Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 11:19 AM EST

PDB ID	:	6X6S
EMDB ID	:	EMD-22081
Title	:	Cryo-EM Structure of the Helicobacter pylori OMC
Authors	:	Sheedlo, M.J.; Chung, J.M.; Sawhney, N.; Durie, C.L.; Cover, T.L.; Ohi, M.D.; Lacy, D.B.
Deposited on	:	2020-05-29
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

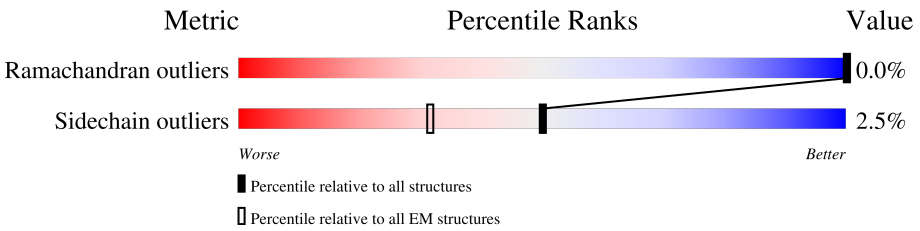
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 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	AA	481	11% 49% • 48%
1	AB	481	• 18% 81%
1	AC	481	• 19% 81%
1	AD	481	7% 19% • 80%
1	AE	481	10% 21% • 78%
1	BA	481	11% 49% • 48%
1	BB	481	• 18% 81%
1	BC	481	• 19% • 81%
1	BD	481	6% 18% • 80%

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Mol	Chain	Length	Quality of chain
1	BE	481	10% 21% 78%
1	CA	481	11% 49% 48%
1	CB	481	18% 81%
1	CC	481	19% 81%
1	CD	481	7% 19% 80%
1	CE	481	10% 21% 78%
1	DA	481	10% 49% 48%
1	DB	481	18% 81%
1	DC	481	18% 81%
1	DD	481	7% 19% 80%
1	DE	481	10% 20% 78%
1	EA	481	11% 49% 48%
1	EB	481	18% 81%
1	EC	481	19% 81%
1	ED	481	7% 18% 80%
1	EE	481	11% 20% 78%
1	FA	481	11% 49% 48%
1	FB	481	18% 81%
1	FC	481	18% 81%
1	FD	481	7% 19% 80%
1	FE	481	10% 20% 78%
1	GA	481	12% 49% 48%
1	GB	481	19% 81%
1	GC	481	18% 81%
1	GD	481	7% 18% 80%

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Mol	Chain	Length	Quality of chain
1	GE	481	10% 20% 78%
1	HA	481	11% 49% 48%
1	HB	481	18% 81%
1	HC	481	19% 81%
1	HD	481	7% 18% 80%
1	HE	481	10% 20% 78%
1	IA	481	11% 49% 48%
1	IB	481	18% 81%
1	IC	481	19% 81%
1	ID	481	6% 18% 80%
1	IE	481	10% 21% 78%
1	JA	481	11% 49% 48%
1	JB	481	18% 81%
1	JC	481	19% 81%
1	JD	481	7% 18% 80%
1	JE	481	10% 21% 78%
1	KA	481	10% 49% 48%
1	KB	481	19% 81%
1	KC	481	18% 81%
1	KD	481	7% 19% 80%
1	KE	481	10% 20% 78%
1	LA	481	12% 49% 48%
1	LB	481	19% 81%
1	LC	481	18% 81%
1	LD	481	7% 19% 80%

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Mol	Chain	Length	Quality of chain
1	LE	481	11% 20% 78%
1	MA	481	11% 49% 48%
1	MB	481	18% 81%
1	MC	481	19% 81%
1	MD	481	7% 19% 80%
1	ME	481	10% 21% 78%
1	NA	481	11% 49% 48%
1	NB	481	18% 81%
1	NC	481	18% 81%
1	ND	481	7% 18% 80%
1	NE	481	11% 21% 78%
2	AM	376	10% 47% 52%
2	Am	376	36% 46% 52%
2	BM	376	10% 47% 52%
2	Bm	376	36% 46% 52%
2	CM	376	10% 47% 52%
2	Cm	376	35% 46% 52%
2	DM	376	11% 47% 52%
2	Dm	376	35% 46% 52%
2	EM	376	10% 47% 52%
2	Em	376	35% 46% 52%
2	FM	376	11% 46% 52%
2	Fm	376	34% 46% 52%
2	GM	376	10% 47% 52%
2	Gm	376	36% 46% 52%

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Mol	Chain	Length	Quality of chain
2	HM	376	10% 47% 52%
2	Hm	376	36% 45% 52%
2	IM	376	10% 47% 52%
2	Im	376	36% 46% 52%
2	JM	376	11% 48% 52%
2	Jm	376	35% 46% 52%
2	KM	376	11% 47% 52%
2	Km	376	35% 47% 52%
2	LM	376	10% 47% 52%
2	Lm	376	35% 46% 52%
2	MM	376	10% 47% 52%
2	Mm	376	34% 47% 52%
2	NM	376	10% 47% 52%
2	Nm	376	35% 46% 52%
3	AT	280	6% 88% 10%
3	At	280	17% 65% 31%
3	BT	280	6% 88% 10%
3	Bt	280	17% 65% 31%
3	CT	280	7% 88% 10%
3	Ct	280	15% 65% 31%
3	DT	280	7% 88% 10%
3	Dt	280	16% 65% 31%
3	ET	280	6% 88% 10%
3	Et	280	16% 65% 31%
3	FT	280	6% 88% 10%

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Mol	Chain	Length	Quality of chain
3	Ft	280	18% 65% 31%
3	GT	280	6% 88% 10%
3	Gt	280	17% 65% 31%
3	HT	280	6% 88% 10%
3	Ht	280	17% 65% 31%
3	IT	280	6% 88% 10%
3	It	280	16% 65% 31%
3	JT	280	7% 88% 10%
3	Jt	280	15% 65% 31%
3	KT	280	6% 88% 10%
3	Kt	280	16% 65% 31%
3	LT	280	6% 88% 10%
3	Lt	280	16% 65% 31%
3	MT	280	7% 88% 10%
3	Mt	280	17% 65% 31%
3	NT	280	6% 88% 10%
3	Nt	280	16% 65% 31%
4	AU	160	58% 100%
4	BU	160	56% 100%
4	CU	160	57% 100%
4	DU	160	59% 100%
4	EU	160	58% 100%
4	FU	160	58% 100%
4	GU	160	58% 100%
4	HU	160	59% 100%

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Mol	Chain	Length	Quality of chain
4	IU	160	56% 100%
4	JU	160	55% 100%
4	KU	160	58% 100%
4	LU	160	58% 100%
4	MU	160	58% 100%
4	NU	160	57% 100%
5	AX	522	30% 68%
5	BX	522	29% 68%
5	CX	522	30% 68%
5	DX	522	30% 68%
5	EX	522	30% 68%
5	FX	522	30% 68%
5	GX	522	30% 68%
5	HX	522	30% 68%
5	IX	522	30% 68%
5	JX	522	30% 68%
5	KX	522	30% 68%
5	LX	522	29% 68%
5	MX	522	30% 68%
5	NX	522	30% 68%
6	AY	1927	10% 89%
6	BY	1927	10% 89%
6	CY	1927	10% 89%
6	DY	1927	10% 89%
6	EY	1927	10% 89%

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Mol	Chain	Length	Quality of chain
6	FY	1927	10% 89%
6	GY	1927	10% 89%
6	HY	1927	10% 89%
6	IY	1927	10% 89%
6	JY	1927	10% 89%
6	KY	1927	10% 89%
6	LY	1927	10% 89%
6	MY	1927	10% 89%
6	NY	1927	10% 89%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 215978 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 Type IV secretion system apparatus protein Cag3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	248	1986	1254	329	395	8	0	0
1	AB	90	728	468	122	135	3	0	0
1	AC	92	741	476	125	137	3	0	0
1	AD	95	778	508	124	143	3	0	0
1	AE	104	847	549	136	159	3	0	0
1	BA	248	1986	1254	329	395	8	0	0
1	BB	90	728	468	122	135	3	0	0
1	BC	92	741	476	125	137	3	0	0
1	BD	95	778	508	124	143	3	0	0
1	BE	104	847	549	136	159	3	0	0
1	CA	248	1986	1254	329	395	8	0	0
1	CB	90	728	468	122	135	3	0	0
1	CC	92	741	476	125	137	3	0	0
1	CD	95	778	508	124	143	3	0	0
1	CE	104	847	549	136	159	3	0	0
1	DA	248	1986	1254	329	395	8	0	0
1	DB	90	728	468	122	135	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	DD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	DE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	EA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	EB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	EC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	ED	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	EE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	FA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	FB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	FC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	FD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	FE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	GA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	GB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	GC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	GD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	GE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	HA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	HB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	HC	92	741	476	125	137	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	HD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	HE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	IA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	IB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	IC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	ID	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	IE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	JA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	JB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	JC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	JD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	JE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	KA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	KB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	KC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	KD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	KE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	LA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	LB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	LC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	LD	95	778	508	124	143	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	LE	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	MA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	MB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	MC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	MD	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	ME	104	847	549	136	159	3	0	0
			Total	C	N	O	S		
1	NA	248	1986	1254	329	395	8	0	0
			Total	C	N	O	S		
1	NB	90	728	468	122	135	3	0	0
			Total	C	N	O	S		
1	NC	92	741	476	125	137	3	0	0
			Total	C	N	O	S		
1	ND	95	778	508	124	143	3	0	0
			Total	C	N	O	S		
1	NE	104	847	549	136	159	3	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
AB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
AC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
AD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
AE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
BA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
BB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
BC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
BD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
BE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
CA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
CB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
CC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
CD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
CE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
DA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
DB	275	ALA	GLN	conflict	UNP A0A2J9KJK3

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Chain	Residue	Modelled	Actual	Comment	Reference
DC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
DD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
DE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
EA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
EB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
EC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
ED	275	ALA	GLN	conflict	UNP A0A2J9KJK3
EE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
FA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
FB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
FC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
FD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
FE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
GA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
GB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
GC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
GD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
GE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
HA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
HB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
HC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
HD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
HE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
IA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
IB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
IC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
ID	275	ALA	GLN	conflict	UNP A0A2J9KJK3
IE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
JA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
JB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
JC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
JD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
JE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
KA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
KB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
KC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
KD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
KE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
LA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
LB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
LC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
LD	275	ALA	GLN	conflict	UNP A0A2J9KJK3

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Chain	Residue	Modelled	Actual	Comment	Reference
LE	275	ALA	GLN	conflict	UNP A0A2J9KJK3
MA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
MB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
MC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
MD	275	ALA	GLN	conflict	UNP A0A2J9KJK3
ME	275	ALA	GLN	conflict	UNP A0A2J9KJK3
NA	275	ALA	GLN	conflict	UNP A0A2J9KJK3
NB	275	ALA	GLN	conflict	UNP A0A2J9KJK3
NC	275	ALA	GLN	conflict	UNP A0A2J9KJK3
ND	275	ALA	GLN	conflict	UNP A0A2J9KJK3
NE	275	ALA	GLN	conflict	UNP A0A2J9KJK3

- Molecule 2 is a protein called Type IV secretion system apparatus protein CagM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	AM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Am	179	1474	939	246	284	5	0	0
			Total	C	N	O	S		
2	BM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Bm	179	1474	939	246	284	5	0	0
			Total	C	N	O	S		
2	CM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Cm	179	1474	939	246	284	5	0	0
			Total	C	N	O	S		
2	DM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Dm	179	1474	939	246	284	5	0	0
			Total	C	N	O	S		
2	EM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Em	179	1474	939	246	284	5	0	0
			Total	C	N	O	S		
2	FM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Fm	179	1474	939	246	284	5	0	0
			Total	C	N	O	S		
2	GM	180	1485	945	250	285	5	0	0
			Total	C	N	O	S		
2	Gm	179	1474	939	246	284	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	HM	180	1485	945	250	285	5	0	0
2	Hm	179	1474	939	246	284	5	0	0
2	IM	180	1485	945	250	285	5	0	0
2	Im	179	1474	939	246	284	5	0	0
2	JM	180	1485	945	250	285	5	0	0
2	Jm	179	1474	939	246	284	5	0	0
2	KM	180	1485	945	250	285	5	0	0
2	Km	179	1474	939	246	284	5	0	0
2	LM	180	1485	945	250	285	5	0	0
2	Lm	179	1474	939	246	284	5	0	0
2	MM	180	1485	945	250	285	5	0	0
2	Mm	179	1474	939	246	284	5	0	0
2	NM	180	1485	945	250	285	5	0	0
2	Nm	179	1474	939	246	284	5	0	0

- Molecule 3 is a protein called Type IV secretion system apparatus protein CagT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AT	253	2083	1308	368	402	5	0	0
3	At	192	1615	1021	283	308	3	0	0
3	BT	253	2083	1308	368	402	5	0	0
3	Bt	192	1615	1021	283	308	3	0	0
3	CT	253	2083	1308	368	402	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Ct	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	DT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Dt	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	ET	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Et	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	FT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Ft	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	GT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Gt	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	HT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Ht	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	IT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	It	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	JT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Jt	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	KT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Kt	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	LT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Lt	192	1615	1021	283	308	3	0	0
			Total	C	N	O	S		
3	MT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Mt	192	1615	1021	283	308	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	NT	253	2083	1308	368	402	5	0	0
			Total	C	N	O	S		
3	Nt	192	1615	1021	283	308	3	0	0

- Molecule 4 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	AU	160	800	480	160	160	0	0
			Total	C	N	O		
4	BU	160	800	480	160	160	0	0
			Total	C	N	O		
4	CU	160	800	480	160	160	0	0
			Total	C	N	O		
4	DU	160	800	480	160	160	0	0
			Total	C	N	O		
4	EU	160	800	480	160	160	0	0
			Total	C	N	O		
4	FU	160	800	480	160	160	0	0
			Total	C	N	O		
4	GU	160	800	480	160	160	0	0
			Total	C	N	O		
4	HU	160	800	480	160	160	0	0
			Total	C	N	O		
4	IU	160	800	480	160	160	0	0
			Total	C	N	O		
4	JU	160	800	480	160	160	0	0
			Total	C	N	O		
4	KU	160	800	480	160	160	0	0
			Total	C	N	O		
4	LU	160	800	480	160	160	0	0
			Total	C	N	O		
4	MU	160	800	480	160	160	0	0
			Total	C	N	O		
4	NU	160	800	480	160	160	0	0

- Molecule 5 is a protein called Type IV secretion system apparatus protein CagX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AX	166	1361	871	237	248	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BX	166	1361	871	237	248	5	0	0
5	CX	166	1361	871	237	248	5	0	0
5	DX	166	1361	871	237	248	5	0	0
5	EX	166	1361	871	237	248	5	0	0
5	FX	166	1361	871	237	248	5	0	0
5	GX	166	1361	871	237	248	5	0	0
5	HX	166	1361	871	237	248	5	0	0
5	IX	166	1361	871	237	248	5	0	0
5	JX	166	1361	871	237	248	5	0	0
5	KX	166	1361	871	237	248	5	0	0
5	LX	166	1361	871	237	248	5	0	0
5	MX	166	1361	871	237	248	5	0	0
5	NX	166	1361	871	237	248	5	0	0

- Molecule 6 is a protein called Cag pathogenicity island protein (Cag7).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AY	203	1529	982	246	292	9	0	0
6	BY	203	1529	982	246	292	9	0	0
6	CY	203	1529	982	246	292	9	0	0
6	DY	203	1529	982	246	292	9	0	0
6	EY	203	1529	982	246	292	9	0	0
6	FY	203	1529	982	246	292	9	0	0

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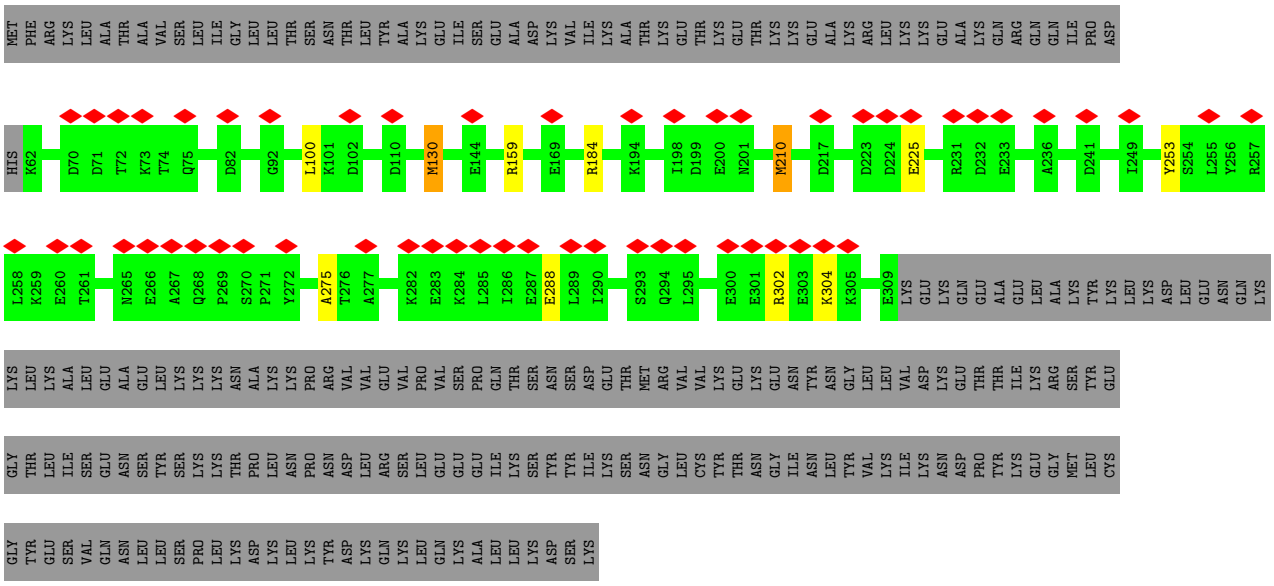
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	GY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	HY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	IY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	JY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	KY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	LY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	MY	203	1529	982	246	292	9	0	0
			Total	C	N	O	S		
6	NY	203	1529	982	246	292	9	0	0

3 Residue-property plots (i)

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

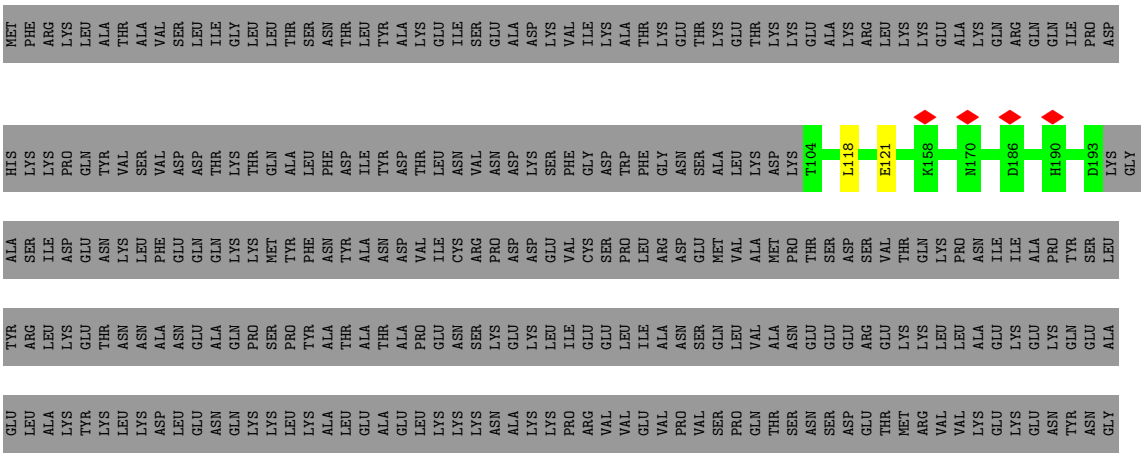
• Molecule 1: Type IV secretion system apparatus protein Cag3

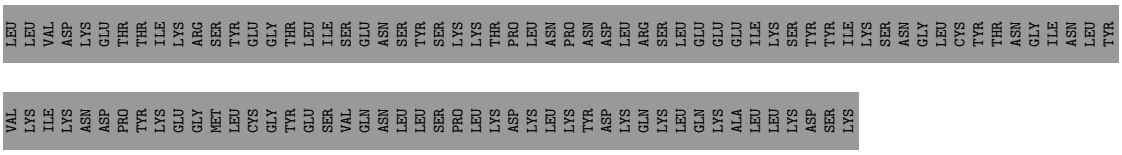
Chain AA:



• Molecule 1: Type IV secretion system apparatus protein Cag3

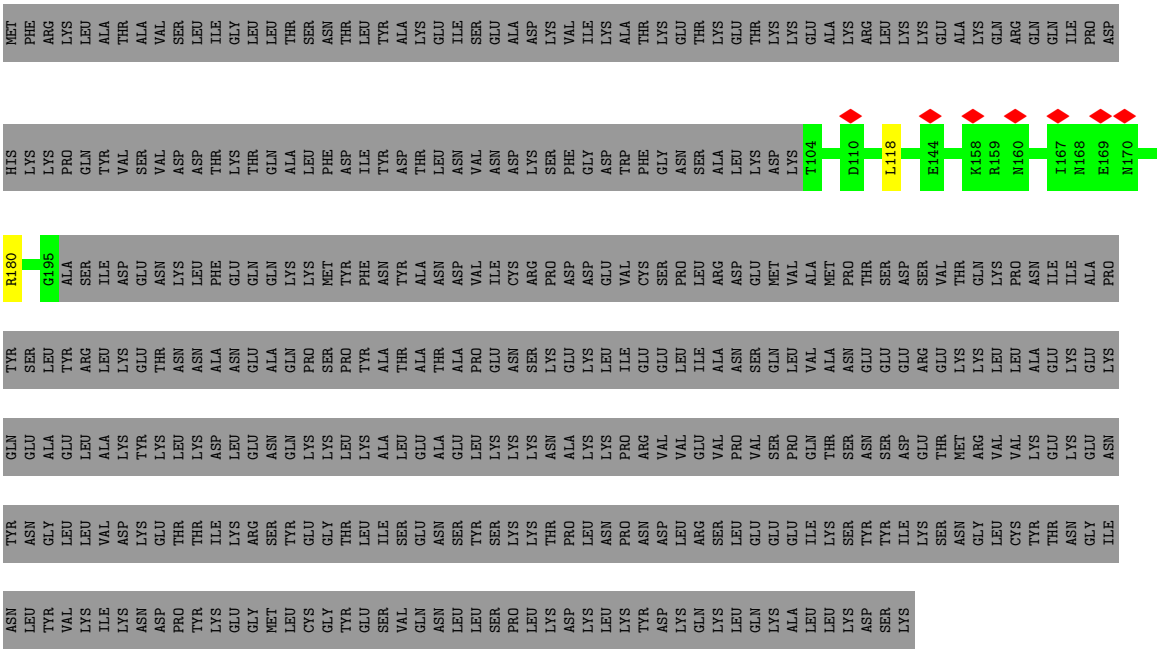
Chain AB:





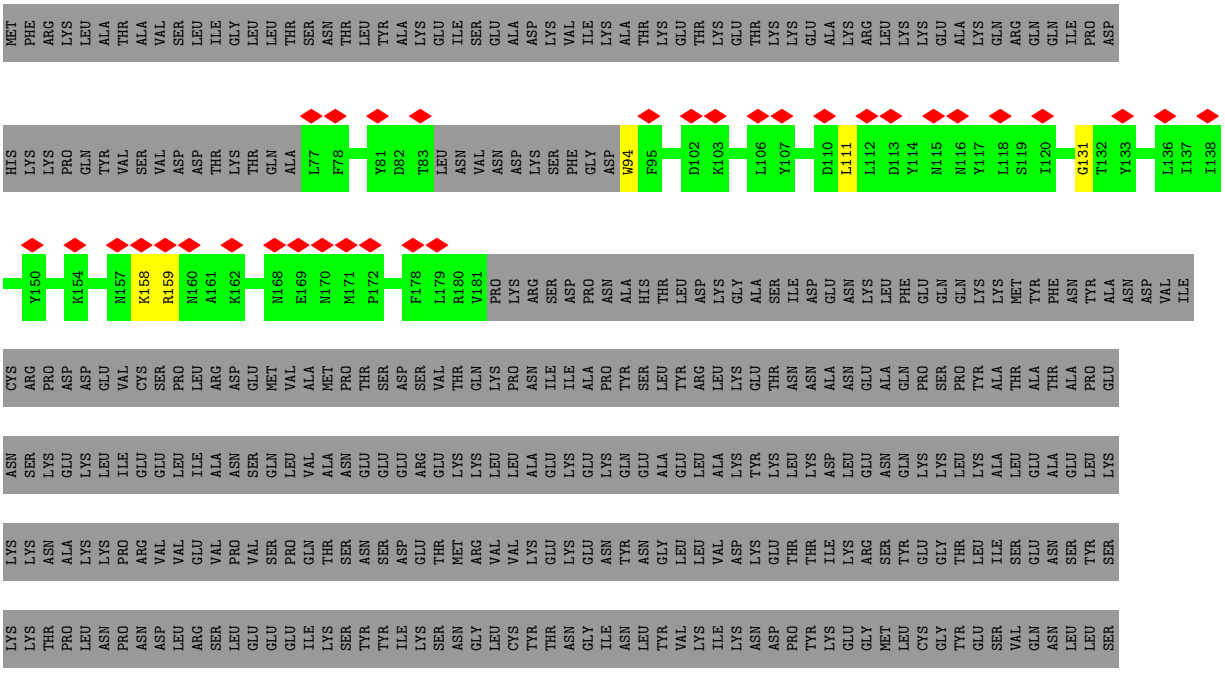
• Molecule 1: Type IV secretion system apparatus protein Cag3

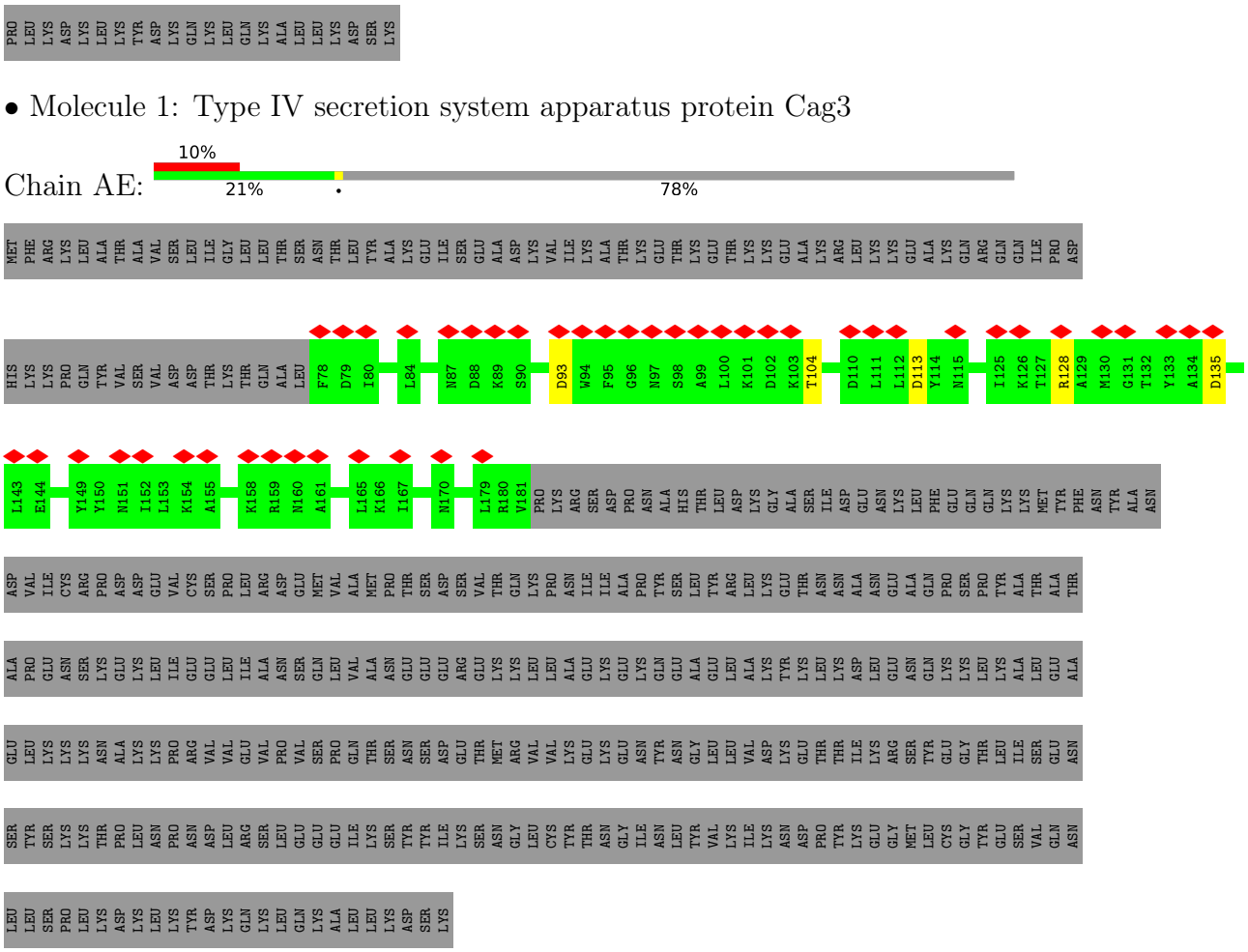
Chain AC:



• Molecule 1: Type IV secretion system apparatus protein Cag3

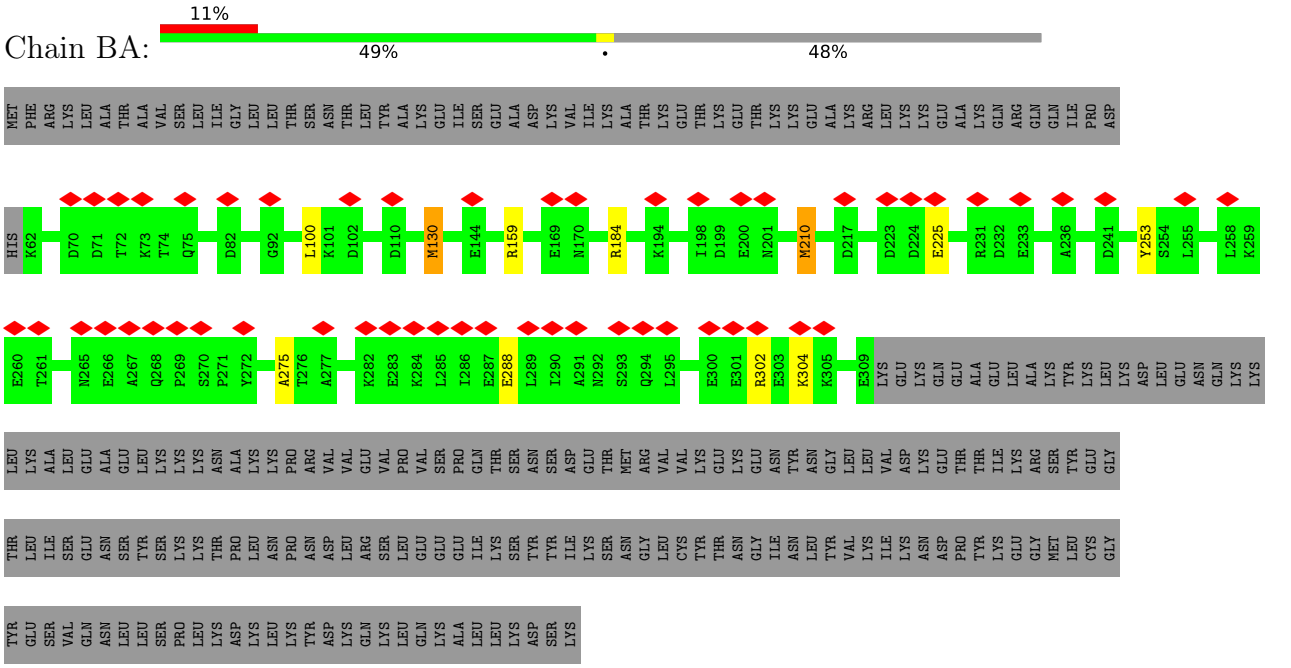
Chain AD:





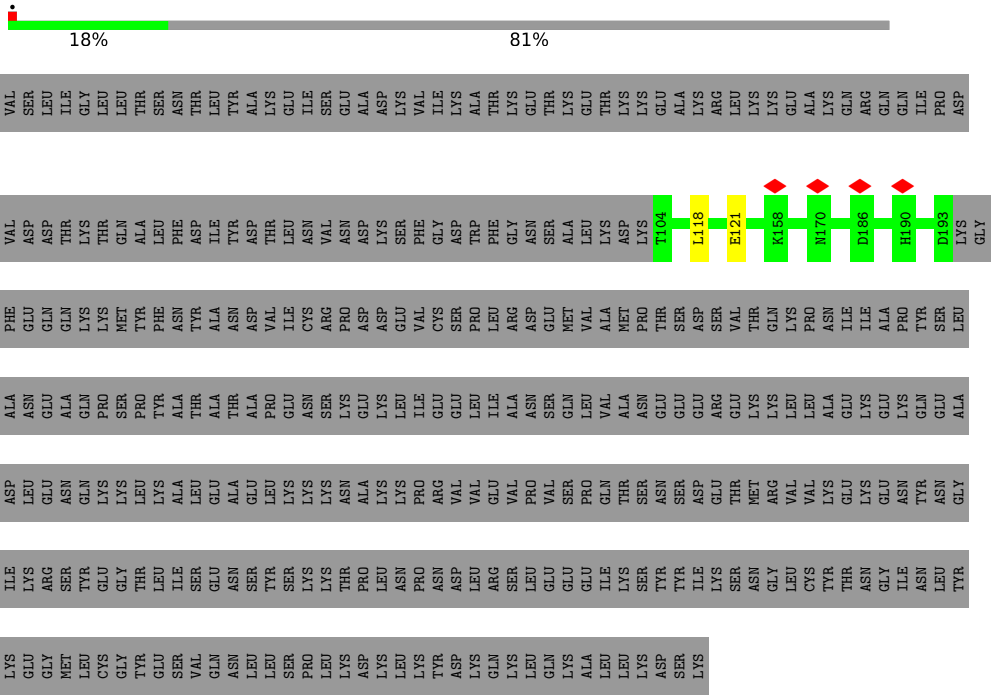
• Molecule 1: Type IV secretion system apparatus protein Cag3

• Molecule 1: Type IV secretion system apparatus protein Cag3



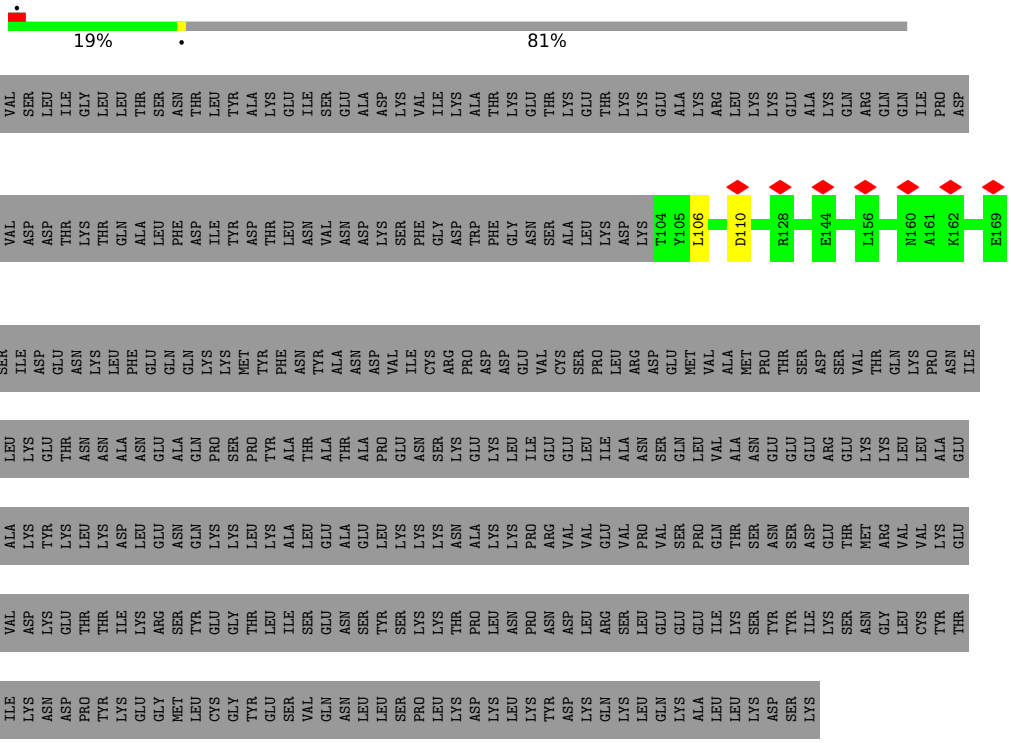
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain BB:



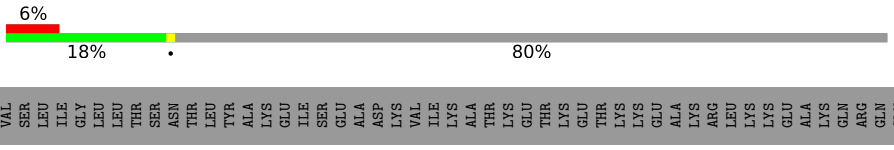
• Molecule 1: Type IV secretion system apparatus protein Cag3

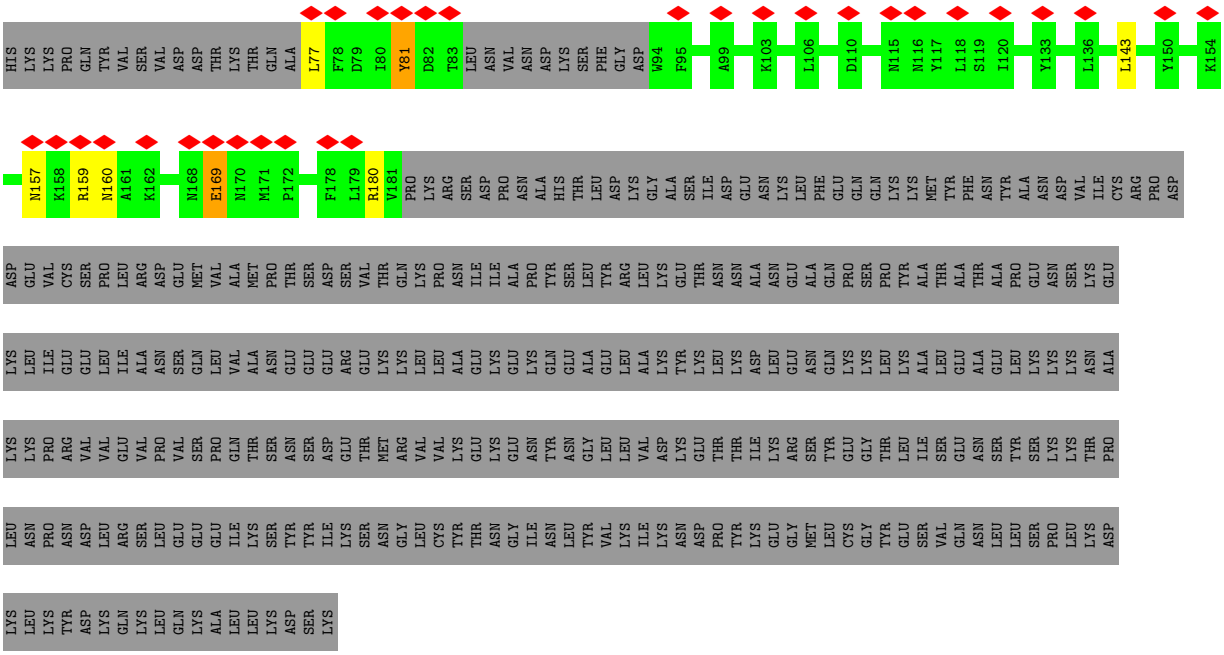
Chain BC:



• Molecule 1: Type IV secretion system apparatus protein Cag3

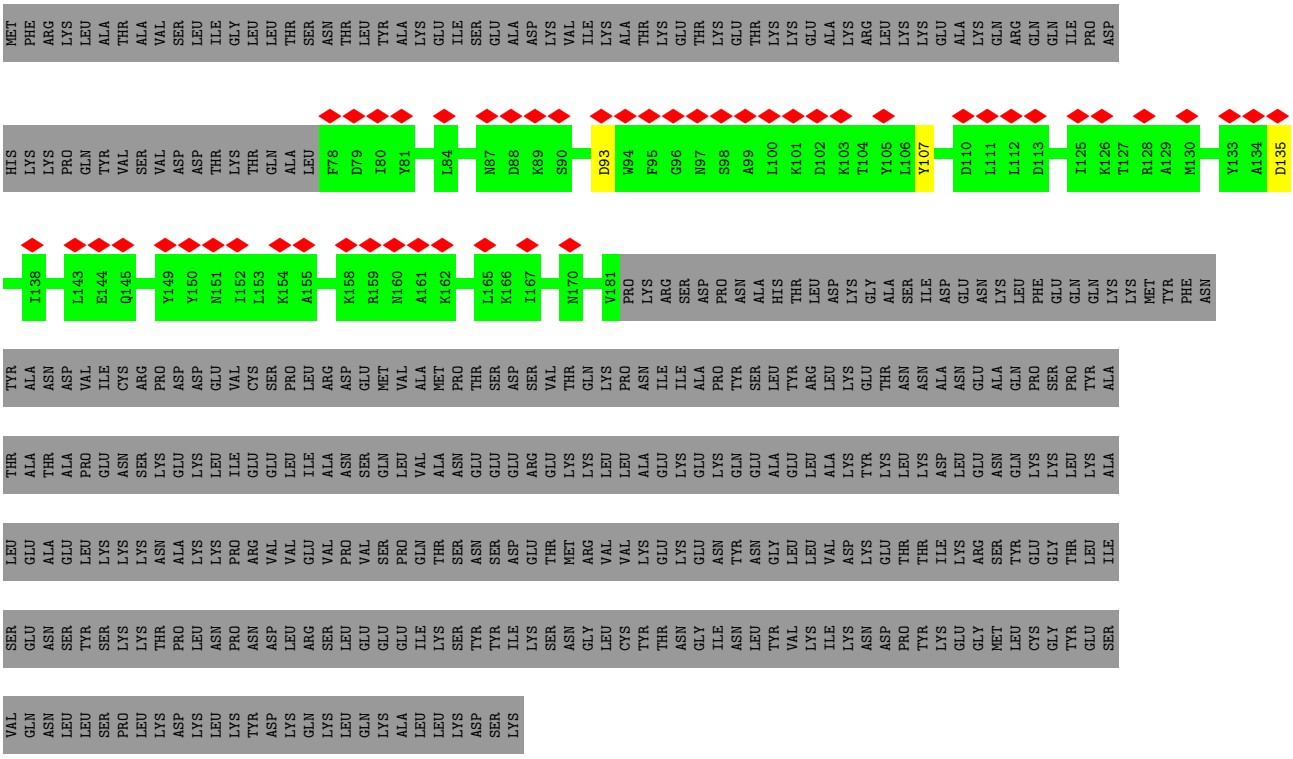
Chain BD:





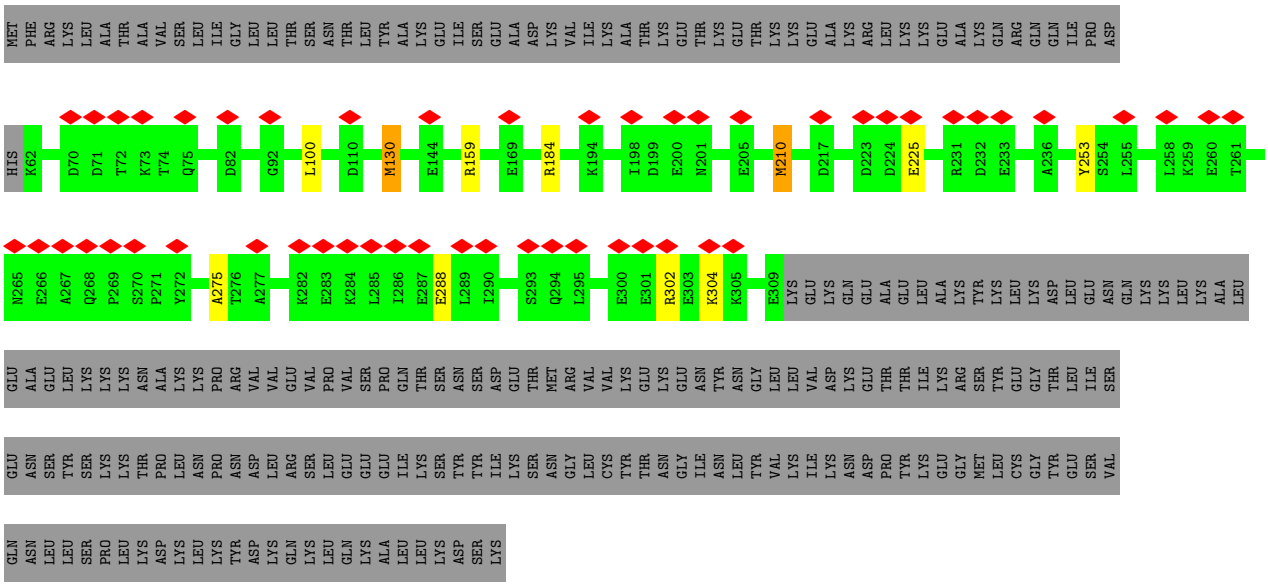
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain BE:



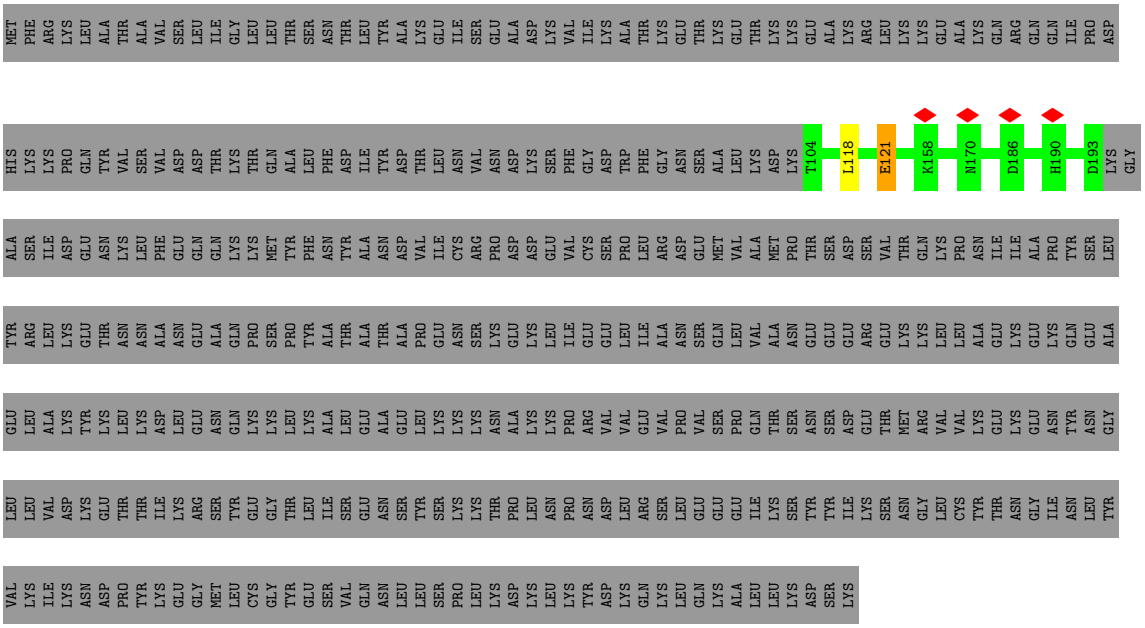
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain CA:



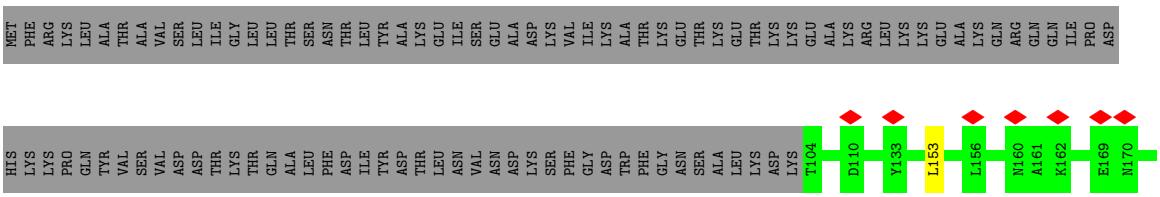
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain CB:



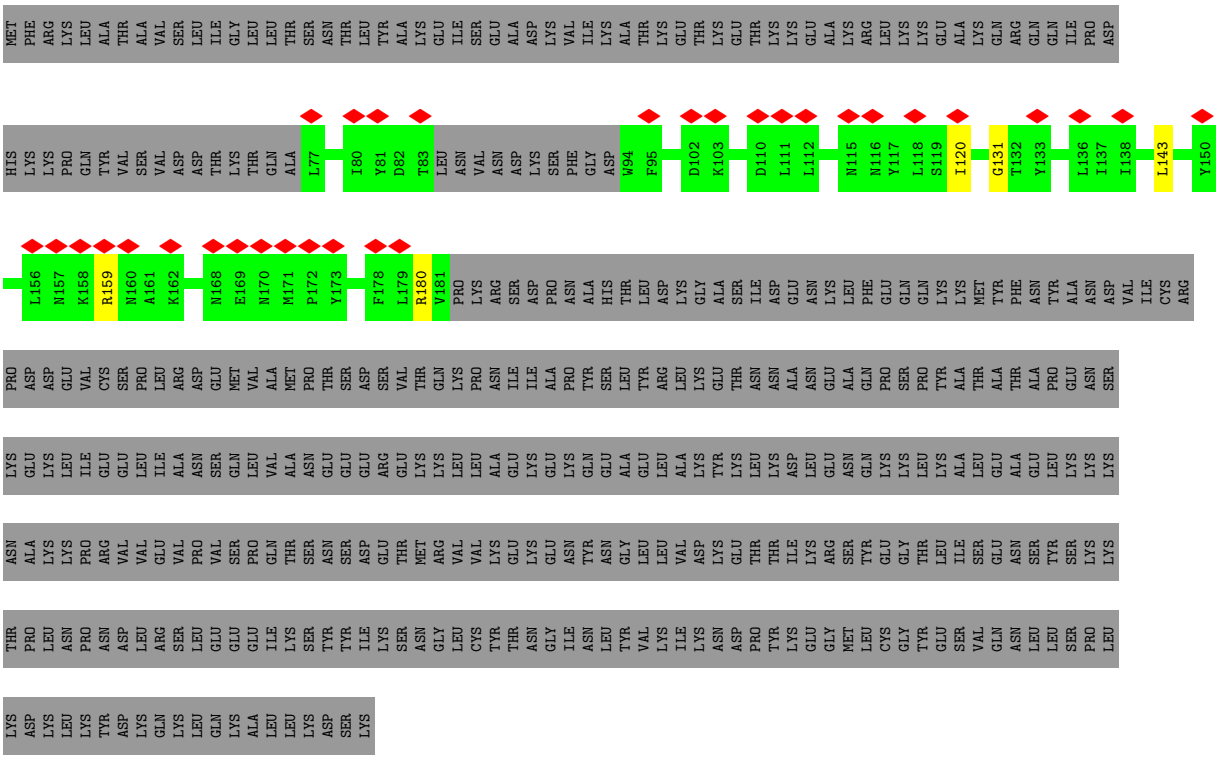
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain CC:



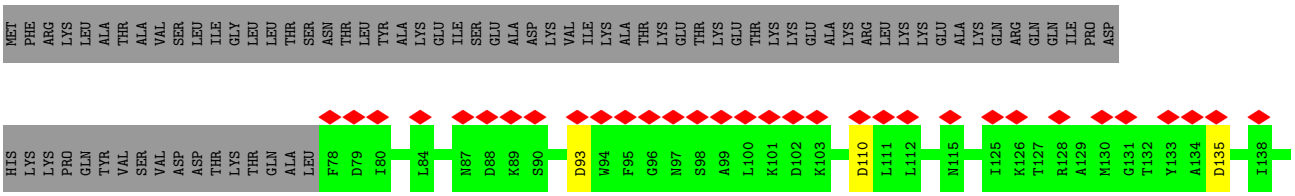
• Molecule 1: Type IV secretion system apparatus protein Cag3

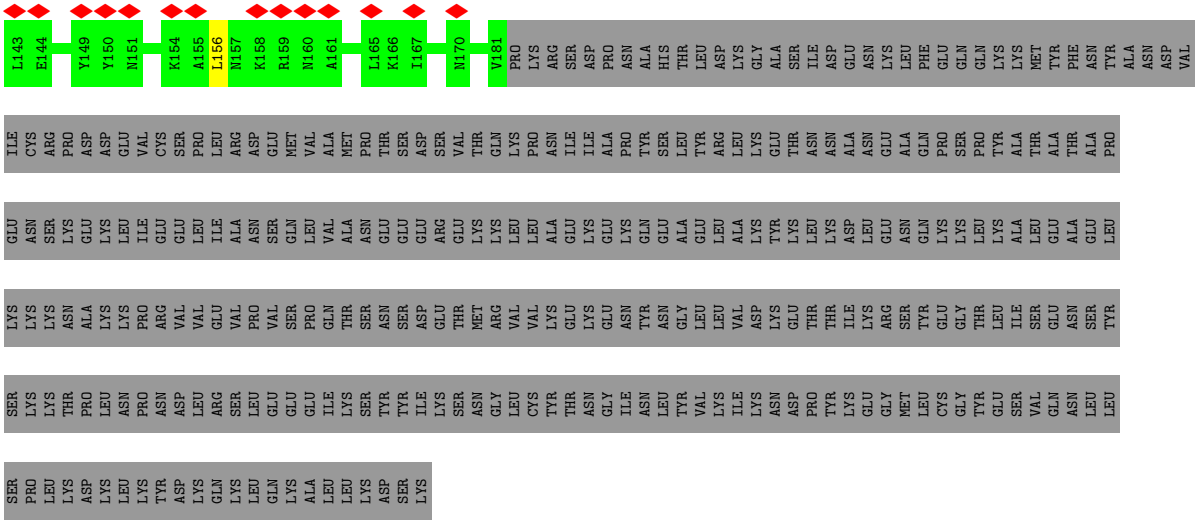
Chain CD:



• Molecule 1: Type IV secretion system apparatus protein Cag3

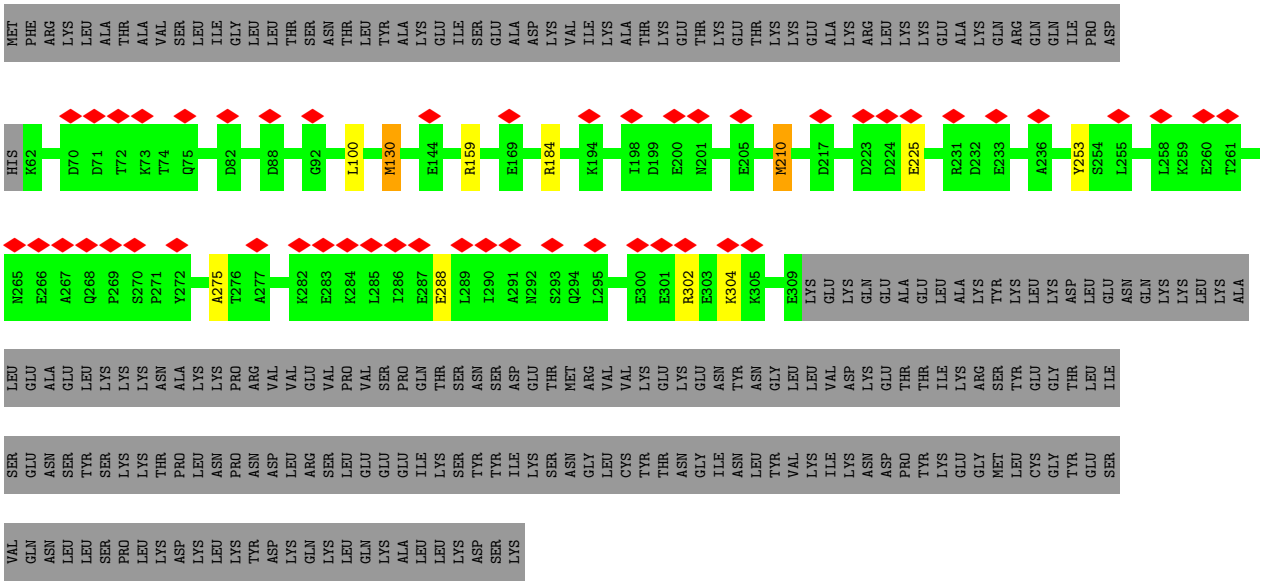
Chain CE:





