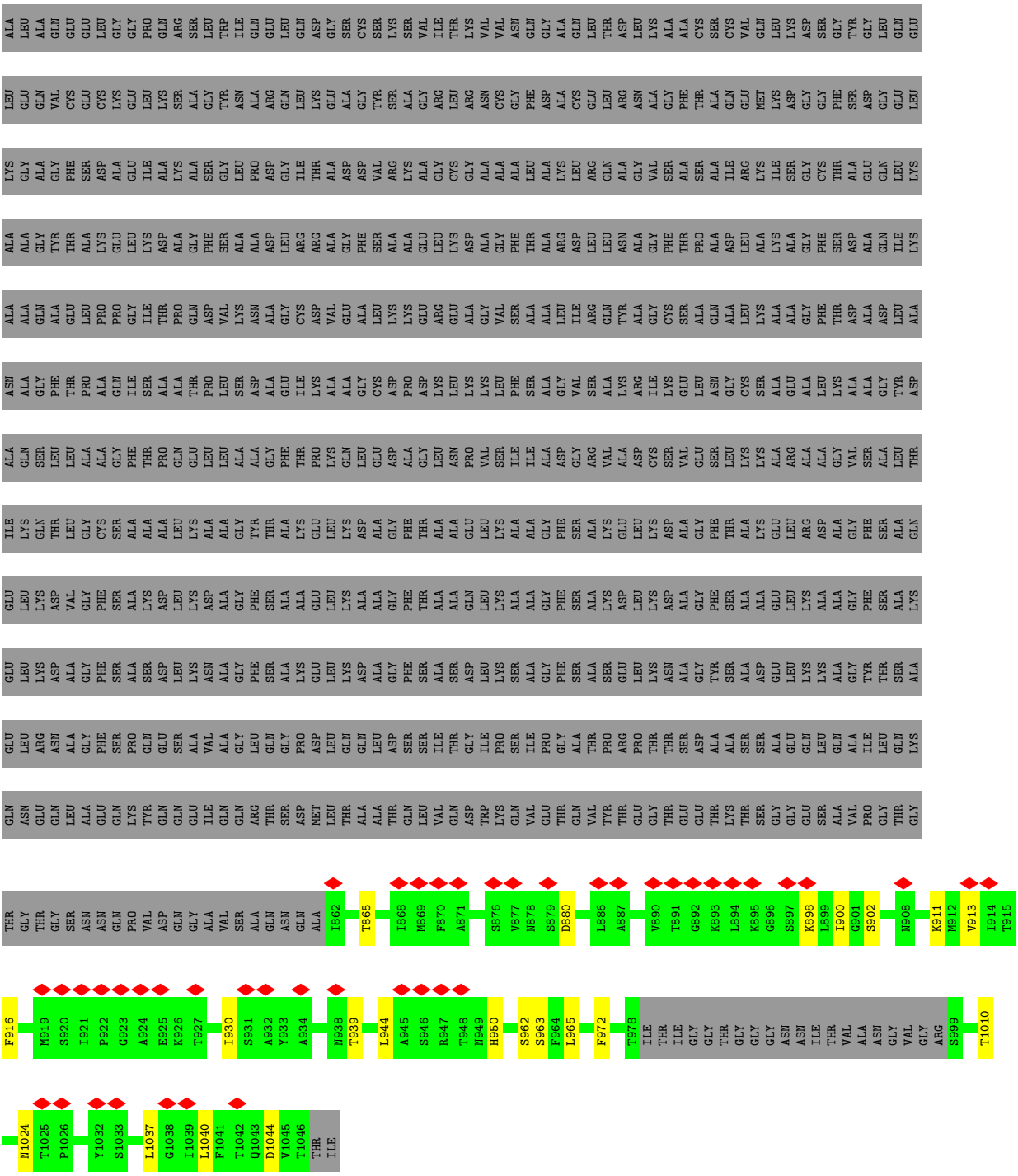




• Molecule 1: IcmE protein

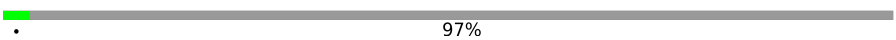
Chain DG:

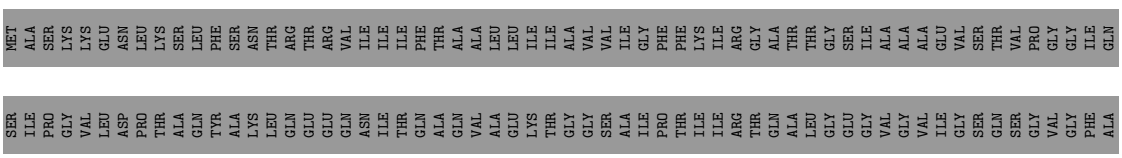


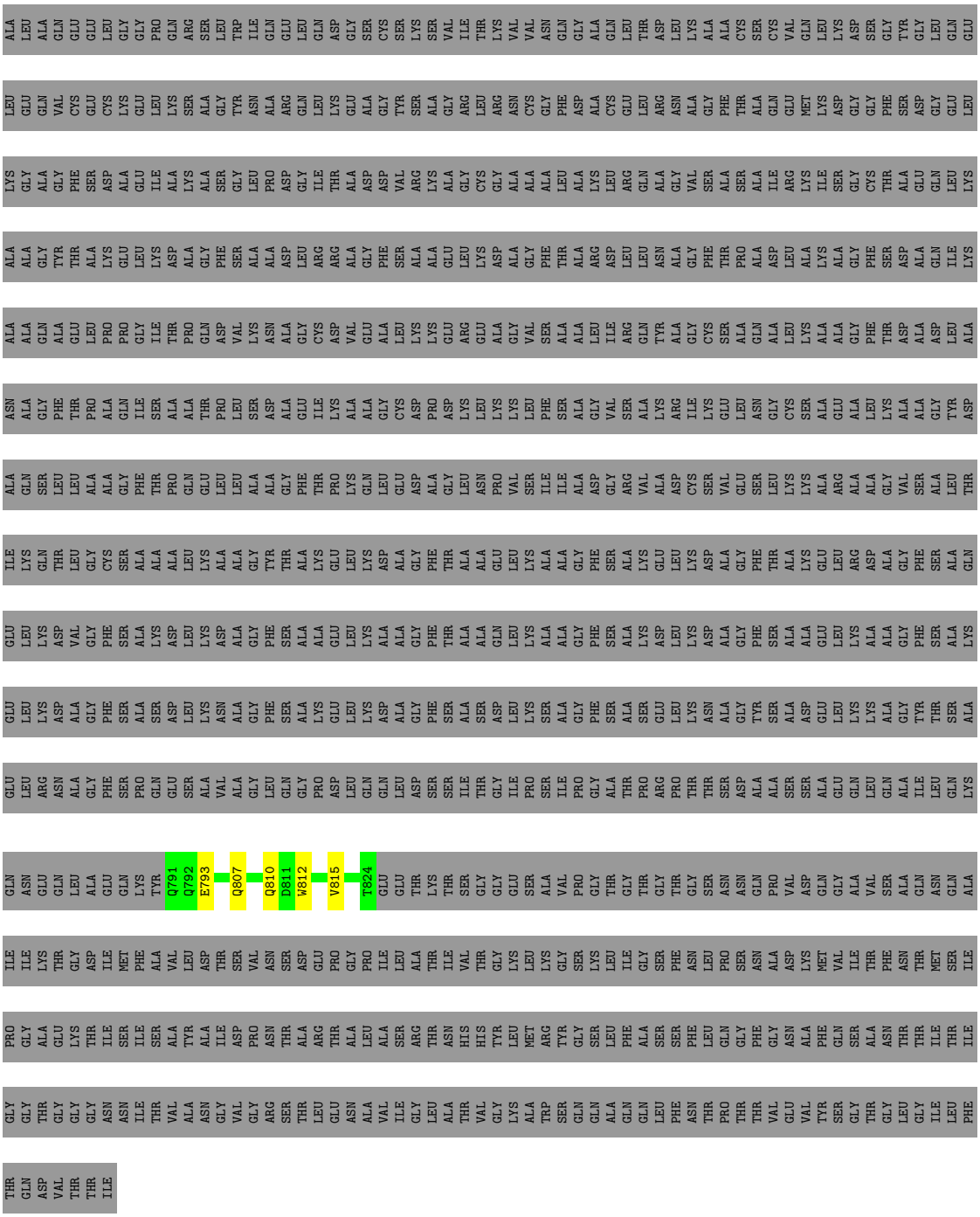


• Molecule 1: IcmE protein

Chain Cg:

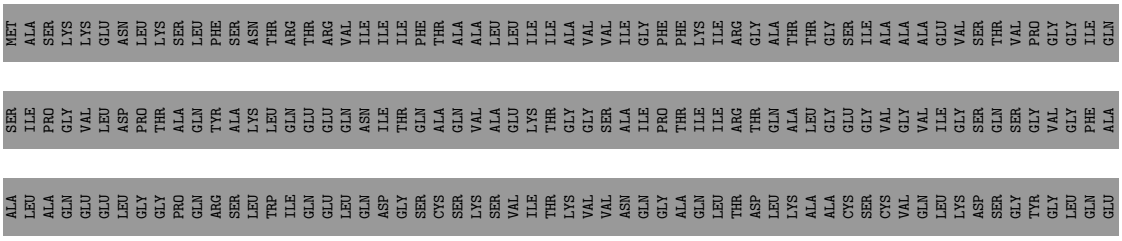


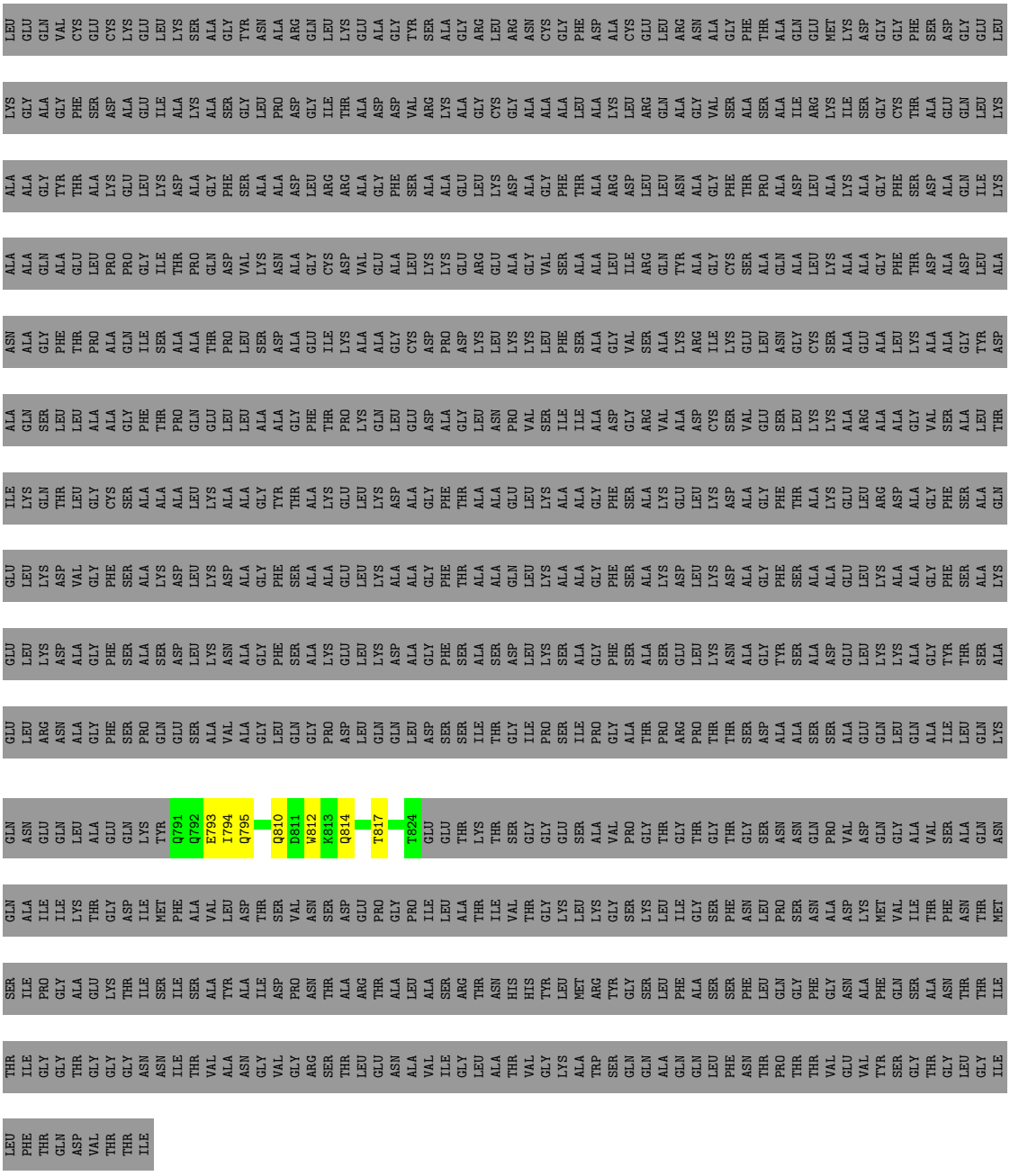




• Molecule 1: IcmE protein

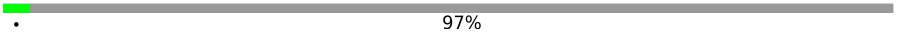
Chain Mg:

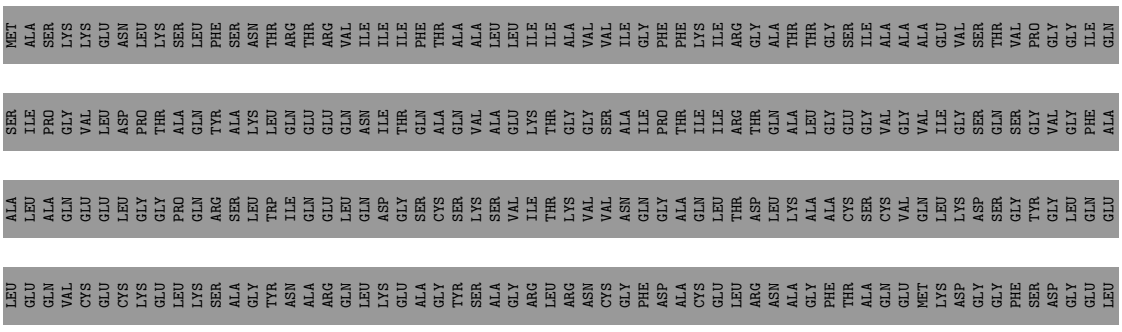


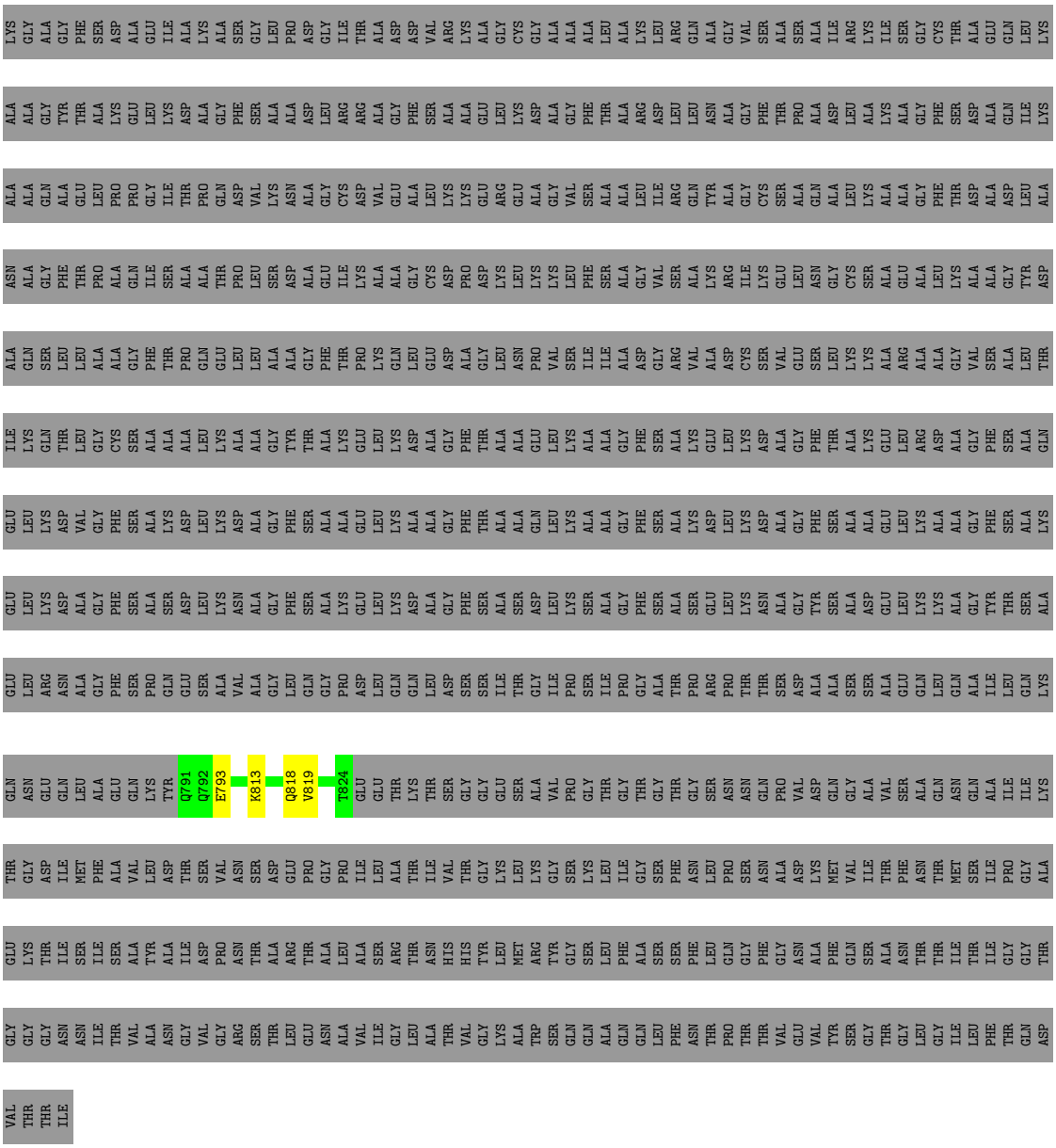


• Molecule 1: IcmE protein

Chain VG:

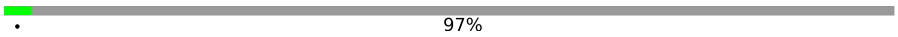


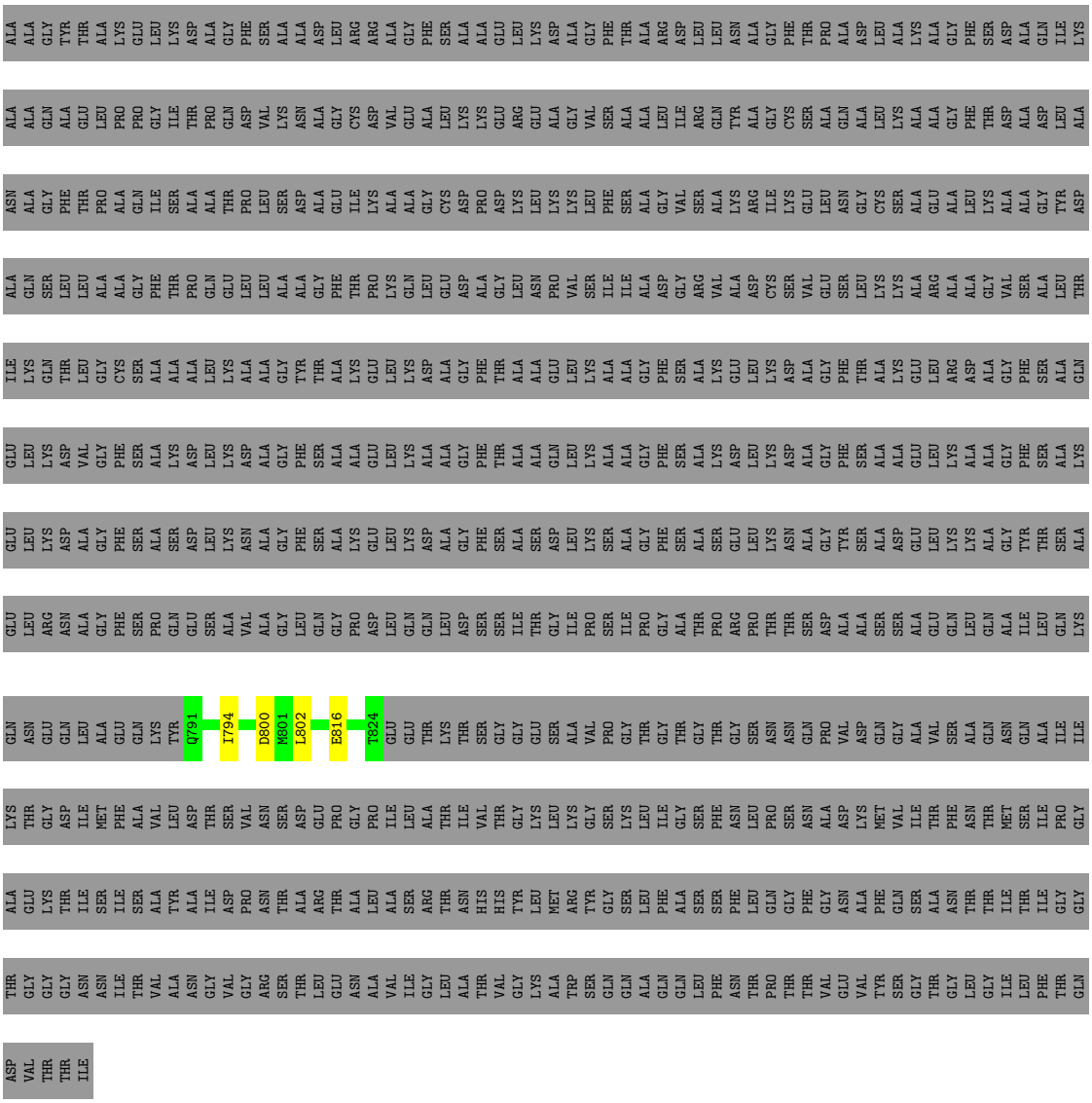




• Molecule 1: IcmE protein

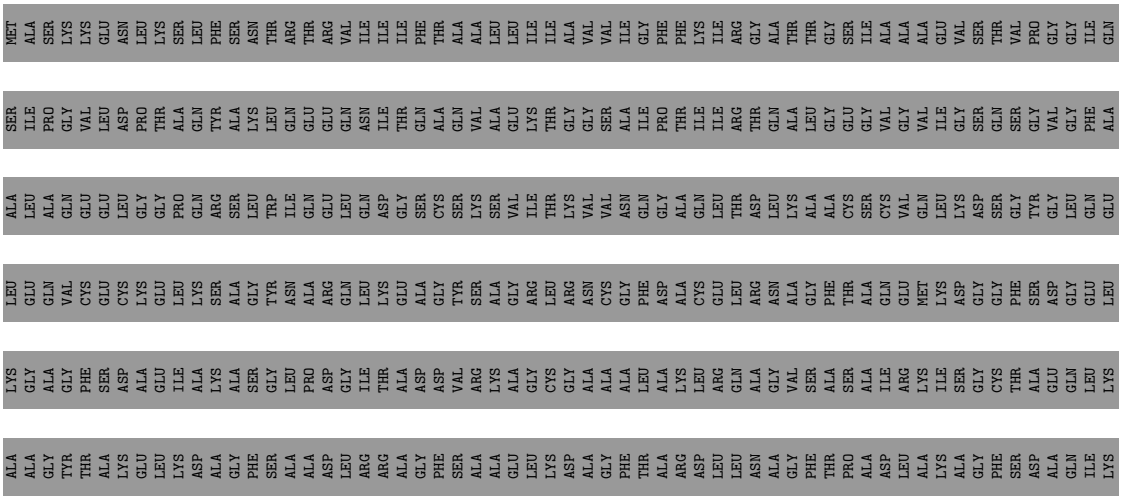
Chain WG:

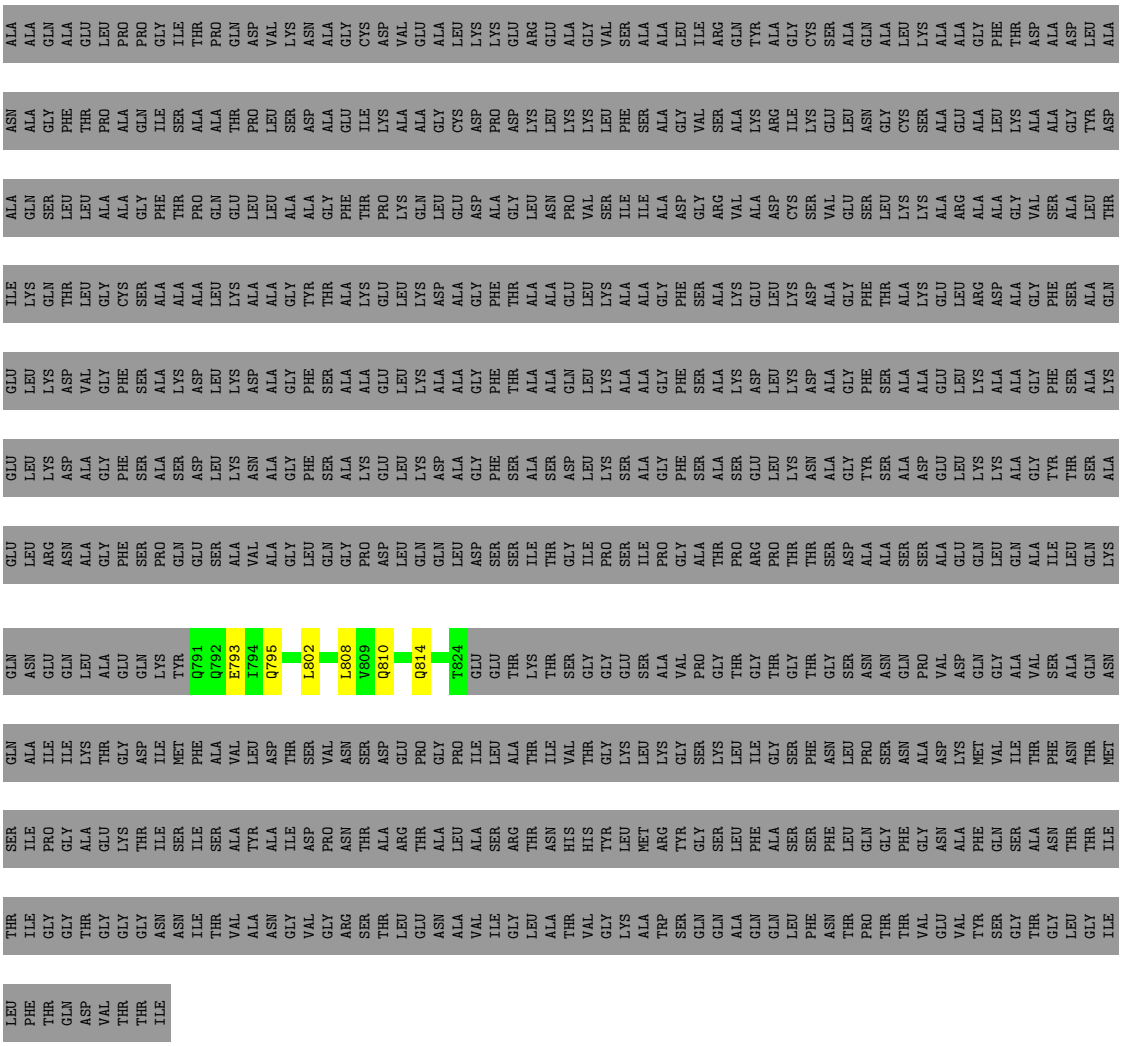




• Molecule 1: IcmE protein

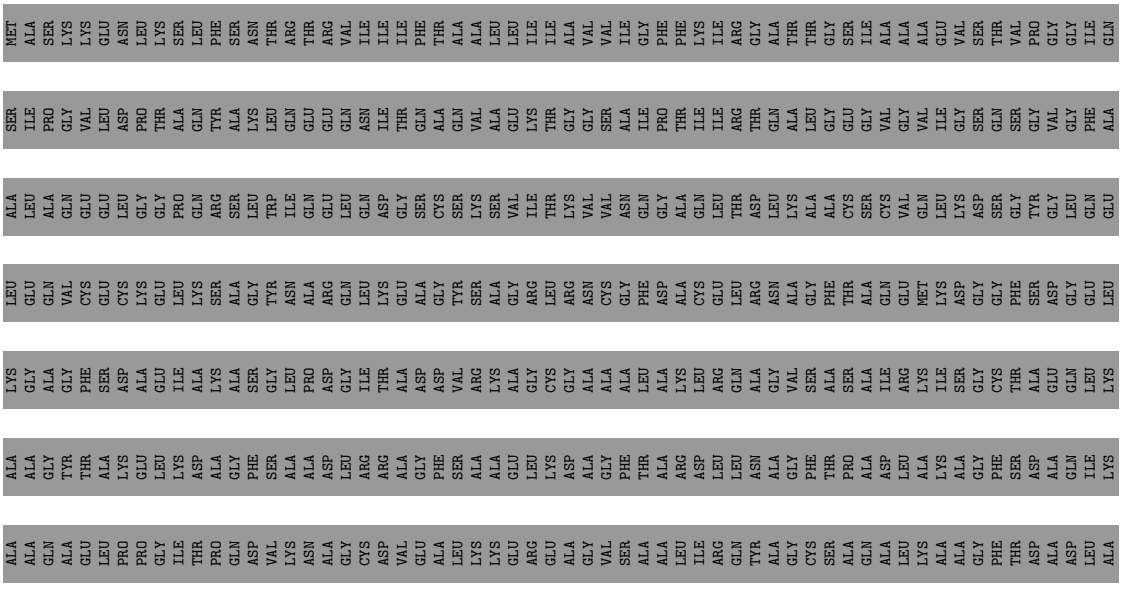
Chain XG: 97%

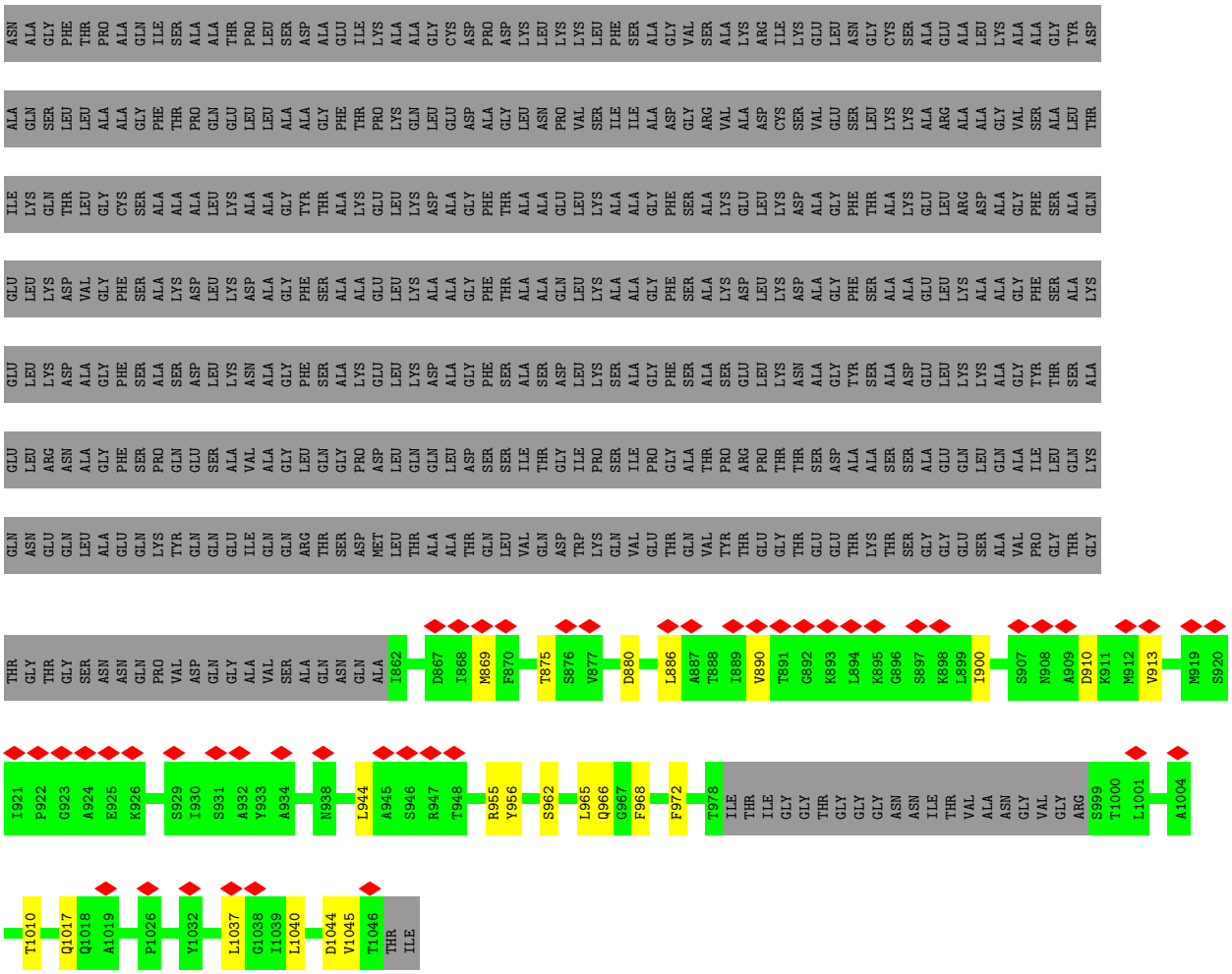




• Molecule 1: IcmE protein

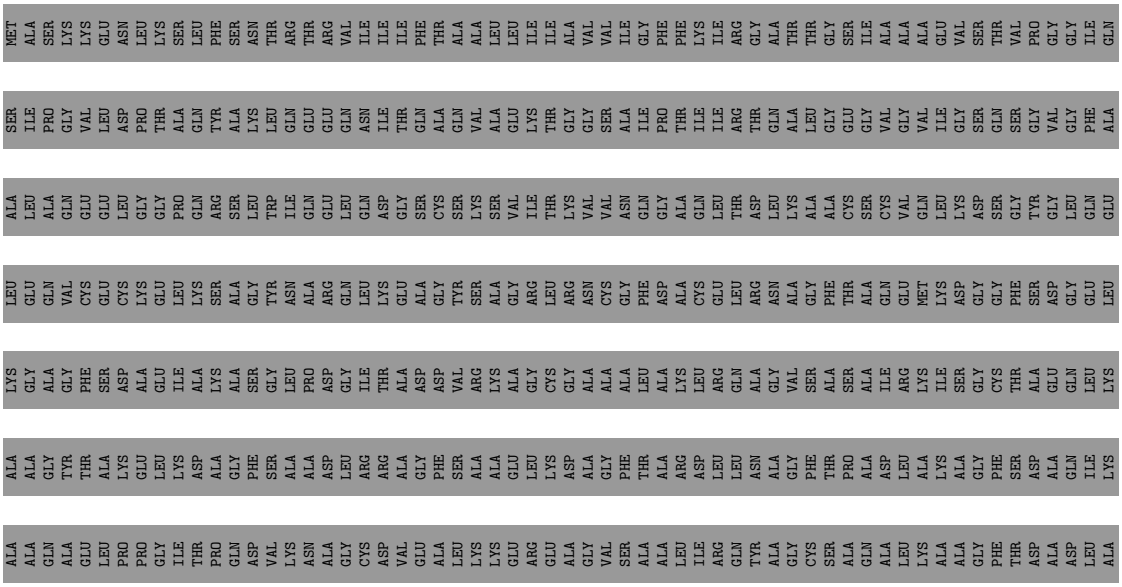
Chain EG:

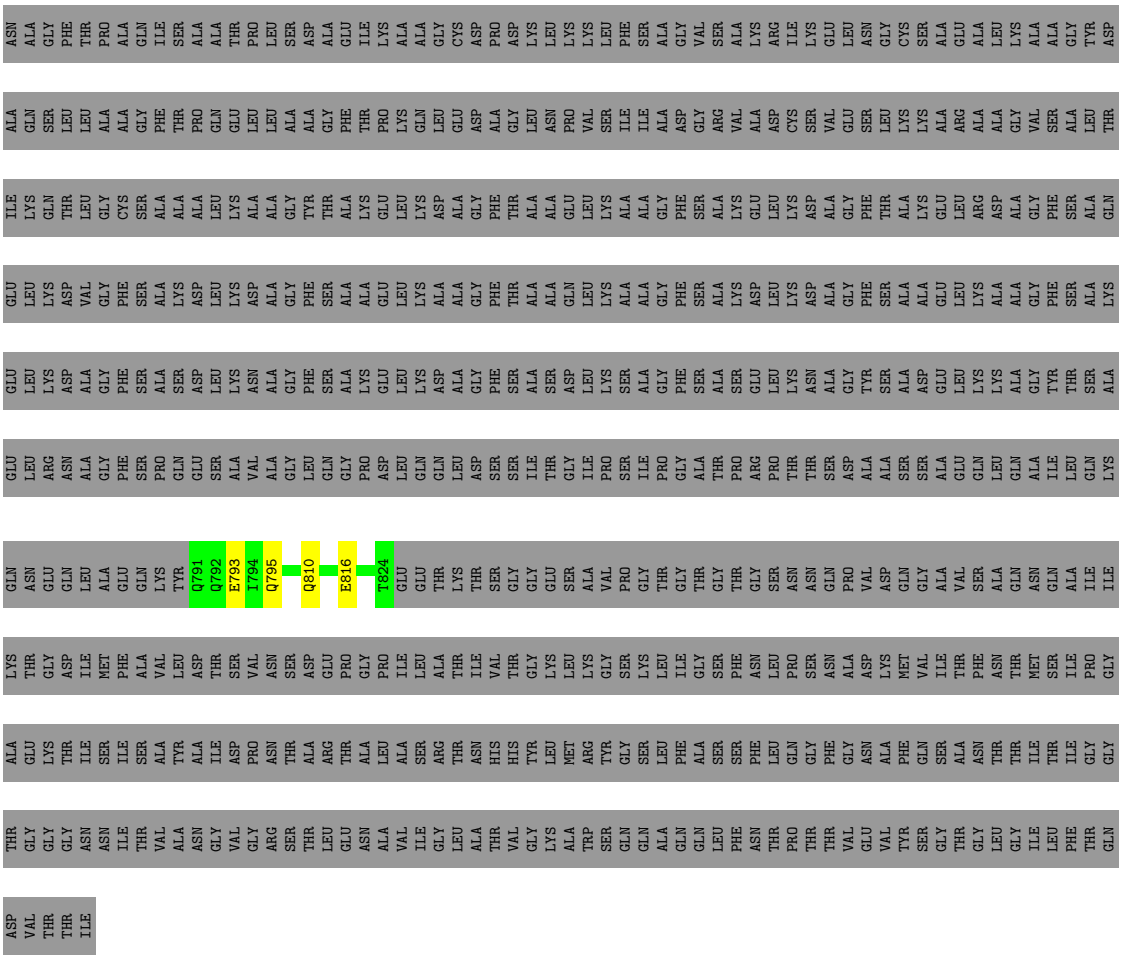




• Molecule 1: IcmE protein

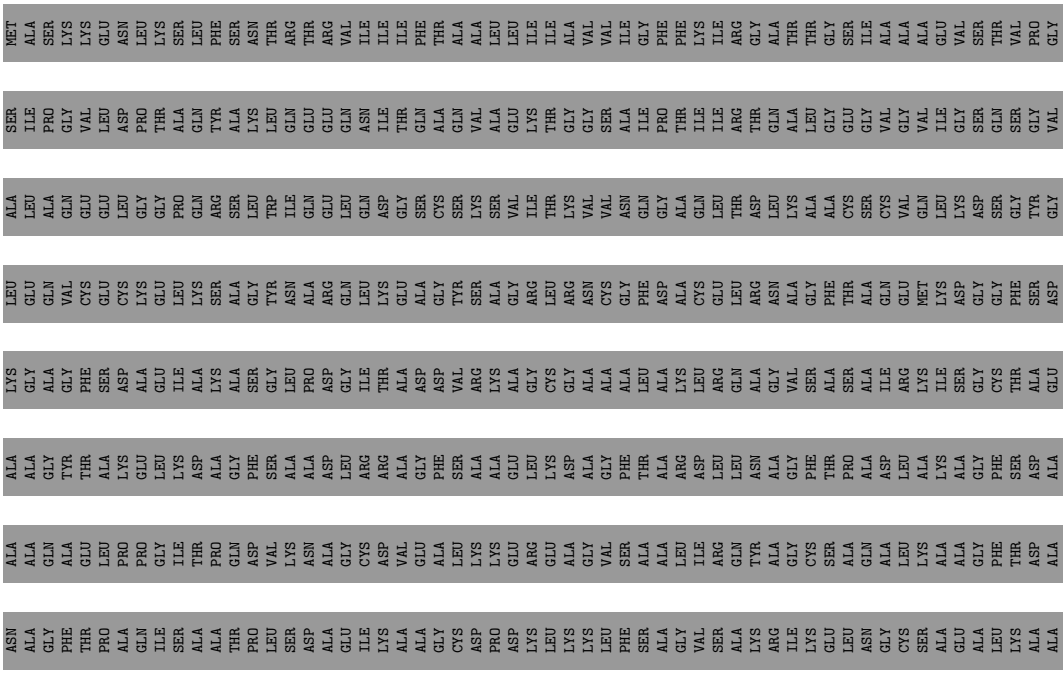
Chain YG: 97%

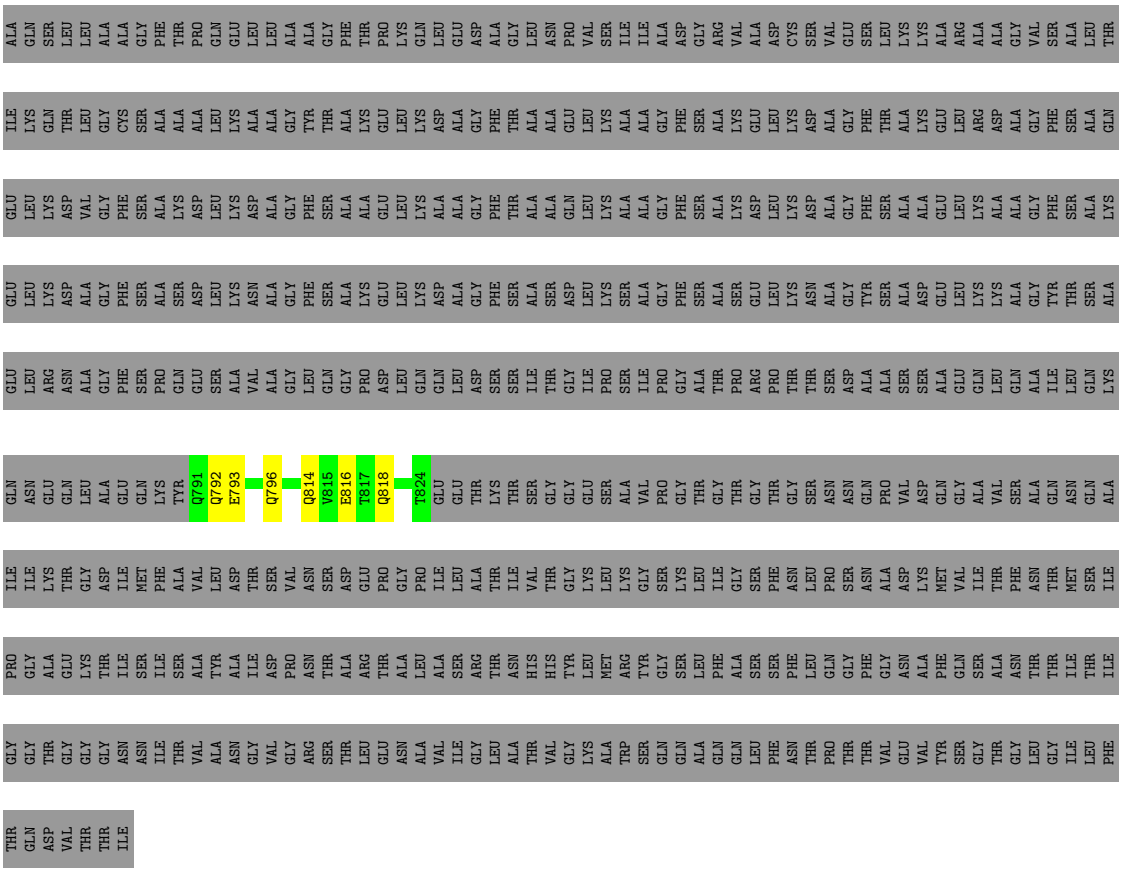




• Molecule 1: IcmE protein

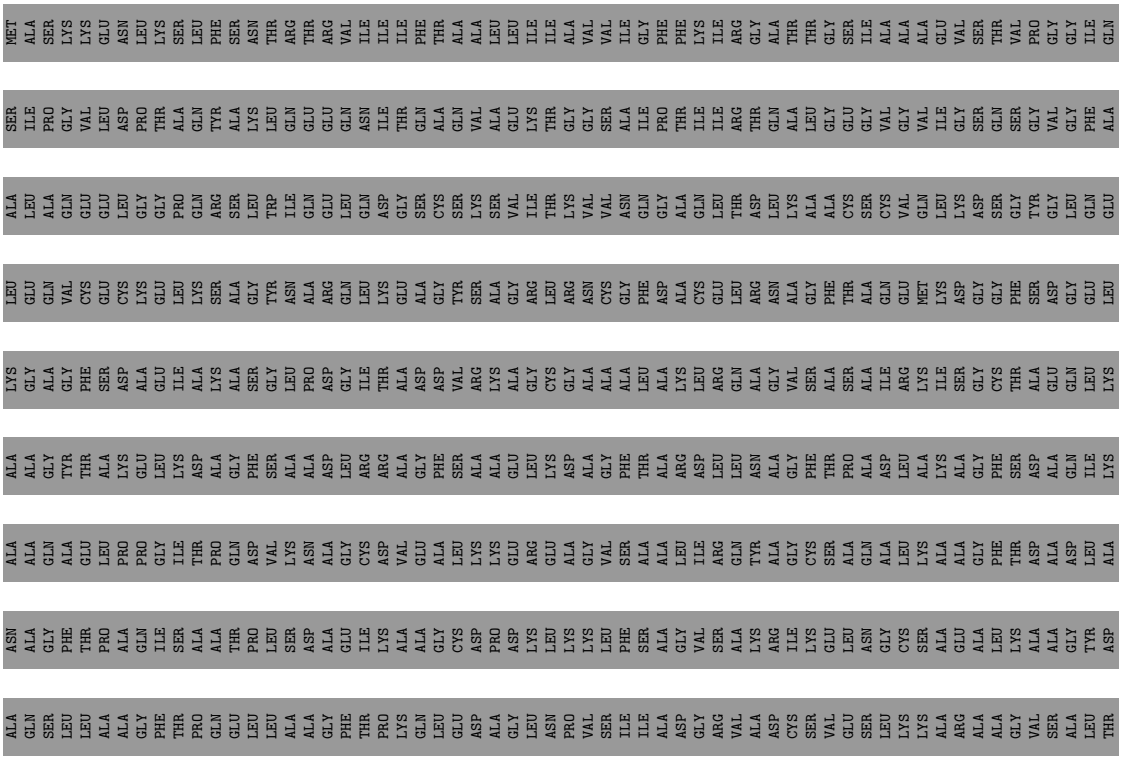
Chain ZG: 97%

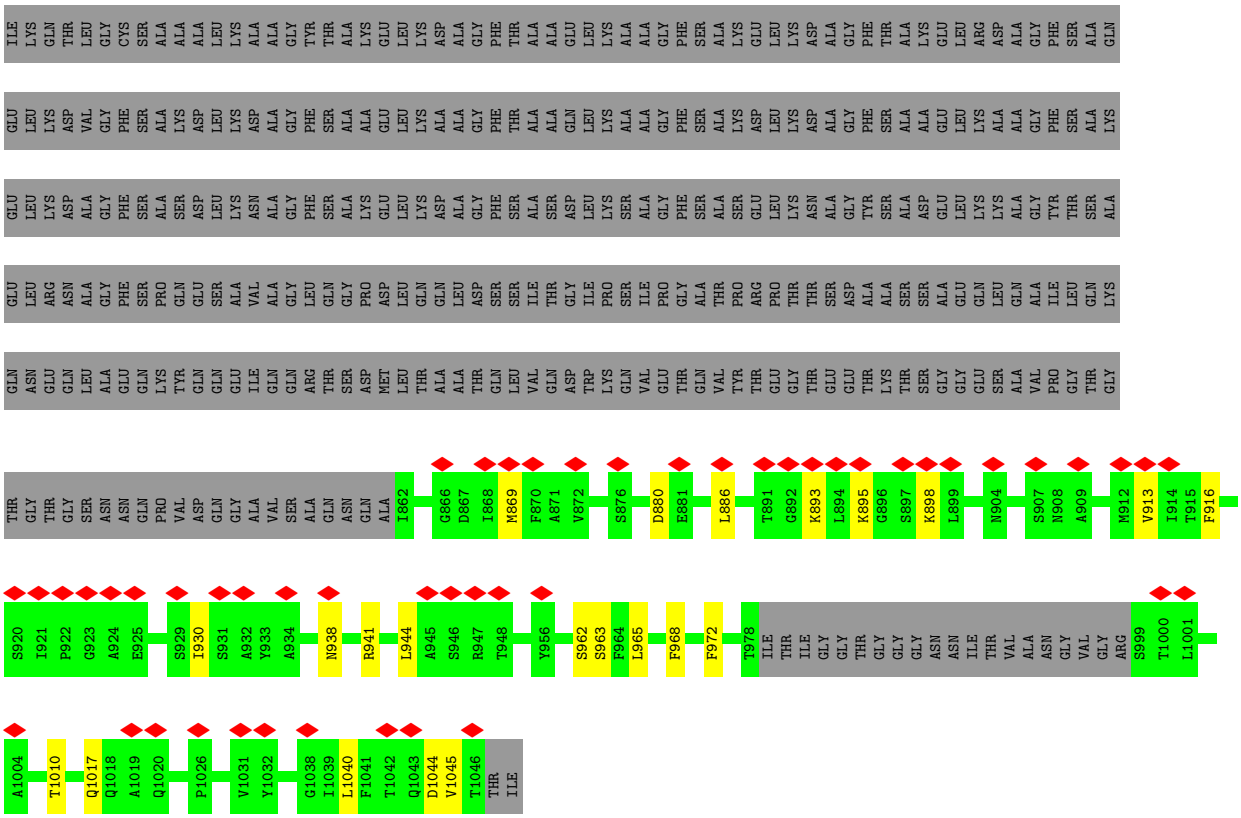




• Molecule 1: IcmE protein

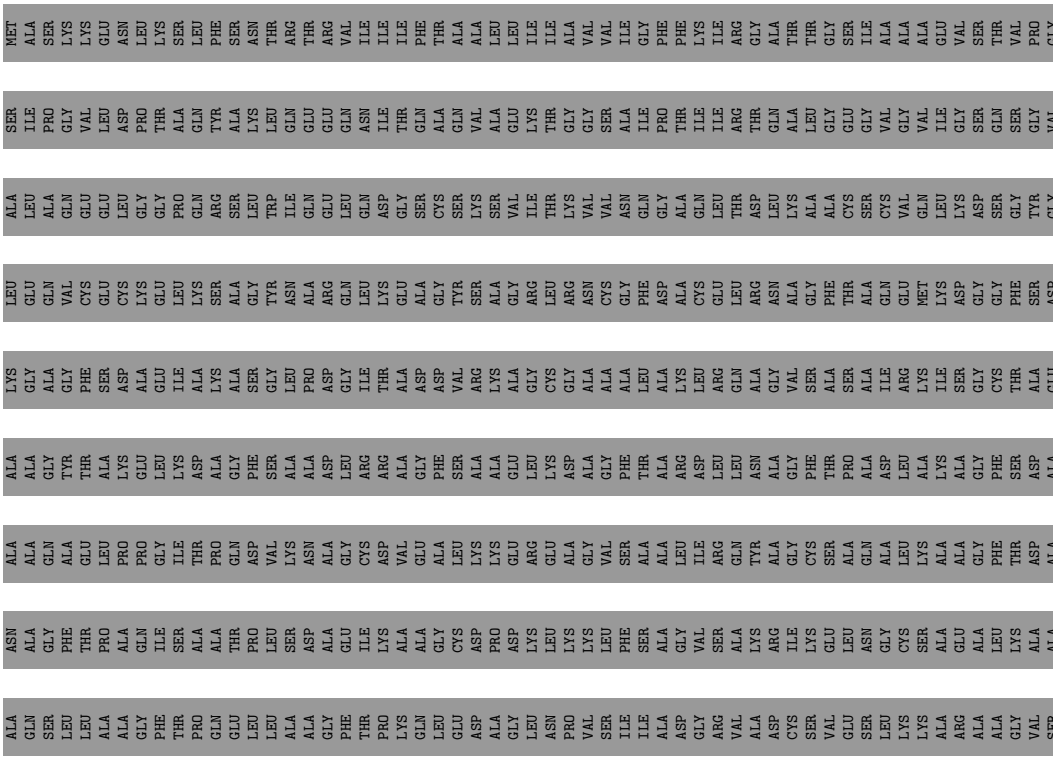
Chain FG:

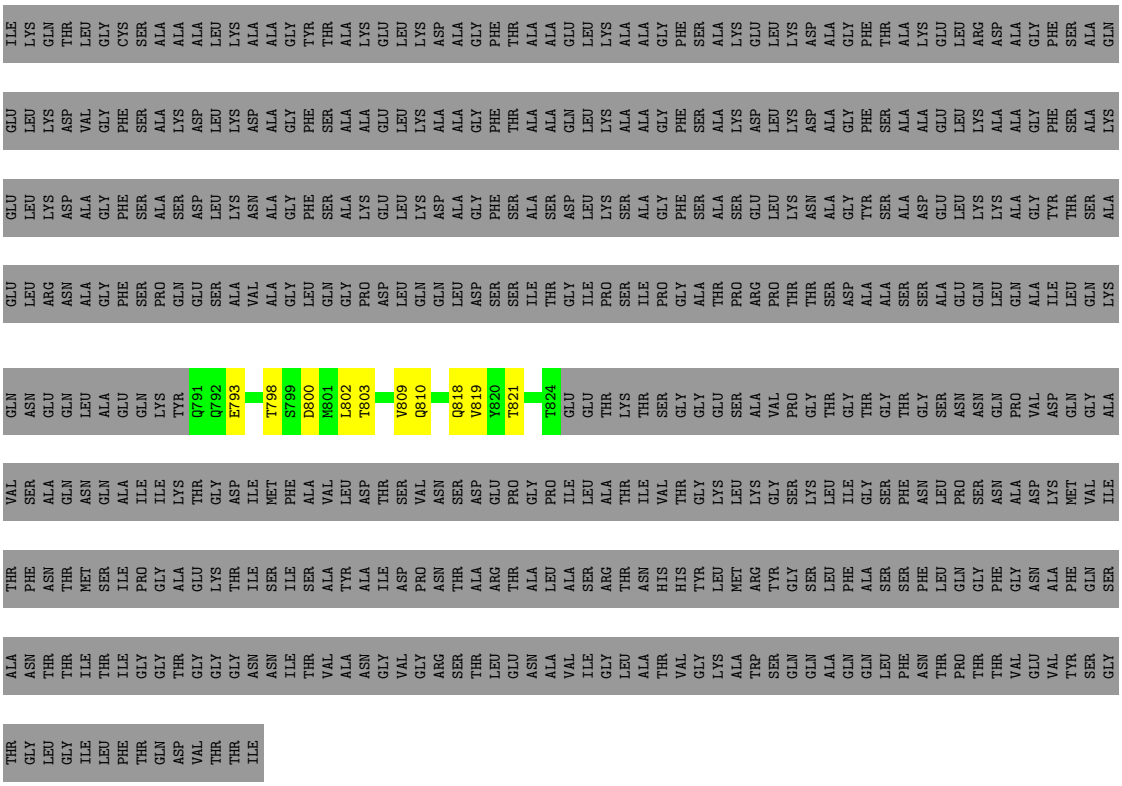




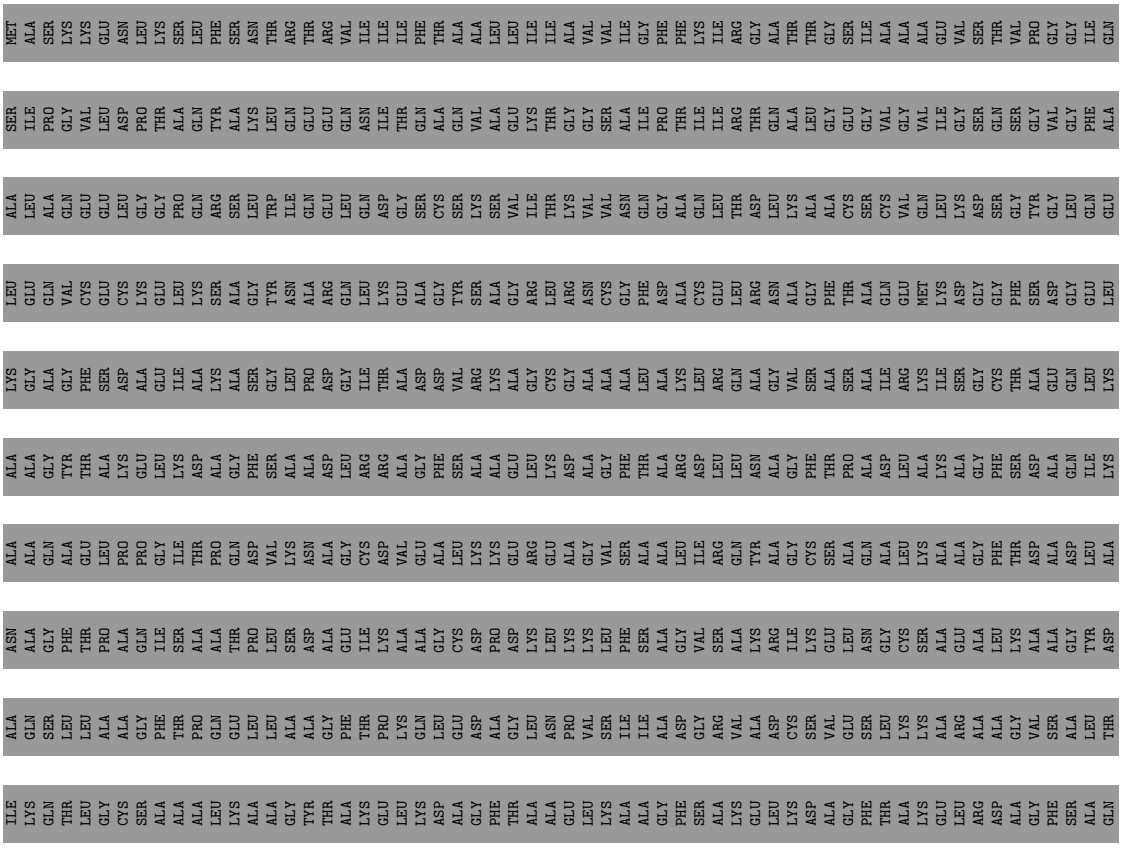
• Molecule 1: IcmE protein

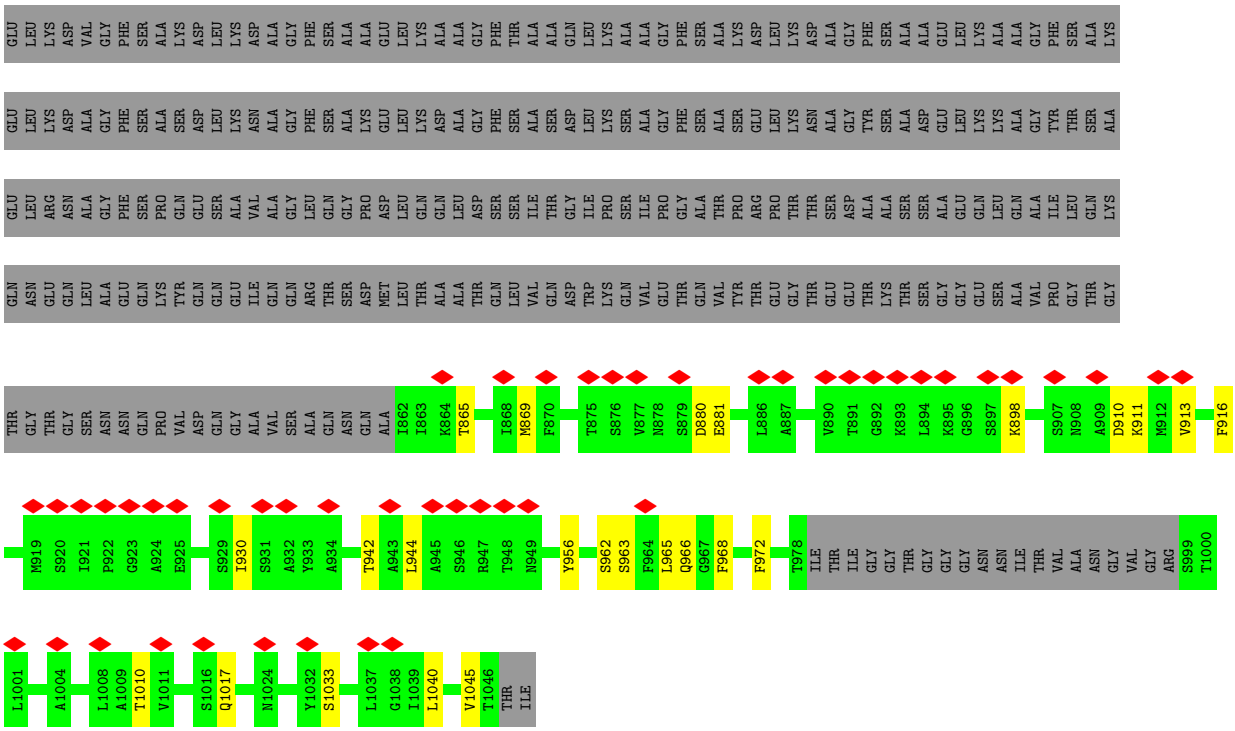
Chain Dg: 97%





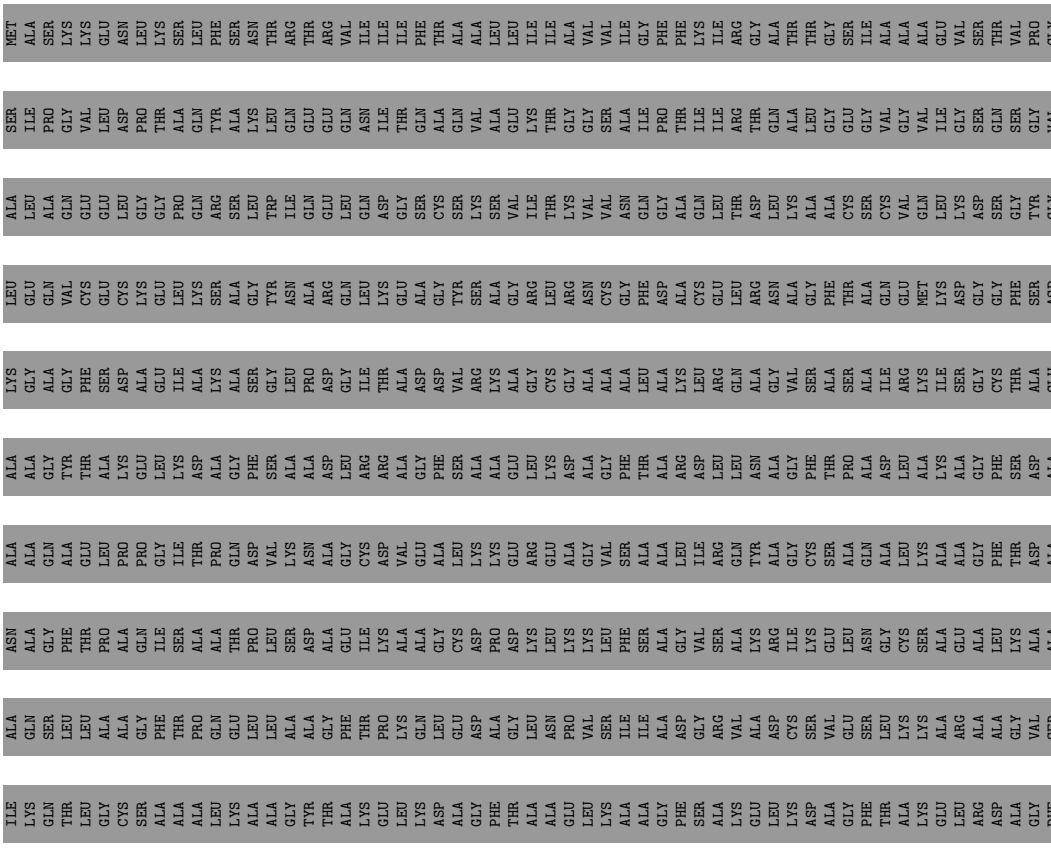
• Molecule 1: IcmE protein

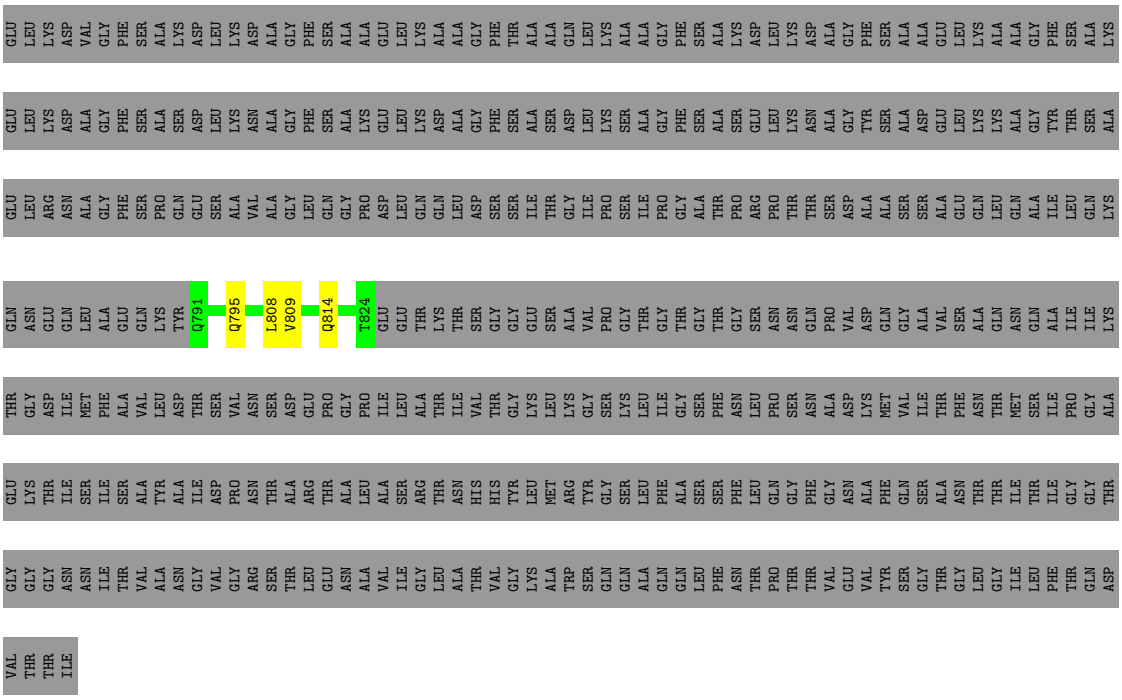




• Molecule 1: IcmE protein

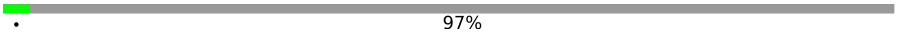
Chain Eg: 97%

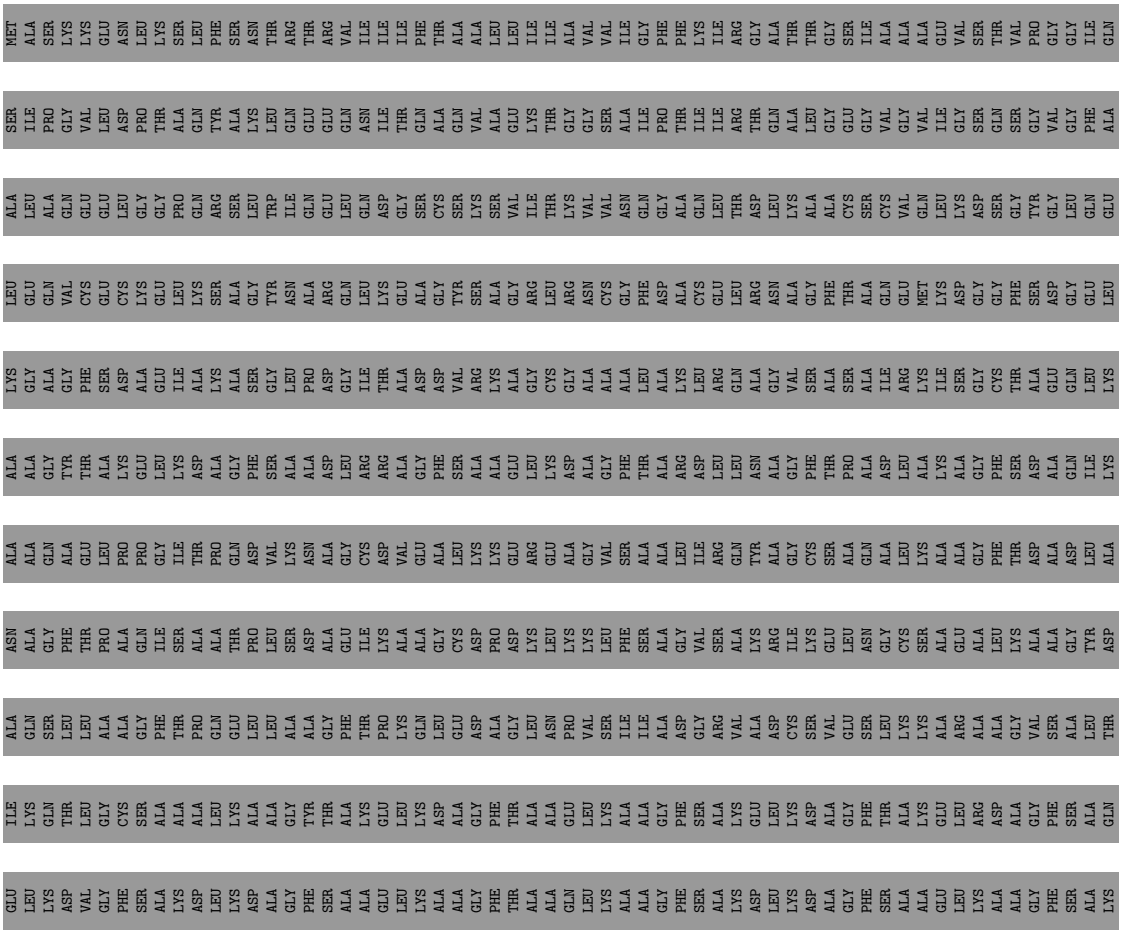


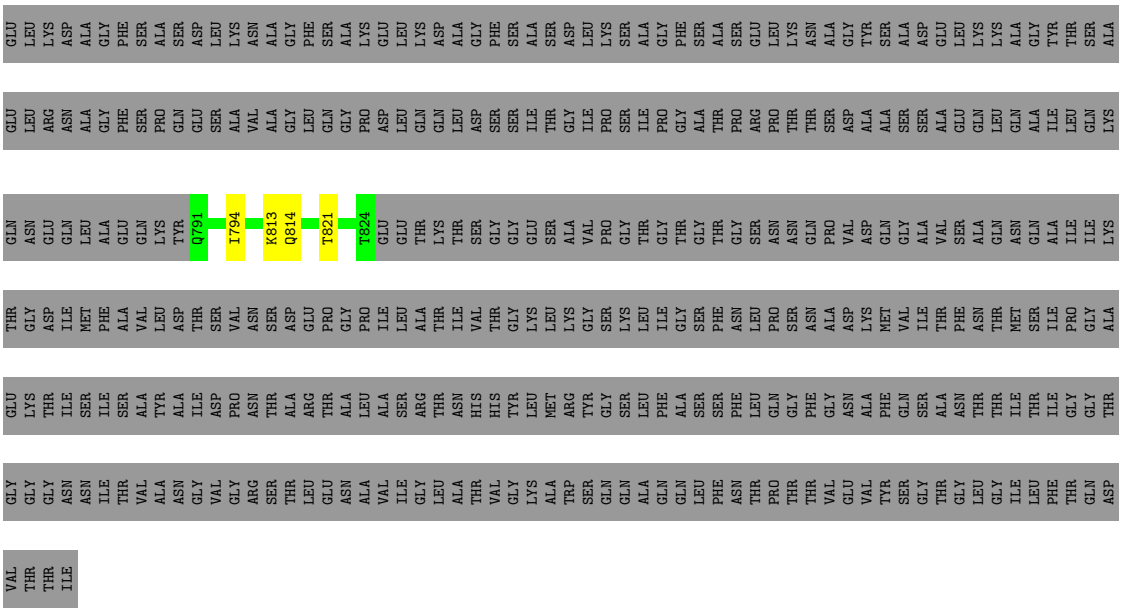


• Molecule 1: IcmE protein

Chain Fg:

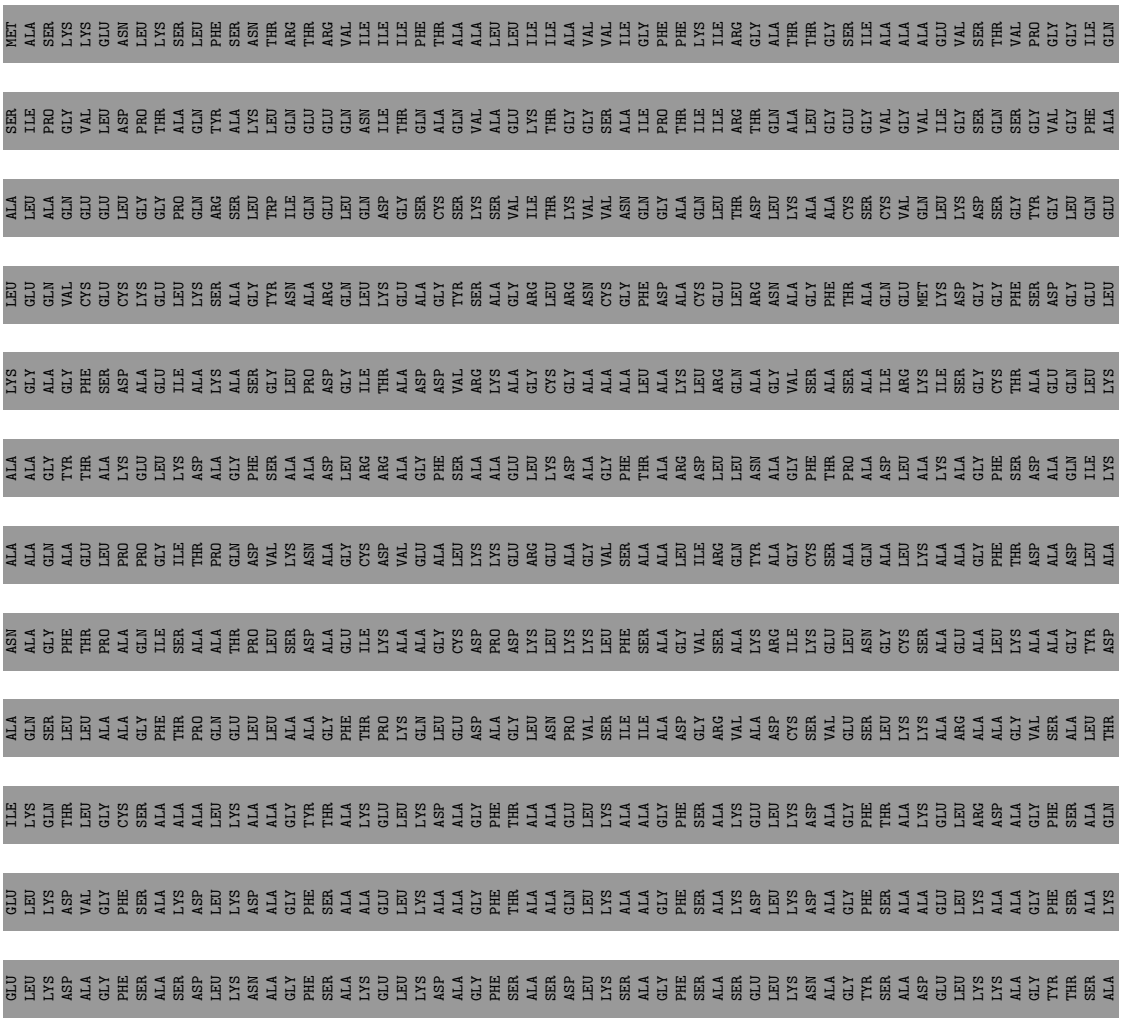






• Molecule 1: IcmE protein

Chain HG:



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

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

THR GLY THR GLY SER ASN ASN GLN PRO VAL ASP GLN GLY ALA VAL SER ALA GLN ASN GLN ALA I862 G866 D867 I868 M869 F870 A871 V872 L873 D874 T875 S876 V877 D880 I885 L886 A887 V890 T891 G892 K893 L894 K895 G896 S897 K898 L899 S902 L905 P906 S907 N908 A909

D910 V913 F916 S920 I921 P922 G923 A924 E925 S929 I930 S931 A932 Y933 A934 I935 N938 L944 A945 S946 R947 T948 L953 S962 S963 F964 L965 Q966 G967 F968 G969 N970 A971 F972 T978 ILE THR ILE GLY GLY THR GLY GLY GLY ASN ASN ILE THR VAL ALA ASN

GLY VAL GLY ARG S999 E1002 G1007 S1016 Q1021 N1024 T1025 P1026 T1027 Y1032 S1033 L1037 G1038 I1039 L1040 D1044 V1045 T1046 THR ILE

- Molecule 1: IcmE protein

Chain IG: 5% 14% • 84%

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

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

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

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

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

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

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

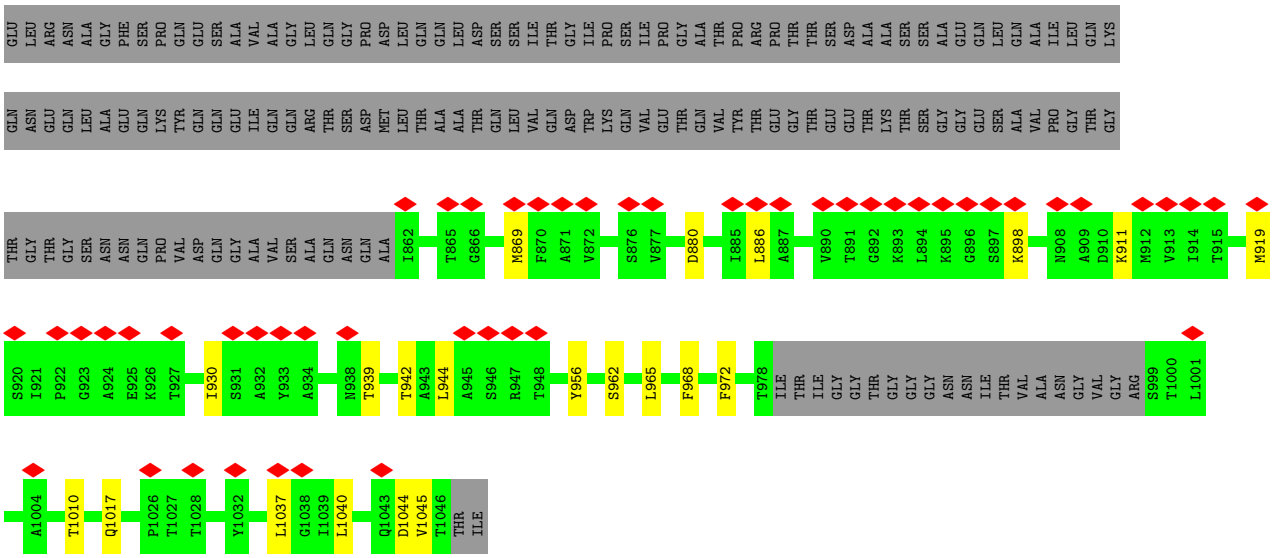
ASN ALA GLY PHE THR PRO ALA GLN ILE SER ALA ALA THR PRO LEU SER ASP ALA GLU ILE LYS ALA ALA GLY CYS ASP PRO ASP LYS LEU LYS LYS LEU PHE SER ALA GLY VAL SER ALA LYS ARG ILE LYS GLU LEU ASN GLY CYS SER ALA GLU GLU ALA LEU LYS ALA ALA GLY TYR ASP

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

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

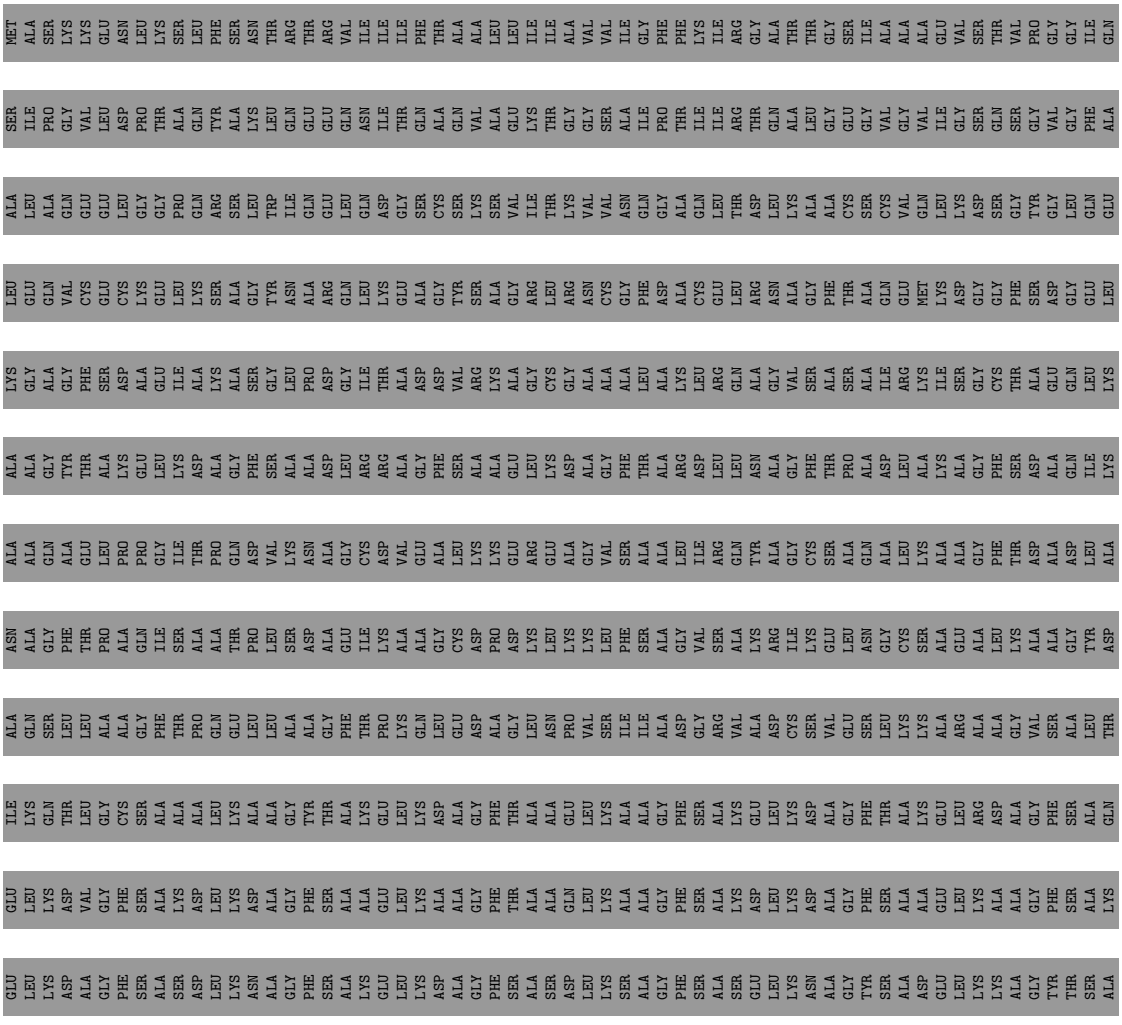
GLU LEU LYS ASP VAL GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA ALA GLU LEU LYS ALA ALA GLY PHE THR ALA ALA GLN LEU LYS ALA ALA GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS

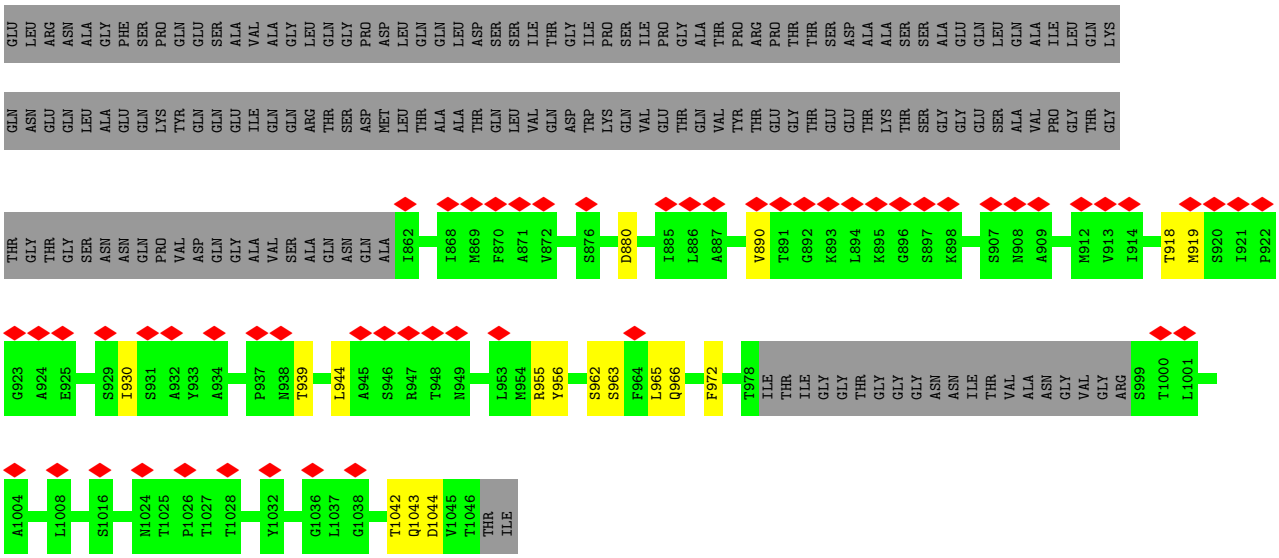
GLU LEU LYS ASP ALA GLY PHE SER ALA SER ASP LEU LYS ASN ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA SER ASP LEU LYS SER ALA GLY PHE SER ALA SER GLU LEU LYS ASN ALA GLY TYR SER ALA ASP GLU LEU LYS LYS ALA GLY TYR THR SER ALA



• Molecule 1: IcmE protein

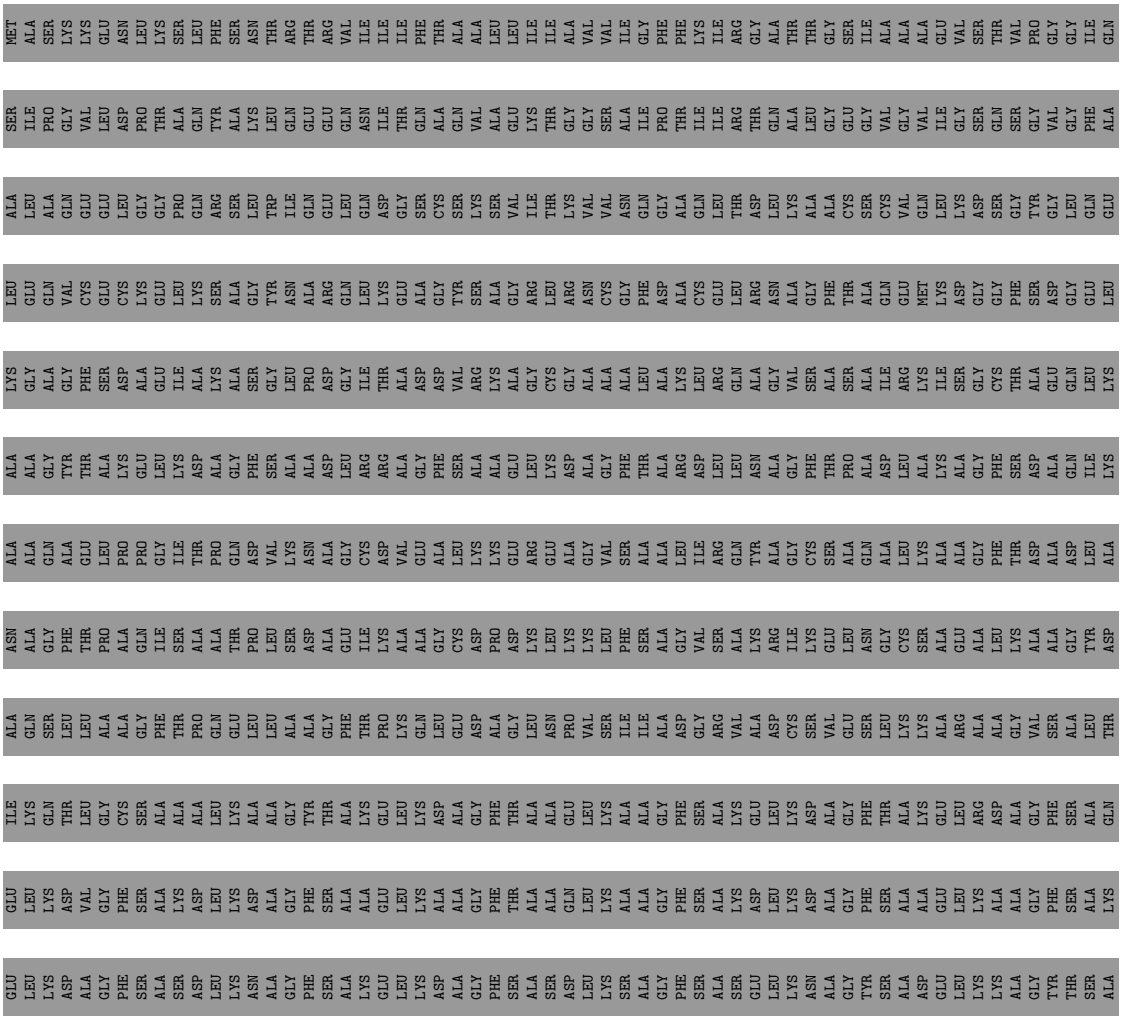
Chain JG:

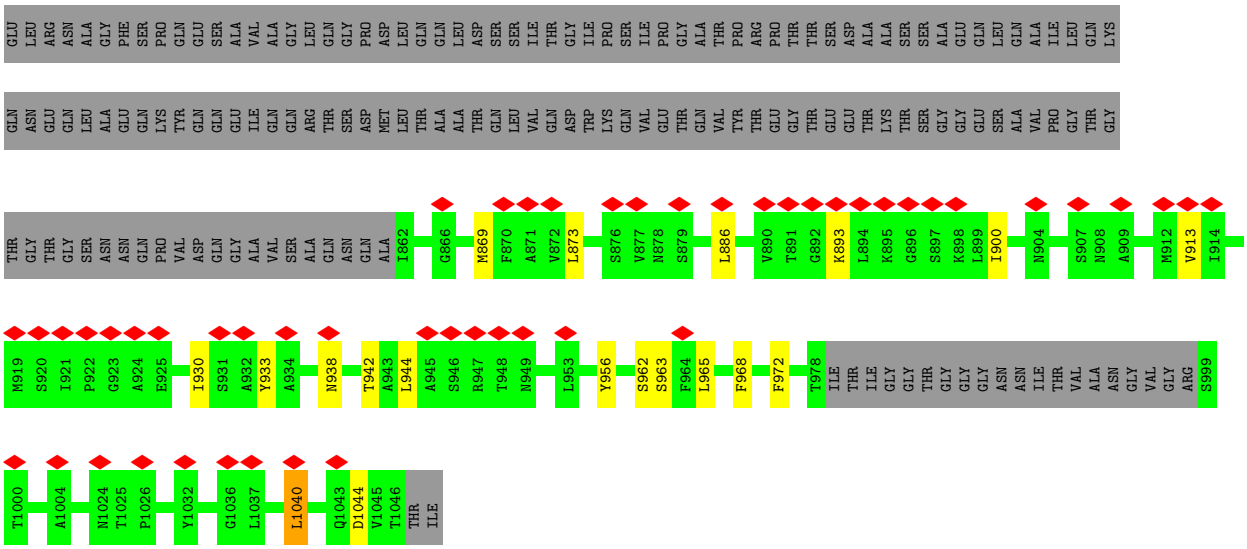




• Molecule 1: IcmE protein

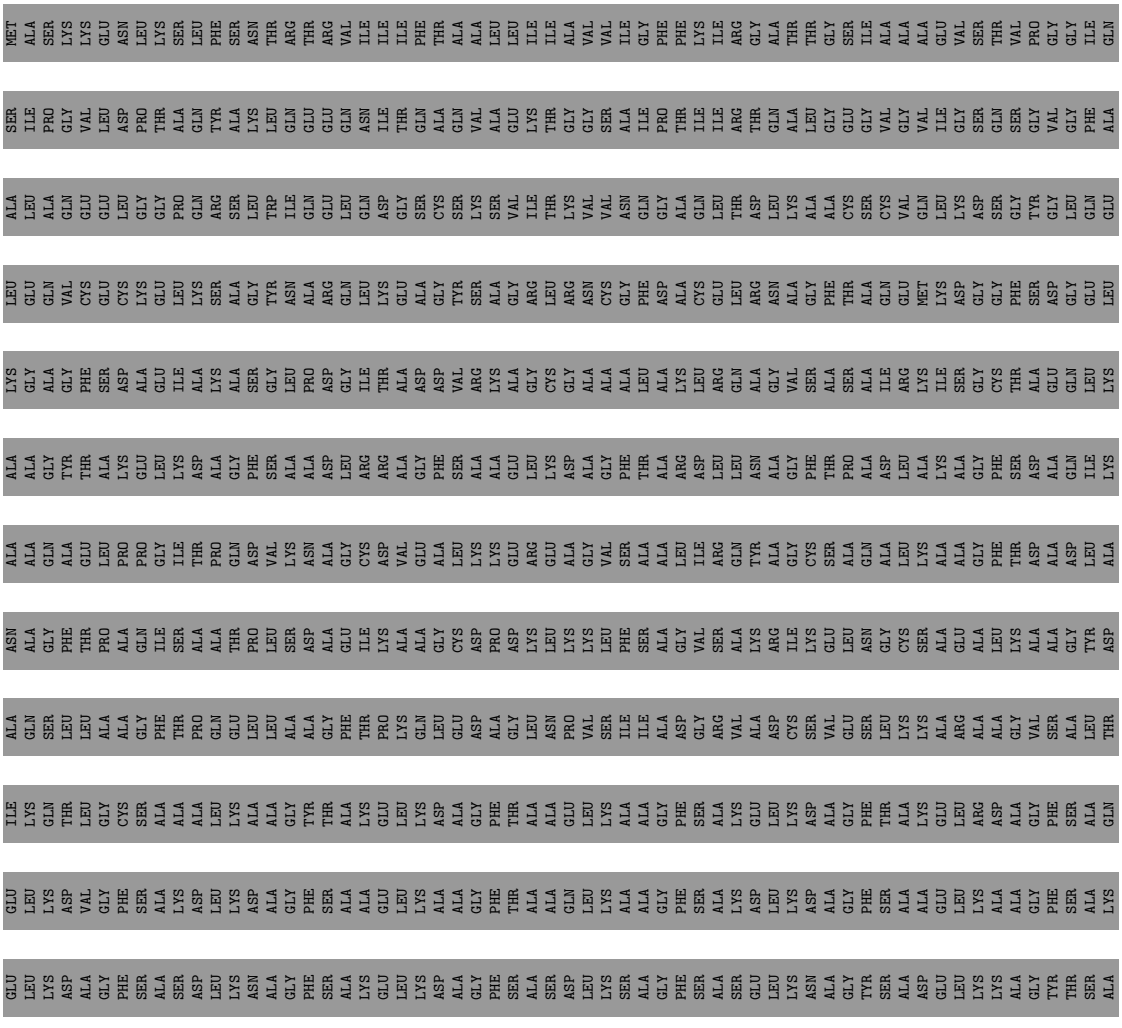
Chain KG:

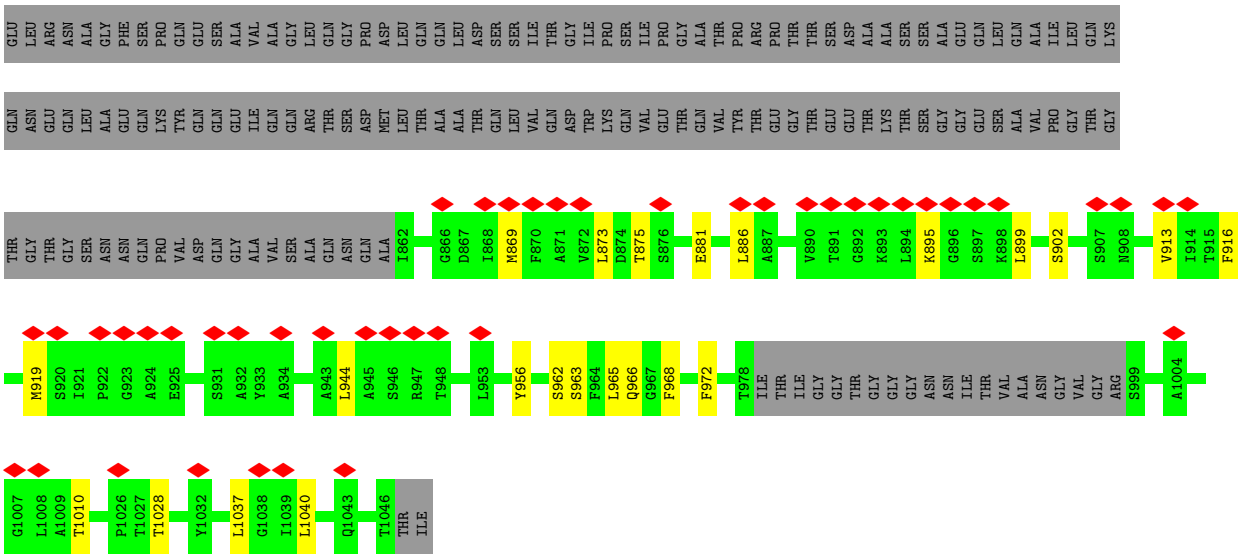


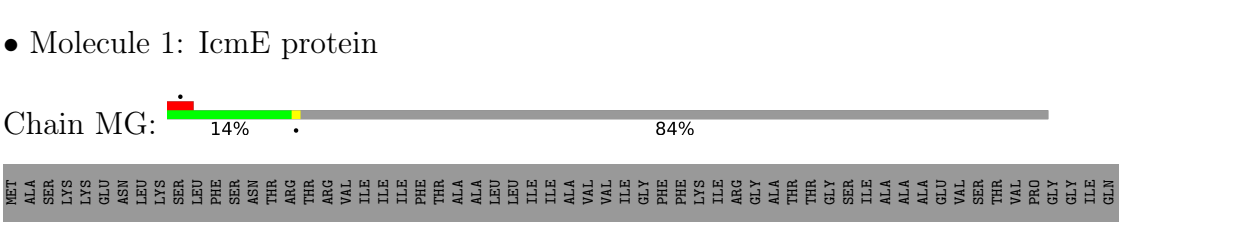


• Molecule 1: IcmE protein

Chain LG:

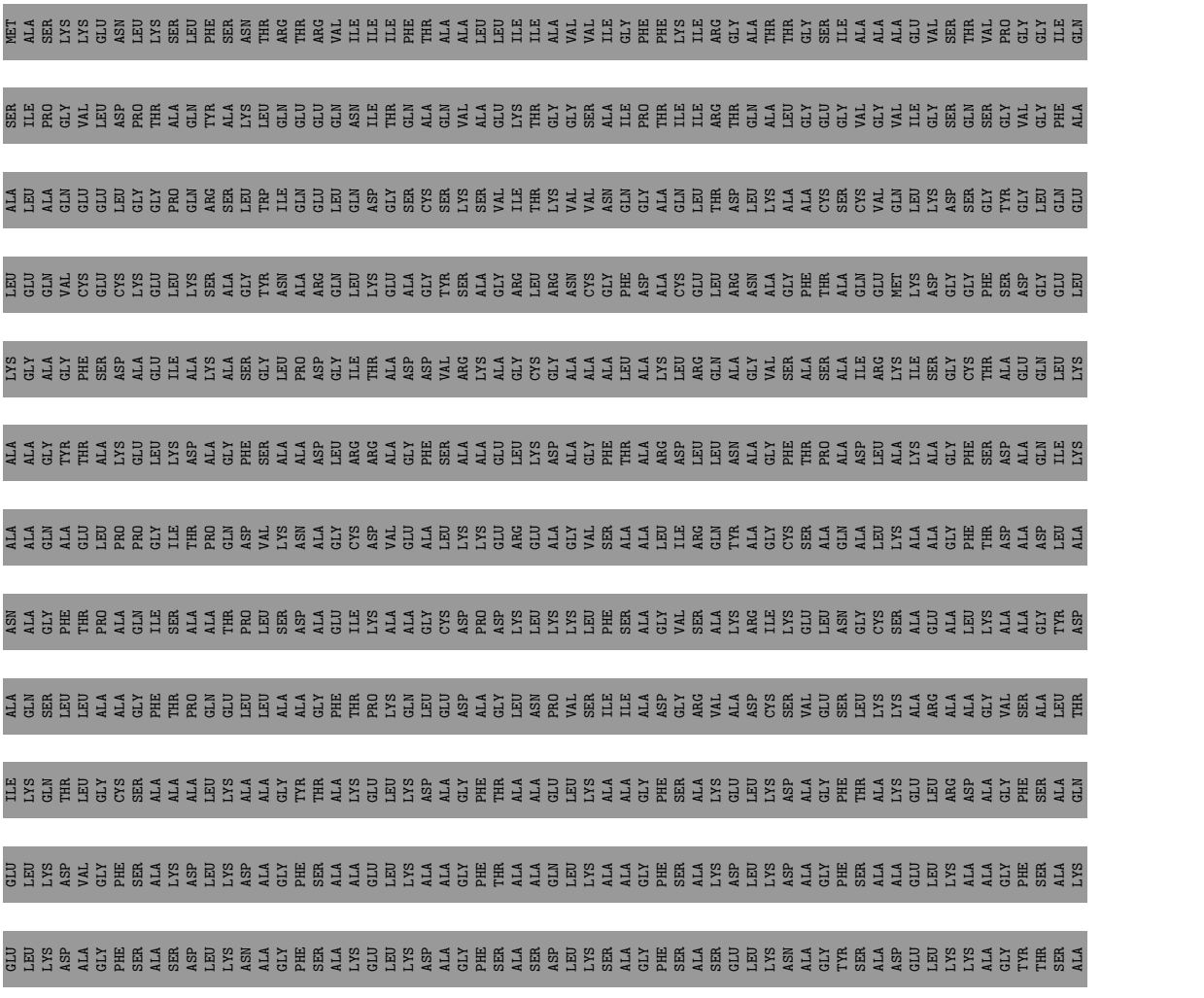


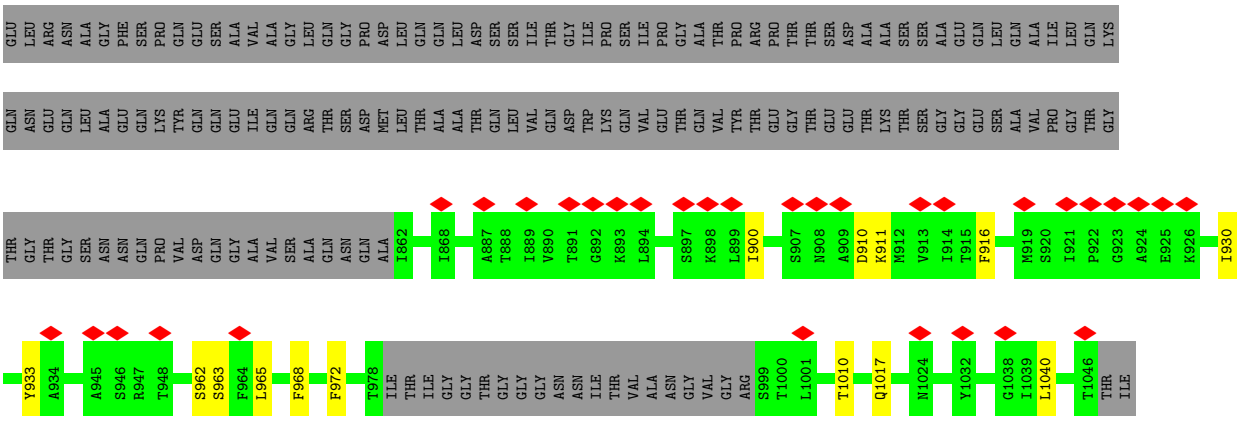




• Molecule 1: IcmE protein

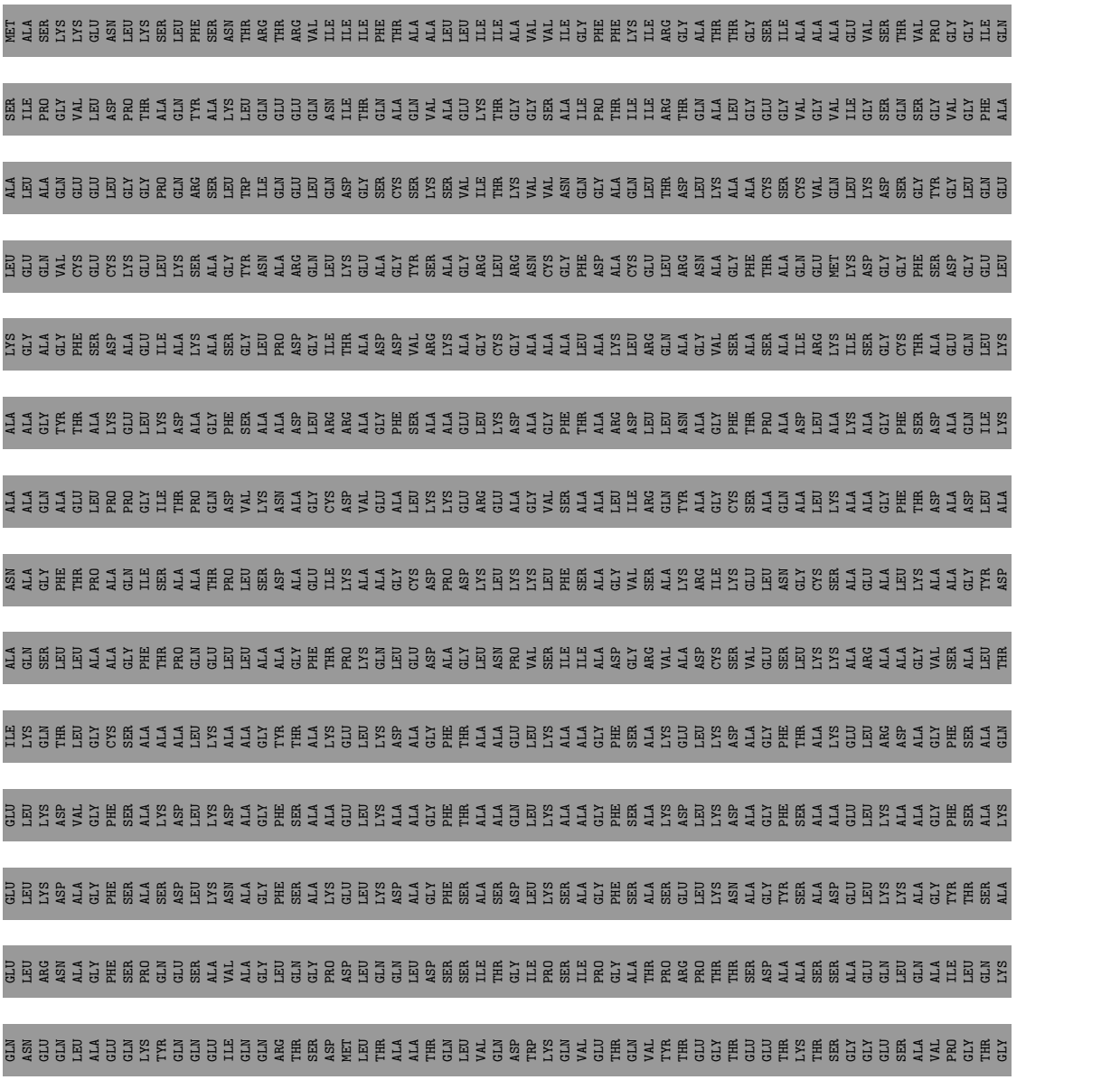
Chain MG:

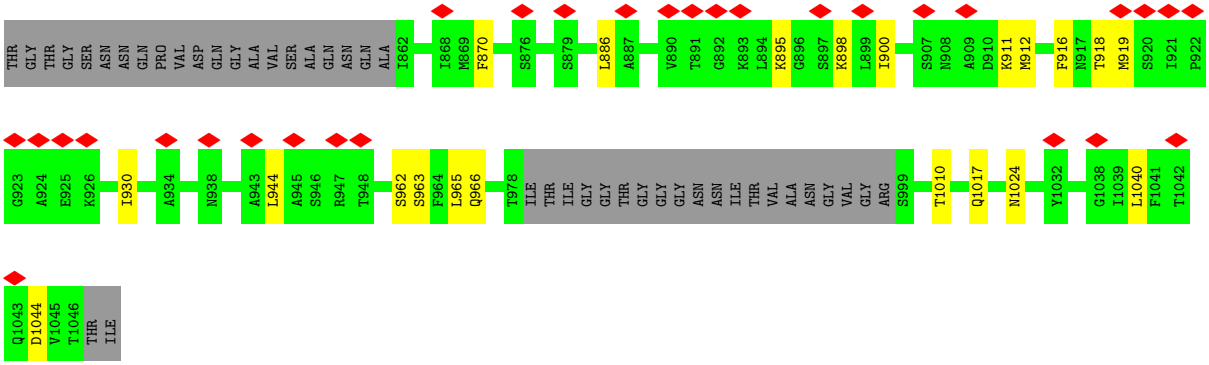




• Molecule 1: IcmE protein

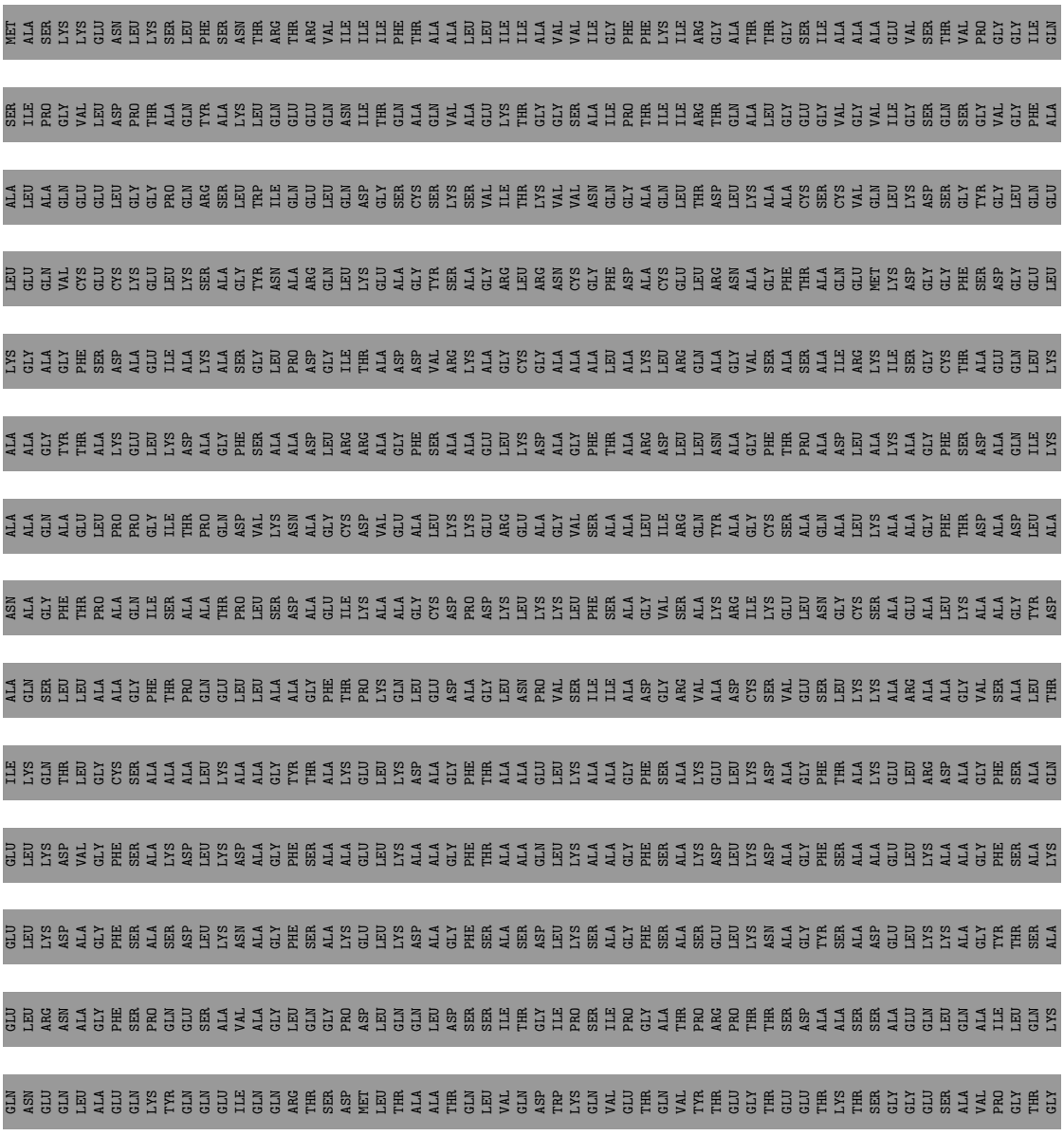
Chain NG:

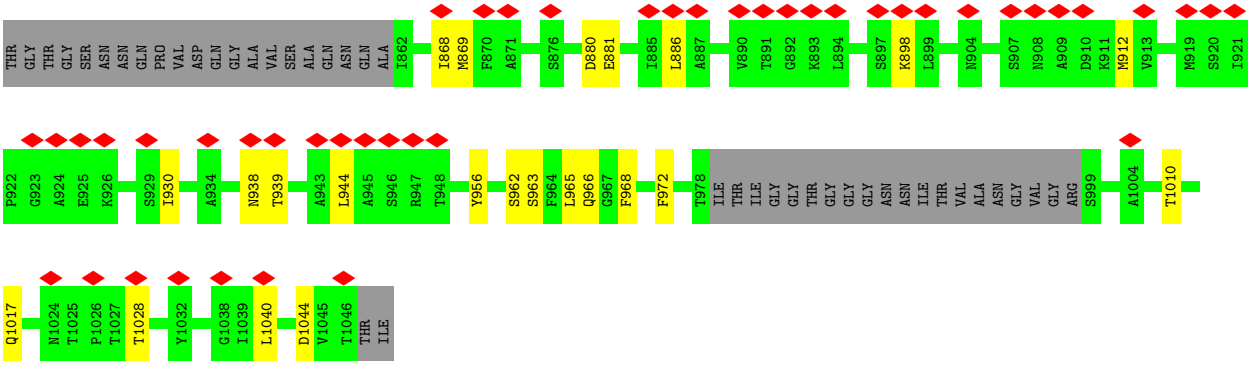




• Molecule 1: IcmE protein

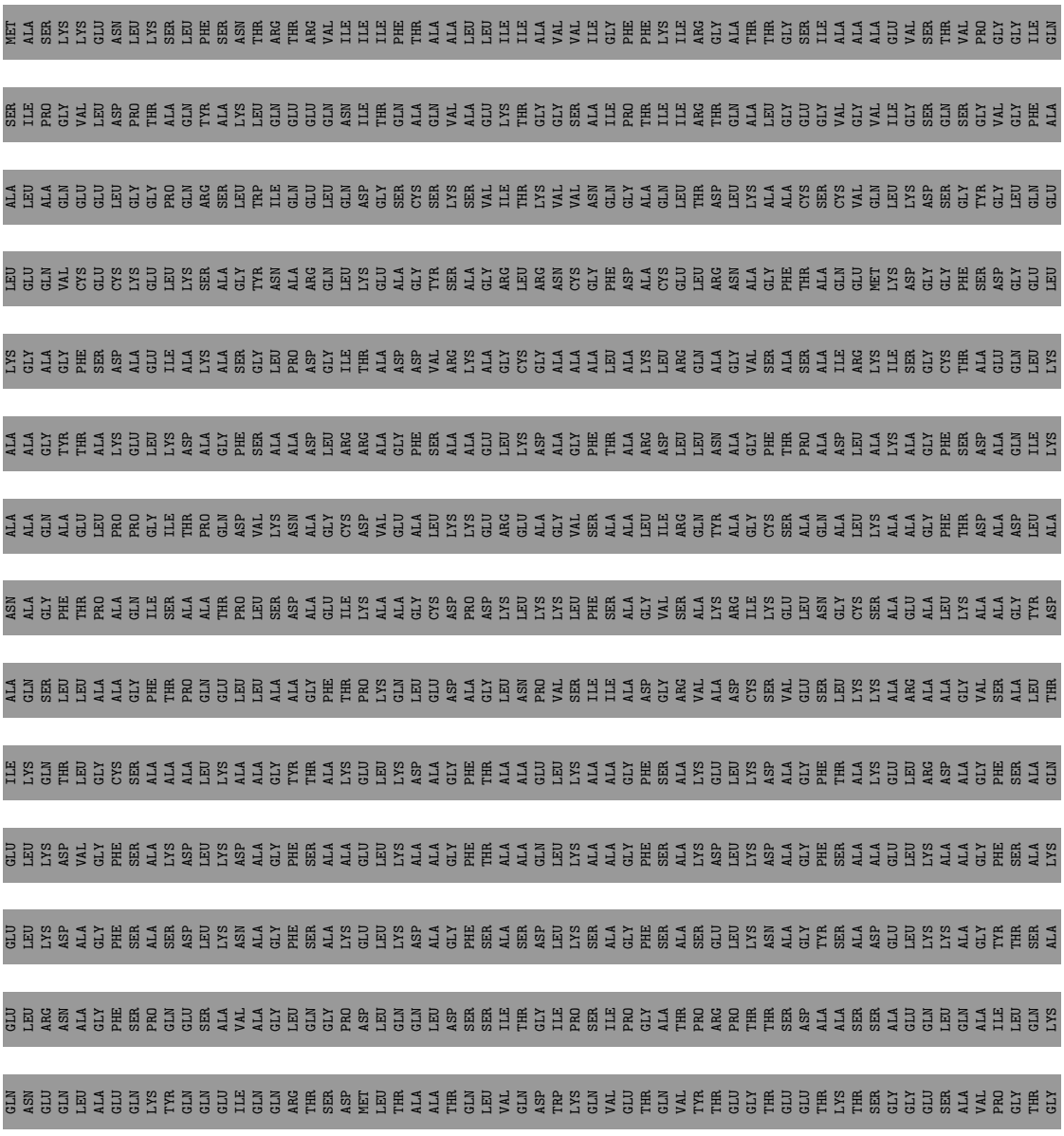
Chain OG:

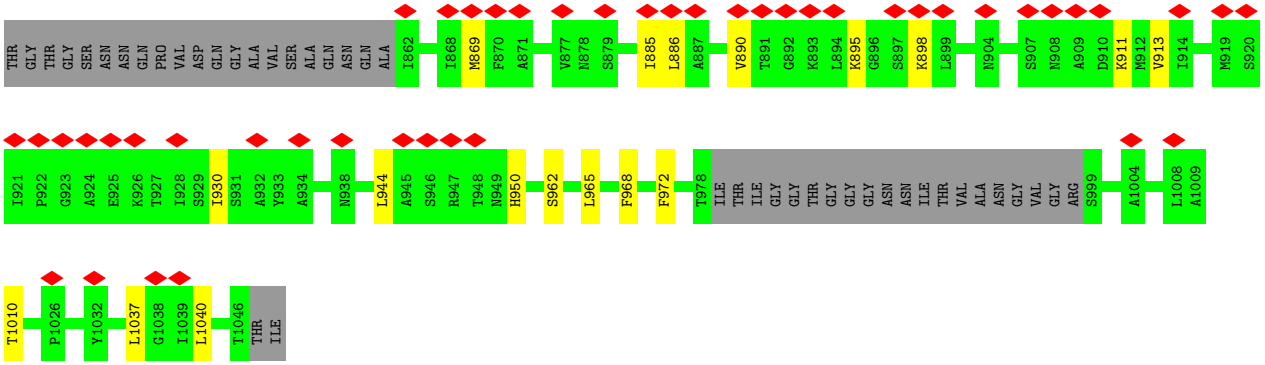




- Molecule 1: IcmE protein

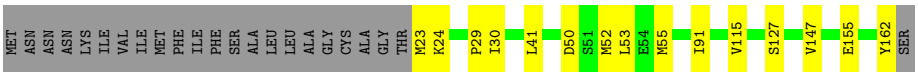
Chain PG: 14% 84%





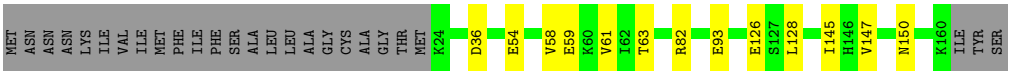
• Molecule 2: DotD

Chain GD:



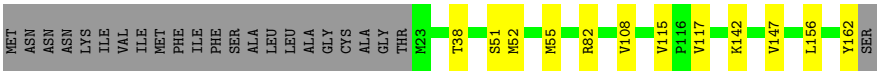
• Molecule 2: DotD

Chain Gd:



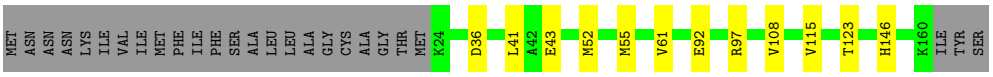
• Molecule 2: DotD

Chain HD:



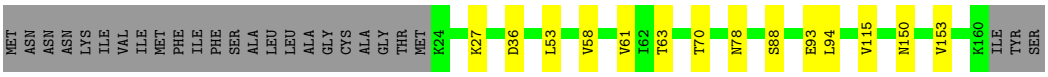
• Molecule 2: DotD

Chain Dd:



• Molecule 2: DotD

Chain Hd:

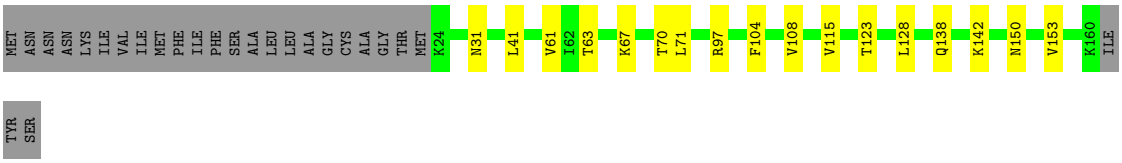


• Molecule 2: DotD

Chain ID:

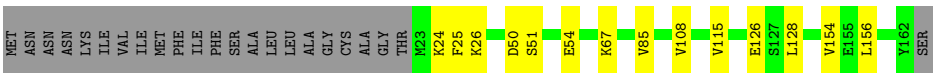
• Molecule 2: DotD

Chain Id:



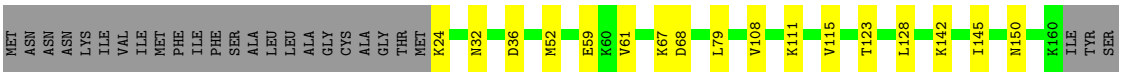
• Molecule 2: DotD

Chain JD:



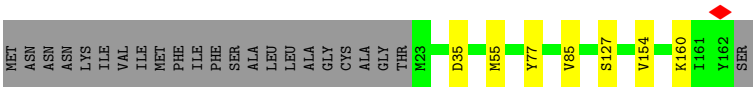
• Molecule 2: DotD

Chain Jd:



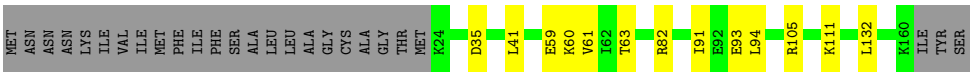
• Molecule 2: DotD

Chain KD:



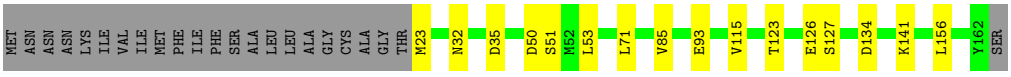
• Molecule 2: DotD

Chain Kd:



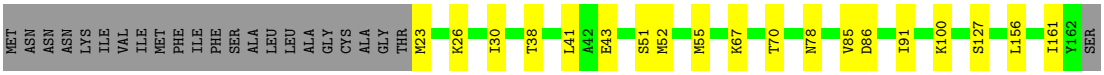
• Molecule 2: DotD

Chain LD:



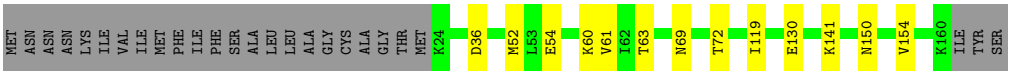
• Molecule 2: DotD

Chain CD:



• Molecule 2: DotD

Chain Ld:

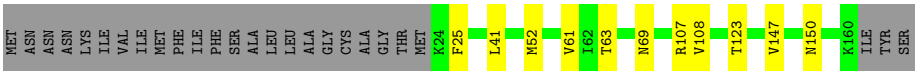


• Molecule 2: DotD

Chain MD:

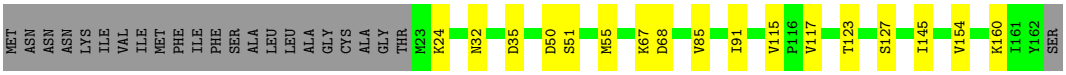
• Molecule 2: DotD

Chain Md:



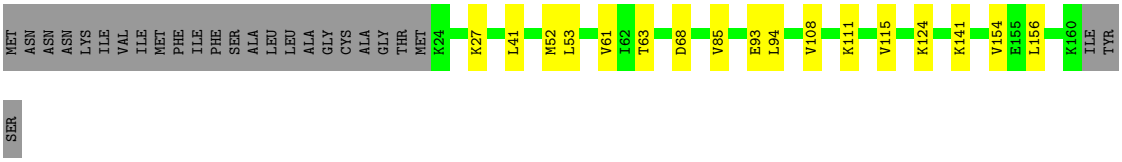
• Molecule 2: DotD

Chain AD:



• Molecule 2: DotD

Chain Ad:

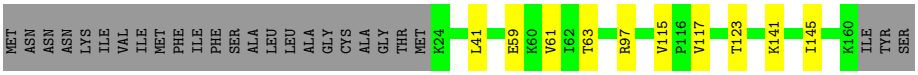


• Molecule 2: DotD

Chain BD:

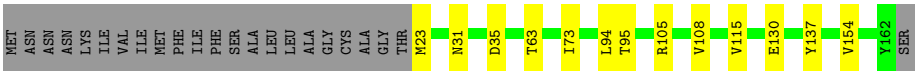
• Molecule 2: DotD

Chain Bd:



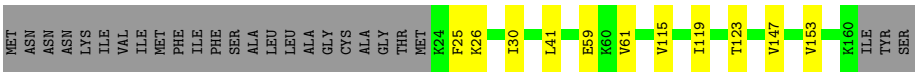
• Molecule 2: DotD

Chain ED:



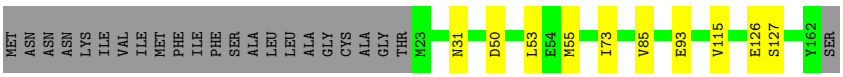
• Molecule 2: DotD

Chain Cd:



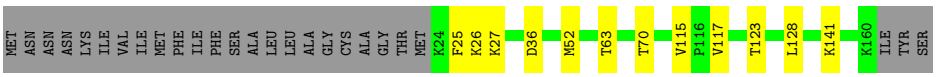
• Molecule 2: DotD

Chain DD:



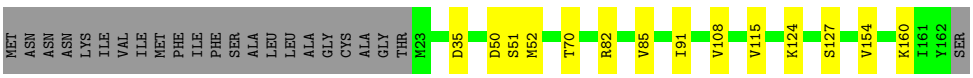
• Molecule 2: DotD

Chain Ed:



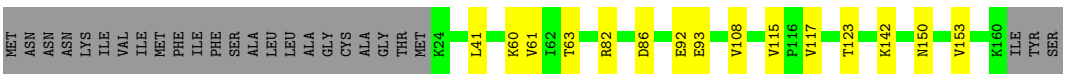
• Molecule 2: DotD

Chain FD:



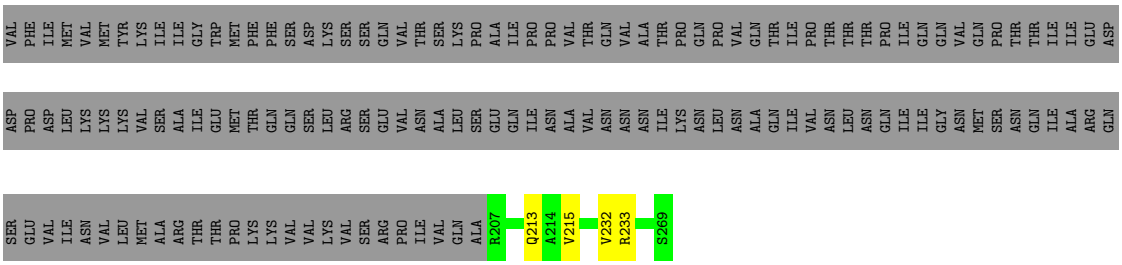
• Molecule 2: DotD

Chain Fd:



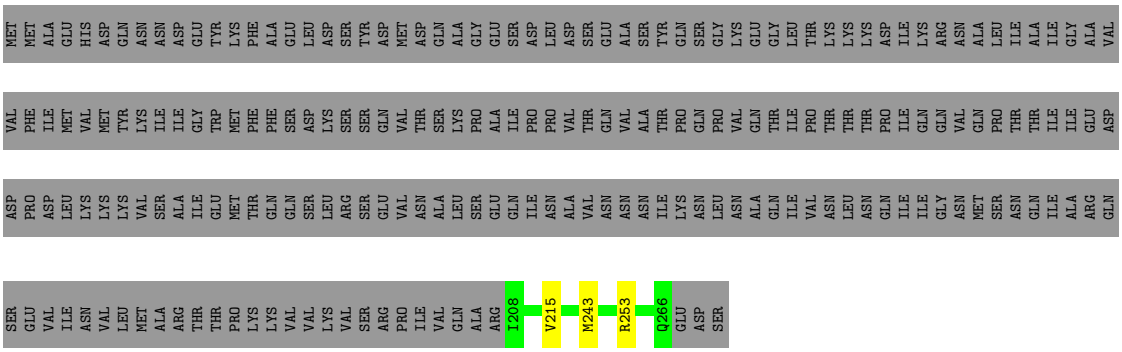
• Molecule 3: DotF

Chain GF:



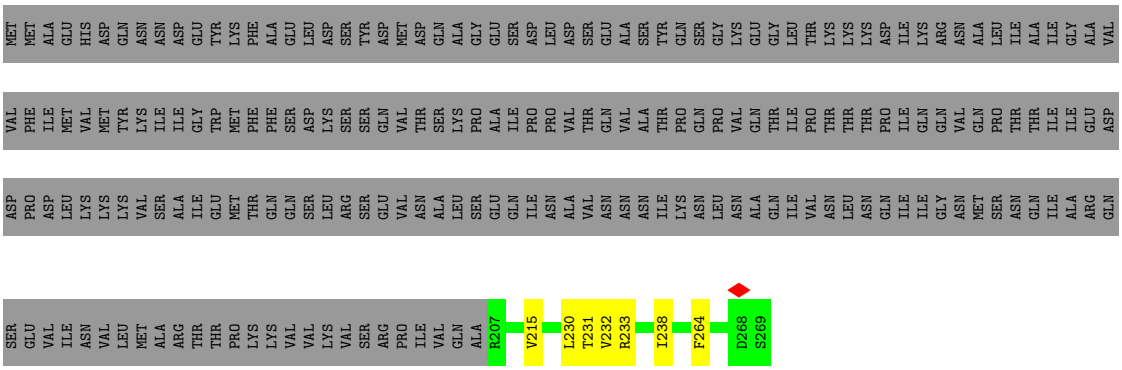
• Molecule 3: DotF

Chain Gf:



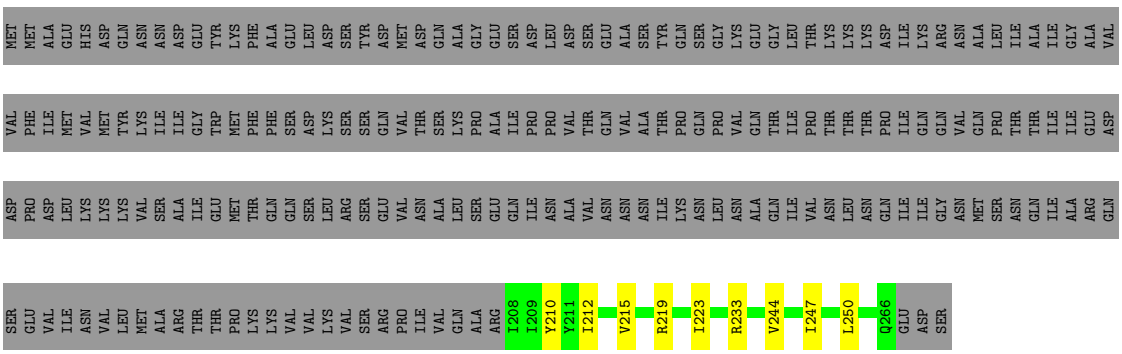
• Molecule 3: DotF

Chain HF:



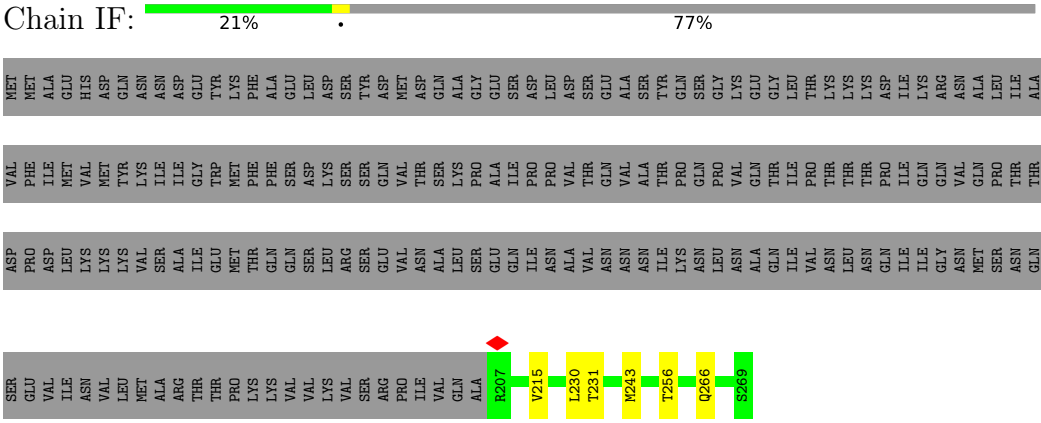
• Molecule 3: DotF

Chain Hf:



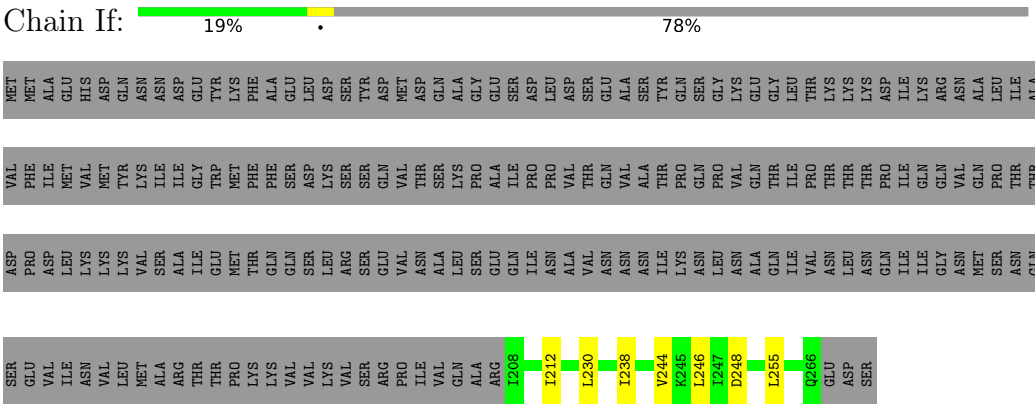
• Molecule 3: DotF

Chain IF:



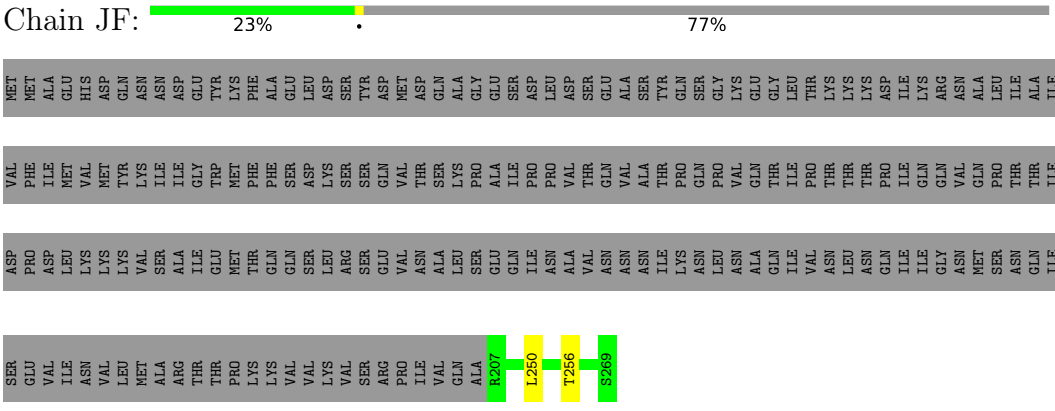
• Molecule 3: DotF

Chain If:



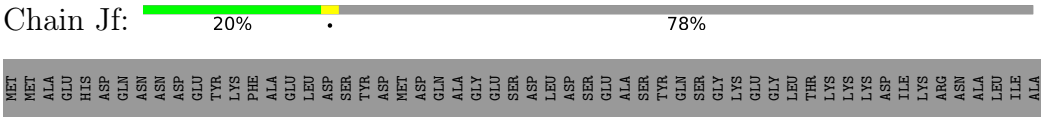
• Molecule 3: DotF

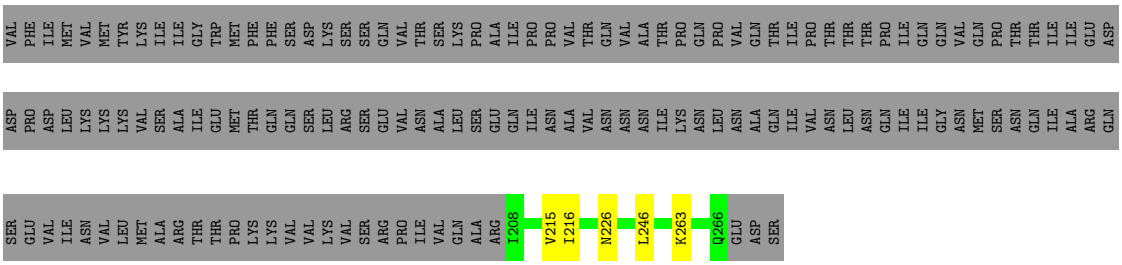
Chain JF:



• Molecule 3: DotF

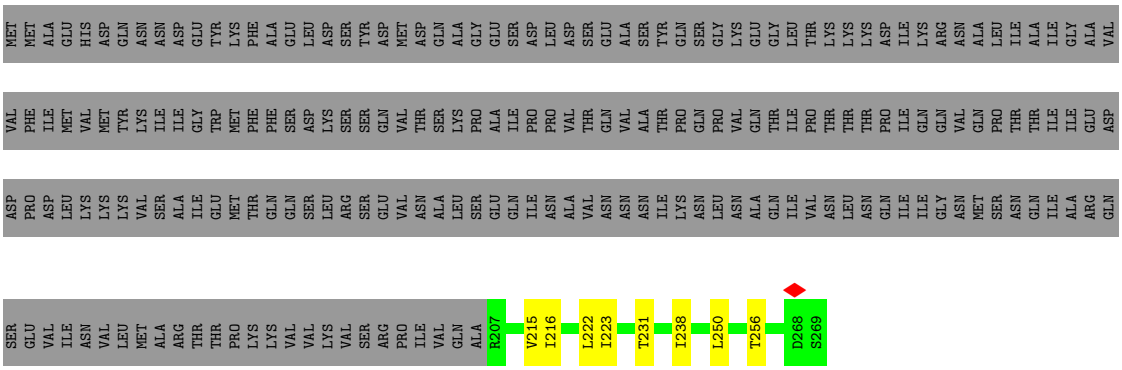
Chain Jf:





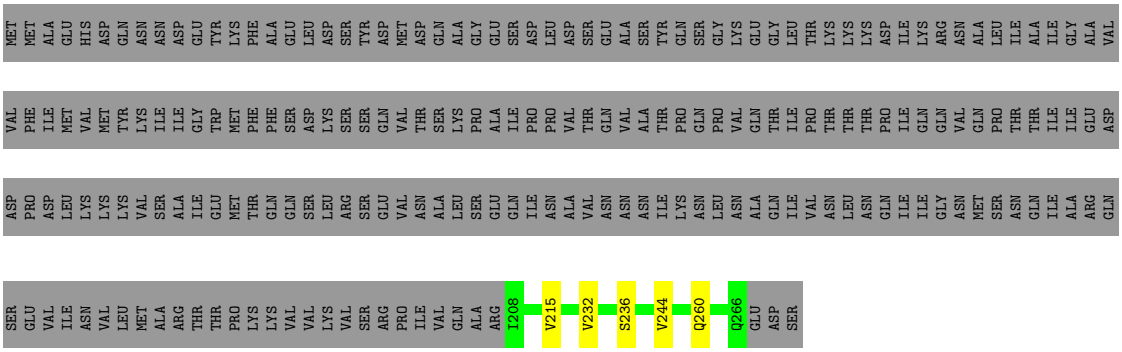
• Molecule 3: DotF

Chain KF:



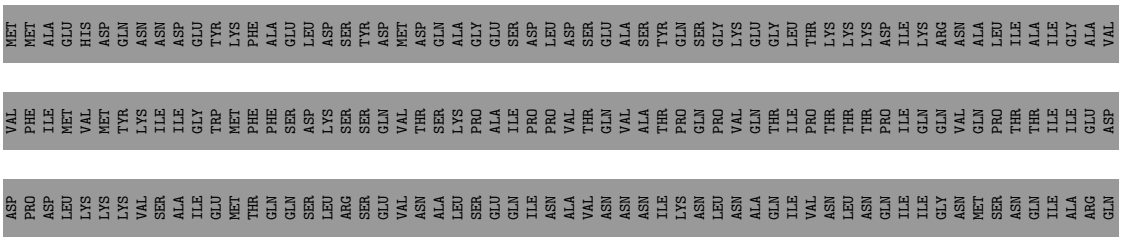
• Molecule 3: DotF

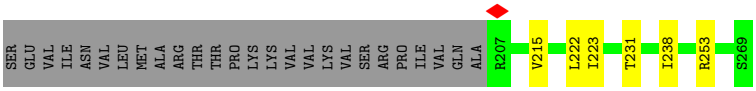
Chain Kf:



• Molecule 3: DotF

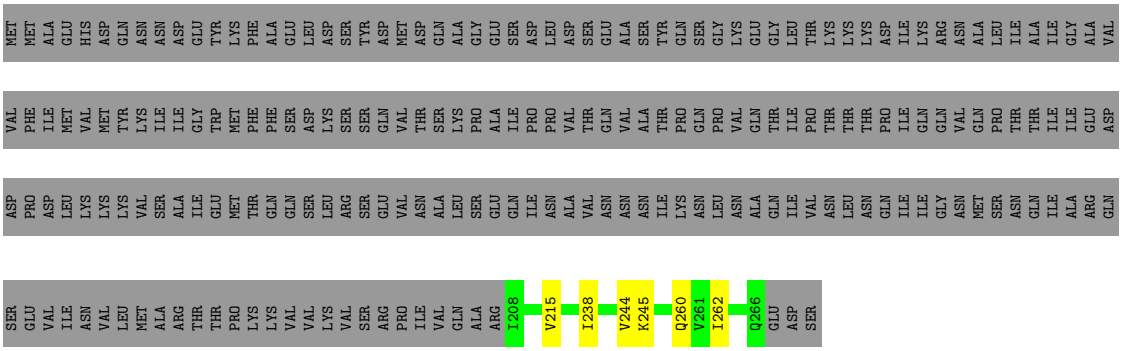
Chain LF:





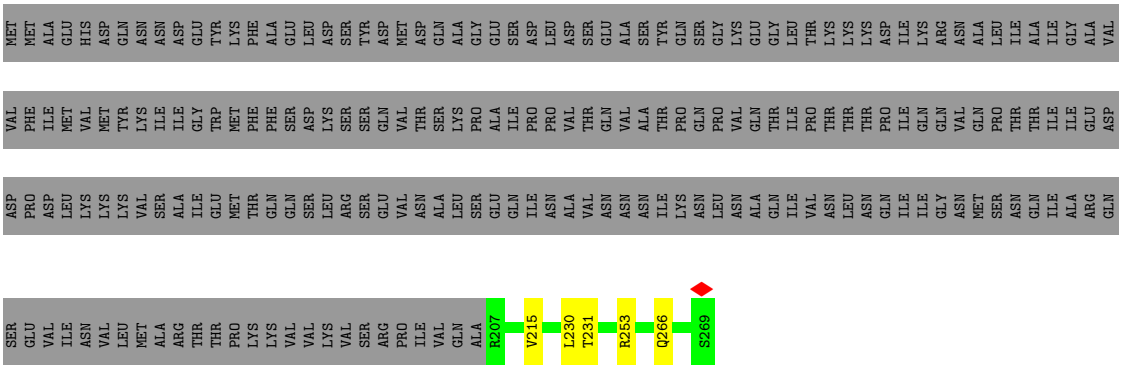
• Molecule 3: DotF

Chain Lf:



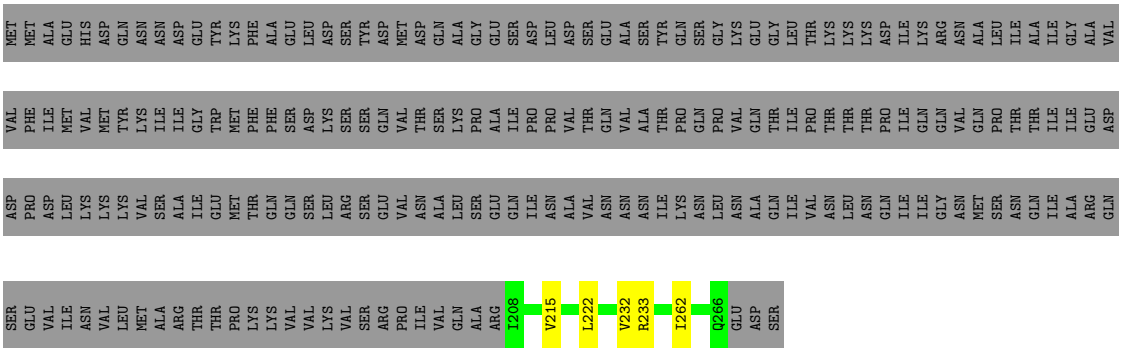
• Molecule 3: DotF

Chain MF:



• Molecule 3: DotF

Chain Df:



• Molecule 3: DotF

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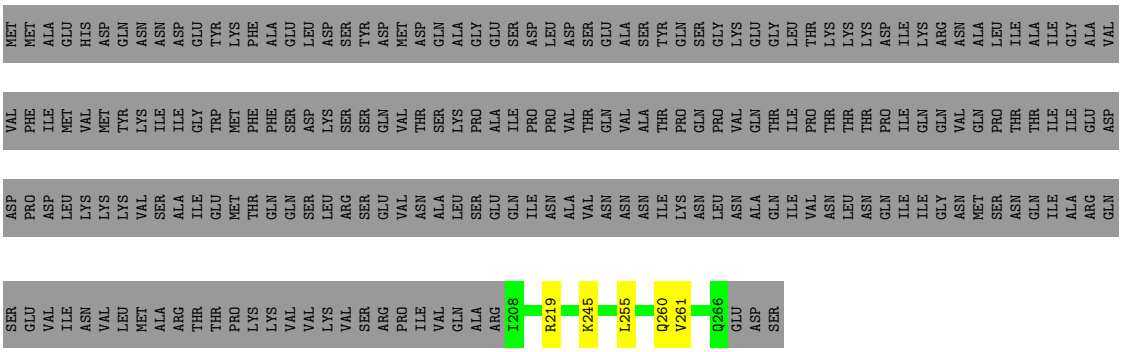
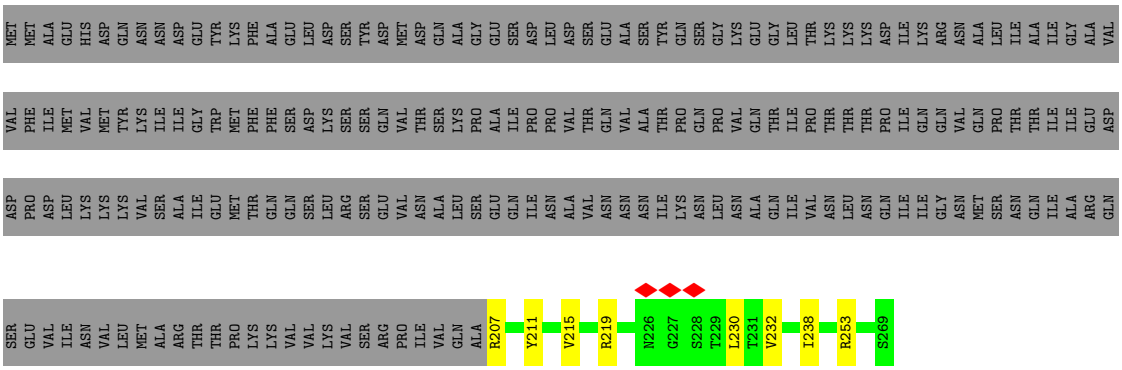


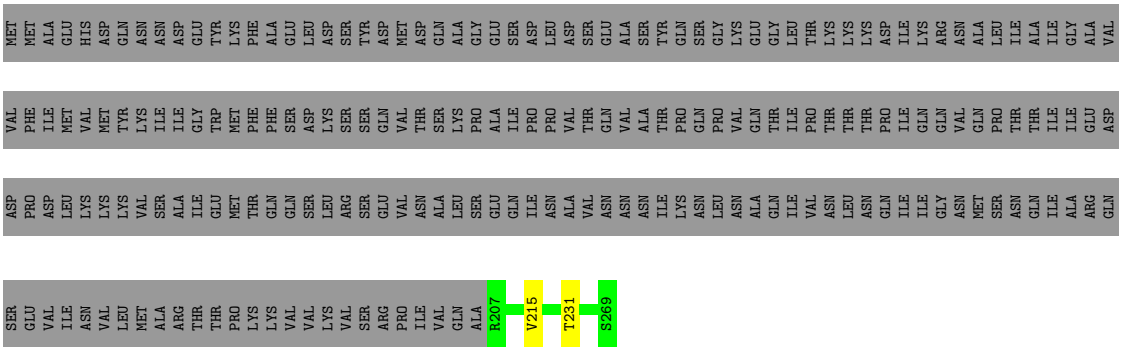
• Molecule 3: DotF

Chain VF:



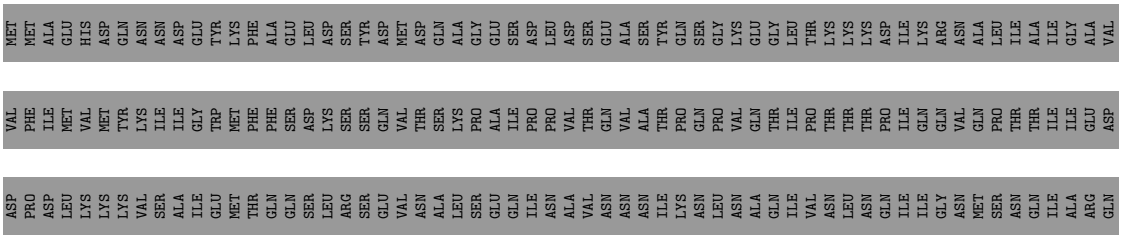
• Molecule 3: DotF

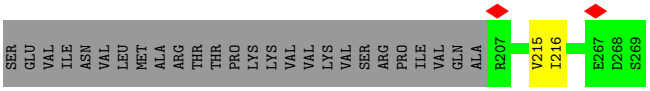
Chain WF:



• Molecule 3: DotF

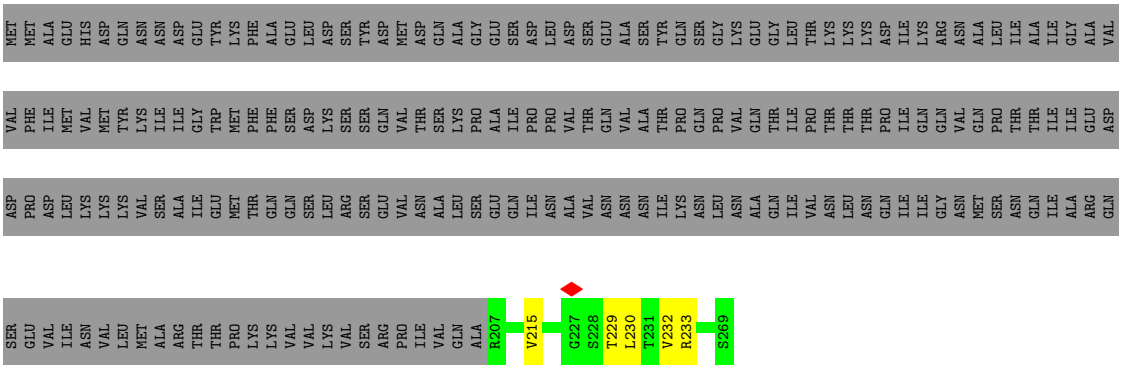
Chain XF:





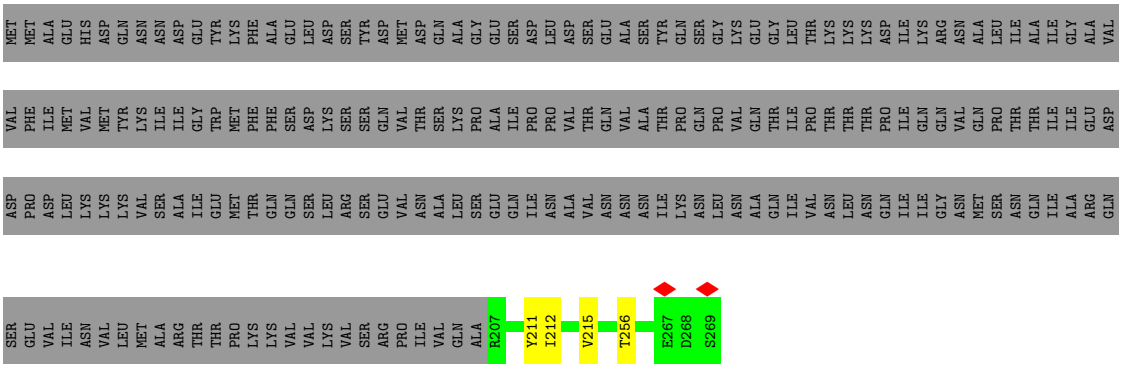
• Molecule 3: DotF

Chain CF:



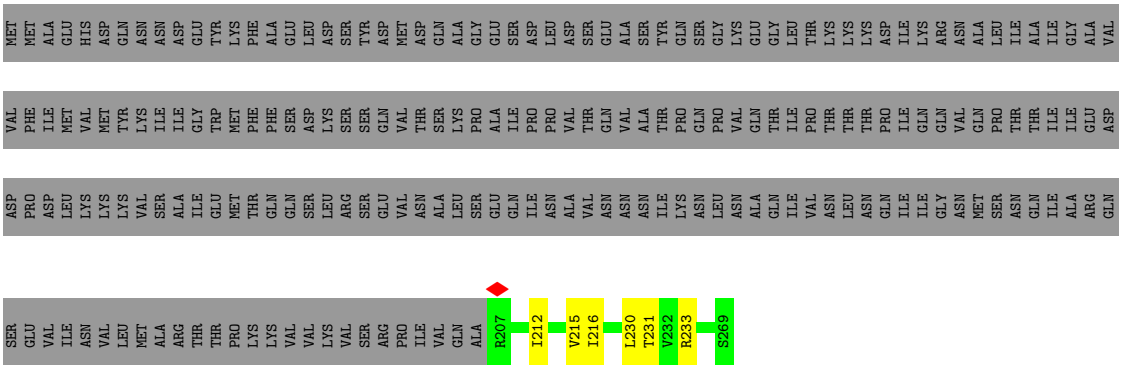
• Molecule 3: DotF

Chain YF:



• Molecule 3: DotF

Chain ZF:



• Molecule 3: DotF

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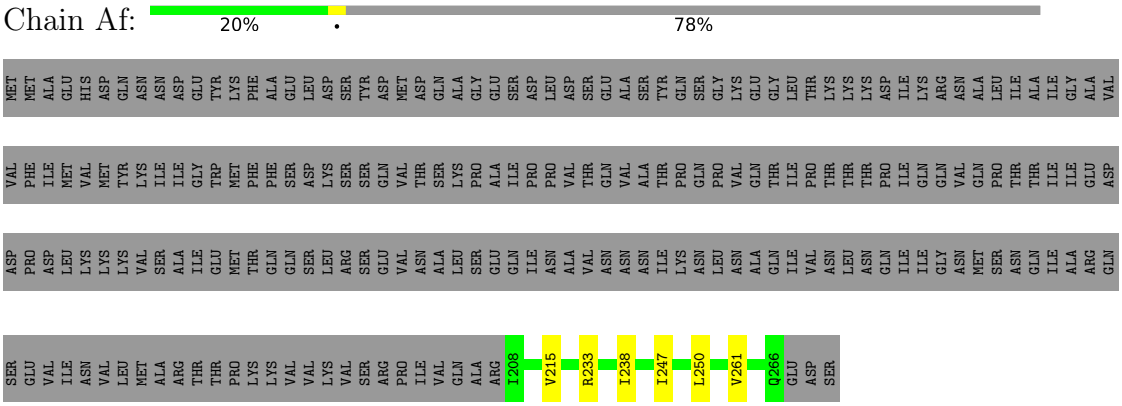
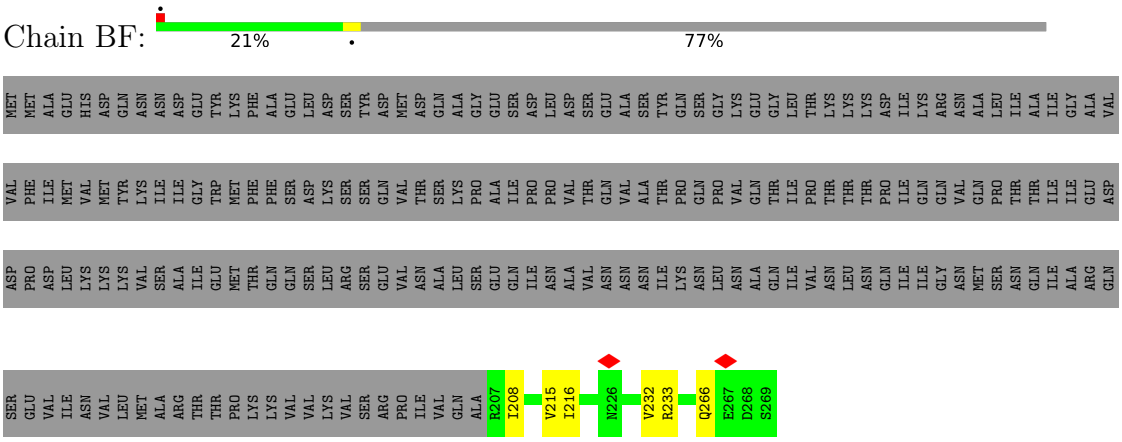


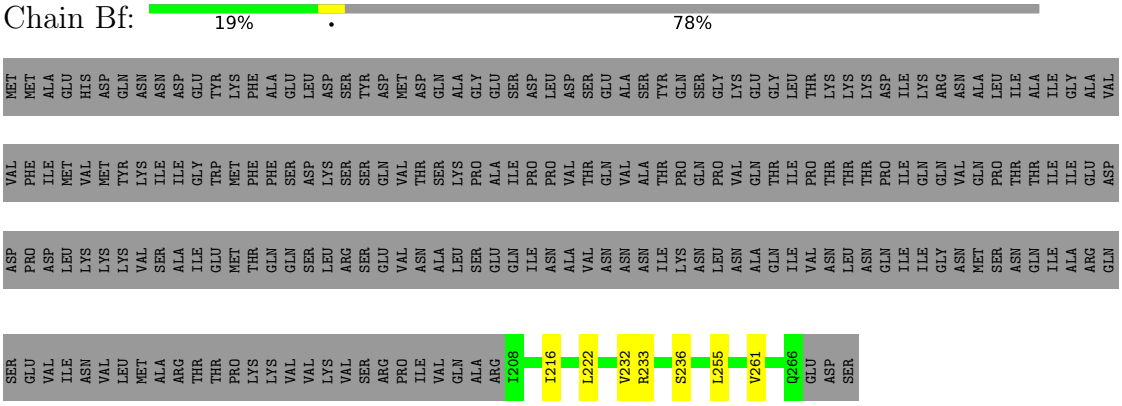
• Molecule 3: DotF

Chain BF:



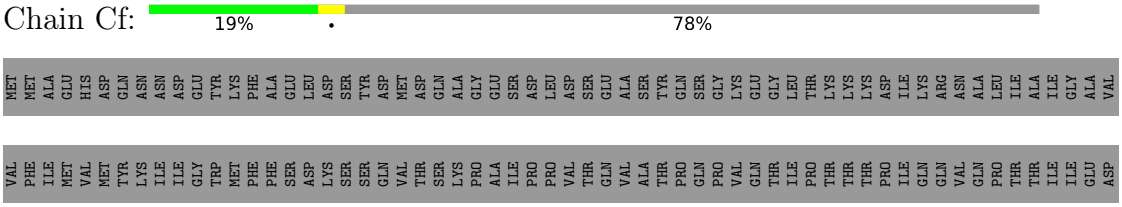
• Molecule 3: DotF

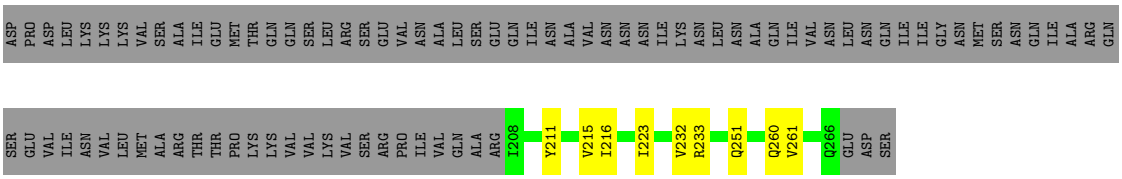
Chain Bf:



• Molecule 3: DotF

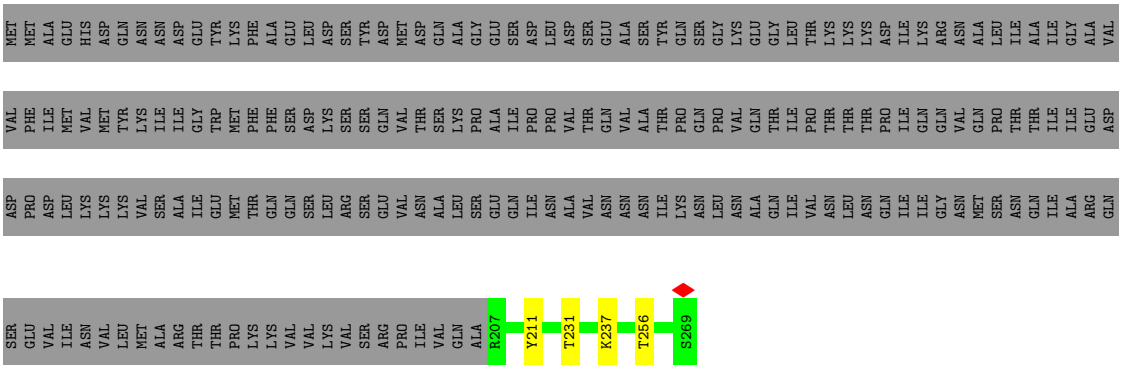
Chain Cf:





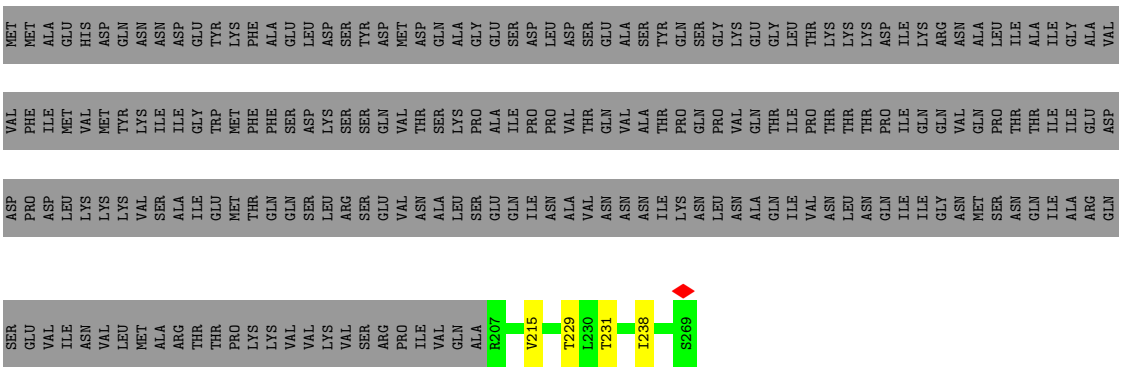
• Molecule 3: DotF

Chain DF:



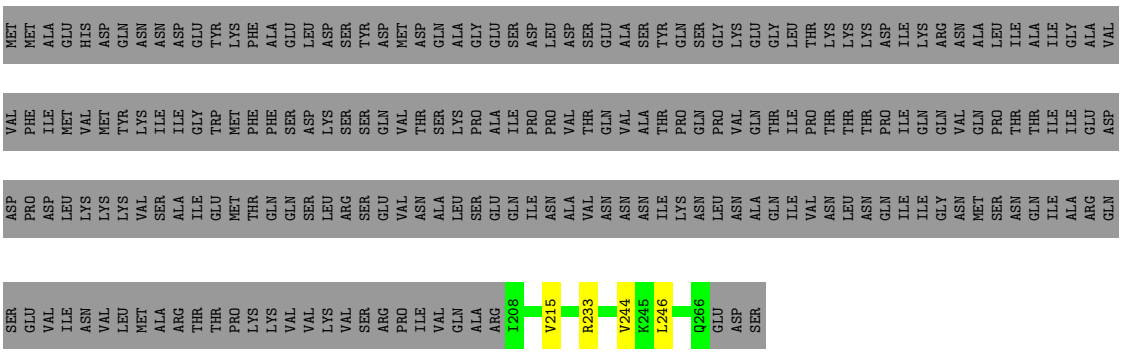
• Molecule 3: DotF

Chain EF:



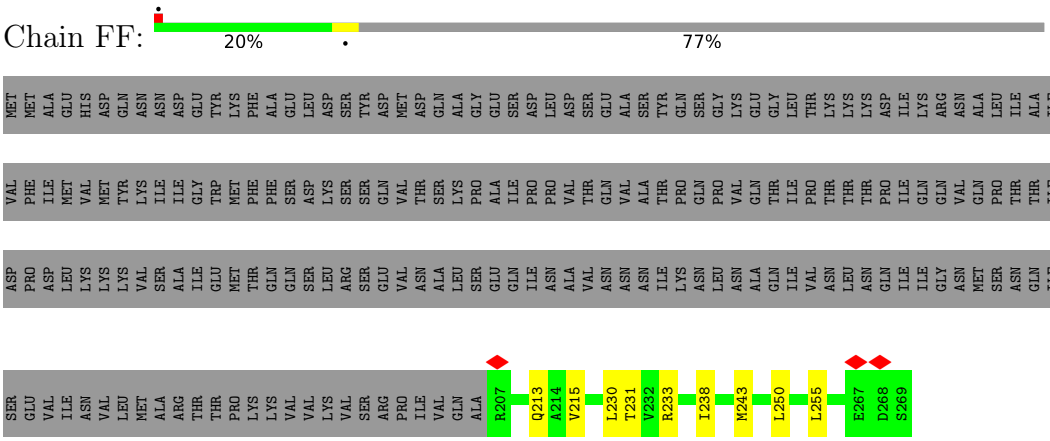
• Molecule 3: DotF

Chain Ef:



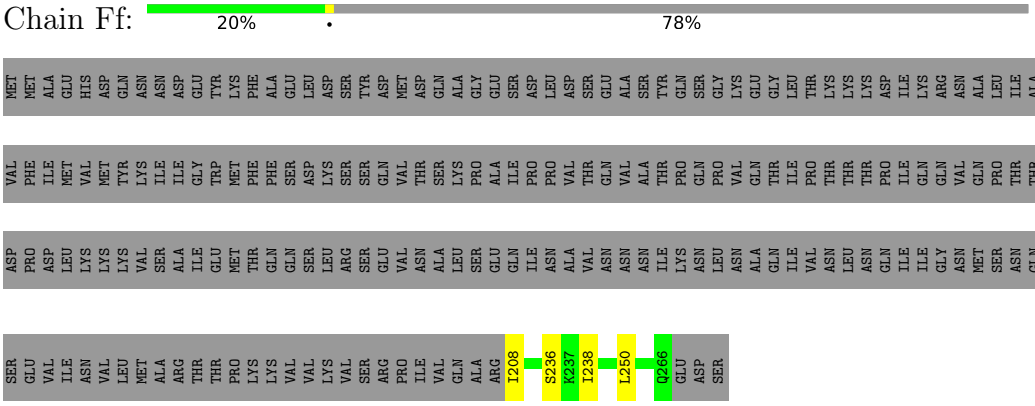
• Molecule 3: DotF

Chain FF:



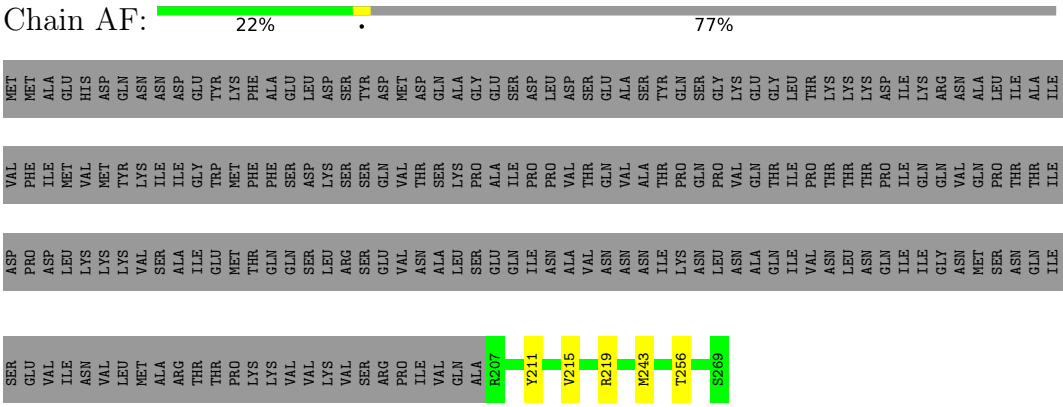
• Molecule 3: DotF

Chain Ff:



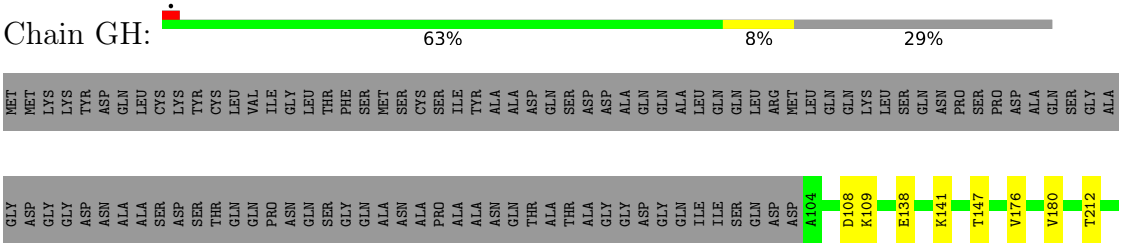
• Molecule 3: DotF

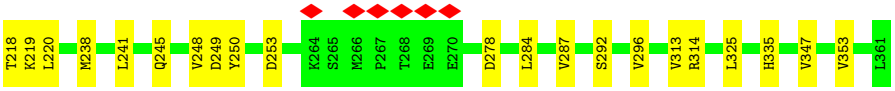
Chain AF:



• Molecule 4: Type IV secretion protein IcmK

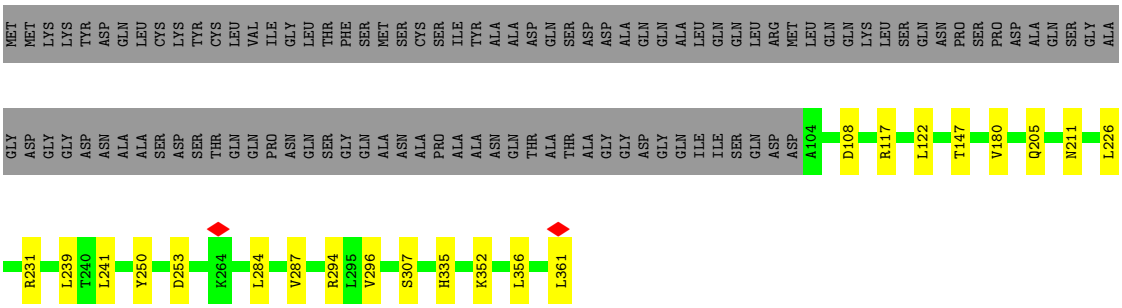
Chain GH:





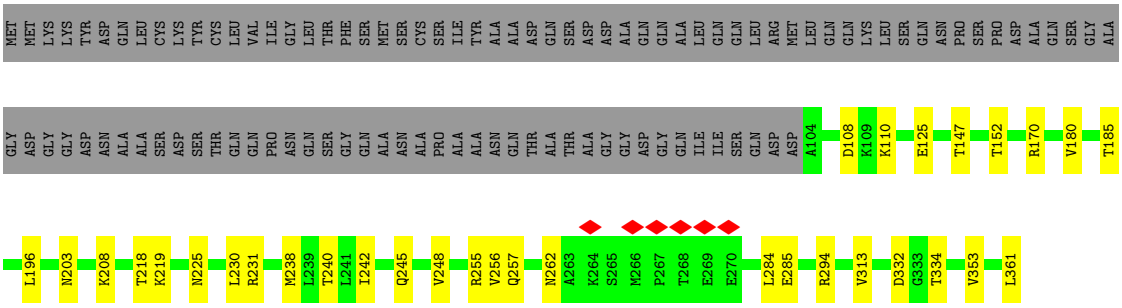
• Molecule 4: Type IV secretion protein IcmK

Chain HH:



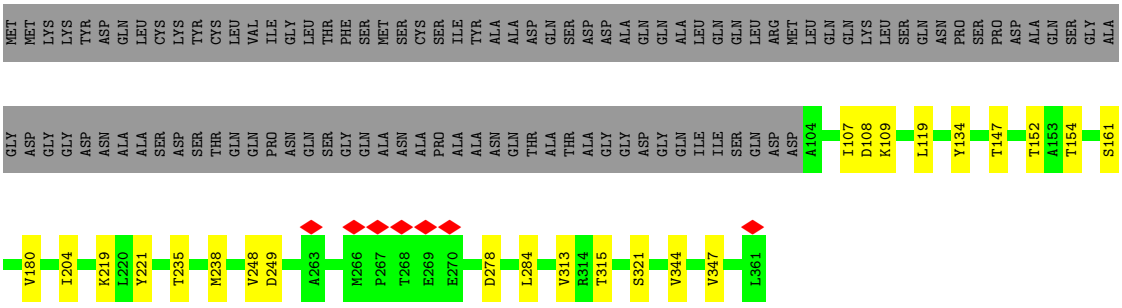
• Molecule 4: Type IV secretion protein IcmK

Chain IH:



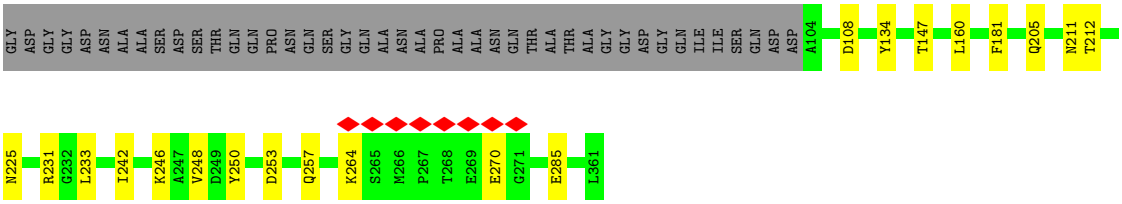
• Molecule 4: Type IV secretion protein IcmK

Chain JH:



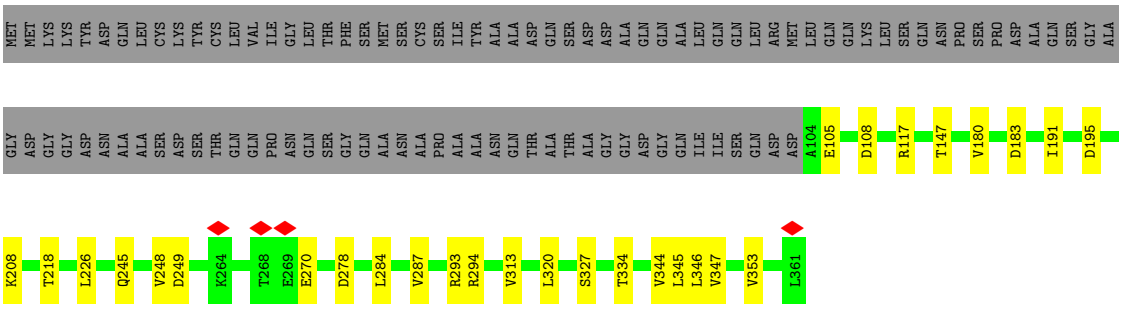
• Molecule 4: Type IV secretion protein IcmK

Chain AH:



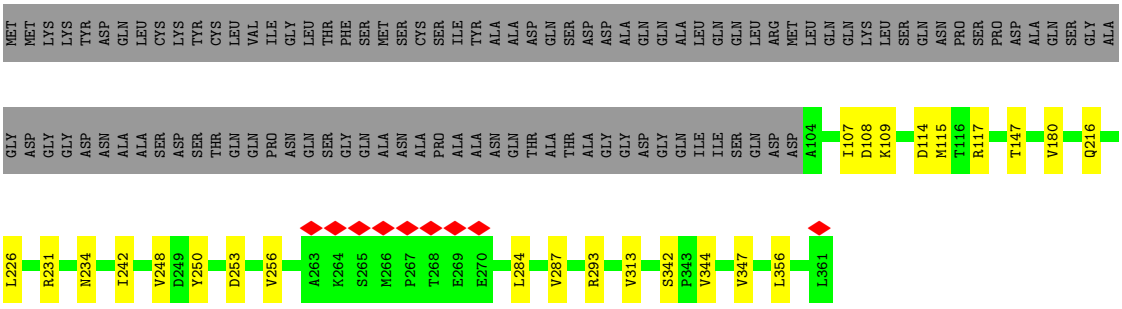
• Molecule 4: Type IV secretion protein IcmK

Chain KH:



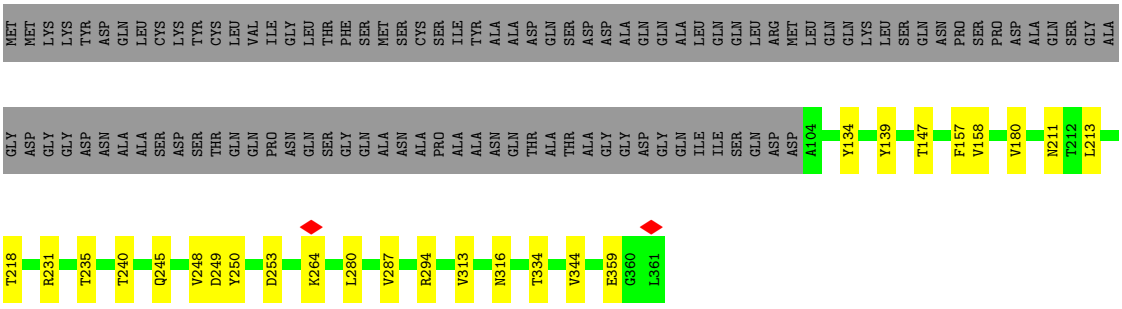
• Molecule 4: Type IV secretion protein IcmK

Chain LH:



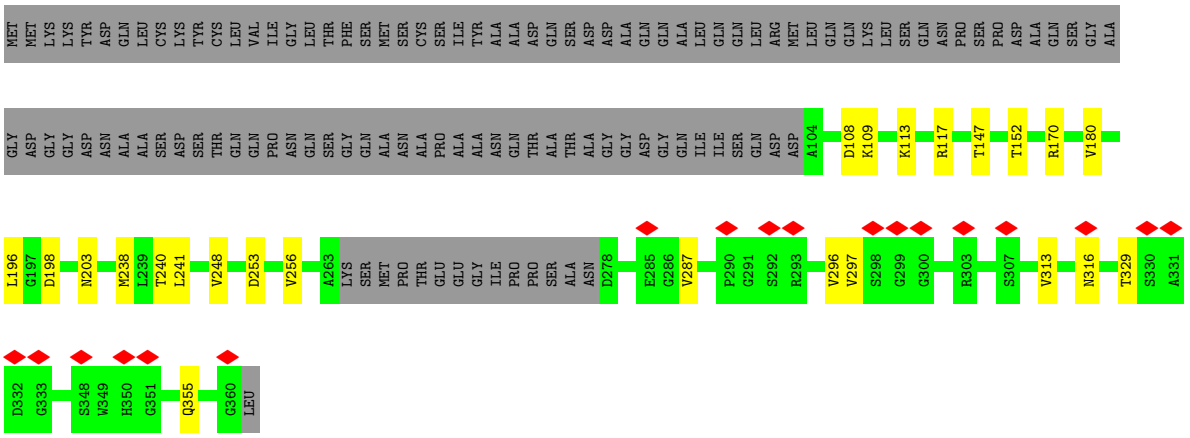
• Molecule 4: Type IV secretion protein IcmK

Chain MH:



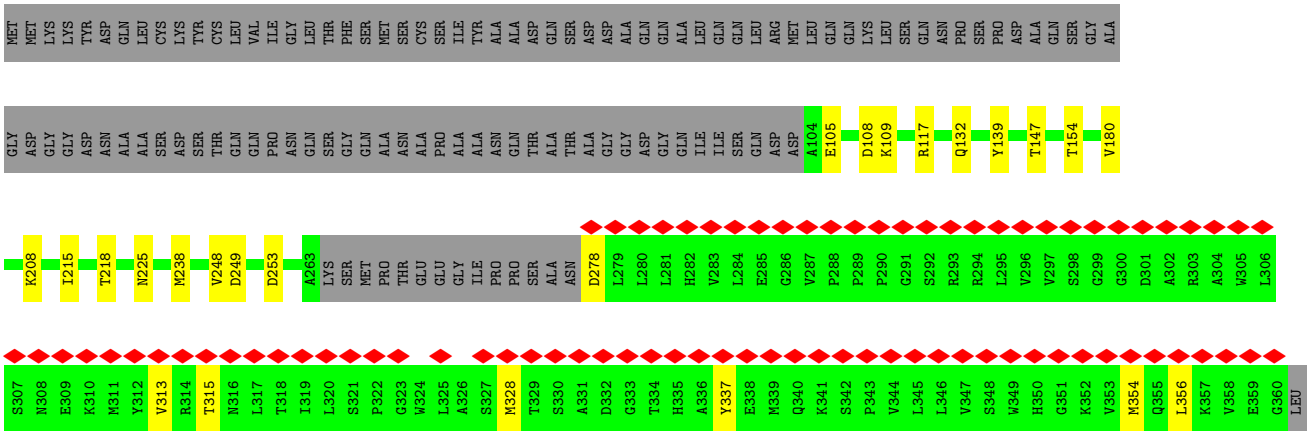
• Molecule 4: Type IV secretion protein IcmK

Chain VH:



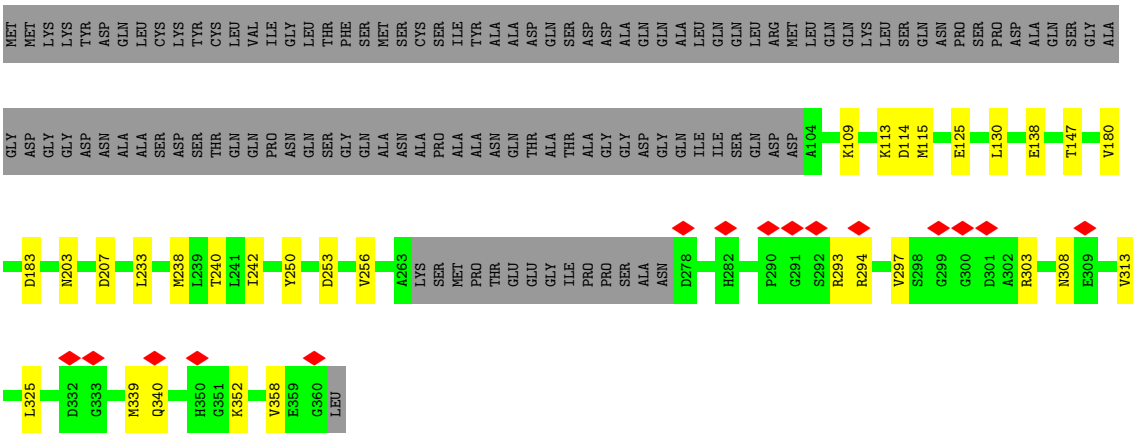
• Molecule 4: Type IV secretion protein IcmK

Chain WH:



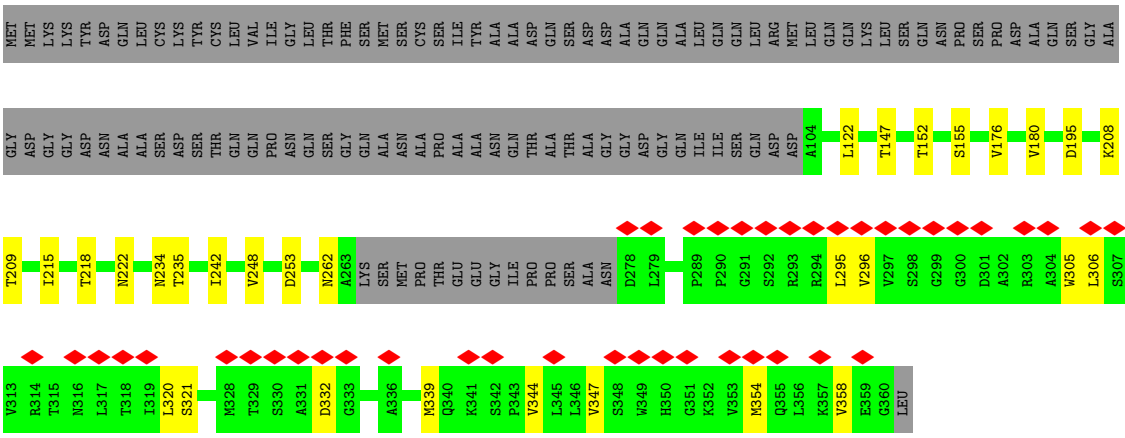
• Molecule 4: Type IV secretion protein IcmK

Chain XH:



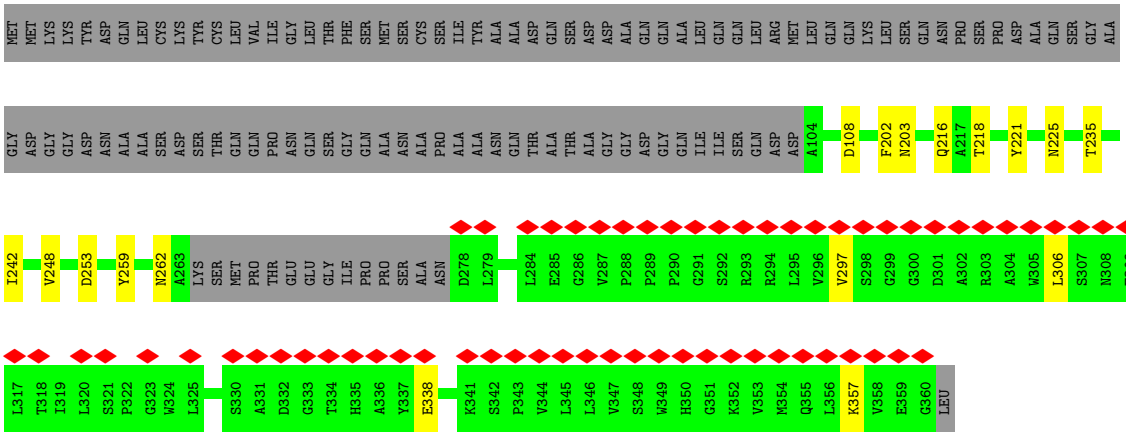
• Molecule 4: Type IV secretion protein IcmK

Chain YH:



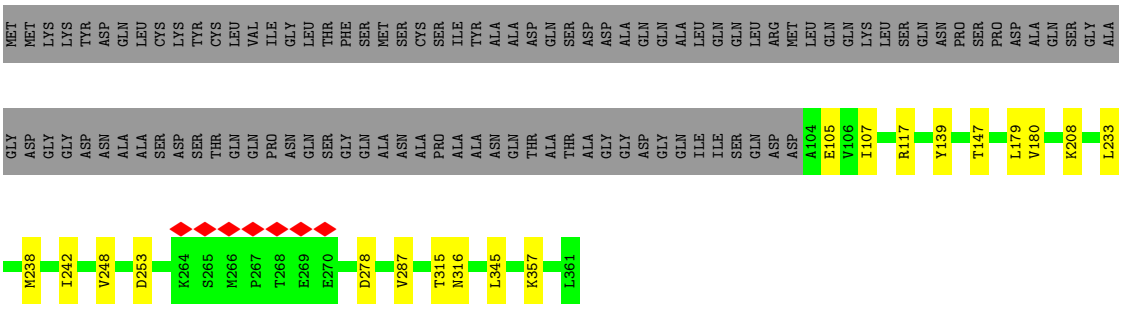
• Molecule 4: Type IV secretion protein IcmK

Chain ZH:



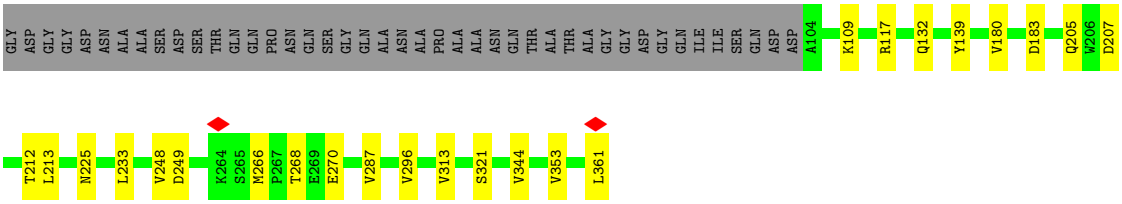
• Molecule 4: Type IV secretion protein IcmK

Chain BH:



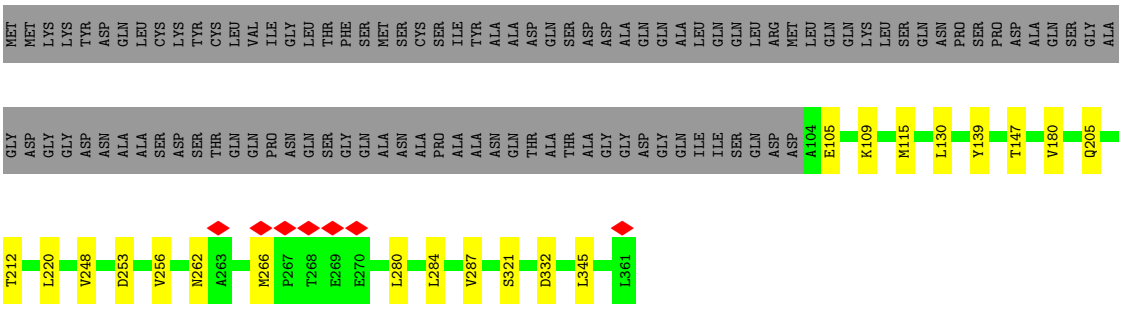
• Molecule 4: Type IV secretion protein IcmK

Chain CH:



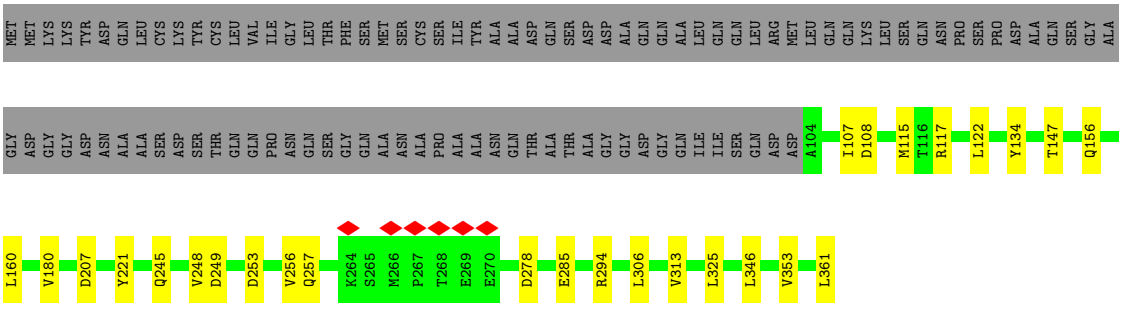
• Molecule 4: Type IV secretion protein IcmK

Chain DH:



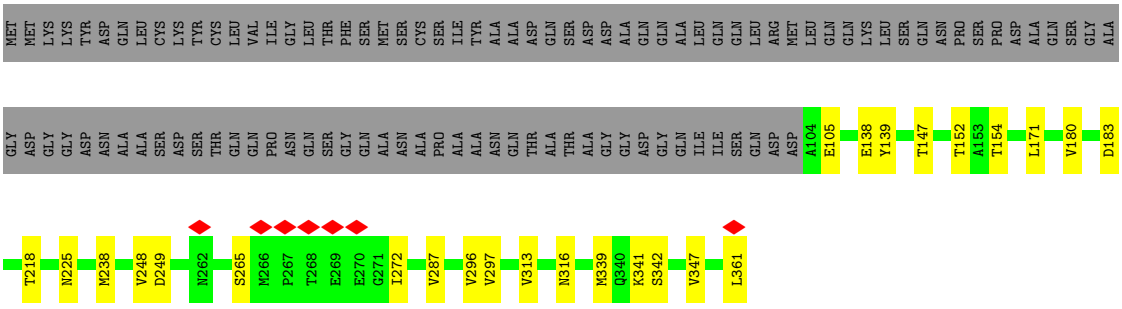
• Molecule 4: Type IV secretion protein IcmK

Chain EH:



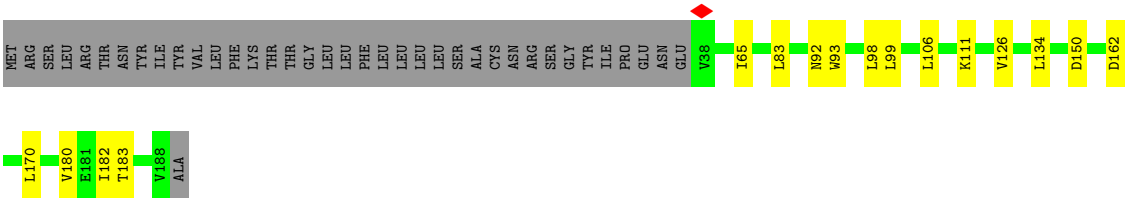
• Molecule 4: Type IV secretion protein IcmK

Chain FH:



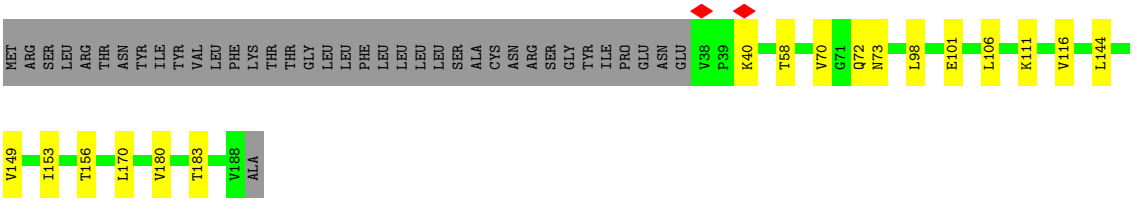
• Molecule 5: Inner membrane lipoprotein YiaD

Chain GK:



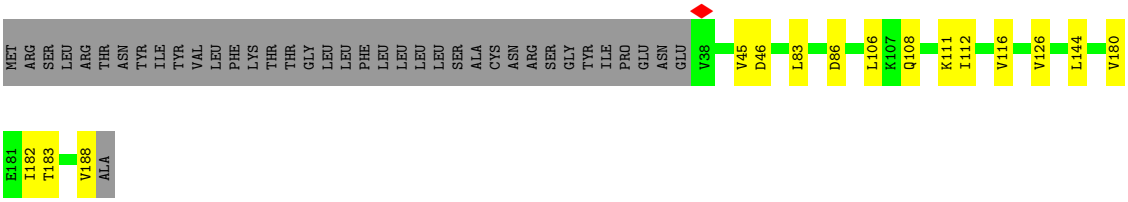
• Molecule 5: Inner membrane lipoprotein YiaD

Chain HK:



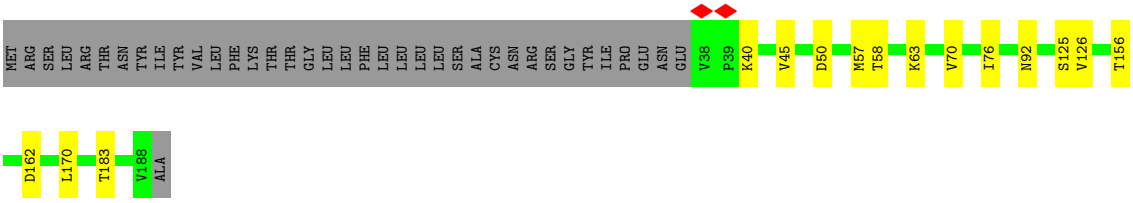
• Molecule 5: Inner membrane lipoprotein YiaD

Chain IK:



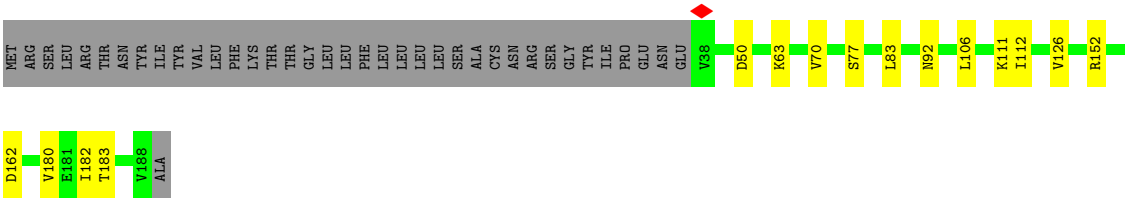
• Molecule 5: Inner membrane lipoprotein YiaD

Chain JK:



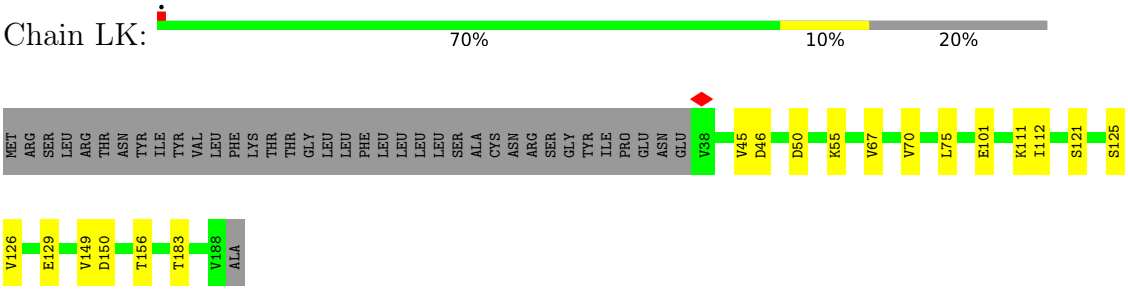
• Molecule 5: Inner membrane lipoprotein YiaD

Chain KK:



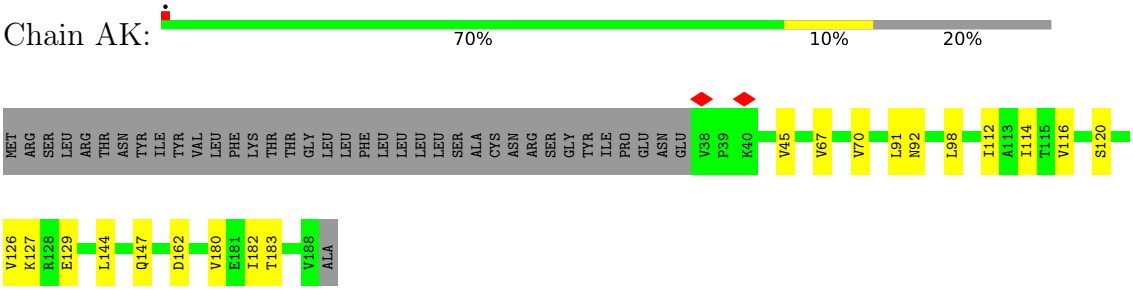
• Molecule 5: Inner membrane lipoprotein YiaD

Chain LK:



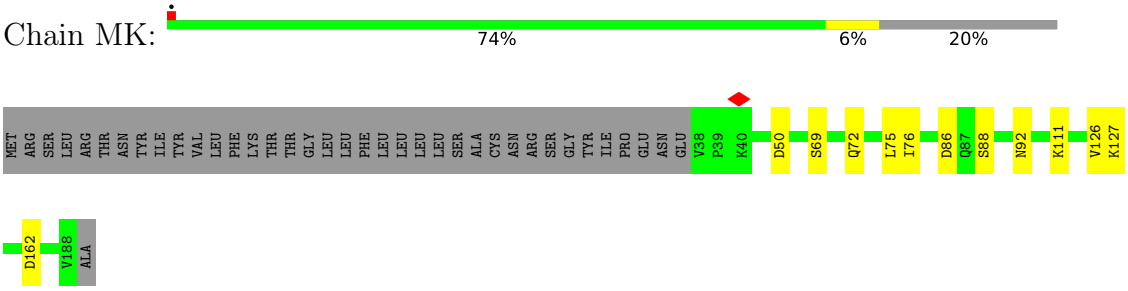
• Molecule 5: Inner membrane lipoprotein YiaD

Chain AK:



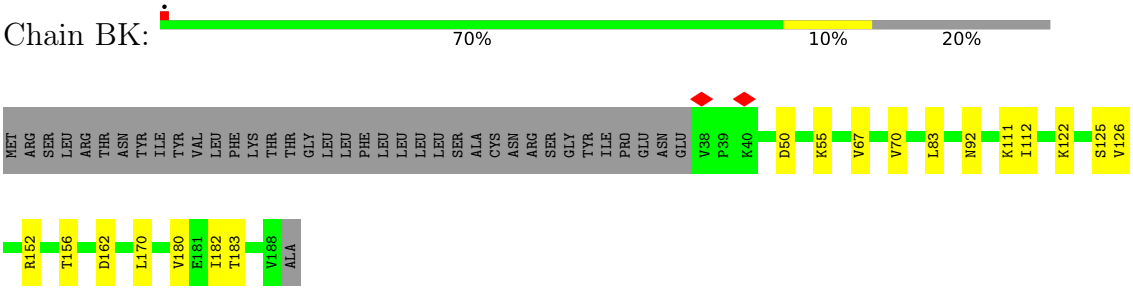
• Molecule 5: Inner membrane lipoprotein YiaD

Chain MK:



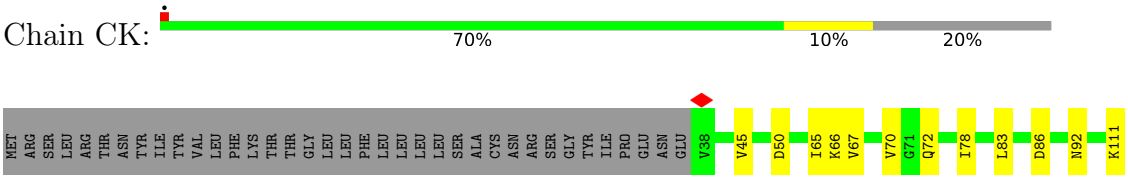
• Molecule 5: Inner membrane lipoprotein YiaD

Chain BK:



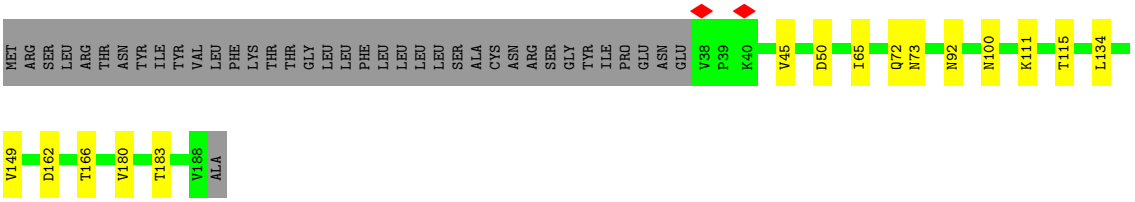
• Molecule 5: Inner membrane lipoprotein YiaD

Chain CK:



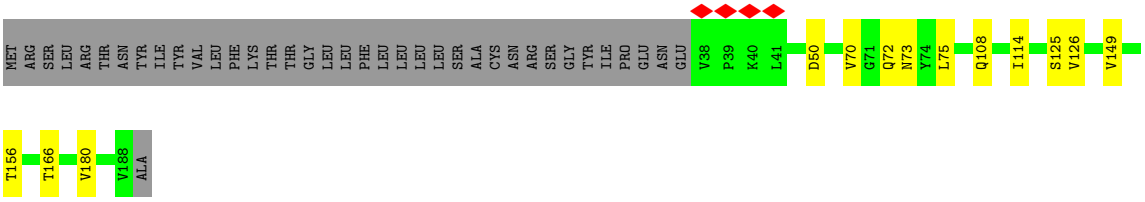
• Molecule 5: Inner membrane lipoprotein YiaD

Chain DK:



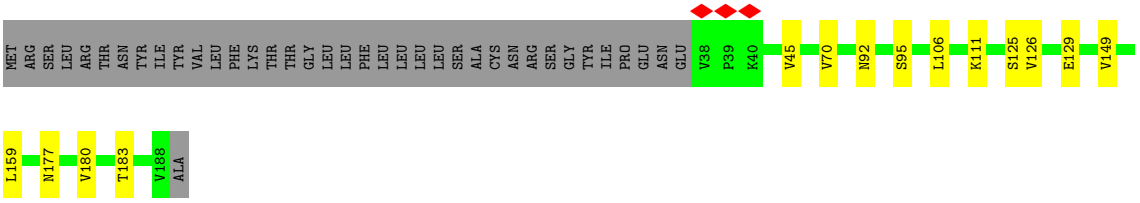
• Molecule 5: Inner membrane lipoprotein YiaD

Chain EK:



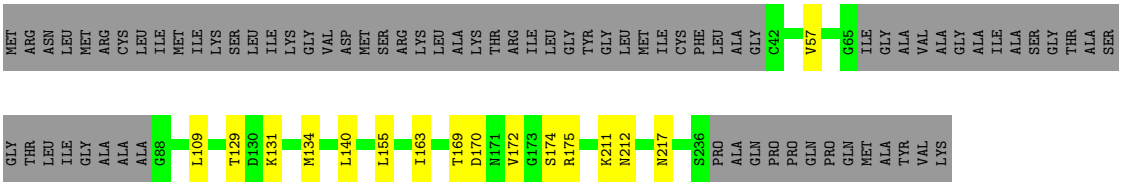
• Molecule 5: Inner membrane lipoprotein YiaD

Chain FK:



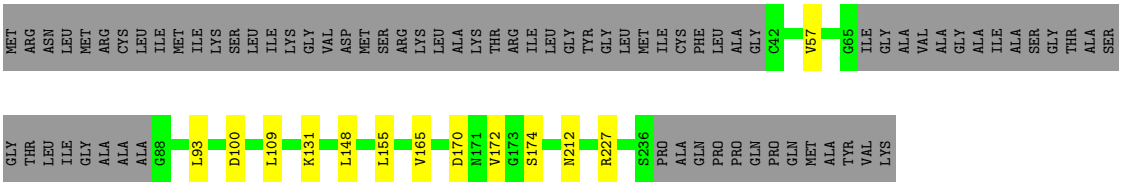
• Molecule 6: Outer membrane protein, OmpA family protein

Chain GL:



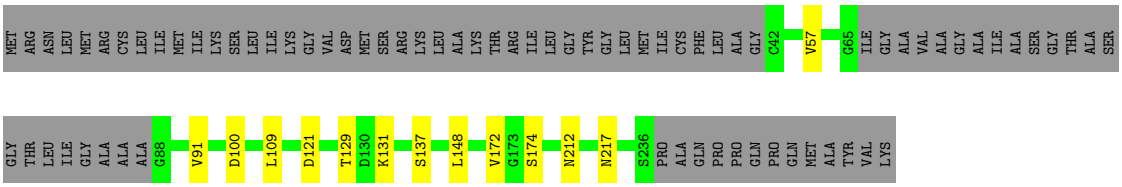
• Molecule 6: Outer membrane protein, OmpA family protein

Chain HL:



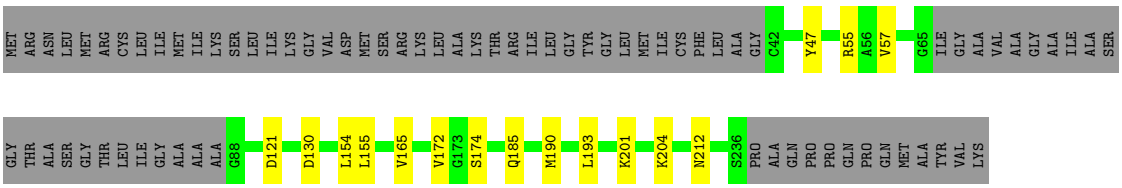
• Molecule 6: Outer membrane protein, OmpA family protein

Chain IL:



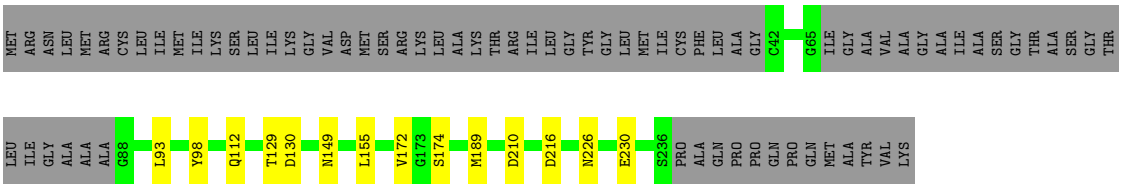
• Molecule 6: Outer membrane protein, OmpA family protein

Chain JL:



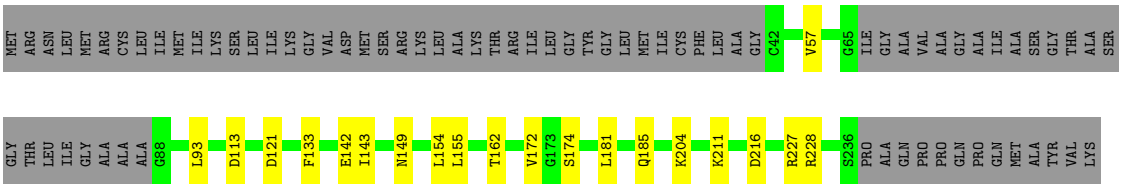
• Molecule 6: Outer membrane protein, OmpA family protein

Chain KL:



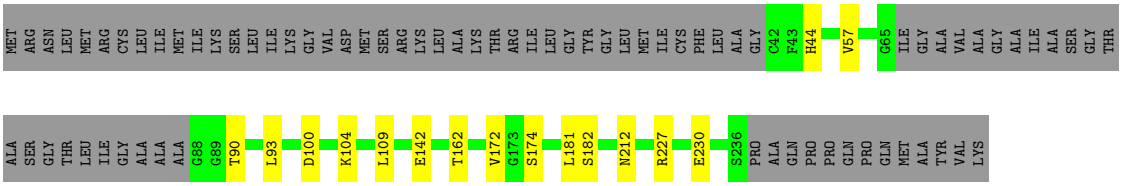
• Molecule 6: Outer membrane protein, OmpA family protein

Chain LL:



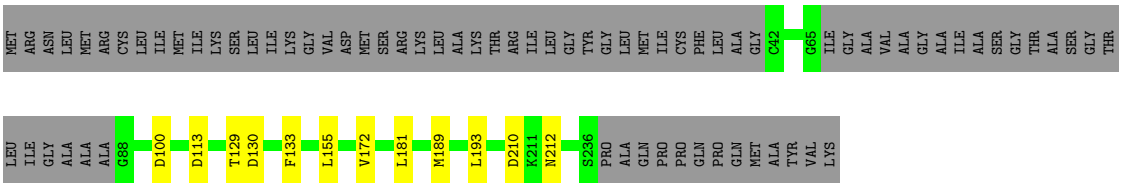
• Molecule 6: Outer membrane protein, OmpA family protein

Chain ML:



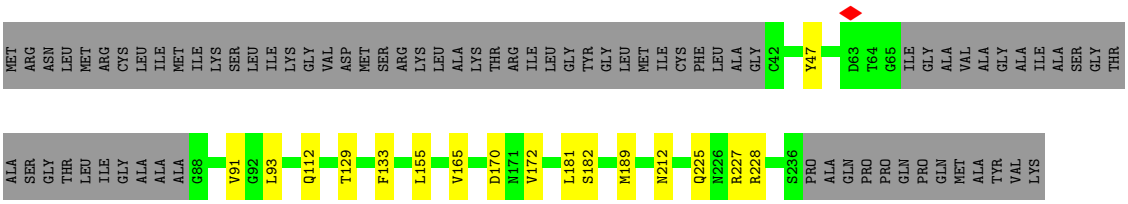
• Molecule 6: Outer membrane protein, OmpA family protein

Chain AL:



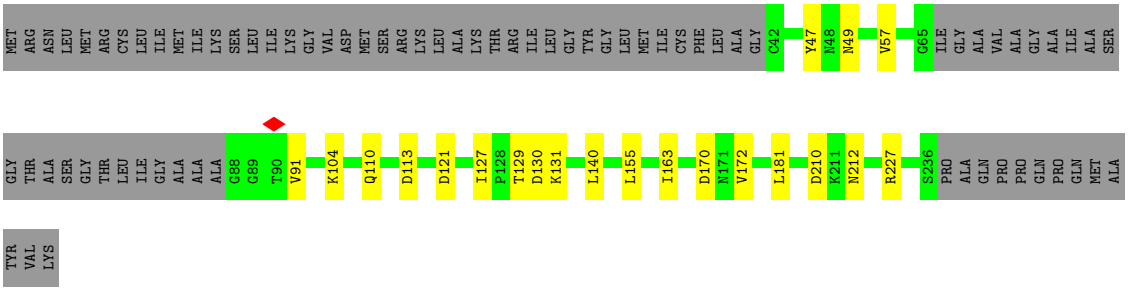
• Molecule 6: Outer membrane protein, OmpA family protein

Chain BL:



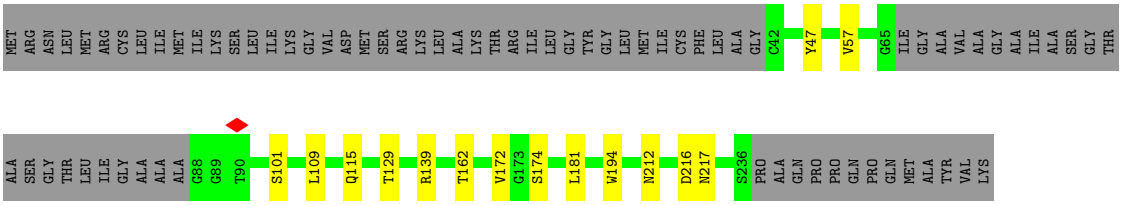
• Molecule 6: Outer membrane protein, OmpA family protein

Chain CL:



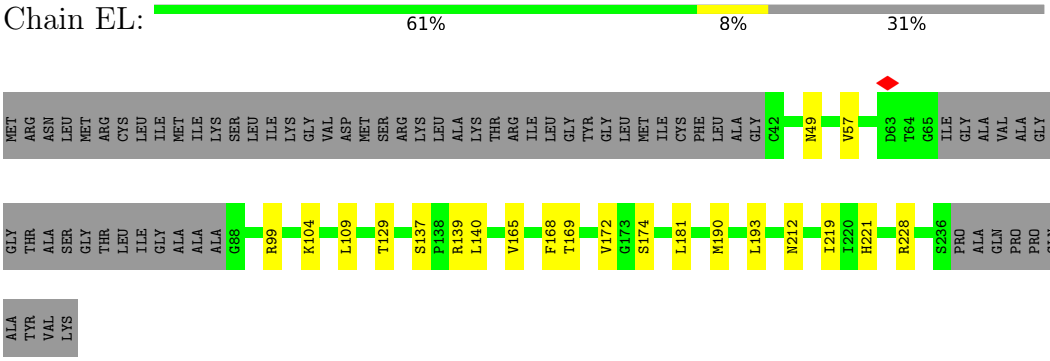
• Molecule 6: Outer membrane protein, OmpA family protein

Chain DL:



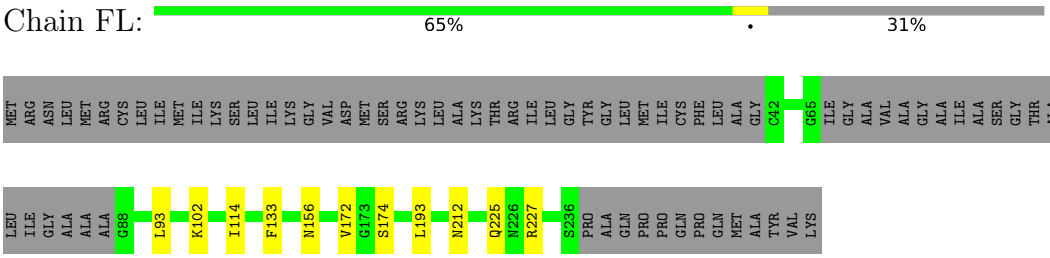
• Molecule 6: Outer membrane protein, OmpA family protein

Chain EL:



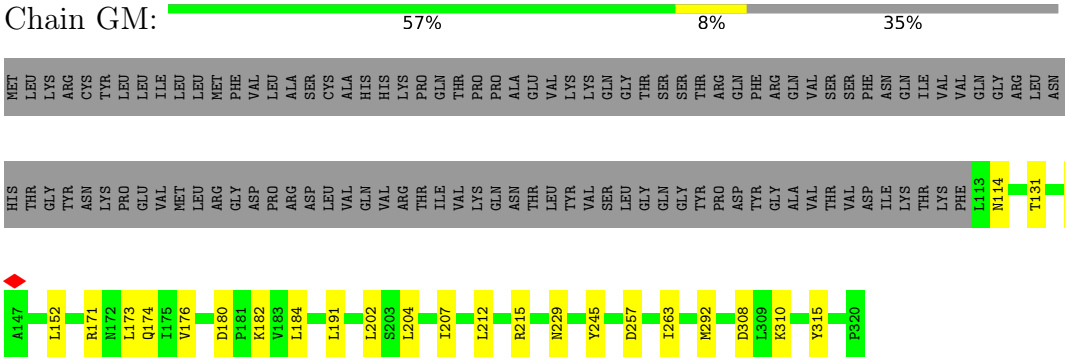
• Molecule 6: Outer membrane protein, OmpA family protein

Chain FL:



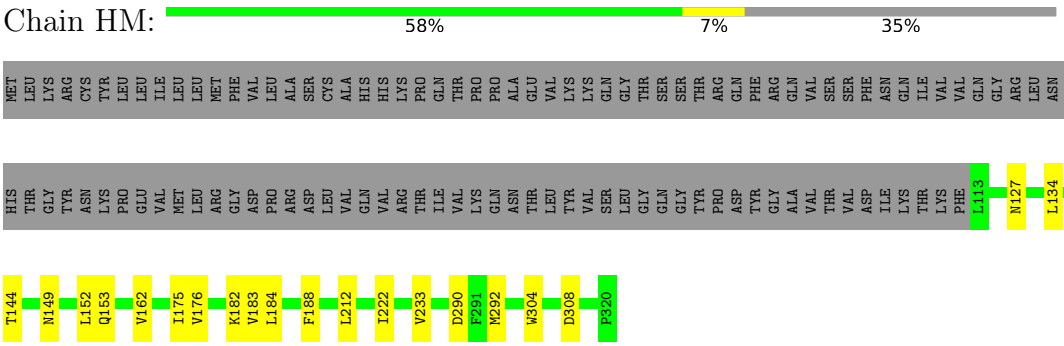
• Molecule 7: DUF2807 domain-containing protein

Chain GM:



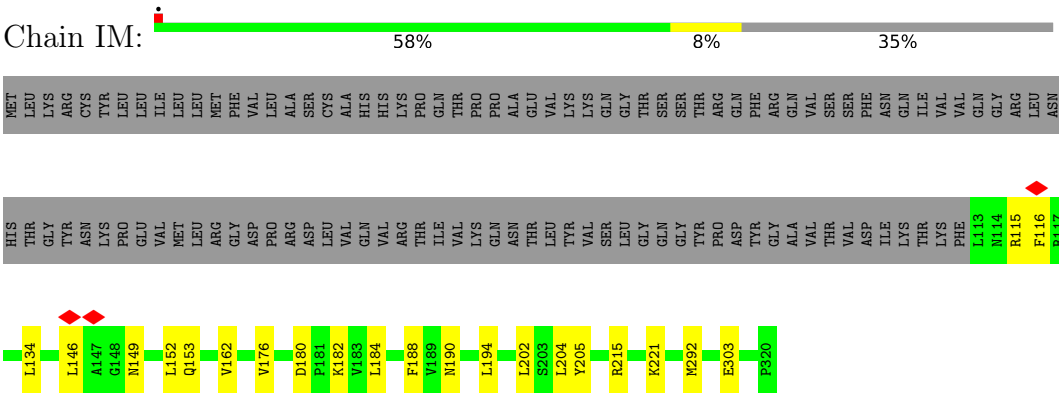
• Molecule 7: DUF2807 domain-containing protein

Chain HM:



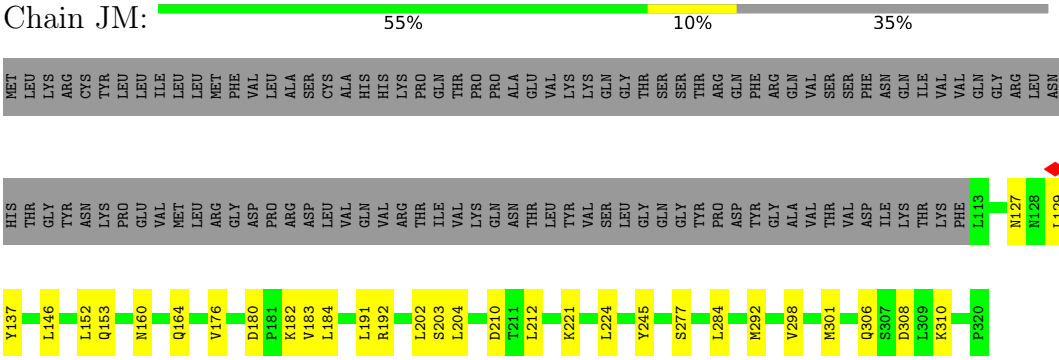
• Molecule 7: DUF2807 domain-containing protein

Chain IM:



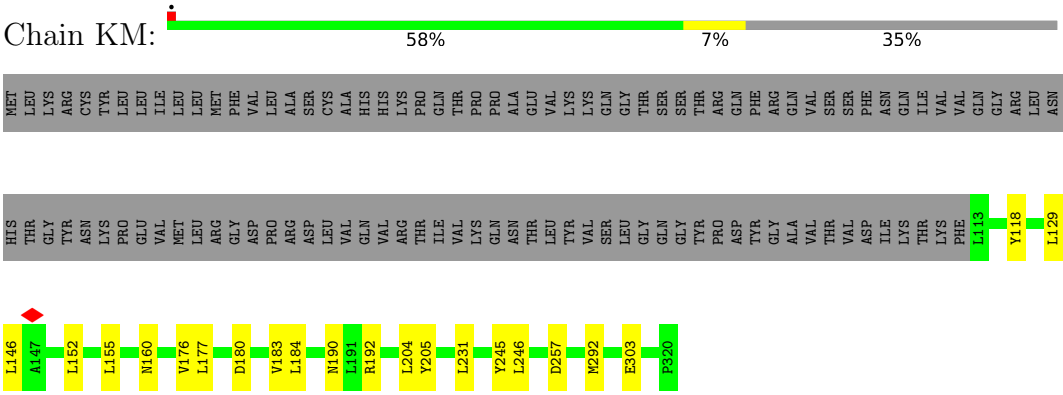
• Molecule 7: DUF2807 domain-containing protein

Chain JM:



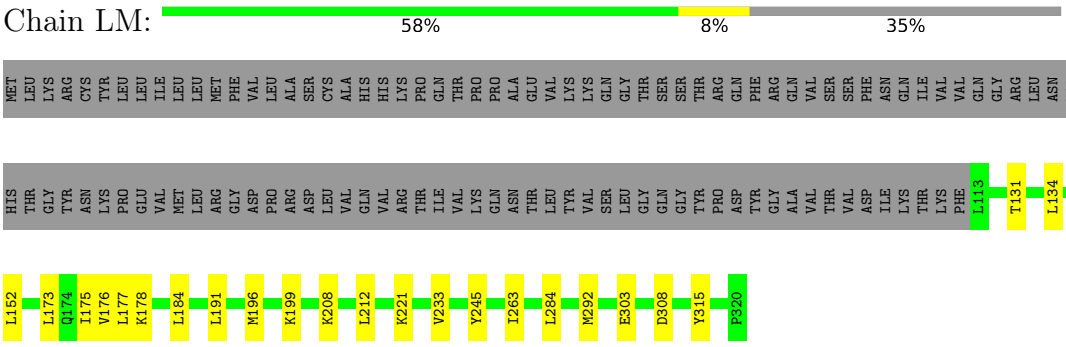
• Molecule 7: DUF2807 domain-containing protein

Chain KM:



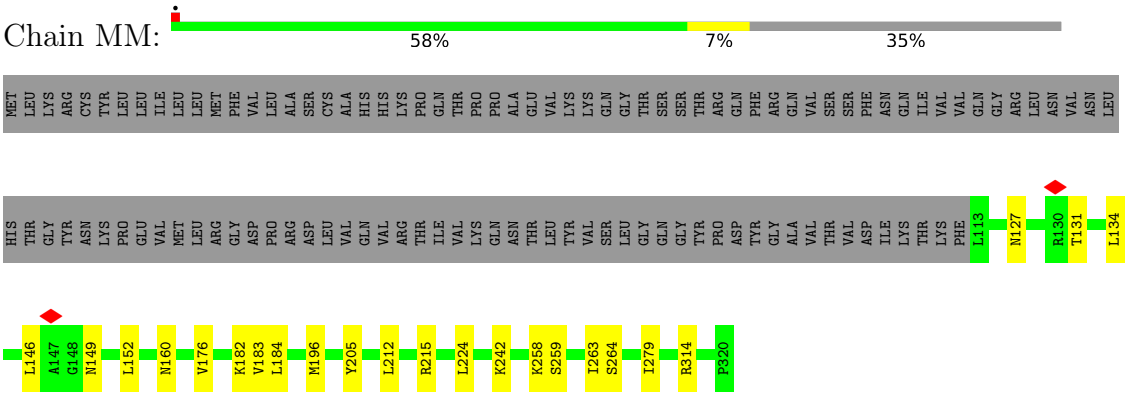
• Molecule 7: DUF2807 domain-containing protein

Chain LM:



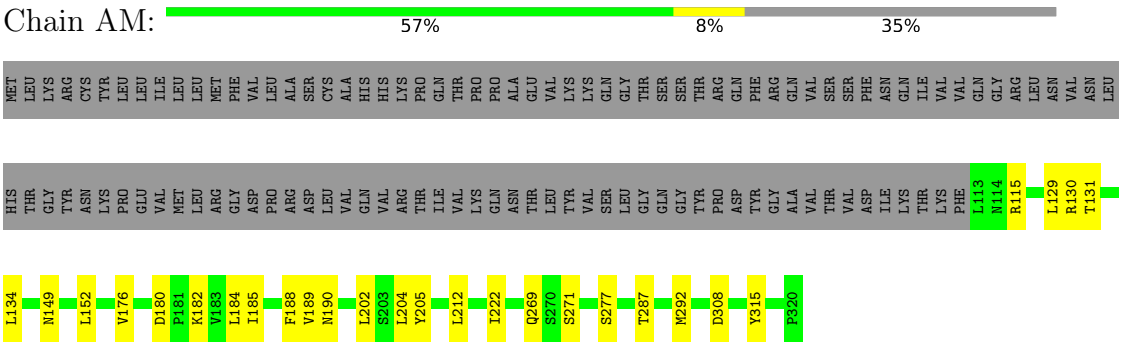
• Molecule 7: DUF2807 domain-containing protein

Chain MM:



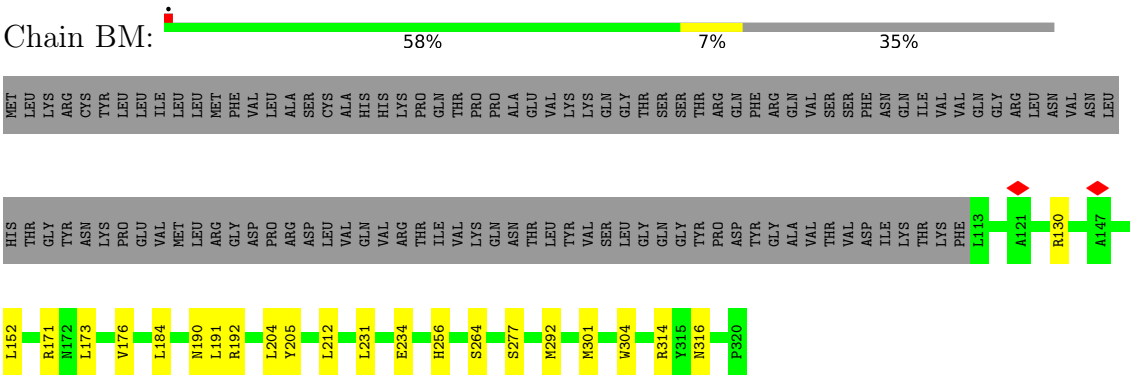
• Molecule 7: DUF2807 domain-containing protein

Chain AM:



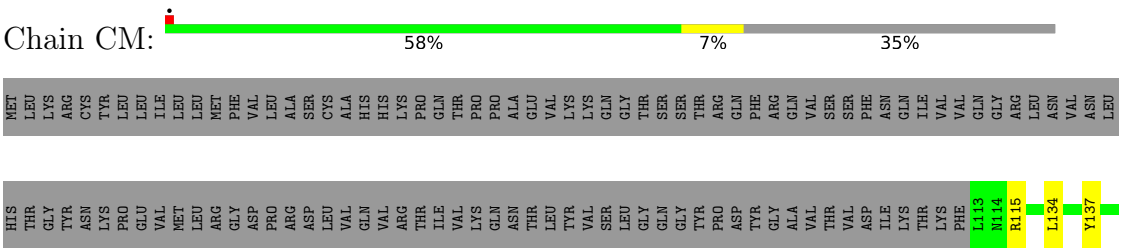
• Molecule 7: DUF2807 domain-containing protein

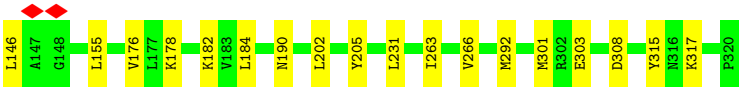
Chain BM:



• Molecule 7: DUF2807 domain-containing protein

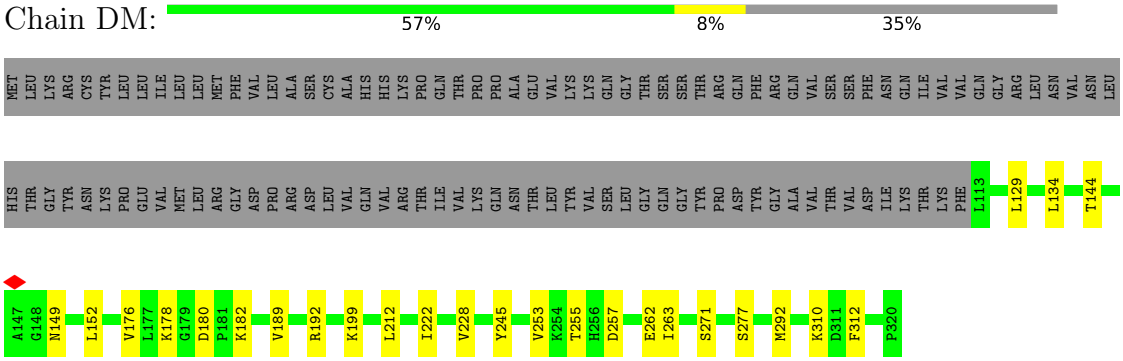
Chain CM:





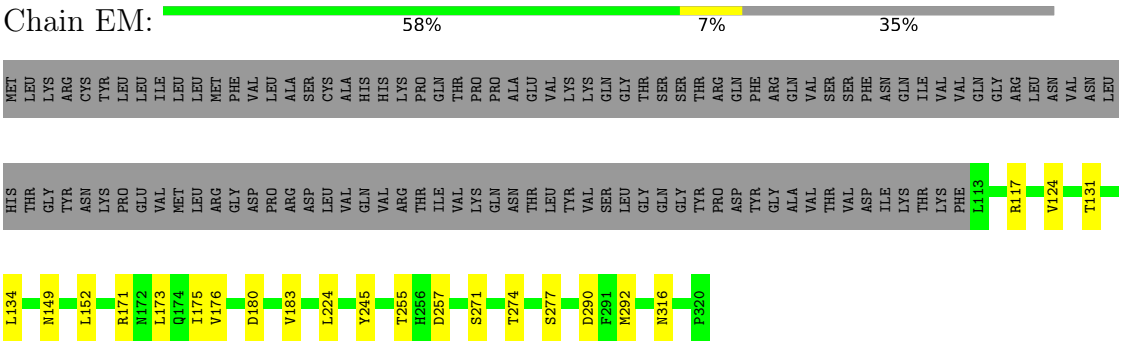
• Molecule 7: DUF2807 domain-containing protein

Chain DM:



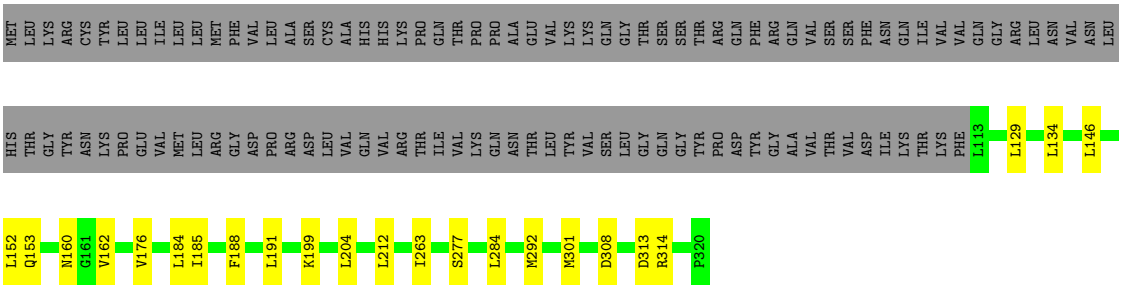
• Molecule 7: DUF2807 domain-containing protein

Chain EM:



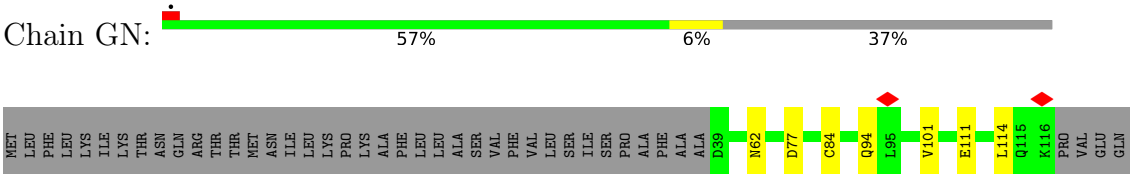
• Molecule 7: DUF2807 domain-containing protein

Chain FM:



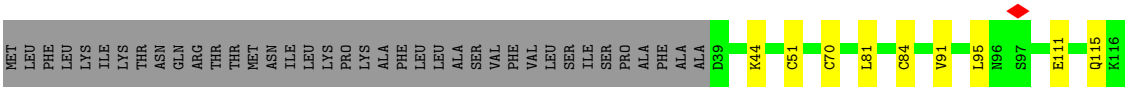
• Molecule 8: Neurogenic locus notch

Chain GN:



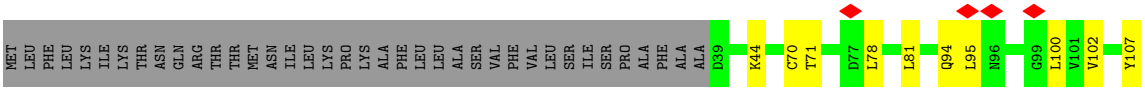
• Molecule 8: Neurogenic locus notch

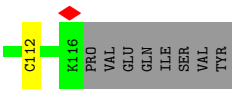
Chain HN:



• Molecule 8: Neurogenic locus notch

Chain IN:





• Molecule 8: Neurogenic locus notch

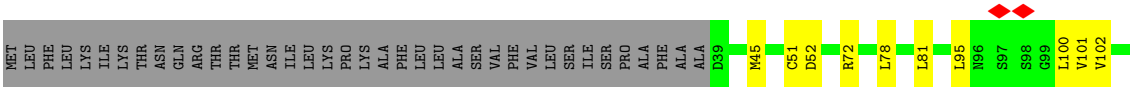
Chain JN:

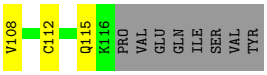
• Molecule 8: Neurogenic locus notch

Chain KN:

• Molecule 8: Neurogenic locus notch

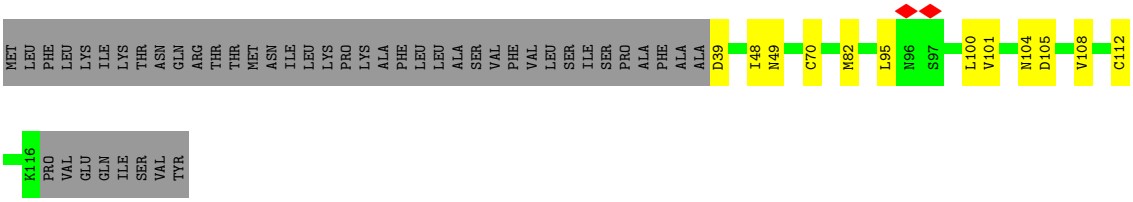
Chain LN:





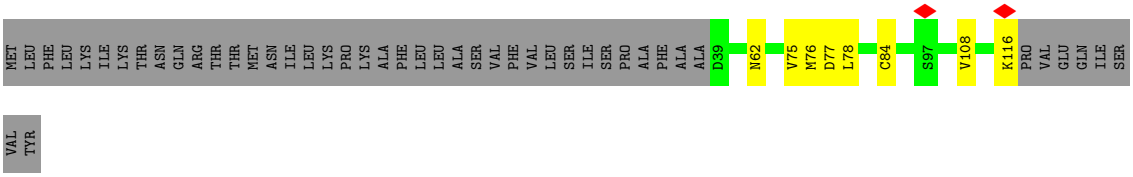
• Molecule 8: Neurogenic locus notch

Chain MN:



• Molecule 8: Neurogenic locus notch

Chain AN:



• Molecule 8: Neurogenic locus notch

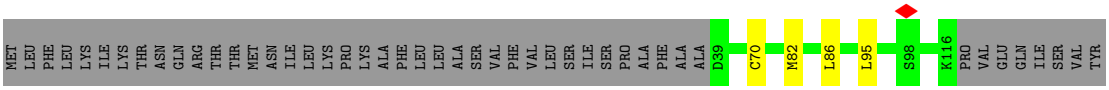
Chain BN:

• Molecule 8: Neurogenic locus notch

Chain CN:

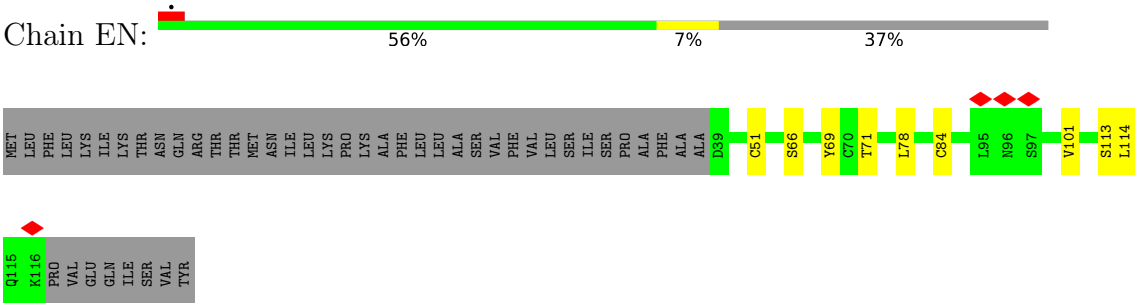
• Molecule 8: Neurogenic locus notch

Chain DN:



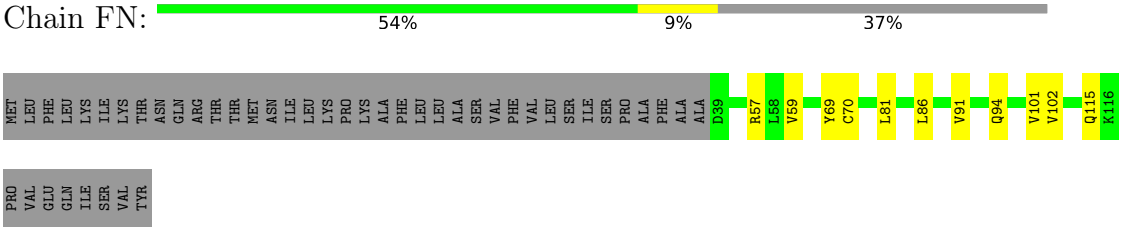
• Molecule 8: Neurogenic locus notch

Chain EN:



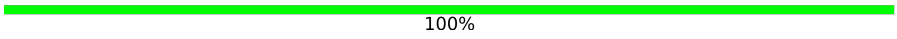
• Molecule 8: Neurogenic locus notch

Chain FN:



• Molecule 9: Unknown protein fragment

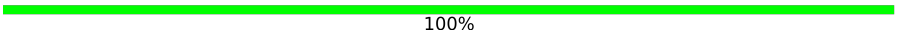
Chain GU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

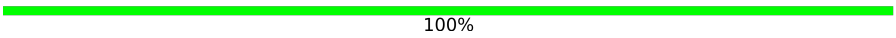
Chain HU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

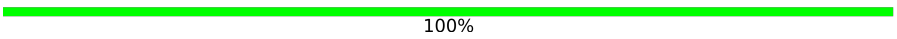
Chain IU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

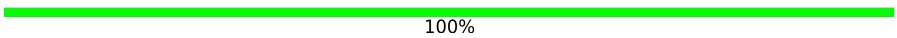
Chain JU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

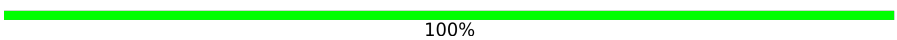
Chain KU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

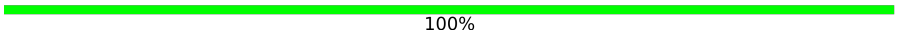
Chain LU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

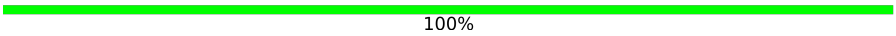
Chain MU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain AU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain BU:

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

Chain CU:

There are no outlier residues recorded for this chain.

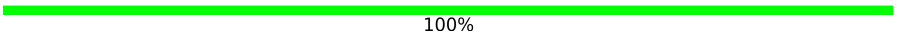
• Molecule 9: Unknown protein fragment

Chain DU:

There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

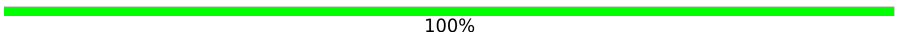
Chain EU:



There are no outlier residues recorded for this chain.

• Molecule 9: Unknown protein fragment

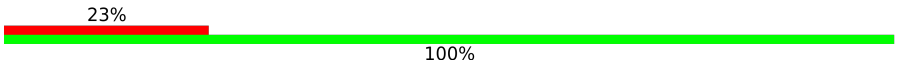
Chain FU:

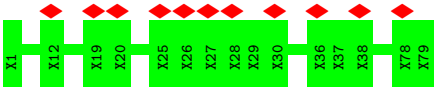


There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

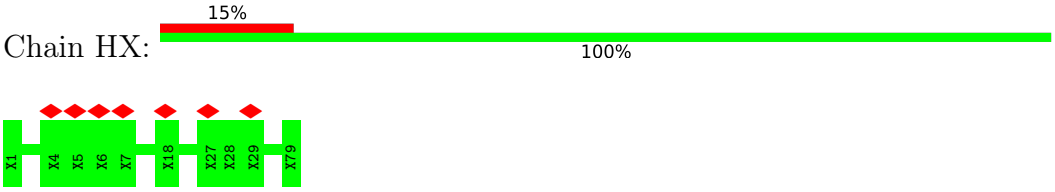
Chain GX:





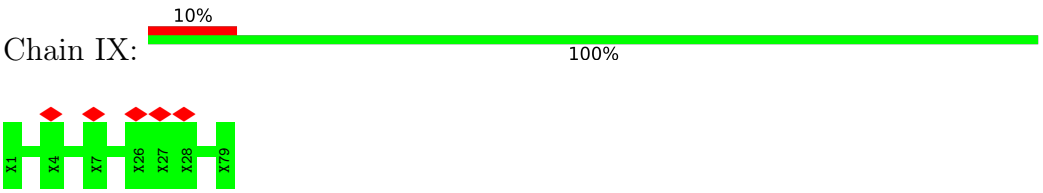
• Molecule 10: Unknown protein fragment

Chain HX:



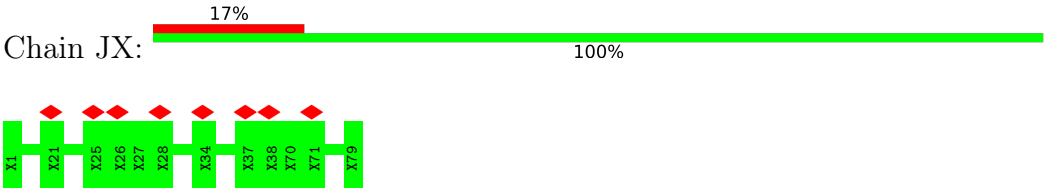
• Molecule 10: Unknown protein fragment

Chain IX:



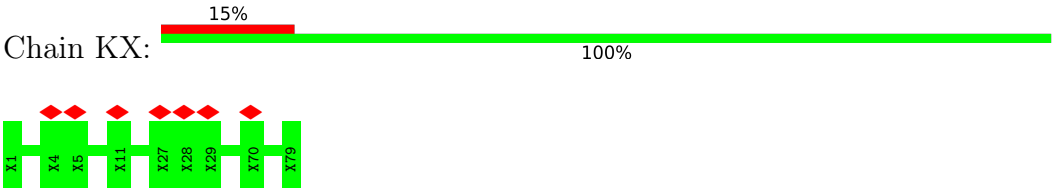
• Molecule 10: Unknown protein fragment

Chain JX:



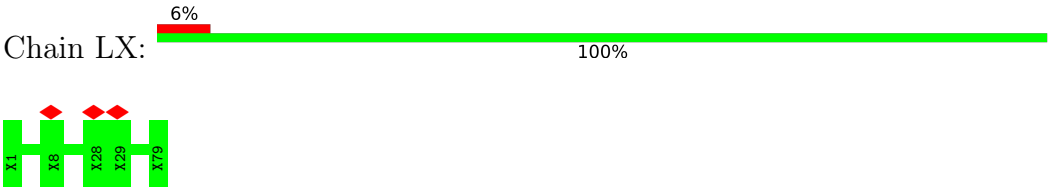
• Molecule 10: Unknown protein fragment

Chain KX:



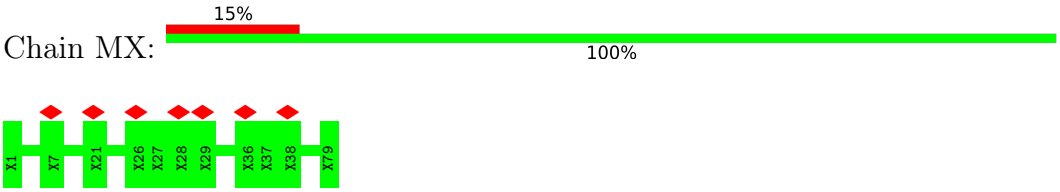
• Molecule 10: Unknown protein fragment

Chain LX:



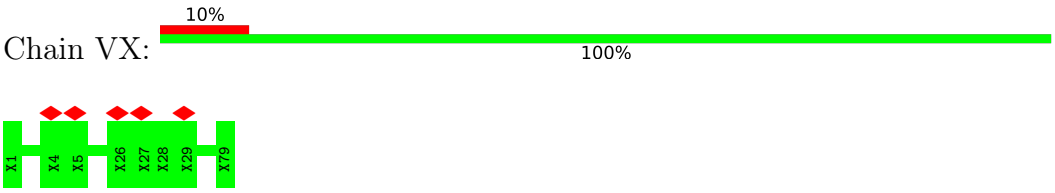
• Molecule 10: Unknown protein fragment

Chain MX:



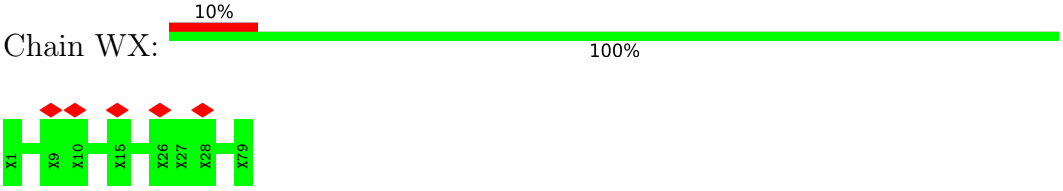
• Molecule 10: Unknown protein fragment

Chain VX:



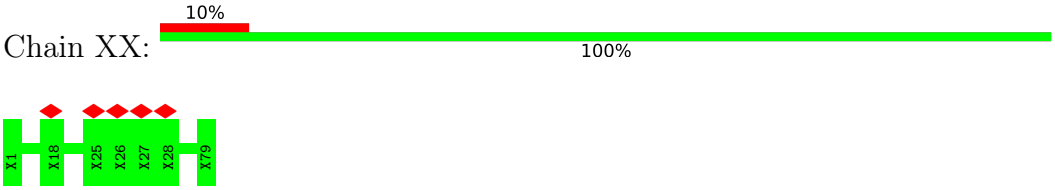
• Molecule 10: Unknown protein fragment

Chain WX:



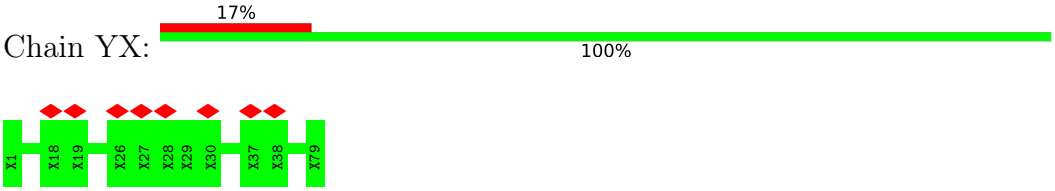
• Molecule 10: Unknown protein fragment

Chain XX:



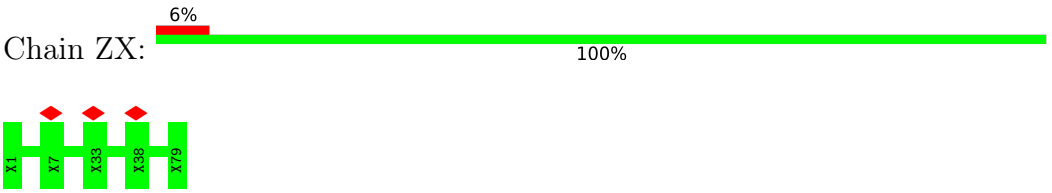
• Molecule 10: Unknown protein fragment

Chain YX:



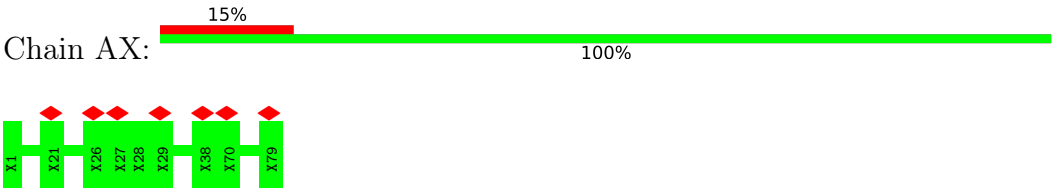
• Molecule 10: Unknown protein fragment

Chain ZX:



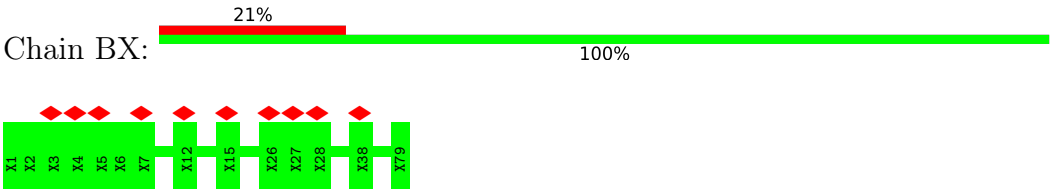
• Molecule 10: Unknown protein fragment

Chain AX:



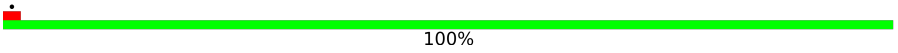
• Molecule 10: Unknown protein fragment

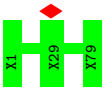
Chain BX:



• Molecule 10: Unknown protein fragment

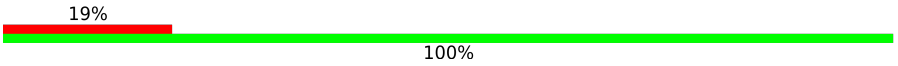
Chain CX:

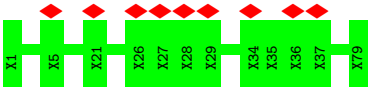




• Molecule 10: Unknown protein fragment

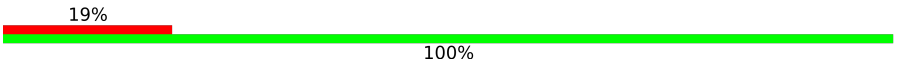
Chain DX:

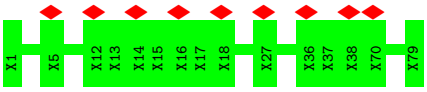




• Molecule 10: Unknown protein fragment

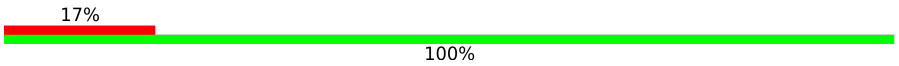
Chain EX:

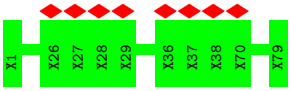




• Molecule 10: Unknown protein fragment

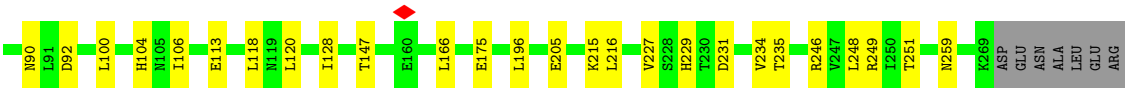
Chain FX:





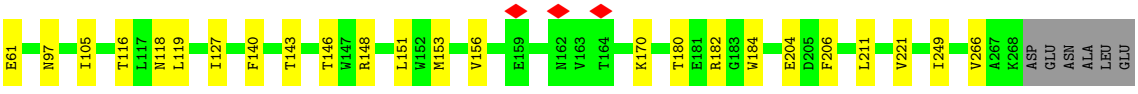
• Molecule 11: DotC

Chain CC:



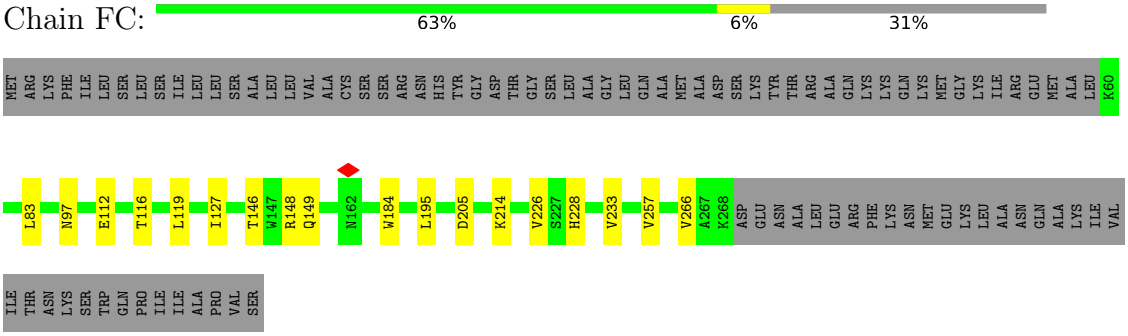
• Molecule 11: DotC

Chain EC:



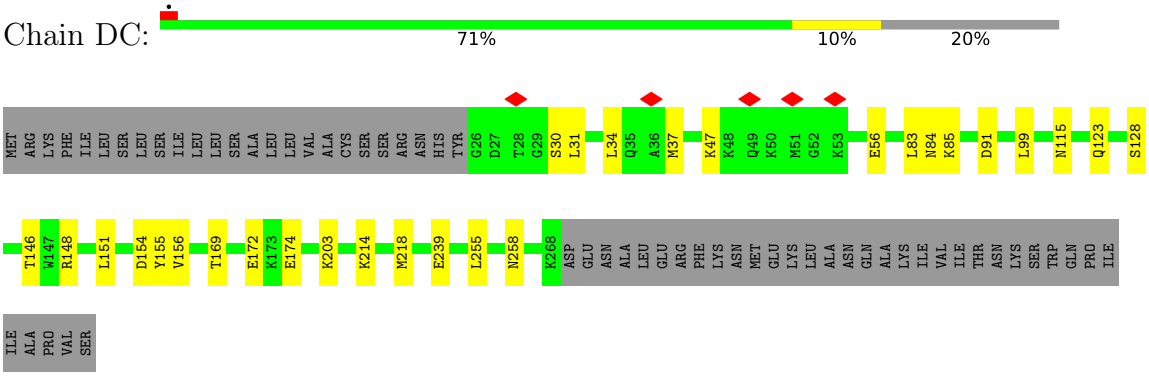
• Molecule 11: DotC

Chain FC:



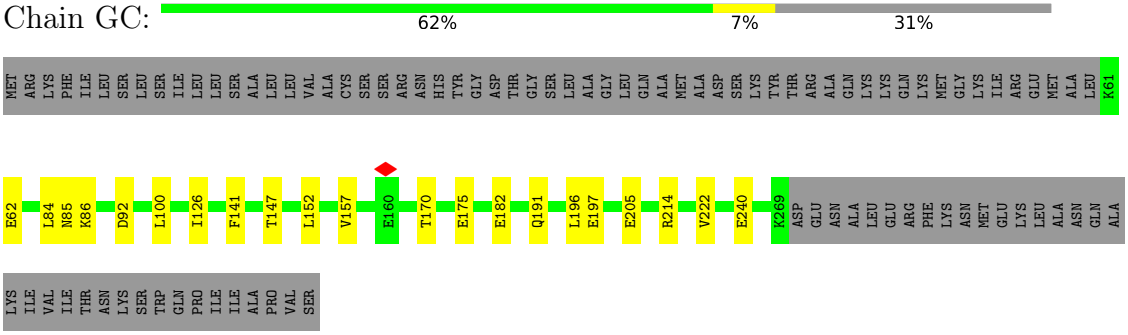
• Molecule 11: DotC

Chain DC:



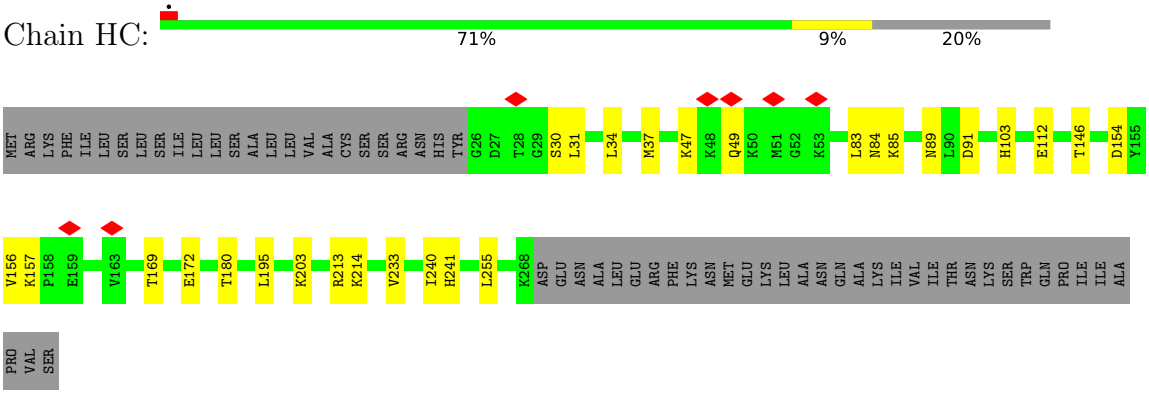
• Molecule 11: DotC

Chain GC:



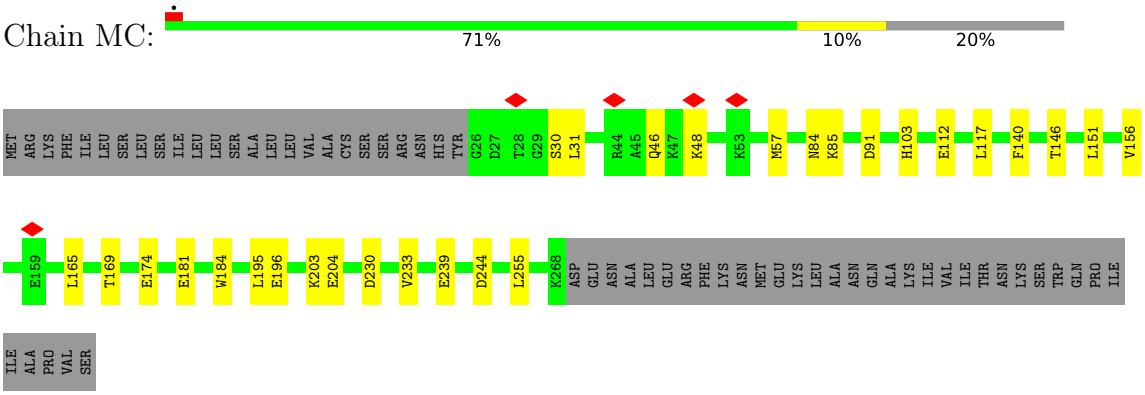
• Molecule 11: DotC

Chain HC:



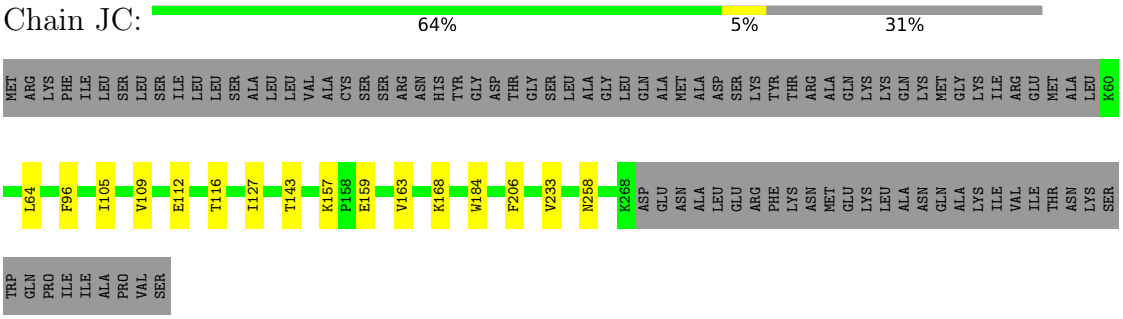
- Molecule 11: DotC

Chain MC:



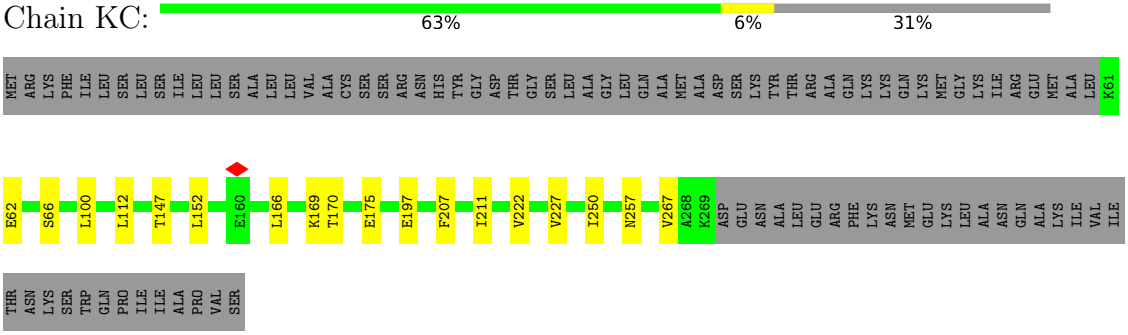
- Molecule 11: DotC

Chain JC:



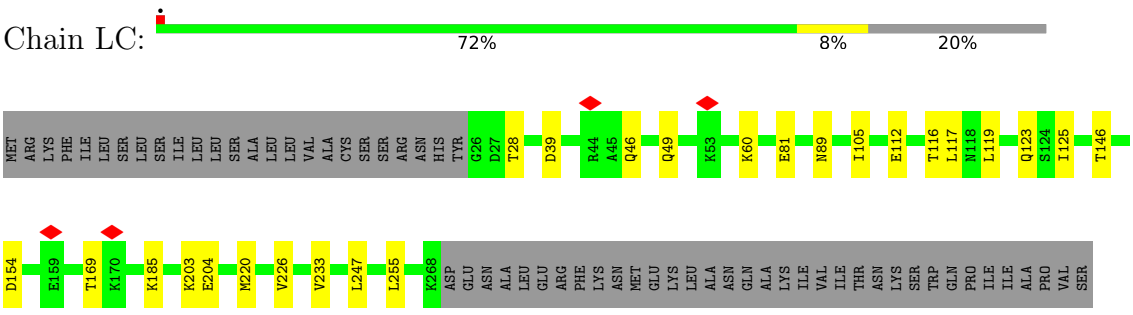
- Molecule 11: DotC

Chain KC:



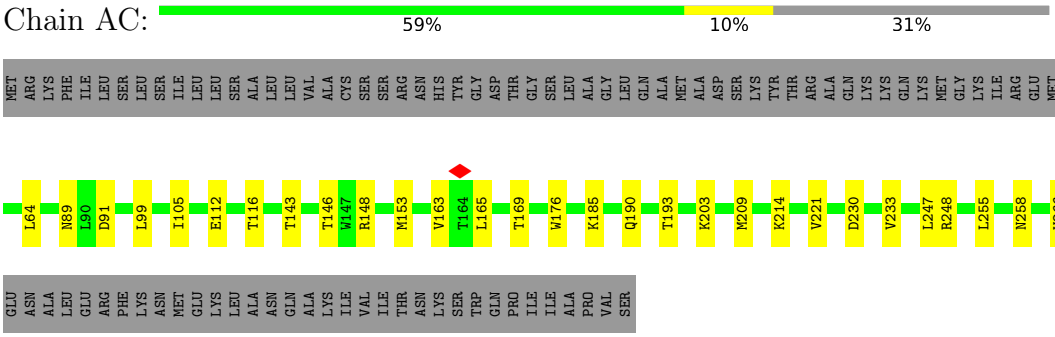
- Molecule 11: DotC

Chain LC:



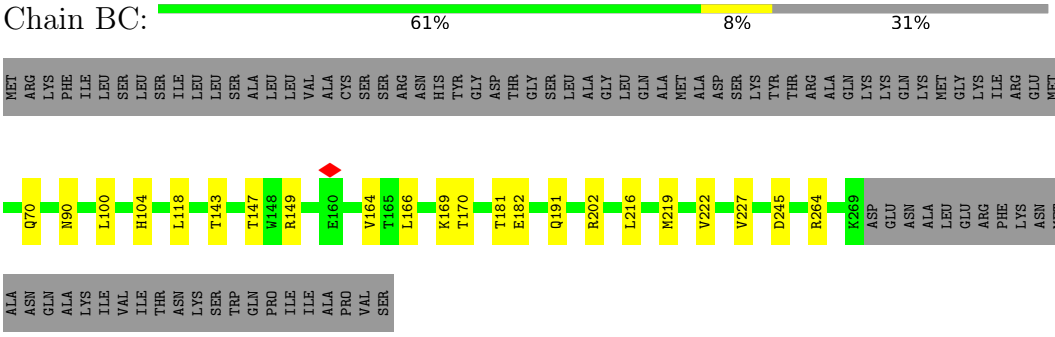
- Molecule 11: DotC

Chain AC:



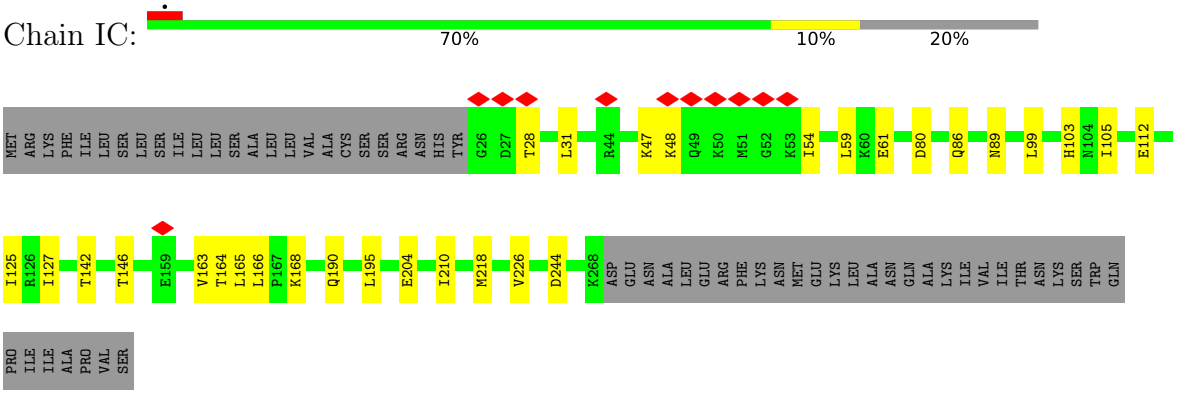
• Molecule 11: DotC

Chain BC:



• Molecule 11: DotC

Chain IC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75959	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	9.010	Depositor
Minimum map value	-4.020	Depositor
Average map value	0.091	Depositor
Map value standard deviation	0.547	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.244, 2.244, 2.244	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AG	0.29	0/1250	0.59	1/1699 (0.1%)
1	Ag	0.26	0/278	0.51	0/377
1	BG	0.30	0/1250	0.60	1/1699 (0.1%)
1	Bg	0.29	0/278	0.49	0/377
1	CG	0.30	0/1250	0.58	1/1699 (0.1%)
1	Cg	0.28	0/278	0.46	0/377
1	DG	0.30	0/1250	0.62	1/1699 (0.1%)
1	Dg	0.27	0/278	0.45	0/377
1	EG	0.29	0/1250	0.57	1/1699 (0.1%)
1	Eg	0.27	0/278	0.48	0/377
1	FG	0.30	0/1250	0.60	1/1699 (0.1%)
1	Fg	0.27	0/278	0.50	0/377
1	GG	0.30	0/1250	0.60	1/1699 (0.1%)
1	Gg	0.29	0/278	0.47	0/377
1	HG	0.29	0/1250	0.59	1/1699 (0.1%)
1	Hg	0.29	0/278	0.50	0/377
1	IG	0.30	0/1250	0.60	1/1699 (0.1%)
1	Ig	0.30	0/278	0.50	0/377
1	JG	0.31	0/1250	0.59	0/1699
1	Jg	0.29	0/278	0.48	0/377
1	KG	0.29	0/1250	0.60	1/1699 (0.1%)
1	Kg	0.28	0/278	0.47	0/377
1	LG	0.30	0/1250	0.59	1/1699 (0.1%)
1	Lg	0.26	0/278	0.47	0/377
1	MG	0.29	0/1250	0.58	0/1699
1	Mg	0.29	0/278	0.49	0/377
1	NG	0.30	0/1250	0.59	0/1699
1	OG	0.29	0/1250	0.60	1/1699 (0.1%)
1	PG	0.30	0/1250	0.59	1/1699 (0.1%)
1	VG	0.31	0/278	0.57	0/377
1	WG	0.28	0/278	0.53	0/377
1	XG	0.28	0/278	0.54	0/377
1	YG	0.29	0/278	0.54	0/377
1	ZG	0.29	0/278	0.55	0/377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AD	0.33	0/1107	0.53	0/1502
2	Ad	0.32	0/1078	0.51	0/1463
2	BD	0.33	0/1107	0.54	0/1502
2	Bd	0.34	0/1078	0.54	0/1463
2	CD	0.34	0/1107	0.54	0/1502
2	Cd	0.31	0/1078	0.51	0/1463
2	DD	0.33	0/1107	0.55	0/1502
2	Dd	0.31	0/1078	0.50	0/1463
2	ED	0.34	0/1107	0.55	0/1502
2	Ed	0.31	0/1078	0.51	0/1463
2	FD	0.33	0/1107	0.54	0/1502
2	Fd	0.32	0/1078	0.50	0/1463
2	GD	0.33	0/1107	0.56	0/1502
2	Gd	0.32	0/1078	0.54	0/1463
2	HD	0.33	0/1107	0.56	0/1502
2	Hd	0.32	0/1078	0.49	0/1463
2	ID	0.33	0/1107	0.55	0/1502
2	Id	0.31	0/1078	0.50	0/1463
2	JD	0.34	0/1107	0.55	0/1502
2	Jd	0.33	0/1078	0.51	0/1463
2	KD	0.33	0/1107	0.56	0/1502
2	Kd	0.31	0/1078	0.53	0/1463
2	LD	0.34	0/1107	0.55	0/1502
2	Ld	0.34	0/1078	0.52	0/1463
2	MD	0.34	0/1107	0.53	0/1502
2	Md	0.31	0/1078	0.51	0/1463
3	AF	0.27	0/490	0.54	0/660
3	Af	0.29	0/456	0.53	0/615
3	BF	0.28	0/490	0.55	0/660
3	Bf	0.29	0/456	0.53	0/615
3	CF	0.28	0/490	0.55	0/660
3	Cf	0.30	0/456	0.55	0/615
3	DF	0.28	0/490	0.57	0/660
3	Df	0.30	0/456	0.53	0/615
3	EF	0.29	0/490	0.52	0/660
3	Ef	0.29	0/456	0.53	0/615
3	FF	0.28	0/490	0.56	0/660
3	Ff	0.30	0/456	0.52	0/615
3	GF	0.28	0/490	0.57	0/660
3	Gf	0.29	0/456	0.53	0/615
3	HF	0.28	0/490	0.55	0/660
3	Hf	0.28	0/456	0.52	0/615
3	IF	0.29	0/490	0.57	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	If	0.28	0/456	0.53	0/615
3	JF	0.27	0/490	0.56	0/660
3	Jf	0.30	0/456	0.52	0/615
3	KF	0.28	0/490	0.54	0/660
3	Kf	0.29	0/456	0.56	0/615
3	LF	0.28	0/490	0.56	0/660
3	Lf	0.30	0/456	0.53	0/615
3	MF	0.28	0/490	0.58	0/660
3	Mf	0.29	0/456	0.54	0/615
3	VF	0.28	0/490	0.53	0/660
3	WF	0.28	0/490	0.55	0/660
3	XF	0.27	0/490	0.55	0/660
3	YF	0.27	0/490	0.56	0/660
3	ZF	0.28	0/490	0.55	0/660
4	AH	0.32	0/2033	0.56	0/2775
4	BH	0.32	0/2033	0.54	0/2775
4	CH	0.31	0/2033	0.54	0/2775
4	DH	0.31	0/2033	0.52	0/2775
4	EH	0.31	0/2033	0.55	0/2775
4	FH	0.31	0/2033	0.54	0/2775
4	GH	0.32	0/2033	0.56	0/2775
4	HH	0.32	0/2033	0.53	0/2775
4	IH	0.32	0/2033	0.53	0/2775
4	JH	0.32	0/2033	0.53	0/2775
4	KH	0.32	0/2033	0.55	0/2775
4	LH	0.32	0/2033	0.56	0/2775
4	MH	0.31	0/2033	0.56	0/2775
4	VH	0.29	0/1921	0.53	0/2620
4	WH	0.28	0/1921	0.51	0/2620
4	XH	0.29	0/1921	0.54	0/2620
4	YH	0.28	0/1921	0.53	0/2620
4	ZH	0.29	0/1921	0.55	0/2620
5	AK	0.34	0/1195	0.54	0/1616
5	BK	0.35	0/1195	0.55	0/1616
5	CK	0.33	0/1195	0.55	0/1616
5	DK	0.34	0/1195	0.55	0/1616
5	EK	0.34	0/1195	0.54	0/1616
5	FK	0.34	0/1195	0.56	0/1616
5	GK	0.33	0/1195	0.56	0/1616
5	HK	0.34	0/1195	0.55	0/1616
5	IK	0.32	0/1195	0.53	0/1616
5	JK	0.33	0/1195	0.55	0/1616
5	KK	0.34	0/1195	0.54	0/1616

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	LK	0.32	0/1195	0.56	0/1616
5	MK	0.33	0/1195	0.56	0/1616
6	AL	0.32	0/1417	0.57	0/1912
6	BL	0.34	0/1417	0.57	0/1912
6	CL	0.34	0/1417	0.56	0/1912
6	DL	0.33	0/1417	0.56	0/1912
6	EL	0.33	0/1417	0.56	0/1912
6	FL	0.33	0/1417	0.57	0/1912
6	GL	0.33	0/1417	0.56	0/1912
6	HL	0.33	0/1417	0.57	0/1912
6	IL	0.33	0/1417	0.58	0/1912
6	JL	0.33	0/1417	0.60	0/1912
6	KL	0.33	0/1417	0.57	0/1912
6	LL	0.33	0/1417	0.57	0/1912
6	ML	0.35	0/1417	0.56	0/1912
7	AM	0.31	0/1678	0.58	0/2262
7	BM	0.31	0/1678	0.61	0/2262
7	CM	0.31	0/1678	0.60	0/2262
7	DM	0.32	0/1678	0.59	0/2262
7	EM	0.31	0/1678	0.59	0/2262
7	FM	0.31	0/1678	0.59	0/2262
7	GM	0.32	0/1678	0.58	0/2262
7	HM	0.31	0/1678	0.56	0/2262
7	IM	0.30	0/1678	0.57	0/2262
7	JM	0.32	0/1678	0.60	0/2262
7	KM	0.32	0/1678	0.58	0/2262
7	LM	0.31	0/1678	0.57	0/2262
7	MM	0.31	0/1678	0.59	0/2262
8	AN	0.34	0/593	0.55	0/799
8	BN	0.36	0/593	0.54	0/799
8	CN	0.35	0/593	0.55	0/799
8	DN	0.37	0/593	0.56	0/799
8	EN	0.35	0/593	0.52	0/799
8	FN	0.34	0/593	0.55	0/799
8	GN	0.36	0/593	0.52	0/799
8	HN	0.37	0/593	0.52	0/799
8	IN	0.35	0/593	0.53	0/799
8	JN	0.35	0/593	0.54	0/799
8	KN	0.36	0/593	0.54	0/799
8	LN	0.36	0/593	0.53	0/799
8	MN	0.32	0/593	0.52	0/799
11	AC	0.34	0/1702	0.55	0/2315
11	BC	0.33	0/1702	0.53	0/2315

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	CC	0.34	0/1702	0.53	0/2315
11	DC	0.33	0/1957	0.53	0/2651
11	EC	0.33	0/1702	0.53	0/2315
11	FC	0.34	0/1702	0.52	0/2315
11	GC	0.33	0/1702	0.53	0/2315
11	HC	0.33	0/1957	0.52	0/2651
11	IC	0.31	0/1957	0.54	0/2651
11	JC	0.35	0/1702	0.54	0/2315
11	KC	0.34	0/1702	0.54	0/2315
11	LC	0.34	0/1957	0.53	0/2651
11	MC	0.33	0/1957	0.53	0/2651
All	All	0.32	0/191071	0.55	13/258997 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	KG	1040	LEU	CA-CB-CG	6.51	130.27	115.30
1	IG	1040	LEU	CA-CB-CG	5.88	128.83	115.30
1	FG	1040	LEU	CA-CB-CG	5.83	128.71	115.30
1	GG	1040	LEU	CA-CB-CG	5.81	128.67	115.30
1	BG	1040	LEU	CA-CB-CG	5.73	128.49	115.30
1	PG	1040	LEU	CA-CB-CG	5.58	128.14	115.30
1	OG	1040	LEU	CA-CB-CG	5.58	128.12	115.30
1	DG	1040	LEU	CA-CB-CG	5.46	127.87	115.30
1	AG	1040	LEU	CA-CB-CG	5.43	127.79	115.30
1	LG	1040	LEU	CA-CB-CG	5.41	127.75	115.30
1	CG	1040	LEU	CA-CB-CG	5.36	127.64	115.30
1	EG	1040	LEU	CA-CB-CG	5.30	127.49	115.30
1	HG	1040	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	Ag	32/1048 (3%)	32 (100%)	0	0	100	100
1	BG	161/1048 (15%)	156 (97%)	5 (3%)	0	100	100
1	Bg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	CG	161/1048 (15%)	151 (94%)	10 (6%)	0	100	100
1	Cg	32/1048 (3%)	32 (100%)	0	0	100	100
1	DG	161/1048 (15%)	155 (96%)	6 (4%)	0	100	100
1	Dg	32/1048 (3%)	32 (100%)	0	0	100	100
1	EG	161/1048 (15%)	157 (98%)	4 (2%)	0	100	100
1	Eg	32/1048 (3%)	32 (100%)	0	0	100	100
1	FG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Fg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	GG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Gg	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	HG	161/1048 (15%)	150 (93%)	11 (7%)	0	100	100
1	Hg	32/1048 (3%)	29 (91%)	3 (9%)	0	100	100
1	IG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Ig	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	JG	161/1048 (15%)	152 (94%)	9 (6%)	0	100	100
1	Jg	32/1048 (3%)	32 (100%)	0	0	100	100
1	KG	161/1048 (15%)	151 (94%)	10 (6%)	0	100	100
1	Kg	32/1048 (3%)	32 (100%)	0	0	100	100
1	LG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	Lg	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
1	MG	161/1048 (15%)	158 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Mg	32/1048 (3%)	32 (100%)	0	0	100	100
1	NG	161/1048 (15%)	154 (96%)	7 (4%)	0	100	100
1	OG	161/1048 (15%)	150 (93%)	11 (7%)	0	100	100
1	PG	161/1048 (15%)	153 (95%)	8 (5%)	0	100	100
1	VG	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	WG	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
1	XG	32/1048 (3%)	32 (100%)	0	0	100	100
1	YG	32/1048 (3%)	32 (100%)	0	0	100	100
1	ZG	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
2	AD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Ad	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
2	BD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Bd	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
2	CD	138/163 (85%)	129 (94%)	9 (6%)	0	100	100
2	Cd	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
2	DD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Dd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ED	138/163 (85%)	135 (98%)	3 (2%)	0	100	100
2	Ed	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
2	FD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Fd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
2	GD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Gd	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
2	HD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Hd	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
2	ID	138/163 (85%)	129 (94%)	9 (6%)	0	100	100
2	Id	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
2	JD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Jd	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
2	KD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Kd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LD	138/163 (85%)	131 (95%)	7 (5%)	0	100	100
2	Ld	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
2	MD	138/163 (85%)	130 (94%)	8 (6%)	0	100	100
2	Md	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
3	AF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Af	57/269 (21%)	56 (98%)	1 (2%)	0	100	100
3	BF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Bf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	CF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
3	Cf	57/269 (21%)	51 (90%)	6 (10%)	0	100	100
3	DF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Df	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	EF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Ef	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	FF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Ff	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	GF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	Gf	57/269 (21%)	50 (88%)	7 (12%)	0	100	100
3	HF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Hf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	IF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	JF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Jf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	KF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Kf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	LF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	Lf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	MF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Mf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	VF	61/269 (23%)	55 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	WF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
3	XF	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
3	YF	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
3	ZF	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
4	AH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
4	BH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
4	CH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100
4	DH	256/361 (71%)	237 (93%)	19 (7%)	0	100	100
4	EH	256/361 (71%)	246 (96%)	10 (4%)	0	100	100
4	FH	256/361 (71%)	248 (97%)	8 (3%)	0	100	100
4	GH	256/361 (71%)	237 (93%)	19 (7%)	0	100	100
4	HH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
4	IH	256/361 (71%)	244 (95%)	12 (5%)	0	100	100
4	JH	256/361 (71%)	239 (93%)	17 (7%)	0	100	100
4	KH	256/361 (71%)	238 (93%)	18 (7%)	0	100	100
4	LH	256/361 (71%)	238 (93%)	18 (7%)	0	100	100
4	MH	256/361 (71%)	235 (92%)	21 (8%)	0	100	100
4	VH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
4	WH	239/361 (66%)	230 (96%)	9 (4%)	0	100	100
4	XH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
4	YH	239/361 (66%)	222 (93%)	17 (7%)	0	100	100
4	ZH	239/361 (66%)	229 (96%)	10 (4%)	0	100	100
5	AK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
5	BK	149/189 (79%)	140 (94%)	9 (6%)	0	100	100
5	CK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
5	DK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
5	EK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
5	FK	149/189 (79%)	143 (96%)	6 (4%)	0	100	100
5	GK	149/189 (79%)	141 (95%)	8 (5%)	0	100	100
5	HK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
5	IK	149/189 (79%)	140 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	JK	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
5	KK	149/189 (79%)	137 (92%)	12 (8%)	0	100	100
5	LK	149/189 (79%)	141 (95%)	8 (5%)	0	100	100
5	MK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	AL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
6	BL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
6	CL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
6	DL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
6	EL	169/249 (68%)	160 (95%)	9 (5%)	0	100	100
6	FL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
6	GL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
6	HL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
6	IL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
6	JL	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
6	KL	169/249 (68%)	163 (96%)	6 (4%)	0	100	100
6	LL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
6	ML	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
7	AM	206/320 (64%)	187 (91%)	19 (9%)	0	100	100
7	BM	206/320 (64%)	183 (89%)	23 (11%)	0	100	100
7	CM	206/320 (64%)	185 (90%)	21 (10%)	0	100	100
7	DM	206/320 (64%)	193 (94%)	13 (6%)	0	100	100
7	EM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
7	FM	206/320 (64%)	188 (91%)	18 (9%)	0	100	100
7	GM	206/320 (64%)	186 (90%)	20 (10%)	0	100	100
7	HM	206/320 (64%)	186 (90%)	20 (10%)	0	100	100
7	IM	206/320 (64%)	188 (91%)	18 (9%)	0	100	100
7	JM	206/320 (64%)	183 (89%)	23 (11%)	0	100	100
7	KM	206/320 (64%)	191 (93%)	15 (7%)	0	100	100
7	LM	206/320 (64%)	186 (90%)	20 (10%)	0	100	100
7	MM	206/320 (64%)	181 (88%)	25 (12%)	0	100	100
8	AN	76/124 (61%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BN	76/124 (61%)	72 (95%)	4 (5%)	0	100	100
8	CN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
8	DN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	EN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
8	FN	76/124 (61%)	67 (88%)	9 (12%)	0	100	100
8	GN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
8	HN	76/124 (61%)	71 (93%)	5 (7%)	0	100	100
8	IN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	JN	76/124 (61%)	67 (88%)	9 (12%)	0	100	100
8	KN	76/124 (61%)	69 (91%)	7 (9%)	0	100	100
8	LN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
8	MN	76/124 (61%)	70 (92%)	6 (8%)	0	100	100
11	AC	207/303 (68%)	195 (94%)	12 (6%)	0	100	100
11	BC	207/303 (68%)	198 (96%)	9 (4%)	0	100	100
11	CC	207/303 (68%)	197 (95%)	10 (5%)	0	100	100
11	DC	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
11	EC	207/303 (68%)	193 (93%)	14 (7%)	0	100	100
11	FC	207/303 (68%)	192 (93%)	15 (7%)	0	100	100
11	GC	207/303 (68%)	188 (91%)	19 (9%)	0	100	100
11	HC	241/303 (80%)	227 (94%)	14 (6%)	0	100	100
11	IC	241/303 (80%)	230 (95%)	11 (5%)	0	100	100
11	JC	207/303 (68%)	196 (95%)	11 (5%)	0	100	100
11	KC	207/303 (68%)	195 (94%)	12 (6%)	0	100	100
11	LC	241/303 (80%)	230 (95%)	11 (5%)	0	100	100
11	MC	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
All	All	23724/70112 (34%)	22355 (94%)	1369 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AG	135/765 (18%)	113 (84%)	22 (16%)	2 14
1	Ag	31/765 (4%)	26 (84%)	5 (16%)	2 15
1	BG	135/765 (18%)	117 (87%)	18 (13%)	4 20
1	Bg	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	CG	135/765 (18%)	118 (87%)	17 (13%)	4 21
1	Cg	31/765 (4%)	26 (84%)	5 (16%)	2 15
1	DG	135/765 (18%)	115 (85%)	20 (15%)	3 17
1	Dg	31/765 (4%)	21 (68%)	10 (32%)	0 2
1	EG	135/765 (18%)	114 (84%)	21 (16%)	2 16
1	Eg	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	FG	135/765 (18%)	114 (84%)	21 (16%)	2 16
1	Fg	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	GG	135/765 (18%)	112 (83%)	23 (17%)	2 13
1	Gg	31/765 (4%)	29 (94%)	2 (6%)	17 44
1	HG	135/765 (18%)	114 (84%)	21 (16%)	2 16
1	Hg	31/765 (4%)	29 (94%)	2 (6%)	17 44
1	IG	135/765 (18%)	115 (85%)	20 (15%)	3 17
1	Ig	31/765 (4%)	23 (74%)	8 (26%)	0 4
1	JG	135/765 (18%)	118 (87%)	17 (13%)	4 21
1	Jg	31/765 (4%)	23 (74%)	8 (26%)	0 4
1	KG	135/765 (18%)	116 (86%)	19 (14%)	3 18
1	Kg	31/765 (4%)	26 (84%)	5 (16%)	2 15
1	LG	135/765 (18%)	113 (84%)	22 (16%)	2 14
1	Lg	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	MG	135/765 (18%)	121 (90%)	14 (10%)	7 27
1	Mg	31/765 (4%)	24 (77%)	7 (23%)	1 6
1	NG	135/765 (18%)	114 (84%)	21 (16%)	2 16
1	OG	135/765 (18%)	113 (84%)	22 (16%)	2 14
1	PG	135/765 (18%)	118 (87%)	17 (13%)	4 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	VG	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	WG	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	XG	31/765 (4%)	25 (81%)	6 (19%)	1 9
1	YG	31/765 (4%)	27 (87%)	4 (13%)	4 20
1	ZG	31/765 (4%)	25 (81%)	6 (19%)	1 9
2	AD	121/139 (87%)	104 (86%)	17 (14%)	3 19
2	Ad	118/139 (85%)	101 (86%)	17 (14%)	3 18
2	BD	121/139 (87%)	106 (88%)	15 (12%)	4 21
2	Bd	118/139 (85%)	108 (92%)	10 (8%)	10 36
2	CD	121/139 (87%)	102 (84%)	19 (16%)	2 15
2	Cd	118/139 (85%)	107 (91%)	11 (9%)	9 30
2	DD	121/139 (87%)	111 (92%)	10 (8%)	11 36
2	Dd	118/139 (85%)	106 (90%)	12 (10%)	7 27
2	ED	121/139 (87%)	108 (89%)	13 (11%)	6 26
2	Ed	118/139 (85%)	106 (90%)	12 (10%)	7 27
2	FD	121/139 (87%)	107 (88%)	14 (12%)	5 23
2	Fd	118/139 (85%)	103 (87%)	15 (13%)	4 21
2	GD	121/139 (87%)	106 (88%)	15 (12%)	4 21
2	Gd	118/139 (85%)	105 (89%)	13 (11%)	6 25
2	HD	121/139 (87%)	109 (90%)	12 (10%)	8 28
2	Hd	118/139 (85%)	104 (88%)	14 (12%)	5 22
2	ID	121/139 (87%)	105 (87%)	16 (13%)	4 20
2	Id	118/139 (85%)	101 (86%)	17 (14%)	3 18
2	JD	121/139 (87%)	107 (88%)	14 (12%)	5 23
2	Jd	118/139 (85%)	101 (86%)	17 (14%)	3 18
2	KD	121/139 (87%)	114 (94%)	7 (6%)	20 47
2	Kd	118/139 (85%)	105 (89%)	13 (11%)	6 25
2	LD	121/139 (87%)	105 (87%)	16 (13%)	4 20
2	Ld	118/139 (85%)	105 (89%)	13 (11%)	6 25
2	MD	121/139 (87%)	106 (88%)	15 (12%)	4 21
2	Md	118/139 (85%)	107 (91%)	11 (9%)	9 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AF	53/237 (22%)	48 (91%)	5 (9%)	8 30
3	Af	49/237 (21%)	43 (88%)	6 (12%)	5 22
3	BF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	Bf	49/237 (21%)	42 (86%)	7 (14%)	3 18
3	CF	53/237 (22%)	48 (91%)	5 (9%)	8 30
3	Cf	49/237 (21%)	40 (82%)	9 (18%)	1 10
3	DF	53/237 (22%)	49 (92%)	4 (8%)	13 40
3	Df	49/237 (21%)	44 (90%)	5 (10%)	7 27
3	EF	53/237 (22%)	49 (92%)	4 (8%)	13 40
3	Ef	49/237 (21%)	45 (92%)	4 (8%)	11 36
3	FF	53/237 (22%)	44 (83%)	9 (17%)	2 13
3	Ff	49/237 (21%)	45 (92%)	4 (8%)	11 36
3	GF	53/237 (22%)	49 (92%)	4 (8%)	13 40
3	Gf	49/237 (21%)	46 (94%)	3 (6%)	18 46
3	HF	53/237 (22%)	46 (87%)	7 (13%)	4 20
3	Hf	49/237 (21%)	40 (82%)	9 (18%)	1 10
3	IF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	If	49/237 (21%)	42 (86%)	7 (14%)	3 18
3	JF	53/237 (22%)	51 (96%)	2 (4%)	33 58
3	Jf	49/237 (21%)	44 (90%)	5 (10%)	7 27
3	KF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	Kf	49/237 (21%)	44 (90%)	5 (10%)	7 27
3	LF	53/237 (22%)	47 (89%)	6 (11%)	6 24
3	Lf	49/237 (21%)	43 (88%)	6 (12%)	5 22
3	MF	53/237 (22%)	48 (91%)	5 (9%)	8 30
3	Mf	49/237 (21%)	44 (90%)	5 (10%)	7 27
3	VF	53/237 (22%)	45 (85%)	8 (15%)	3 16
3	WF	53/237 (22%)	51 (96%)	2 (4%)	33 58
3	XF	53/237 (22%)	51 (96%)	2 (4%)	33 58
3	YF	53/237 (22%)	49 (92%)	4 (8%)	13 40
3	ZF	53/237 (22%)	47 (89%)	6 (11%)	6 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	AH	220/300 (73%)	200 (91%)	20 (9%)	9 31
4	BH	220/300 (73%)	201 (91%)	19 (9%)	10 35
4	CH	220/300 (73%)	196 (89%)	24 (11%)	6 25
4	DH	220/300 (73%)	199 (90%)	21 (10%)	8 29
4	EH	220/300 (73%)	193 (88%)	27 (12%)	4 22
4	FH	220/300 (73%)	194 (88%)	26 (12%)	5 23
4	GH	220/300 (73%)	191 (87%)	29 (13%)	4 20
4	HH	220/300 (73%)	198 (90%)	22 (10%)	7 28
4	IH	220/300 (73%)	187 (85%)	33 (15%)	3 16
4	JH	220/300 (73%)	196 (89%)	24 (11%)	6 25
4	KH	220/300 (73%)	191 (87%)	29 (13%)	4 20
4	LH	220/300 (73%)	195 (89%)	25 (11%)	5 24
4	MH	220/300 (73%)	194 (88%)	26 (12%)	5 23
4	VH	207/300 (69%)	183 (88%)	24 (12%)	5 23
4	WH	207/300 (69%)	183 (88%)	24 (12%)	5 23
4	XH	207/300 (69%)	176 (85%)	31 (15%)	3 16
4	YH	207/300 (69%)	177 (86%)	30 (14%)	3 17
4	ZH	207/300 (69%)	190 (92%)	17 (8%)	11 36
5	AK	129/163 (79%)	110 (85%)	19 (15%)	3 17
5	BK	129/163 (79%)	111 (86%)	18 (14%)	3 19
5	CK	129/163 (79%)	110 (85%)	19 (15%)	3 17
5	DK	129/163 (79%)	114 (88%)	15 (12%)	5 23
5	EK	129/163 (79%)	116 (90%)	13 (10%)	7 27
5	FK	129/163 (79%)	115 (89%)	14 (11%)	6 25
5	GK	129/163 (79%)	113 (88%)	16 (12%)	4 21
5	HK	129/163 (79%)	112 (87%)	17 (13%)	4 20
5	IK	129/163 (79%)	114 (88%)	15 (12%)	5 23
5	JK	129/163 (79%)	114 (88%)	15 (12%)	5 23
5	KK	129/163 (79%)	114 (88%)	15 (12%)	5 23
5	LK	129/163 (79%)	111 (86%)	18 (14%)	3 19
5	MK	129/163 (79%)	117 (91%)	12 (9%)	9 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	AL	148/203 (73%)	136 (92%)	12 (8%)	11 37
6	BL	148/203 (73%)	131 (88%)	17 (12%)	5 23
6	CL	148/203 (73%)	127 (86%)	21 (14%)	3 18
6	DL	148/203 (73%)	133 (90%)	15 (10%)	7 27
6	EL	148/203 (73%)	127 (86%)	21 (14%)	3 18
6	FL	148/203 (73%)	137 (93%)	11 (7%)	13 40
6	GL	148/203 (73%)	132 (89%)	16 (11%)	6 26
6	HL	148/203 (73%)	135 (91%)	13 (9%)	10 33
6	IL	148/203 (73%)	135 (91%)	13 (9%)	10 33
6	JL	148/203 (73%)	132 (89%)	16 (11%)	6 26
6	KL	148/203 (73%)	134 (90%)	14 (10%)	8 29
6	LL	148/203 (73%)	128 (86%)	20 (14%)	4 19
6	ML	148/203 (73%)	132 (89%)	16 (11%)	6 26
7	AM	175/276 (63%)	148 (85%)	27 (15%)	2 16
7	BM	175/276 (63%)	153 (87%)	22 (13%)	4 21
7	CM	175/276 (63%)	154 (88%)	21 (12%)	5 22
7	DM	175/276 (63%)	149 (85%)	26 (15%)	3 16
7	EM	175/276 (63%)	153 (87%)	22 (13%)	4 21
7	FM	175/276 (63%)	152 (87%)	23 (13%)	4 20
7	GM	175/276 (63%)	149 (85%)	26 (15%)	3 16
7	HM	175/276 (63%)	154 (88%)	21 (12%)	5 22
7	IM	175/276 (63%)	151 (86%)	24 (14%)	3 19
7	JM	175/276 (63%)	143 (82%)	32 (18%)	1 11
7	KM	175/276 (63%)	154 (88%)	21 (12%)	5 22
7	LM	175/276 (63%)	151 (86%)	24 (14%)	3 19
7	MM	175/276 (63%)	152 (87%)	23 (13%)	4 20
8	AN	66/107 (62%)	58 (88%)	8 (12%)	5 22
8	BN	66/107 (62%)	60 (91%)	6 (9%)	9 31
8	CN	66/107 (62%)	57 (86%)	9 (14%)	3 19
8	DN	66/107 (62%)	62 (94%)	4 (6%)	18 46
8	EN	66/107 (62%)	57 (86%)	9 (14%)	3 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	FN	66/107 (62%)	55 (83%)	11 (17%)	2	14
8	GN	66/107 (62%)	59 (89%)	7 (11%)	6	26
8	HN	66/107 (62%)	57 (86%)	9 (14%)	3	19
8	IN	66/107 (62%)	55 (83%)	11 (17%)	2	14
8	JN	66/107 (62%)	59 (89%)	7 (11%)	6	26
8	KN	66/107 (62%)	53 (80%)	13 (20%)	1	9
8	LN	66/107 (62%)	53 (80%)	13 (20%)	1	9
8	MN	66/107 (62%)	54 (82%)	12 (18%)	1	11
11	AC	178/257 (69%)	149 (84%)	29 (16%)	2	14
11	BC	178/257 (69%)	155 (87%)	23 (13%)	4	20
11	CC	178/257 (69%)	152 (85%)	26 (15%)	3	17
11	DC	203/257 (79%)	174 (86%)	29 (14%)	3	18
11	EC	178/257 (69%)	154 (86%)	24 (14%)	4	19
11	FC	178/257 (69%)	160 (90%)	18 (10%)	7	27
11	GC	178/257 (69%)	157 (88%)	21 (12%)	5	23
11	HC	203/257 (79%)	175 (86%)	28 (14%)	3	19
11	IC	203/257 (79%)	173 (85%)	30 (15%)	3	17
11	JC	178/257 (69%)	162 (91%)	16 (9%)	9	32
11	KC	178/257 (69%)	160 (90%)	18 (10%)	7	27
11	LC	203/257 (79%)	178 (88%)	25 (12%)	4	22
11	MC	203/257 (79%)	174 (86%)	29 (14%)	3	18
All	All	20484/55449 (37%)	17938 (88%)	2546 (12%)	8	21

All (2546) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AG	865	THR
1	AG	867	ASP
1	AG	869	MET
1	AG	880	ASP
1	AG	885	ILE
1	AG	900	ILE
1	AG	902	SER
1	AG	910	ASP
1	AG	911	LYS

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Mol	Chain	Res	Type
1	AG	913	VAL
1	AG	939	THR
1	AG	944	LEU
1	AG	947	ARG
1	AG	962	SER
1	AG	965	LEU
1	AG	968	PHE
1	AG	972	PHE
1	AG	1010	THR
1	AG	1017	GLN
1	AG	1037	LEU
1	AG	1044	ASP
1	AG	1045	VAL
2	GD	23	MET
2	GD	24	LYS
2	GD	29	PRO
2	GD	30	ILE
2	GD	41	LEU
2	GD	50	ASP
2	GD	52	MET
2	GD	53	LEU
2	GD	55	MET
2	GD	91	ILE
2	GD	115	VAL
2	GD	127	SER
2	GD	147	VAL
2	GD	155	GLU
2	GD	162	TYR
3	GF	213	GLN
3	GF	215	VAL
3	GF	232	VAL
3	GF	233	ARG
1	Gg	817	THR
1	Gg	819	VAL
4	GH	108	ASP
4	GH	109	LYS
4	GH	138	GLU
4	GH	141	LYS
4	GH	147	THR
4	GH	176	VAL
4	GH	180	VAL
4	GH	212	THR