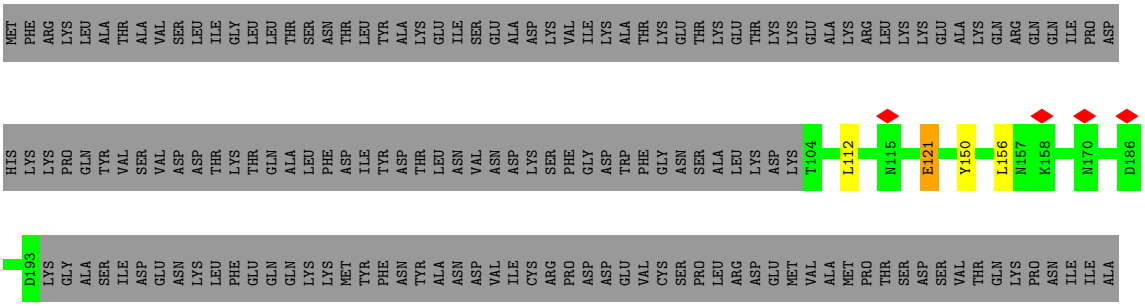
• Molecule 1: Type IV secretion system apparatus protein Cag3

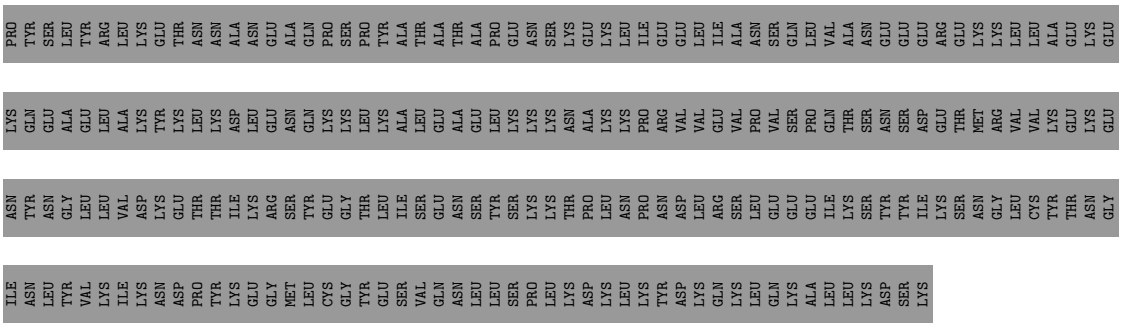
Chain DA:



• Molecule 1: Type IV secretion system apparatus protein Cag3

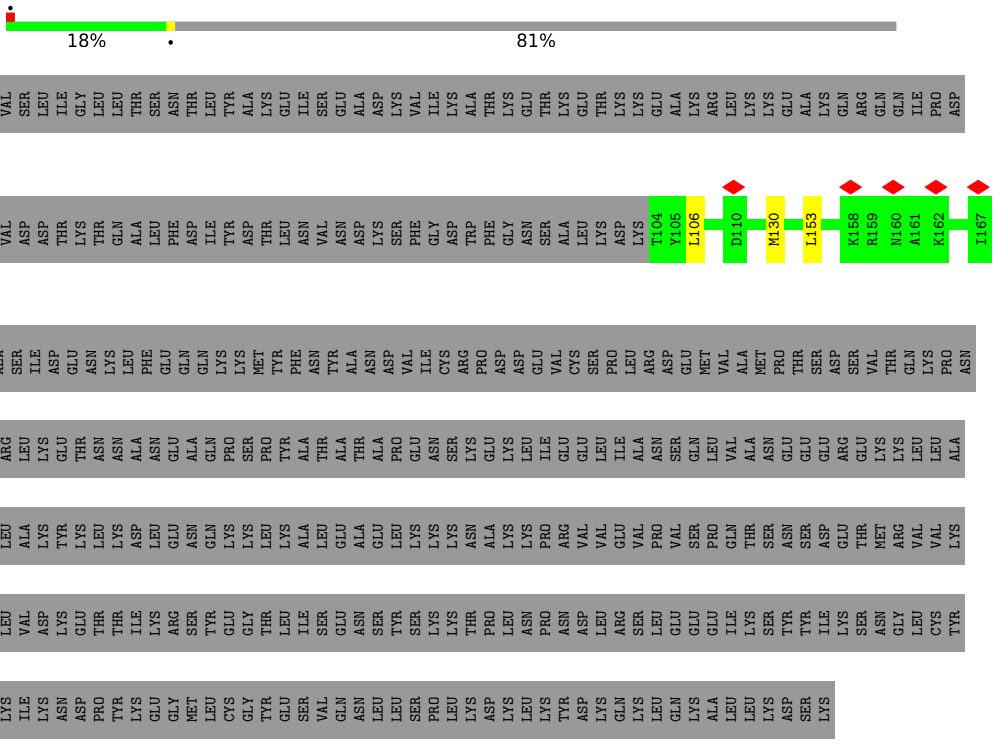
Chain DB:





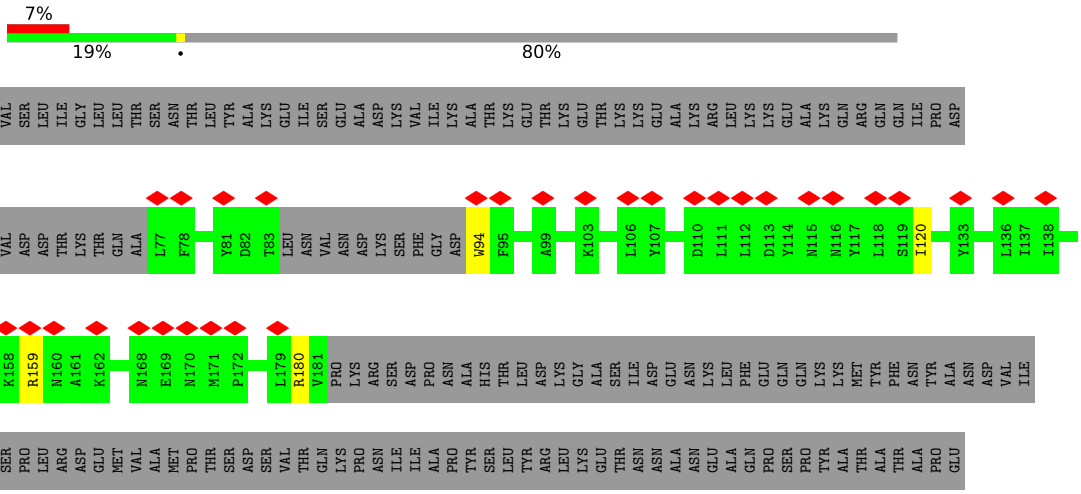
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain DC:



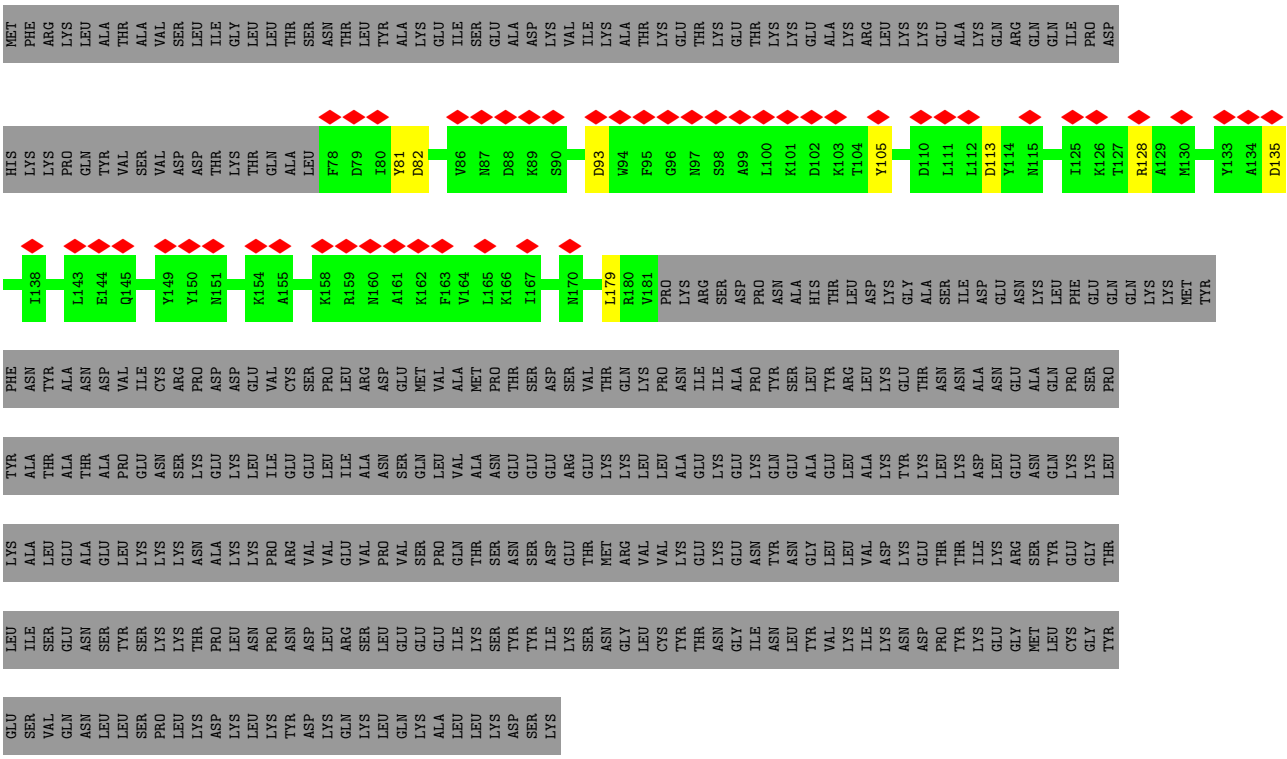
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain DD:



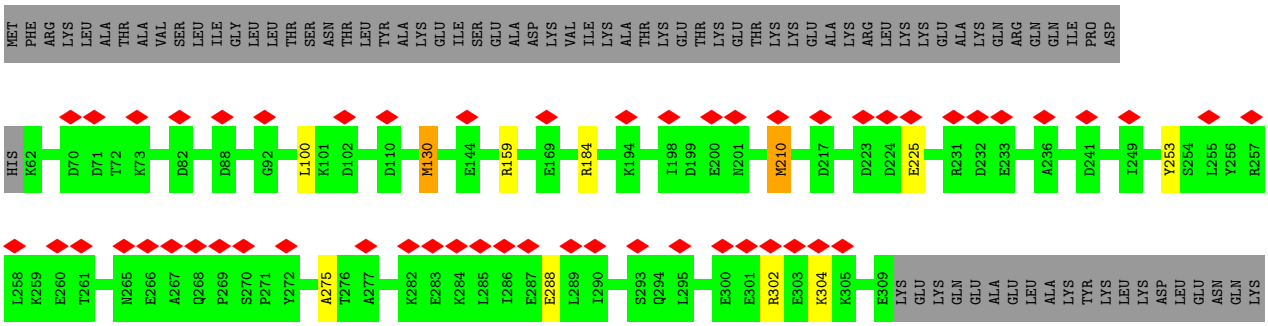
• Molecule 1: Type IV secretion system apparatus protein Cag3

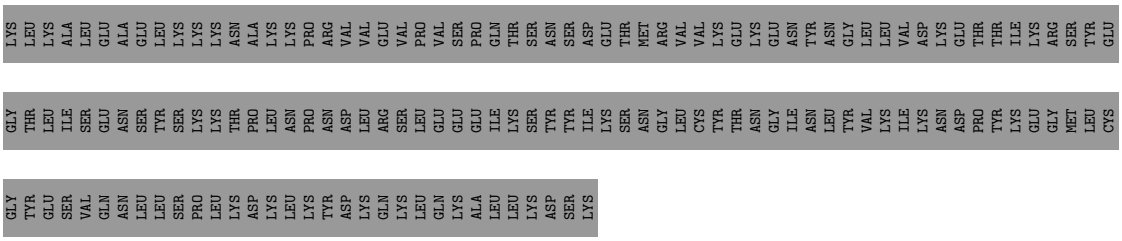
Chain DE:



• Molecule 1: Type IV secretion system apparatus protein Cag3

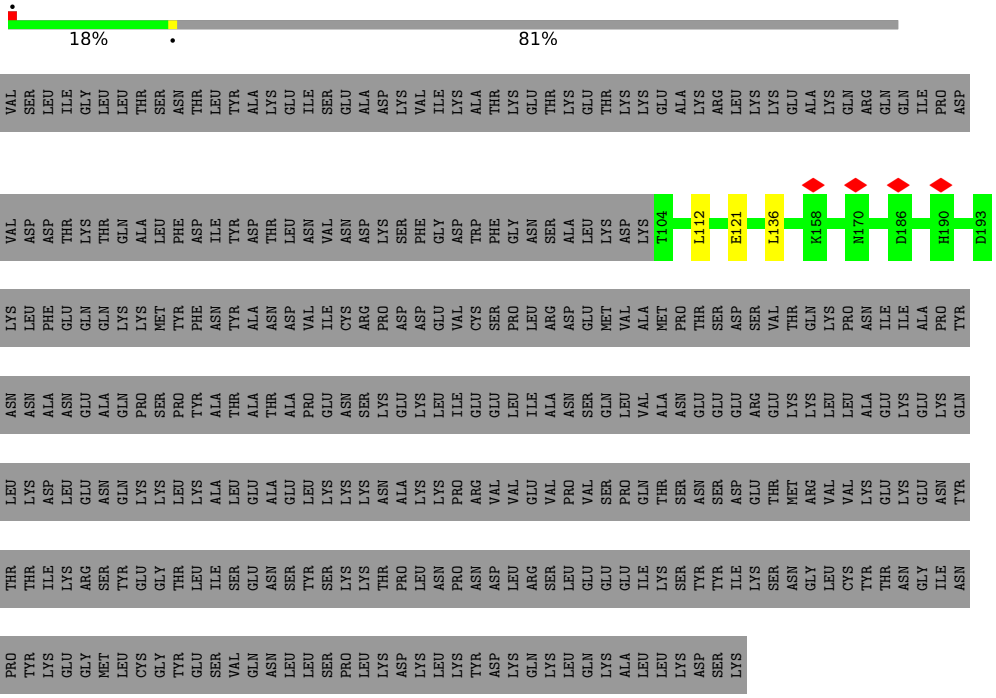
Chain EA:





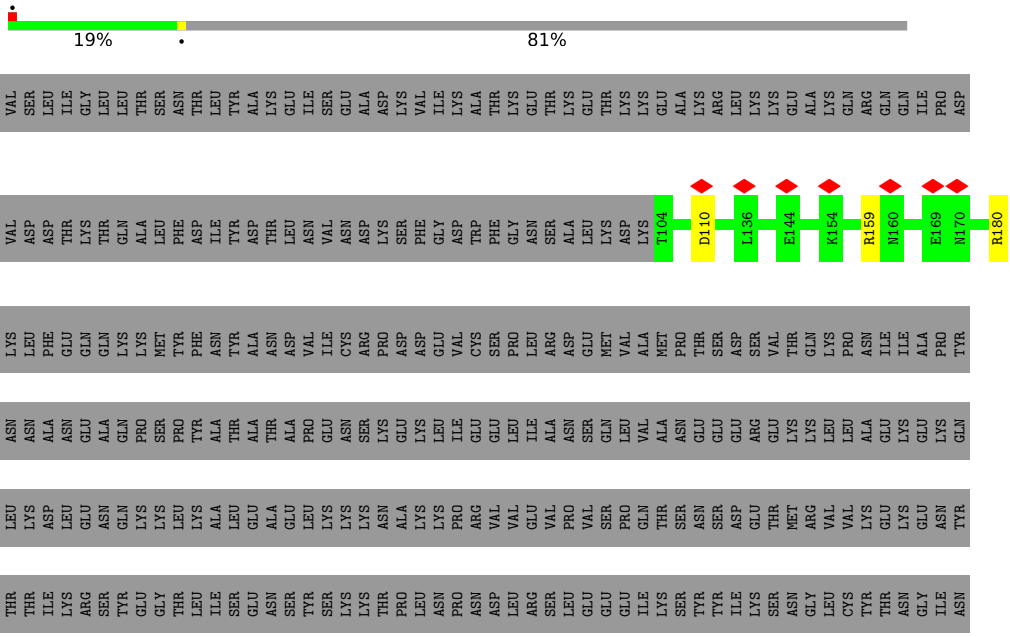
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain EB:

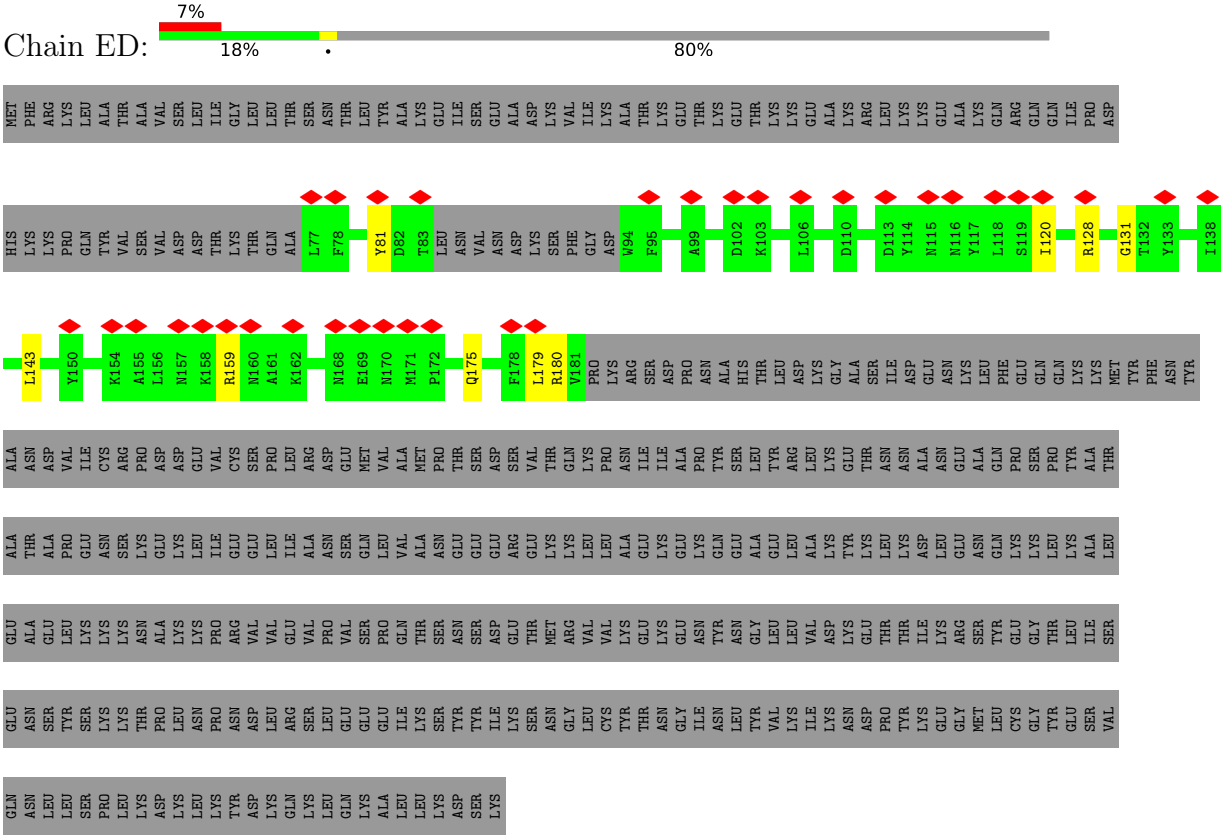


• Molecule 1: Type IV secretion system apparatus protein Cag3

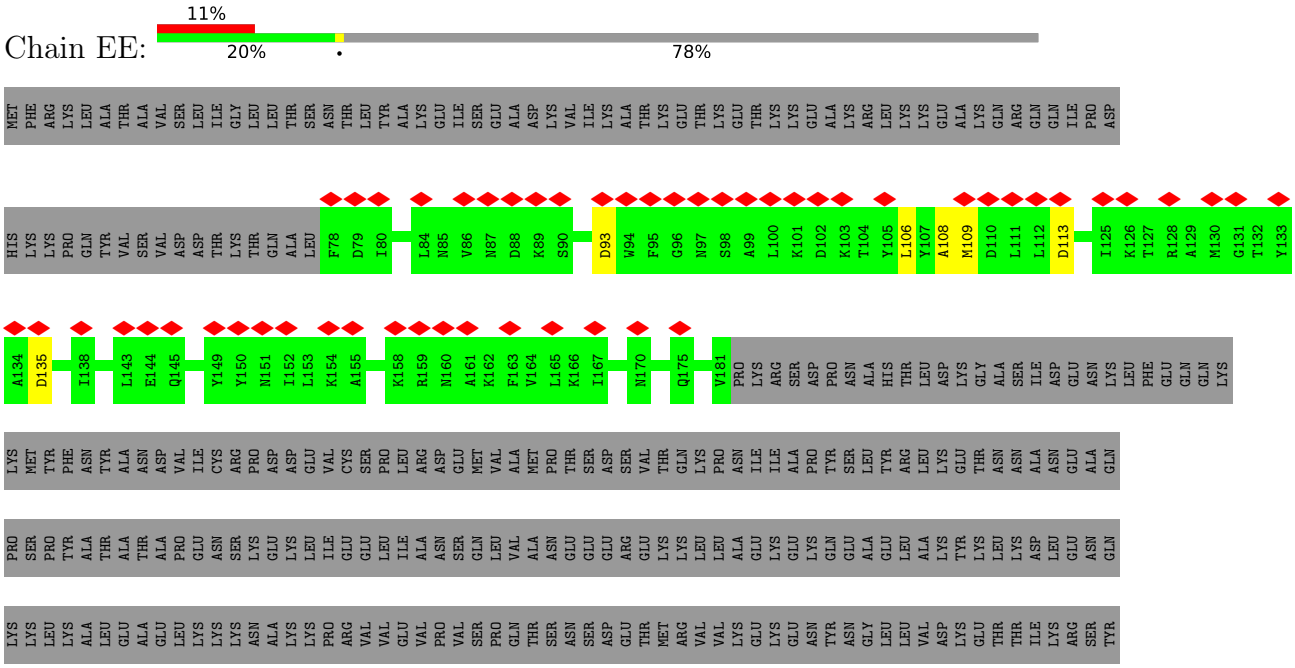
Chain EC:

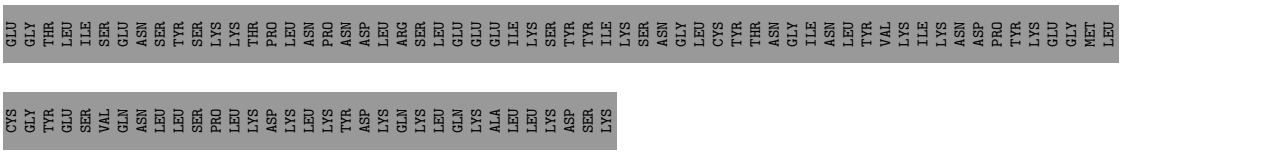


• Molecule 1: Type IV secretion system apparatus protein Cag3



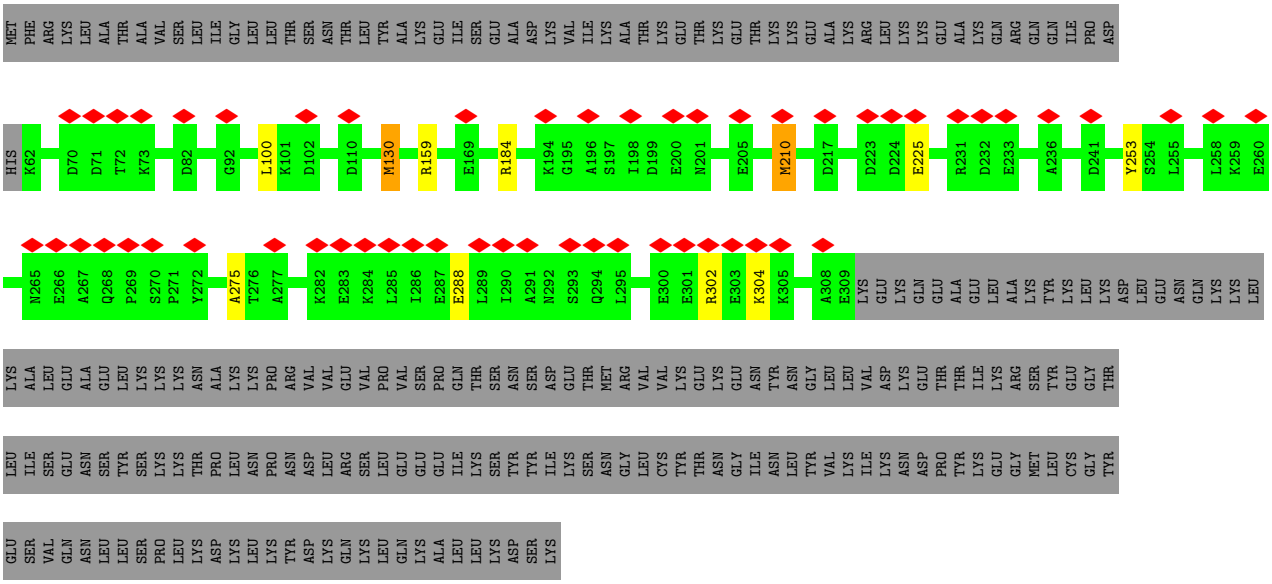
• Molecule 1: Type IV secretion system apparatus protein Cag3





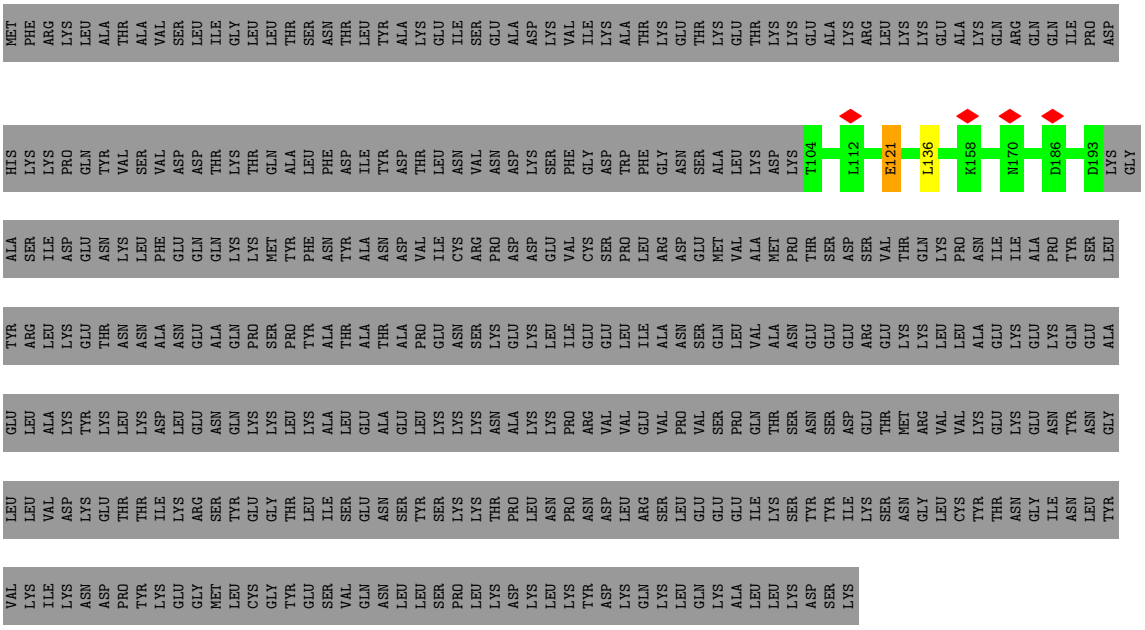
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain FA:



• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain FB:



• Molecule 1: Type IV secretion system apparatus protein Cag3

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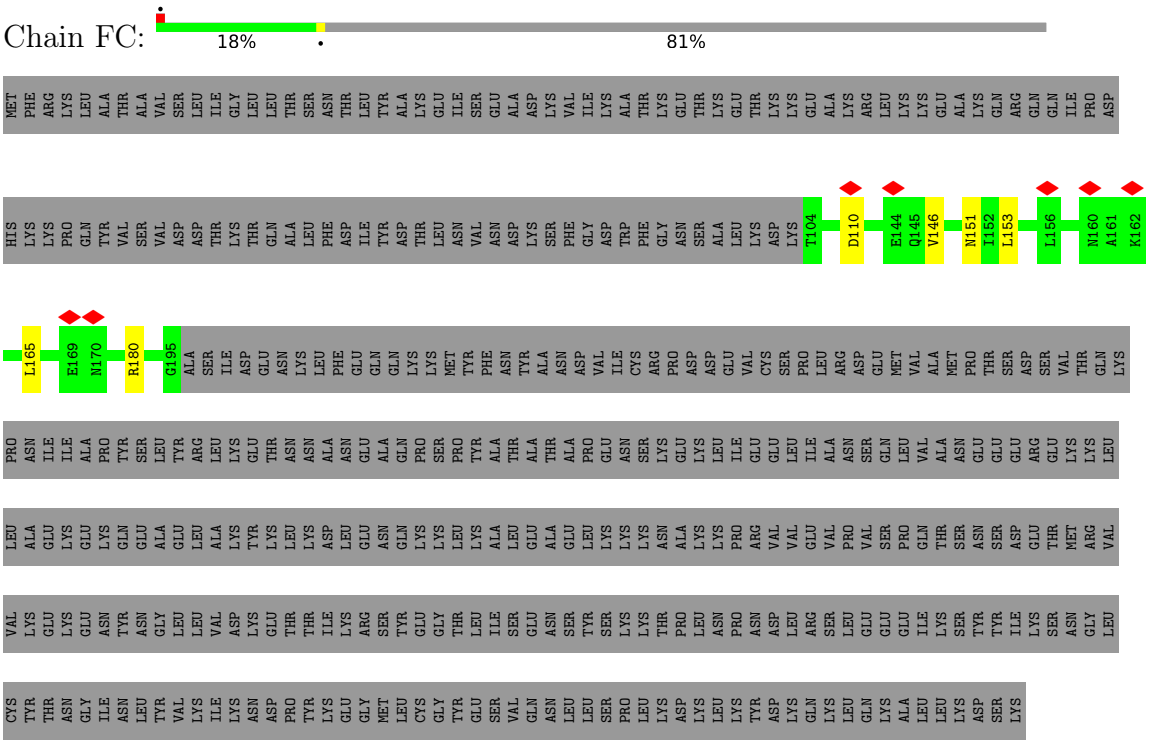

• Molecule 1: Type IV secretion system apparatus protein Cag3

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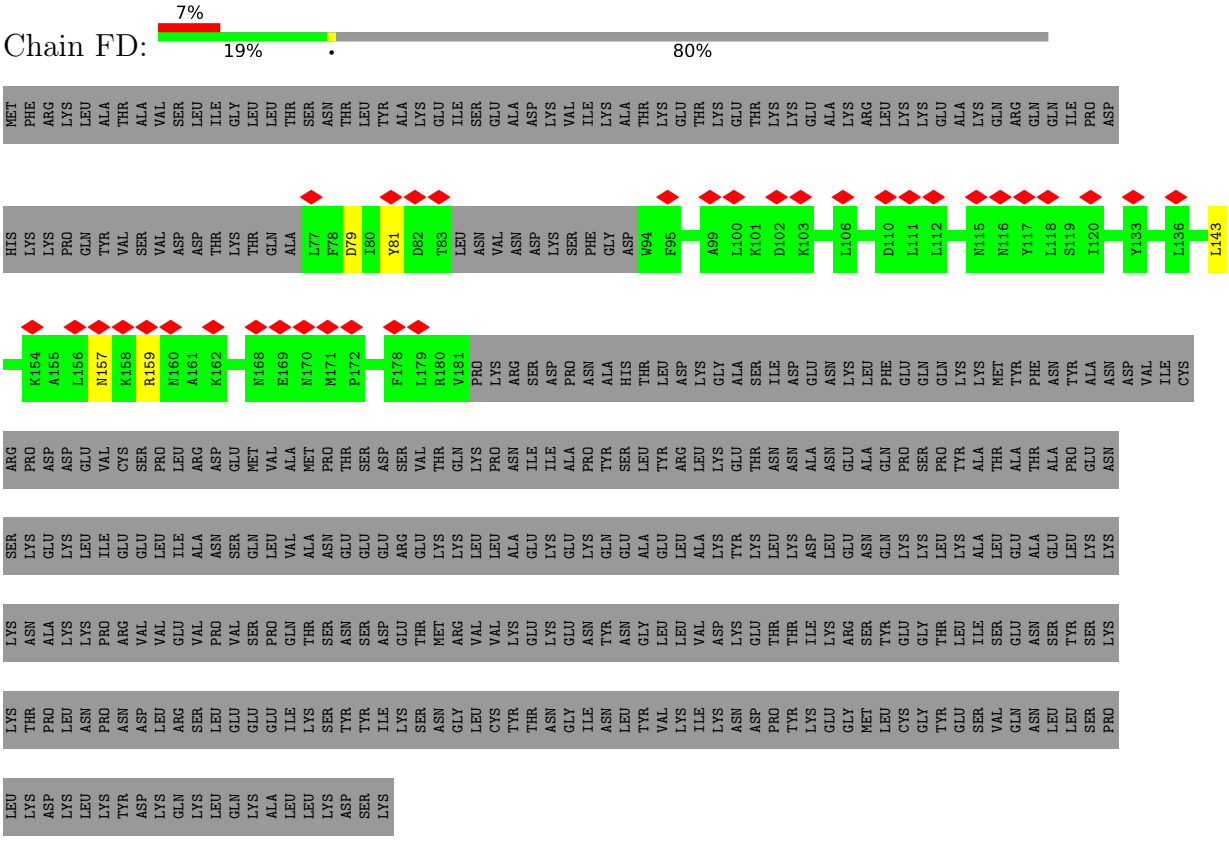

• Molecule 1: Type IV secretion system apparatus protein Cag3

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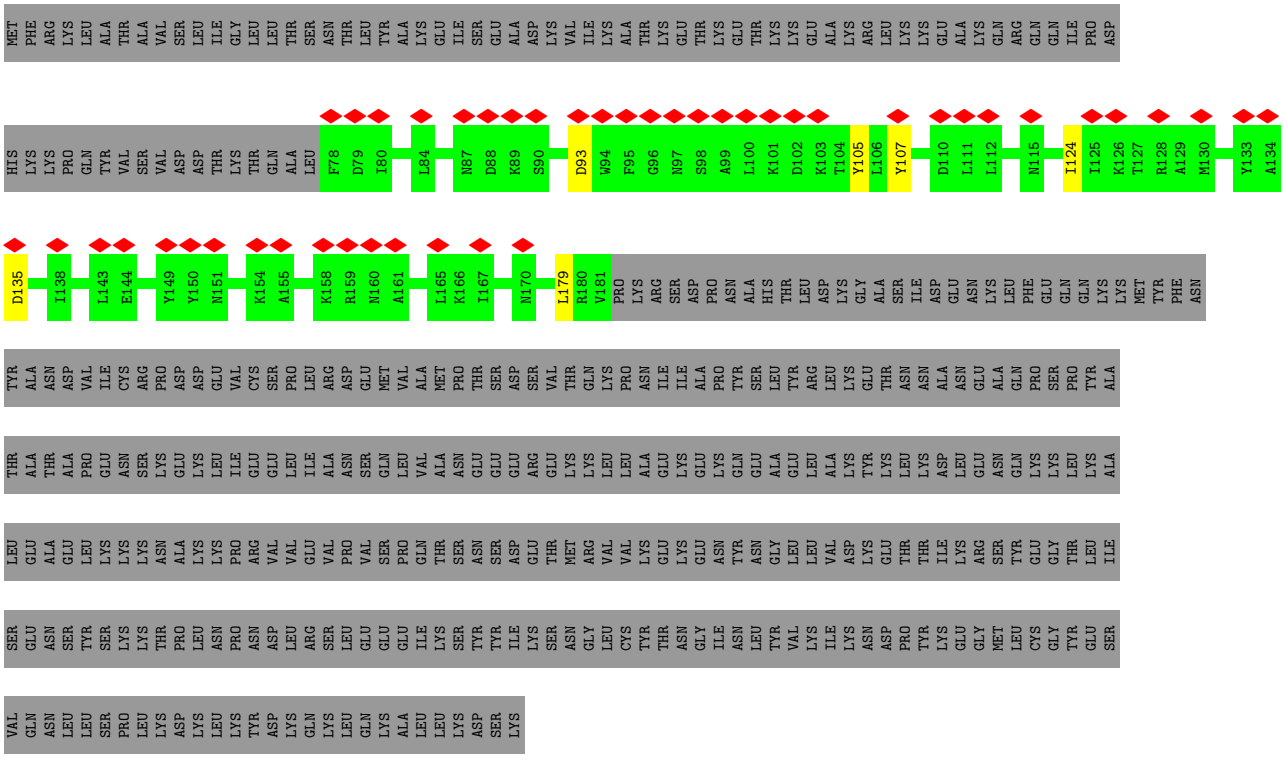

• Molecule 1: Type IV secretion system apparatus protein Cag3

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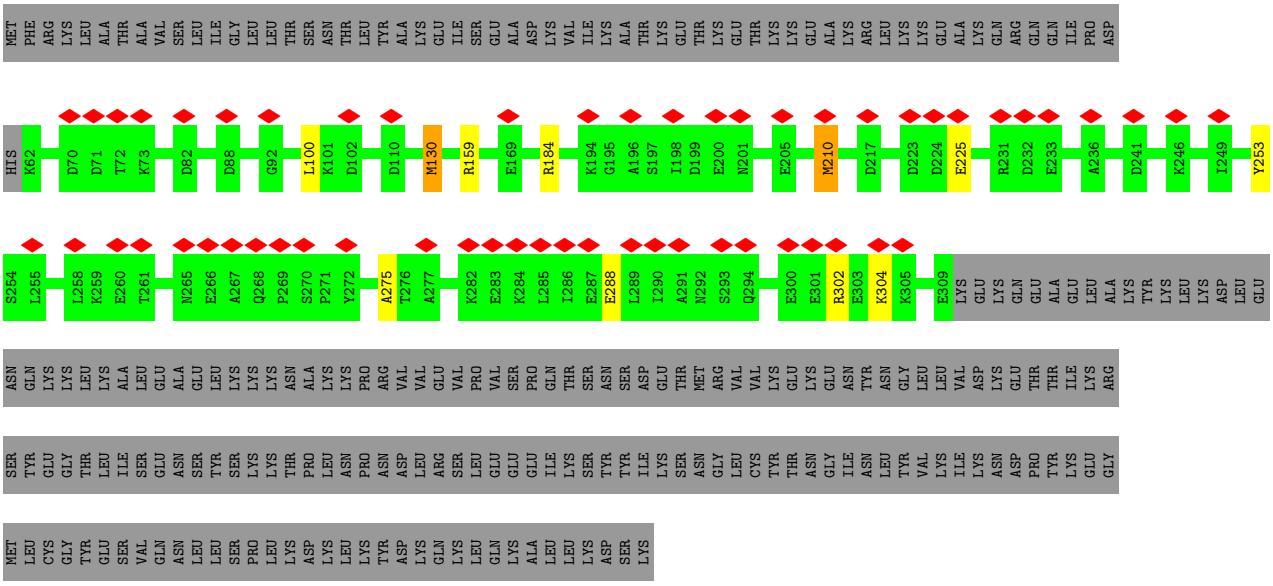
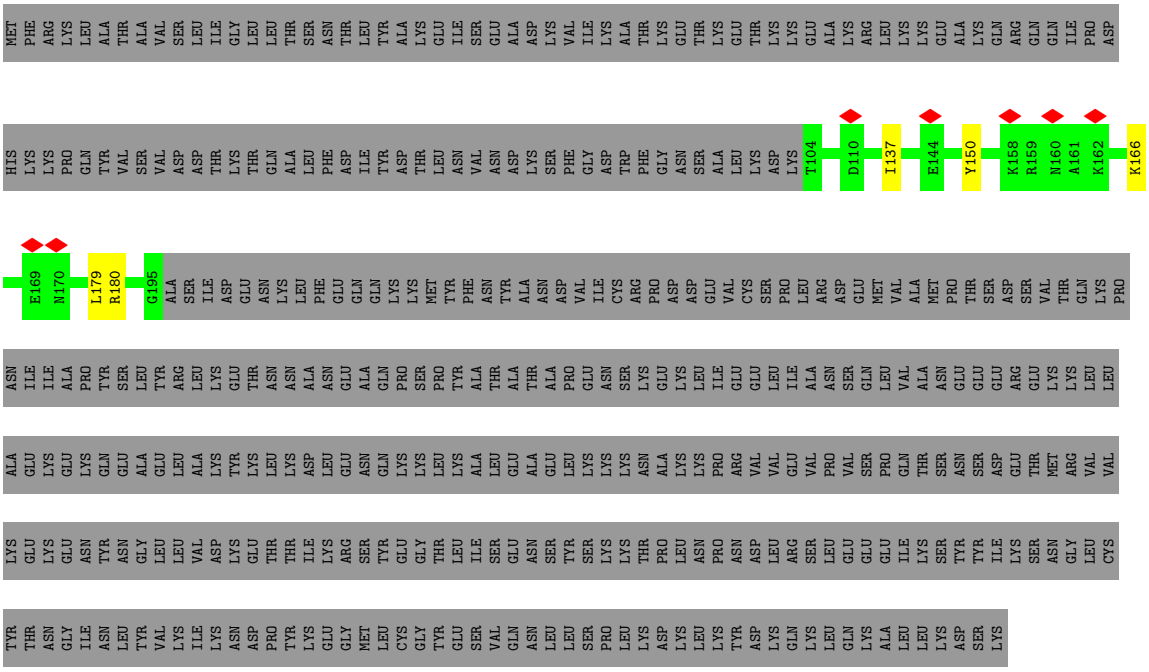


• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain GB:

• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain GC:



• Molecule 1: Type IV secretion system apparatus protein Cag3

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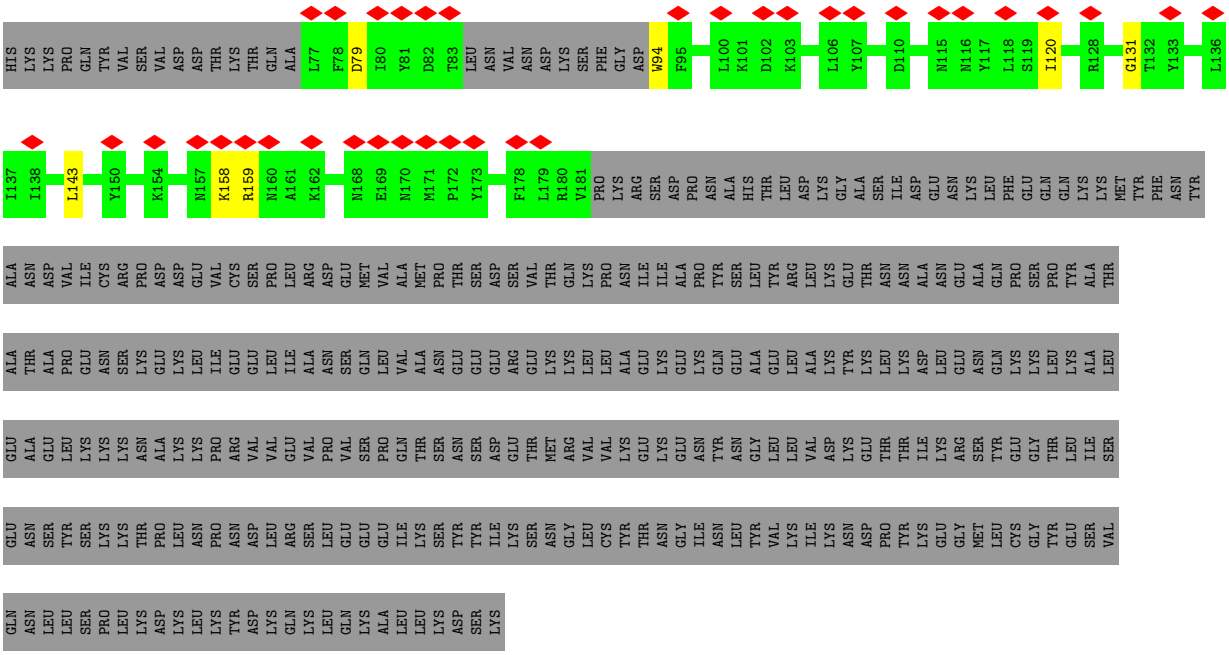

• Molecule 1: Type IV secretion system apparatus protein Cag3

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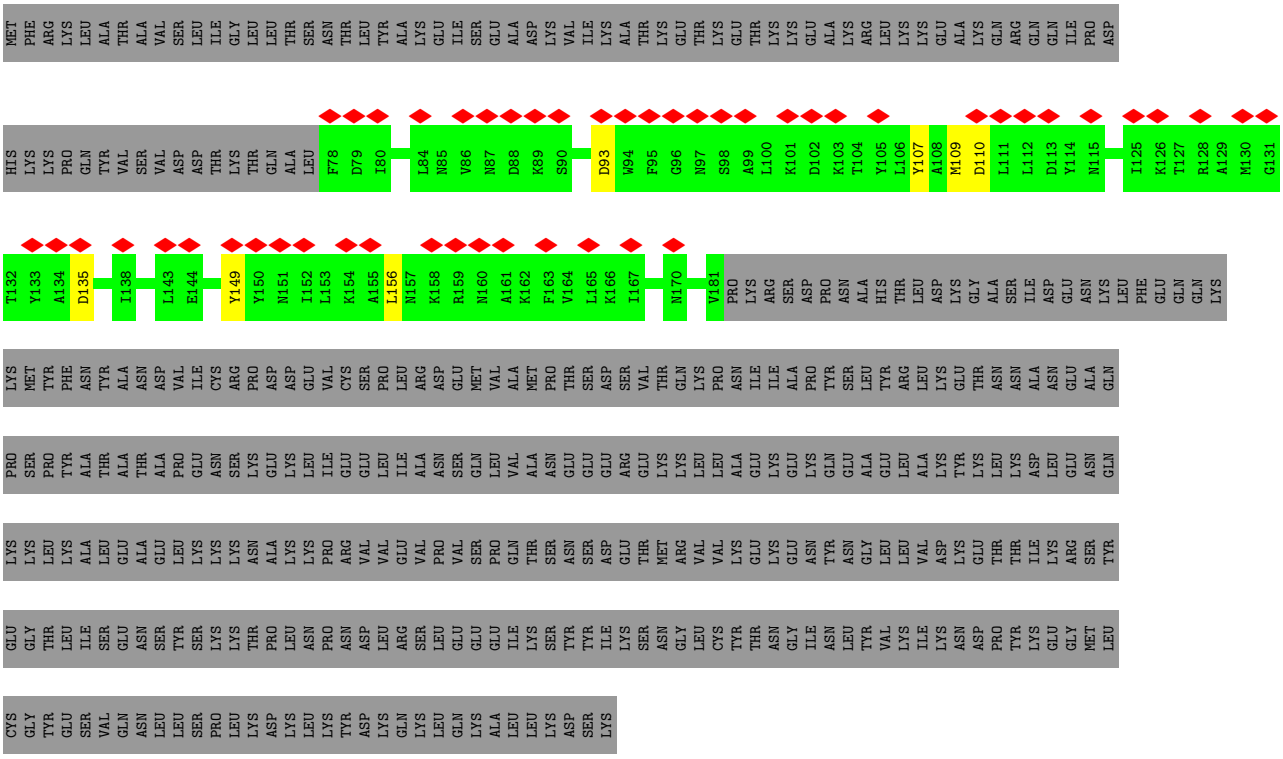

• Molecule 1: Type IV secretion system apparatus protein Cag3

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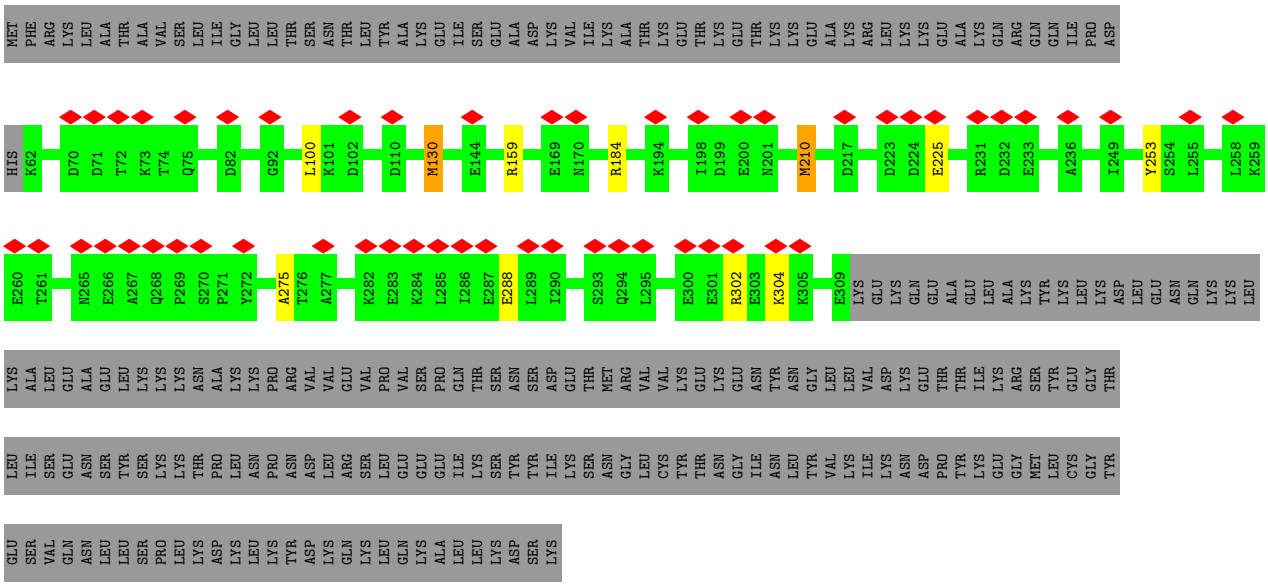

• Molecule 1: Type IV secretion system apparatus protein Cag3

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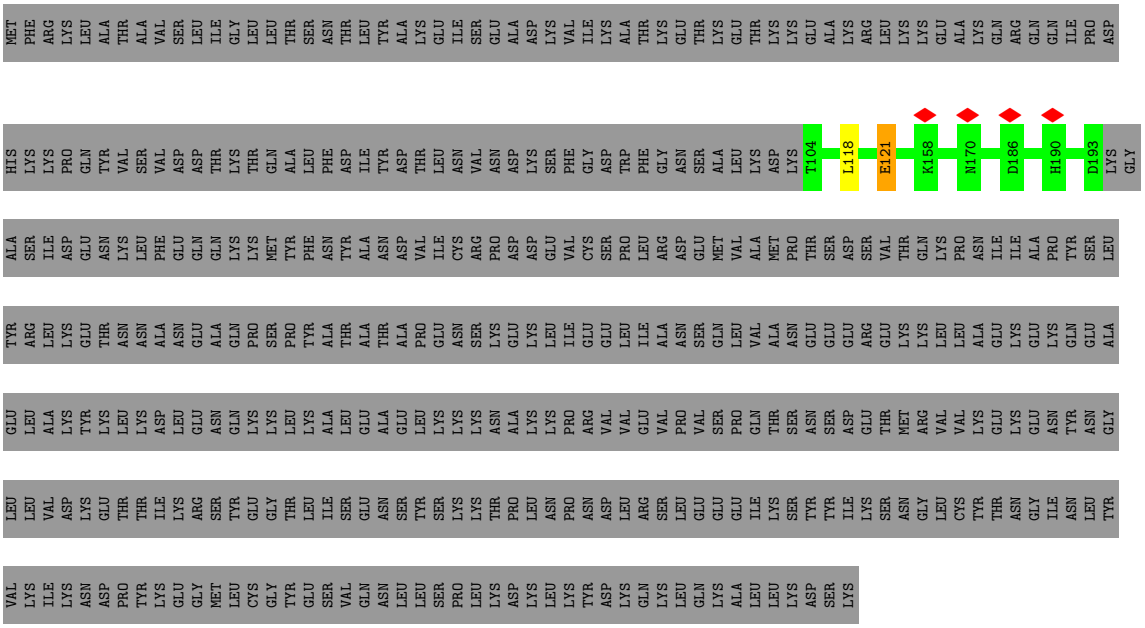

• Molecule 1: Type IV secretion system apparatus protein Cag3

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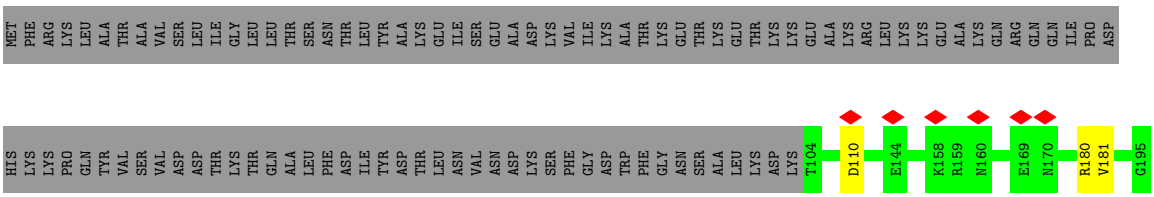

• Molecule 1: Type IV secretion system apparatus protein Cag3

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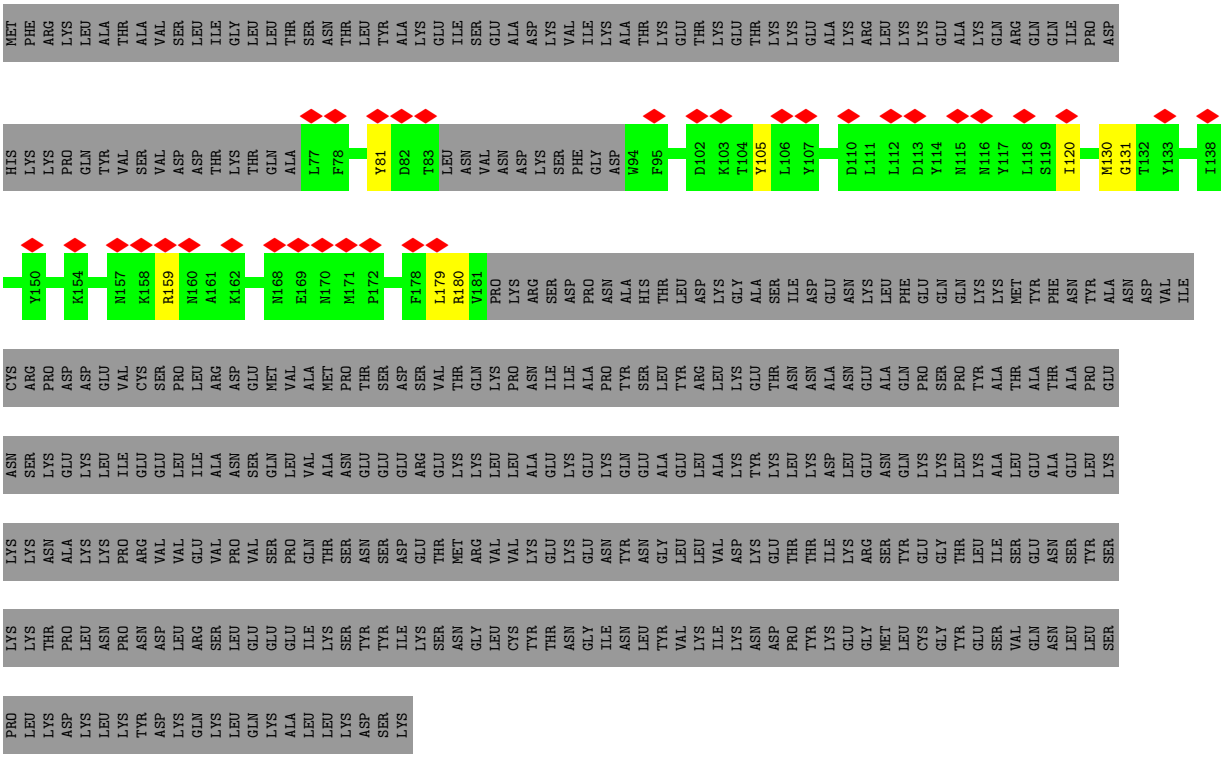

• Molecule 1: Type IV secretion system apparatus protein Cag3

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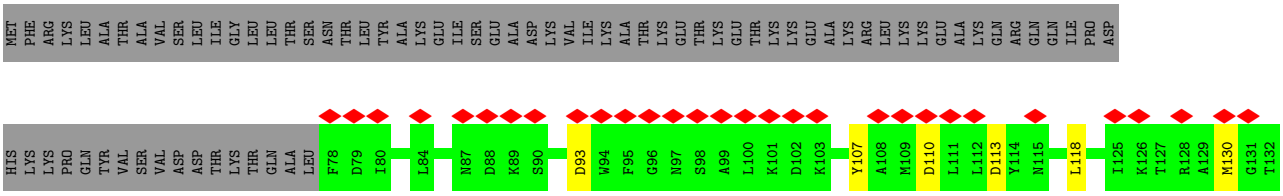
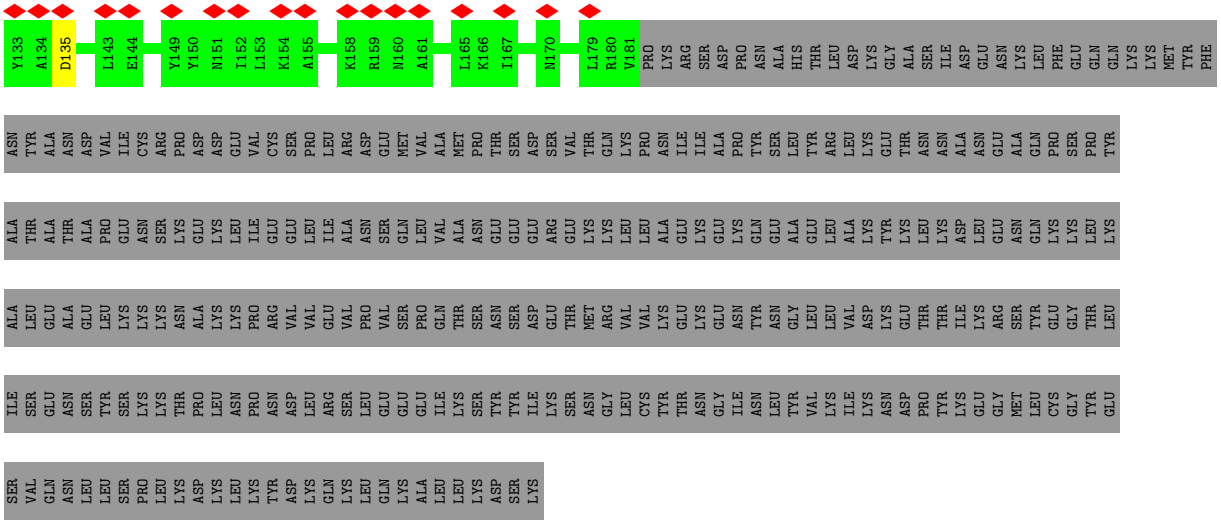
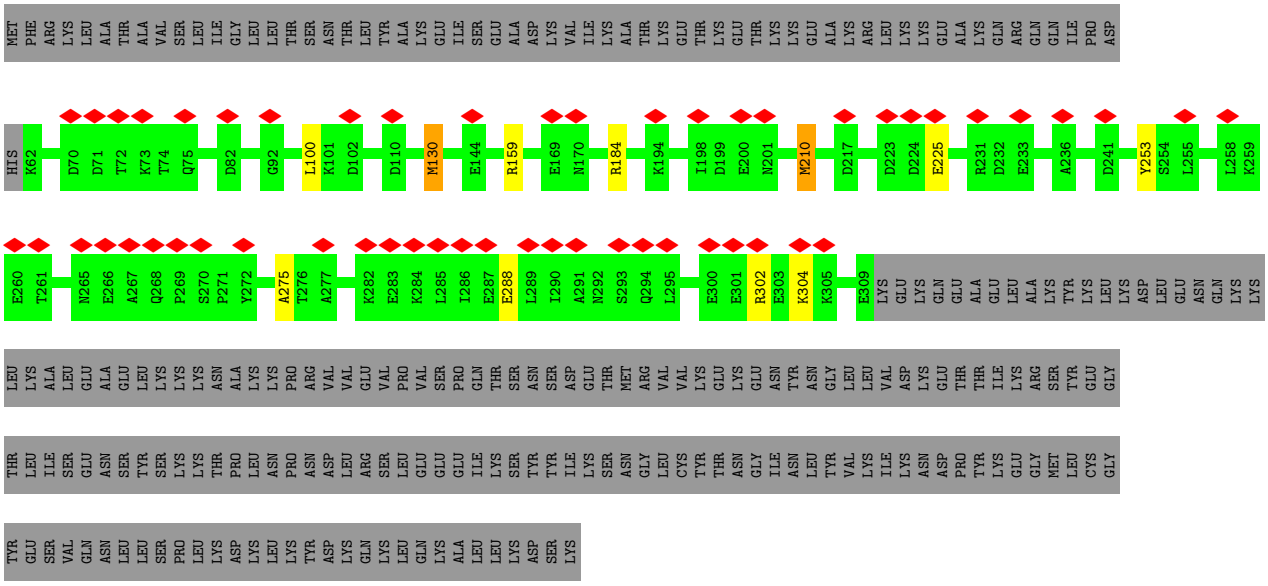




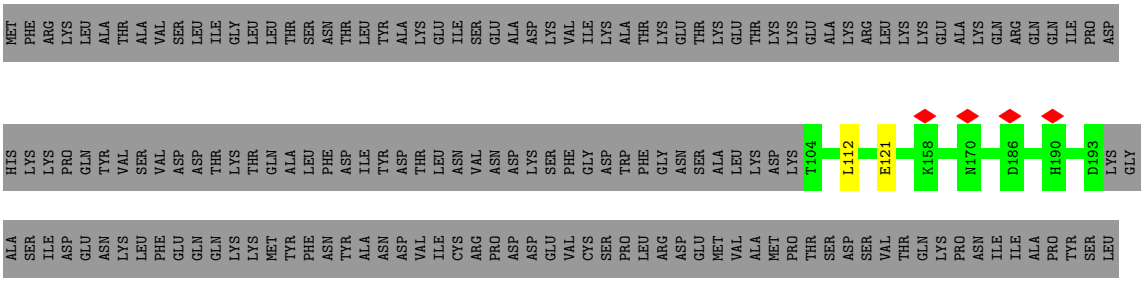
• Molecule 1: Type IV secretion system apparatus protein Cag3

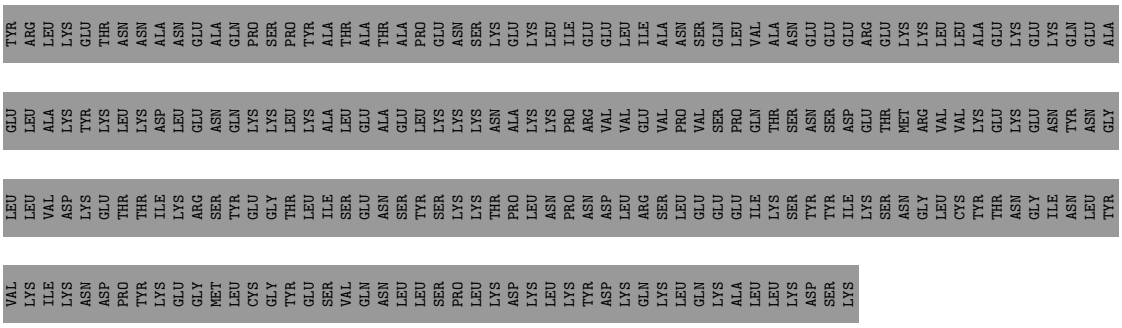
Chain IA:



• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain IB:





• Molecule 1: Type IV secretion system apparatus protein Cag3

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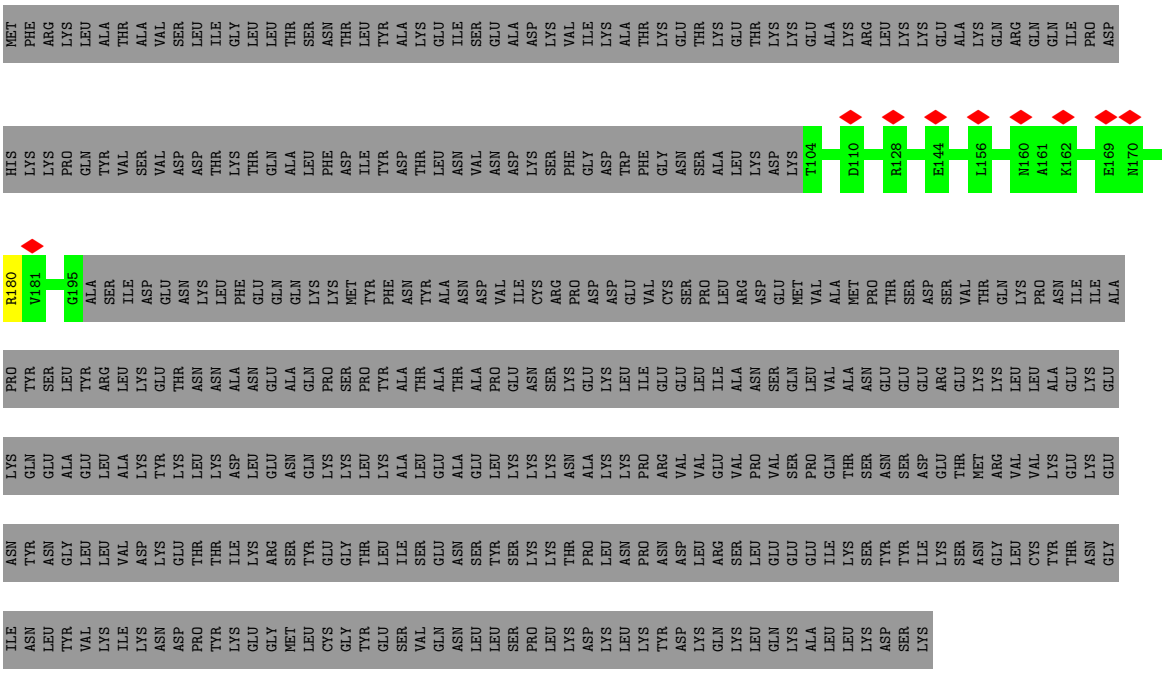

• Molecule 1: Type IV secretion system apparatus protein Cag3

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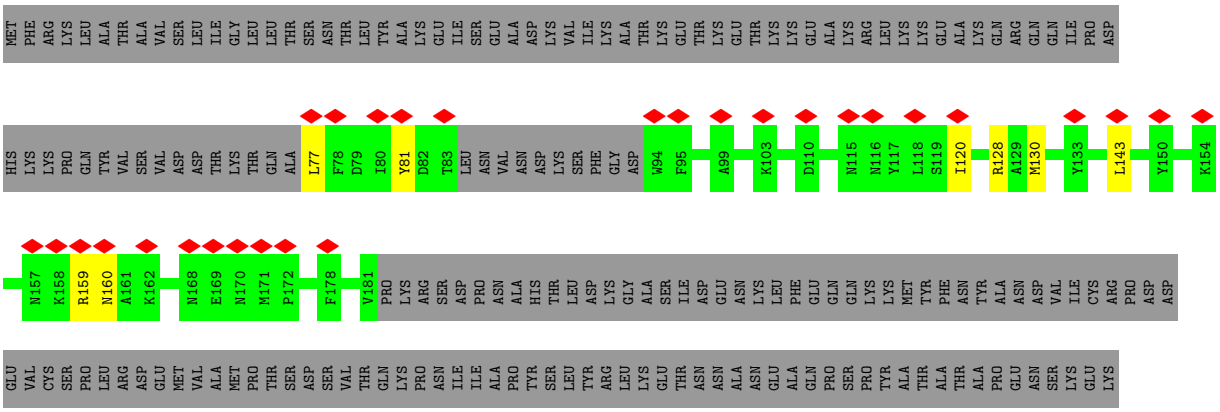

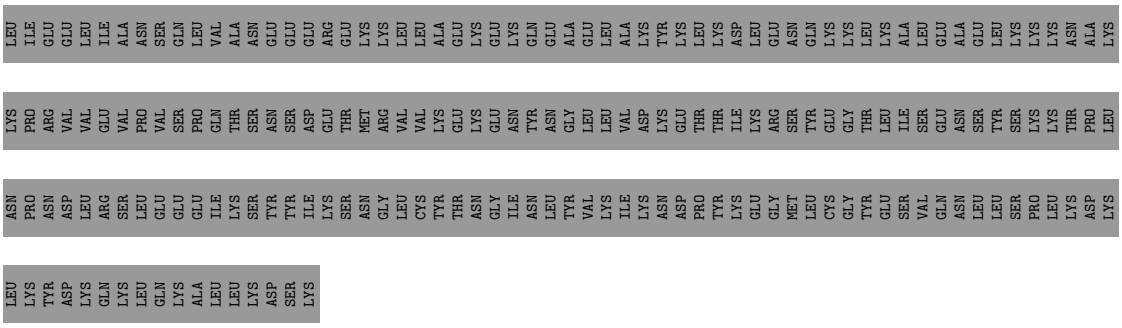

- Molecule 1: Type IV secretion system apparatus protein Cag3

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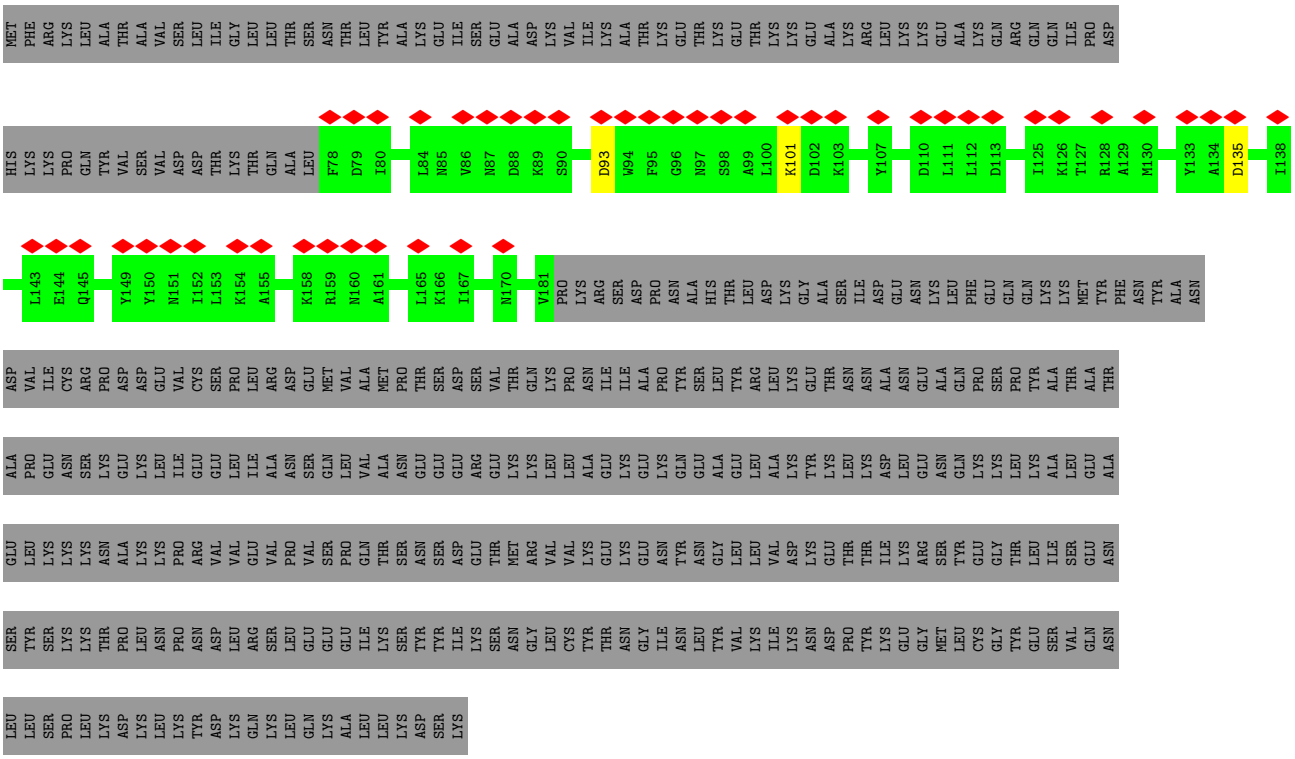

- Molecule 1: Type IV secretion system apparatus protein Cag3

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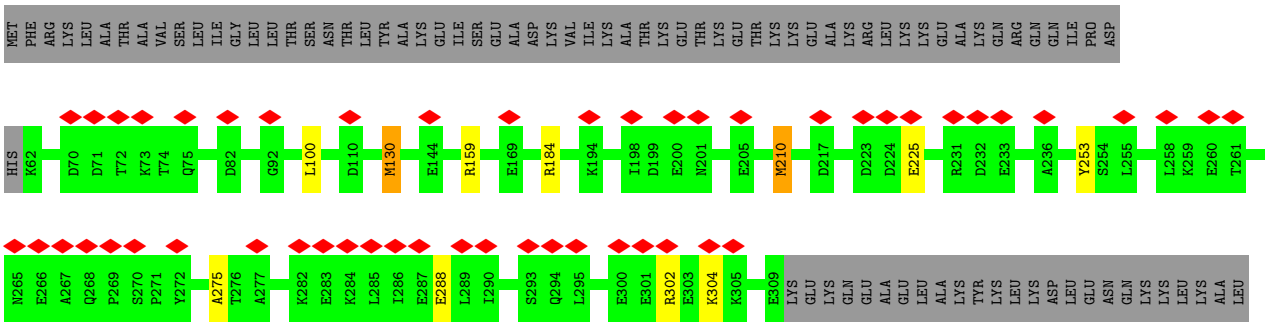

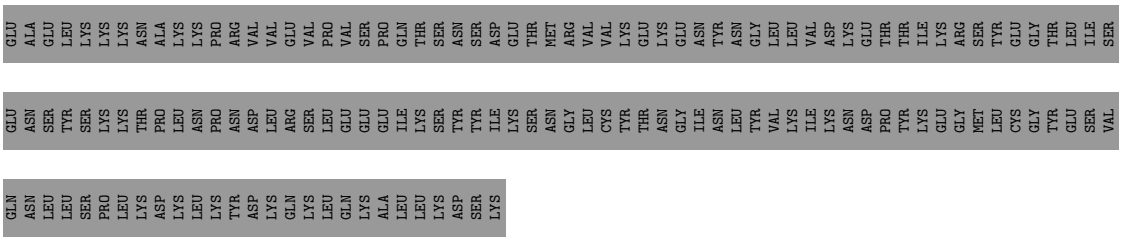

• Molecule 1: Type IV secretion system apparatus protein Cag3

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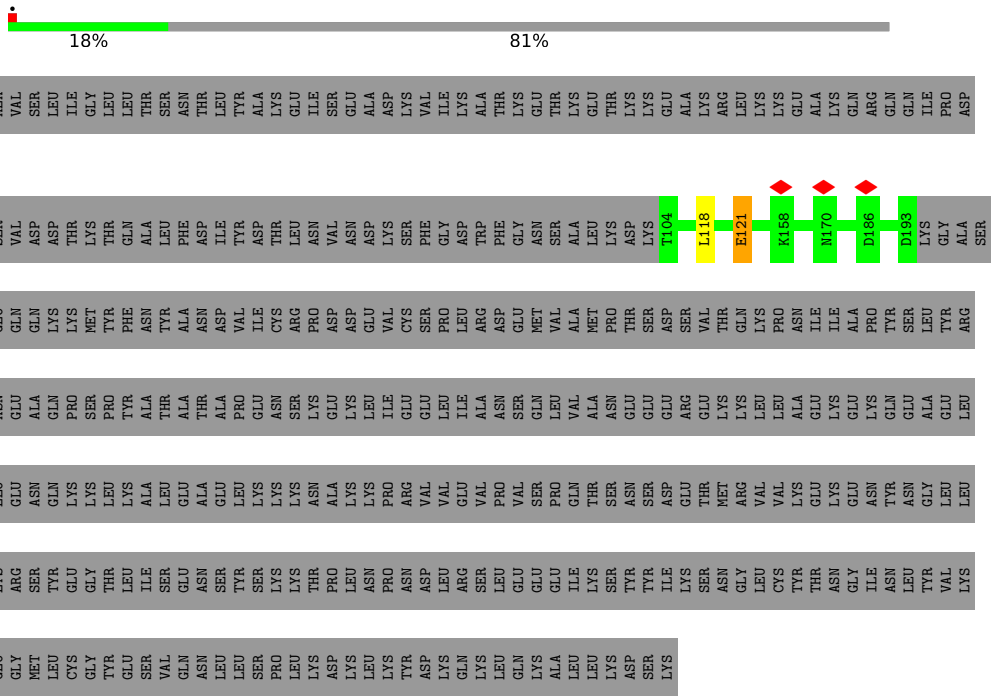
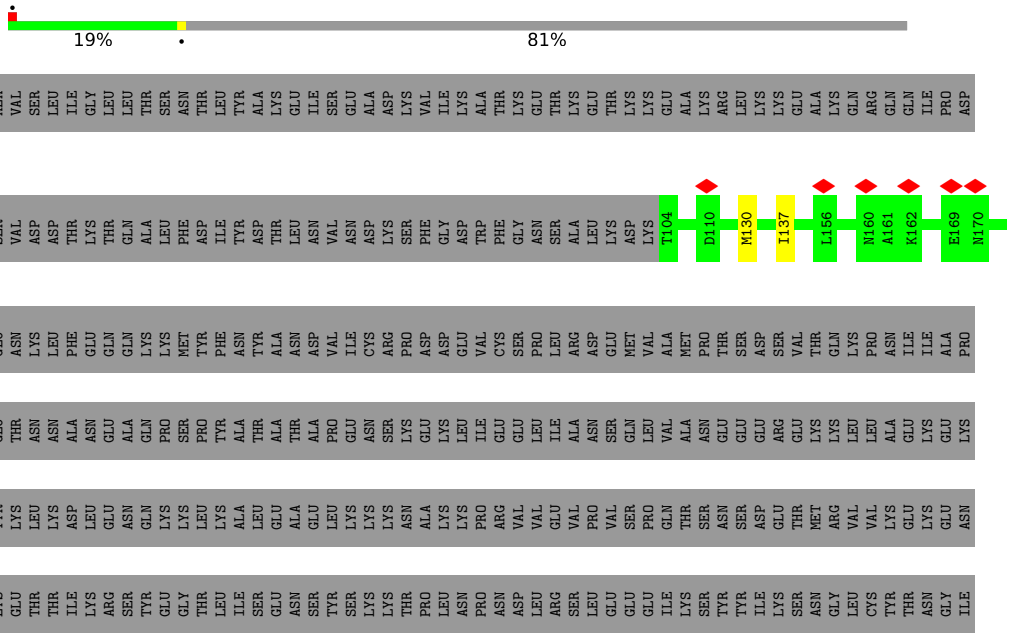
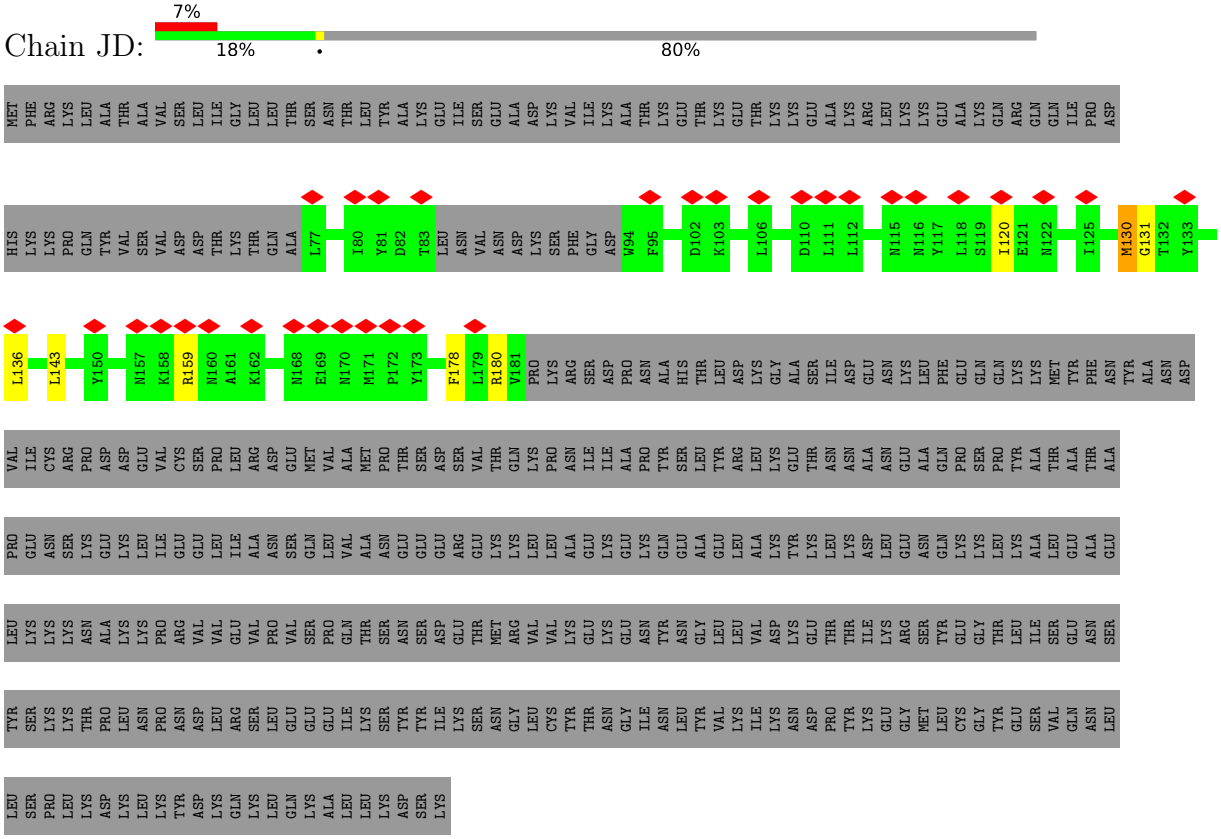


• Molecule 1: Type IV secretion system apparatus protein Cag3

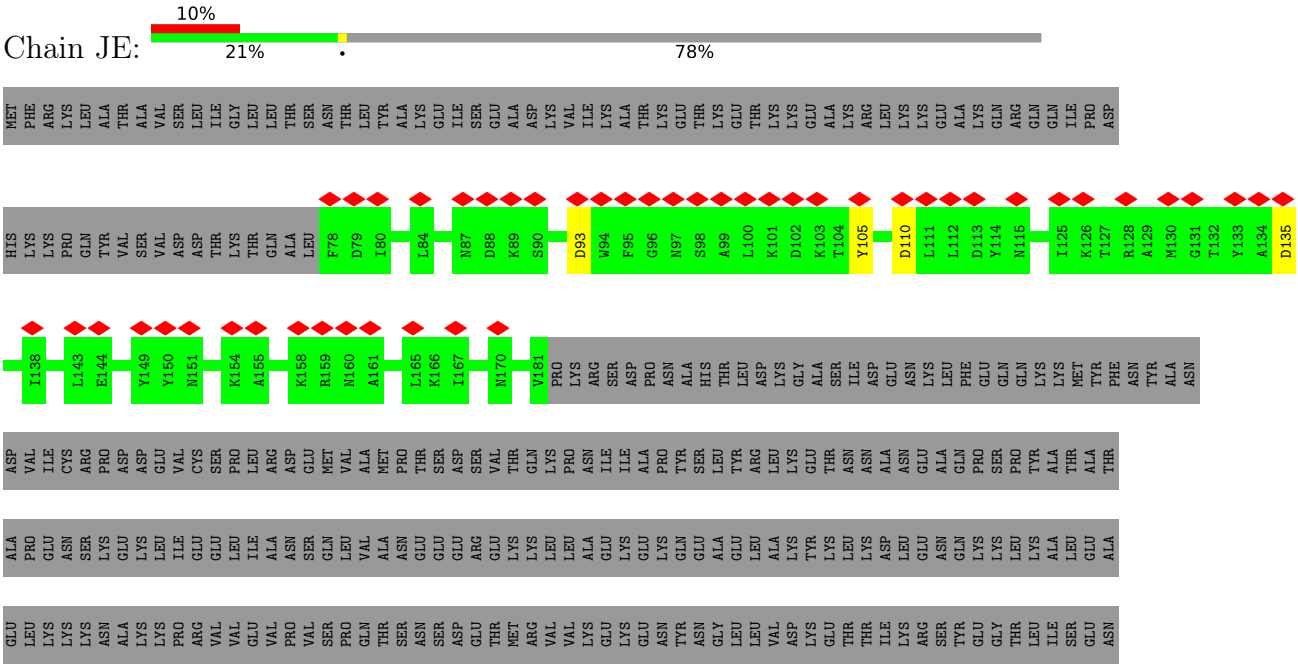
Chain JC:

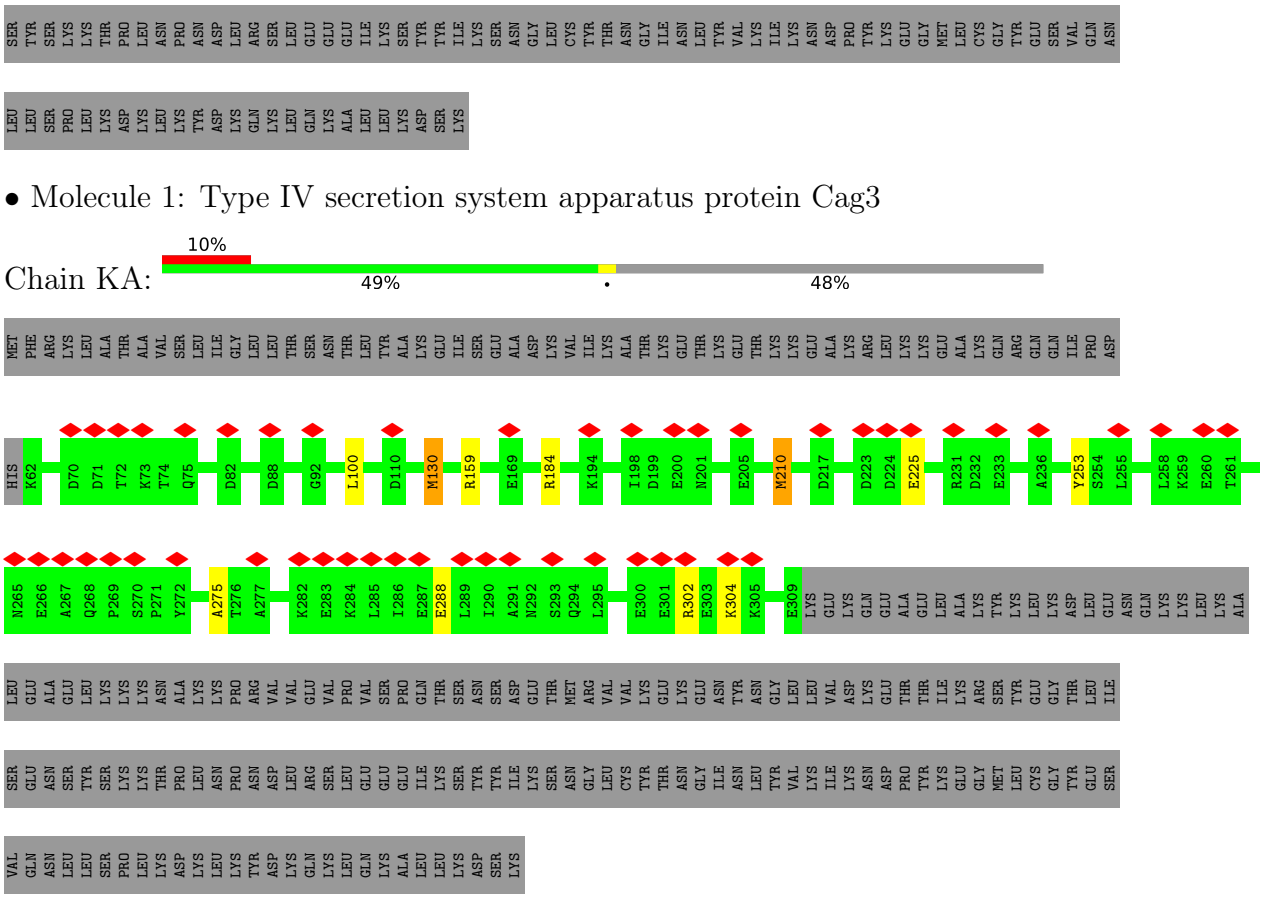


• Molecule 1: Type IV secretion system apparatus protein Cag3

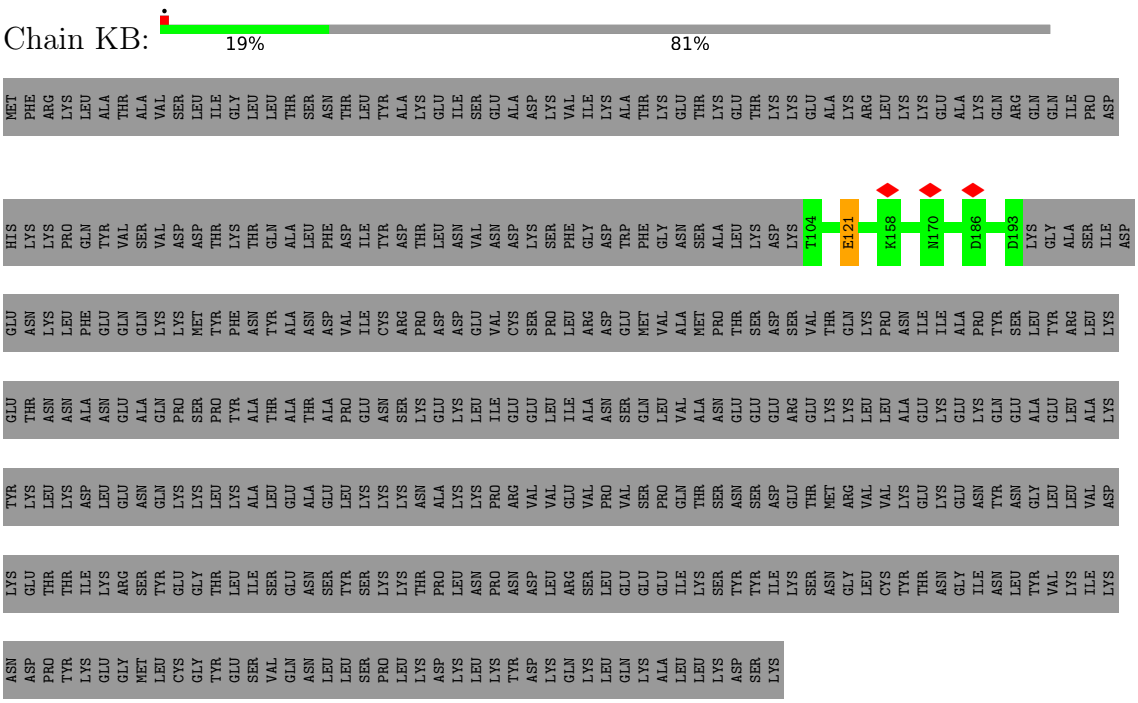


• Molecule 1: Type IV secretion system apparatus protein Cag3





• Molecule 1: Type IV secretion system apparatus protein Cag3



• Molecule 1: Type IV secretion system apparatus protein Cag3

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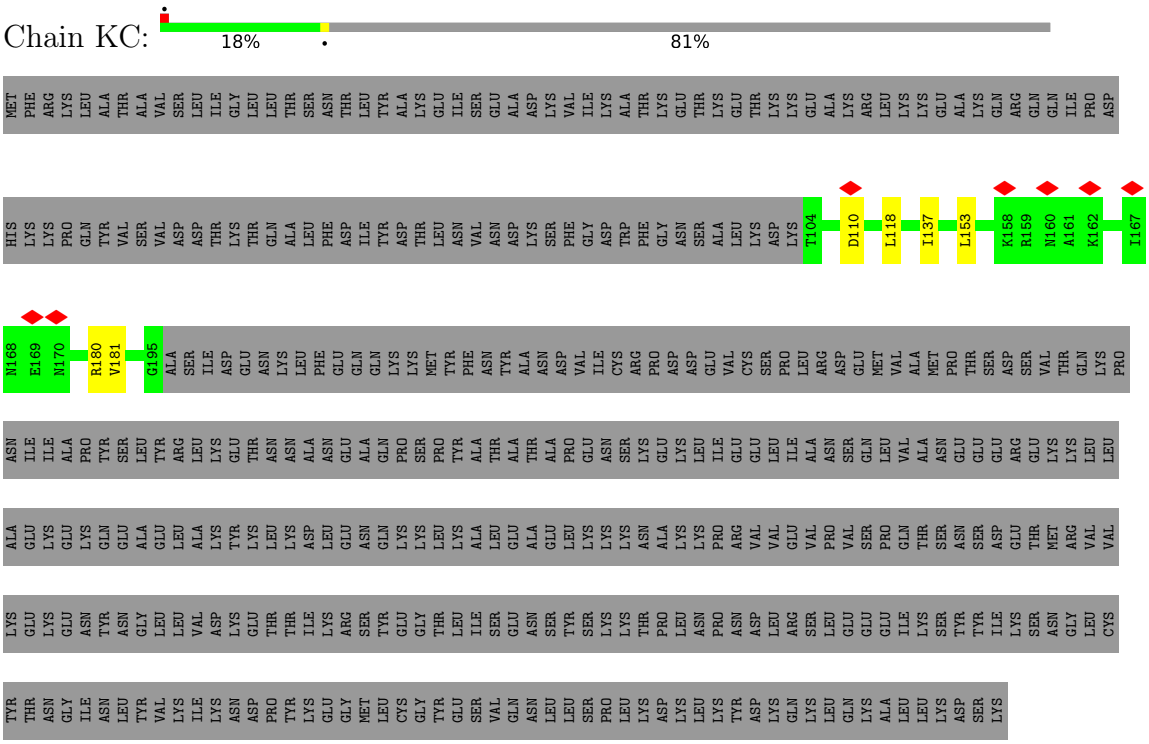

- Molecule 1: Type IV secretion system apparatus protein Cag3

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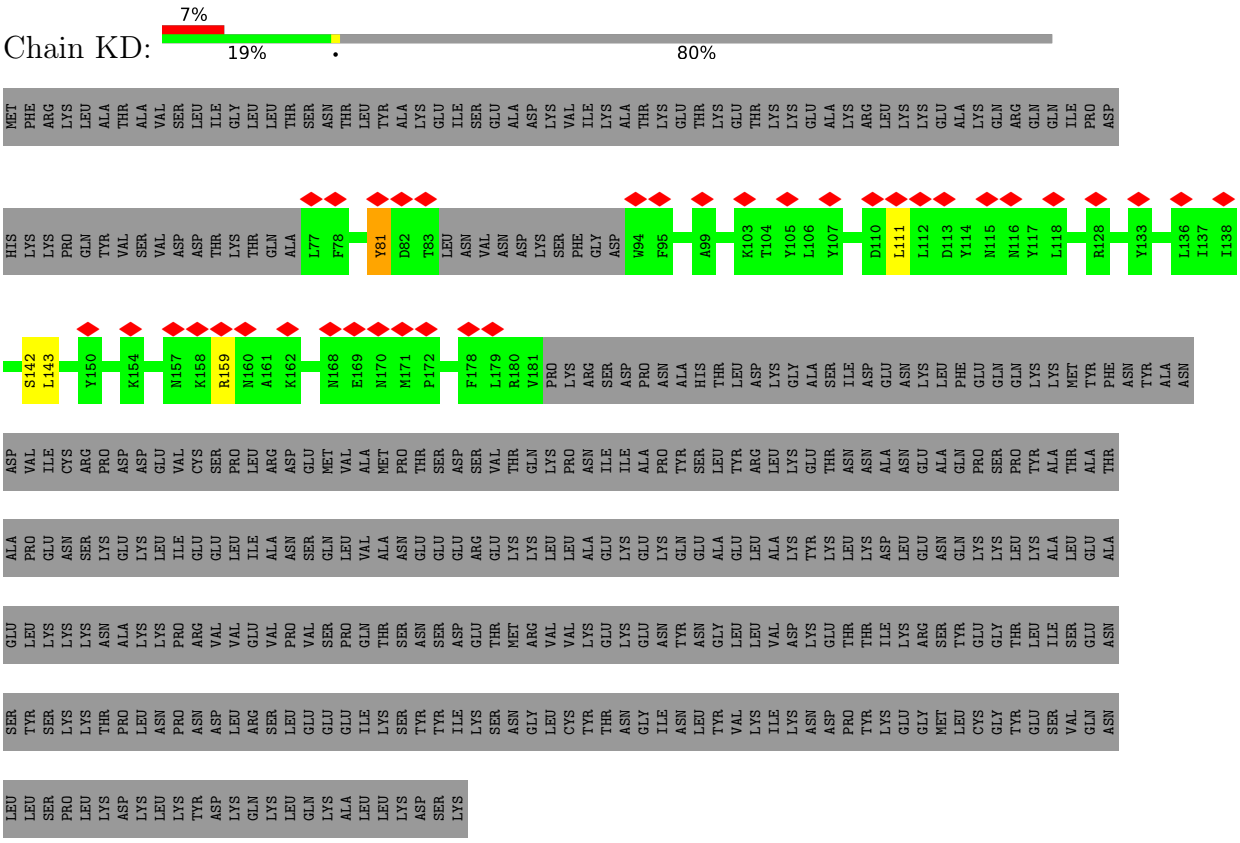

- Molecule 1: Type IV secretion system apparatus protein Cag3

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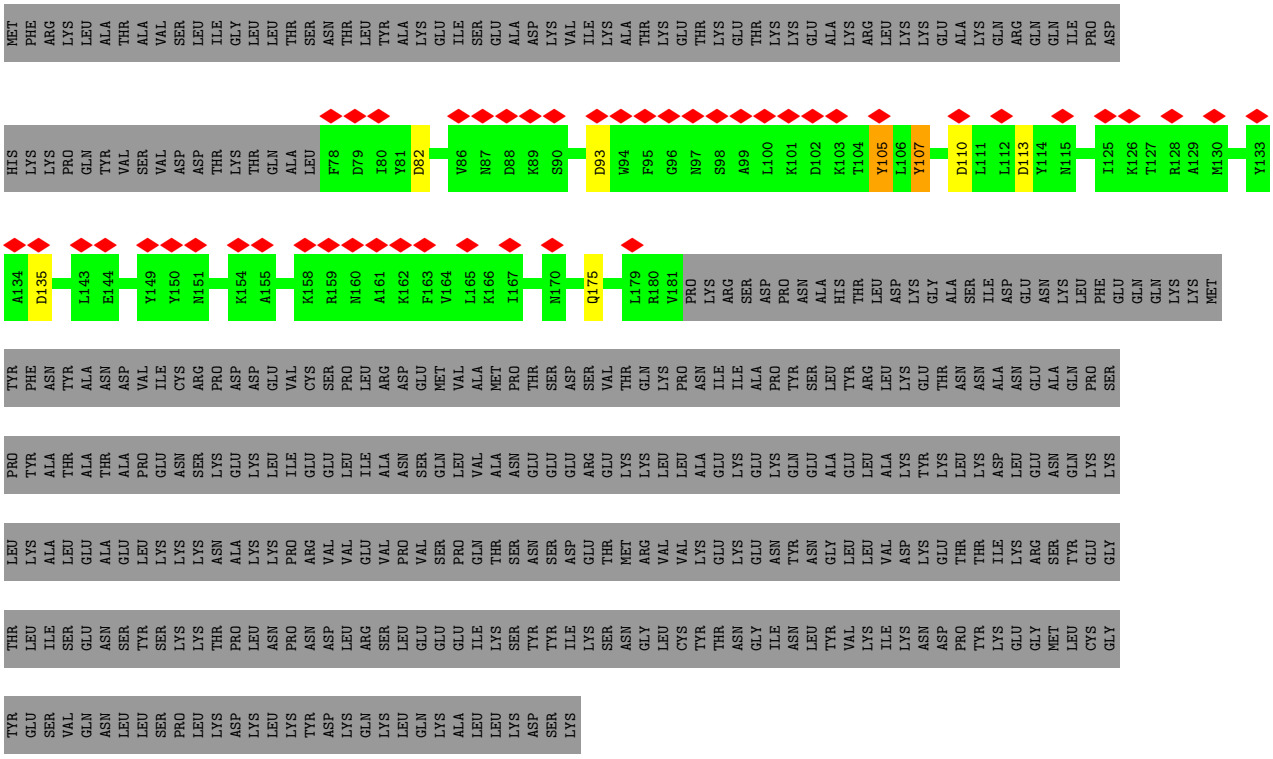

• Molecule 1: Type IV secretion system apparatus protein Cag3

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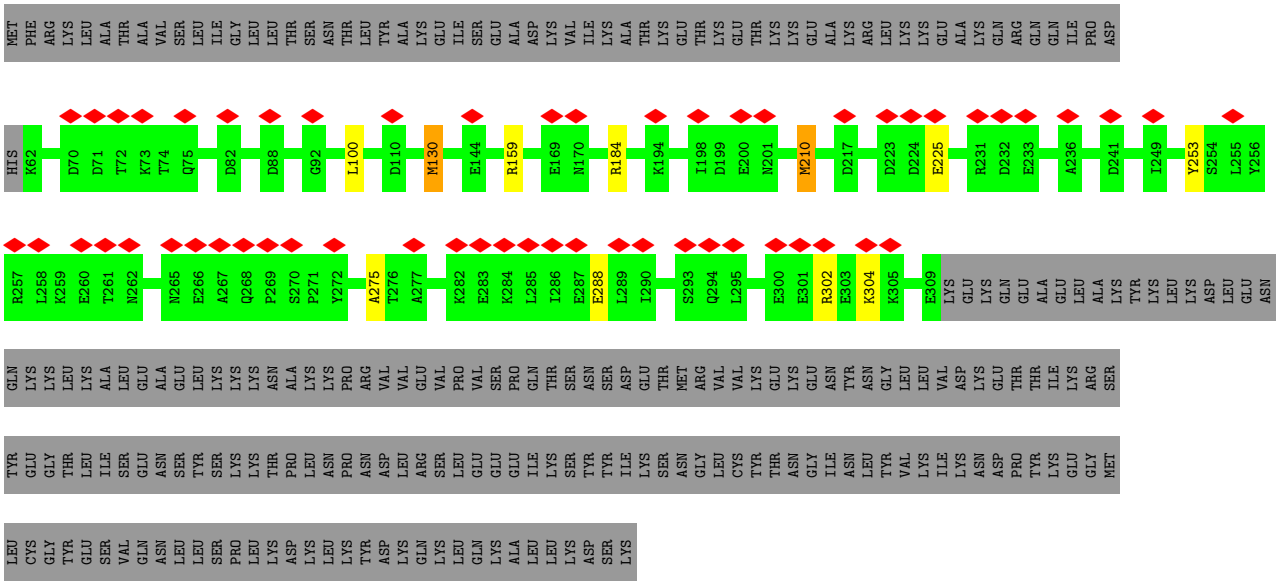

• Molecule 1: Type IV secretion system apparatus protein Cag3

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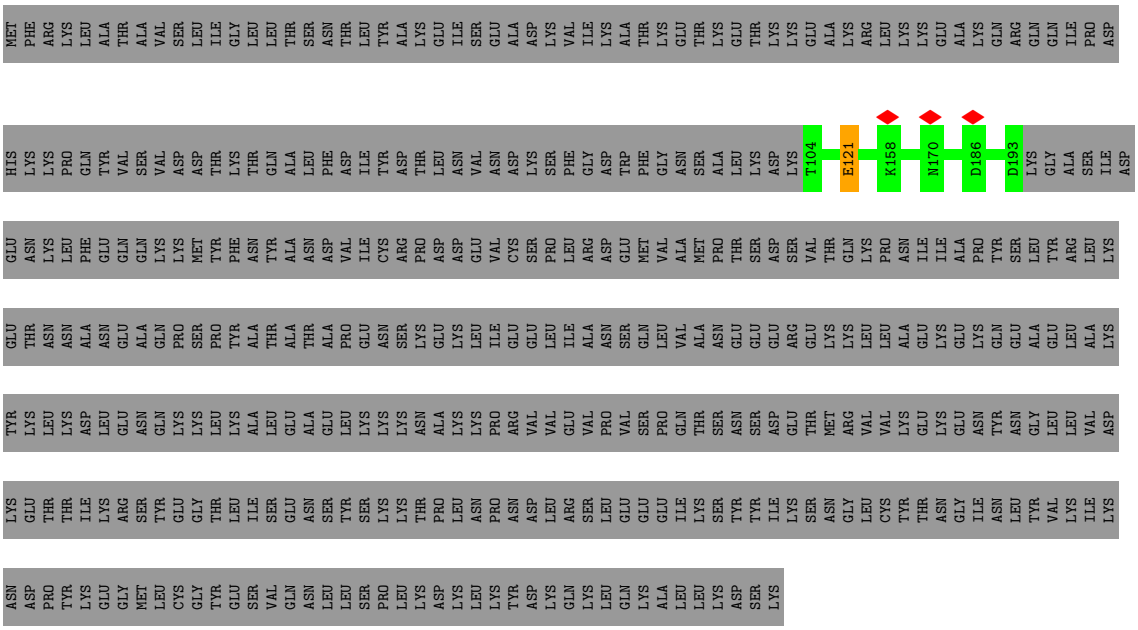

• Molecule 1: Type IV secretion system apparatus protein Cag3

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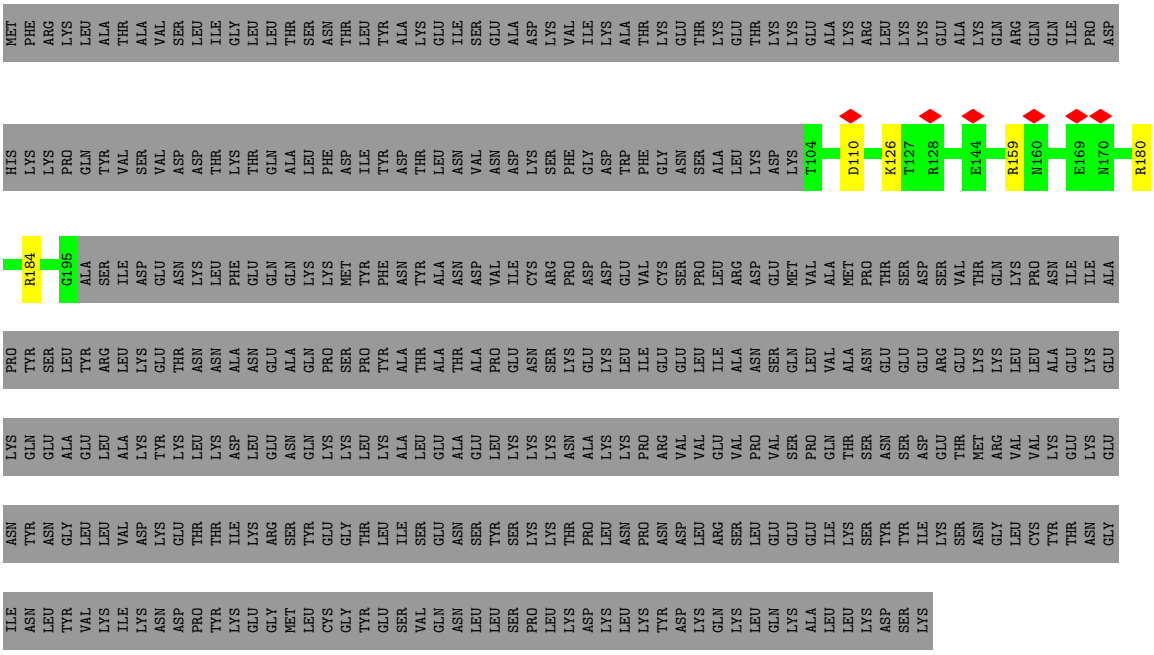

• Molecule 1: Type IV secretion system apparatus protein Cag3

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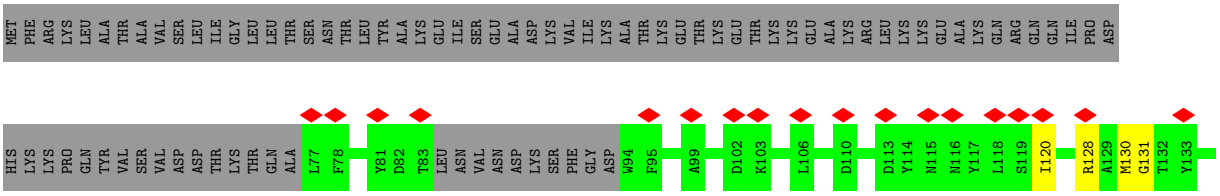

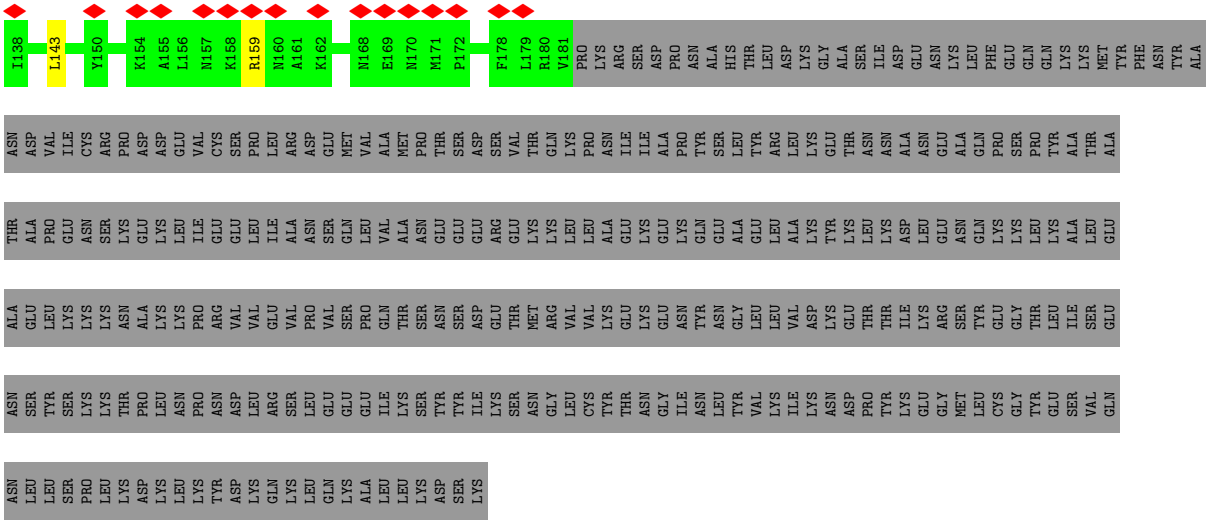

• Molecule 1: Type IV secretion system apparatus protein Cag3

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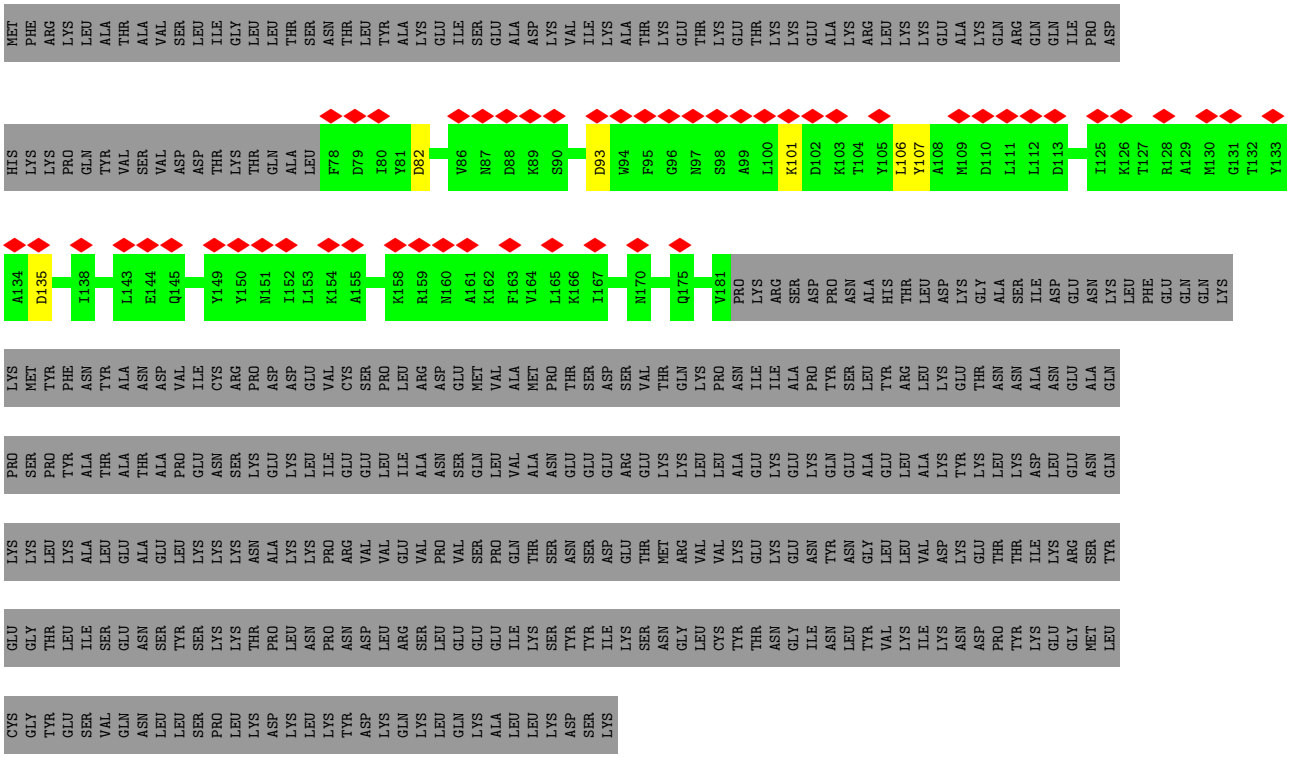