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Mol	Chain	Res	Type
4	GH	218	THR
4	GH	219	LYS
4	GH	220	LEU
4	GH	238	MET
4	GH	241	LEU
4	GH	245	GLN
4	GH	248	VAL
4	GH	249	ASP
4	GH	250	TYR
4	GH	253	ASP
4	GH	278	ASP
4	GH	284	LEU
4	GH	287	VAL
4	GH	292	SER
4	GH	296	VAL
4	GH	313	VAL
4	GH	314	ARG
4	GH	325	LEU
4	GH	335	HIS
4	GH	347	VAL
4	GH	353	VAL
5	GK	65	ILE
5	GK	83	LEU
5	GK	92	ASN
5	GK	93	TRP
5	GK	98	LEU
5	GK	99	LEU
5	GK	106	LEU
5	GK	111	LYS
5	GK	126	VAL
5	GK	134	LEU
5	GK	150	ASP
5	GK	162	ASP
5	GK	170	LEU
5	GK	180	VAL
5	GK	182	ILE
5	GK	183	THR
6	GL	57	VAL
6	GL	109	LEU
6	GL	129	THR
6	GL	131	LYS
6	GL	134	MET

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Mol	Chain	Res	Type
6	GL	140	LEU
6	GL	155	LEU
6	GL	163	ILE
6	GL	169	THR
6	GL	170	ASP
6	GL	172	VAL
6	GL	174	SER
6	GL	175	ARG
6	GL	211	LYS
6	GL	212	ASN
6	GL	217	ASN
7	GM	114	ASN
7	GM	131	THR
7	GM	134	LEU
7	GM	146	LEU
7	GM	152	LEU
7	GM	171	ARG
7	GM	173	LEU
7	GM	174	GLN
7	GM	176	VAL
7	GM	180	ASP
7	GM	182	LYS
7	GM	184	LEU
7	GM	191	LEU
7	GM	202	LEU
7	GM	204	LEU
7	GM	207	ILE
7	GM	212	LEU
7	GM	215	ARG
7	GM	229	ASN
7	GM	245	TYR
7	GM	257	ASP
7	GM	263	ILE
7	GM	292	MET
7	GM	308	ASP
7	GM	310	LYS
7	GM	315	TYR
8	GN	62	ASN
8	GN	77	ASP
8	GN	84	CYS
8	GN	94	GLN
8	GN	101	VAL

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Mol	Chain	Res	Type
8	GN	111	GLU
8	GN	114	LEU
2	Gd	36	ASP
2	Gd	54	GLU
2	Gd	58	VAL
2	Gd	59	GLU
2	Gd	61	VAL
2	Gd	63	THR
2	Gd	82	ARG
2	Gd	93	GLU
2	Gd	126	GLU
2	Gd	128	LEU
2	Gd	145	ILE
2	Gd	147	VAL
2	Gd	150	ASN
3	Gf	215	VAL
3	Gf	243	MET
3	Gf	253	ARG
2	HD	38	THR
2	HD	51	SER
2	HD	52	MET
2	HD	55	MET
2	HD	82	ARG
2	HD	108	VAL
2	HD	115	VAL
2	HD	117	VAL
2	HD	142	LYS
2	HD	147	VAL
2	HD	156	LEU
2	HD	162	TYR
3	HF	215	VAL
3	HF	230	LEU
3	HF	231	THR
3	HF	232	VAL
3	HF	233	ARG
3	HF	238	ILE
3	HF	264	PHE
1	Hg	800	ASP
1	Hg	820	TYR
2	Dd	36	ASP
2	Dd	41	LEU
2	Dd	43	GLU

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Mol	Chain	Res	Type
2	Dd	52	MET
2	Dd	55	MET
2	Dd	61	VAL
2	Dd	92	GLU
2	Dd	97	ARG
2	Dd	108	VAL
2	Dd	115	VAL
2	Dd	123	THR
2	Dd	146	HIS
4	HH	108	ASP
4	HH	117	ARG
4	HH	122	LEU
4	HH	147	THR
4	HH	180	VAL
4	HH	205	GLN
4	HH	211	ASN
4	HH	226	LEU
4	HH	231	ARG
4	HH	239	LEU
4	HH	241	LEU
4	HH	250	TYR
4	HH	253	ASP
4	HH	284	LEU
4	HH	287	VAL
4	HH	294	ARG
4	HH	296	VAL
4	HH	307	SER
4	HH	335	HIS
4	HH	352	LYS
4	HH	356	LEU
4	HH	361	LEU
5	HK	40	LYS
5	HK	58	THR
5	HK	70	VAL
5	HK	72	GLN
5	HK	73	ASN
5	HK	98	LEU
5	HK	101	GLU
5	HK	106	LEU
5	HK	111	LYS
5	HK	116	VAL
5	HK	144	LEU

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Mol	Chain	Res	Type
5	HK	149	VAL
5	HK	153	ILE
5	HK	156	THR
5	HK	170	LEU
5	HK	180	VAL
5	HK	183	THR
6	HL	57	VAL
6	HL	93	LEU
6	HL	100	ASP
6	HL	109	LEU
6	HL	131	LYS
6	HL	148	LEU
6	HL	155	LEU
6	HL	165	VAL
6	HL	170	ASP
6	HL	172	VAL
6	HL	174	SER
6	HL	212	ASN
6	HL	227	ARG
7	HM	127	ASN
7	HM	134	LEU
7	HM	137	TYR
7	HM	144	THR
7	HM	149	ASN
7	HM	152	LEU
7	HM	153	GLN
7	HM	162	VAL
7	HM	175	ILE
7	HM	176	VAL
7	HM	182	LYS
7	HM	183	VAL
7	HM	184	LEU
7	HM	188	PHE
7	HM	212	LEU
7	HM	222	ILE
7	HM	233	VAL
7	HM	290	ASP
7	HM	292	MET
7	HM	304	TRP
7	HM	308	ASP
8	HN	44	LYS
8	HN	51	CYS

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Mol	Chain	Res	Type
8	HN	70	CYS
8	HN	81	LEU
8	HN	84	CYS
8	HN	91	VAL
8	HN	95	LEU
8	HN	111	GLU
8	HN	115	GLN
2	Hd	27	LYS
2	Hd	36	ASP
2	Hd	53	LEU
2	Hd	58	VAL
2	Hd	61	VAL
2	Hd	63	THR
2	Hd	70	THR
2	Hd	78	ASN
2	Hd	88	SER
2	Hd	93	GLU
2	Hd	94	LEU
2	Hd	115	VAL
2	Hd	150	ASN
2	Hd	153	VAL
3	Hf	210	TYR
3	Hf	212	ILE
3	Hf	215	VAL
3	Hf	219	ARG
3	Hf	223	ILE
3	Hf	233	ARG
3	Hf	244	VAL
3	Hf	247	ILE
3	Hf	250	LEU
1	Bg	792	GLN
1	Bg	796	GLN
1	Bg	800	ASP
1	Bg	809	VAL
1	Bg	815	VAL
1	Bg	819	VAL
1	BG	864	LYS
1	BG	865	THR
1	BG	880	ASP
1	BG	885	ILE
1	BG	900	ILE
1	BG	910	ASP

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Mol	Chain	Res	Type
1	BG	911	LYS
1	BG	912	MET
1	BG	913	VAL
1	BG	916	PHE
1	BG	930	ILE
1	BG	944	LEU
1	BG	962	SER
1	BG	965	LEU
1	BG	972	PHE
1	BG	1010	THR
1	BG	1028	THR
1	BG	1040	LEU
2	ID	23	MET
2	ID	51	SER
2	ID	55	MET
2	ID	73	ILE
2	ID	78	ASN
2	ID	85	VAL
2	ID	86	ASP
2	ID	108	VAL
2	ID	115	VAL
2	ID	124	LYS
2	ID	126	GLU
2	ID	134	ASP
2	ID	147	VAL
2	ID	152	GLN
2	ID	154	VAL
2	ID	160	LYS
3	IF	215	VAL
3	IF	230	LEU
3	IF	231	THR
3	IF	243	MET
3	IF	256	THR
3	IF	266	GLN
1	Ig	793	GLU
1	Ig	795	GLN
1	Ig	808	LEU
1	Ig	809	VAL
1	Ig	810	GLN
1	Ig	814	GLN
1	Ig	817	THR
1	Ig	819	VAL

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Mol	Chain	Res	Type
4	IH	108	ASP
4	IH	110	LYS
4	IH	125	GLU
4	IH	147	THR
4	IH	152	THR
4	IH	170	ARG
4	IH	180	VAL
4	IH	185	THR
4	IH	196	LEU
4	IH	203	ASN
4	IH	208	LYS
4	IH	218	THR
4	IH	219	LYS
4	IH	225	ASN
4	IH	230	LEU
4	IH	231	ARG
4	IH	238	MET
4	IH	240	THR
4	IH	242	ILE
4	IH	245	GLN
4	IH	248	VAL
4	IH	255	ARG
4	IH	256	VAL
4	IH	257	GLN
4	IH	262	ASN
4	IH	284	LEU
4	IH	285	GLU
4	IH	294	ARG
4	IH	313	VAL
4	IH	332	ASP
4	IH	334	THR
4	IH	353	VAL
4	IH	361	LEU
5	IK	45	VAL
5	IK	46	ASP
5	IK	83	LEU
5	IK	86	ASP
5	IK	106	LEU
5	IK	108	GLN
5	IK	111	LYS
5	IK	112	ILE
5	IK	116	VAL

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Mol	Chain	Res	Type
5	IK	126	VAL
5	IK	144	LEU
5	IK	180	VAL
5	IK	182	ILE
5	IK	183	THR
5	IK	188	VAL
6	IL	57	VAL
6	IL	91	VAL
6	IL	100	ASP
6	IL	109	LEU
6	IL	121	ASP
6	IL	129	THR
6	IL	131	LYS
6	IL	137	SER
6	IL	148	LEU
6	IL	172	VAL
6	IL	174	SER
6	IL	212	ASN
6	IL	217	ASN
7	IM	115	ARG
7	IM	116	PHE
7	IM	118	TYR
7	IM	131	THR
7	IM	134	LEU
7	IM	146	LEU
7	IM	149	ASN
7	IM	152	LEU
7	IM	153	GLN
7	IM	162	VAL
7	IM	176	VAL
7	IM	180	ASP
7	IM	182	LYS
7	IM	184	LEU
7	IM	188	PHE
7	IM	190	ASN
7	IM	194	LEU
7	IM	202	LEU
7	IM	204	LEU
7	IM	205	TYR
7	IM	215	ARG
7	IM	221	LYS
7	IM	292	MET

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Mol	Chain	Res	Type
7	IM	303	GLU
8	IN	44	LYS
8	IN	70	CYS
8	IN	71	THR
8	IN	78	LEU
8	IN	81	LEU
8	IN	94	GLN
8	IN	95	LEU
8	IN	100	LEU
8	IN	102	VAL
8	IN	107	TYR
8	IN	112	CYS
2	Id	31	ASN
2	Id	41	LEU
2	Id	61	VAL
2	Id	63	THR
2	Id	67	LYS
2	Id	70	THR
2	Id	71	LEU
2	Id	97	ARG
2	Id	104	PHE
2	Id	108	VAL
2	Id	115	VAL
2	Id	123	THR
2	Id	128	LEU
2	Id	138	GLN
2	Id	142	LYS
2	Id	150	ASN
2	Id	153	VAL
3	If	212	ILE
3	If	230	LEU
3	If	238	ILE
3	If	244	VAL
3	If	246	LEU
3	If	248	ASP
3	If	255	LEU
2	JD	24	LYS
2	JD	25	PHE
2	JD	26	LYS
2	JD	50	ASP
2	JD	51	SER
2	JD	54	GLU

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Mol	Chain	Res	Type
2	JD	67	LYS
2	JD	85	VAL
2	JD	108	VAL
2	JD	115	VAL
2	JD	126	GLU
2	JD	128	LEU
2	JD	154	VAL
2	JD	156	LEU
3	JF	250	LEU
3	JF	256	THR
1	Jg	800	ASP
1	Jg	802	LEU
1	Jg	808	LEU
1	Jg	809	VAL
1	Jg	814	GLN
1	Jg	817	THR
1	Jg	819	VAL
1	Jg	821	THR
4	JH	107	ILE
4	JH	108	ASP
4	JH	109	LYS
4	JH	119	LEU
4	JH	134	TYR
4	JH	147	THR
4	JH	152	THR
4	JH	154	THR
4	JH	161	SER
4	JH	180	VAL
4	JH	204	ILE
4	JH	219	LYS
4	JH	221	TYR
4	JH	235	THR
4	JH	238	MET
4	JH	248	VAL
4	JH	249	ASP
4	JH	278	ASP
4	JH	284	LEU
4	JH	313	VAL
4	JH	315	THR
4	JH	321	SER
4	JH	344	VAL
4	JH	347	VAL

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Mol	Chain	Res	Type
5	JK	40	LYS
5	JK	45	VAL
5	JK	50	ASP
5	JK	57	MET
5	JK	58	THR
5	JK	63	LYS
5	JK	70	VAL
5	JK	76	ILE
5	JK	92	ASN
5	JK	125	SER
5	JK	126	VAL
5	JK	156	THR
5	JK	162	ASP
5	JK	170	LEU
5	JK	183	THR
6	JL	47	TYR
6	JL	55	ARG
6	JL	57	VAL
6	JL	121	ASP
6	JL	130	ASP
6	JL	154	LEU
6	JL	155	LEU
6	JL	165	VAL
6	JL	172	VAL
6	JL	174	SER
6	JL	185	GLN
6	JL	190	MET
6	JL	193	LEU
6	JL	201	LYS
6	JL	204	LYS
6	JL	212	ASN
7	JM	127	ASN
7	JM	129	LEU
7	JM	134	LEU
7	JM	137	TYR
7	JM	146	LEU
7	JM	152	LEU
7	JM	153	GLN
7	JM	160	ASN
7	JM	164	GLN
7	JM	176	VAL
7	JM	180	ASP

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Mol	Chain	Res	Type
7	JM	182	LYS
7	JM	183	VAL
7	JM	184	LEU
7	JM	191	LEU
7	JM	192	ARG
7	JM	202	LEU
7	JM	203	SER
7	JM	204	LEU
7	JM	210	ASP
7	JM	212	LEU
7	JM	221	LYS
7	JM	224	LEU
7	JM	245	TYR
7	JM	277	SER
7	JM	284	LEU
7	JM	292	MET
7	JM	298	VAL
7	JM	301	MET
7	JM	306	GLN
7	JM	308	ASP
7	JM	310	LYS
8	JN	62	ASN
8	JN	82	MET
8	JN	84	CYS
8	JN	91	VAL
8	JN	95	LEU
8	JN	101	VAL
8	JN	115	GLN
2	Jd	24	LYS
2	Jd	32	ASN
2	Jd	36	ASP
2	Jd	52	MET
2	Jd	59	GLU
2	Jd	61	VAL
2	Jd	67	LYS
2	Jd	68	ASP
2	Jd	79	LEU
2	Jd	108	VAL
2	Jd	111	LYS
2	Jd	115	VAL
2	Jd	123	THR
2	Jd	128	LEU

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Mol	Chain	Res	Type
2	Jd	142	LYS
2	Jd	145	ILE
2	Jd	150	ASN
3	Jf	215	VAL
3	Jf	216	ILE
3	Jf	226	ASN
3	Jf	246	LEU
3	Jf	263	LYS
4	AH	108	ASP
4	AH	134	TYR
4	AH	147	THR
4	AH	160	LEU
4	AH	181	PHE
4	AH	205	GLN
4	AH	211	ASN
4	AH	212	THR
4	AH	225	ASN
4	AH	231	ARG
4	AH	233	LEU
4	AH	242	ILE
4	AH	246	LYS
4	AH	248	VAL
4	AH	250	TYR
4	AH	253	ASP
4	AH	257	GLN
4	AH	264	LYS
4	AH	270	GLU
4	AH	285	GLU
2	KD	35	ASP
2	KD	55	MET
2	KD	77	TYR
2	KD	85	VAL
2	KD	127	SER
2	KD	154	VAL
2	KD	160	LYS
1	CG	865	THR
1	CG	880	ASP
1	CG	886	LEU
1	CG	895	LYS
1	CG	898	LYS
1	CG	900	ILE
1	CG	910	ASP

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Mol	Chain	Res	Type
1	CG	913	VAL
1	CG	916	PHE
1	CG	918	THR
1	CG	930	ILE
1	CG	944	LEU
1	CG	962	SER
1	CG	965	LEU
1	CG	972	PHE
1	CG	1010	THR
1	CG	1028	THR
11	CC	90	ASN
11	CC	92	ASP
11	CC	100	LEU
11	CC	104	HIS
11	CC	106	ILE
11	CC	113	GLU
11	CC	118	LEU
11	CC	120	LEU
11	CC	128	ILE
11	CC	147	THR
11	CC	166	LEU
11	CC	175	GLU
11	CC	196	LEU
11	CC	205	GLU
11	CC	215	LYS
11	CC	216	LEU
11	CC	227	VAL
11	CC	229	HIS
11	CC	231	ASP
11	CC	234	VAL
11	CC	235	THR
11	CC	246	ARG
11	CC	248	LEU
11	CC	249	ARG
11	CC	251	THR
11	CC	259	ASN
3	KF	215	VAL
3	KF	216	ILE
3	KF	222	LEU
3	KF	223	ILE
3	KF	231	THR
3	KF	238	ILE

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Mol	Chain	Res	Type
3	KF	250	LEU
3	KF	256	THR
1	Kg	794	ILE
1	Kg	795	GLN
1	Kg	802	LEU
1	Kg	814	GLN
1	Kg	819	VAL
4	KH	105	GLU
4	KH	108	ASP
4	KH	117	ARG
4	KH	147	THR
4	KH	180	VAL
4	KH	183	ASP
4	KH	191	ILE
4	KH	195	ASP
4	KH	208	LYS
4	KH	218	THR
4	KH	226	LEU
4	KH	245	GLN
4	KH	248	VAL
4	KH	249	ASP
4	KH	270	GLU
4	KH	278	ASP
4	KH	284	LEU
4	KH	287	VAL
4	KH	293	ARG
4	KH	294	ARG
4	KH	313	VAL
4	KH	320	LEU
4	KH	327	SER
4	KH	334	THR
4	KH	344	VAL
4	KH	345	LEU
4	KH	346	LEU
4	KH	347	VAL
4	KH	353	VAL
5	KK	50	ASP
5	KK	63	LYS
5	KK	70	VAL
5	KK	77	SER
5	KK	83	LEU
5	KK	92	ASN

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Mol	Chain	Res	Type
5	KK	106	LEU
5	KK	111	LYS
5	KK	112	ILE
5	KK	126	VAL
5	KK	152	ARG
5	KK	162	ASP
5	KK	180	VAL
5	KK	182	ILE
5	KK	183	THR
6	KL	93	LEU
6	KL	98	TYR
6	KL	112	GLN
6	KL	129	THR
6	KL	130	ASP
6	KL	149	ASN
6	KL	155	LEU
6	KL	172	VAL
6	KL	174	SER
6	KL	189	MET
6	KL	210	ASP
6	KL	216	ASP
6	KL	226	ASN
6	KL	230	GLU
7	KM	118	TYR
7	KM	129	LEU
7	KM	146	LEU
7	KM	152	LEU
7	KM	155	LEU
7	KM	160	ASN
7	KM	176	VAL
7	KM	177	LEU
7	KM	180	ASP
7	KM	183	VAL
7	KM	184	LEU
7	KM	190	ASN
7	KM	192	ARG
7	KM	204	LEU
7	KM	205	TYR
7	KM	231	LEU
7	KM	245	TYR
7	KM	246	LEU
7	KM	257	ASP

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Mol	Chain	Res	Type
7	KM	292	MET
7	KM	303	GLU
8	KN	62	ASN
8	KN	67	THR
8	KN	69	TYR
8	KN	71	THR
8	KN	80	PHE
8	KN	84	CYS
8	KN	94	GLN
8	KN	105	ASP
8	KN	107	TYR
8	KN	108	VAL
8	KN	111	GLU
8	KN	112	CYS
8	KN	115	GLN
1	Ag	801	MET
1	Ag	808	LEU
1	Ag	814	GLN
1	Ag	817	THR
1	Ag	822	GLU
2	Kd	35	ASP
2	Kd	41	LEU
2	Kd	59	GLU
2	Kd	60	LYS
2	Kd	61	VAL
2	Kd	63	THR
2	Kd	82	ARG
2	Kd	91	ILE
2	Kd	93	GLU
2	Kd	94	LEU
2	Kd	105	ARG
2	Kd	111	LYS
2	Kd	132	LEU
3	Kf	215	VAL
3	Kf	232	VAL
3	Kf	236	SER
3	Kf	244	VAL
3	Kf	260	GLN
2	LD	23	MET
2	LD	32	ASN
2	LD	35	ASP
2	LD	50	ASP

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Mol	Chain	Res	Type
2	LD	51	SER
2	LD	53	LEU
2	LD	71	LEU
2	LD	85	VAL
2	LD	93	GLU
2	LD	115	VAL
2	LD	123	THR
2	LD	126	GLU
2	LD	127	SER
2	LD	134	ASP
2	LD	141	LYS
2	LD	156	LEU
3	LF	215	VAL
3	LF	222	LEU
3	LF	223	ILE
3	LF	231	THR
3	LF	238	ILE
3	LF	253	ARG
1	Lg	793	GLU
1	Lg	795	GLN
1	Lg	808	LEU
1	Lg	814	GLN
1	Lg	815	VAL
1	Lg	821	THR
4	LH	107	ILE
4	LH	108	ASP
4	LH	109	LYS
4	LH	114	ASP
4	LH	115	MET
4	LH	117	ARG
4	LH	147	THR
4	LH	180	VAL
4	LH	216	GLN
4	LH	226	LEU
4	LH	231	ARG
4	LH	234	ASN
4	LH	242	ILE
4	LH	248	VAL
4	LH	250	TYR
4	LH	253	ASP
4	LH	256	VAL
4	LH	284	LEU

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Mol	Chain	Res	Type
4	LH	287	VAL
4	LH	293	ARG
4	LH	313	VAL
4	LH	342	SER
4	LH	344	VAL
4	LH	347	VAL
4	LH	356	LEU
5	LK	45	VAL
5	LK	46	ASP
5	LK	50	ASP
5	LK	55	LYS
5	LK	67	VAL
5	LK	70	VAL
5	LK	75	LEU
5	LK	101	GLU
5	LK	111	LYS
5	LK	112	ILE
5	LK	121	SER
5	LK	125	SER
5	LK	126	VAL
5	LK	129	GLU
5	LK	149	VAL
5	LK	150	ASP
5	LK	156	THR
5	LK	183	THR
6	LL	57	VAL
6	LL	93	LEU
6	LL	113	ASP
6	LL	121	ASP
6	LL	133	PHE
6	LL	142	GLU
6	LL	143	ILE
6	LL	149	ASN
6	LL	154	LEU
6	LL	155	LEU
6	LL	162	THR
6	LL	172	VAL
6	LL	174	SER
6	LL	181	LEU
6	LL	185	GLN
6	LL	204	LYS
6	LL	211	LYS

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Mol	Chain	Res	Type
6	LL	216	ASP
6	LL	227	ARG
6	LL	228	ARG
7	LM	131	THR
7	LM	134	LEU
7	LM	146	LEU
7	LM	152	LEU
7	LM	173	LEU
7	LM	175	ILE
7	LM	176	VAL
7	LM	177	LEU
7	LM	178	LYS
7	LM	184	LEU
7	LM	191	LEU
7	LM	196	MET
7	LM	199	LYS
7	LM	208	LYS
7	LM	212	LEU
7	LM	221	LYS
7	LM	233	VAL
7	LM	245	TYR
7	LM	263	ILE
7	LM	284	LEU
7	LM	292	MET
7	LM	303	GLU
7	LM	308	ASP
7	LM	315	TYR
8	LN	45	MET
8	LN	51	CYS
8	LN	52	ASP
8	LN	72	ARG
8	LN	78	LEU
8	LN	81	LEU
8	LN	95	LEU
8	LN	100	LEU
8	LN	101	VAL
8	LN	102	VAL
8	LN	108	VAL
8	LN	112	CYS
8	LN	115	GLN
2	CD	23	MET
2	CD	26	LYS

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Mol	Chain	Res	Type
2	CD	30	ILE
2	CD	38	THR
2	CD	41	LEU
2	CD	43	GLU
2	CD	51	SER
2	CD	52	MET
2	CD	55	MET
2	CD	67	LYS
2	CD	70	THR
2	CD	78	ASN
2	CD	85	VAL
2	CD	86	ASP
2	CD	91	ILE
2	CD	100	LYS
2	CD	127	SER
2	CD	156	LEU
2	CD	161	ILE
2	Ld	36	ASP
2	Ld	52	MET
2	Ld	54	GLU
2	Ld	60	LYS
2	Ld	61	VAL
2	Ld	63	THR
2	Ld	69	ASN
2	Ld	72	THR
2	Ld	119	ILE
2	Ld	130	GLU
2	Ld	141	LYS
2	Ld	150	ASN
2	Ld	154	VAL
3	Lf	215	VAL
3	Lf	238	ILE
3	Lf	244	VAL
3	Lf	245	LYS
3	Lf	260	GLN
3	Lf	262	ILE
1	DG	865	THR
1	DG	880	ASP
1	DG	898	LYS
1	DG	900	ILE
1	DG	902	SER
1	DG	911	LYS

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Mol	Chain	Res	Type
1	DG	913	VAL
1	DG	916	PHE
1	DG	930	ILE
1	DG	939	THR
1	DG	944	LEU
1	DG	950	HIS
1	DG	962	SER
1	DG	963	SER
1	DG	965	LEU
1	DG	972	PHE
1	DG	1010	THR
1	DG	1024	ASN
1	DG	1037	LEU
1	DG	1044	ASP
5	AK	45	VAL
5	AK	67	VAL
5	AK	70	VAL
5	AK	91	LEU
5	AK	92	ASN
5	AK	98	LEU
5	AK	112	ILE
5	AK	114	ILE
5	AK	116	VAL
5	AK	120	SER
5	AK	126	VAL
5	AK	127	LYS
5	AK	129	GLU
5	AK	144	LEU
5	AK	147	GLN
5	AK	162	ASP
5	AK	180	VAL
5	AK	182	ILE
5	AK	183	THR
2	MD	29	PRO
2	MD	32	ASN
2	MD	55	MET
2	MD	61	VAL
2	MD	67	LYS
2	MD	73	ILE
2	MD	86	ASP
2	MD	115	VAL
2	MD	123	THR

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Mol	Chain	Res	Type
2	MD	127	SER
2	MD	136	ASP
2	MD	145	ILE
2	MD	147	VAL
2	MD	154	VAL
2	MD	160	LYS
3	MF	215	VAL
3	MF	230	LEU
3	MF	231	THR
3	MF	253	ARG
3	MF	266	GLN
1	Cg	793	GLU
1	Cg	807	GLN
1	Cg	810	GLN
1	Cg	812	TRP
1	Cg	815	VAL
1	Mg	793	GLU
1	Mg	794	ILE
1	Mg	795	GLN
1	Mg	810	GLN
1	Mg	812	TRP
1	Mg	814	GLN
1	Mg	817	THR
4	MH	134	TYR
4	MH	139	TYR
4	MH	147	THR
4	MH	157	PHE
4	MH	158	VAL
4	MH	180	VAL
4	MH	211	ASN
4	MH	213	LEU
4	MH	218	THR
4	MH	231	ARG
4	MH	235	THR
4	MH	240	THR
4	MH	245	GLN
4	MH	248	VAL
4	MH	249	ASP
4	MH	250	TYR
4	MH	253	ASP
4	MH	264	LYS
4	MH	280	LEU

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Mol	Chain	Res	Type
4	MH	287	VAL
4	MH	294	ARG
4	MH	313	VAL
4	MH	316	ASN
4	MH	334	THR
4	MH	344	VAL
4	MH	359	GLU
5	MK	50	ASP
5	MK	69	SER
5	MK	72	GLN
5	MK	75	LEU
5	MK	76	ILE
5	MK	86	ASP
5	MK	88	SER
5	MK	92	ASN
5	MK	111	LYS
5	MK	126	VAL
5	MK	127	LYS
5	MK	162	ASP
3	Df	215	VAL
3	Df	222	LEU
3	Df	232	VAL
3	Df	233	ARG
3	Df	262	ILE
6	ML	44	HIS
6	ML	57	VAL
6	ML	90	THR
6	ML	93	LEU
6	ML	100	ASP
6	ML	104	LYS
6	ML	109	LEU
6	ML	142	GLU
6	ML	162	THR
6	ML	172	VAL
6	ML	174	SER
6	ML	181	LEU
6	ML	182	SER
6	ML	212	ASN
6	ML	227	ARG
6	ML	230	GLU
7	MM	127	ASN
7	MM	131	THR

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Mol	Chain	Res	Type
7	MM	134	LEU
7	MM	146	LEU
7	MM	149	ASN
7	MM	152	LEU
7	MM	160	ASN
7	MM	176	VAL
7	MM	182	LYS
7	MM	183	VAL
7	MM	184	LEU
7	MM	196	MET
7	MM	205	TYR
7	MM	212	LEU
7	MM	215	ARG
7	MM	224	LEU
7	MM	242	LYS
7	MM	258	LYS
7	MM	259	SER
7	MM	263	ILE
7	MM	264	SER
7	MM	279	ILE
7	MM	314	ARG
8	MN	39	ASP
8	MN	48	ILE
8	MN	49	ASN
8	MN	70	CYS
8	MN	82	MET
8	MN	95	LEU
8	MN	100	LEU
8	MN	101	VAL
8	MN	104	ASN
8	MN	105	ASP
8	MN	108	VAL
8	MN	112	CYS
2	Md	25	PHE
2	Md	41	LEU
2	Md	52	MET
2	Md	61	VAL
2	Md	63	THR
2	Md	69	ASN
2	Md	107	ARG
2	Md	108	VAL
2	Md	123	THR

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Mol	Chain	Res	Type
2	Md	147	VAL
2	Md	150	ASN
3	Mf	219	ARG
3	Mf	245	LYS
3	Mf	255	LEU
3	Mf	260	GLN
3	Mf	261	VAL
3	VF	207	ARG
3	VF	211	TYR
3	VF	215	VAL
3	VF	219	ARG
3	VF	230	LEU
3	VF	232	VAL
3	VF	238	ILE
3	VF	253	ARG
1	VG	793	GLU
1	VG	813	LYS
1	VG	818	GLN
1	VG	819	VAL
4	VH	108	ASP
4	VH	109	LYS
4	VH	113	LYS
4	VH	117	ARG
4	VH	147	THR
4	VH	152	THR
4	VH	170	ARG
4	VH	180	VAL
4	VH	196	LEU
4	VH	198	ASP
4	VH	203	ASN
4	VH	238	MET
4	VH	240	THR
4	VH	241	LEU
4	VH	248	VAL
4	VH	253	ASP
4	VH	256	VAL
4	VH	287	VAL
4	VH	296	VAL
4	VH	297	VAL
4	VH	313	VAL
4	VH	316	ASN
4	VH	329	THR

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Mol	Chain	Res	Type
4	VH	355	GLN
3	WF	215	VAL
3	WF	231	THR
1	WG	794	ILE
1	WG	800	ASP
1	WG	802	LEU
1	WG	816	GLU
4	WH	105	GLU
4	WH	108	ASP
4	WH	109	LYS
4	WH	117	ARG
4	WH	132	GLN
4	WH	139	TYR
4	WH	147	THR
4	WH	154	THR
4	WH	180	VAL
4	WH	208	LYS
4	WH	215	ILE
4	WH	218	THR
4	WH	225	ASN
4	WH	238	MET
4	WH	248	VAL
4	WH	249	ASP
4	WH	253	ASP
4	WH	278	ASP
4	WH	313	VAL
4	WH	315	THR
4	WH	328	MET
4	WH	337	TYR
4	WH	354	MET
4	WH	356	LEU
3	XF	215	VAL
3	XF	216	ILE
1	XG	793	GLU
1	XG	795	GLN
1	XG	802	LEU
1	XG	808	LEU
1	XG	810	GLN
1	XG	814	GLN
3	CF	215	VAL
3	CF	229	THR
3	CF	230	LEU

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Mol	Chain	Res	Type
3	CF	232	VAL
3	CF	233	ARG
1	EG	869	MET
1	EG	875	THR
1	EG	880	ASP
1	EG	886	LEU
1	EG	890	VAL
1	EG	900	ILE
1	EG	910	ASP
1	EG	913	VAL
1	EG	944	LEU
1	EG	955	ARG
1	EG	956	TYR
1	EG	962	SER
1	EG	965	LEU
1	EG	966	GLN
1	EG	968	PHE
1	EG	972	PHE
1	EG	1010	THR
1	EG	1017	GLN
1	EG	1037	LEU
1	EG	1044	ASP
1	EG	1045	VAL
4	XH	109	LYS
4	XH	113	LYS
4	XH	114	ASP
4	XH	115	MET
4	XH	125	GLU
4	XH	130	LEU
4	XH	138	GLU
4	XH	147	THR
4	XH	180	VAL
4	XH	183	ASP
4	XH	203	ASN
4	XH	207	ASP
4	XH	233	LEU
4	XH	238	MET
4	XH	240	THR
4	XH	242	ILE
4	XH	250	TYR
4	XH	253	ASP
4	XH	256	VAL

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Mol	Chain	Res	Type
4	XH	293	ARG
4	XH	294	ARG
4	XH	297	VAL
4	XH	303	ARG
4	XH	308	ASN
4	XH	313	VAL
4	XH	319	ILE
4	XH	325	LEU
4	XH	339	MET
4	XH	340	GLN
4	XH	352	LYS
4	XH	358	VAL
3	YF	211	TYR
3	YF	212	ILE
3	YF	215	VAL
3	YF	256	THR
6	AL	100	ASP
6	AL	113	ASP
6	AL	129	THR
6	AL	130	ASP
6	AL	133	PHE
6	AL	155	LEU
6	AL	172	VAL
6	AL	181	LEU
6	AL	189	MET
6	AL	193	LEU
6	AL	210	ASP
6	AL	212	ASN
1	YG	793	GLU
1	YG	795	GLN
1	YG	810	GLN
1	YG	816	GLU
4	YH	122	LEU
4	YH	147	THR
4	YH	152	THR
4	YH	155	SER
4	YH	176	VAL
4	YH	180	VAL
4	YH	195	ASP
4	YH	208	LYS
4	YH	209	THR
4	YH	215	ILE

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Mol	Chain	Res	Type
4	YH	218	THR
4	YH	222	ASN
4	YH	234	ASN
4	YH	235	THR
4	YH	242	ILE
4	YH	248	VAL
4	YH	253	ASP
4	YH	262	ASN
4	YH	295	LEU
4	YH	296	VAL
4	YH	305	TRP
4	YH	306	LEU
4	YH	320	LEU
4	YH	321	SER
4	YH	332	ASP
4	YH	339	MET
4	YH	344	VAL
4	YH	347	VAL
4	YH	354	MET
4	YH	358	VAL
3	ZF	212	ILE
3	ZF	215	VAL
3	ZF	216	ILE
3	ZF	230	LEU
3	ZF	231	THR
3	ZF	233	ARG
2	AD	24	LYS
2	AD	32	ASN
2	AD	35	ASP
2	AD	50	ASP
2	AD	51	SER
2	AD	55	MET
2	AD	67	LYS
2	AD	68	ASP
2	AD	85	VAL
2	AD	91	ILE
2	AD	115	VAL
2	AD	117	VAL
2	AD	123	THR
2	AD	127	SER
2	AD	145	ILE
2	AD	154	VAL

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Mol	Chain	Res	Type
2	AD	160	LYS
1	ZG	792	GLN
1	ZG	793	GLU
1	ZG	796	GLN
1	ZG	814	GLN
1	ZG	816	GLU
1	ZG	818	GLN
4	ZH	108	ASP
4	ZH	202	PHE
4	ZH	203	ASN
4	ZH	216	GLN
4	ZH	218	THR
4	ZH	221	TYR
4	ZH	225	ASN
4	ZH	235	THR
4	ZH	242	ILE
4	ZH	248	VAL
4	ZH	253	ASP
4	ZH	259	TYR
4	ZH	262	ASN
4	ZH	297	VAL
4	ZH	306	LEU
4	ZH	338	GLU
4	ZH	357	LYS
7	AM	115	ARG
7	AM	129	LEU
7	AM	130	ARG
7	AM	131	THR
7	AM	134	LEU
7	AM	149	ASN
7	AM	152	LEU
7	AM	176	VAL
7	AM	180	ASP
7	AM	182	LYS
7	AM	184	LEU
7	AM	185	ILE
7	AM	188	PHE
7	AM	189	VAL
7	AM	190	ASN
7	AM	202	LEU
7	AM	204	LEU
7	AM	205	TYR

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Mol	Chain	Res	Type
7	AM	212	LEU
7	AM	222	ILE
7	AM	269	GLN
7	AM	271	SER
7	AM	277	SER
7	AM	287	THR
7	AM	292	MET
7	AM	308	ASP
7	AM	315	TYR
8	AN	62	ASN
8	AN	75	VAL
8	AN	76	MET
8	AN	77	ASP
8	AN	78	LEU
8	AN	84	CYS
8	AN	108	VAL
8	AN	116	LYS
2	Ad	27	LYS
2	Ad	41	LEU
2	Ad	52	MET
2	Ad	53	LEU
2	Ad	61	VAL
2	Ad	63	THR
2	Ad	68	ASP
2	Ad	85	VAL
2	Ad	93	GLU
2	Ad	94	LEU
2	Ad	108	VAL
2	Ad	111	LYS
2	Ad	115	VAL
2	Ad	124	LYS
2	Ad	141	LYS
2	Ad	154	VAL
2	Ad	156	LEU
3	Af	215	VAL
3	Af	233	ARG
3	Af	238	ILE
3	Af	247	ILE
3	Af	250	LEU
3	Af	261	VAL
2	BD	25	PHE
2	BD	32	ASN

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Mol	Chain	Res	Type
2	BD	46	VAL
2	BD	50	ASP
2	BD	51	SER
2	BD	55	MET
2	BD	71	LEU
2	BD	73	ILE
2	BD	78	ASN
2	BD	85	VAL
2	BD	108	VAL
2	BD	115	VAL
2	BD	123	THR
2	BD	131	ILE
2	BD	137	TYR
3	BF	208	ILE
3	BF	215	VAL
3	BF	216	ILE
3	BF	232	VAL
3	BF	233	ARG
3	BF	266	GLN
4	BH	105	GLU
4	BH	107	ILE
4	BH	117	ARG
4	BH	139	TYR
4	BH	147	THR
4	BH	179	LEU
4	BH	180	VAL
4	BH	208	LYS
4	BH	233	LEU
4	BH	238	MET
4	BH	242	ILE
4	BH	248	VAL
4	BH	253	ASP
4	BH	278	ASP
4	BH	287	VAL
4	BH	315	THR
4	BH	316	ASN
4	BH	345	LEU
4	BH	357	LYS
5	BK	50	ASP
5	BK	55	LYS
5	BK	67	VAL
5	BK	70	VAL

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Mol	Chain	Res	Type
5	BK	83	LEU
5	BK	92	ASN
5	BK	111	LYS
5	BK	112	ILE
5	BK	122	LYS
5	BK	125	SER
5	BK	126	VAL
5	BK	152	ARG
5	BK	156	THR
5	BK	162	ASP
5	BK	170	LEU
5	BK	180	VAL
5	BK	182	ILE
5	BK	183	THR
6	BL	47	TYR
6	BL	91	VAL
6	BL	93	LEU
6	BL	112	GLN
6	BL	129	THR
6	BL	133	PHE
6	BL	155	LEU
6	BL	165	VAL
6	BL	170	ASP
6	BL	172	VAL
6	BL	181	LEU
6	BL	182	SER
6	BL	189	MET
6	BL	212	ASN
6	BL	225	GLN
6	BL	227	ARG
6	BL	228	ARG
7	BM	130	ARG
7	BM	152	LEU
7	BM	171	ARG
7	BM	173	LEU
7	BM	176	VAL
7	BM	184	LEU
7	BM	190	ASN
7	BM	191	LEU
7	BM	192	ARG
7	BM	204	LEU
7	BM	205	TYR

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Mol	Chain	Res	Type
7	BM	212	LEU
7	BM	231	LEU
7	BM	234	GLU
7	BM	256	HIS
7	BM	264	SER
7	BM	277	SER
7	BM	292	MET
7	BM	301	MET
7	BM	304	TRP
7	BM	314	ARG
7	BM	316	ASN
8	BN	44	LYS
8	BN	65	TYR
8	BN	68	CYS
8	BN	78	LEU
8	BN	94	GLN
8	BN	115	GLN
1	FG	869	MET
1	FG	880	ASP
1	FG	886	LEU
1	FG	893	LYS
1	FG	895	LYS
1	FG	898	LYS
1	FG	913	VAL
1	FG	916	PHE
1	FG	930	ILE
1	FG	938	ASN
1	FG	941	ARG
1	FG	944	LEU
1	FG	962	SER
1	FG	963	SER
1	FG	965	LEU
1	FG	968	PHE
1	FG	972	PHE
1	FG	1010	THR
1	FG	1017	GLN
1	FG	1044	ASP
1	FG	1045	VAL
2	Bd	41	LEU
2	Bd	59	GLU
2	Bd	61	VAL
2	Bd	63	THR

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Mol	Chain	Res	Type
2	Bd	97	ARG
2	Bd	115	VAL
2	Bd	117	VAL
2	Bd	123	THR
2	Bd	141	LYS
2	Bd	145	ILE
3	Bf	216	ILE
3	Bf	222	LEU
3	Bf	232	VAL
3	Bf	233	ARG
3	Bf	236	SER
3	Bf	255	LEU
3	Bf	261	VAL
1	Dg	793	GLU
1	Dg	798	THR
1	Dg	800	ASP
1	Dg	802	LEU
1	Dg	803	THR
1	Dg	809	VAL
1	Dg	810	GLN
1	Dg	818	GLN
1	Dg	819	VAL
1	Dg	821	THR
11	EC	61	GLU
11	EC	97	ASN
11	EC	105	ILE
11	EC	116	THR
11	EC	118	ASN
11	EC	119	LEU
11	EC	127	ILE
11	EC	140	PHE
11	EC	143	THR
11	EC	146	THR
11	EC	148	ARG
11	EC	151	LEU
11	EC	153	MET
11	EC	156	VAL
11	EC	170	LYS
11	EC	180	THR
11	EC	182	ARG
11	EC	184	TRP
11	EC	204	GLU

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Mol	Chain	Res	Type
11	EC	206	PHE
11	EC	211	LEU
11	EC	221	VAL
11	EC	249	ILE
11	EC	266	VAL
11	FC	83	LEU
11	FC	97	ASN
11	FC	112	GLU
11	FC	116	THR
11	FC	119	LEU
11	FC	127	ILE
11	FC	146	THR
11	FC	148	ARG
11	FC	149	GLN
11	FC	184	TRP
11	FC	195	LEU
11	FC	205	ASP
11	FC	214	LYS
11	FC	226	VAL
11	FC	228	HIS
11	FC	233	VAL
11	FC	257	VAL
11	FC	266	VAL
11	DC	30	SER
11	DC	31	LEU
11	DC	34	LEU
11	DC	37	MET
11	DC	47	LYS
11	DC	56	GLU
11	DC	83	LEU
11	DC	84	ASN
11	DC	85	LYS
11	DC	91	ASP
11	DC	99	LEU
11	DC	115	ASN
11	DC	123	GLN
11	DC	128	SER
11	DC	146	THR
11	DC	148	ARG
11	DC	151	LEU
11	DC	154	ASP
11	DC	155	TYR

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Mol	Chain	Res	Type
11	DC	156	VAL
11	DC	169	THR
11	DC	172	GLU
11	DC	174	GLU
11	DC	203	LYS
11	DC	214	LYS
11	DC	218	MET
11	DC	239	GLU
11	DC	255	LEU
11	DC	258	ASN
11	GC	62	GLU
11	GC	84	LEU
11	GC	85	ASN
11	GC	86	LYS
11	GC	92	ASP
11	GC	100	LEU
11	GC	126	ILE
11	GC	141	PHE
11	GC	147	THR
11	GC	152	LEU
11	GC	157	VAL
11	GC	170	THR
11	GC	175	GLU
11	GC	182	GLU
11	GC	191	GLN
11	GC	196	LEU
11	GC	197	GLU
11	GC	205	GLU
11	GC	214	ARG
11	GC	222	VAL
11	GC	240	GLU
2	ED	23	MET
2	ED	31	ASN
2	ED	35	ASP
2	ED	63	THR
2	ED	73	ILE
2	ED	94	LEU
2	ED	95	THR
2	ED	105	ARG
2	ED	108	VAL
2	ED	115	VAL
2	ED	130	GLU

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Mol	Chain	Res	Type
2	ED	137	TYR
2	ED	154	VAL
11	HC	30	SER
11	HC	31	LEU
11	HC	34	LEU
11	HC	37	MET
11	HC	47	LYS
11	HC	49	GLN
11	HC	83	LEU
11	HC	84	ASN
11	HC	85	LYS
11	HC	89	ASN
11	HC	91	ASP
11	HC	103	HIS
11	HC	112	GLU
11	HC	146	THR
11	HC	154	ASP
11	HC	156	VAL
11	HC	157	LYS
11	HC	169	THR
11	HC	172	GLU
11	HC	180	THR
11	HC	195	LEU
11	HC	203	LYS
11	HC	213	ARG
11	HC	214	LYS
11	HC	233	VAL
11	HC	240	ILE
11	HC	241	HIS
11	HC	255	LEU
11	MC	30	SER
11	MC	31	LEU
11	MC	46	GLN
11	MC	48	LYS
11	MC	57	MET
11	MC	84	ASN
11	MC	85	LYS
11	MC	91	ASP
11	MC	103	HIS
11	MC	112	GLU
11	MC	117	LEU
11	MC	140	PHE

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Mol	Chain	Res	Type
11	MC	146	THR
11	MC	151	LEU
11	MC	156	VAL
11	MC	165	LEU
11	MC	169	THR
11	MC	174	GLU
11	MC	181	GLU
11	MC	184	TRP
11	MC	195	LEU
11	MC	196	GLU
11	MC	203	LYS
11	MC	204	GLU
11	MC	230	ASP
11	MC	233	VAL
11	MC	239	GLU
11	MC	244	ASP
11	MC	255	LEU
11	JC	64	LEU
11	JC	96	PHE
11	JC	105	ILE
11	JC	109	VAL
11	JC	112	GLU
11	JC	116	THR
11	JC	127	ILE
11	JC	143	THR
11	JC	157	LYS
11	JC	159	GLU
11	JC	163	VAL
11	JC	168	LYS
11	JC	184	TRP
11	JC	206	PHE
11	JC	233	VAL
11	JC	258	ASN
11	KC	62	GLU
11	KC	66	SER
11	KC	100	LEU
11	KC	112	LEU
11	KC	147	THR
11	KC	152	LEU
11	KC	166	LEU
11	KC	169	LYS
11	KC	170	THR

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Mol	Chain	Res	Type
11	KC	175	GLU
11	KC	197	GLU
11	KC	207	PHE
11	KC	211	ILE
11	KC	222	VAL
11	KC	227	VAL
11	KC	250	ILE
11	KC	257	ASN
11	KC	267	VAL
11	LC	28	THR
11	LC	39	ASP
11	LC	46	GLN
11	LC	49	GLN
11	LC	60	LYS
11	LC	81	GLU
11	LC	89	ASN
11	LC	105	ILE
11	LC	112	GLU
11	LC	116	THR
11	LC	117	LEU
11	LC	119	LEU
11	LC	123	GLN
11	LC	125	ILE
11	LC	146	THR
11	LC	154	ASP
11	LC	169	THR
11	LC	185	LYS
11	LC	203	LYS
11	LC	204	GLU
11	LC	220	MET
11	LC	226	VAL
11	LC	233	VAL
11	LC	247	LEU
11	LC	255	LEU
4	CH	109	LYS
4	CH	117	ARG
4	CH	132	GLN
4	CH	139	TYR
4	CH	180	VAL
4	CH	183	ASP
4	CH	205	GLN
4	CH	207	ASP

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Mol	Chain	Res	Type
4	CH	212	THR
4	CH	213	LEU
4	CH	225	ASN
4	CH	233	LEU
4	CH	248	VAL
4	CH	249	ASP
4	CH	266	MET
4	CH	268	THR
4	CH	270	GLU
4	CH	287	VAL
4	CH	296	VAL
4	CH	313	VAL
4	CH	321	SER
4	CH	344	VAL
4	CH	353	VAL
4	CH	361	LEU
5	CK	45	VAL
5	CK	50	ASP
5	CK	65	ILE
5	CK	66	LYS
5	CK	67	VAL
5	CK	70	VAL
5	CK	72	GLN
5	CK	78	ILE
5	CK	83	LEU
5	CK	86	ASP
5	CK	92	ASN
5	CK	111	LYS
5	CK	124	VAL
5	CK	126	VAL
5	CK	132	LEU
5	CK	144	LEU
5	CK	162	ASP
5	CK	180	VAL
5	CK	183	THR
6	CL	47	TYR
6	CL	49	ASN
6	CL	57	VAL
6	CL	91	VAL
6	CL	104	LYS
6	CL	110	GLN
6	CL	113	ASP

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Mol	Chain	Res	Type
6	CL	121	ASP
6	CL	127	ILE
6	CL	129	THR
6	CL	130	ASP
6	CL	131	LYS
6	CL	140	LEU
6	CL	155	LEU
6	CL	163	ILE
6	CL	170	ASP
6	CL	172	VAL
6	CL	181	LEU
6	CL	210	ASP
6	CL	212	ASN
6	CL	227	ARG
7	CM	115	ARG
7	CM	134	LEU
7	CM	137	TYR
7	CM	146	LEU
7	CM	155	LEU
7	CM	176	VAL
7	CM	178	LYS
7	CM	182	LYS
7	CM	184	LEU
7	CM	190	ASN
7	CM	202	LEU
7	CM	205	TYR
7	CM	231	LEU
7	CM	263	ILE
7	CM	266	VAL
7	CM	292	MET
7	CM	301	MET
7	CM	303	GLU
7	CM	308	ASP
7	CM	315	TYR
7	CM	317	LYS
8	CN	48	ILE
8	CN	59	VAL
8	CN	64	PHE
8	CN	65	TYR
8	CN	69	TYR
8	CN	85	CYS
8	CN	94	GLN

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Mol	Chain	Res	Type
8	CN	95	LEU
8	CN	108	VAL
2	Cd	25	PHE
2	Cd	26	LYS
2	Cd	30	ILE
2	Cd	41	LEU
2	Cd	59	GLU
2	Cd	61	VAL
2	Cd	115	VAL
2	Cd	119	ILE
2	Cd	123	THR
2	Cd	147	VAL
2	Cd	153	VAL
3	Cf	211	TYR
3	Cf	215	VAL
3	Cf	216	ILE
3	Cf	223	ILE
3	Cf	232	VAL
3	Cf	233	ARG
3	Cf	251	GLN
3	Cf	260	GLN
3	Cf	261	VAL
2	DD	31	ASN
2	DD	50	ASP
2	DD	53	LEU
2	DD	55	MET
2	DD	73	ILE
2	DD	85	VAL
2	DD	93	GLU
2	DD	115	VAL
2	DD	126	GLU
2	DD	127	SER
3	DF	211	TYR
3	DF	231	THR
3	DF	237	LYS
3	DF	256	THR
4	DH	105	GLU
4	DH	109	LYS
4	DH	115	MET
4	DH	130	LEU
4	DH	139	TYR
4	DH	147	THR