• Molecule 1: Type IV secretion system apparatus protein Cag3

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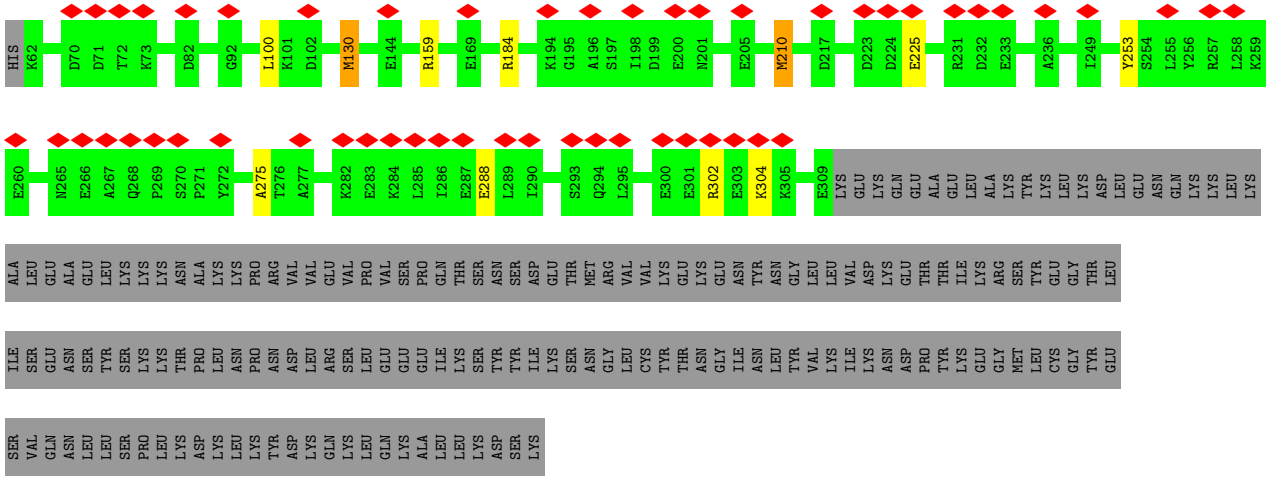
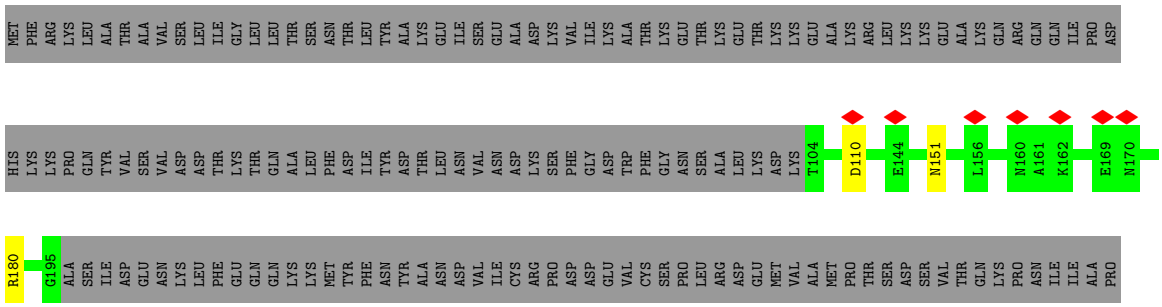


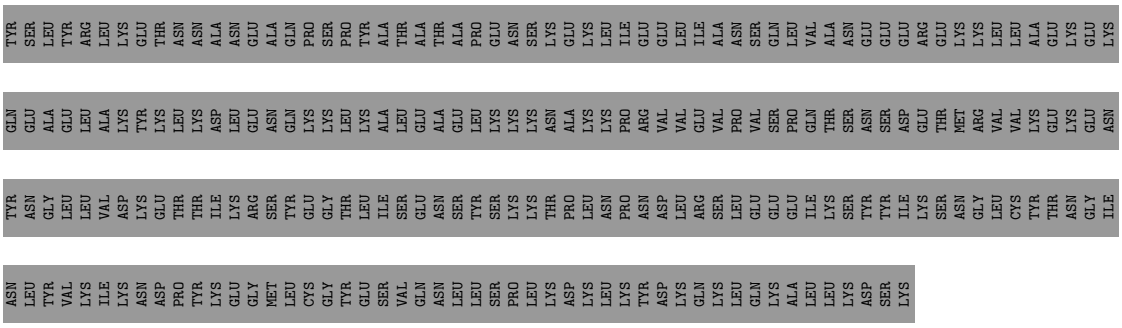
• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain MB:

• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain MC:





• Molecule 1: Type IV secretion system apparatus protein Cag3

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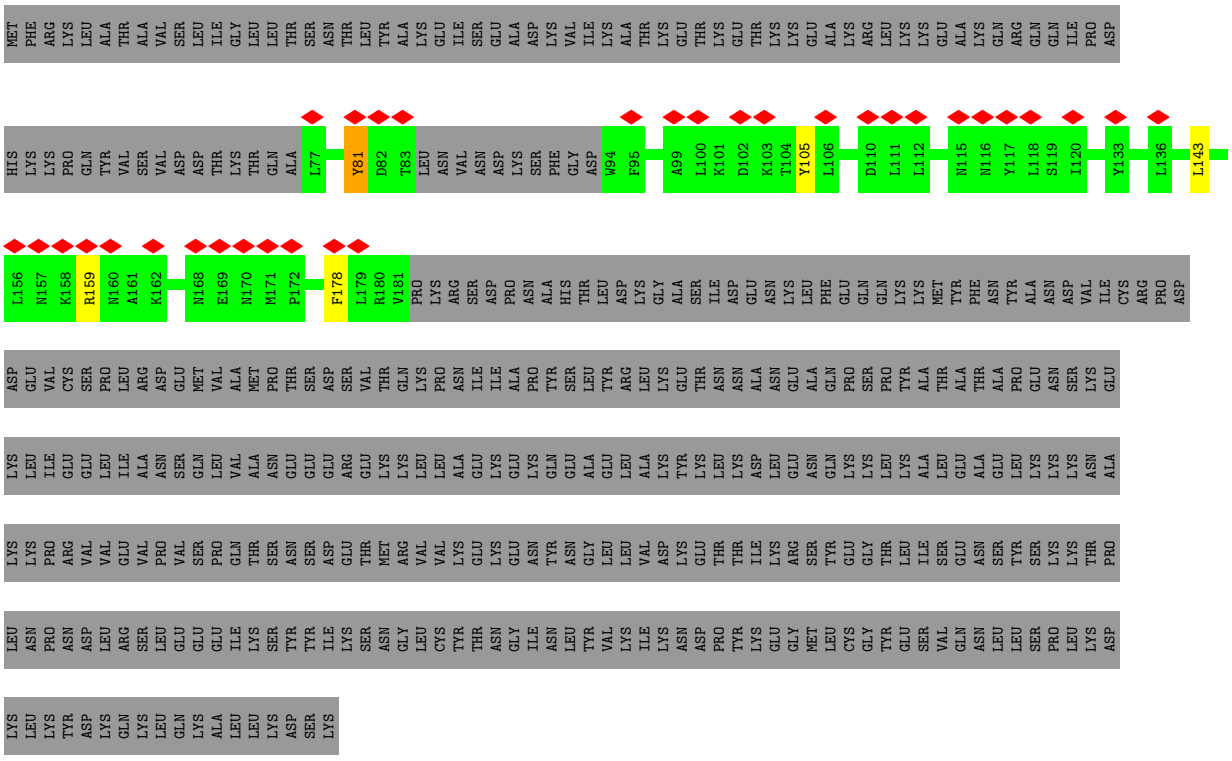

• Molecule 1: Type IV secretion system apparatus protein Cag3

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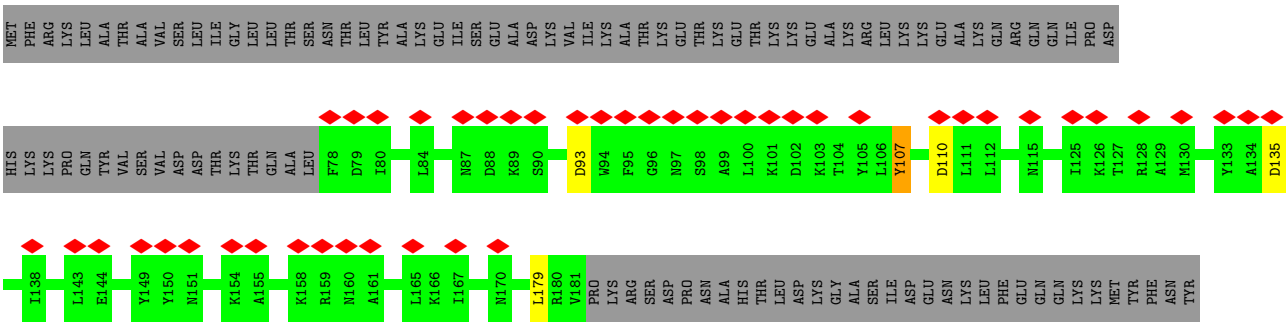

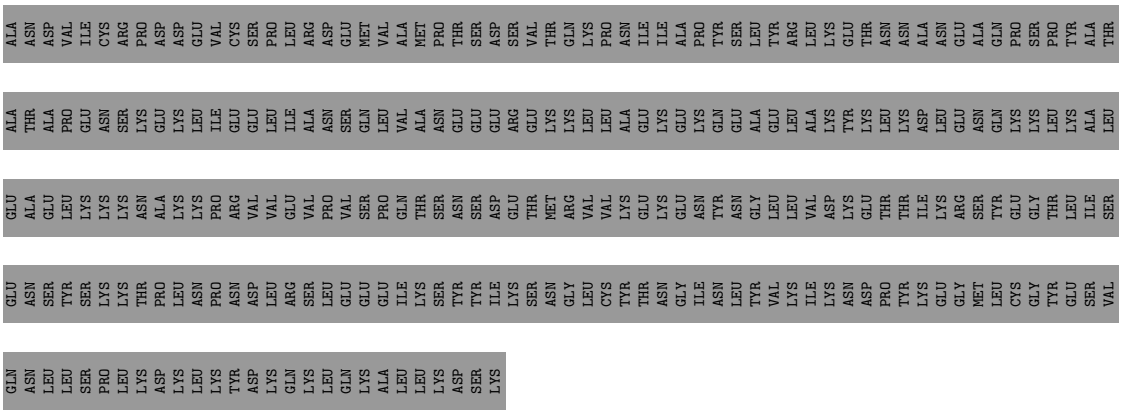

• Molecule 1: Type IV secretion system apparatus protein Cag3

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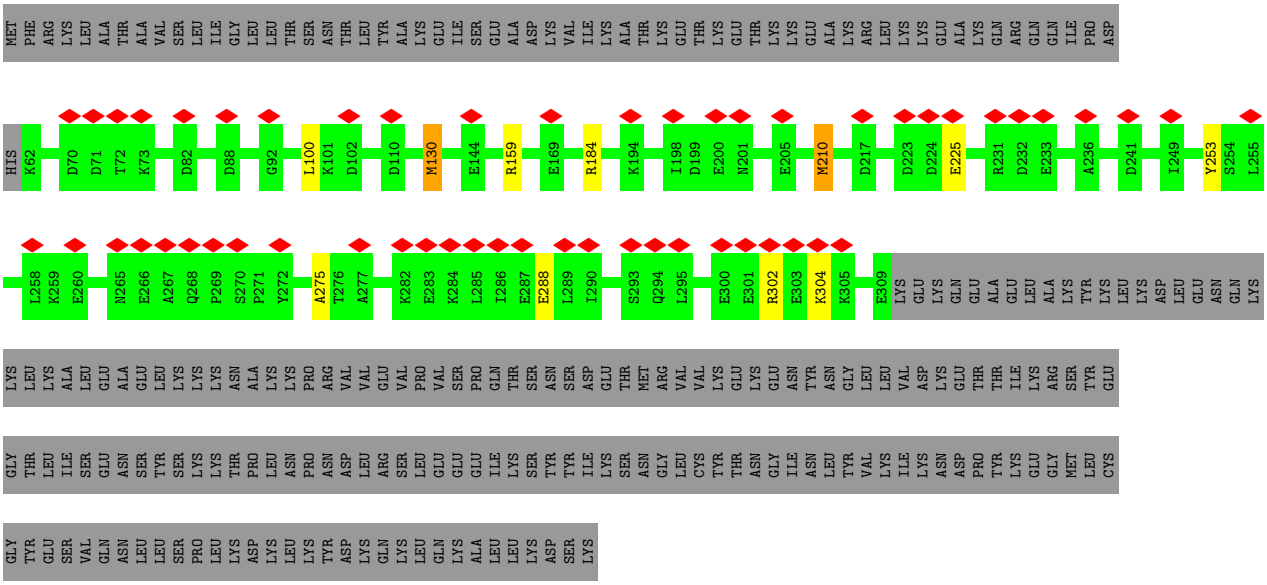
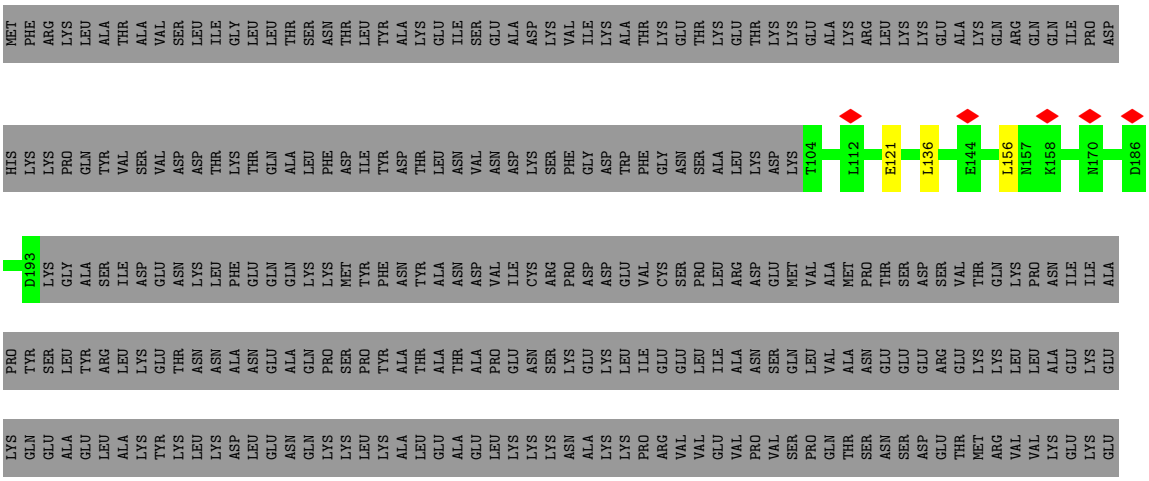
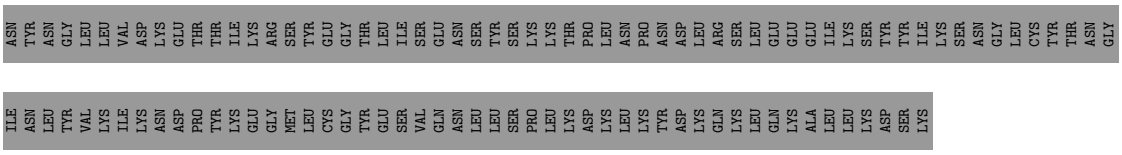


• Molecule 1: Type IV secretion system apparatus protein Cag3

Chain NB:





• Molecule 1: Type IV secretion system apparatus protein Cag3

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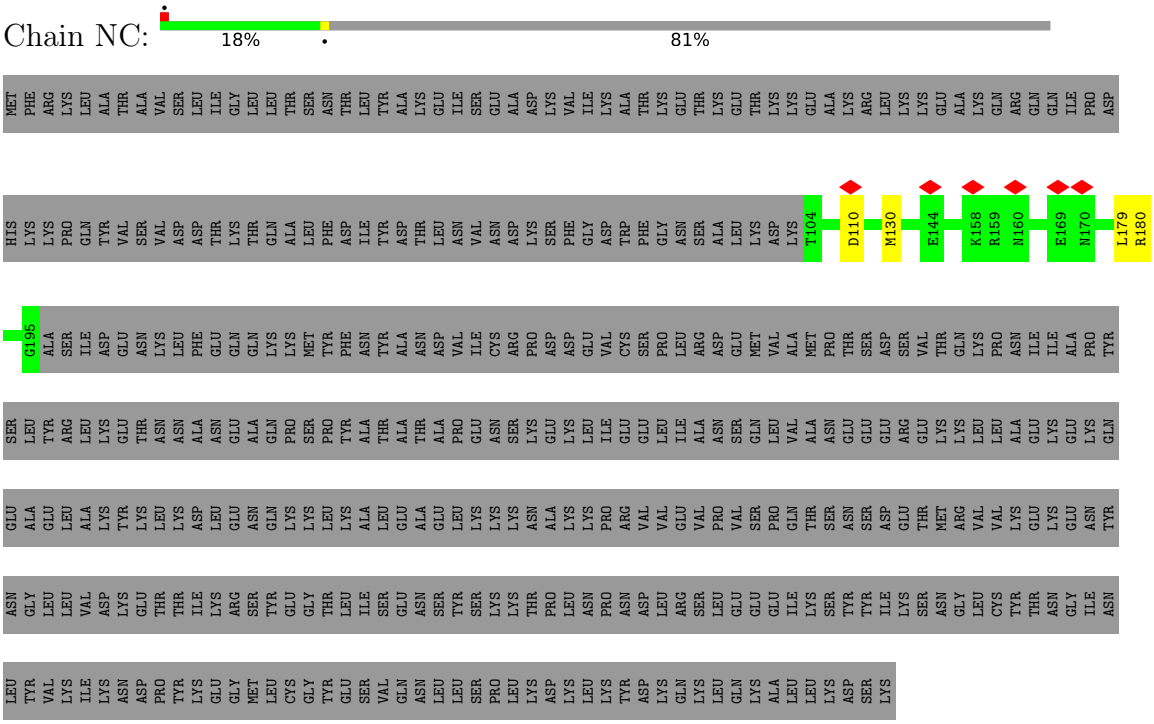

• Molecule 1: Type IV secretion system apparatus protein Cag3

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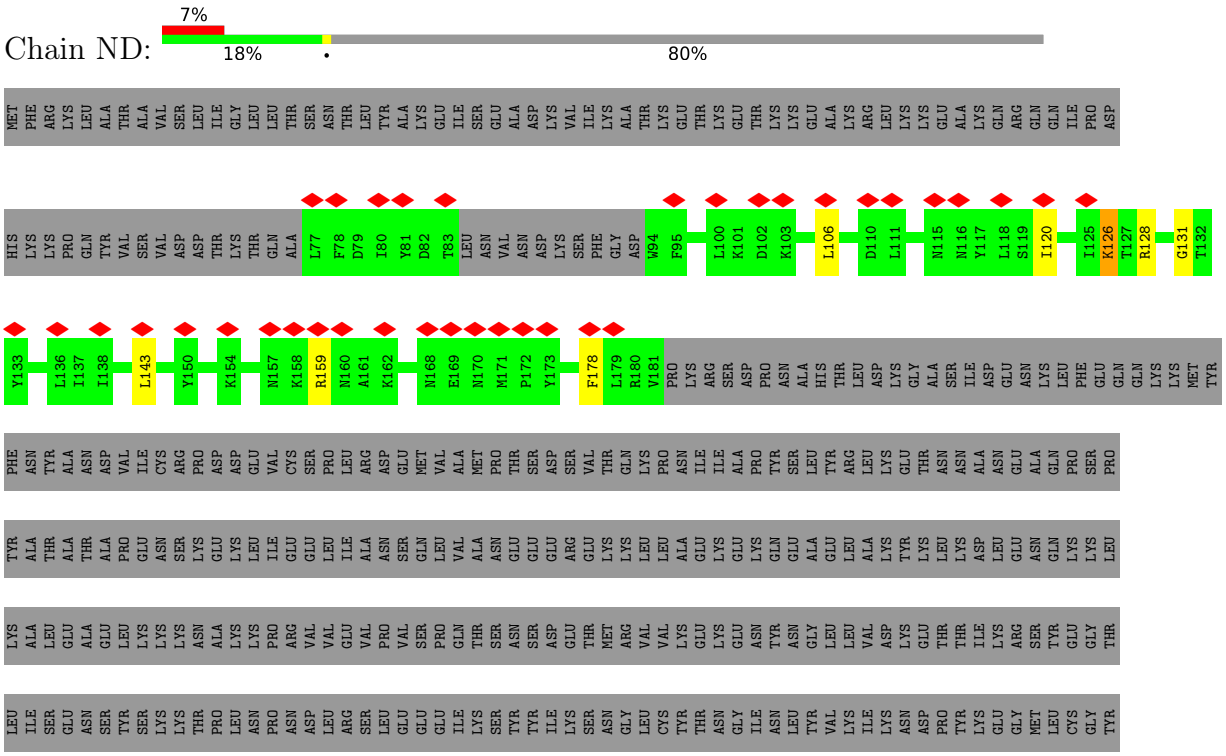
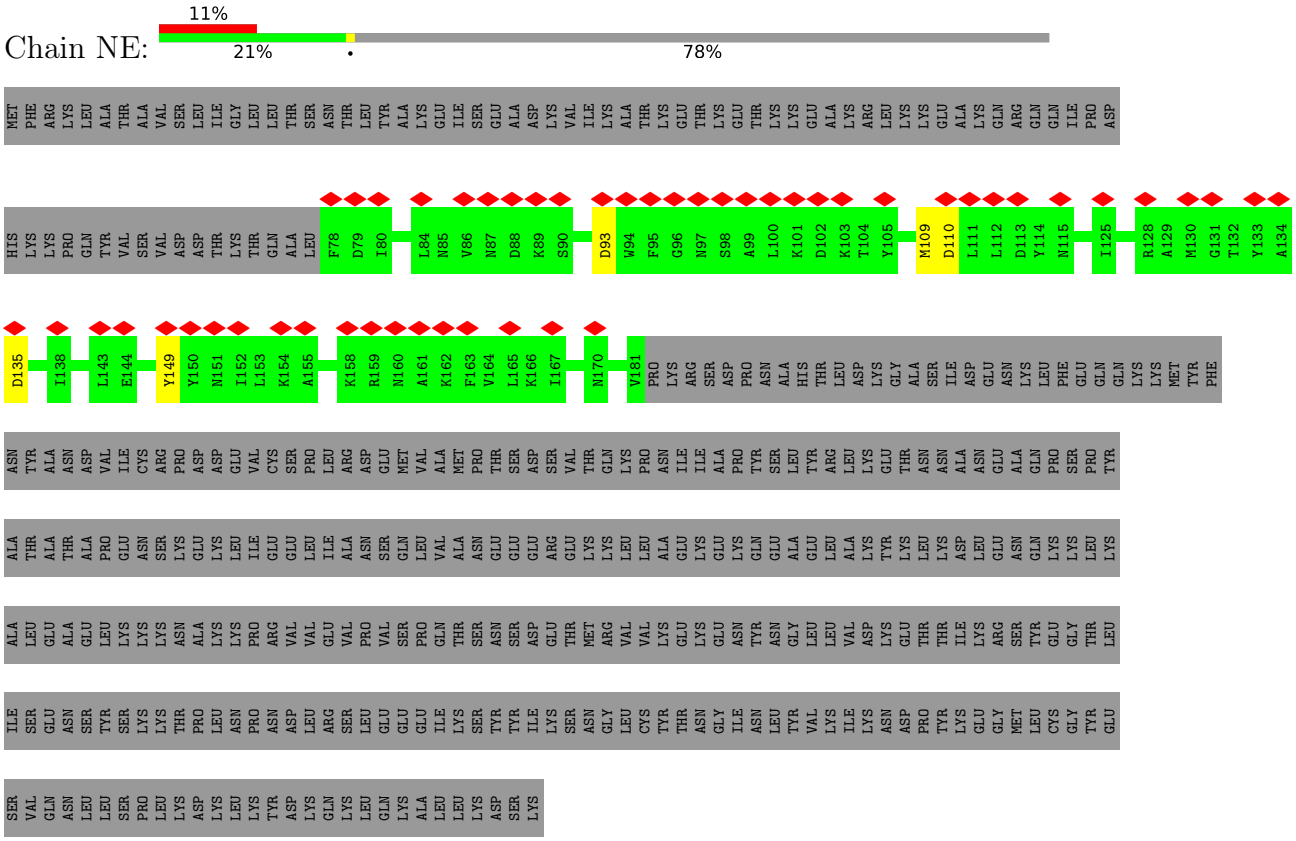
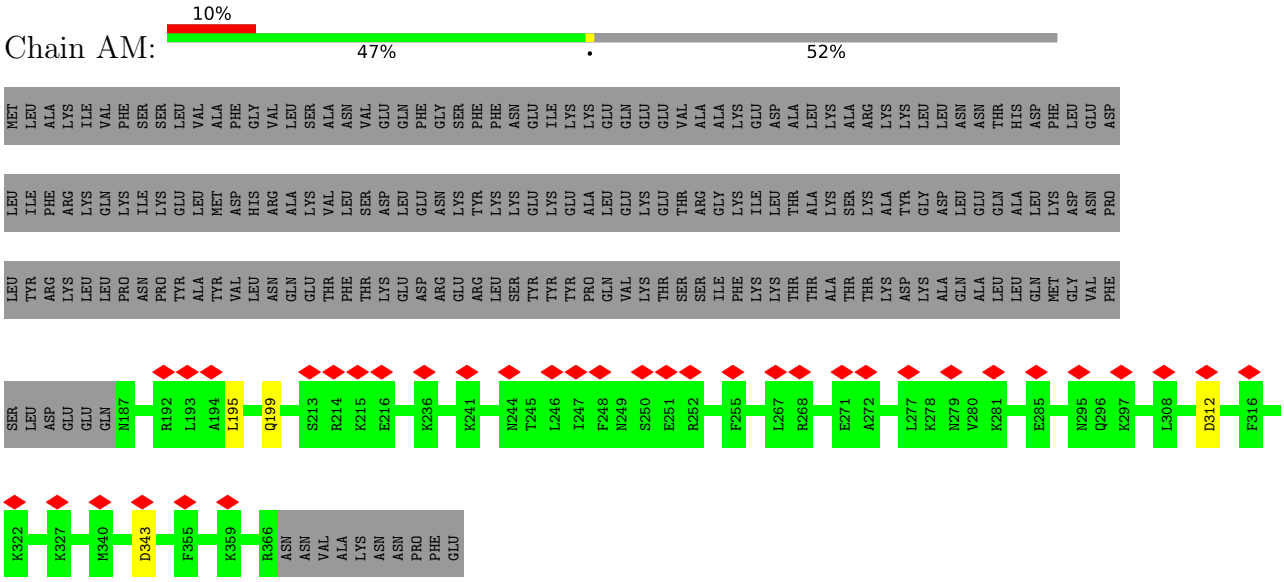


• Molecule 1: Type IV secretion system apparatus protein Cag3



• Molecule 2: Type IV secretion system apparatus protein CagM



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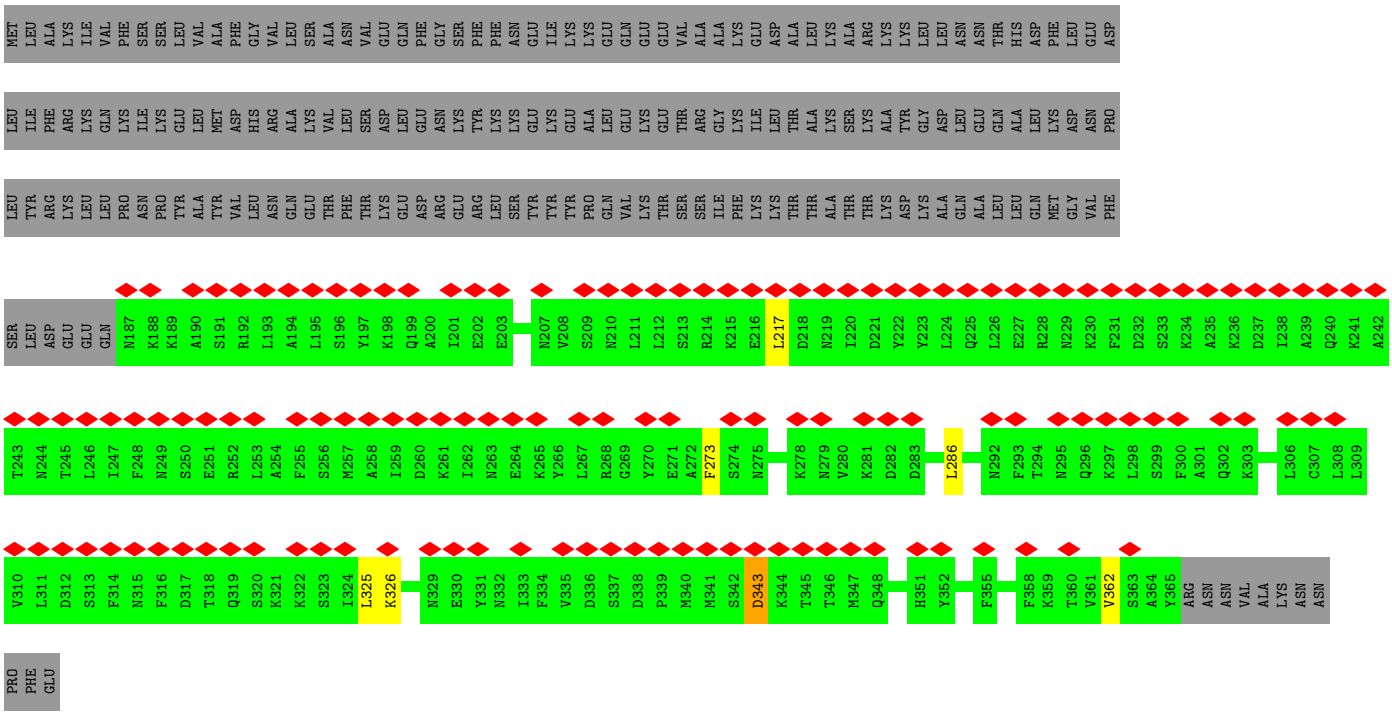

• Molecule 2: Type IV secretion system apparatus protein CagM

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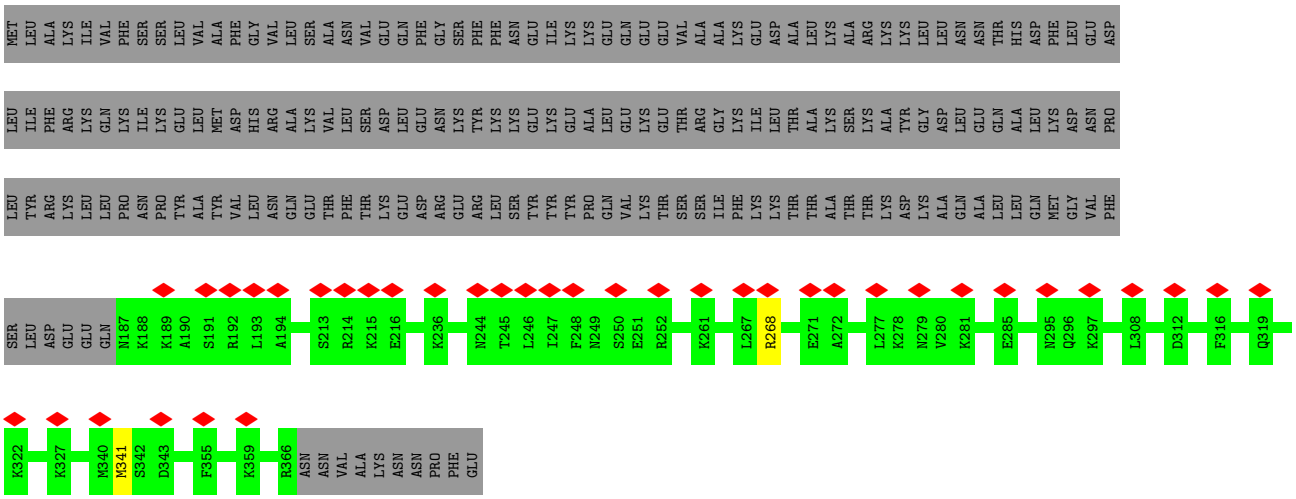

• Molecule 2: Type IV secretion system apparatus protein CagM

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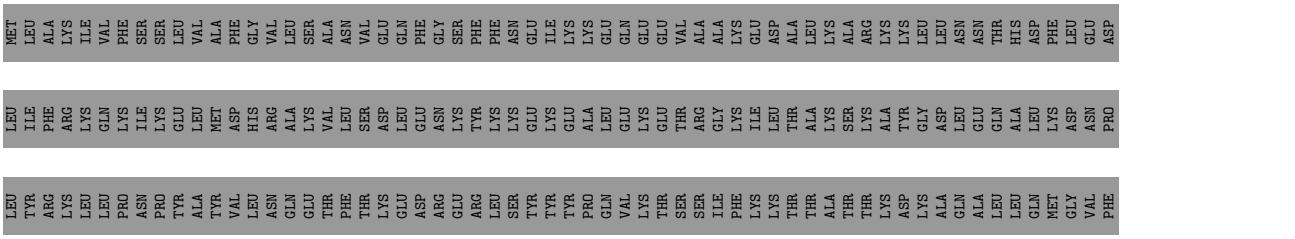

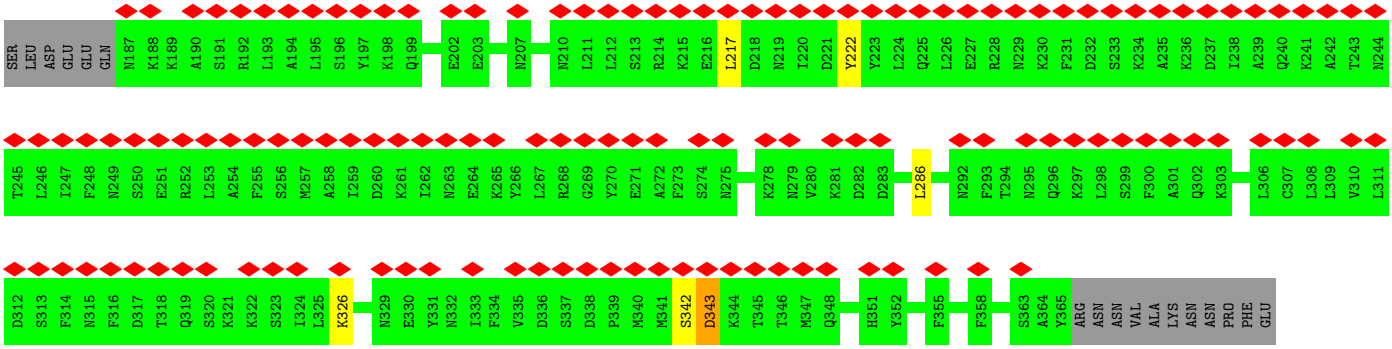

• Molecule 2: Type IV secretion system apparatus protein CagM

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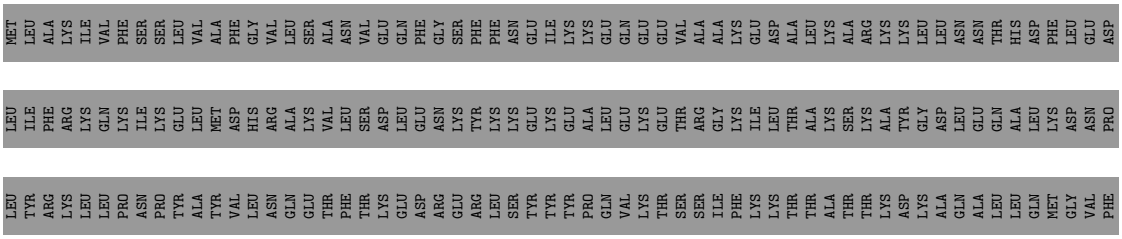

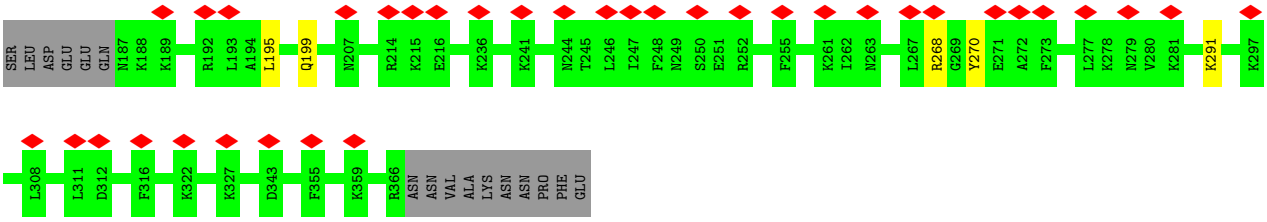

• Molecule 2: Type IV secretion system apparatus protein CagM

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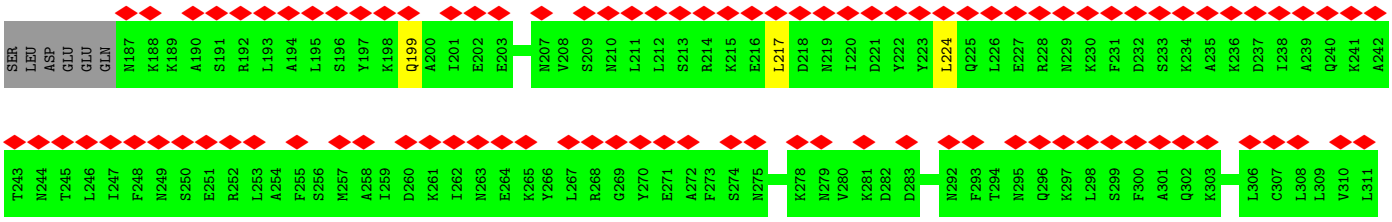

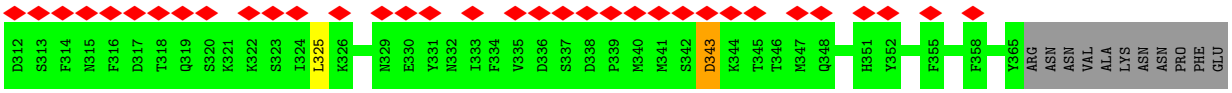

• Molecule 2: Type IV secretion system apparatus protein CagM

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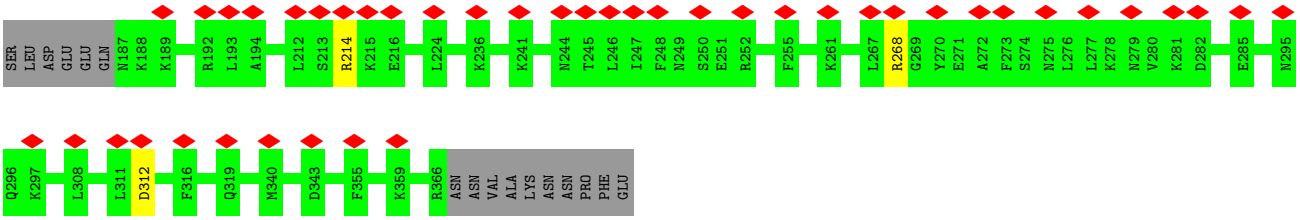

• Molecule 2: Type IV secretion system apparatus protein CagM

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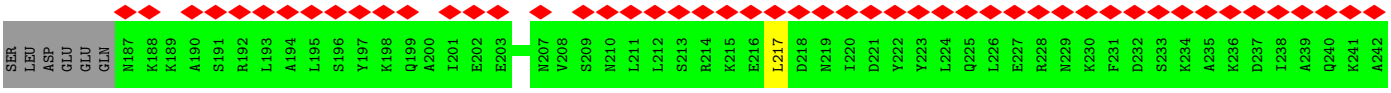

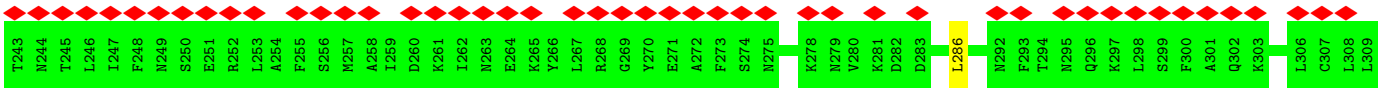

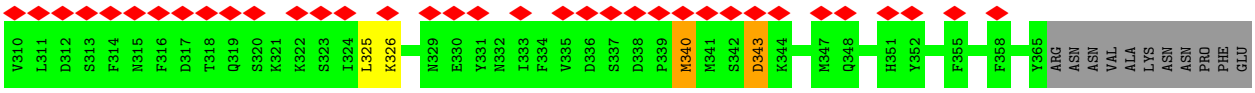

• Molecule 2: Type IV secretion system apparatus protein CagM

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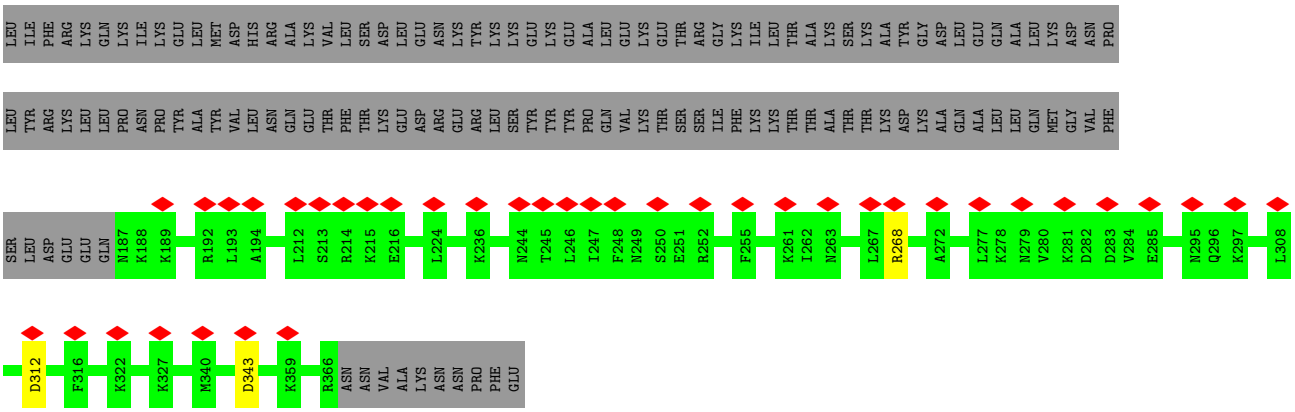
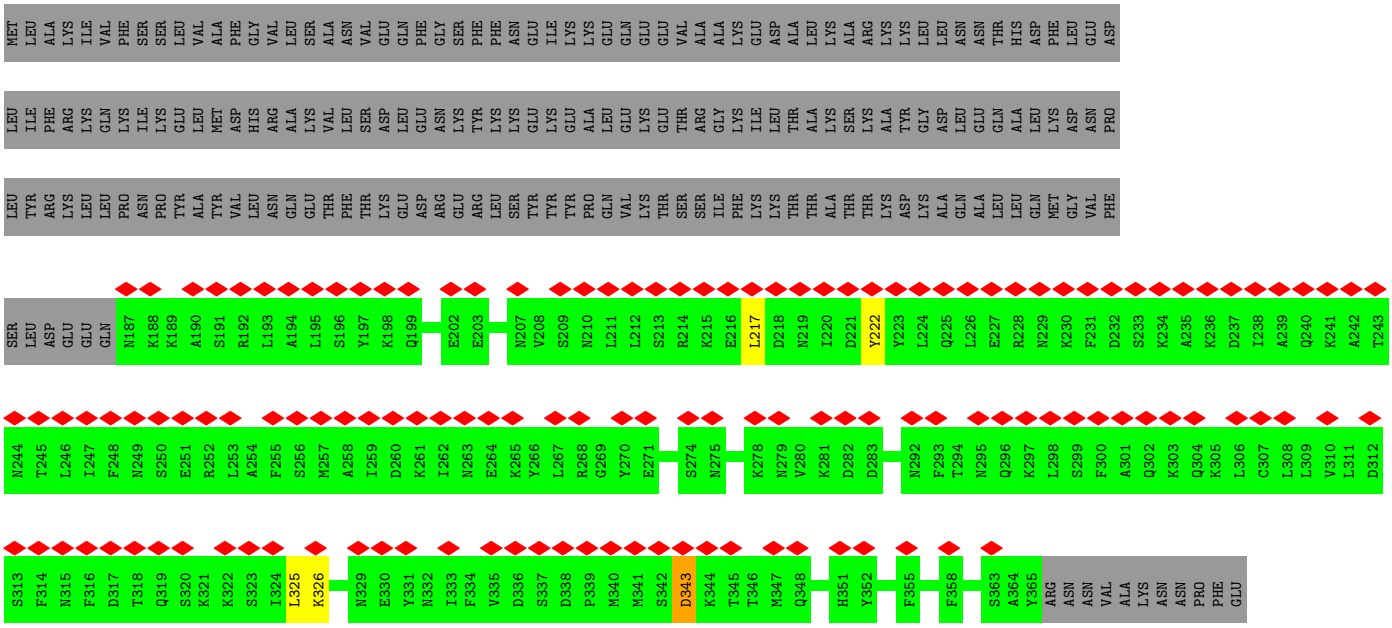


• Molecule 2: Type IV secretion system apparatus protein CagM

Chain Em:



• Molecule 2: Type IV secretion system apparatus protein CagM

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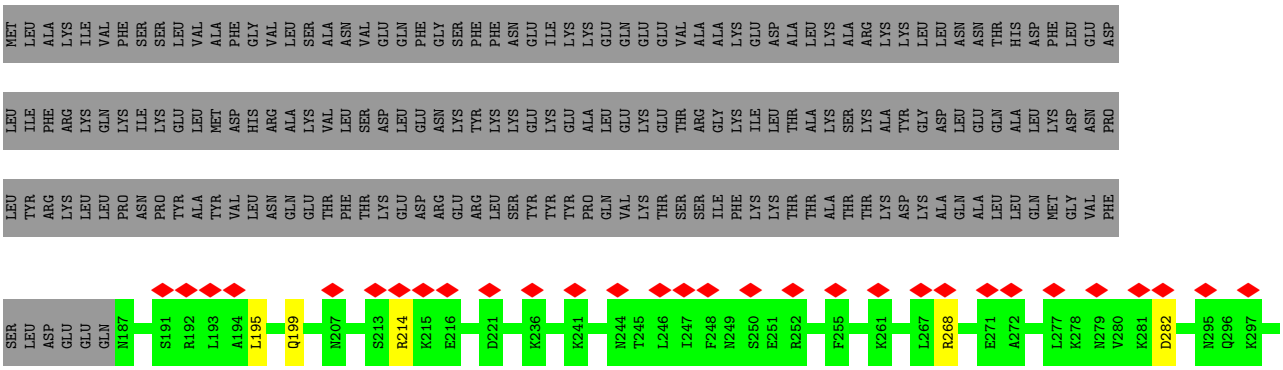

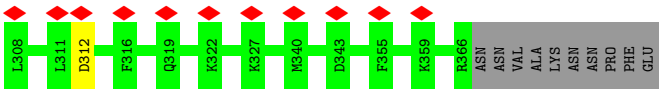

• Molecule 2: Type IV secretion system apparatus protein CagM

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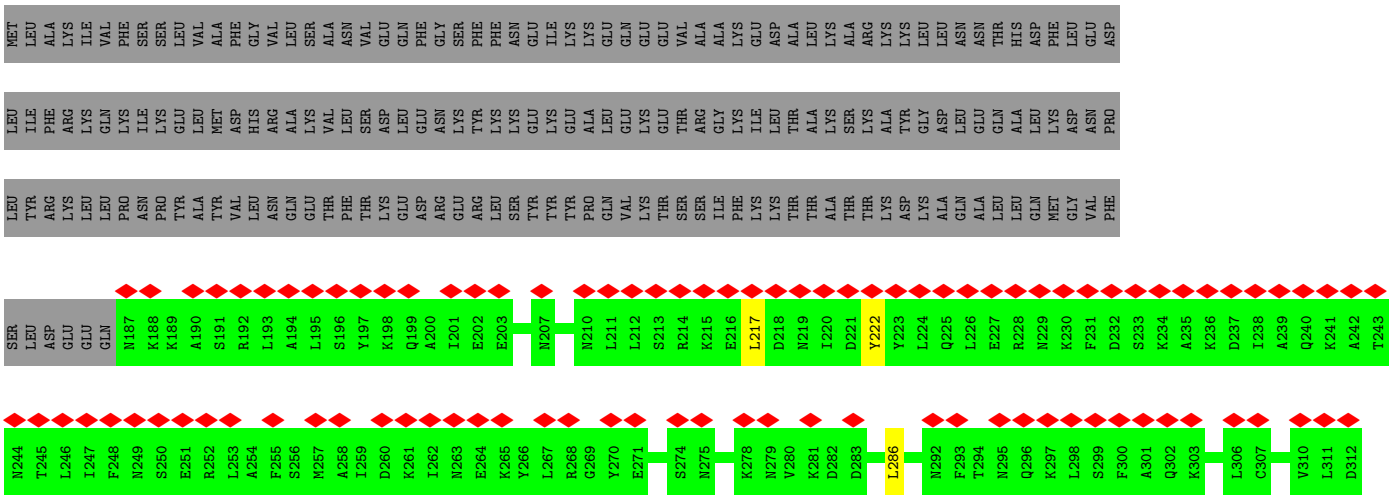

• Molecule 2: Type IV secretion system apparatus protein CagM

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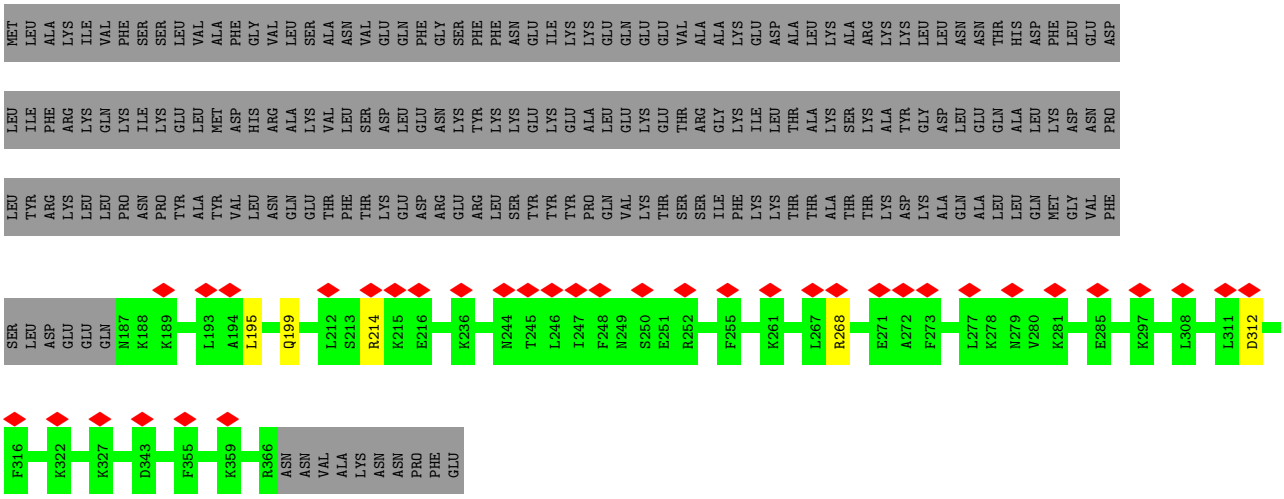

• Molecule 2: Type IV secretion system apparatus protein CagM

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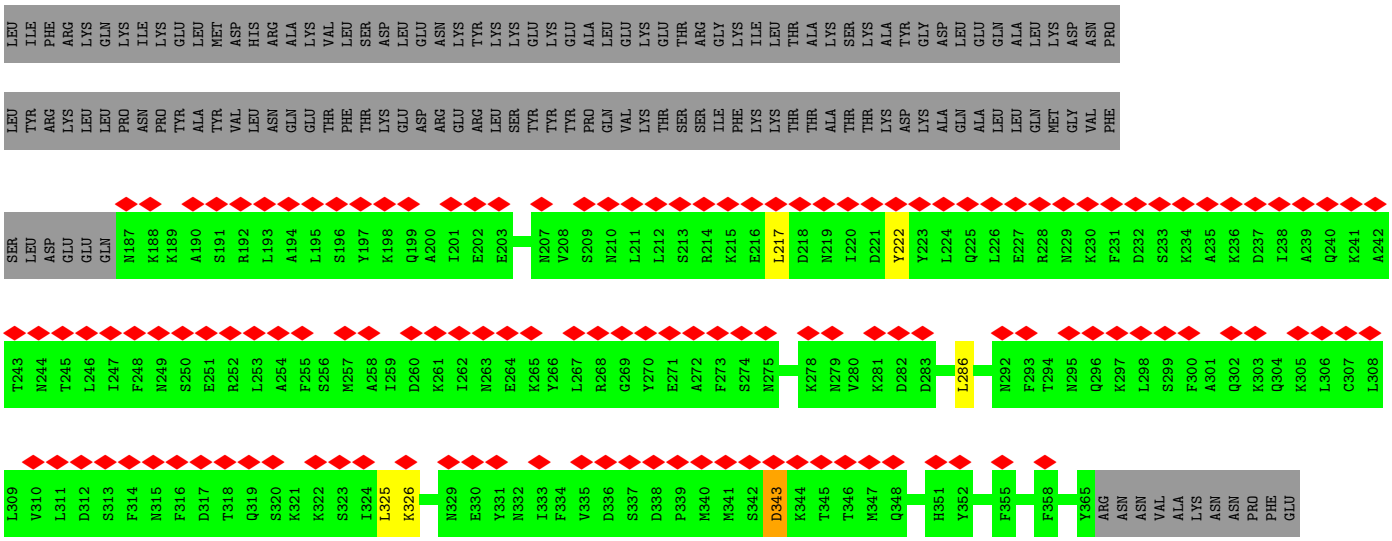

- Molecule 2: Type IV secretion system apparatus protein CagM

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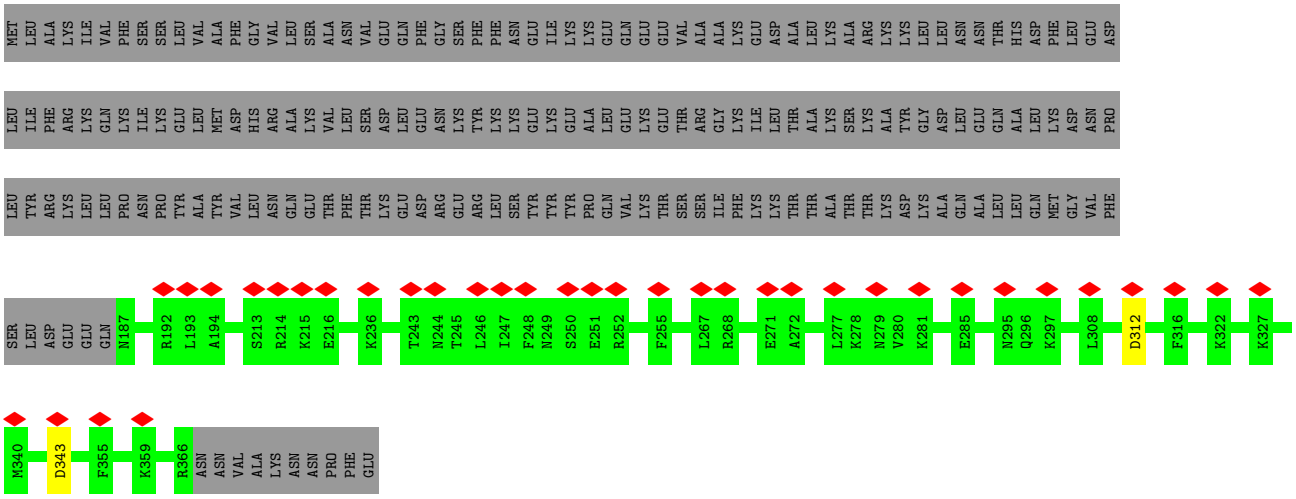

- Molecule 2: Type IV secretion system apparatus protein CagM

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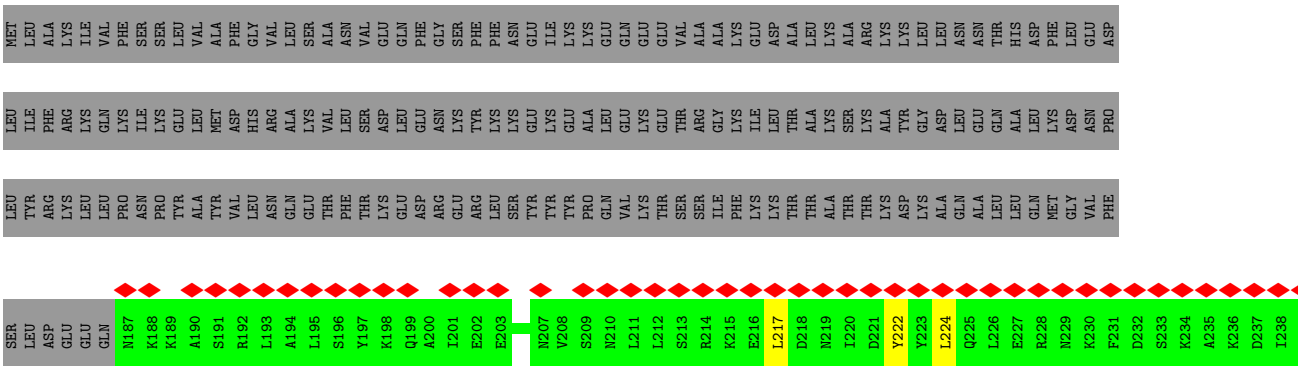