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Mol	Chain	Res	Type
4	DH	180	VAL
4	DH	205	GLN
4	DH	212	THR
4	DH	220	LEU
4	DH	248	VAL
4	DH	253	ASP
4	DH	256	VAL
4	DH	262	ASN
4	DH	266	MET
4	DH	280	LEU
4	DH	284	LEU
4	DH	287	VAL
4	DH	321	SER
4	DH	332	ASP
4	DH	345	LEU
1	GG	865	THR
1	GG	869	MET
1	GG	880	ASP
1	GG	881	GLU
1	GG	898	LYS
1	GG	910	ASP
1	GG	911	LYS
1	GG	913	VAL
1	GG	916	PHE
1	GG	930	ILE
1	GG	942	THR
1	GG	944	LEU
1	GG	956	TYR
1	GG	962	SER
1	GG	963	SER
1	GG	965	LEU
1	GG	966	GLN
1	GG	968	PHE
1	GG	972	PHE
1	GG	1010	THR
1	GG	1017	GLN
1	GG	1033	SER
1	GG	1045	VAL
5	DK	45	VAL
5	DK	50	ASP
5	DK	65	ILE
5	DK	72	GLN

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Mol	Chain	Res	Type
5	DK	73	ASN
5	DK	92	ASN
5	DK	100	ASN
5	DK	111	LYS
5	DK	115	THR
5	DK	134	LEU
5	DK	149	VAL
5	DK	162	ASP
5	DK	166	THR
5	DK	180	VAL
5	DK	183	THR
6	DL	47	TYR
6	DL	57	VAL
6	DL	101	SER
6	DL	109	LEU
6	DL	115	GLN
6	DL	129	THR
6	DL	139	ARG
6	DL	162	THR
6	DL	172	VAL
6	DL	174	SER
6	DL	181	LEU
6	DL	194	TRP
6	DL	212	ASN
6	DL	216	ASP
6	DL	217	ASN
7	DM	129	LEU
7	DM	134	LEU
7	DM	144	THR
7	DM	149	ASN
7	DM	152	LEU
7	DM	176	VAL
7	DM	178	LYS
7	DM	180	ASP
7	DM	182	LYS
7	DM	189	VAL
7	DM	192	ARG
7	DM	199	LYS
7	DM	212	LEU
7	DM	222	ILE
7	DM	228	VAL
7	DM	245	TYR

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Mol	Chain	Res	Type
7	DM	253	VAL
7	DM	255	THR
7	DM	257	ASP
7	DM	262	GLU
7	DM	263	ILE
7	DM	271	SER
7	DM	277	SER
7	DM	292	MET
7	DM	310	LYS
7	DM	312	PHE
8	DN	70	CYS
8	DN	82	MET
8	DN	86	LEU
8	DN	95	LEU
3	EF	215	VAL
3	EF	229	THR
3	EF	231	THR
3	EF	238	ILE
1	Eg	795	GLN
1	Eg	808	LEU
1	Eg	809	VAL
1	Eg	814	GLN
4	EH	107	ILE
4	EH	108	ASP
4	EH	115	MET
4	EH	117	ARG
4	EH	122	LEU
4	EH	134	TYR
4	EH	147	THR
4	EH	156	GLN
4	EH	160	LEU
4	EH	180	VAL
4	EH	207	ASP
4	EH	221	TYR
4	EH	245	GLN
4	EH	248	VAL
4	EH	249	ASP
4	EH	253	ASP
4	EH	256	VAL
4	EH	257	GLN
4	EH	278	ASP
4	EH	285	GLU

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Mol	Chain	Res	Type
4	EH	294	ARG
4	EH	306	LEU
4	EH	313	VAL
4	EH	325	LEU
4	EH	346	LEU
4	EH	353	VAL
4	EH	361	LEU
5	EK	50	ASP
5	EK	70	VAL
5	EK	72	GLN
5	EK	73	ASN
5	EK	75	LEU
5	EK	108	GLN
5	EK	114	ILE
5	EK	125	SER
5	EK	126	VAL
5	EK	149	VAL
5	EK	156	THR
5	EK	166	THR
5	EK	180	VAL
6	EL	49	ASN
6	EL	57	VAL
6	EL	99	ARG
6	EL	104	LYS
6	EL	109	LEU
6	EL	129	THR
6	EL	137	SER
6	EL	139	ARG
6	EL	140	LEU
6	EL	165	VAL
6	EL	168	PHE
6	EL	169	THR
6	EL	172	VAL
6	EL	174	SER
6	EL	181	LEU
6	EL	190	MET
6	EL	193	LEU
6	EL	212	ASN
6	EL	219	ILE
6	EL	221	HIS
6	EL	228	ARG
7	EM	117	ARG

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Mol	Chain	Res	Type
7	EM	124	VAL
7	EM	131	THR
7	EM	134	LEU
7	EM	149	ASN
7	EM	152	LEU
7	EM	171	ARG
7	EM	173	LEU
7	EM	175	ILE
7	EM	176	VAL
7	EM	180	ASP
7	EM	183	VAL
7	EM	224	LEU
7	EM	245	TYR
7	EM	255	THR
7	EM	257	ASP
7	EM	271	SER
7	EM	274	THR
7	EM	277	SER
7	EM	290	ASP
7	EM	292	MET
7	EM	316	ASN
8	EN	51	CYS
8	EN	66	SER
8	EN	69	TYR
8	EN	71	THR
8	EN	78	LEU
8	EN	84	CYS
8	EN	101	VAL
8	EN	113	SER
8	EN	114	LEU
2	Ed	25	PHE
2	Ed	26	LYS
2	Ed	27	LYS
2	Ed	36	ASP
2	Ed	52	MET
2	Ed	63	THR
2	Ed	70	THR
2	Ed	115	VAL
2	Ed	117	VAL
2	Ed	123	THR
2	Ed	128	LEU
2	Ed	141	LYS

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Mol	Chain	Res	Type
3	Ef	215	VAL
3	Ef	233	ARG
3	Ef	244	VAL
3	Ef	246	LEU
2	FD	35	ASP
2	FD	50	ASP
2	FD	51	SER
2	FD	52	MET
2	FD	70	THR
2	FD	82	ARG
2	FD	85	VAL
2	FD	91	ILE
2	FD	108	VAL
2	FD	115	VAL
2	FD	124	LYS
2	FD	127	SER
2	FD	154	VAL
2	FD	160	LYS
3	FF	213	GLN
3	FF	215	VAL
3	FF	230	LEU
3	FF	231	THR
3	FF	233	ARG
3	FF	238	ILE
3	FF	243	MET
3	FF	250	LEU
3	FF	255	LEU
1	Fg	794	ILE
1	Fg	813	LYS
1	Fg	814	GLN
1	Fg	821	THR
4	FH	105	GLU
4	FH	138	GLU
4	FH	139	TYR
4	FH	147	THR
4	FH	152	THR
4	FH	154	THR
4	FH	171	LEU
4	FH	180	VAL
4	FH	183	ASP
4	FH	218	THR
4	FH	225	ASN

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Mol	Chain	Res	Type
4	FH	238	MET
4	FH	248	VAL
4	FH	249	ASP
4	FH	265	SER
4	FH	272	ILE
4	FH	287	VAL
4	FH	296	VAL
4	FH	297	VAL
4	FH	313	VAL
4	FH	316	ASN
4	FH	339	MET
4	FH	341	LYS
4	FH	342	SER
4	FH	347	VAL
4	FH	361	LEU
5	FK	45	VAL
5	FK	70	VAL
5	FK	92	ASN
5	FK	95	SER
5	FK	106	LEU
5	FK	111	LYS
5	FK	125	SER
5	FK	126	VAL
5	FK	129	GLU
5	FK	149	VAL
5	FK	159	LEU
5	FK	177	ASN
5	FK	180	VAL
5	FK	183	THR
6	FL	93	LEU
6	FL	102	LYS
6	FL	114	ILE
6	FL	133	PHE
6	FL	156	ASN
6	FL	172	VAL
6	FL	174	SER
6	FL	193	LEU
6	FL	212	ASN
6	FL	225	GLN
6	FL	227	ARG
1	HG	869	MET
1	HG	874	ASP

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Mol	Chain	Res	Type
1	HG	880	ASP
1	HG	886	LEU
1	HG	898	LYS
1	HG	905	LEU
1	HG	916	PHE
1	HG	930	ILE
1	HG	944	LEU
1	HG	962	SER
1	HG	963	SER
1	HG	965	LEU
1	HG	966	GLN
1	HG	968	PHE
1	HG	972	PHE
1	HG	1002	GLU
1	HG	1021	GLN
1	HG	1024	ASN
1	HG	1033	SER
1	HG	1037	LEU
1	HG	1044	ASP
1	IG	869	MET
1	IG	880	ASP
1	IG	886	LEU
1	IG	898	LYS
1	IG	911	LYS
1	IG	919	MET
1	IG	930	ILE
1	IG	939	THR
1	IG	942	THR
1	IG	944	LEU
1	IG	956	TYR
1	IG	962	SER
1	IG	965	LEU
1	IG	968	PHE
1	IG	972	PHE
1	IG	1010	THR
1	IG	1017	GLN
1	IG	1037	LEU
1	IG	1044	ASP
1	IG	1045	VAL
1	JG	880	ASP
1	JG	890	VAL
1	JG	918	THR

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Mol	Chain	Res	Type
1	JG	919	MET
1	JG	930	ILE
1	JG	939	THR
1	JG	944	LEU
1	JG	955	ARG
1	JG	956	TYR
1	JG	962	SER
1	JG	963	SER
1	JG	965	LEU
1	JG	966	GLN
1	JG	972	PHE
1	JG	1042	THR
1	JG	1043	GLN
1	JG	1044	ASP
1	KG	869	MET
1	KG	873	LEU
1	KG	886	LEU
1	KG	893	LYS
1	KG	900	ILE
1	KG	913	VAL
1	KG	930	ILE
1	KG	933	TYR
1	KG	938	ASN
1	KG	942	THR
1	KG	944	LEU
1	KG	956	TYR
1	KG	962	SER
1	KG	963	SER
1	KG	965	LEU
1	KG	968	PHE
1	KG	972	PHE
1	KG	1040	LEU
1	KG	1044	ASP
1	LG	869	MET
1	LG	873	LEU
1	LG	875	THR
1	LG	881	GLU
1	LG	886	LEU
1	LG	895	LYS
1	LG	899	LEU
1	LG	902	SER
1	LG	913	VAL

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Mol	Chain	Res	Type
1	LG	916	PHE
1	LG	919	MET
1	LG	944	LEU
1	LG	956	TYR
1	LG	962	SER
1	LG	963	SER
1	LG	965	LEU
1	LG	966	GLN
1	LG	968	PHE
1	LG	972	PHE
1	LG	1010	THR
1	LG	1028	THR
1	LG	1037	LEU
1	MG	900	ILE
1	MG	910	ASP
1	MG	911	LYS
1	MG	916	PHE
1	MG	930	ILE
1	MG	933	TYR
1	MG	962	SER
1	MG	963	SER
1	MG	965	LEU
1	MG	968	PHE
1	MG	972	PHE
1	MG	1010	THR
1	MG	1017	GLN
1	MG	1040	LEU
1	NG	870	PHE
1	NG	886	LEU
1	NG	895	LYS
1	NG	898	LYS
1	NG	900	ILE
1	NG	911	LYS
1	NG	912	MET
1	NG	916	PHE
1	NG	918	THR
1	NG	919	MET
1	NG	930	ILE
1	NG	944	LEU
1	NG	962	SER
1	NG	963	SER
1	NG	965	LEU

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Mol	Chain	Res	Type
1	NG	966	GLN
1	NG	1010	THR
1	NG	1017	GLN
1	NG	1024	ASN
1	NG	1040	LEU
1	NG	1044	ASP
1	OG	868	ILE
1	OG	869	MET
1	OG	880	ASP
1	OG	881	GLU
1	OG	886	LEU
1	OG	898	LYS
1	OG	912	MET
1	OG	930	ILE
1	OG	938	ASN
1	OG	939	THR
1	OG	944	LEU
1	OG	956	TYR
1	OG	962	SER
1	OG	963	SER
1	OG	965	LEU
1	OG	966	GLN
1	OG	968	PHE
1	OG	972	PHE
1	OG	1010	THR
1	OG	1017	GLN
1	OG	1028	THR
1	OG	1044	ASP
1	PG	869	MET
1	PG	885	ILE
1	PG	886	LEU
1	PG	890	VAL
1	PG	895	LYS
1	PG	898	LYS
1	PG	911	LYS
1	PG	913	VAL
1	PG	930	ILE
1	PG	944	LEU
1	PG	950	HIS
1	PG	962	SER
1	PG	965	LEU
1	PG	968	PHE

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Mol	Chain	Res	Type
1	PG	972	PHE
1	PG	1010	THR
1	PG	1037	LEU
11	AC	64	LEU
11	AC	89	ASN
11	AC	91	ASP
11	AC	99	LEU
11	AC	105	ILE
11	AC	112	GLU
11	AC	116	THR
11	AC	143	THR
11	AC	146	THR
11	AC	148	ARG
11	AC	153	MET
11	AC	163	VAL
11	AC	165	LEU
11	AC	169	THR
11	AC	176	TRP
11	AC	185	LYS
11	AC	190	GLN
11	AC	193	THR
11	AC	203	LYS
11	AC	209	MET
11	AC	214	LYS
11	AC	221	VAL
11	AC	230	ASP
11	AC	233	VAL
11	AC	247	LEU
11	AC	248	ARG
11	AC	255	LEU
11	AC	258	ASN
11	AC	266	VAL
7	FM	129	LEU
7	FM	134	LEU
7	FM	146	LEU
7	FM	152	LEU
7	FM	153	GLN
7	FM	160	ASN
7	FM	162	VAL
7	FM	176	VAL
7	FM	184	LEU
7	FM	185	ILE

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Mol	Chain	Res	Type
7	FM	188	PHE
7	FM	191	LEU
7	FM	199	LYS
7	FM	204	LEU
7	FM	212	LEU
7	FM	263	ILE
7	FM	277	SER
7	FM	284	LEU
7	FM	292	MET
7	FM	301	MET
7	FM	308	ASP
7	FM	313	ASP
7	FM	314	ARG
8	FN	57	ARG
8	FN	59	VAL
8	FN	69	TYR
8	FN	70	CYS
8	FN	81	LEU
8	FN	86	LEU
8	FN	91	VAL
8	FN	94	GLN
8	FN	101	VAL
8	FN	102	VAL
8	FN	115	GLN
2	Fd	41	LEU
2	Fd	60	LYS
2	Fd	61	VAL
2	Fd	63	THR
2	Fd	82	ARG
2	Fd	86	ASP
2	Fd	92	GLU
2	Fd	93	GLU
2	Fd	108	VAL
2	Fd	115	VAL
2	Fd	117	VAL
2	Fd	123	THR
2	Fd	142	LYS
2	Fd	150	ASN
2	Fd	153	VAL
3	Ff	208	ILE
3	Ff	236	SER
3	Ff	238	ILE

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Mol	Chain	Res	Type
3	Ff	250	LEU
11	BC	61	LYS
11	BC	70	GLN
11	BC	90	ASN
11	BC	100	LEU
11	BC	104	HIS
11	BC	118	LEU
11	BC	143	THR
11	BC	147	THR
11	BC	149	ARG
11	BC	164	VAL
11	BC	166	LEU
11	BC	169	LYS
11	BC	170	THR
11	BC	181	THR
11	BC	182	GLU
11	BC	191	GLN
11	BC	202	ARG
11	BC	216	LEU
11	BC	219	MET
11	BC	222	VAL
11	BC	227	VAL
11	BC	245	ASP
11	BC	264	ARG
11	IC	28	THR
11	IC	31	LEU
11	IC	47	LYS
11	IC	48	LYS
11	IC	54	ILE
11	IC	59	LEU
11	IC	61	GLU
11	IC	80	ASP
11	IC	86	GLN
11	IC	89	ASN
11	IC	99	LEU
11	IC	103	HIS
11	IC	105	ILE
11	IC	112	GLU
11	IC	125	ILE
11	IC	127	ILE
11	IC	142	THR
11	IC	146	THR

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Mol	Chain	Res	Type
11	IC	163	VAL
11	IC	164	THR
11	IC	165	LEU
11	IC	166	LEU
11	IC	168	LYS
11	IC	190	GLN
11	IC	195	LEU
11	IC	204	GLU
11	IC	210	ILE
11	IC	218	MET
11	IC	226	VAL
11	IC	244	ASP
3	AF	211	TYR
3	AF	215	VAL
3	AF	219	ARG
3	AF	243	MET
3	AF	256	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
6	GL	110	GLN
7	GM	267	ASN
6	HL	226	ASN
1	BG	1017	GLN
4	IH	245	GLN
7	IM	318	GLN
2	Id	138	GLN
7	JM	190	ASN
8	JN	115	GLN
1	CG	1018	GLN
11	CC	124	GLN
1	Kg	810	GLN
4	KH	159	ASN
4	KH	257	GLN
7	KM	267	ASN
2	Kd	32	ASN
4	LH	216	GLN
8	LN	49	ASN
1	DG	1017	GLN
1	Cg	810	GLN
7	MM	267	ASN

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Mol	Chain	Res	Type
4	WH	257	GLN
1	EG	966	GLN
1	EG	1020	GLN
4	XH	257	GLN
4	YH	205	GLN
7	AM	267	ASN
7	AM	316	ASN
8	AN	61	ASN
7	BM	249	GLN
7	BM	267	ASN
8	BN	61	ASN
11	DC	49	GLN
11	GC	105	ASN
11	GC	124	GLN
11	GC	193	ASN
11	HC	104	ASN
11	HC	123	GLN
11	MC	69	GLN
11	MC	198	ASN
4	CH	118	ASN
4	CH	132	GLN
4	CH	159	ASN
4	CH	257	GLN
6	CL	232	GLN
7	CM	249	GLN
4	DH	203	ASN
4	DH	205	GLN
4	DH	216	GLN
8	DN	115	GLN
6	EL	183	GLN
6	EL	196	ASN
1	HG	966	GLN
1	JG	966	GLN
1	JG	1017	GLN
1	KG	1017	GLN
1	LG	1018	GLN
1	MG	1020	GLN
1	NG	966	GLN
8	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

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Mol	Chain	Number of breaks
10	DX	1
10	XX	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	IX	38:UNK	C	70:UNK	N	26.35
1	GX	38:UNK	C	70:UNK	N	25.37
1	AX	38:UNK	C	70:UNK	N	25.35
1	ZX	38:UNK	C	70:UNK	N	24.93
1	CX	38:UNK	C	70:UNK	N	24.93
1	WX	38:UNK	C	70:UNK	N	24.81
1	YX	38:UNK	C	70:UNK	N	24.75
1	EX	38:UNK	C	70:UNK	N	24.39
1	MX	38:UNK	C	70:UNK	N	24.13
1	HX	38:UNK	C	70:UNK	N	24.03
1	LX	38:UNK	C	70:UNK	N	23.91
1	VX	38:UNK	C	70:UNK	N	23.13
1	BX	38:UNK	C	70:UNK	N	23.09
1	KX	38:UNK	C	70:UNK	N	22.88
1	JX	38:UNK	C	70:UNK	N	22.83
1	FX	38:UNK	C	70:UNK	N	22.82
1	DX	38:UNK	C	70:UNK	N	22.14
1	XX	38:UNK	C	70:UNK	N	21.04

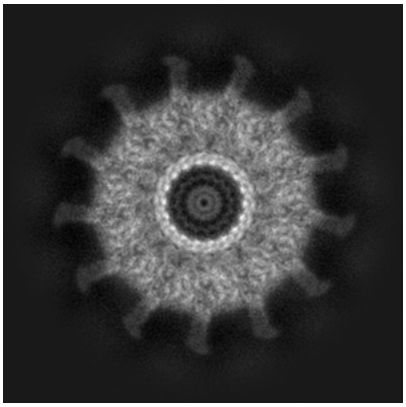
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24020. These allow visual inspection of the internal detail of the map and identification of artifacts.

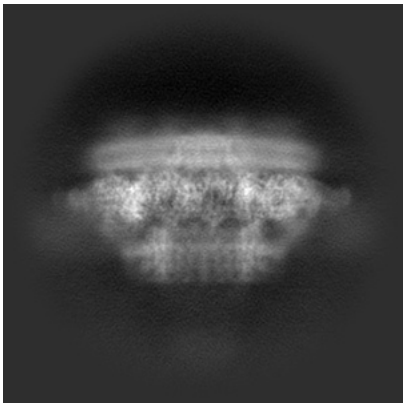
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

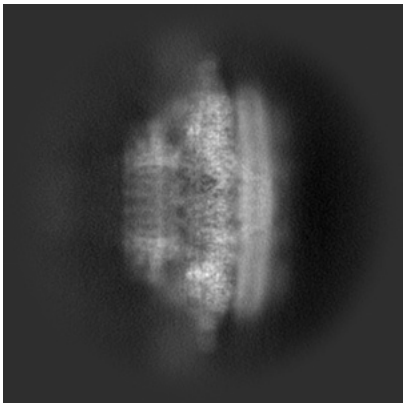
6.1.1 Primary map



X



Y

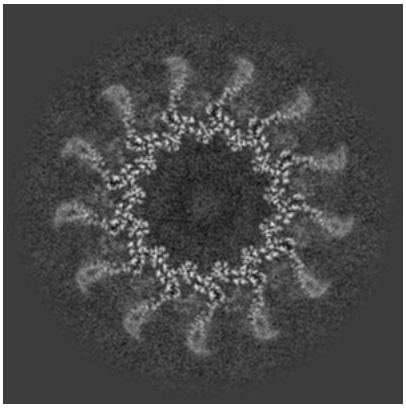


Z

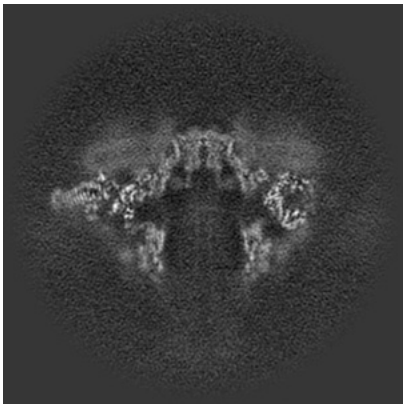
The images above show the map projected in three orthogonal directions.

6.2 Central slices

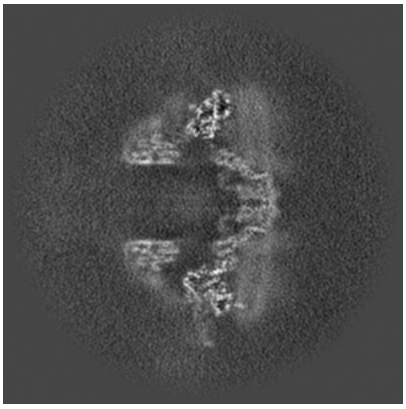
6.2.1 Primary map



X Index: 125



Y Index: 125

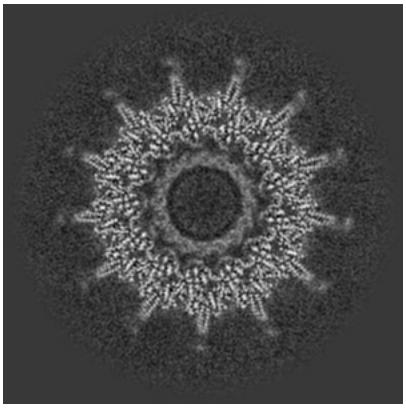


Z Index: 125

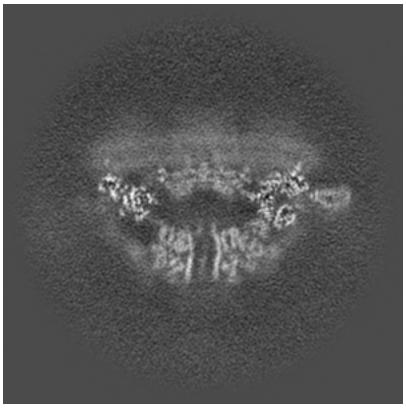
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

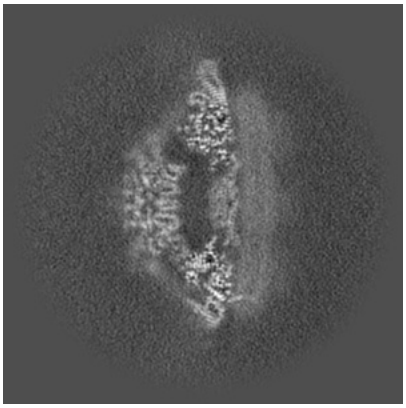
6.3.1 Primary map



X Index: 134



Y Index: 149



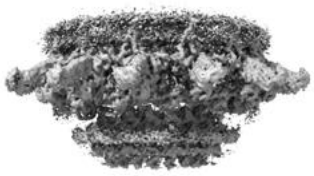
Z Index: 152

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

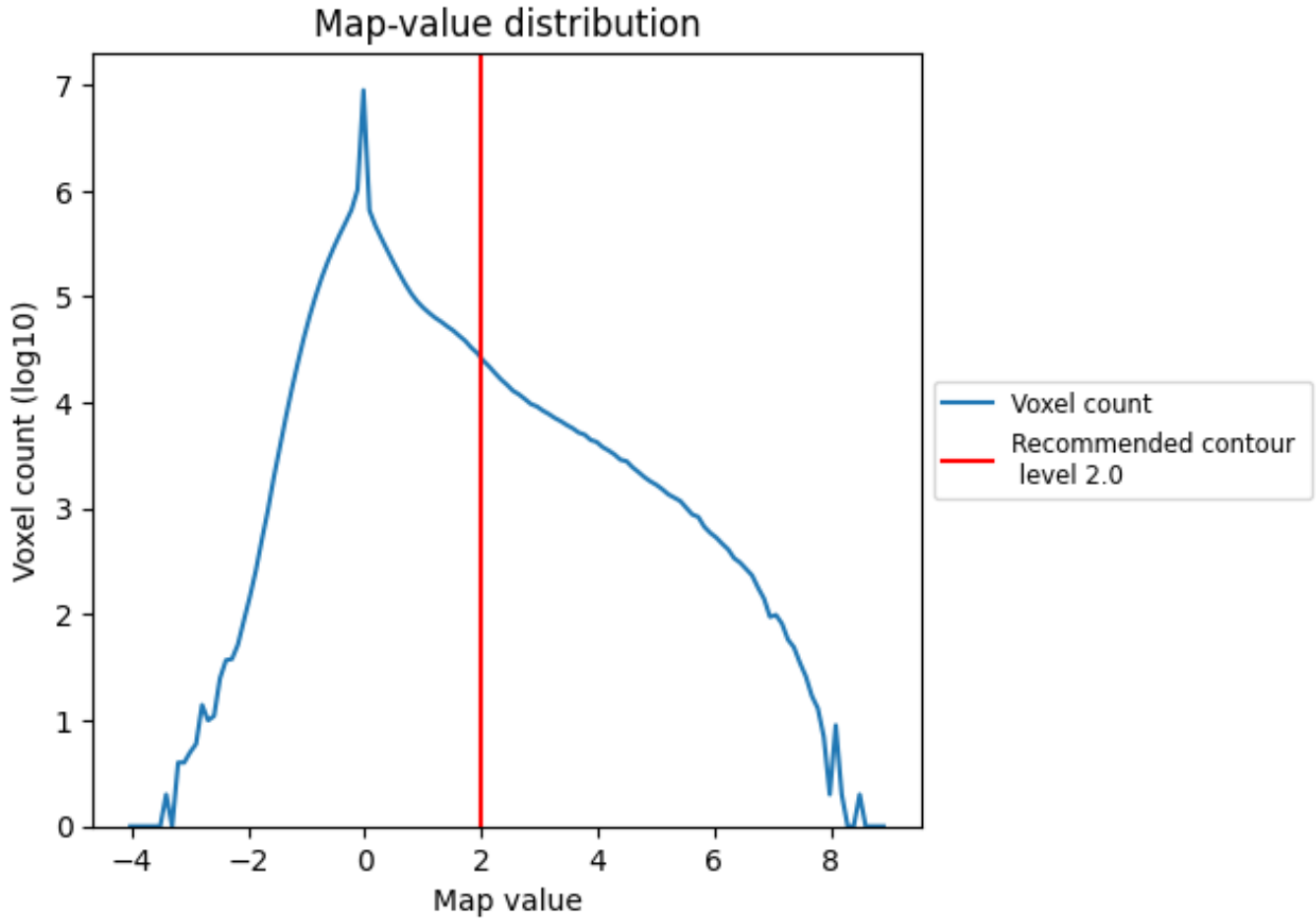
6.5 Mask visualisation (i)

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

7 Map analysis

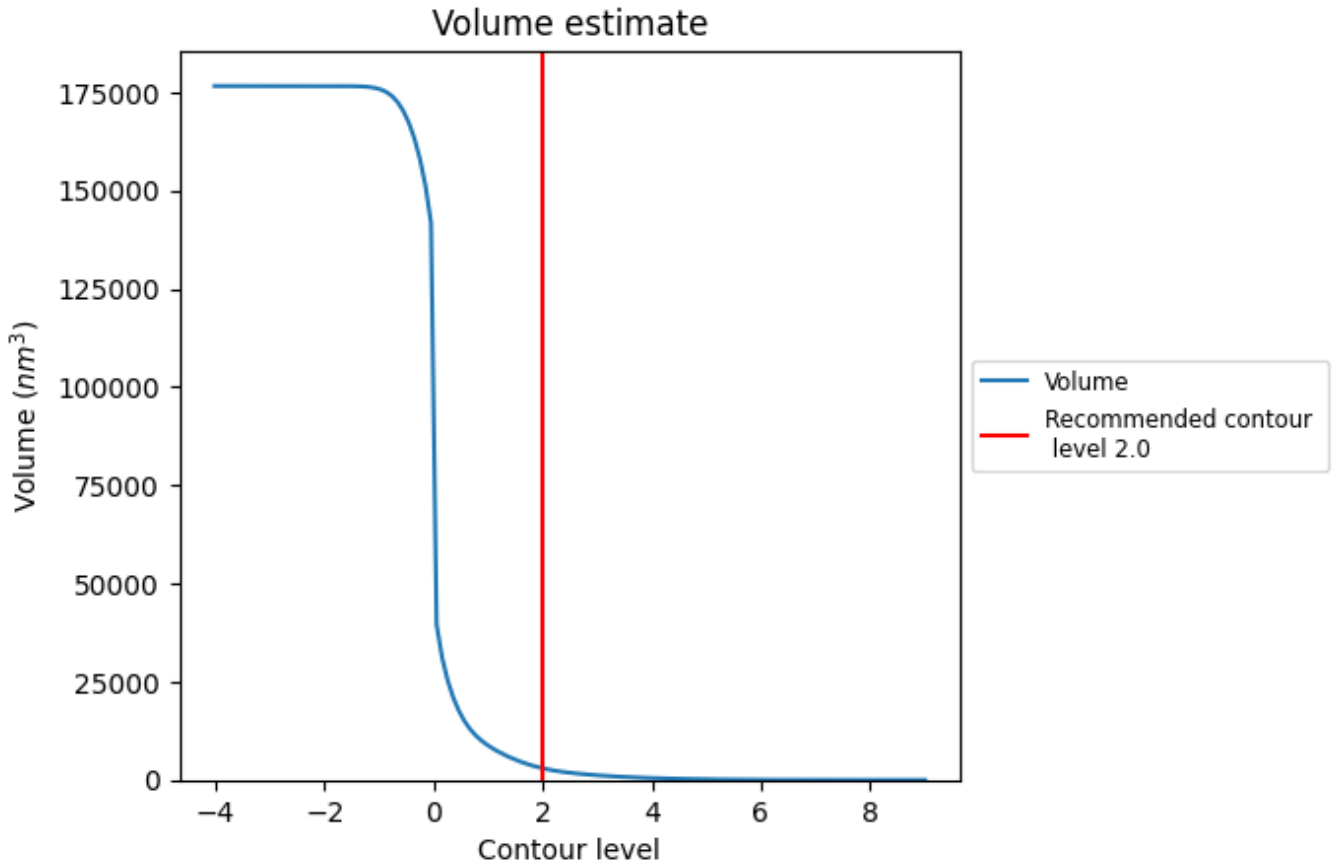
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

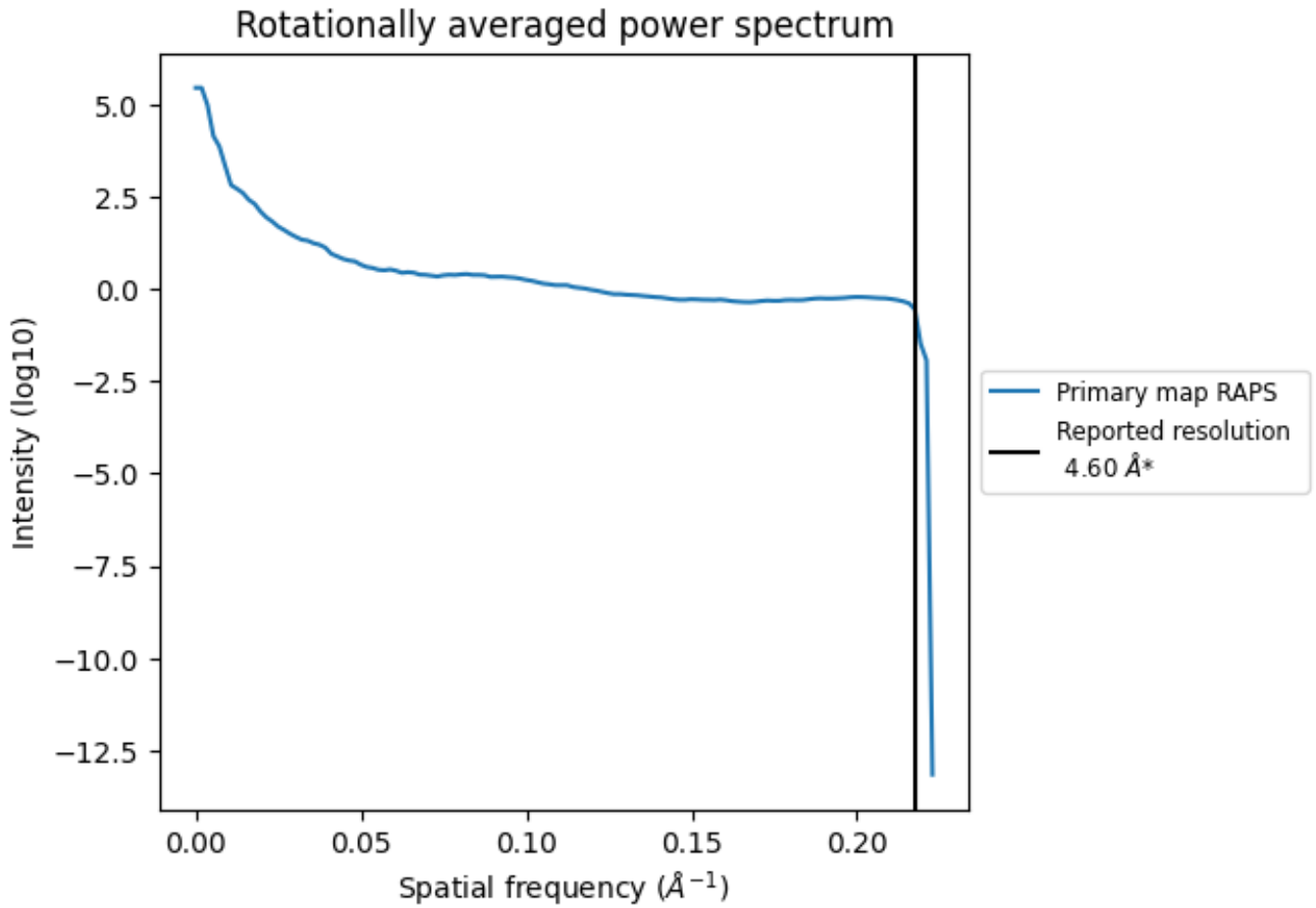
7.2 Volume estimate



The volume at the recommended contour level is 2956 nm^3; this corresponds to an approximate mass of 2670 kDa.

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

7.3 Rotationally averaged power spectrum (i)



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

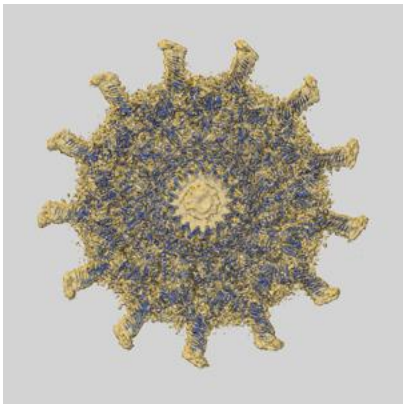
8 Fourier-Shell correlation (i)

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

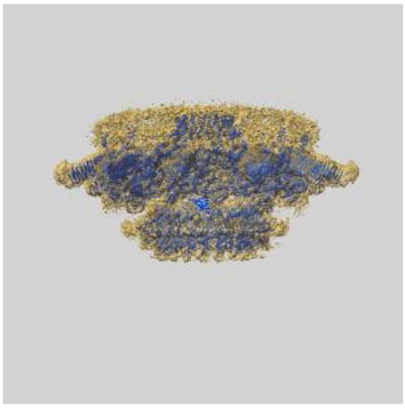
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24020 and PDB model 7MUS. Per-residue inclusion information can be found in section 3 on page 22.

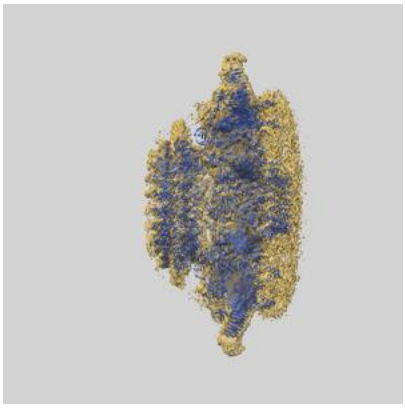
9.1 Map-model overlay



X



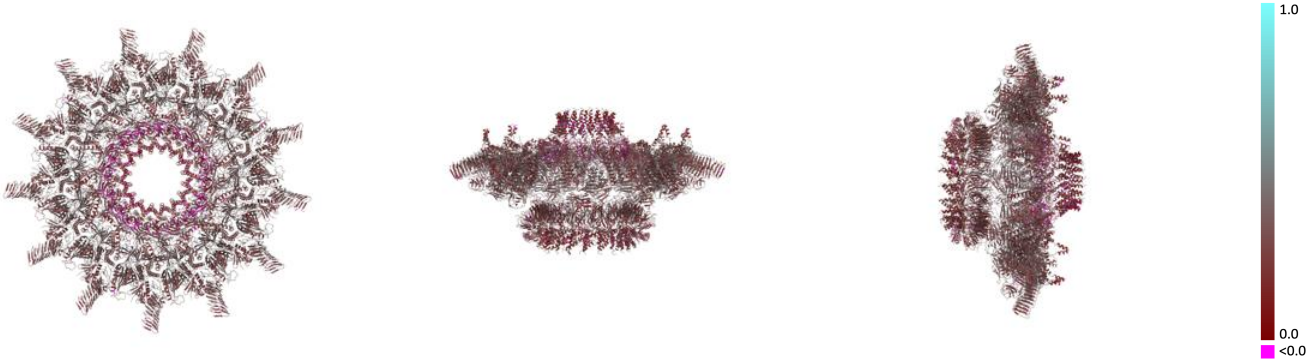
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

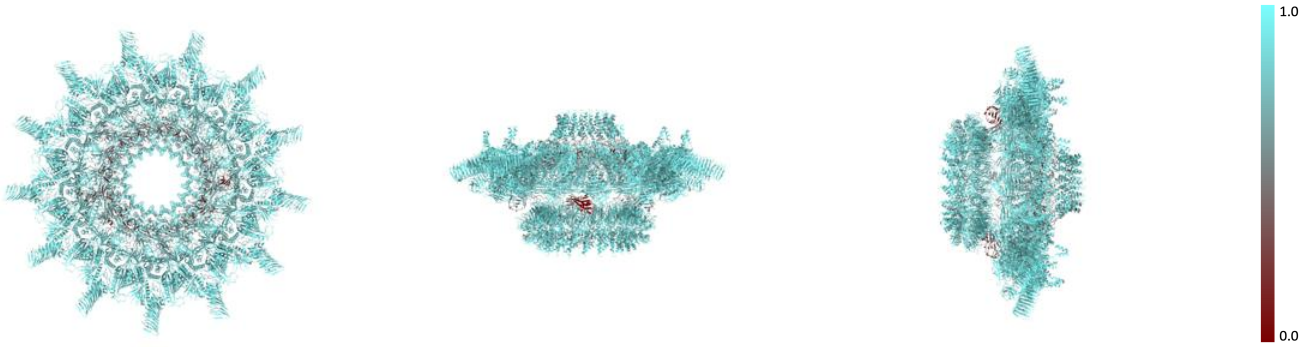
9.2 Q-score mapped to coordinate model (i)



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.

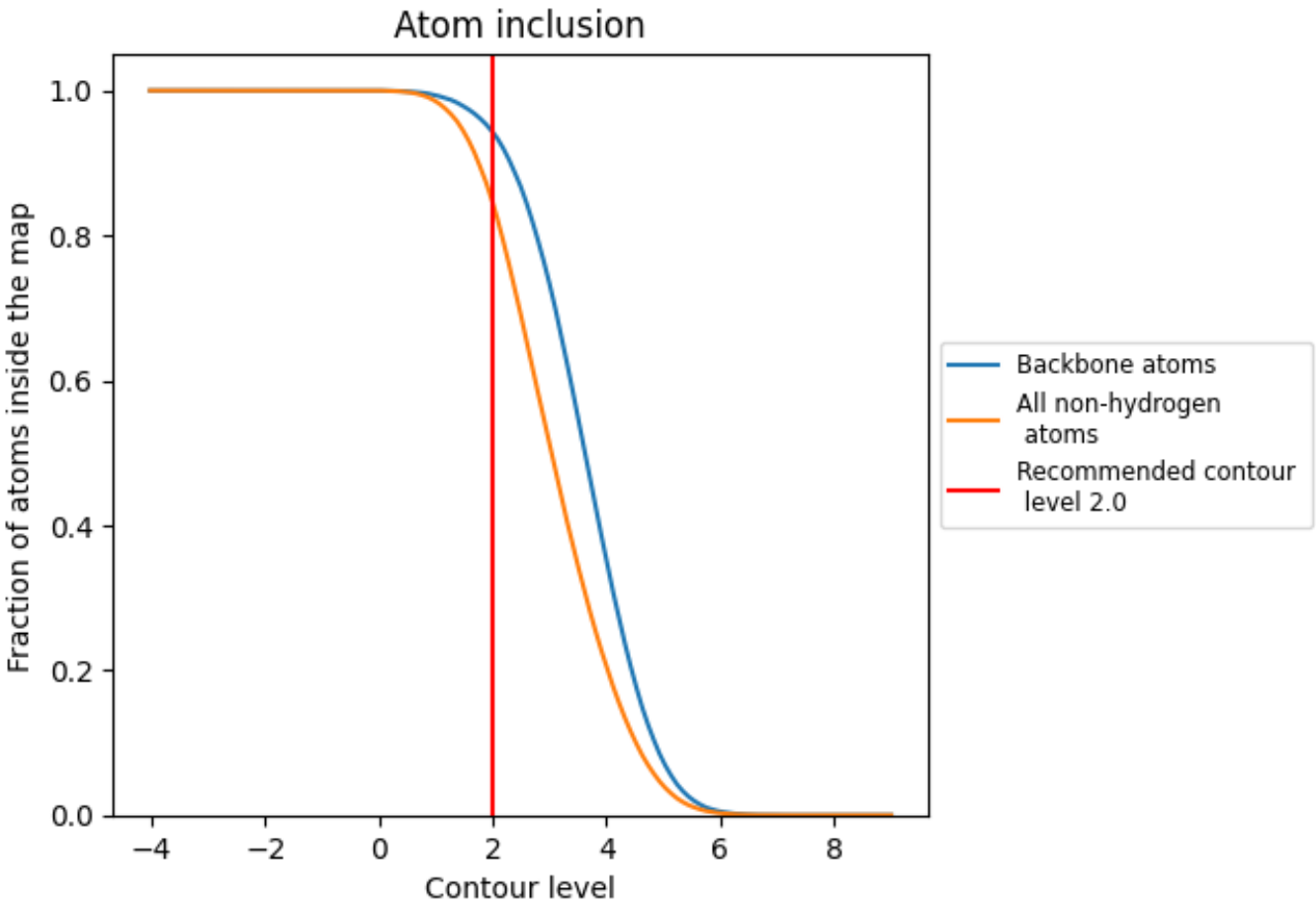
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8461	0.3050
AC	0.8871	0.3340
AD	0.8839	0.3450
AF	0.8854	0.2740
AG	0.6667	0.1580
AH	0.8727	0.3080
AK	0.8898	0.3440
AL	0.8925	0.3310
AM	0.8963	0.3180
AN	0.8776	0.3560
AU	1.0000	0.4820
AX	0.7458	0.2770
Ad	0.8809	0.3330
Af	0.9157	0.3180
Ag	0.9044	0.2670
BC	0.8773	0.3380
BD	0.8727	0.3400
BF	0.8514	0.2650
BG	0.6675	0.1480
BH	0.8686	0.3090
BK	0.8845	0.3480
BL	0.8962	0.3300
BM	0.8783	0.3330
BN	0.8934	0.3620
BU	1.0000	0.5020
BX	0.7708	0.2630
Bd	0.8876	0.3350
Bf	0.8474	0.3060
Bg	0.9118	0.2750
CC	0.8742	0.3420
CD	0.8933	0.3380
CF	0.8577	0.2620
CG	0.6585	0.1580
CH	0.8701	0.3140
CK	0.8933	0.3450

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Chain	Atom inclusion	Q-score
CL	0.8933	0.3230
CM	0.8845	0.3280
CN	0.8741	0.3690
CU	1.0000	0.4640
CX	0.9083	0.3150
Cd	0.8895	0.3380
Cf	0.9089	0.3330
Cg	0.9007	0.2640
DC	0.8526	0.3270
DD	0.8764	0.3520
DF	0.9087	0.2730
DG	0.6478	0.1630
DH	0.8686	0.3050
DK	0.8976	0.3500
DL	0.8925	0.3280
DM	0.9056	0.3280
DN	0.8654	0.3550
DU	1.0000	0.4930
DX	0.8208	0.2710
Dd	0.8847	0.3290
Df	0.8975	0.3220
Dg	0.9338	0.2730
EC	0.8675	0.3290
ED	0.8727	0.3480
EF	0.8896	0.2630
EG	0.6133	0.1540
EH	0.8676	0.3130
EK	0.8679	0.3470
EL	0.8977	0.3210
EM	0.8901	0.3270
EN	0.8217	0.3610
EU	1.0000	0.4890
EX	0.7750	0.2630
Ed	0.8742	0.3280
Ef	0.8884	0.3140
Eg	0.9081	0.2710
FC	0.8767	0.3360
FD	0.8848	0.3540
FF	0.8726	0.2570
FG	0.6141	0.1400
FH	0.8506	0.3120
FK	0.8836	0.3530

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Chain	Atom inclusion	Q-score
FL	0.8984	0.3280
FM	0.8864	0.3250
FN	0.8986	0.3660
FU	0.9778	0.4360
FX	0.7125	0.3110
Fd	0.8934	0.3350
Ff	0.8679	0.3000
Fg	0.9154	0.2540
GC	0.8761	0.3370
GD	0.8923	0.3570
GF	0.8726	0.2720
GG	0.6429	0.1470
GH	0.8593	0.3090
GK	0.8933	0.3460
GL	0.9014	0.3270
GM	0.9038	0.3290
GN	0.8724	0.3520
GU	1.0000	0.4720
GX	0.7250	0.2490
Gd	0.8742	0.3380
Gf	0.8679	0.3190
Gg	0.9007	0.2890
HC	0.8510	0.3210
HD	0.8783	0.3500
HF	0.8641	0.2590
HG	0.6125	0.1320
HH	0.8978	0.3230
HK	0.8898	0.3510
HL	0.9118	0.3350
HM	0.8802	0.3240
HN	0.8636	0.3590
HU	1.0000	0.4480
HX	0.8292	0.2900
Hd	0.8857	0.3380
Hf	0.8747	0.3050
Hg	0.9007	0.2850
IC	0.8446	0.3220
ID	0.8811	0.3400
IF	0.8790	0.2550
IG	0.5895	0.1260
IH	0.8681	0.3160
IK	0.8880	0.3510

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Chain	Atom inclusion	Q-score
IL	0.8999	0.3280
IM	0.8814	0.3330
IN	0.8199	0.3590
IU	1.0000	0.4820
IX	0.8500	0.2470
Id	0.8982	0.3360
If	0.8861	0.2960
Ig	0.9154	0.2920
JC	0.8804	0.3360
JD	0.8699	0.3430
JF	0.9002	0.2540
JG	0.5911	0.1270
JH	0.8634	0.3200
JK	0.8871	0.3490
JL	0.9036	0.3290
JM	0.8908	0.3290
JN	0.8794	0.3670
JU	1.0000	0.4660
JX	0.8125	0.2640
Jd	0.8732	0.3350
Jf	0.8702	0.3140
Jg	0.8897	0.2910
KC	0.8896	0.3370
KD	0.8642	0.3500
KF	0.8854	0.2420
KG	0.6190	0.1290
KH	0.8604	0.3080
KK	0.8906	0.3510
KL	0.9133	0.3310
KM	0.8883	0.3320
KN	0.8934	0.3620
KU	1.0000	0.4740
KX	0.7917	0.2790
Kd	0.8722	0.3340
Kf	0.8724	0.3060
Kg	0.9228	0.2820
LC	0.8536	0.3280
LD	0.8876	0.3540
LF	0.8832	0.2480
LG	0.6445	0.1470
LH	0.8511	0.2990
LK	0.8863	0.3420

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Chain	Atom inclusion	Q-score
LL	0.8940	0.3250
LM	0.8678	0.3300
LN	0.8706	0.3570
LU	0.9778	0.4540
LX	0.8708	0.2500
Ld	0.8895	0.3440
Lf	0.8519	0.3100
Lg	0.9301	0.2840
MC	0.8425	0.3130
MD	0.8727	0.3530
MF	0.8769	0.2620
MG	0.6897	0.1860
MH	0.8747	0.3080
MK	0.9003	0.3540
ML	0.9185	0.3380
MM	0.8963	0.3260
MN	0.8462	0.3680
MU	0.9778	0.4600
MX	0.8208	0.2570
Md	0.9020	0.3410
Mf	0.8998	0.3340
Mg	0.8971	0.2710
NG	0.7167	0.1890
OG	0.6453	0.1520
PG	0.6363	0.1390
VF	0.8854	0.2410
VG	0.8860	0.2540
VH	0.7935	0.2830
VX	0.8167	0.2590
WF	0.8981	0.2750
WG	0.8971	0.2680
WH	0.5886	0.2720
WX	0.8000	0.2850
XF	0.8386	0.2520
XG	0.9007	0.2810
XH	0.7967	0.2930
XX	0.8375	0.2630
YF	0.8493	0.2570
YG	0.8603	0.2550
YH	0.7092	0.2860
YX	0.7833	0.2410
ZF	0.8641	0.2570

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Chain	Atom inclusion	Q-score
ZG	0.8934	0.2640
ZH	0.6571	0.2640
ZX	0.8500	0.2450