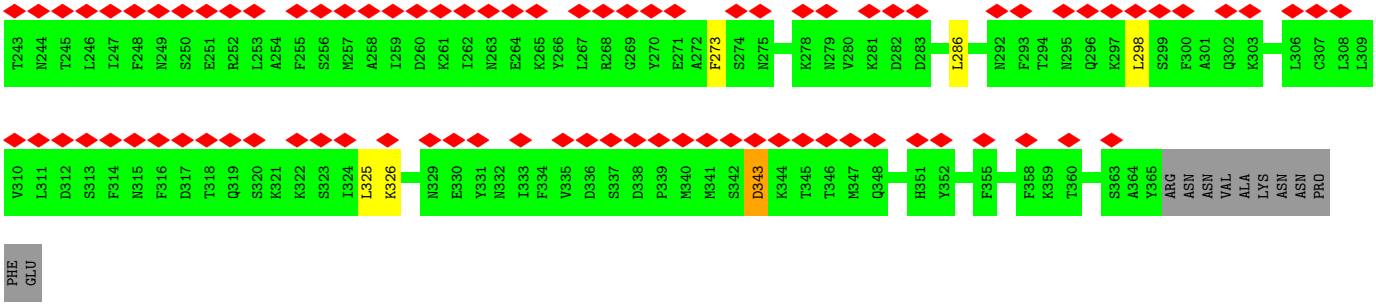

- Molecule 2: Type IV secretion system apparatus protein CagM

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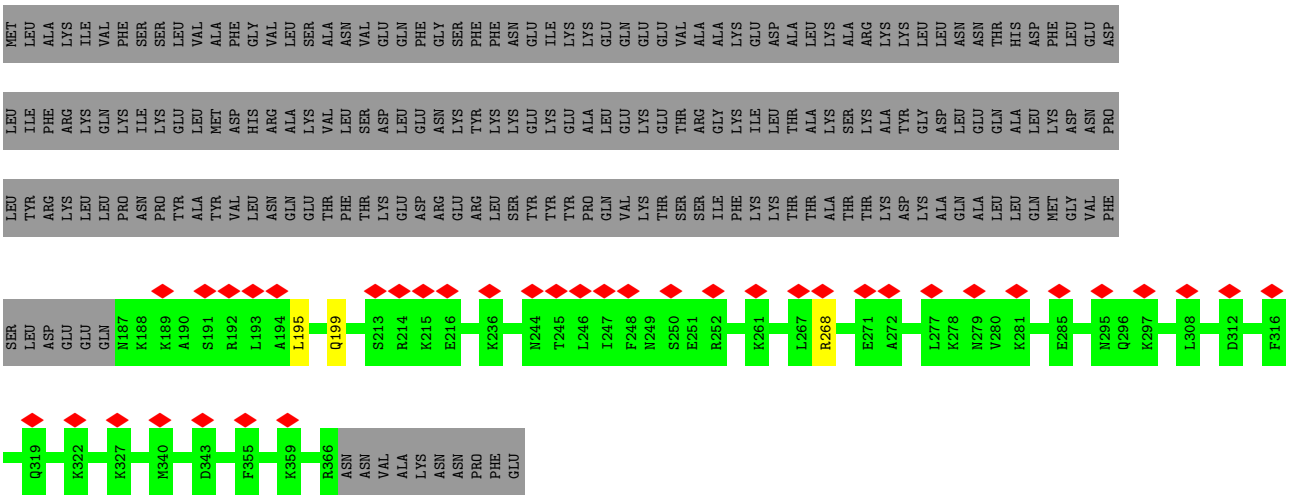

- Molecule 2: Type IV secretion system apparatus protein CagM

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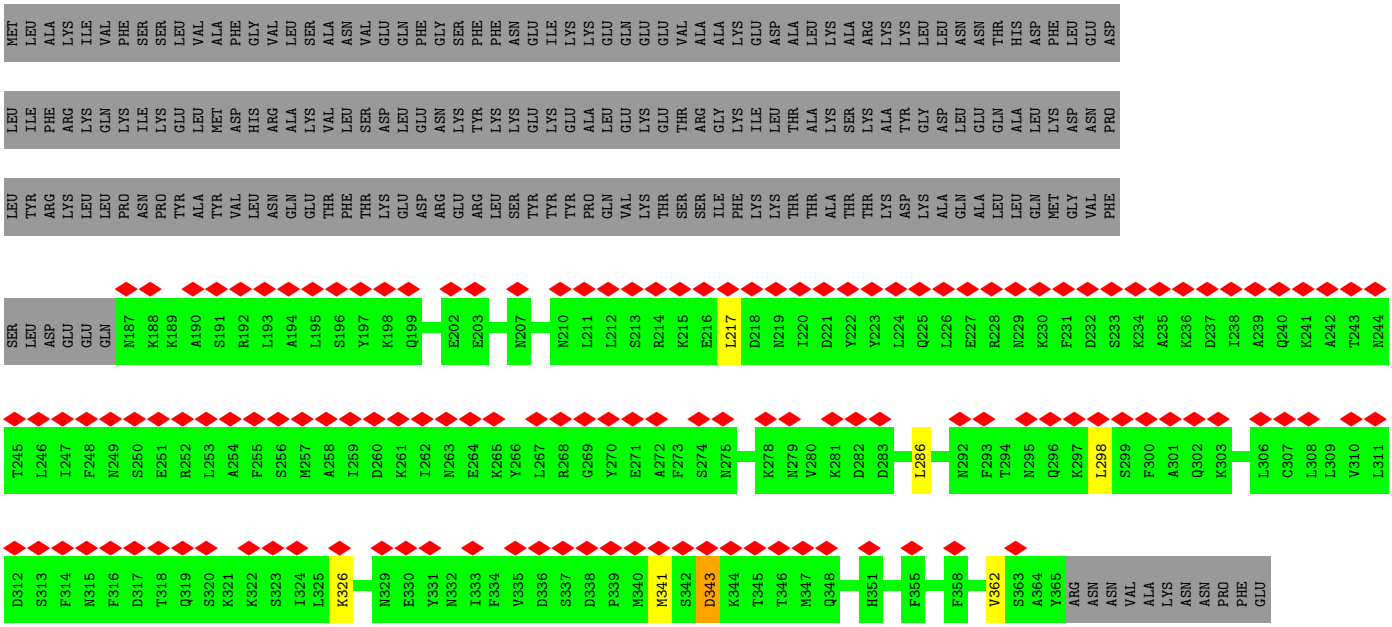

• Molecule 2: Type IV secretion system apparatus protein CagM

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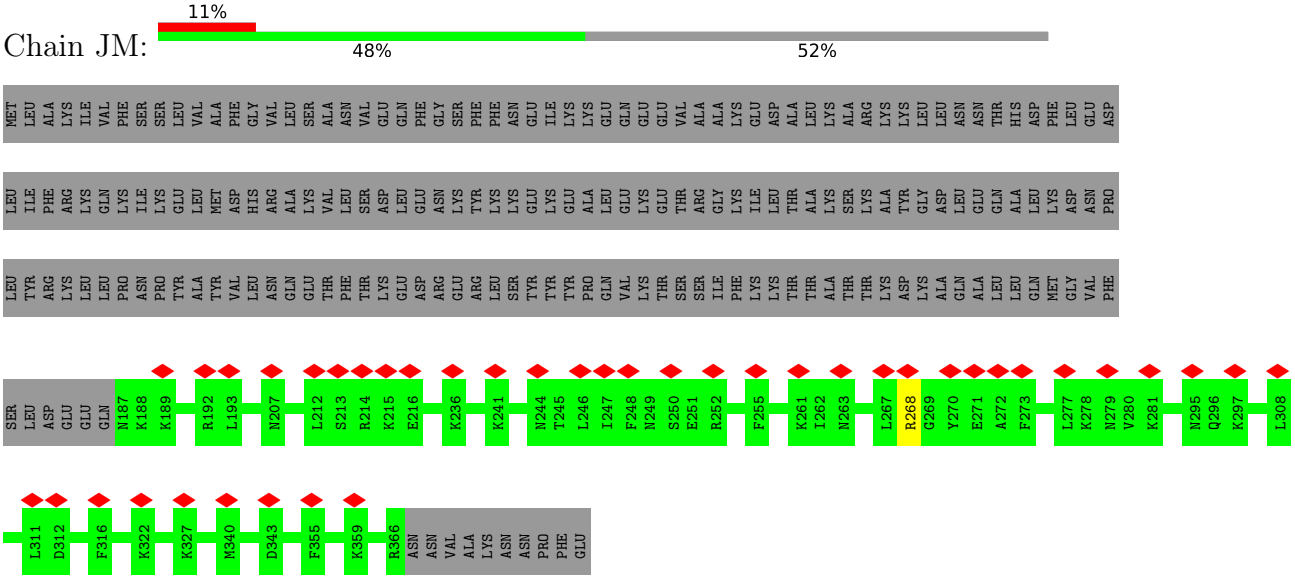

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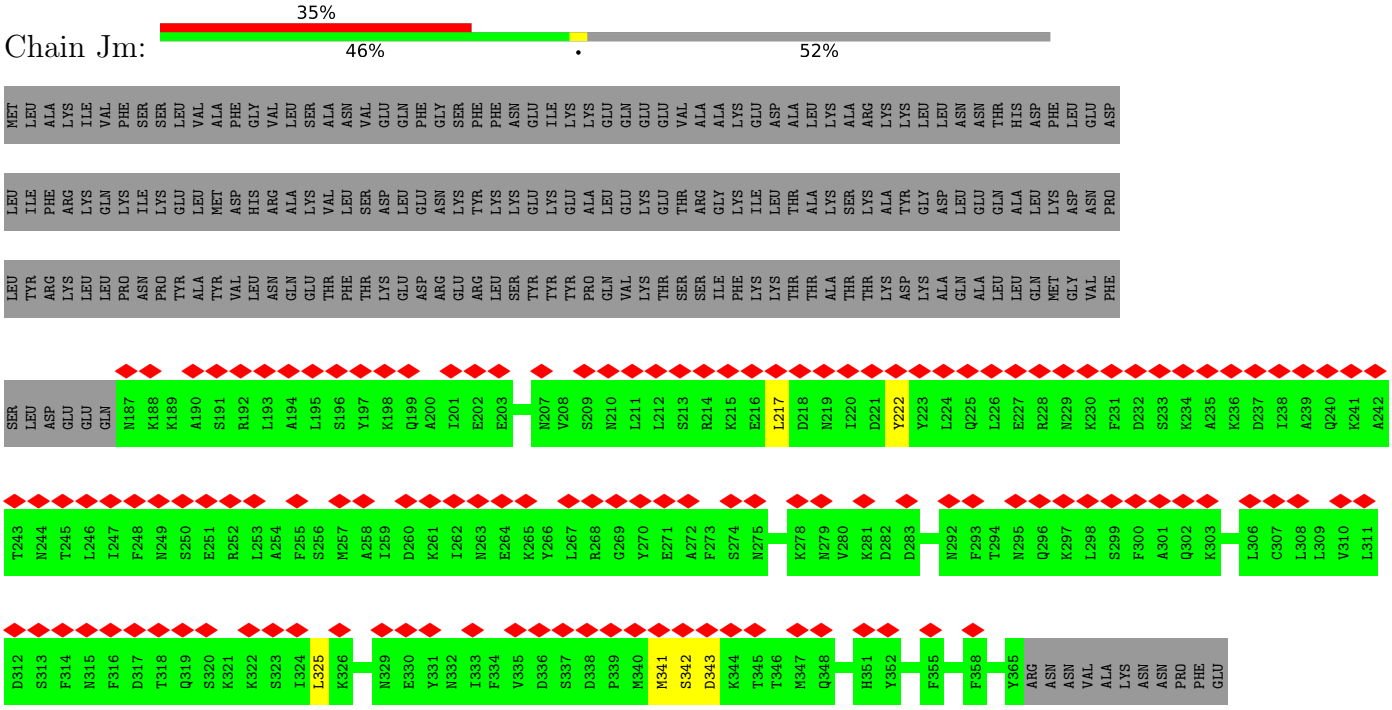

• Molecule 2: Type IV secretion system apparatus protein CagM

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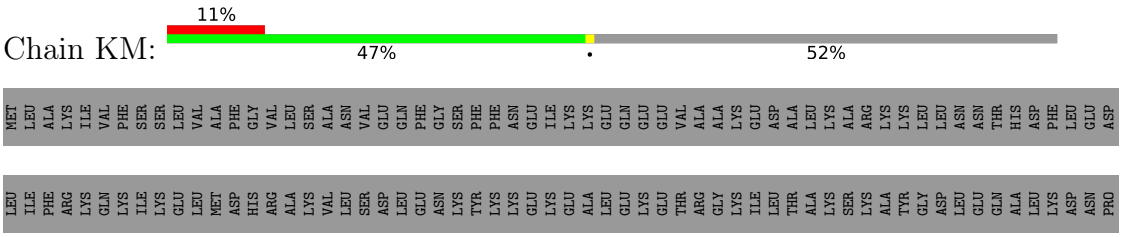

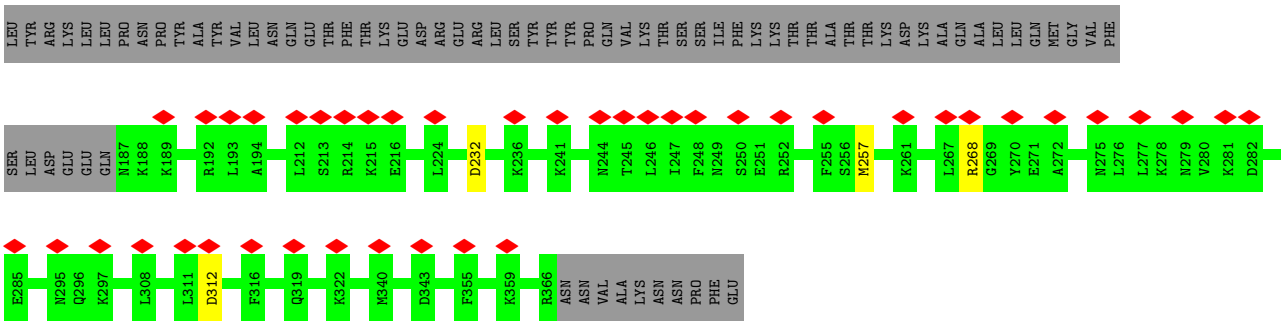

- Molecule 2: Type IV secretion system apparatus protein CagM

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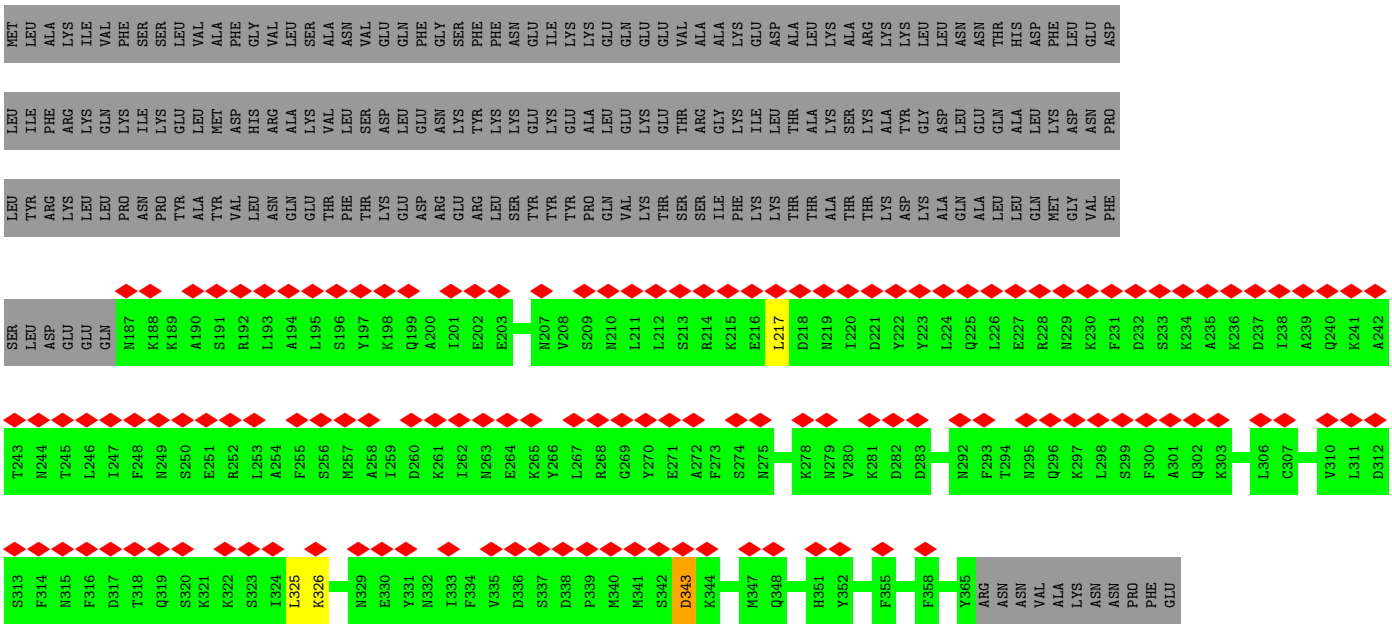

- Molecule 2: Type IV secretion system apparatus protein CagM

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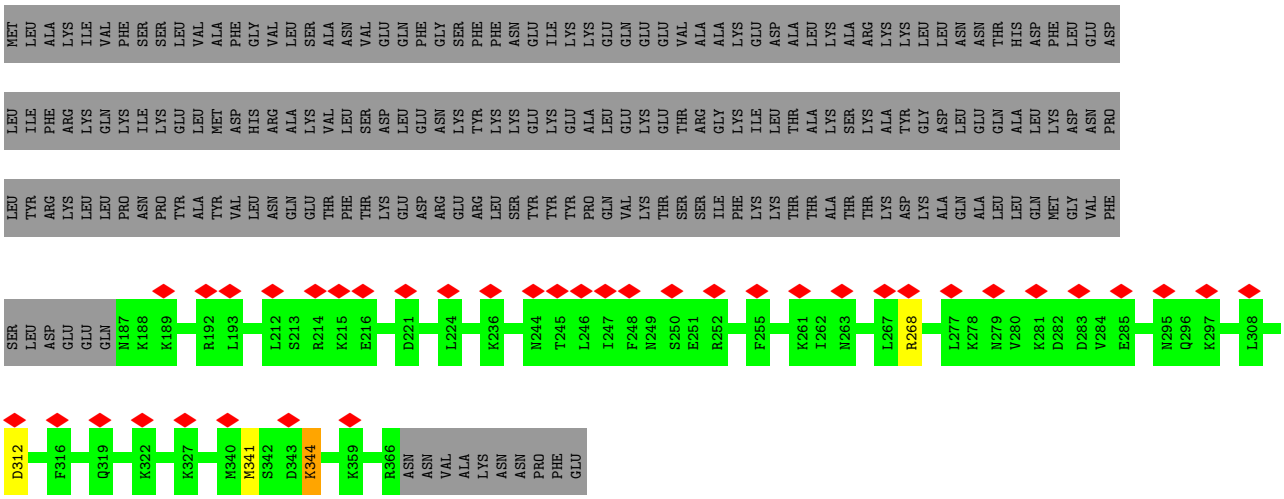

• Molecule 2: Type IV secretion system apparatus protein CagM

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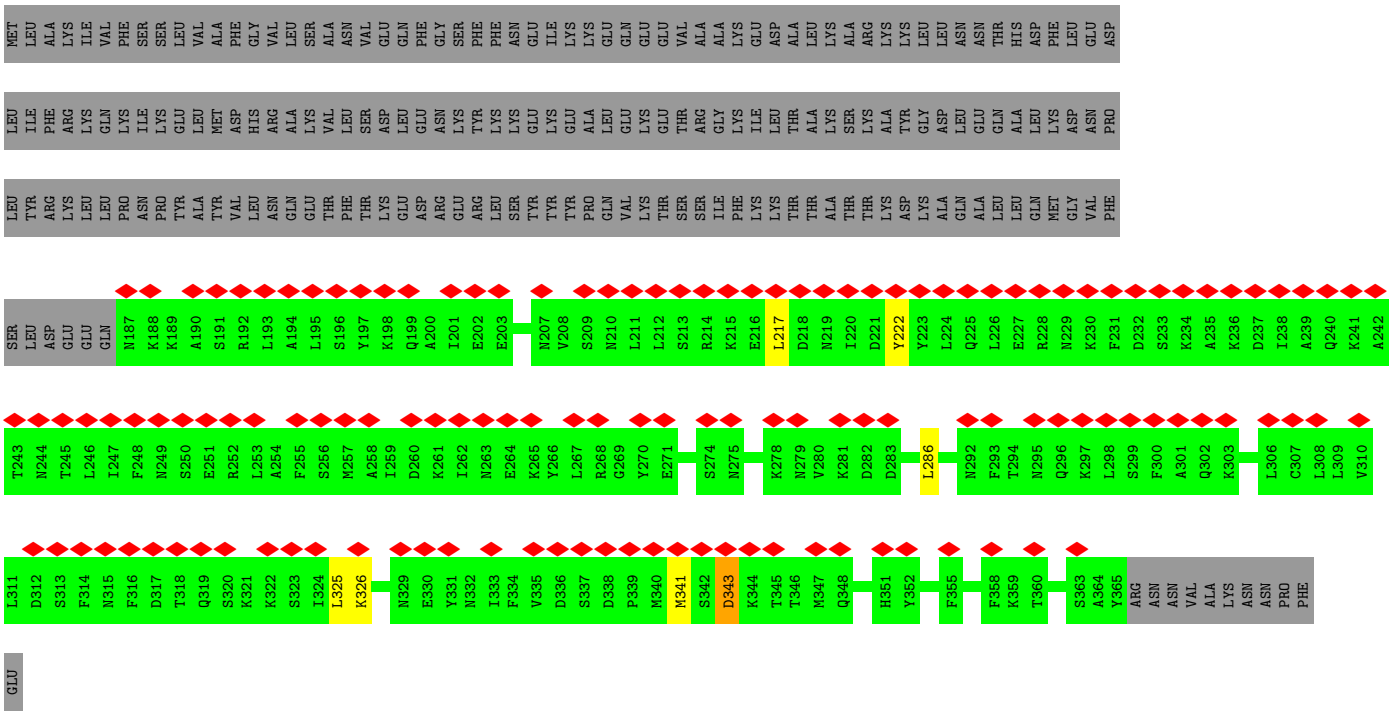

• Molecule 2: Type IV secretion system apparatus protein CagM

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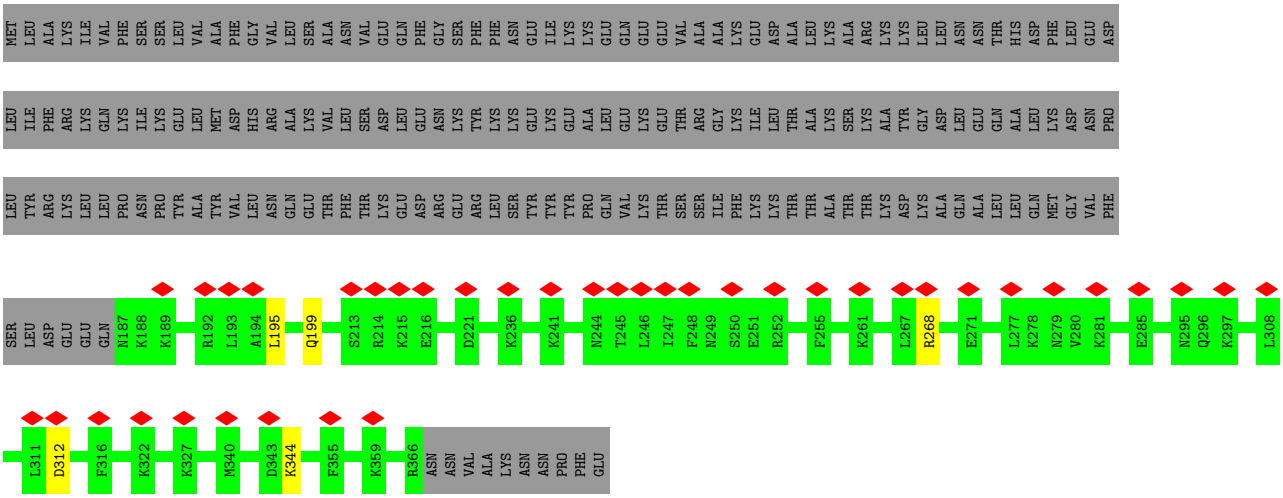

• Molecule 2: Type IV secretion system apparatus protein CagM

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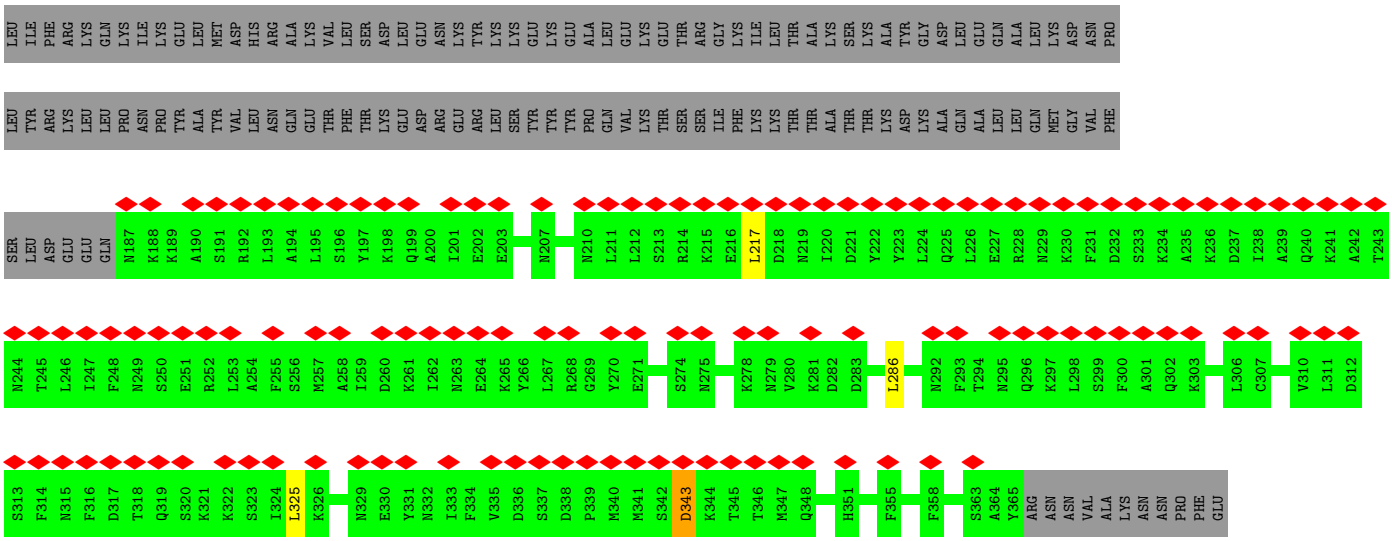

- Molecule 2: Type IV secretion system apparatus protein CagM

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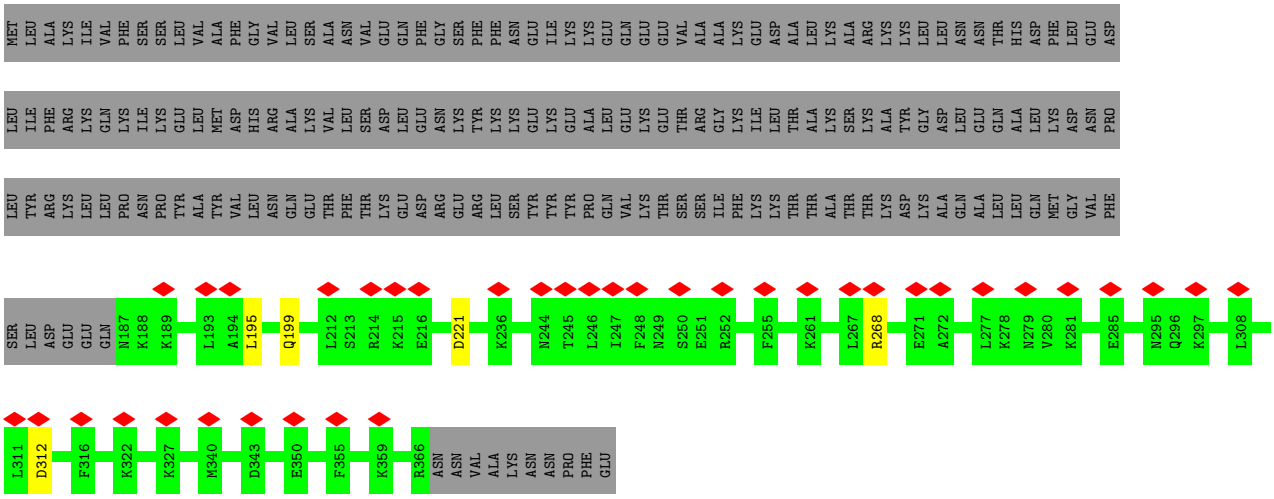

- Molecule 2: Type IV secretion system apparatus protein CagM

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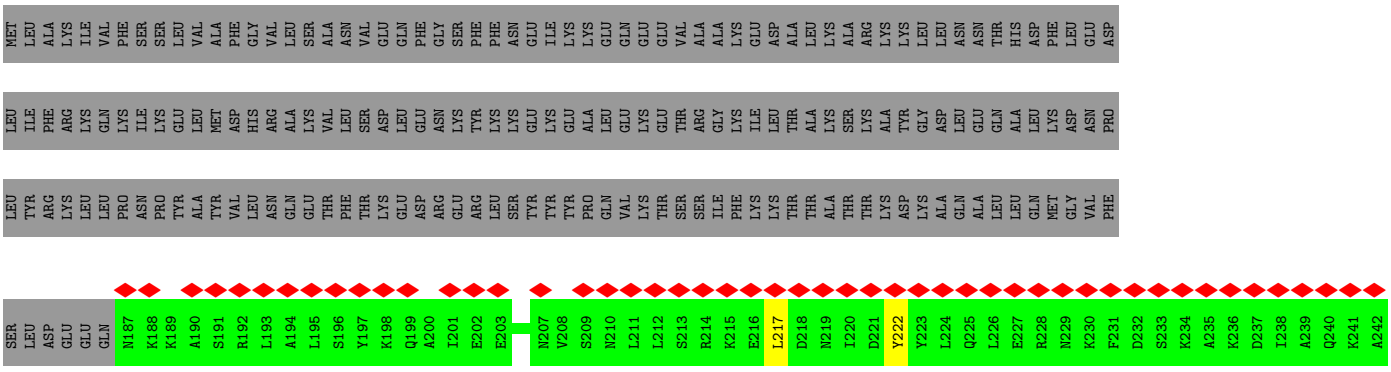

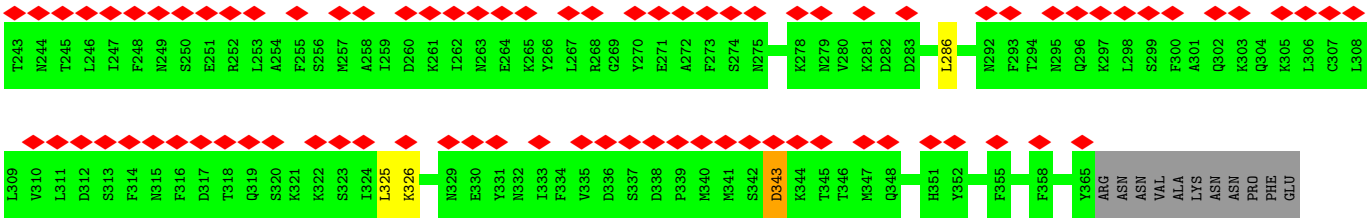

• Molecule 3: Type IV secretion system apparatus protein CagT

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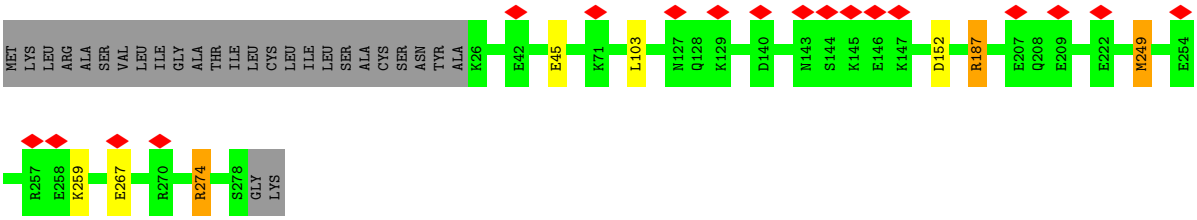

• Molecule 3: Type IV secretion system apparatus protein CagT

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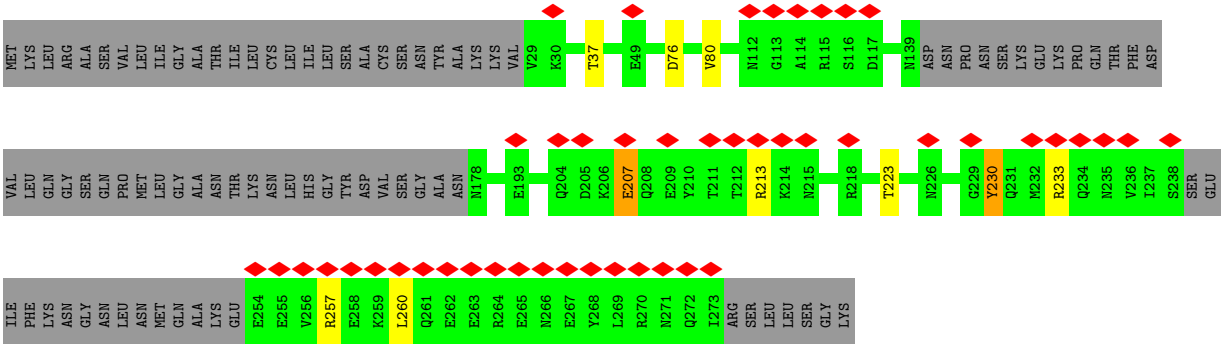

• Molecule 3: Type IV secretion system apparatus protein CagT

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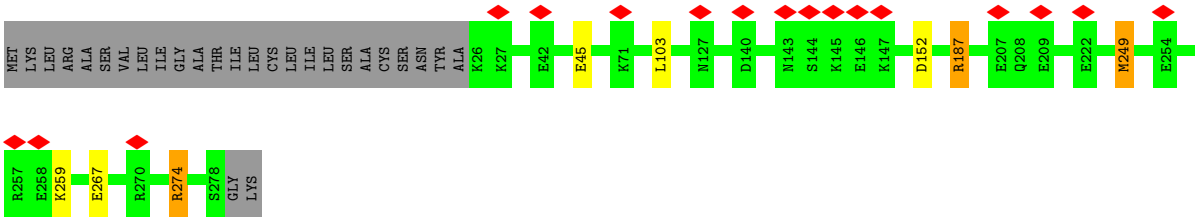

• Molecule 3: Type IV secretion system apparatus protein CagT

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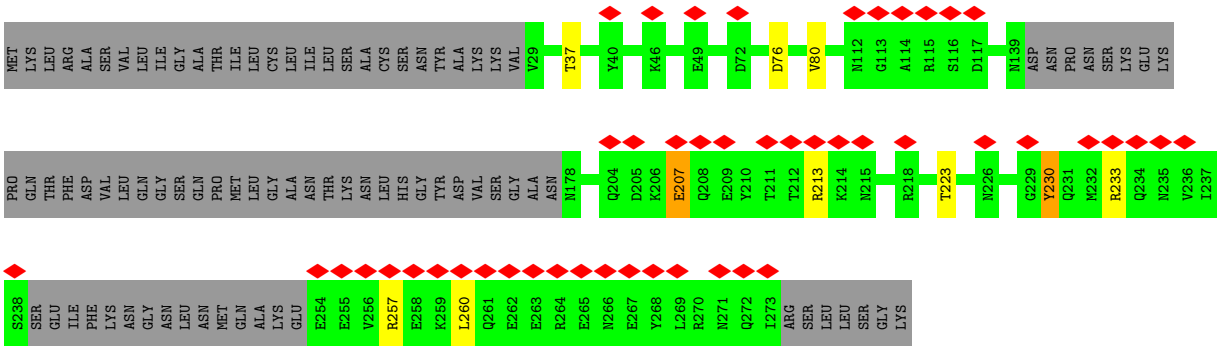

• Molecule 3: Type IV secretion system apparatus protein CagT

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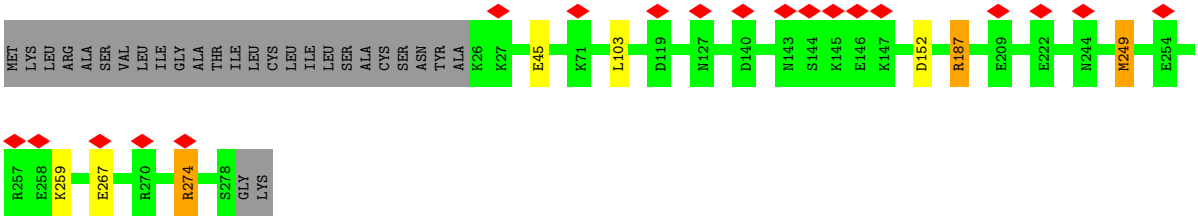

• Molecule 3: Type IV secretion system apparatus protein CagT

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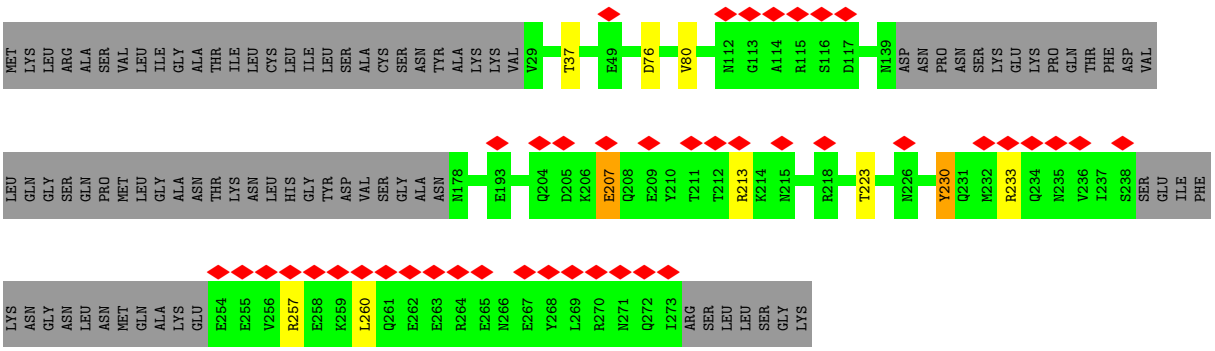

• Molecule 3: Type IV secretion system apparatus protein CagT

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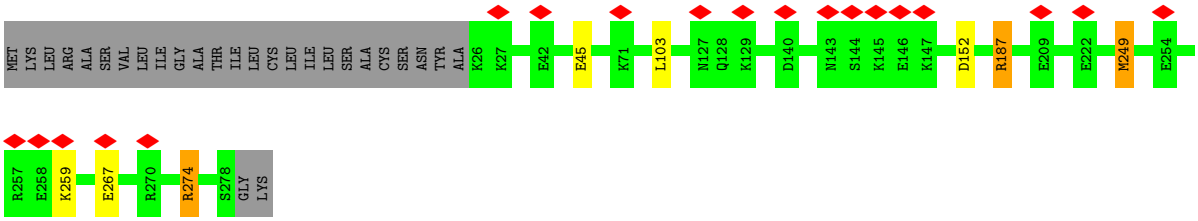

• Molecule 3: Type IV secretion system apparatus protein CagT

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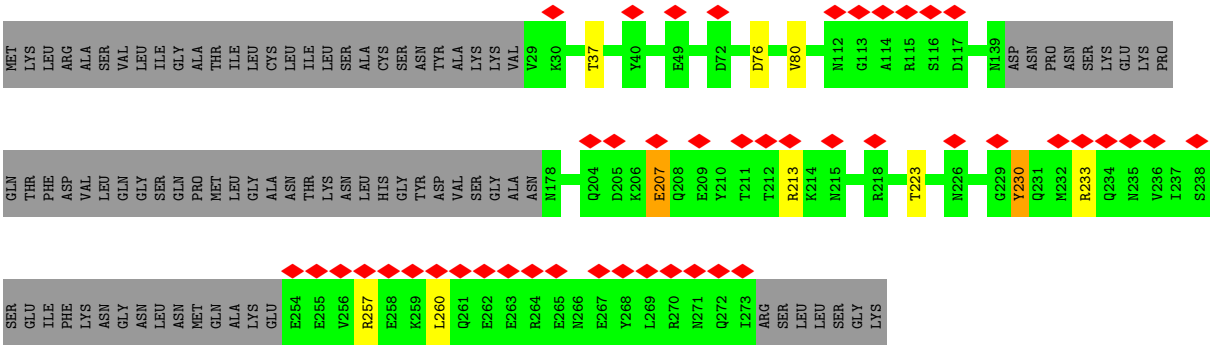

• Molecule 3: Type IV secretion system apparatus protein CagT

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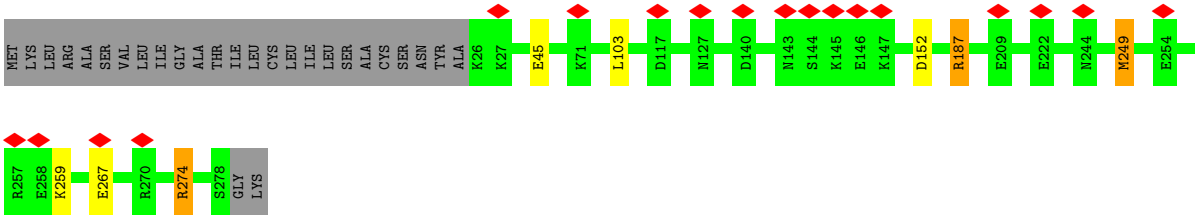

• Molecule 3: Type IV secretion system apparatus protein CagT

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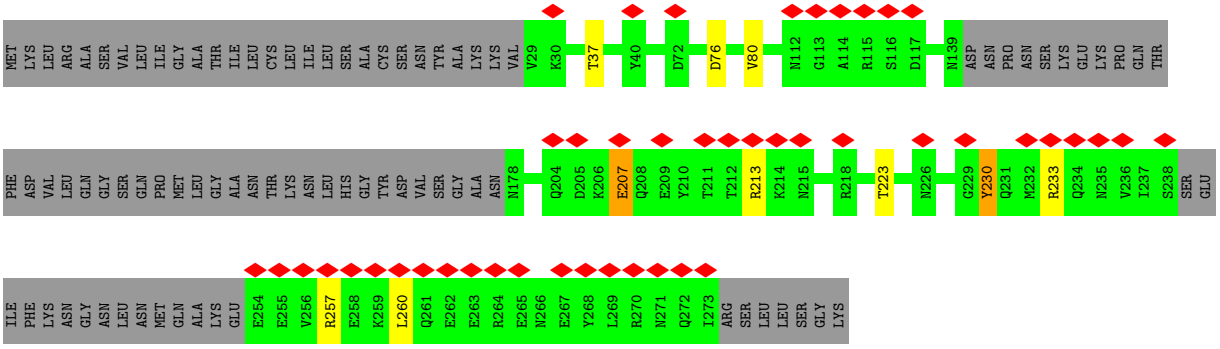

• Molecule 3: Type IV secretion system apparatus protein CagT

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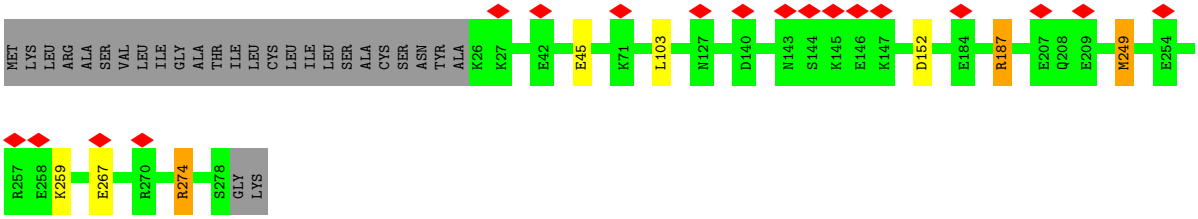

• Molecule 3: Type IV secretion system apparatus protein CagT

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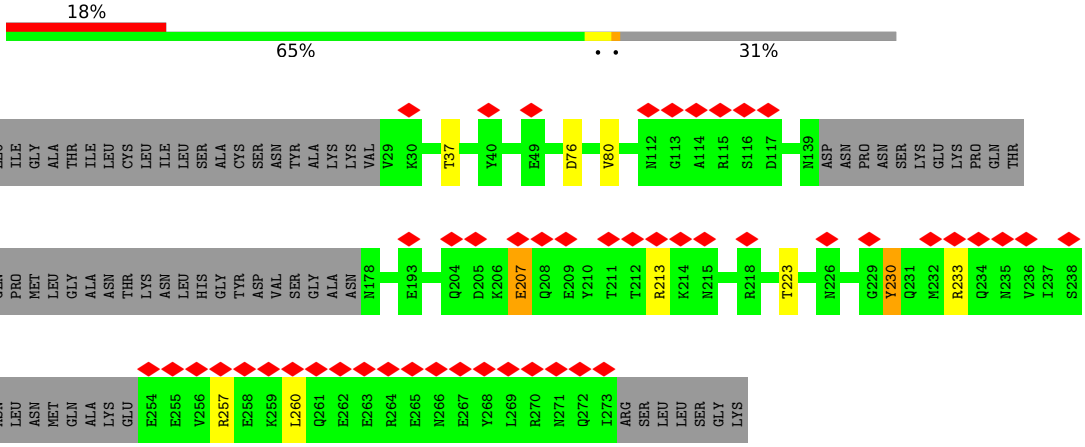

• Molecule 3: Type IV secretion system apparatus protein CagT

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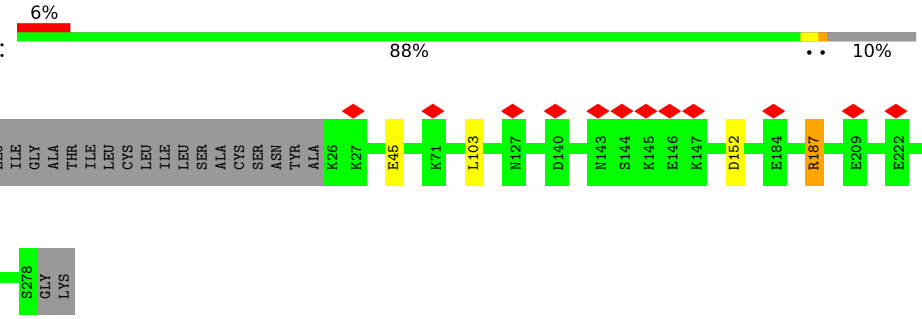
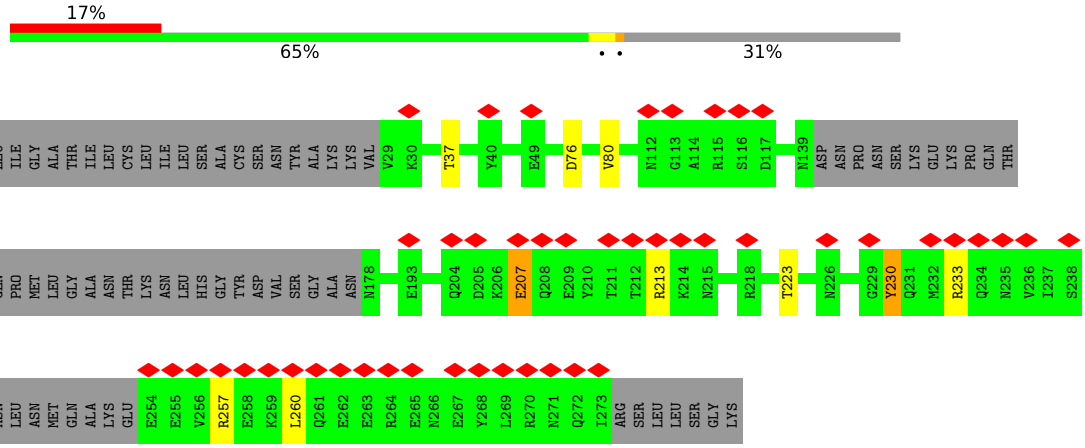


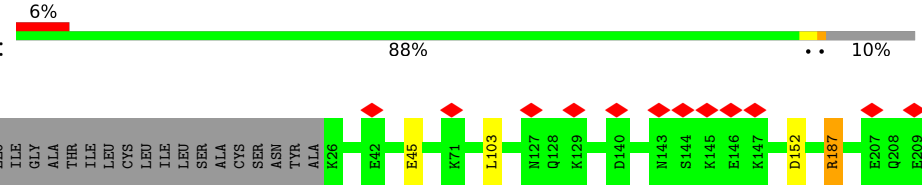
• Molecule 3: Type IV secretion system apparatus protein CagT

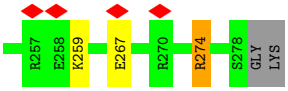
Chain Gt:



• Molecule 3: Type IV secretion system apparatus protein CagT

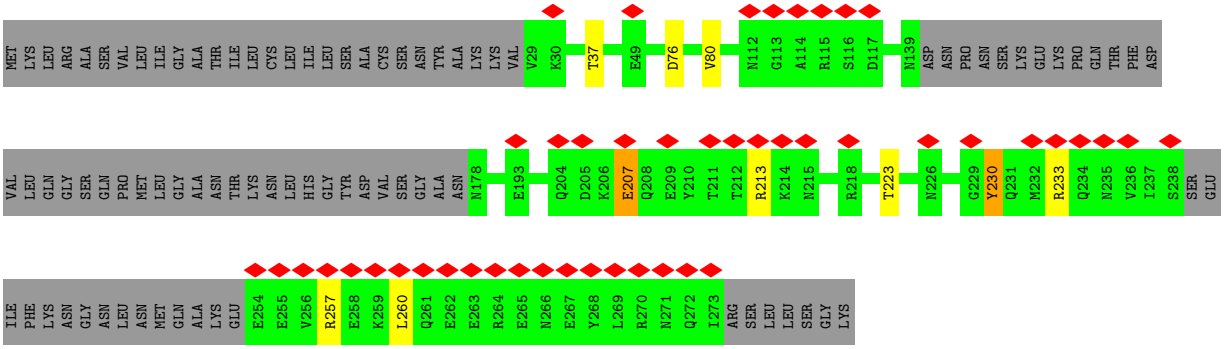
Chain HT:





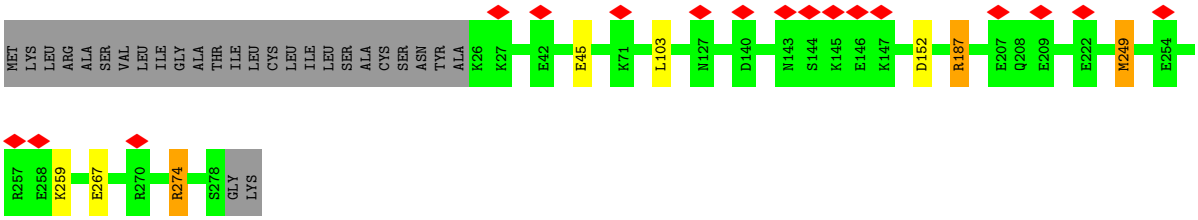
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain Ht:



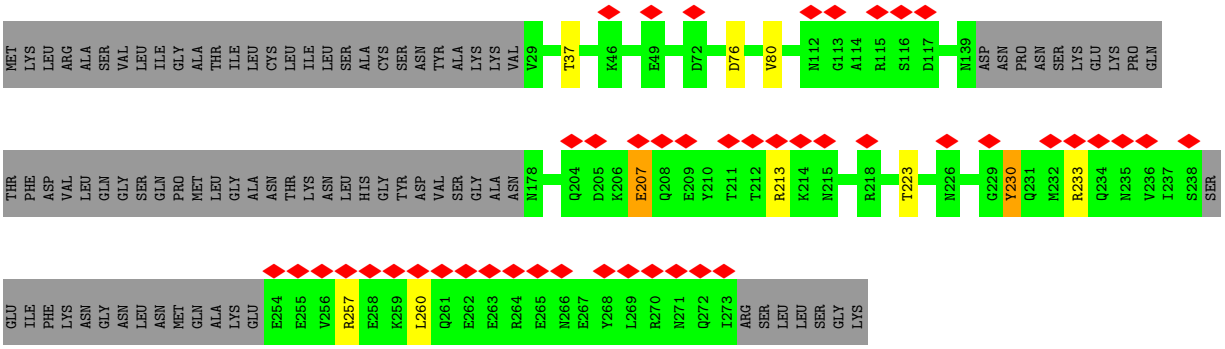
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain IT:



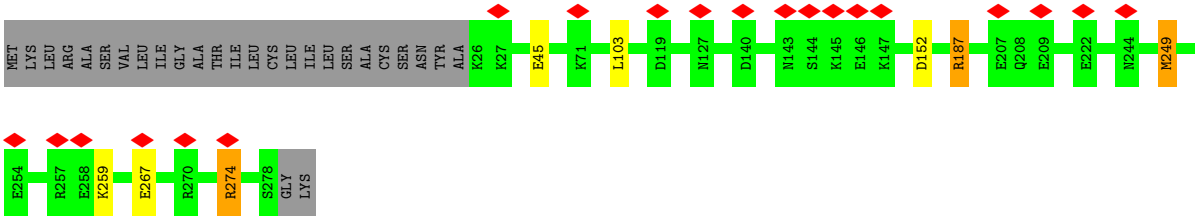
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain It:



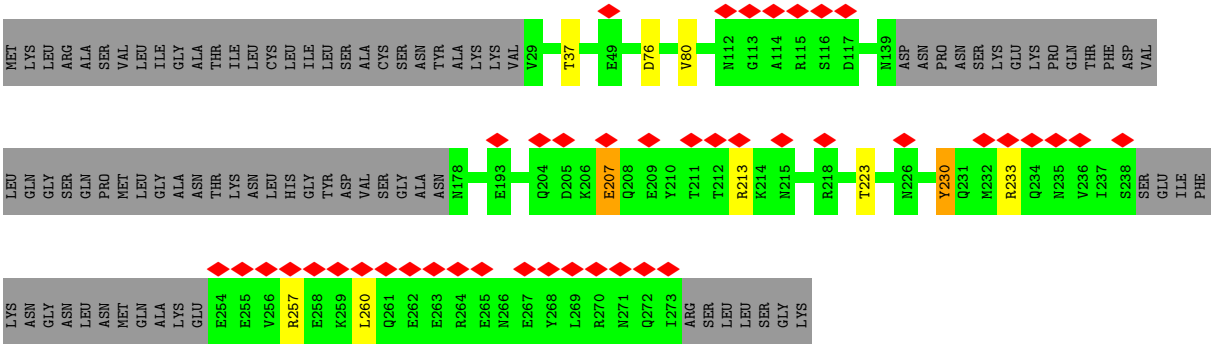
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain JT:



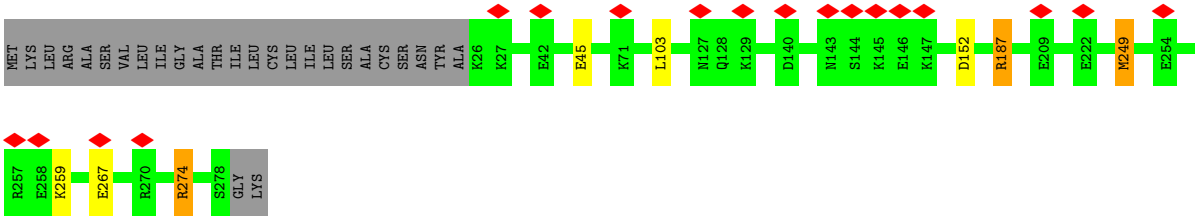
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain Jt:



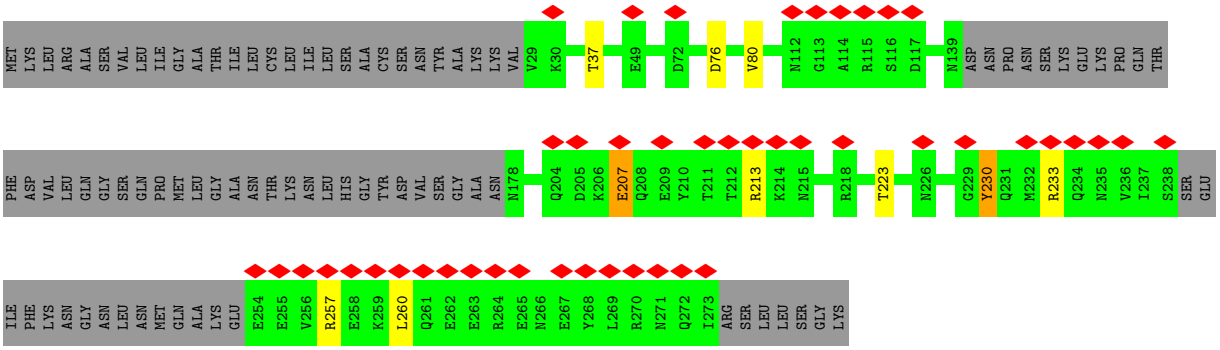
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain KT:



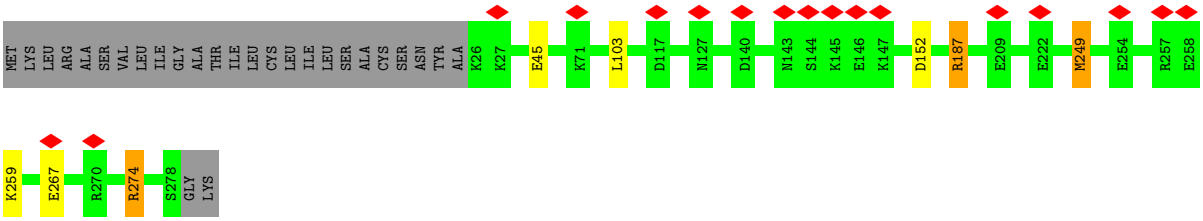
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain Kt:



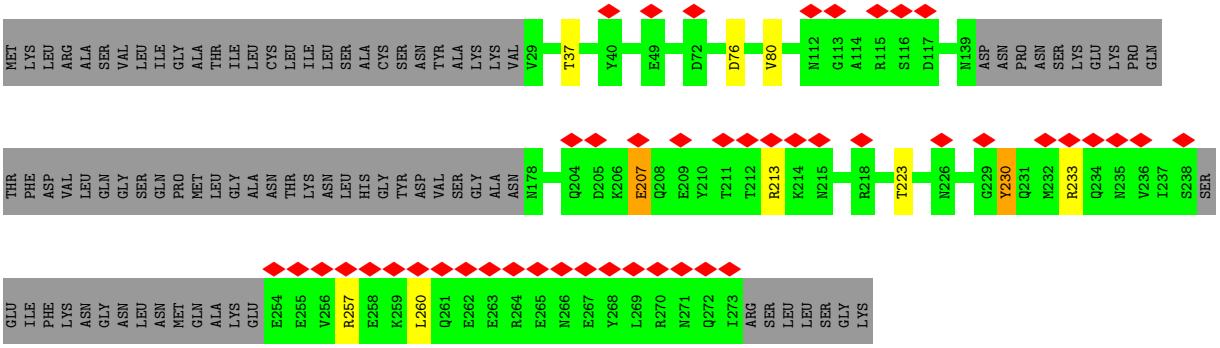
• Molecule 3: Type IV secretion system apparatus protein CagT

Chain LT:



- Molecule 3: Type IV secretion system apparatus protein CagT

Chain Lt:



- Molecule 3: Type IV secretion system apparatus protein CagT

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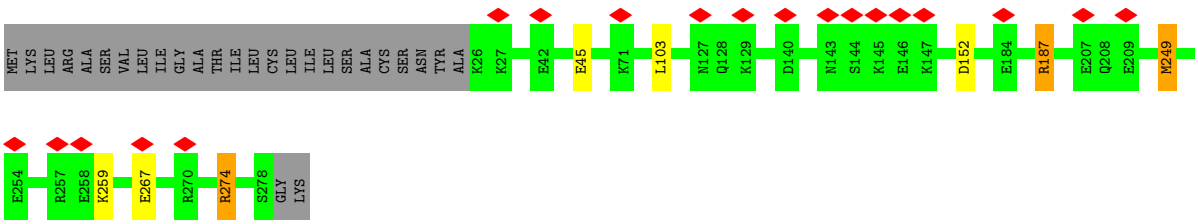

- Molecule 3: Type IV secretion system apparatus protein CagT

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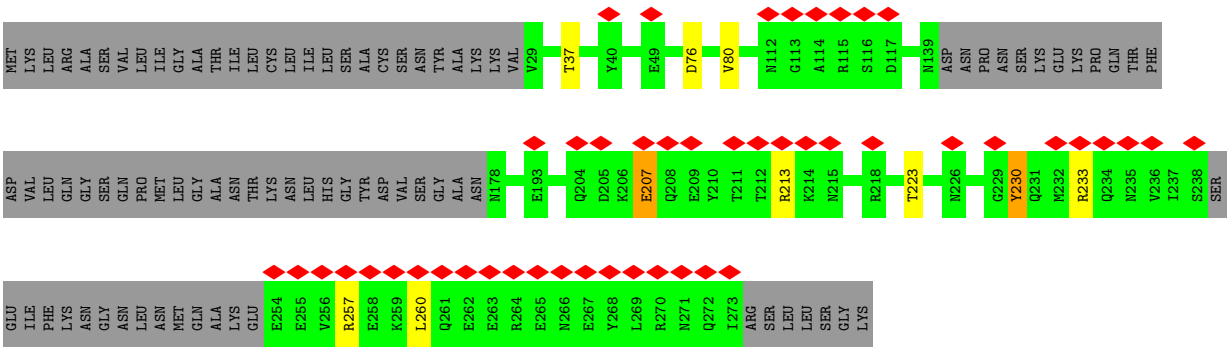
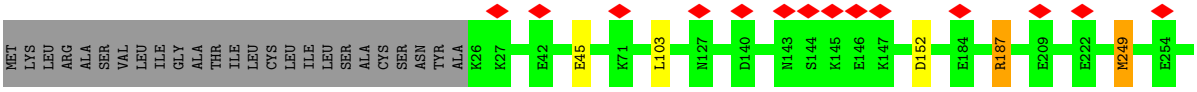
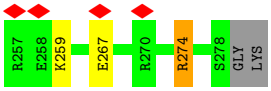


• Molecule 3: Type IV secretion system apparatus protein CagT

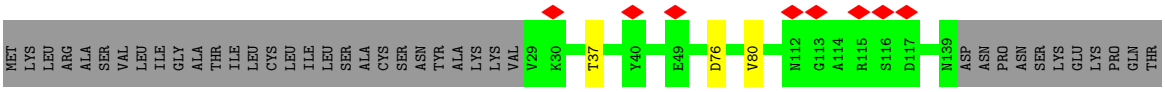
Chain NT:

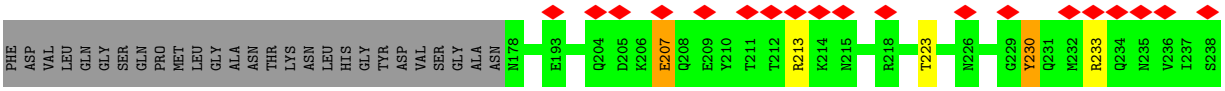


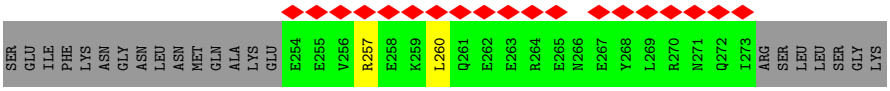


• Molecule 3: Type IV secretion system apparatus protein CagT

Chain Nt:

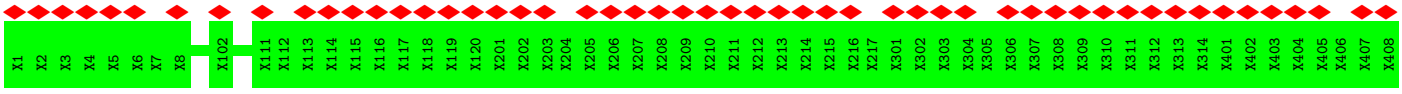


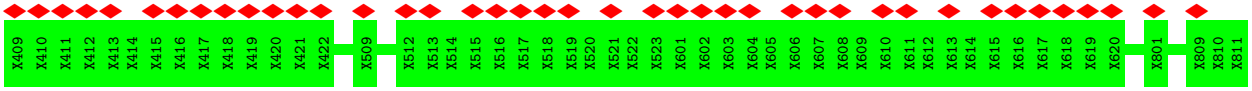




• Molecule 4: Unknown protein fragment

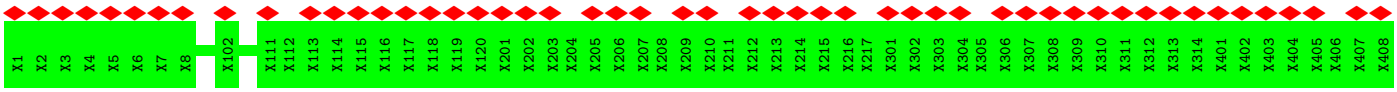
Chain AU:

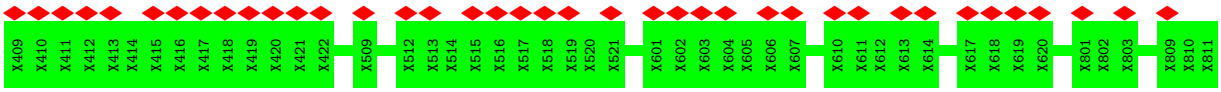




• Molecule 4: Unknown protein fragment

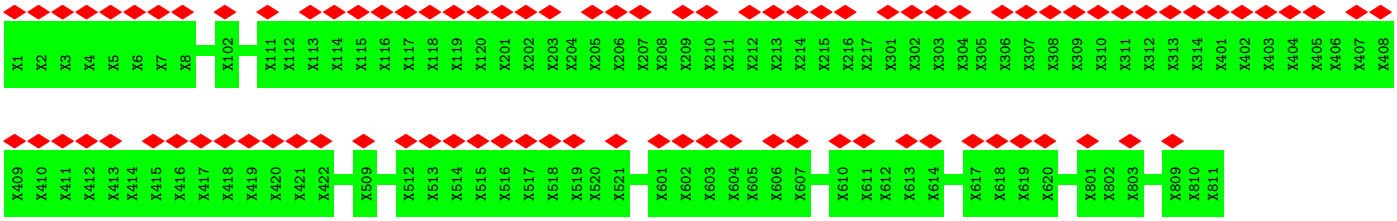
Chain BU:





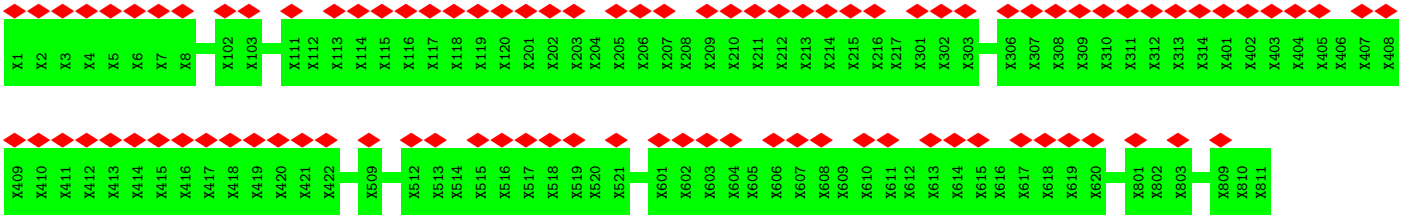
• Molecule 4: Unknown protein fragment

Chain CU: 57% 100%



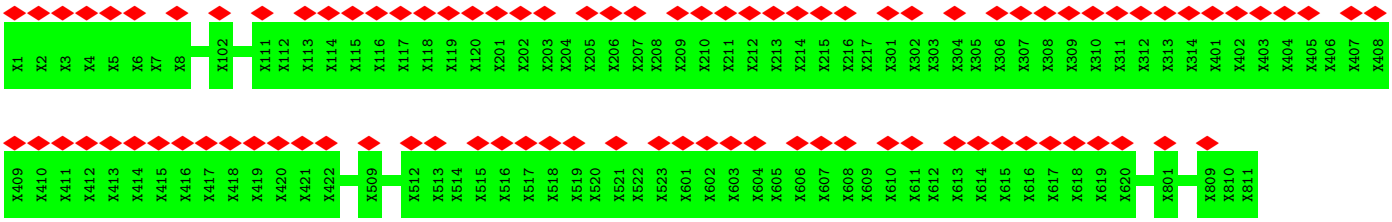
- Molecule 4: Unknown protein fragment

Chain DU: 59% 100%



- Molecule 4: Unknown protein fragment

Chain EU: 58% 100%

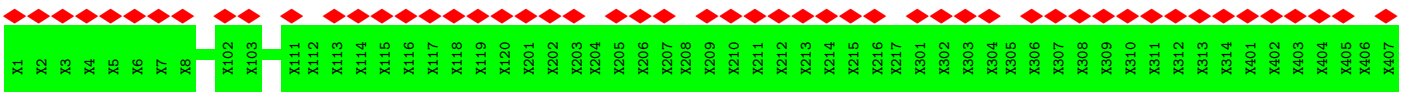


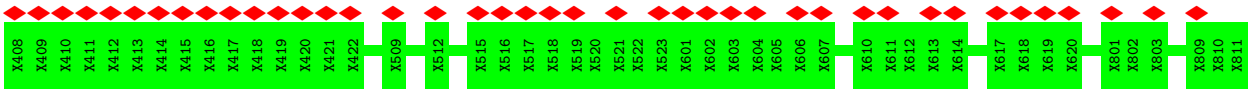
- Molecule 4: Unknown protein fragment

Chain FU: 58% 100%

- Molecule 4: Unknown protein fragment

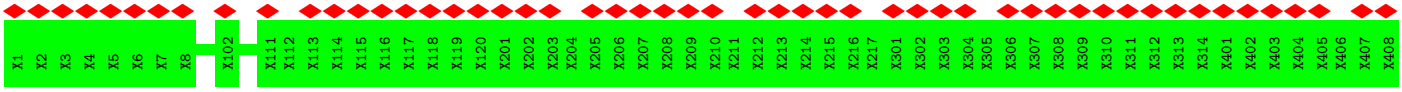
Chain GU: 58% 100%

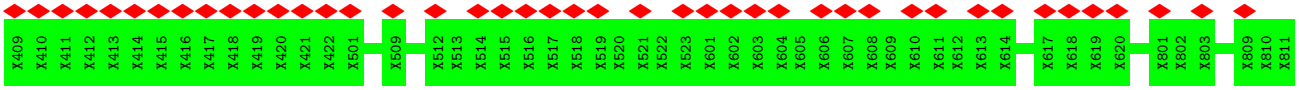




• Molecule 4: Unknown protein fragment

Chain HU:





• Molecule 4: Unknown protein fragment

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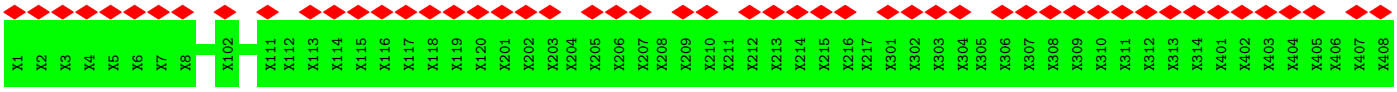

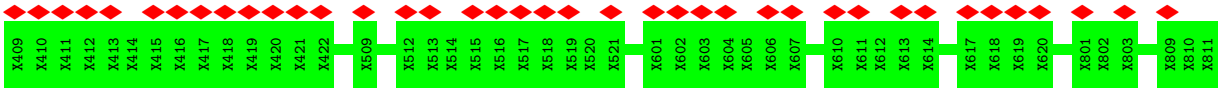

• Molecule 4: Unknown protein fragment

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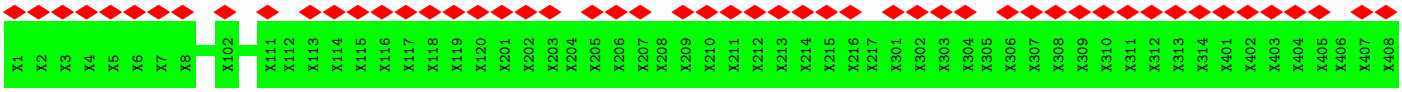

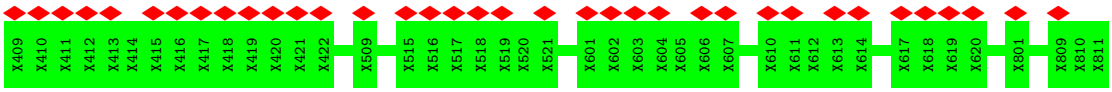

• Molecule 4: Unknown protein fragment

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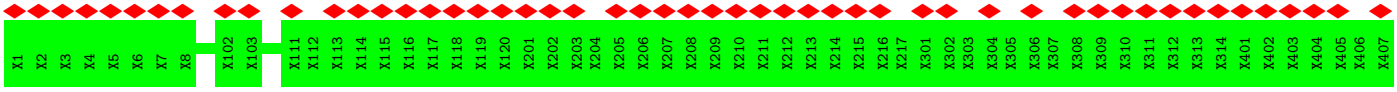

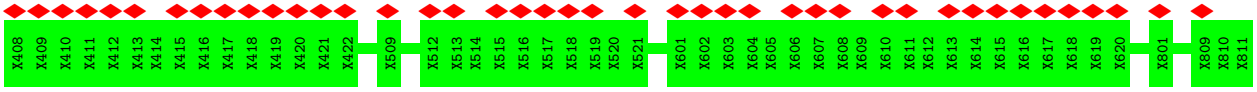

• Molecule 4: Unknown protein fragment

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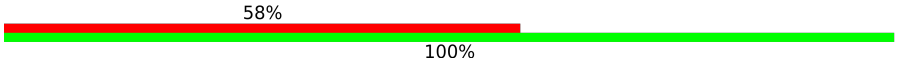

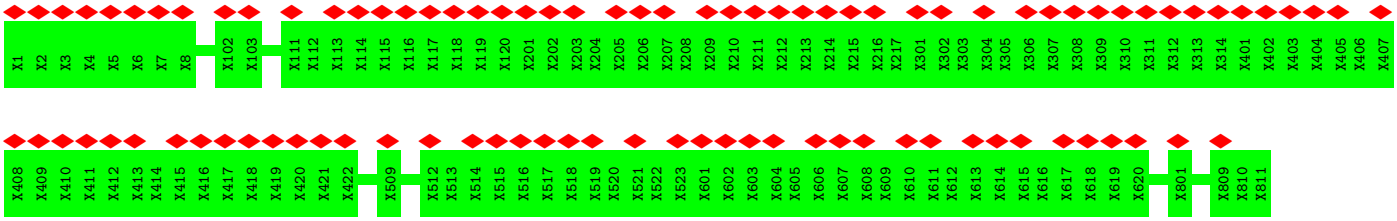

- Molecule 4: Unknown protein fragment

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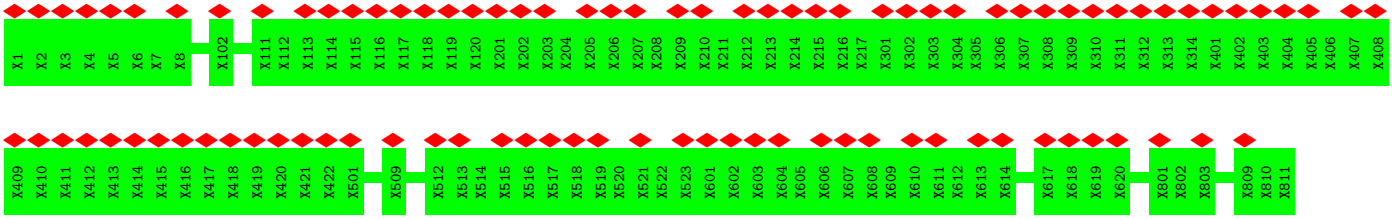
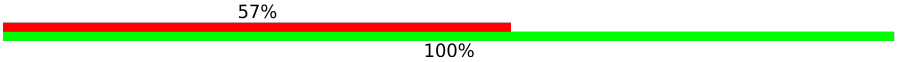
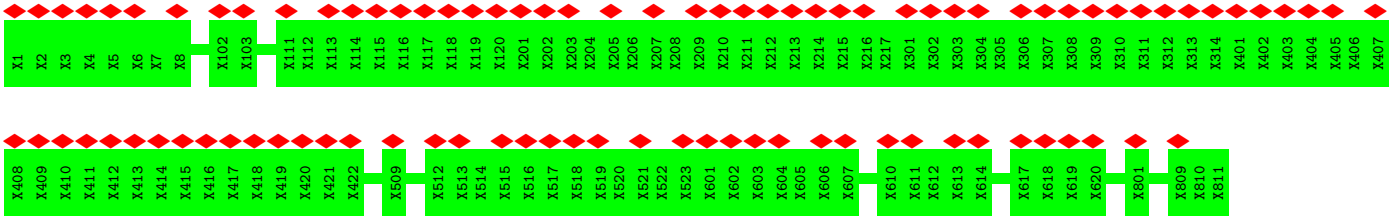


- Molecule 4: Unknown protein fragment

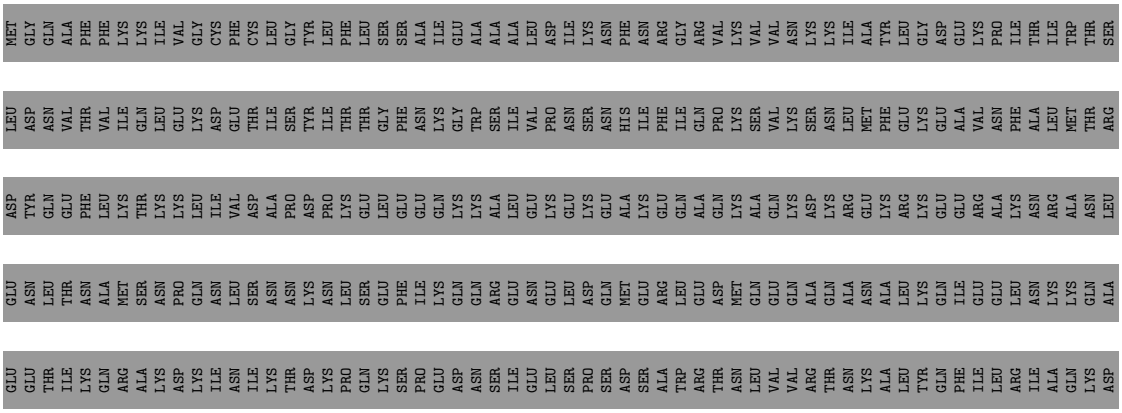
Chain NU:

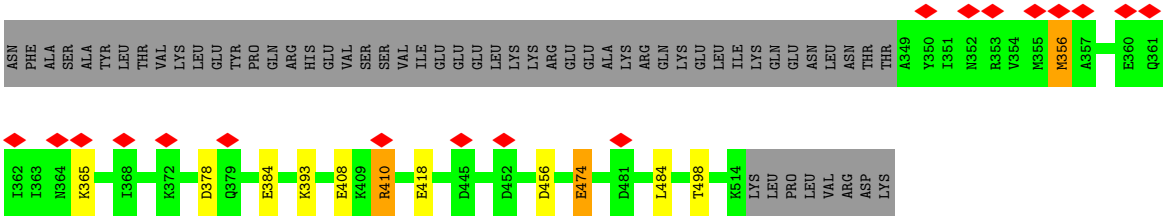




- Molecule 5: Type IV secretion system apparatus protein CagX

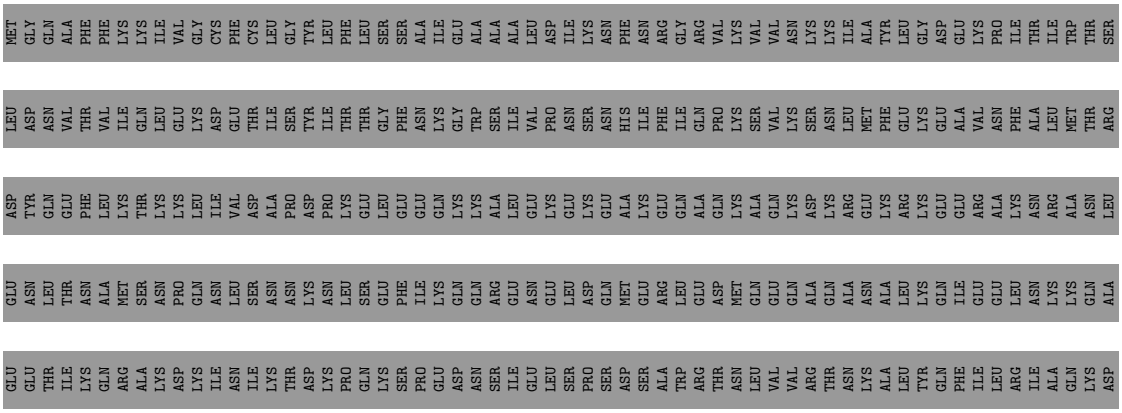
Chain AX:

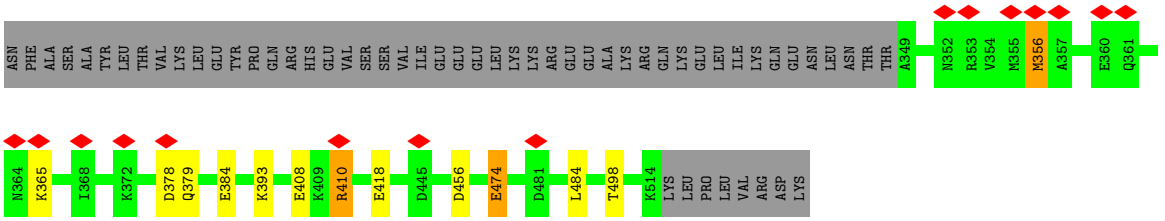




• Molecule 5: Type IV secretion system apparatus protein CagX

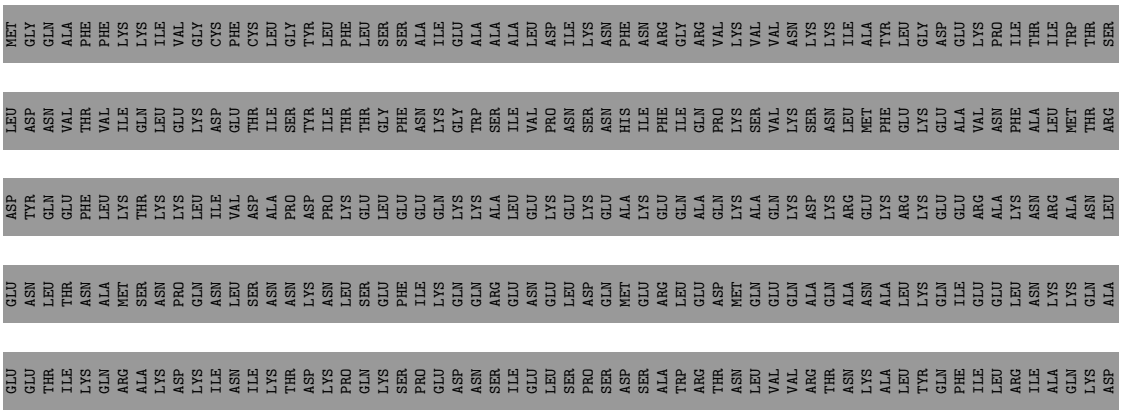
Chain BX:

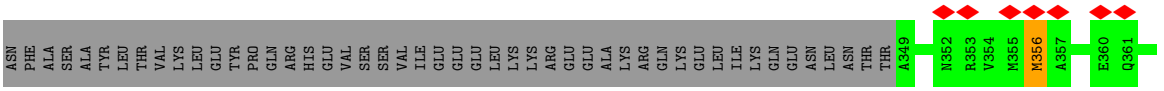


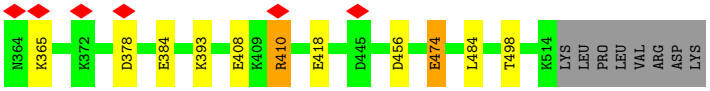


• Molecule 5: Type IV secretion system apparatus protein CagX

Chain CX:

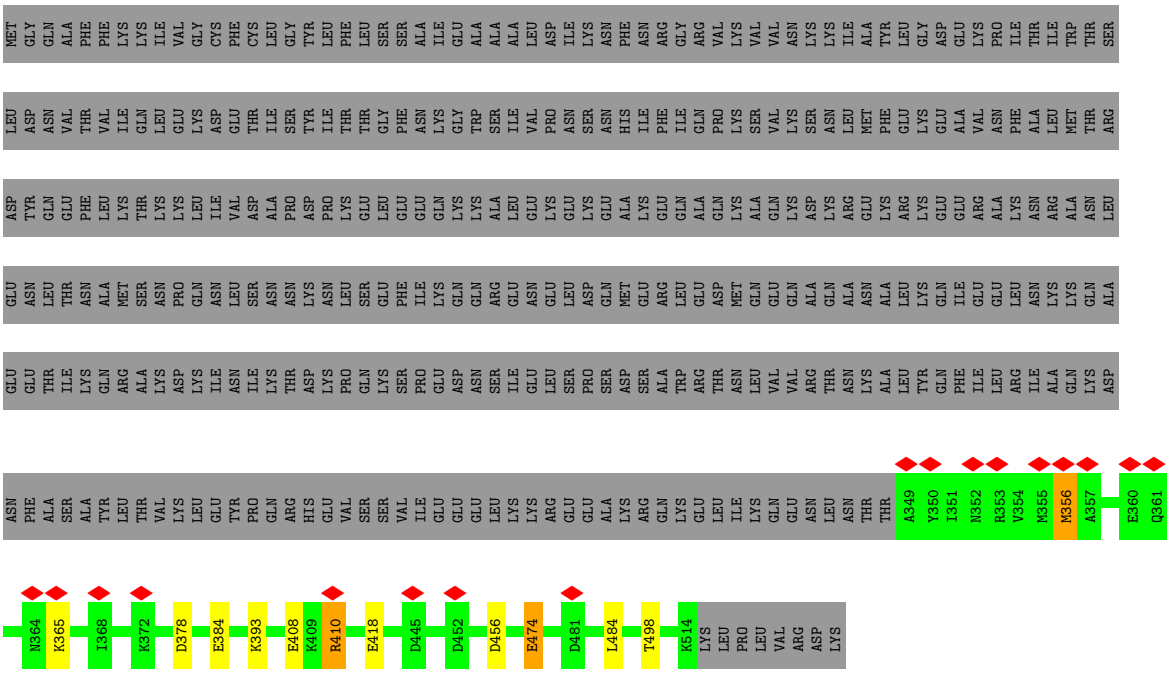






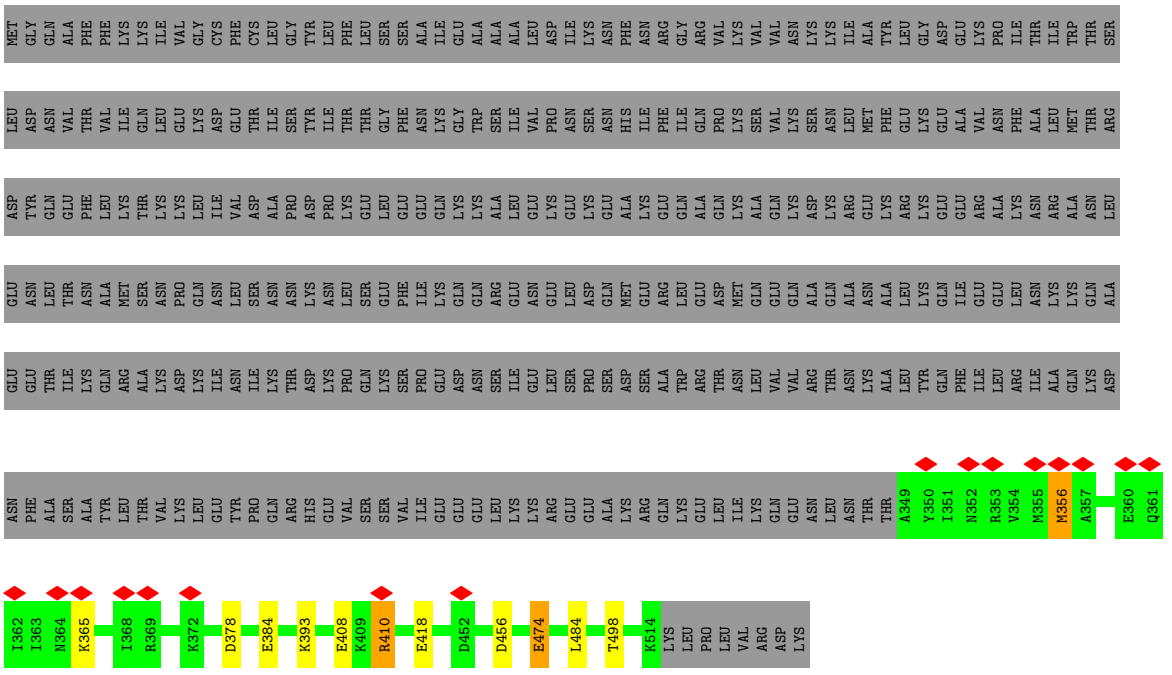
• Molecule 5: Type IV secretion system apparatus protein CagX

Chain DX:



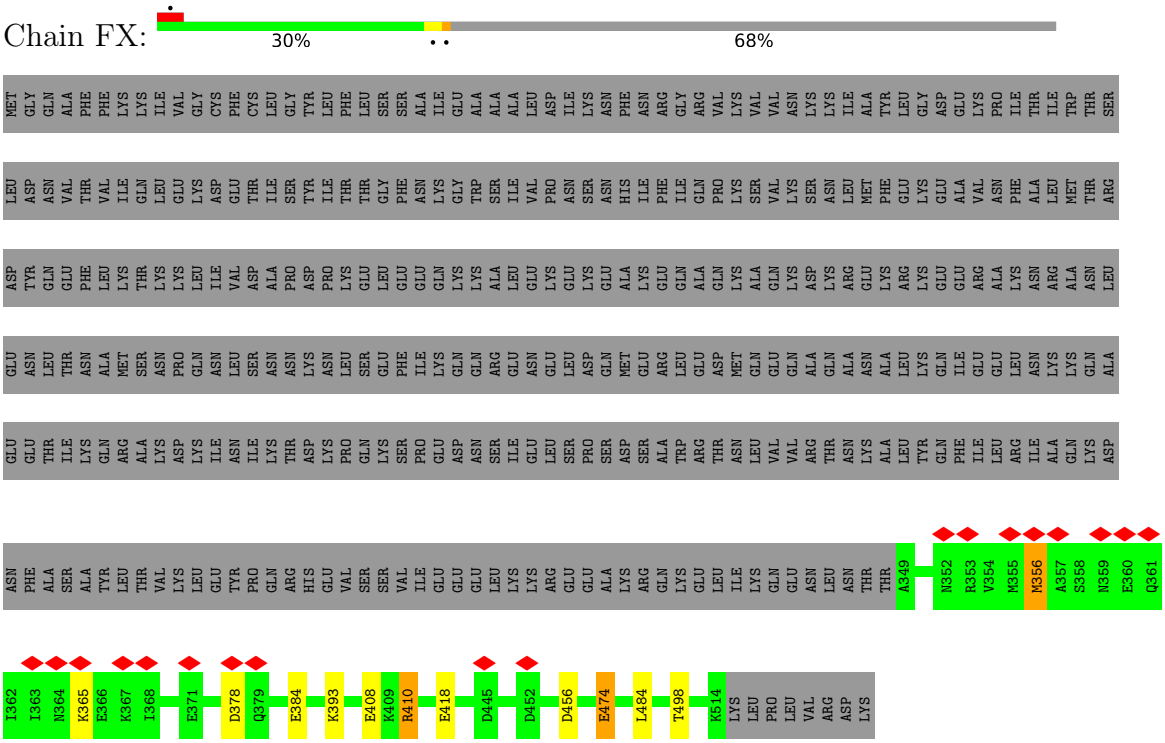
• Molecule 5: Type IV secretion system apparatus protein CagX

Chain EX:



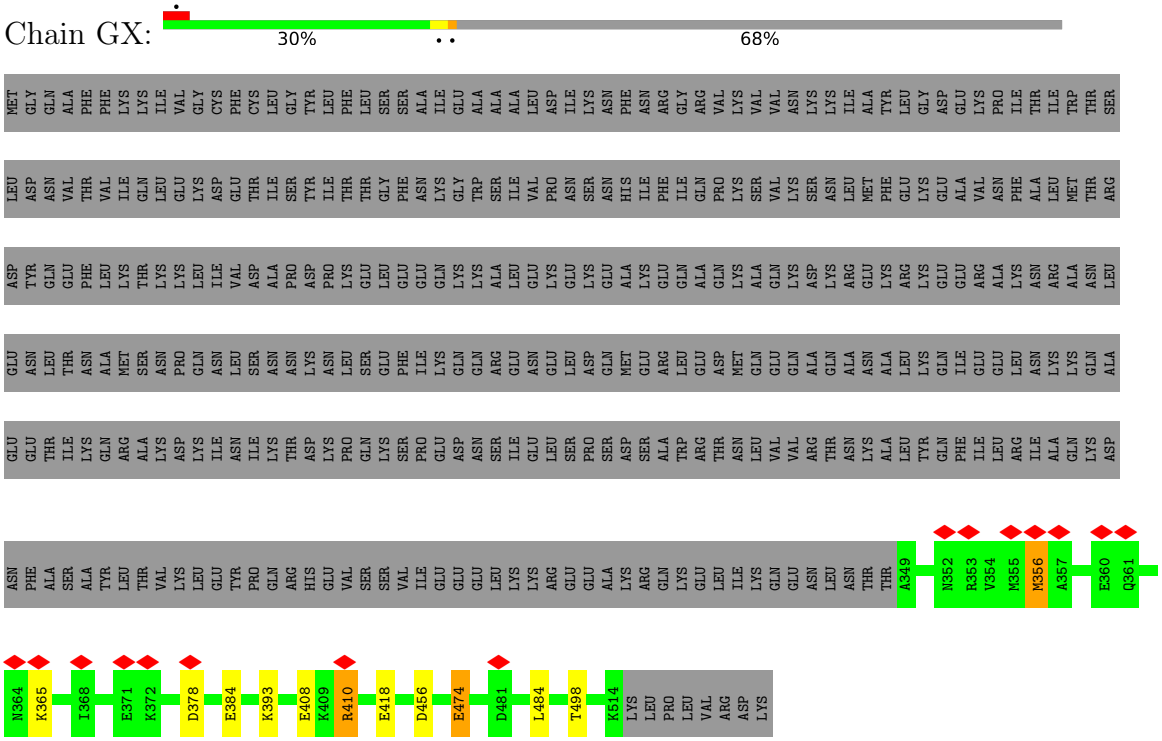
• Molecule 5: Type IV secretion system apparatus protein CagX

Chain FX:



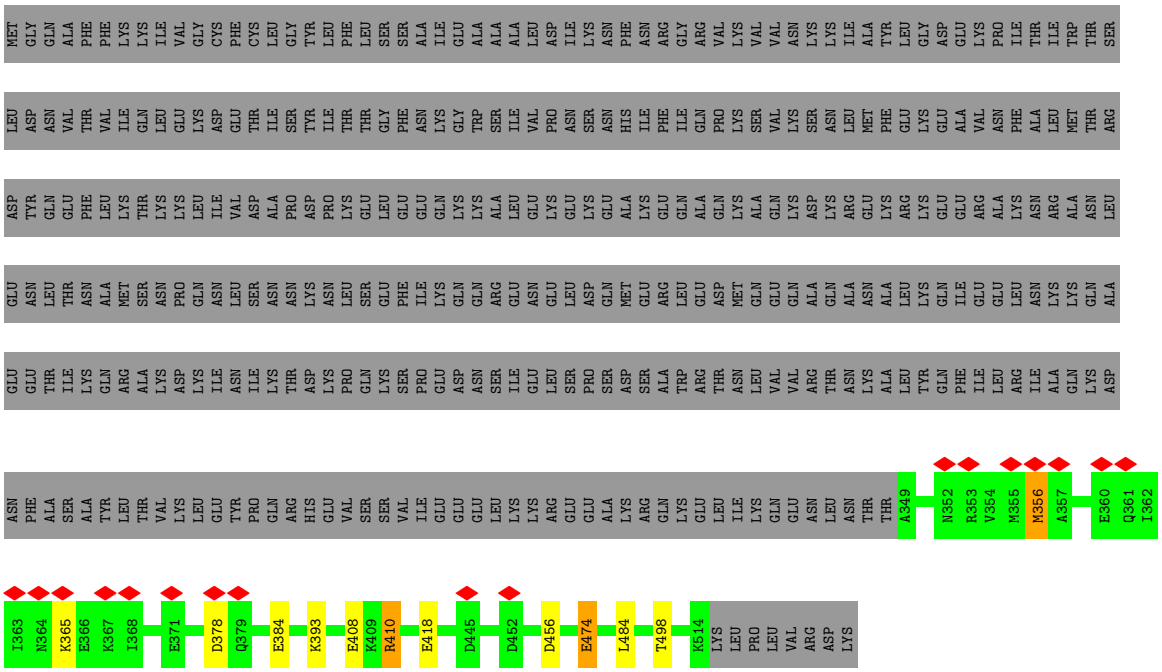
• Molecule 5: Type IV secretion system apparatus protein CagX

Chain GX:



• Molecule 5: Type IV secretion system apparatus protein CagX

Chain HX:



• Molecule 5: Type IV secretion system apparatus protein CagX

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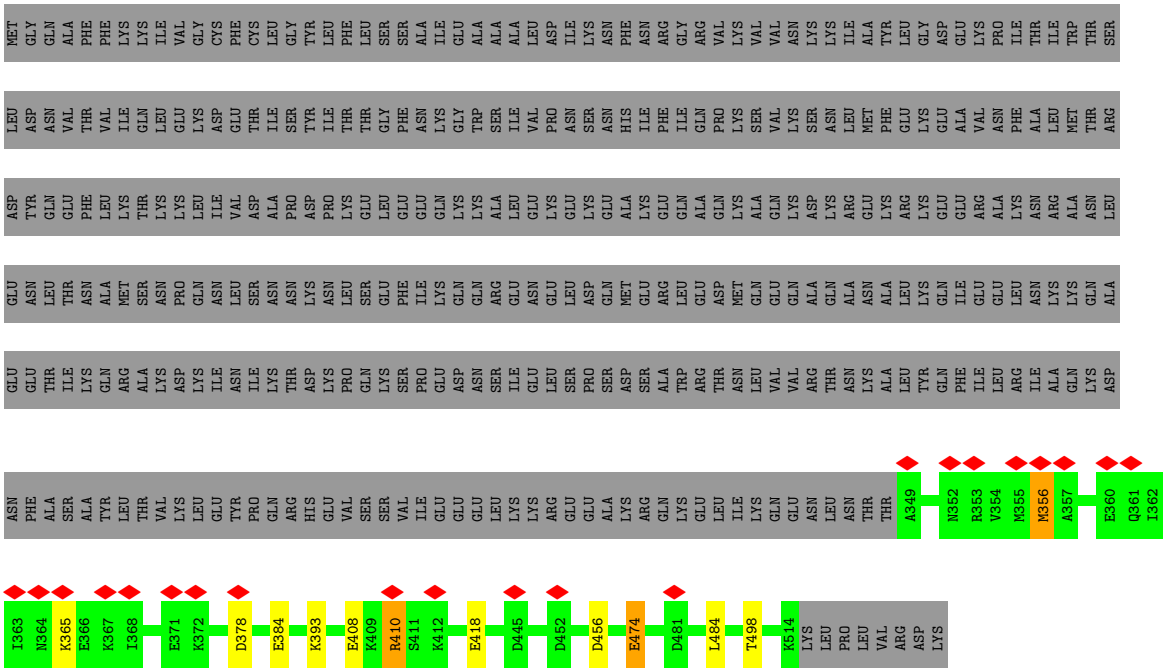

• Molecule 5: Type IV secretion system apparatus protein CagX

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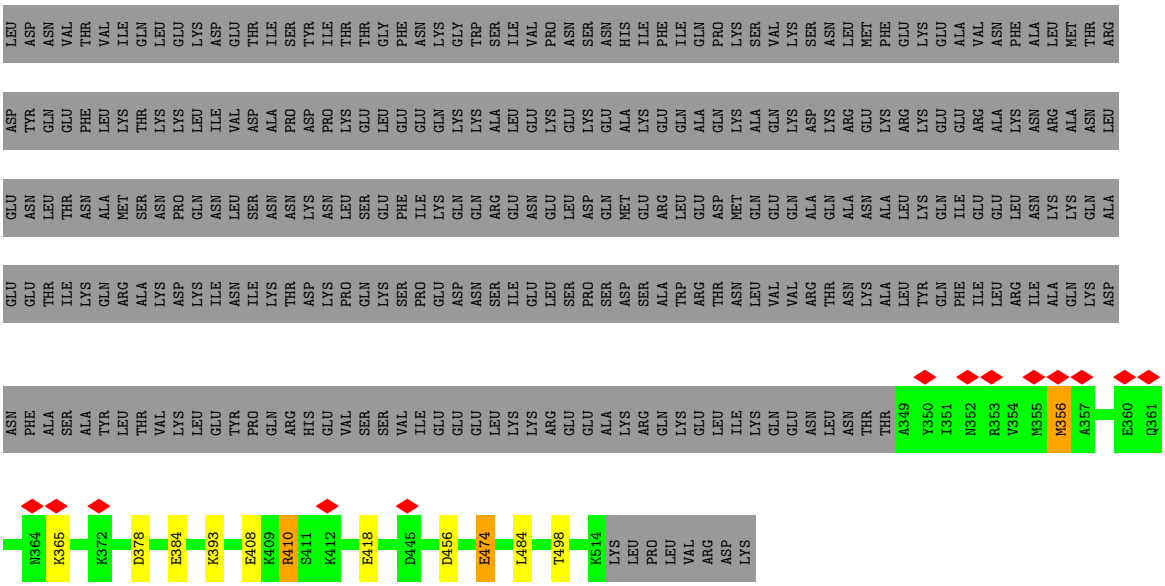

• Molecule 5: Type IV secretion system apparatus protein CagX

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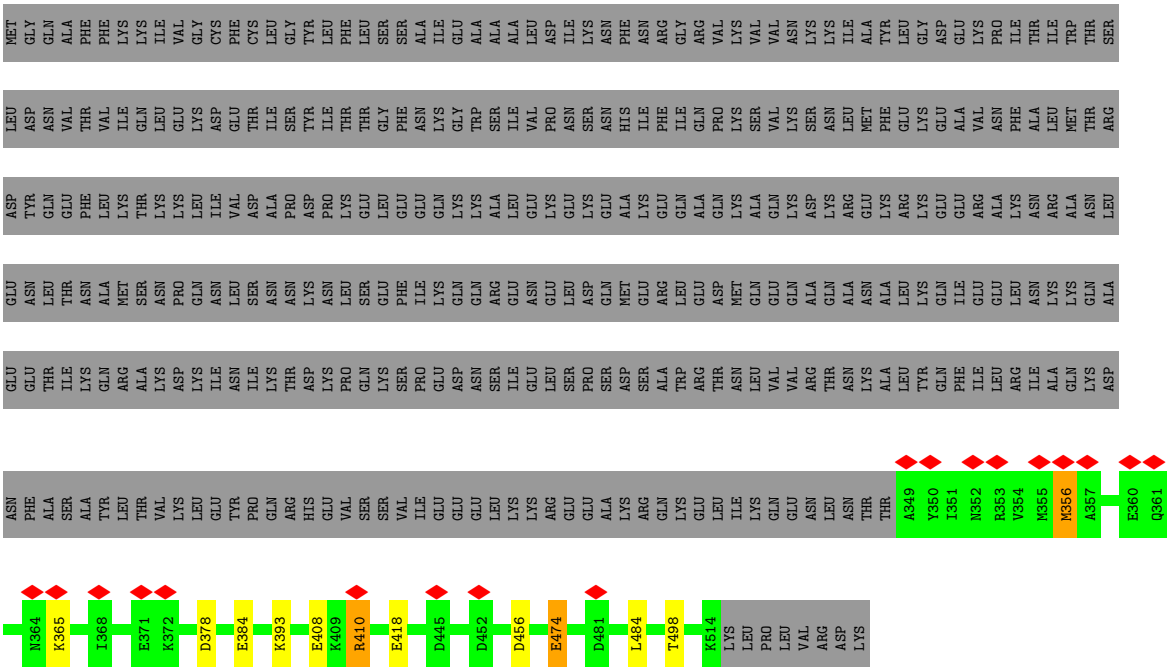

• Molecule 5: Type IV secretion system apparatus protein CagX

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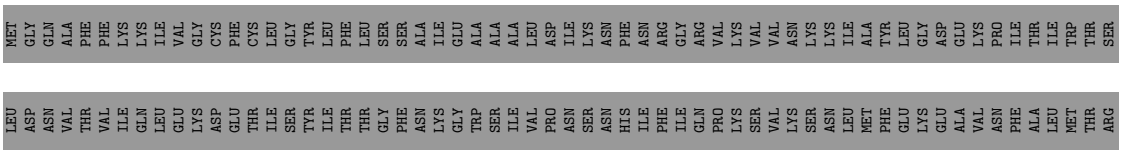

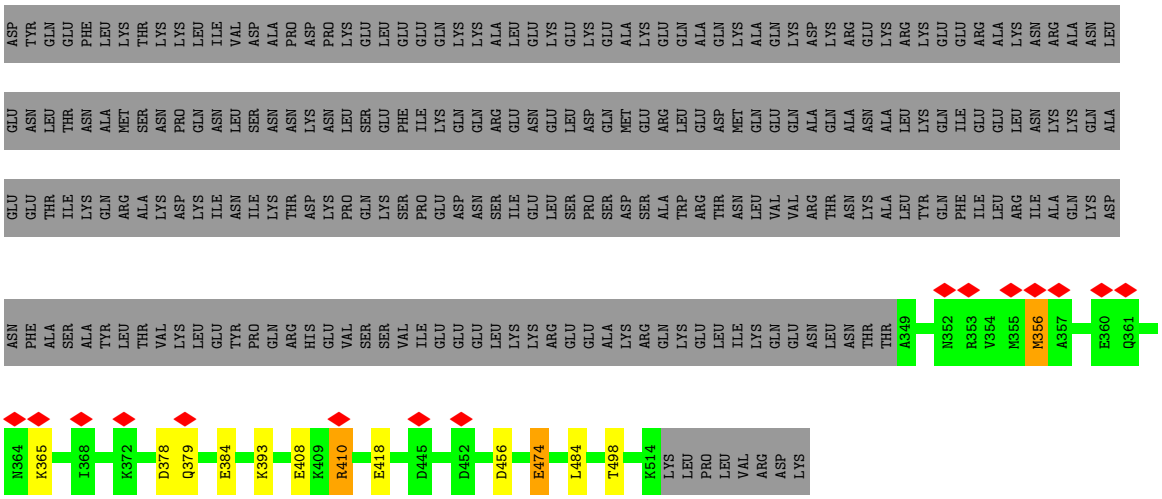

• Molecule 5: Type IV secretion system apparatus protein CagX

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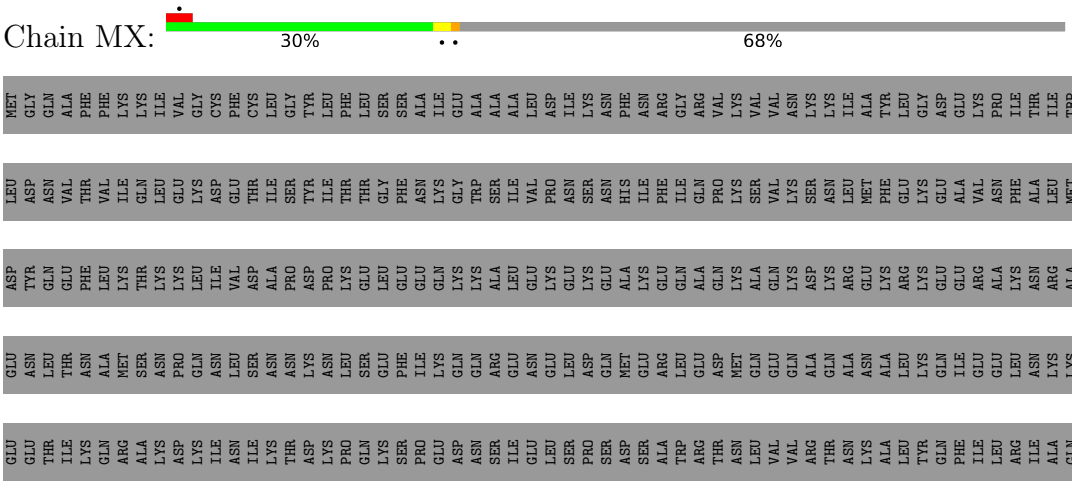

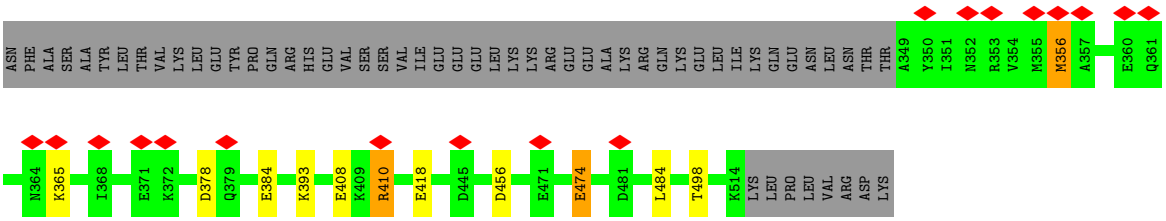

• Molecule 5: Type IV secretion system apparatus protein CagX

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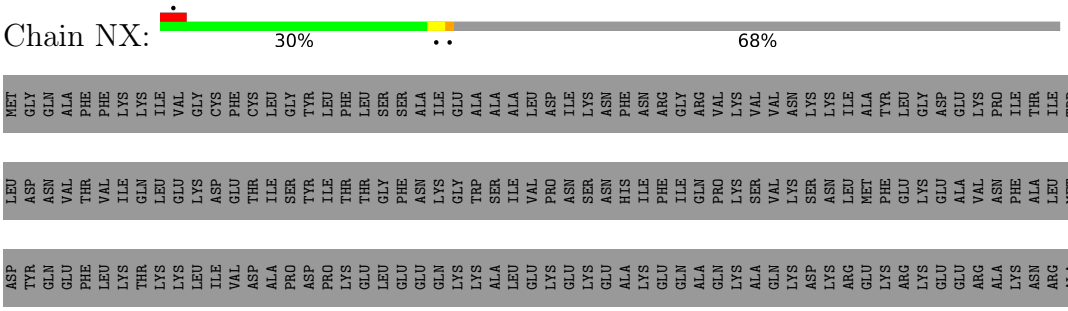
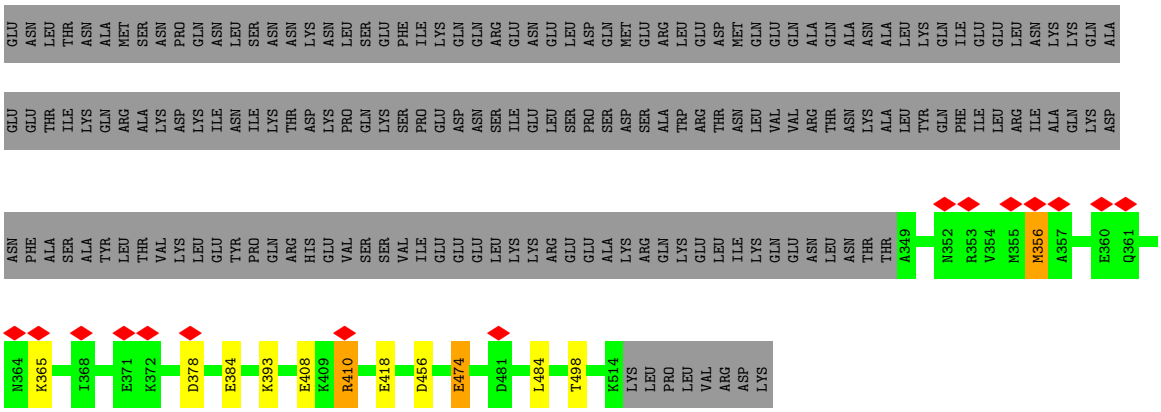
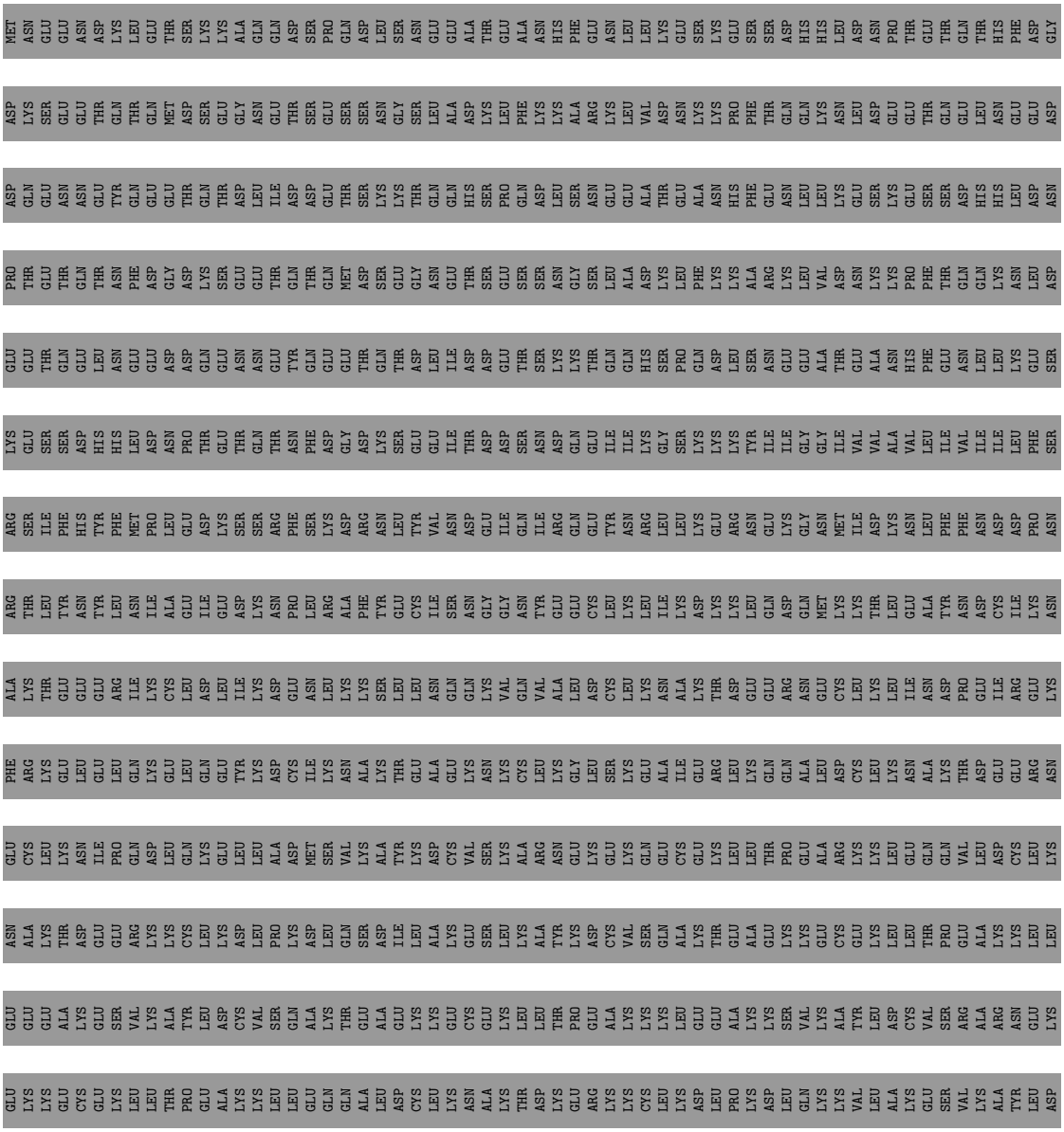
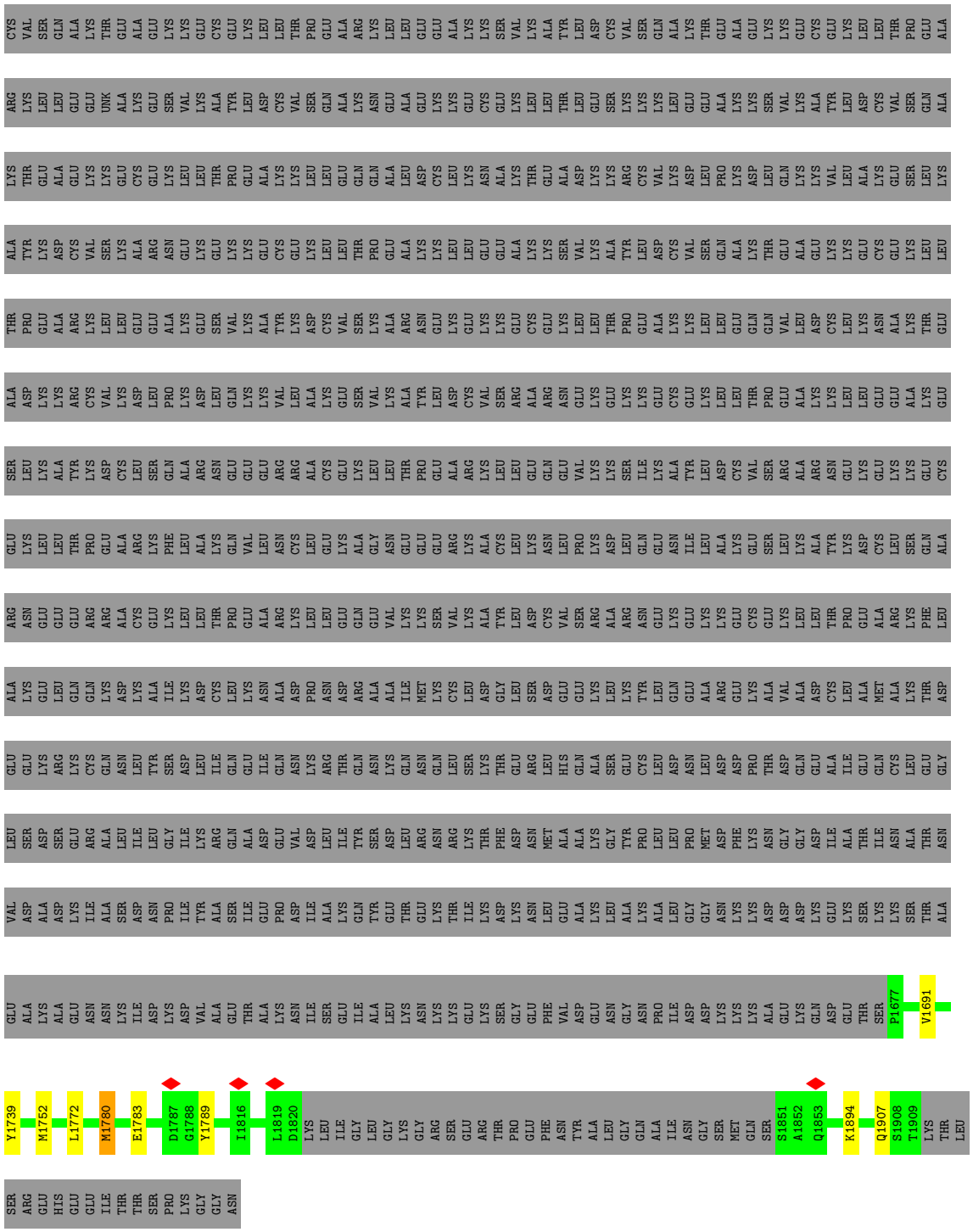




• Molecule 6: Cag pathogenicity island protein (Cag7)

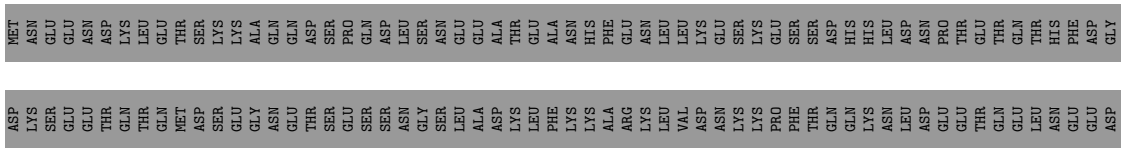
Chain AY: 10% 89%





• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain BY: 10% 89%



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

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

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

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

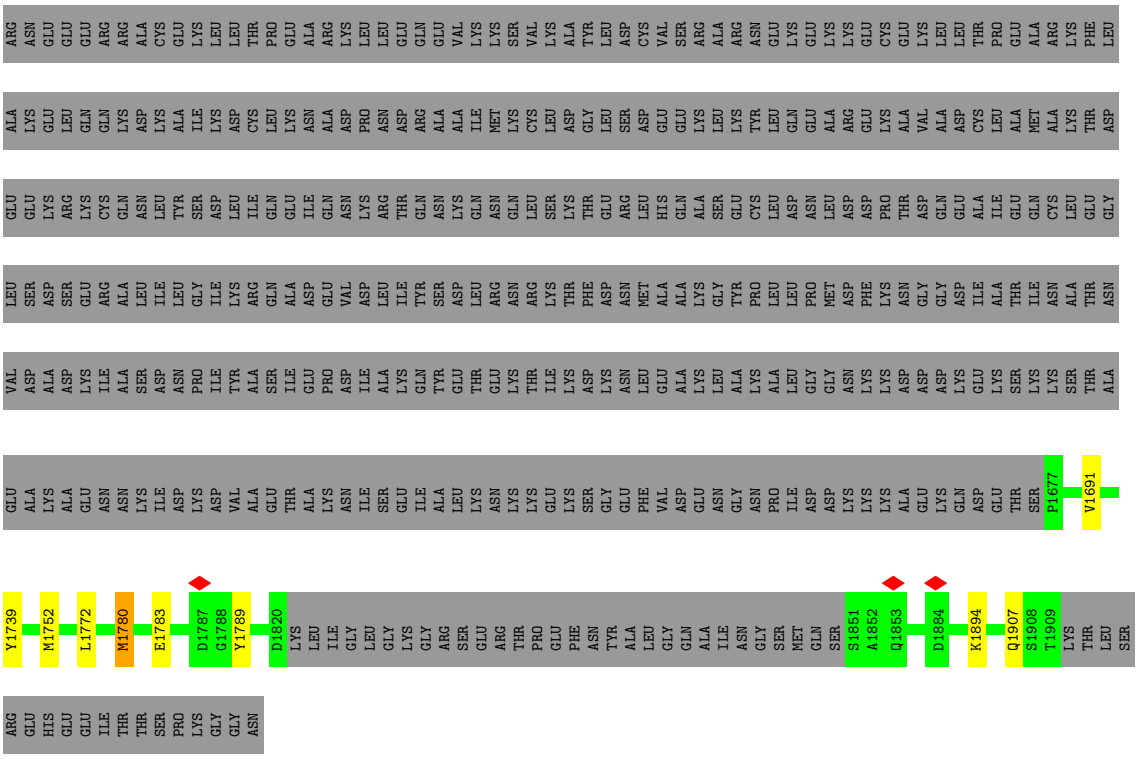
ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU

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

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

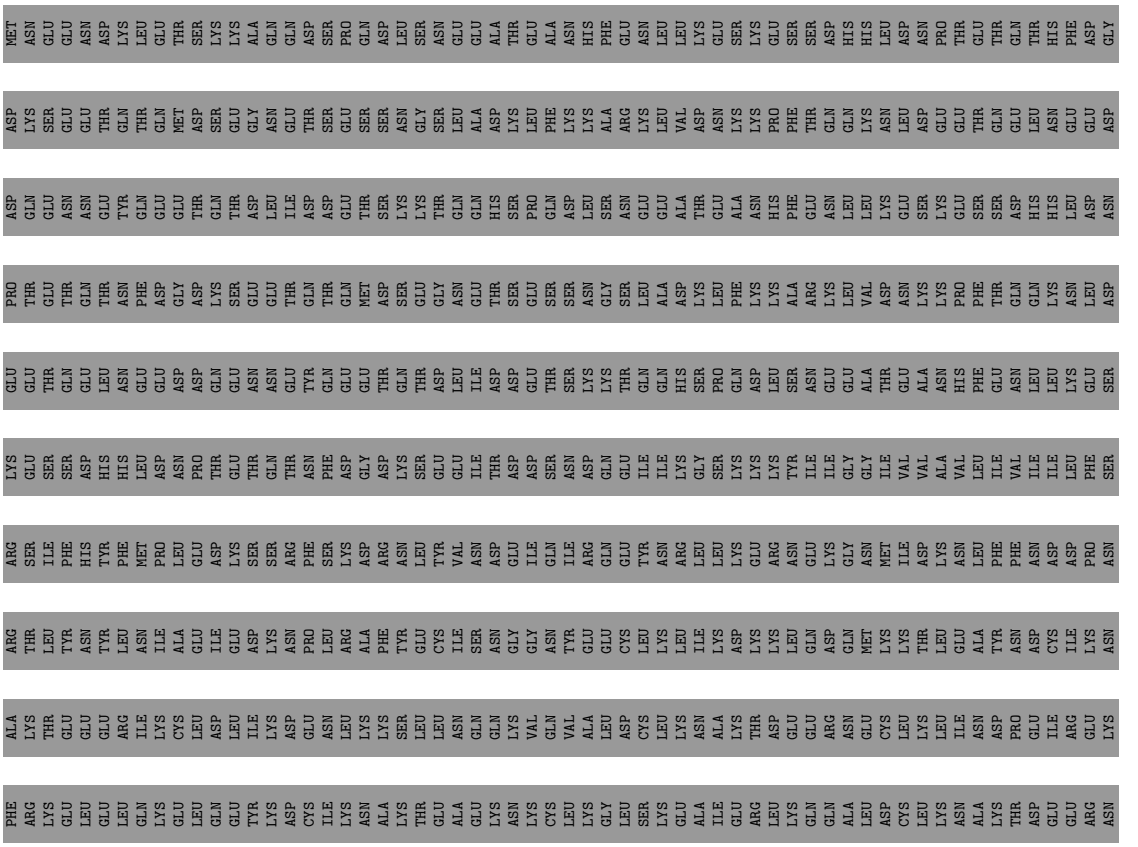
SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLN GLU VAL LYS LYS SER ILE LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ASN GLU LYS GLU LYS GLU CYS

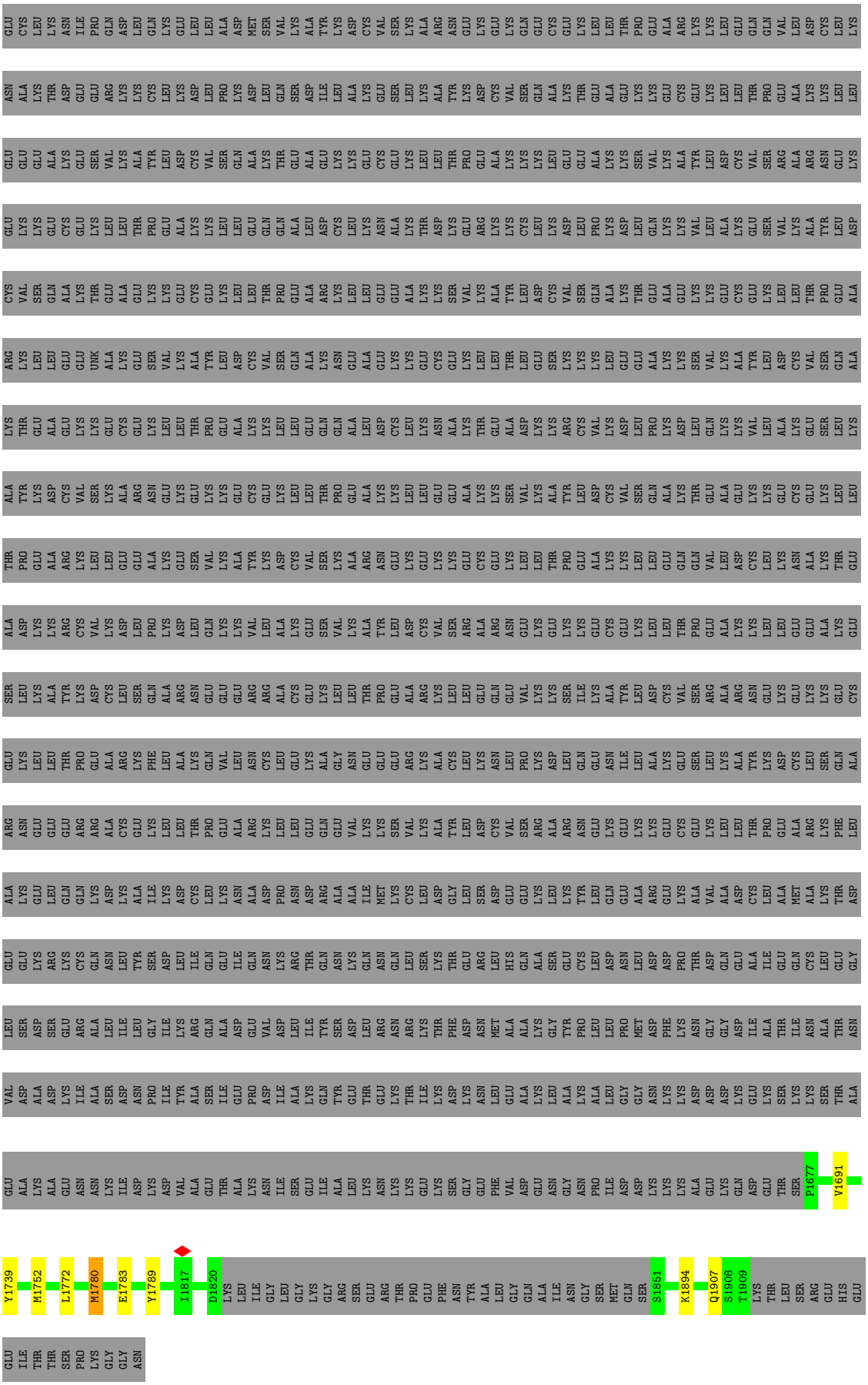
GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU ALA LYS GLN VAL LEU ASN CYS LEU GLU LYS ALA GLY ASN GLU GLU ARG LYS ALA CYS LEU LYS ASN LEU PRO LYS ASP LEU GLN GLU ASN ILE LEU ALA LYS GLU SER LEU LYS ALA TYR LYS ASP CYS LEU SER GLN ALA



• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain CY: 10% 89%

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P1677
V1691

• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain DY:

MET ASN GLU GLU ASN ASP LYS LEU GLU THR SER LYS LYS ALA GLN GLN ASP SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN PRO THR GLU THR GLN THR HIS PHE ASP GLY

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

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

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

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

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

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

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

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

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

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

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

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

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

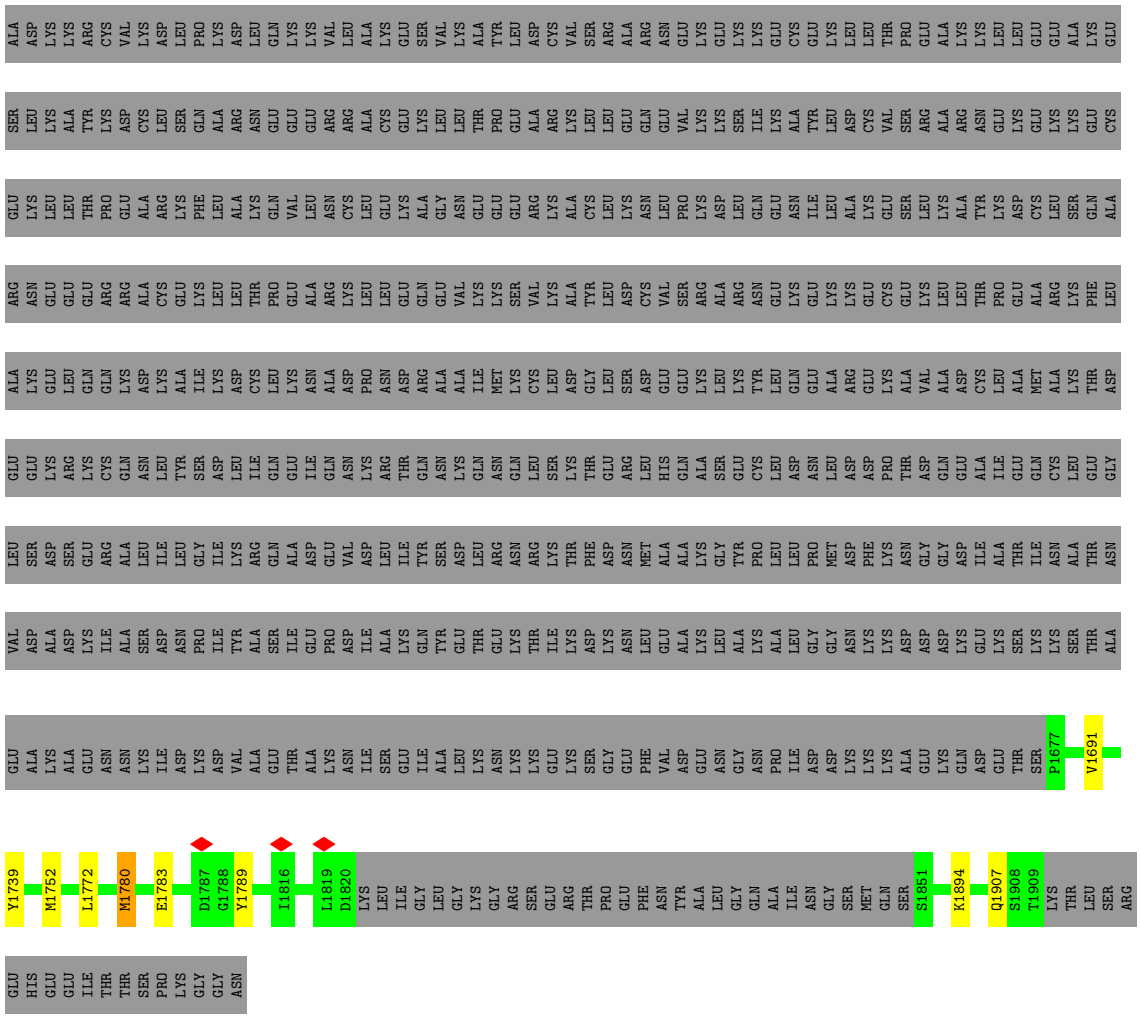
CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

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

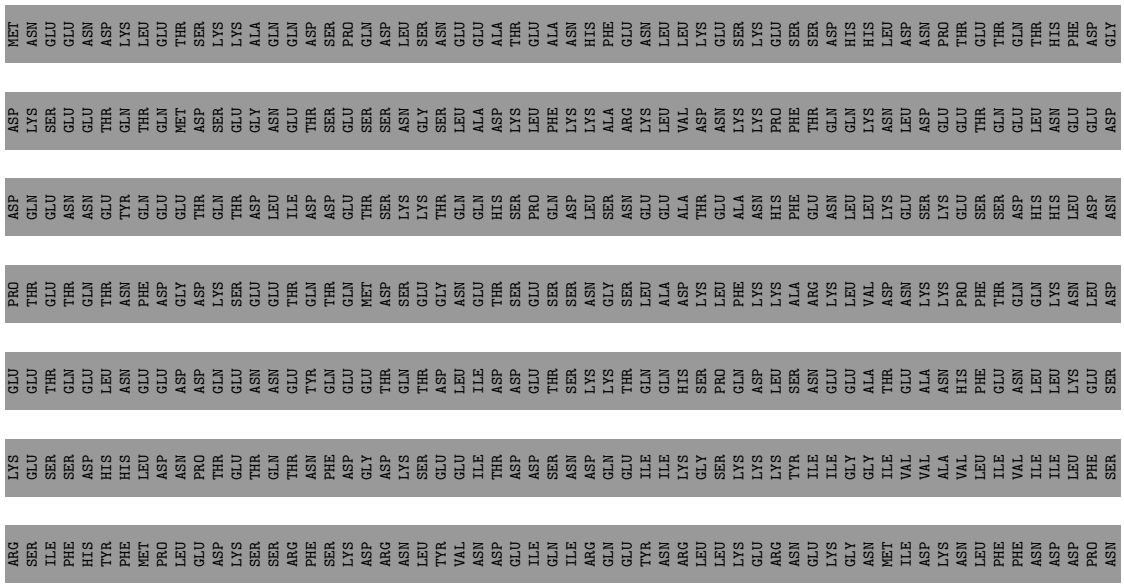
ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU

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



• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain EY: 10% 89%



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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

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

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

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

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

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

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

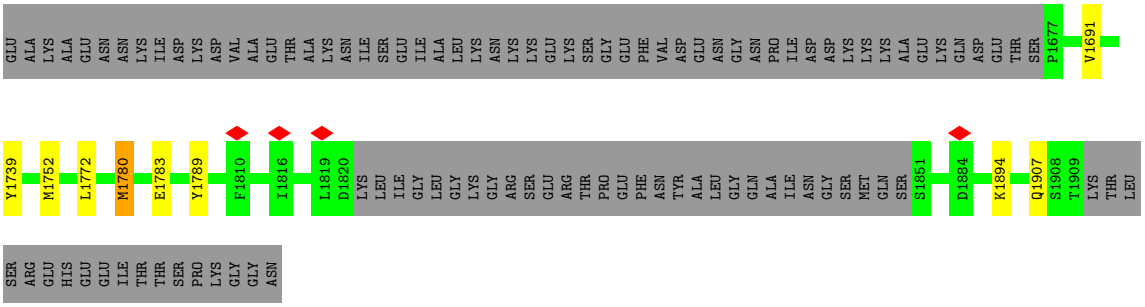
ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLN GLU VAL LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU

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

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

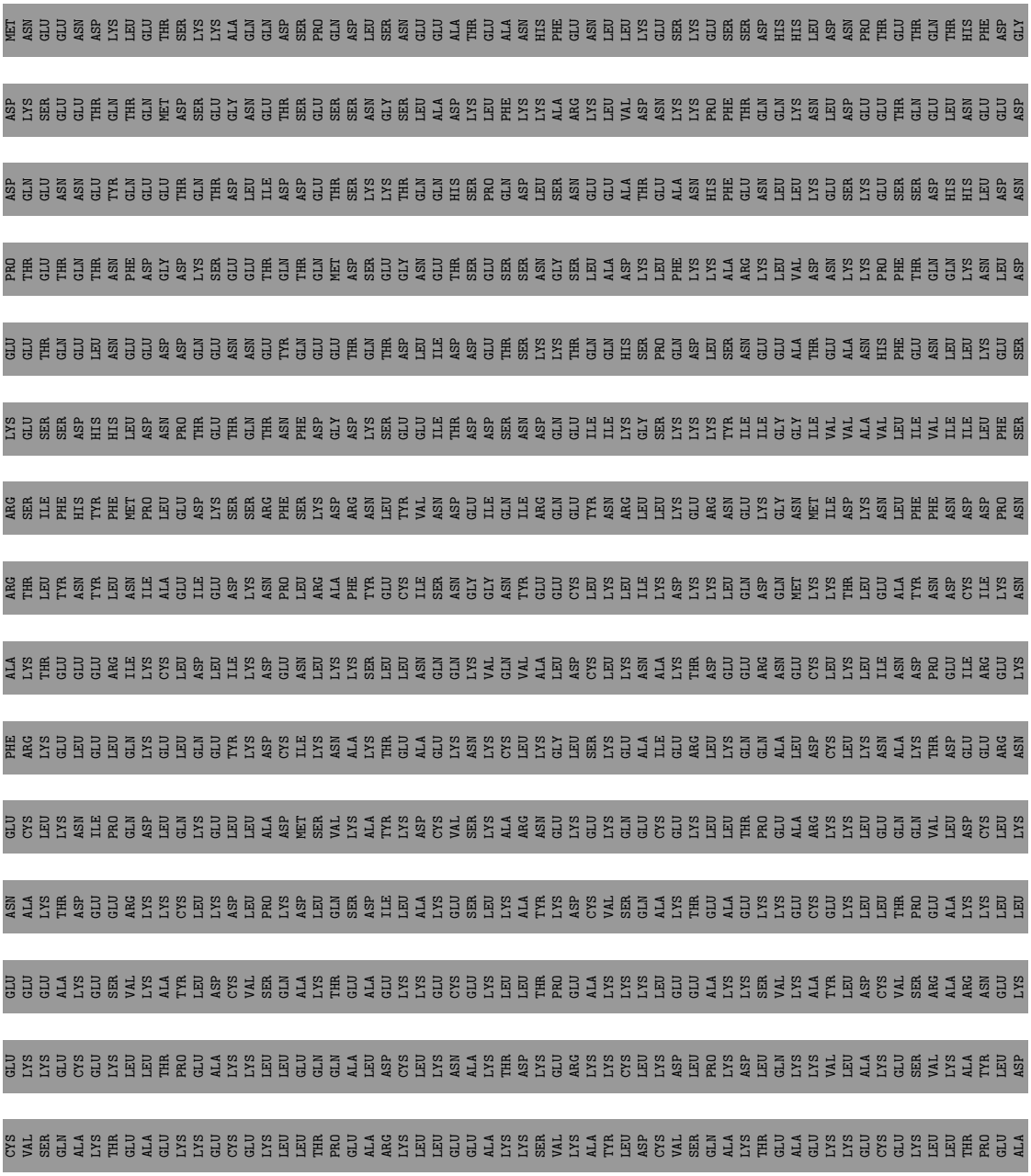
LEU SER ASP SER GLU ARG ALA LEU ILE LEU GLY ILE LYS ARG GLN ALA ASP GLU VAL ASP LEU ILE TYR SER ASP LEU ARG ASN ARG LYS THR PHE ASP ASN MET ALA ALA LYS GLY TYR PRO LEU LEU PRO MET ASP PHE LYS ASN GLY GLY ASP ILE ALA THR ILE ASN ALA THR ASN

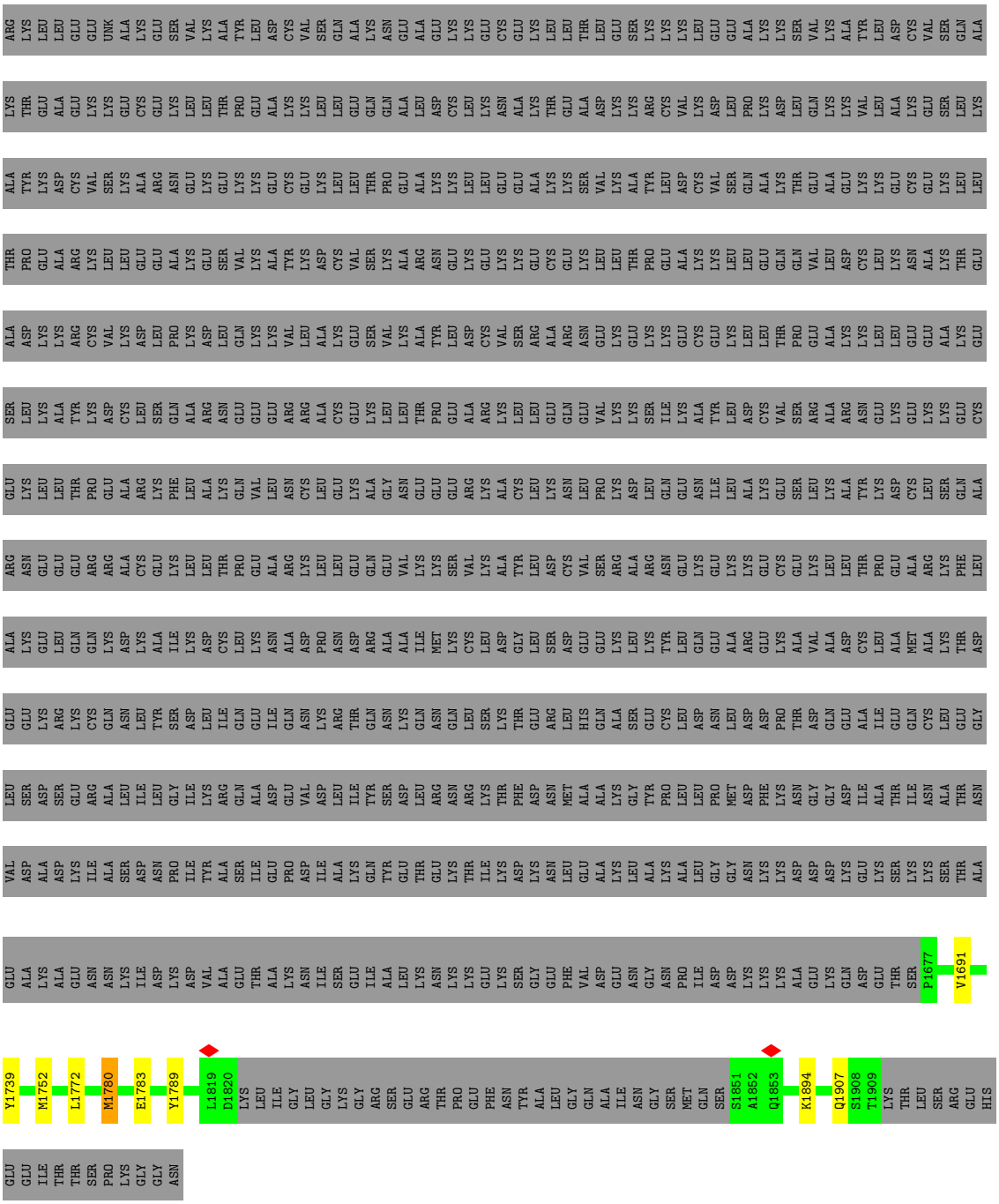
VAL ASP ALA ASP LYS ILE ALA SER ASP ASN PRO ILE TYR ALA SER ILE GLU PRO ASP ILE ALA LYS GLN TYR GLU THR GLU LYS THR ILE LYS ASP LYS ASN LEU GLU ALA LYS LEU ALA LYS ALA LEU GLY GLY ASN LYS LYS ASP ASP ASP LYS GLU LYS SER LYS LYS SER THR ALA



• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain FY: 10% 89%





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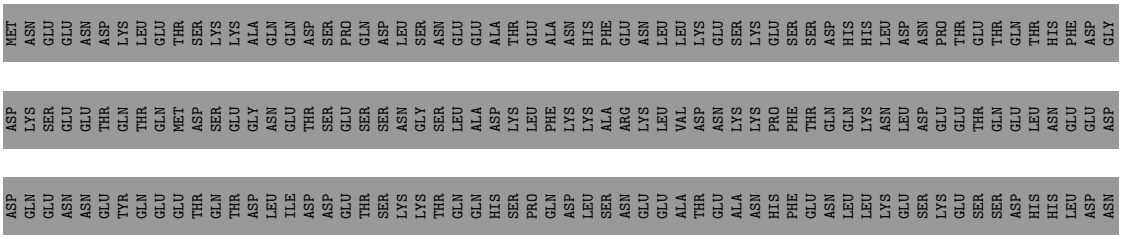

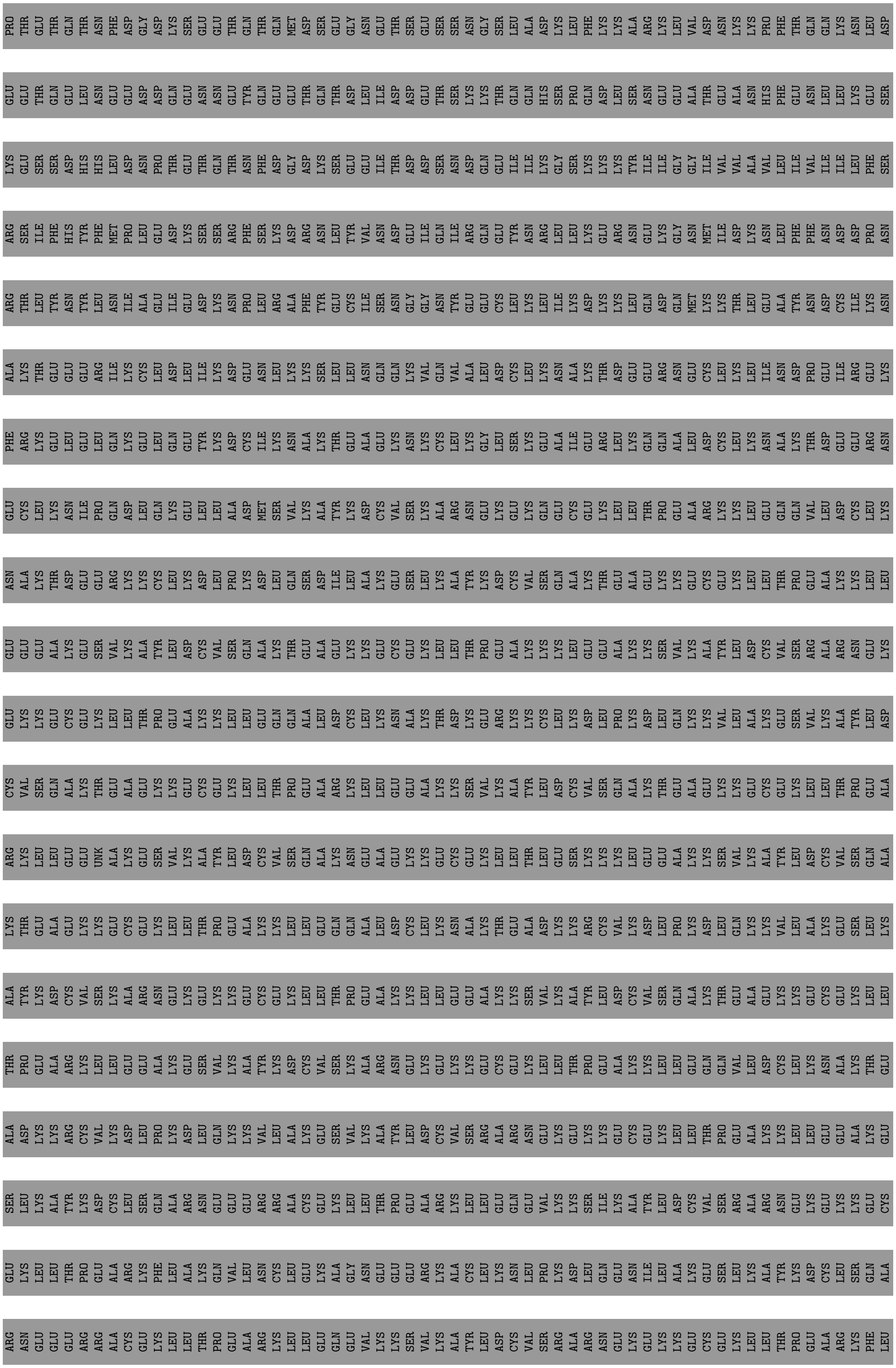
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GLU GLU THR GLN GLU LEU ASN GLU GLU ASP ASP GLN GLU ASN ASN GLU TYR GLN GLU GLU THR GLN THR ASP LEU ILE ASP ASP GLU THR SER LYS LYS THR GLN GLN HIS SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER
LYS GLU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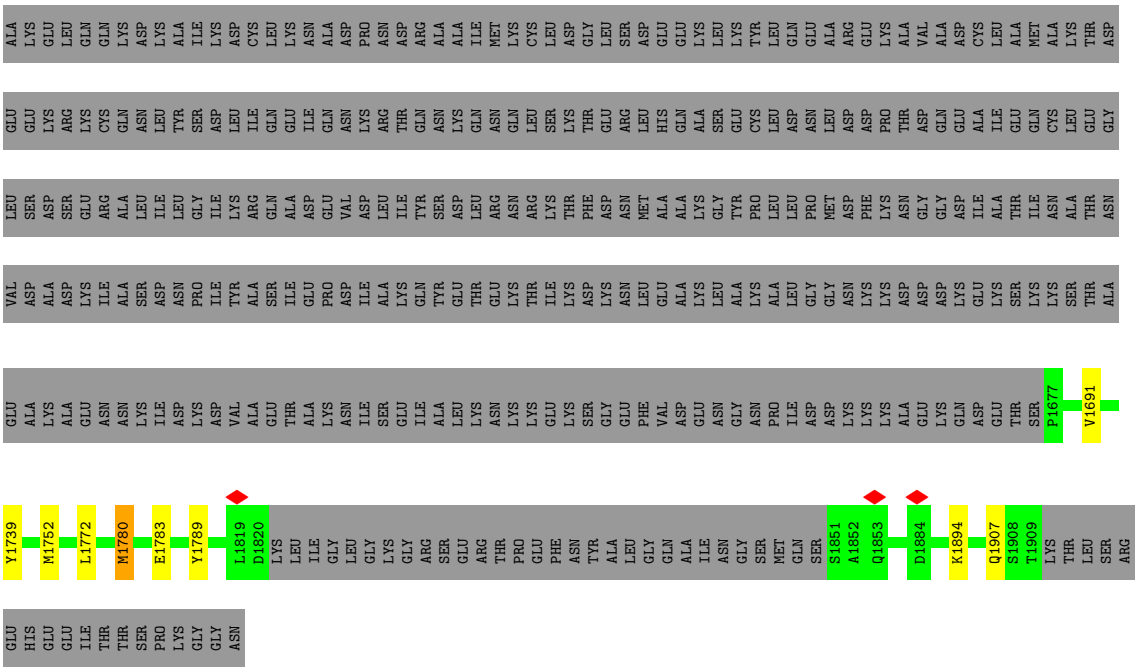
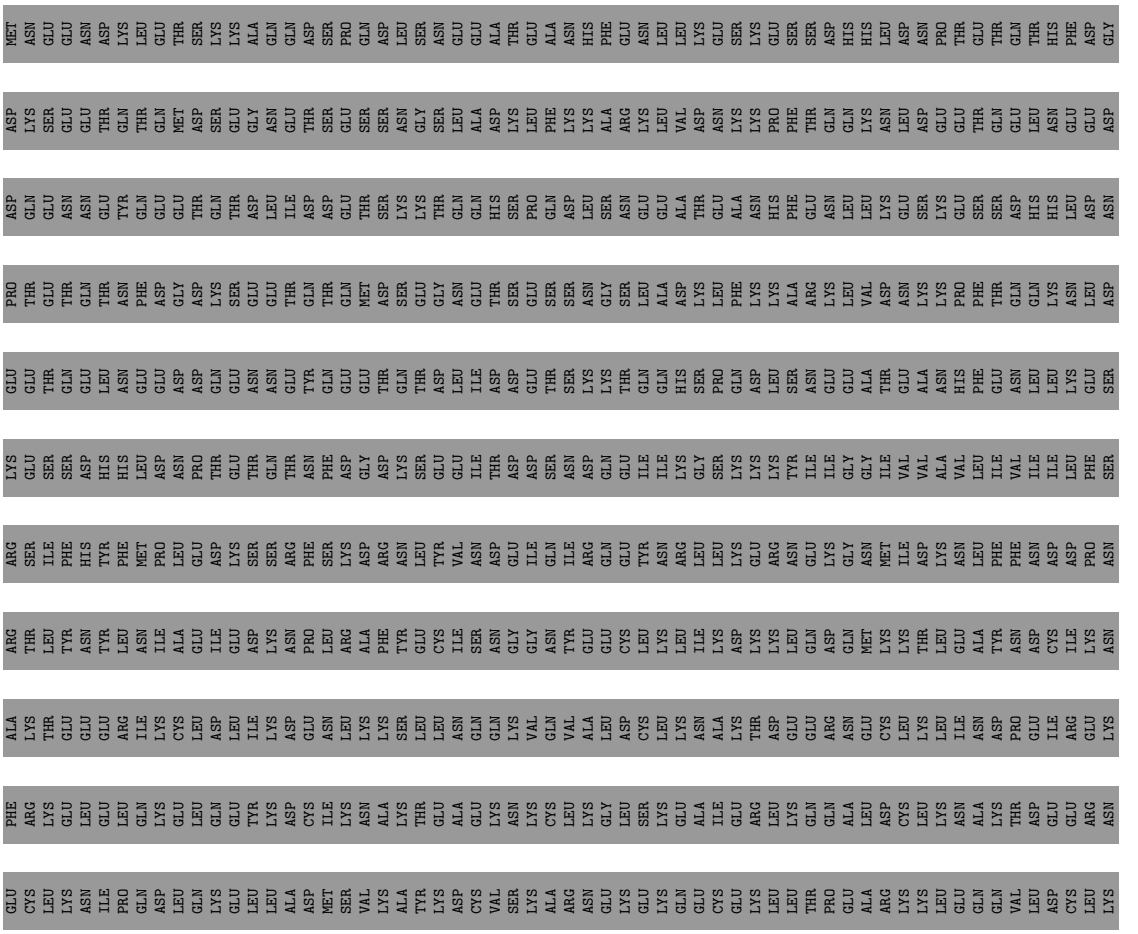
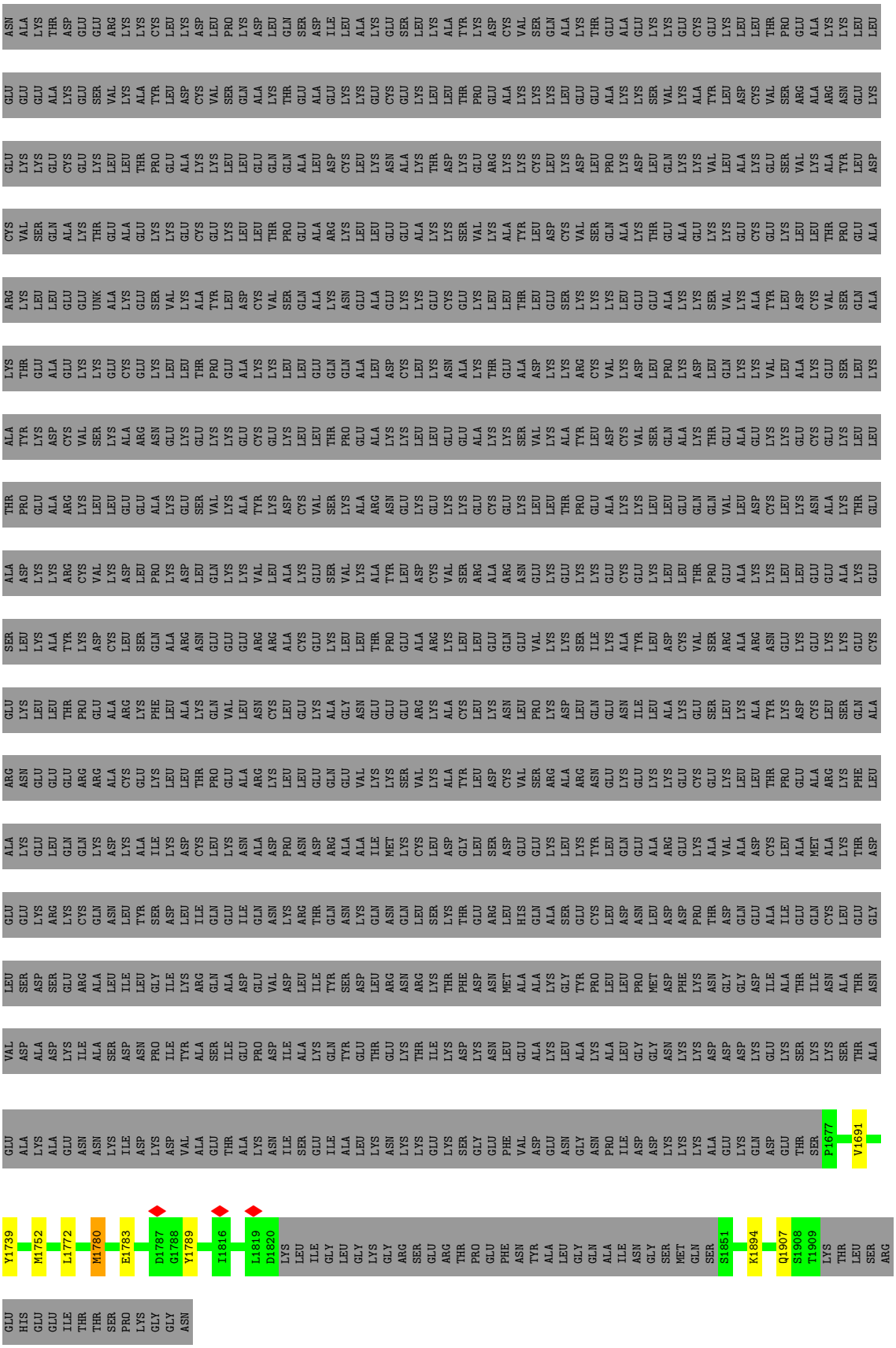
ALA TYR LYS ASP CYS VAL SER LYS ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU
THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS GLU SER VAL LYS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



- Molecule 6: Cag pathogenicity island protein (Cag7)

Chain HY: 10% 89%





- Molecule 6: Cag pathogenicity island protein (Cag7)

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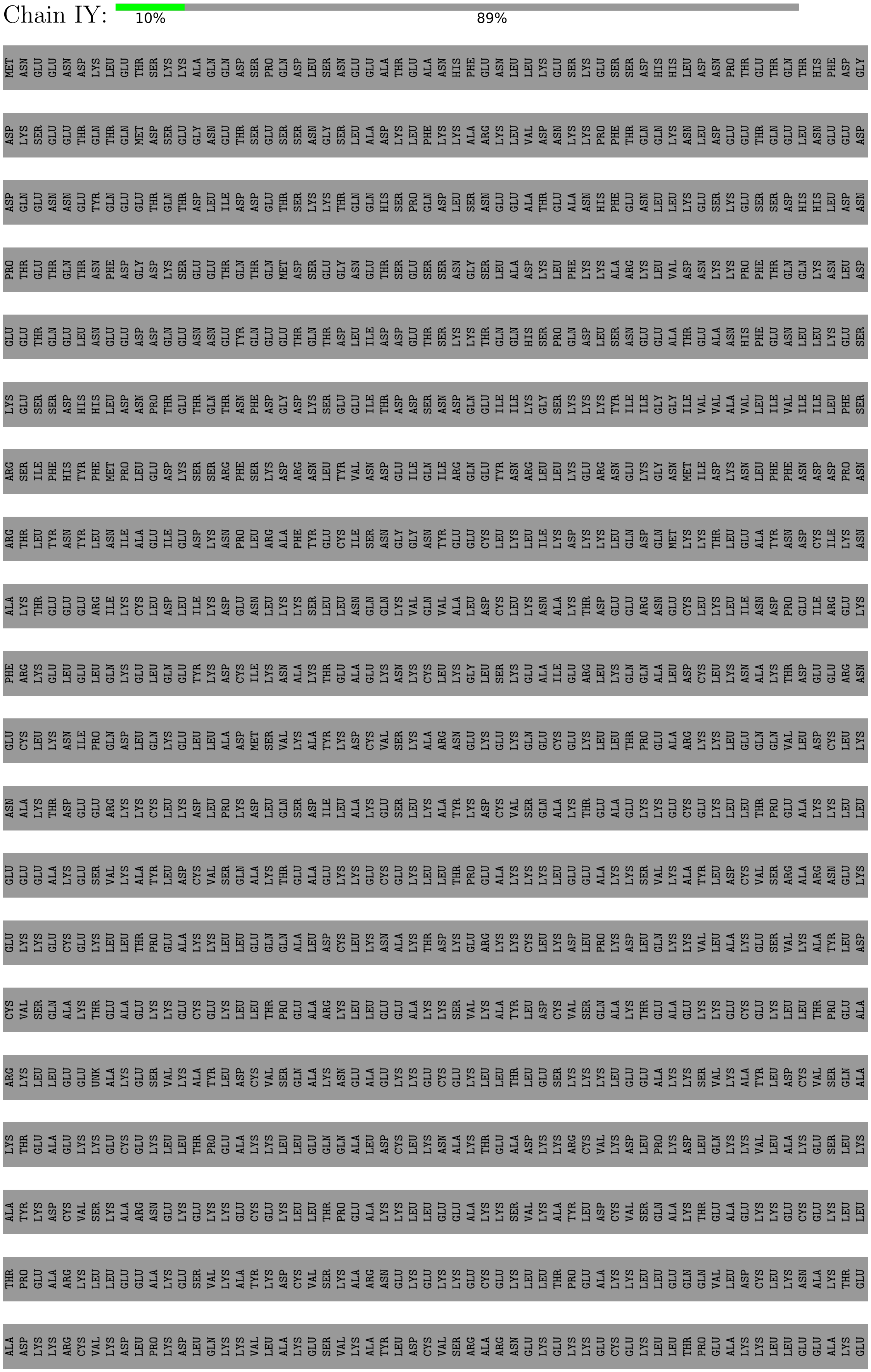

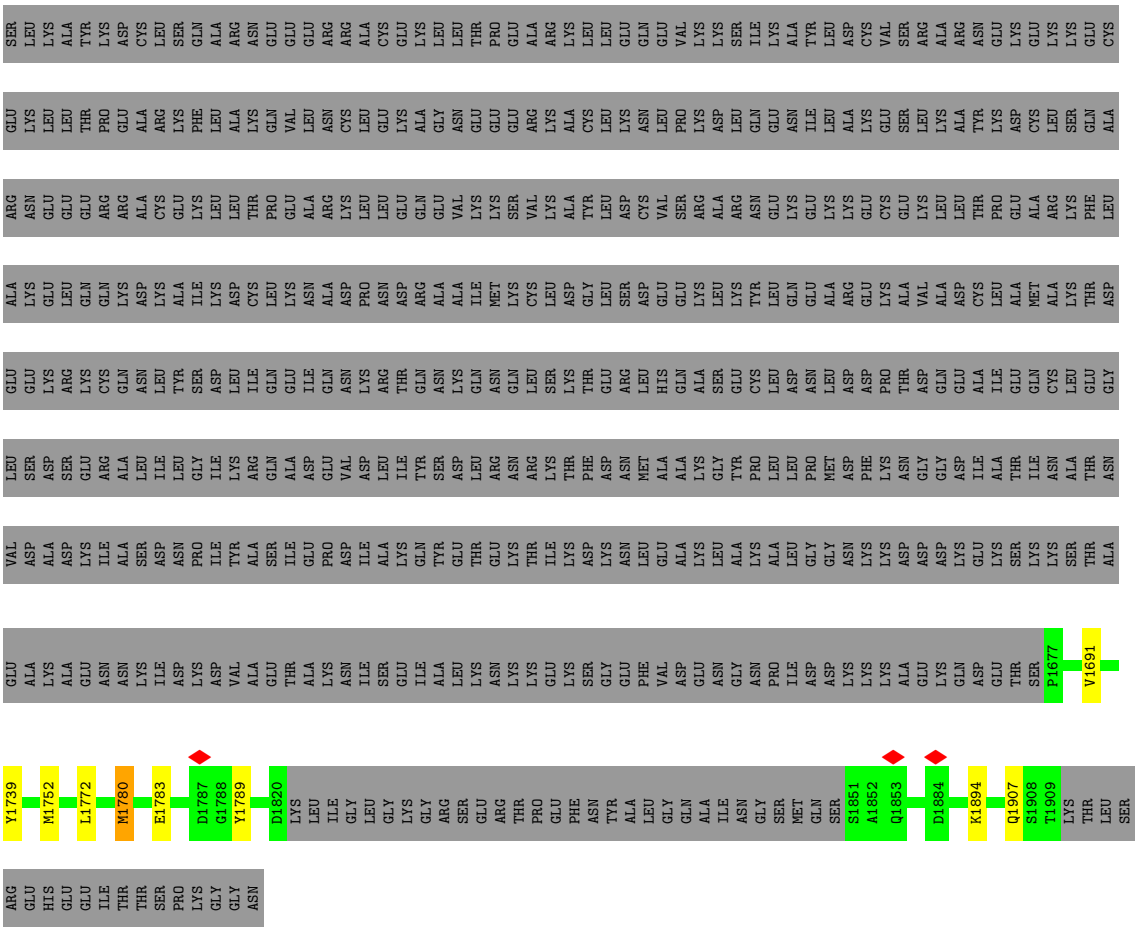

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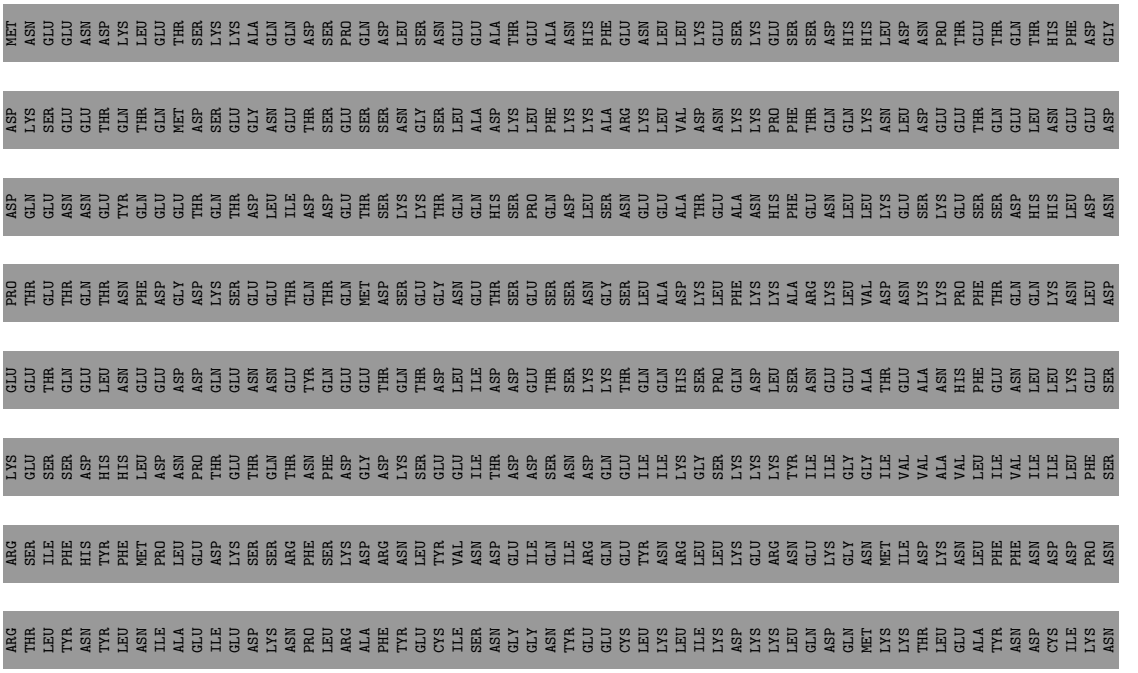

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ILE	LEU	LEU	ASP	GLN	LYS	ASN	ALA	CYS	LYS	CYS	LYS	LEU	ALA	LYS	LYS	ALA	LEU	LYS	GLU
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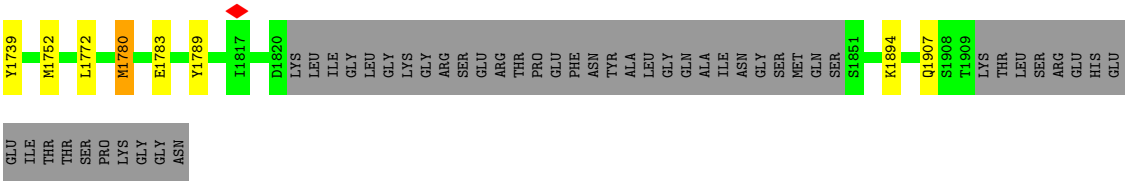
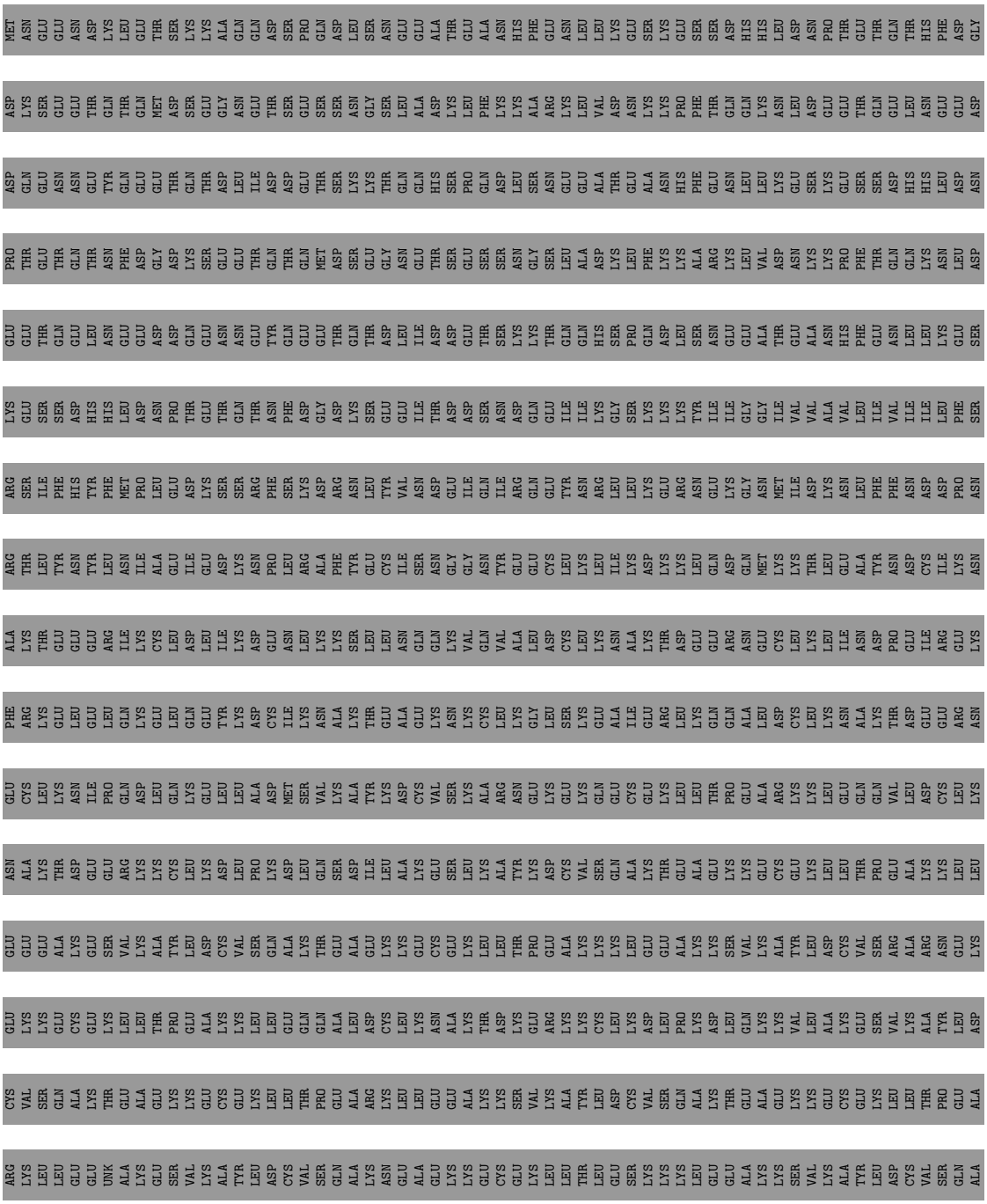
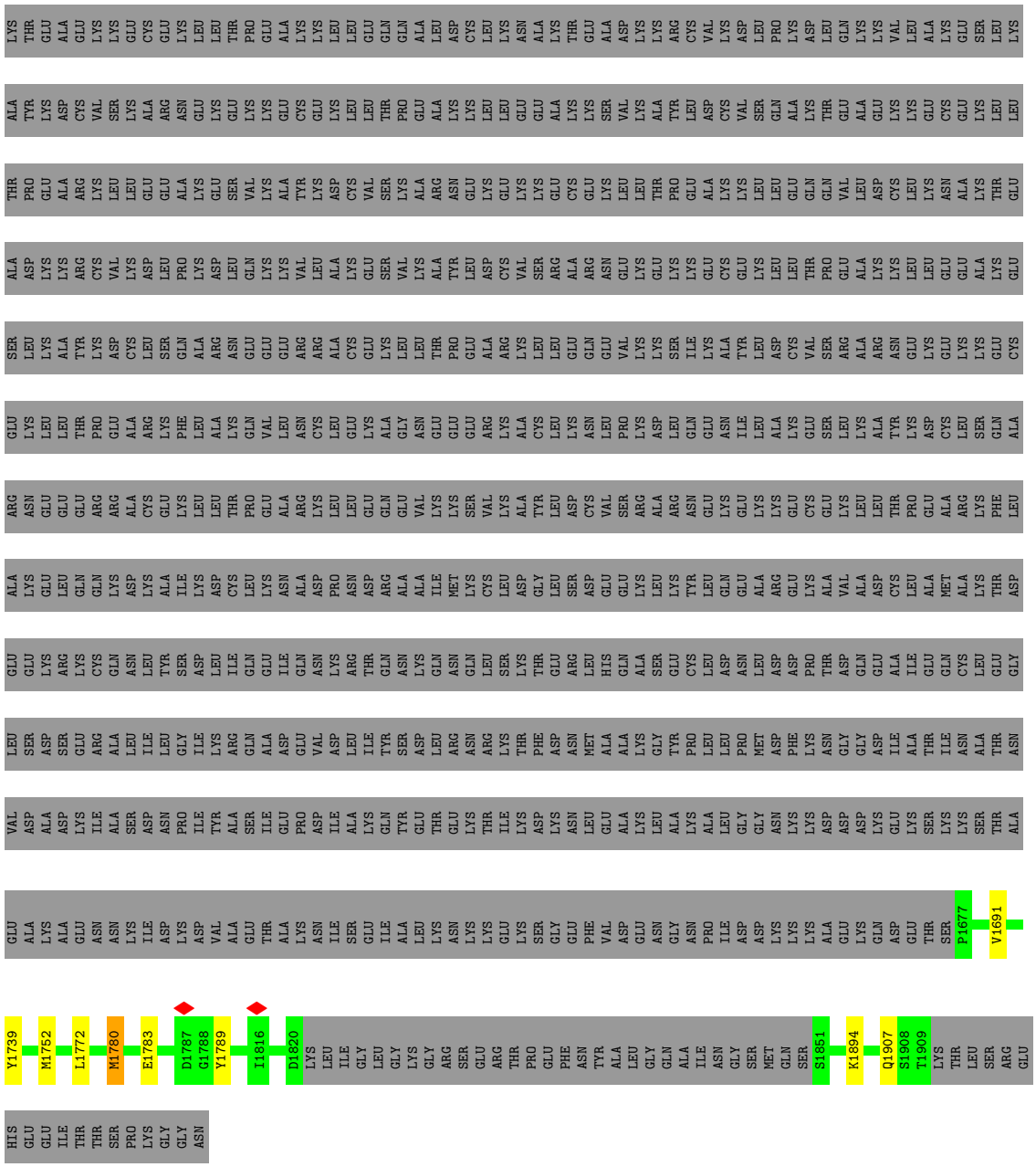
LYS	LYS	PHE	ASP	GLU	GLU	LYS	CYS	LEU	GLU	ALA	LYS	LYS	ALA	LYS	LYS	GLU	ALA	LEU	GLU
LYS	LYS	LYS	PRO	LYS	CYS	GLU	VAL	THR	GLN	LYS	ASP	LYS	GLU	LYS	ALA	CYS	ARG	ASP	CYS
ALA	ASP	ASN	THR	ALA	GLU	SER	SER	PRO	GLN	THR	LEU	SER	LYS	VAL	TYR	GLU	LYS	CYS	LEU
GLU	ASP	GLY	ASP	VAL	LYS	LEU	ARG	GLU	VAL	GLU	GLN	VAL	LYS	LEU	LEU	LYS	LYS	LEU	LYS
LYS	ASP	GLY	GLN	ALA	LEU	LYS	ALA	ALA	LEU	ALA	LYS	LYS	GLU	ALA	ASP	LEU	LEU	LYS	LEU
GLN	LYS	ASP	GLU	ASP	LEU	ALA	ARG	LYS	ASP	GLU	LYS	ALA	CYS	LYS	CYS	LEU	GLU	ASN	ILE
ASP	GLU	ILE	ALA	CYS	THR	TYR	ASN	LYS	CYS	LYS	VAL	TYR	GLU	GLU	VAL	THR	GLN	ALA	ASN
GLU	LYS	ALA	ILE	LEU	PRO	LYS	GLU	LEU	LEU	LYS	LEU	LEU	LYS	SER	SER	PRO	GLN	LYS	ASP
THR	SER	THR	GLU	ALA	GLU	ASP	LYS	LEU	LYS	GLU	ALA	ASP	LEU	VAL	ARG	GLU	VAL	THR	PRO
SER	LYS	ILE	GLN	MET	ALA	CYS	GLU	GLU	ASN	CYS	LYS	CYS	LEU	LYS	ALA	ALA	ALA	ASP	GLU
P1677	LYS	ASN	CYS	ALA	ARG	LEU	LYS	GLU	ALA	GLU	GLU	VAL	THR	ALA	ARG	LYS	LEU	ASP	ILE
	SER	ALA	LEU	LYS	LYS	SER	LYS	ALA	LYS	LYS	SER	SER	PRO	TYR	ASN	LYS	CYS	GLU	ARG
V1691	THR	THR	GLU	THR	PHE	GLN	GLU	LYS	THR	LEU	LEU	GLN	GLU	LEU	GLU	LEU	LEU	ARG	GLU
	ALA	ASN	GLY	ASP	LEU	ALA	CYS	GLU	GLU	LEU	LYS	ALA	ALA	ASP	LYS	LEU	LYS	ASN	LYS



• Molecule 6: Cag pathogenicity island protein (Cag7)

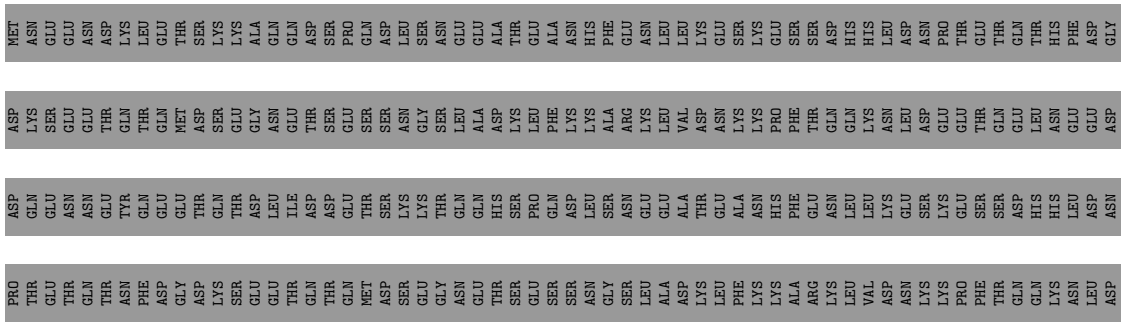
Chain KY: 10% 89%





• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain LY: 10% 89%



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

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

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

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

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

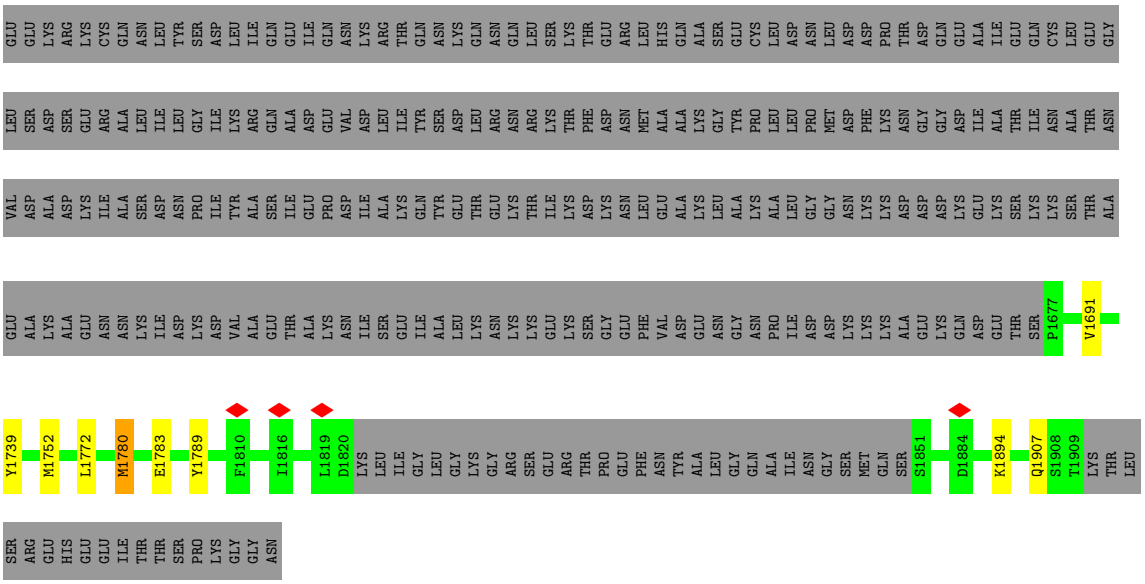
ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS GLU

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

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

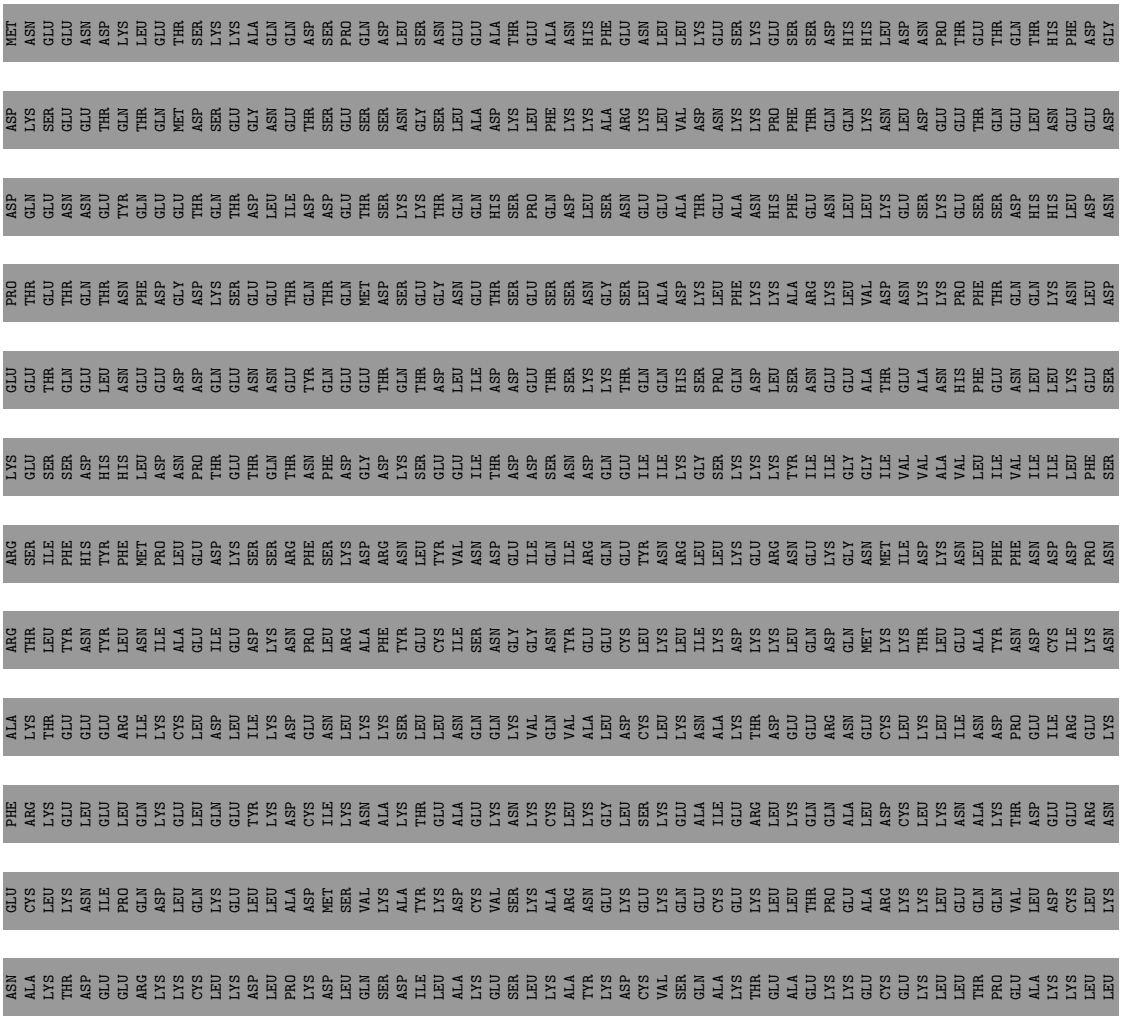
ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLN GLU VAL LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU

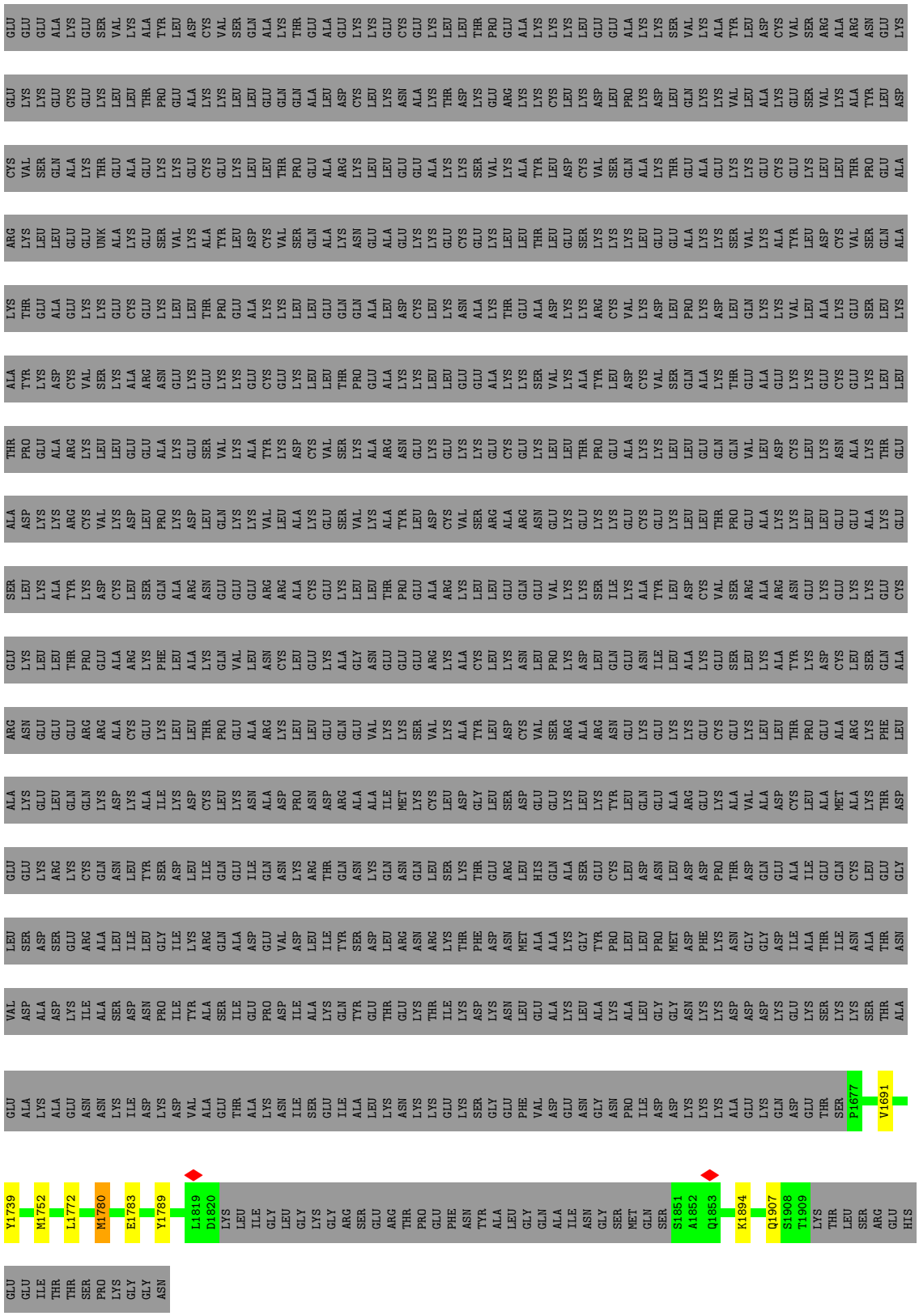
ALA LYS GLU LEU GLN GLN LYS ASP LYS ALA ILE LYS ASP CYS LEU LYS ASN ALA ASP PRO ASN ASP ARG ALA ALA ILE MET LYS CYS LEU ASP GLY LEU SER ASP GLU GLU LYS LEU LYS TYR LEU GLN GLU ALA ARG GLU LYS ALA VAL ALA ASP CYS LEU ALA MET ALA LYS THR ASP



- Molecule 6: Cag pathogenicity island protein (Cag7)

Chain MY: 10% 89%





• Molecule 6: Cag pathogenicity island protein (Cag7)

Chain NY: 10% 89%

MET ASN GLU GLU ASN ASP LYS LEU GLU THR SER LYS LYS ALA GLN GLN ASP SER PRO GLN ASP LEU SER ASN GLU GLU ALA THR GLU ALA ASN HIS PHE GLU ASN LEU LEU LYS GLU SER LYS GLU SER SER ASP HIS HIS LEU ASP ASN PRO THR GLU THR GLN THR HIS PHE ASP GLY

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

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

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

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

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

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

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

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

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

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

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

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

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

CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS THR GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA

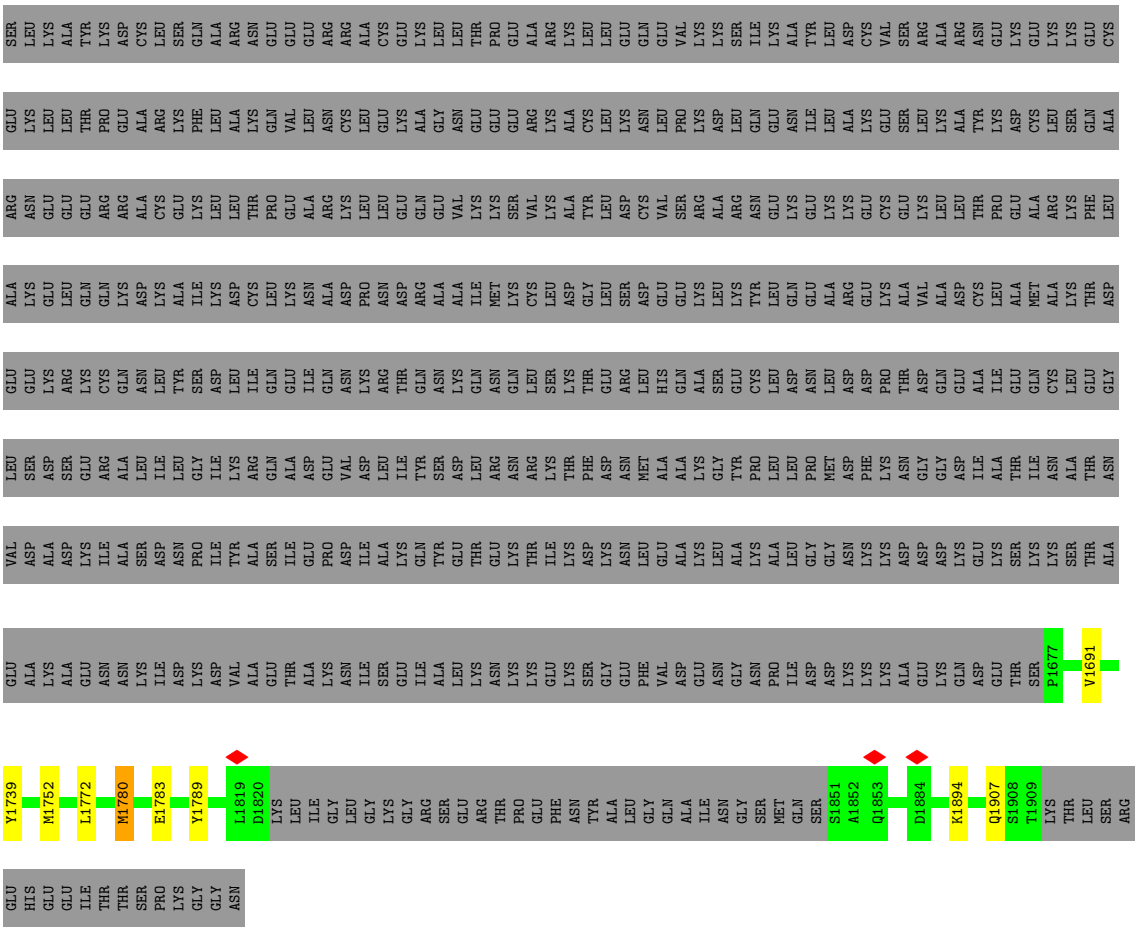
ARG LYS LEU LEU GLU GLU UNK ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA LYS ASN GLU ALA GLU LYS LYS GLU CYS GLU LYS LEU LEU THR LEU GLU SER LYS LYS LEU GLU GLU ALA LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER GLN ALA

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

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

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

ALA ASP LYS LYS ARG CYS VAL LYS ASP LEU PRO LYS ASP LEU GLN LYS LYS VAL LEU ALA LYS GLU SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA LYS LYS LEU LEU GLU GLU ALA LYS GLU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GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU ALA LYS GLN VAL LEU ASN CYS LEU GLU LYS ALA GLY ASN GLU GLU GLU GLU ARG LYS ALA CYS LEU LYS ASN LEU PRO LYS ASP LEU GLN GLU ASN ILE LEU ALA LYS GLU SER LEU LYS ALA TYR LEU GLN GLU LYS SER GLN ALA
ARG ASN GLU GLU GLU ARG ARG ALA CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS LEU LEU GLU GLU GLU VAL LYS LYS SER VAL LYS ALA TYR LEU ASP CYS VAL SER ARG ALA ARG ASN GLU LYS GLU LYS GLU CYS GLU LYS LEU LEU THR PRO GLU ALA ARG LYS PHE LEU
ALA LYS GLU LEU GLN GLN LYS ASP LYS ALA ILE LYS ASP CYS LEU LYS ASN ALA ASP PRO ASN ASP ARG ALA ALA ILE MET LYS CYS LEU ASP GLY LEU SER ASP GLU GLU LYS TYR LEU GLN GLU ALA ARG GLU LYS ALA ALA VAL ALA ASP CYS LEU ALA MET ALA LYS THR ASP
GLU GLU LYS ARG LYS CYS GLN ASN LEU TYR SER ASP LEU ILE GLN GLU ILE GLN ASN LYS GLN ASN GLN LEU SER LYS THR GLU ARG LEU HIS GLN ALA SER GLU CYS LEU ASP ASN LEU ASP ASP PRO THR ASP GLN GLU ALA ILE GLU GLN CYS LEU GLU GLY
LEU SER ASP SER GLU ARG ALA ILE LEU LYS ARG GLN ALA ASP GLU VAL ASP LEU ILE TYR SER ASP LEU ILE LYS THR PHE ASP ASN MET ALA ALA LYS GLY TYR PRO LEU LEU PRO MET ASP PHE LYS ASN GLY GLY ASP ILE ALA THR ASN
VAL ASP ALA ASP LYS ILE ALA SER ASP ASN PRO ILE TYR ALA SER ILE GLU PRO ASP ILE ALA LYS GLN TYR GLU THR GLU LYS THR ILE LYS ASP LYS ASN LEU GLU ALA LYS LEU ALA ALA LEU GLY GLY ASN LYS LYS ASP ASP LYS GLU LYS SER LYS LYS SER THR ALA
GLU ALA LYS ALA GLU ASN ASN LYS ILE ASP LYS ASP VAL ALA GLU THR ALA LYS ASN ILE SER GLU ILE ALA LEU LYS ASN LYS LYS GLU LYS SER GLY GLU PHE VAL ASP GLU ASN GLY ASN PRO ILE ASP ASP LYS LYS LYS ALA GLU LYS GLN ASP GLU THR SER P1677 V1691
Y1739 M1752 L1772 M1780 E1783 Y1789 L1819 D1820 LYS LEU ILE GLY LEU GLY LYS GLY ARG SER GLU ARG THR PRO GLU PHE ASN TYR ALA LEU GLY GLN ALA ILE ASN GLY SER MET GLN SER S1851 A1852 Q1853 D1884 K1894 Q1907 S1908 T1909 LYS THR LEU SER ARG
GLU HIS GLU GLU ILE THR THR SER PRO LYS GLY GLY ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C14	Depositor
Number of particles used	47440	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 ($e^-/Å^2$)	59.2, 59.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	AA	0.50	0/2023	0.83	6/2742 (0.2%)
1	AB	0.56	1/742 (0.1%)	0.87	2/1007 (0.2%)
1	AC	0.58	0/755	0.90	1/1023 (0.1%)
1	AD	0.62	0/793	0.99	2/1073 (0.2%)
1	AE	0.59	1/864 (0.1%)	0.94	3/1170 (0.3%)
1	BA	0.50	0/2023	0.83	6/2742 (0.2%)
1	BB	0.54	1/742 (0.1%)	0.82	1/1007 (0.1%)
1	BC	0.54	0/755	0.90	2/1023 (0.2%)
1	BD	0.69	2/793 (0.3%)	1.11	7/1073 (0.7%)
1	BE	0.52	1/864 (0.1%)	0.83	2/1170 (0.2%)
1	CA	0.50	0/2023	0.83	6/2742 (0.2%)
1	CB	0.73	3/742 (0.4%)	0.92	4/1007 (0.4%)
1	CC	0.55	0/755	0.94	1/1023 (0.1%)
1	CD	0.56	0/793	1.01	4/1073 (0.4%)
1	CE	0.44	0/864	0.92	4/1170 (0.3%)
1	DA	0.50	0/2023	0.83	6/2742 (0.2%)
1	DB	0.81	3/742 (0.4%)	1.04	4/1007 (0.4%)
1	DC	0.56	0/755	0.96	3/1023 (0.3%)
1	DD	0.64	0/793	0.98	4/1073 (0.4%)
1	DE	0.46	0/864	1.01	9/1170 (0.8%)
1	EA	0.50	0/2023	0.83	6/2742 (0.2%)
1	EB	0.73	2/742 (0.3%)	0.99	4/1007 (0.4%)
1	EC	0.55	0/755	0.95	2/1023 (0.2%)
1	ED	0.64	0/793	1.14	7/1073 (0.7%)
1	EE	0.48	0/864	0.93	5/1170 (0.4%)
1	FA	0.50	0/2023	0.83	6/2742 (0.2%)
1	FB	0.71	3/742 (0.4%)	0.95	4/1007 (0.4%)
1	FC	0.65	1/755 (0.1%)	1.03	5/1023 (0.5%)
1	FD	0.68	0/793	1.03	5/1073 (0.5%)
1	FE	0.49	0/864	0.87	5/1170 (0.4%)
1	GA	0.50	0/2023	0.83	6/2742 (0.2%)
1	GB	0.58	1/742 (0.1%)	0.85	0/1007
1	GC	0.63	1/755 (0.1%)	0.95	2/1023 (0.2%)
1	GD	0.57	0/793	1.05	5/1073 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	GE	0.58	1/864 (0.1%)	0.90	5/1170 (0.4%)
1	HA	0.50	0/2023	0.83	6/2742 (0.2%)
1	HB	0.73	2/742 (0.3%)	0.89	3/1007 (0.3%)
1	HC	0.61	1/755 (0.1%)	0.90	1/1023 (0.1%)
1	HD	0.60	1/793 (0.1%)	1.05	5/1073 (0.5%)
1	HE	0.53	1/864 (0.1%)	0.98	7/1170 (0.6%)
1	IA	0.50	0/2023	0.83	6/2742 (0.2%)
1	IB	0.53	1/742 (0.1%)	0.81	1/1007 (0.1%)
1	IC	0.51	0/755	0.85	0/1023
1	ID	0.63	0/793	1.12	8/1073 (0.7%)
1	IE	0.50	0/864	0.85	3/1170 (0.3%)
1	JA	0.50	0/2023	0.83	6/2742 (0.2%)
1	JB	0.75	3/742 (0.4%)	0.93	4/1007 (0.4%)
1	JC	0.56	0/755	0.98	2/1023 (0.2%)
1	JD	0.67	1/793 (0.1%)	1.13	6/1073 (0.6%)
1	JE	0.50	0/864	0.87	4/1170 (0.3%)
1	KA	0.50	0/2023	0.83	6/2742 (0.2%)
1	KB	0.76	2/742 (0.3%)	0.96	2/1007 (0.2%)
1	KC	0.56	1/755 (0.1%)	0.93	4/1023 (0.4%)
1	KD	1.61	7/793 (0.9%)	1.45	10/1073 (0.9%)
1	KE	1.00	4/864 (0.5%)	1.32	14/1170 (1.2%)
1	LA	0.50	0/2023	0.83	6/2742 (0.2%)
1	LB	0.71	2/742 (0.3%)	0.93	2/1007 (0.2%)
1	LC	0.59	0/755	0.98	5/1023 (0.5%)
1	LD	0.60	0/793	1.10	4/1073 (0.4%)
1	LE	0.46	0/864	0.94	6/1170 (0.5%)
1	MA	0.50	0/2023	0.83	6/2742 (0.2%)
1	MB	0.76	2/742 (0.3%)	0.92	3/1007 (0.3%)
1	MC	0.57	0/755	0.95	2/1023 (0.2%)
1	MD	0.71	2/793 (0.3%)	1.10	5/1073 (0.5%)
1	ME	0.61	2/864 (0.2%)	0.91	5/1170 (0.4%)
1	NA	0.50	0/2023	0.83	6/2742 (0.2%)
1	NB	0.62	1/742 (0.1%)	0.90	2/1007 (0.2%)
1	NC	0.55	0/755	0.91	2/1023 (0.2%)
1	ND	0.72	3/793 (0.4%)	1.11	6/1073 (0.6%)
1	NE	0.52	0/864	0.90	4/1170 (0.3%)
2	AM	0.43	0/1507	0.72	4/2019 (0.2%)
2	Am	0.48	2/1496 (0.1%)	0.77	4/2005 (0.2%)
2	BM	0.41	0/1507	0.67	1/2019 (0.0%)
2	Bm	0.41	1/1496 (0.1%)	0.75	4/2005 (0.2%)
2	CM	0.42	0/1507	0.68	3/2019 (0.1%)
2	Cm	0.37	0/1496	0.73	4/2005 (0.2%)
2	DM	0.45	0/1507	0.76	2/2019 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Dm	0.47	0/1496	0.83	6/2005 (0.3%)
2	EM	0.44	0/1507	0.75	2/2019 (0.1%)
2	Em	0.45	1/1496 (0.1%)	0.78	5/2005 (0.2%)
2	FM	0.47	0/1507	0.79	5/2019 (0.2%)
2	Fm	0.49	1/1496 (0.1%)	0.79	5/2005 (0.2%)
2	GM	0.43	0/1507	0.72	5/2019 (0.2%)
2	Gm	0.44	1/1496 (0.1%)	0.83	6/2005 (0.3%)
2	HM	0.42	0/1507	0.71	2/2019 (0.1%)
2	Hm	0.51	2/1496 (0.1%)	0.83	8/2005 (0.4%)
2	IM	0.42	0/1507	0.67	2/2019 (0.1%)
2	Im	0.43	1/1496 (0.1%)	0.77	5/2005 (0.2%)
2	JM	0.42	0/1507	0.68	0/2019
2	Jm	0.41	1/1496 (0.1%)	0.78	4/2005 (0.2%)
2	KM	0.41	0/1507	0.72	3/2019 (0.1%)
2	Km	0.45	0/1496	0.77	3/2005 (0.1%)
2	LM	0.52	2/1507 (0.1%)	0.82	3/2019 (0.1%)
2	Lm	0.46	0/1496	0.81	7/2005 (0.3%)
2	MM	0.49	1/1507 (0.1%)	0.76	3/2019 (0.1%)
2	Mm	0.45	0/1496	0.76	4/2005 (0.2%)
2	NM	0.44	0/1507	0.72	4/2019 (0.2%)
2	Nm	0.47	1/1496 (0.1%)	0.77	5/2005 (0.2%)
3	AT	0.58	0/2115	0.80	10/2847 (0.4%)
3	At	0.49	1/1638 (0.1%)	0.78	5/2203 (0.2%)
3	BT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Bt	0.49	1/1638 (0.1%)	0.78	6/2203 (0.3%)
3	CT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Ct	0.49	1/1638 (0.1%)	0.79	6/2203 (0.3%)
3	DT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Dt	0.49	1/1638 (0.1%)	0.79	6/2203 (0.3%)
3	ET	0.58	0/2115	0.80	10/2847 (0.4%)
3	Et	0.49	1/1638 (0.1%)	0.78	6/2203 (0.3%)
3	FT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Ft	0.49	1/1638 (0.1%)	0.79	6/2203 (0.3%)
3	GT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Gt	0.49	1/1638 (0.1%)	0.78	5/2203 (0.2%)
3	HT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Ht	0.49	1/1638 (0.1%)	0.78	6/2203 (0.3%)
3	IT	0.58	0/2115	0.80	10/2847 (0.4%)
3	It	0.49	1/1638 (0.1%)	0.79	6/2203 (0.3%)
3	JT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Jt	0.49	1/1638 (0.1%)	0.79	6/2203 (0.3%)
3	KT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Kt	0.49	1/1638 (0.1%)	0.78	6/2203 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	LT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Lt	0.49	1/1638 (0.1%)	0.79	6/2203 (0.3%)
3	MT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Mt	0.49	1/1638 (0.1%)	0.78	6/2203 (0.3%)
3	NT	0.58	0/2115	0.80	10/2847 (0.4%)
3	Nt	0.49	1/1638 (0.1%)	0.78	6/2203 (0.3%)
5	AX	0.67	0/1388	0.89	9/1870 (0.5%)
5	BX	0.67	0/1388	0.89	9/1870 (0.5%)
5	CX	0.67	0/1388	0.89	9/1870 (0.5%)
5	DX	0.67	0/1388	0.89	9/1870 (0.5%)
5	EX	0.67	0/1388	0.89	9/1870 (0.5%)
5	FX	0.67	0/1388	0.89	9/1870 (0.5%)
5	GX	0.67	0/1388	0.89	9/1870 (0.5%)
5	HX	0.67	0/1388	0.89	9/1870 (0.5%)
5	IX	0.67	0/1388	0.89	9/1870 (0.5%)
5	JX	0.67	0/1388	0.89	9/1870 (0.5%)
5	KX	0.67	0/1388	0.89	9/1870 (0.5%)
5	LX	0.67	0/1388	0.89	9/1870 (0.5%)
5	MX	0.67	0/1388	0.89	9/1870 (0.5%)
5	NX	0.67	0/1388	0.89	9/1870 (0.5%)
6	AY	0.64	0/1553	0.75	3/2106 (0.1%)
6	BY	0.64	0/1553	0.75	3/2106 (0.1%)
6	CY	0.64	0/1553	0.76	3/2106 (0.1%)
6	DY	0.64	0/1553	0.75	3/2106 (0.1%)
6	EY	0.64	0/1553	0.75	3/2106 (0.1%)
6	FY	0.64	0/1553	0.75	3/2106 (0.1%)
6	GY	0.64	0/1553	0.75	3/2106 (0.1%)
6	HY	0.64	0/1553	0.75	3/2106 (0.1%)
6	IY	0.64	0/1553	0.75	3/2106 (0.1%)
6	JY	0.64	0/1553	0.75	3/2106 (0.1%)
6	KY	0.64	0/1553	0.75	3/2106 (0.1%)
6	LY	0.64	0/1553	0.76	3/2106 (0.1%)
6	MY	0.64	0/1553	0.75	3/2106 (0.1%)
6	NY	0.64	0/1553	0.75	3/2106 (0.1%)
All	All	0.57	85/208236 (0.0%)	0.84	805/280910 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AD	0	2
1	AE	0	1
1	BA	0	3
1	BD	0	2
1	CA	0	3
1	CB	0	1
1	CD	0	1
1	DA	0	3
1	DB	0	1
1	EA	0	3
1	ED	0	1
1	EE	0	1
1	FA	0	3
1	FB	0	1
1	FE	0	1
1	GA	0	3
1	GC	0	1
1	GD	0	2
1	GE	0	1
1	HA	0	3
1	HB	0	1
1	HD	0	2
1	IA	0	3
1	JA	0	3
1	JB	0	1
1	JD	0	2
1	KA	0	3
1	KB	0	1
1	KD	0	2
1	KE	0	2
1	LA	0	3
1	LB	0	1
1	LD	0	1
1	MA	0	3
1	MB	0	1
1	MD	0	1
1	ME	0	1
1	NA	0	3
1	NC	0	1
1	ND	0	1
1	NE	0	1
2	Am	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Bm	0	2
2	Cm	0	1
2	Dm	0	1
2	Em	0	1
2	Fm	0	1
2	Gm	0	1
2	Hm	0	1
2	Im	0	1
2	Jm	0	1
2	Km	0	1
2	LM	0	1
2	Lm	0	1
2	Mm	0	1
2	Nm	0	1
5	AX	0	1
5	BX	0	1
5	CX	0	1
5	DX	0	1
5	EX	0	1
5	FX	0	1
5	GX	0	1
5	HX	0	1
5	IX	0	1
5	JX	0	1
5	KX	0	1
5	LX	0	1
5	MX	0	1
5	NX	0	1
All	All	0	107

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	KD	81	TYR	CE2-CZ	21.33	1.66	1.38
1	KD	81	TYR	CD2-CE2	21.19	1.71	1.39
1	KD	81	TYR	CG-CD2	18.52	1.63	1.39
1	KE	107	TYR	CB-CG	16.40	1.76	1.51
1	KD	81	TYR	CG-CD1	-14.30	1.20	1.39
1	KE	107	TYR	CE1-CZ	-12.74	1.22	1.38
1	KD	81	TYR	CE1-CZ	-11.45	1.23	1.38
1	HB	121	GLU	CB-CG	-11.32	1.30	1.52
1	JB	121	GLU	CB-CG	-11.29	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	MB	121	GLU	CB-CG	-11.21	1.30	1.52
1	CB	121	GLU	CB-CG	-11.05	1.31	1.52
1	EB	121	GLU	CB-CG	-10.58	1.32	1.52
1	KB	121	GLU	CB-CG	-10.15	1.32	1.52
1	DB	121	GLU	CB-CG	-10.07	1.33	1.52
1	LB	121	GLU	CB-CG	-10.05	1.33	1.52
1	FB	121	GLU	CB-CG	-9.49	1.34	1.52
2	Nm	222	TYR	CD2-CE2	-9.41	1.25	1.39
1	MB	121	GLU	CG-CD	-9.24	1.38	1.51
1	ME	107	TYR	CE2-CZ	-9.21	1.26	1.38
1	HB	121	GLU	CG-CD	-9.02	1.38	1.51
1	KB	121	GLU	CG-CD	-8.54	1.39	1.51
1	KE	107	TYR	CG-CD2	8.51	1.50	1.39
1	DB	121	GLU	CG-CD	-8.34	1.39	1.51
1	LB	121	GLU	CG-CD	-8.08	1.39	1.51
1	JB	121	GLU	CG-CD	-8.07	1.39	1.51
1	CB	121	GLU	CG-CD	-7.98	1.40	1.51
1	KD	81	TYR	CZ-OH	7.76	1.51	1.37
2	Hm	222	TYR	CD2-CE2	-7.71	1.27	1.39
1	FB	121	GLU	CG-CD	-7.66	1.40	1.51
1	EB	121	GLU	CG-CD	-7.61	1.40	1.51
1	HD	105	TYR	CD1-CE1	-7.60	1.27	1.39
1	NB	121	GLU	CD-OE1	-7.39	1.17	1.25
1	KE	107	TYR	CD1-CE1	7.38	1.50	1.39
1	GB	121	GLU	CD-OE1	-7.37	1.17	1.25
1	AB	121	GLU	CD-OE1	-7.33	1.17	1.25
1	JD	178	PHE	CD1-CE1	-6.99	1.25	1.39
1	MD	178	PHE	CD1-CE1	-6.84	1.25	1.39
1	GE	107	TYR	CD2-CE2	-6.70	1.29	1.39
1	ND	126	LYS	CE-NZ	-6.68	1.32	1.49
1	KD	81	TYR	CB-CG	6.68	1.61	1.51
1	BE	107	TYR	CE1-CZ	-6.48	1.30	1.38
2	Fm	222	TYR	CD2-CE2	-6.35	1.29	1.39
2	LM	344	LYS	CD-CE	-6.33	1.35	1.51
1	ND	126	LYS	CD-CE	-6.33	1.35	1.51
1	ME	107	TYR	CG-CD2	-6.16	1.31	1.39
1	BD	169	GLU	CD-OE2	-6.12	1.19	1.25
2	Gm	222	TYR	CD2-CE2	-6.08	1.30	1.39
1	DB	150	TYR	CD2-CE2	-5.97	1.30	1.39
2	Hm	273	PHE	CB-CG	-5.92	1.41	1.51
1	FC	146	VAL	CB-CG1	-5.85	1.40	1.52
1	GC	150	TYR	CD1-CE1	-5.77	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HE	107	TYR	CE2-CZ	-5.68	1.31	1.38
1	MD	105	TYR	CD1-CE1	-5.62	1.30	1.39
2	Em	222	TYR	CD2-CE2	-5.58	1.30	1.39
2	Bm	222	TYR	CD2-CE2	-5.55	1.31	1.39
1	JB	121	GLU	CD-OE2	-5.48	1.19	1.25
1	KC	181	VAL	C-N	5.40	1.44	1.34
2	Am	362	VAL	CB-CG2	-5.39	1.41	1.52
1	IB	121	GLU	CD-OE1	-5.34	1.19	1.25
1	BD	169	GLU	CD-OE1	-5.32	1.19	1.25
1	BB	121	GLU	CD-OE1	-5.31	1.19	1.25
2	MM	344	LYS	CE-NZ	-5.25	1.35	1.49
1	AE	128	ARG	CB-CG	-5.23	1.38	1.52
3	Jt	80	VAL	CB-CG1	-5.18	1.42	1.52
3	Dt	80	VAL	CB-CG1	-5.17	1.42	1.52
3	Kt	80	VAL	CB-CG1	-5.17	1.42	1.52
3	Et	80	VAL	CB-CG1	-5.17	1.42	1.52
3	Lt	80	VAL	CB-CG1	-5.17	1.42	1.52
3	Ct	80	VAL	CB-CG1	-5.16	1.42	1.52
3	Ft	80	VAL	CB-CG1	-5.16	1.42	1.52
3	Mt	80	VAL	CB-CG1	-5.16	1.42	1.52
1	ND	178	PHE	CD1-CE1	-5.15	1.28	1.39
3	It	80	VAL	CB-CG1	-5.15	1.42	1.52
2	Im	362	VAL	CB-CG2	-5.15	1.42	1.52
3	Bt	80	VAL	CB-CG1	-5.14	1.42	1.52
3	At	80	VAL	CB-CG1	-5.14	1.42	1.52
2	Jm	222	TYR	CD2-CE2	-5.14	1.31	1.39
3	Gt	80	VAL	CB-CG1	-5.14	1.42	1.52
1	HC	181	VAL	C-N	5.14	1.44	1.34
1	CB	121	GLU	CD-OE2	-5.13	1.20	1.25
1	FB	121	GLU	CD-OE2	-5.13	1.20	1.25
3	Nt	80	VAL	CB-CG1	-5.12	1.42	1.52
3	Ht	80	VAL	CB-CG1	-5.12	1.42	1.52
2	LM	341	MET	CA-CB	5.10	1.65	1.53
2	Am	273	PHE	CB-CG	-5.02	1.42	1.51

All (805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	KE	107	TYR	CB-CG-CD1	19.20	132.52	121.00
1	KD	81	TYR	CB-CG-CD2	16.50	130.90	121.00
2	LM	344	LYS	CD-CE-NZ	-15.77	75.43	111.70
1	KD	81	TYR	CZ-CE2-CD2	-14.49	106.76	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	KD	81	TYR	CD1-CE1-CZ	14.21	132.59	119.80
1	ND	143	LEU	CB-CG-CD1	-14.15	86.94	111.00
1	KE	107	TYR	CA-CB-CG	14.11	140.22	113.40
1	KD	81	TYR	CA-CB-CG	13.19	138.47	113.40
1	KD	81	TYR	CB-CG-CD1	-12.25	113.65	121.00
1	LD	143	LEU	CB-CG-CD2	-11.82	90.90	111.00
1	JD	143	LEU	CB-CG-CD2	-11.60	91.29	111.00
1	CD	143	LEU	CB-CG-CD1	-11.48	91.49	111.00
1	CE	110	ASP	CB-CG-OD1	11.35	128.51	118.30
1	DE	82	ASP	CB-CG-OD1	11.12	128.31	118.30
1	KE	107	TYR	CD1-CG-CD2	-11.09	105.70	117.90
2	Dm	286	LEU	CA-CB-CG	11.02	140.64	115.30
1	ID	143	LEU	CB-CG-CD2	-10.98	92.34	111.00
1	JD	143	LEU	CA-CB-CG	10.88	140.32	115.30
1	BD	143	LEU	CB-CG-CD2	-10.85	92.56	111.00
1	ED	143	LEU	CB-CG-CD2	-10.63	92.92	111.00
5	LX	410	ARG	NE-CZ-NH2	10.63	125.62	120.30
5	HX	410	ARG	NE-CZ-NH2	10.62	125.61	120.30
5	MX	410	ARG	NE-CZ-NH2	10.61	125.61	120.30
5	NX	410	ARG	NE-CZ-NH2	10.61	125.61	120.30
5	EX	410	ARG	NE-CZ-NH2	10.59	125.59	120.30
5	JX	410	ARG	NE-CZ-NH2	10.58	125.59	120.30
5	BX	410	ARG	NE-CZ-NH2	10.57	125.59	120.30
5	IX	410	ARG	NE-CZ-NH2	10.56	125.58	120.30
5	KX	410	ARG	NE-CZ-NH2	10.52	125.56	120.30
5	DX	410	ARG	NE-CZ-NH2	10.52	125.56	120.30
5	GX	410	ARG	NE-CZ-NH2	10.52	125.56	120.30
5	CX	410	ARG	NE-CZ-NH2	10.50	125.55	120.30
5	FX	410	ARG	NE-CZ-NH2	10.49	125.55	120.30
5	AX	410	ARG	NE-CZ-NH2	10.45	125.53	120.30
2	Gm	286	LEU	CA-CB-CG	10.40	139.22	115.30
1	BD	143	LEU	CA-CB-CG	10.37	139.14	115.30
1	ID	143	LEU	CA-CB-CG	10.35	139.11	115.30
1	DA	210	MET	CA-CB-CG	10.32	130.84	113.30
1	LA	210	MET	CA-CB-CG	10.31	130.83	113.30
1	BA	210	MET	CA-CB-CG	10.30	130.82	113.30
1	EA	210	MET	CA-CB-CG	10.30	130.81	113.30
1	KA	210	MET	CA-CB-CG	10.30	130.81	113.30
1	AA	210	MET	CA-CB-CG	10.30	130.81	113.30
1	GA	210	MET	CA-CB-CG	10.30	130.81	113.30
1	IA	210	MET	CA-CB-CG	10.30	130.81	113.30
1	FA	210	MET	CA-CB-CG	10.29	130.80	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	MA	210	MET	CA-CB-CG	10.29	130.78	113.30
1	HA	210	MET	CA-CB-CG	10.28	130.78	113.30
1	CA	210	MET	CA-CB-CG	10.28	130.77	113.30
1	JA	210	MET	CA-CB-CG	10.28	130.77	113.30
1	NA	210	MET	CA-CB-CG	10.27	130.76	113.30
1	HE	130	MET	CG-SD-CE	-9.98	84.23	100.20
3	HT	274	ARG	NE-CZ-NH1	9.71	125.15	120.30
3	DT	274	ARG	NE-CZ-NH1	9.70	125.15	120.30
3	KT	274	ARG	NE-CZ-NH1	9.70	125.15	120.30
3	CT	274	ARG	NE-CZ-NH1	9.68	125.14	120.30
3	GT	274	ARG	NE-CZ-NH1	9.68	125.14	120.30
3	LT	274	ARG	NE-CZ-NH1	9.65	125.12	120.30
3	AT	274	ARG	NE-CZ-NH1	9.59	125.10	120.30
3	JT	274	ARG	NE-CZ-NH1	9.59	125.09	120.30
3	MT	274	ARG	NE-CZ-NH1	9.59	125.09	120.30
3	FT	274	ARG	NE-CZ-NH1	9.57	125.08	120.30
3	BT	274	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	FD	143	LEU	CB-CG-CD2	-9.51	94.83	111.00
3	IT	274	ARG	NE-CZ-NH1	9.51	125.05	120.30
3	ET	274	ARG	NE-CZ-NH1	9.48	125.04	120.30
3	NT	274	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	MD	81	TYR	CA-CB-CG	9.44	131.33	113.40
1	HA	210	MET	CB-CG-SD	9.31	140.34	112.40
1	CA	210	MET	CB-CG-SD	9.31	140.33	112.40
1	JA	210	MET	CB-CG-SD	9.31	140.33	112.40
1	AA	210	MET	CB-CG-SD	9.31	140.32	112.40
1	FA	210	MET	CB-CG-SD	9.31	140.32	112.40
1	KA	210	MET	CB-CG-SD	9.31	140.32	112.40
1	IA	210	MET	CB-CG-SD	9.30	140.31	112.40
1	GA	210	MET	CB-CG-SD	9.30	140.31	112.40
1	LA	210	MET	CB-CG-SD	9.30	140.31	112.40
1	NA	210	MET	CB-CG-SD	9.30	140.30	112.40
1	BA	210	MET	CB-CG-SD	9.30	140.29	112.40
1	EA	210	MET	CB-CG-SD	9.30	140.29	112.40
1	MA	210	MET	CB-CG-SD	9.30	140.29	112.40
1	DA	210	MET	CB-CG-SD	9.29	140.27	112.40
1	MD	143	LEU	CB-CG-CD2	-9.22	95.33	111.00
1	ID	130	MET	CG-SD-CE	-9.06	85.70	100.20
1	NE	110	ASP	CB-CG-OD1	9.06	126.45	118.30
2	Hm	222	TYR	CB-CG-CD2	-9.03	115.58	121.00
1	HD	81	TYR	CB-CA-C	8.98	128.35	110.40
1	HD	81	TYR	CA-CB-CG	8.84	130.20	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	MX	410	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	JC	130	MET	CG-SD-CE	-8.80	86.12	100.20
5	HX	410	ARG	NE-CZ-NH1	-8.75	115.92	120.30
5	FX	410	ARG	NE-CZ-NH1	-8.75	115.93	120.30
5	LX	410	ARG	NE-CZ-NH1	-8.74	115.93	120.30
5	JX	410	ARG	NE-CZ-NH1	-8.72	115.94	120.30
5	IX	410	ARG	NE-CZ-NH1	-8.71	115.95	120.30
5	CX	410	ARG	NE-CZ-NH1	-8.69	115.95	120.30
5	BX	410	ARG	NE-CZ-NH1	-8.67	115.96	120.30
5	EX	410	ARG	NE-CZ-NH1	-8.67	115.96	120.30
5	NX	410	ARG	NE-CZ-NH1	-8.67	115.97	120.30
5	DX	410	ARG	NE-CZ-NH1	-8.66	115.97	120.30
5	GX	410	ARG	NE-CZ-NH1	-8.66	115.97	120.30
5	AX	410	ARG	NE-CZ-NH1	-8.65	115.97	120.30
5	KX	410	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	MD	81	TYR	CB-CA-C	8.53	127.46	110.40
1	GD	79	ASP	CB-CG-OD2	8.48	125.94	118.30
1	ND	143	LEU	CA-CB-CG	8.47	134.78	115.30
1	KE	107	TYR	N-CA-CB	8.45	125.82	110.60
1	KE	113	ASP	CB-CG-OD1	8.43	125.89	118.30
1	CE	93	ASP	CB-CG-OD2	8.41	125.87	118.30
1	HC	110	ASP	CB-CG-OD2	8.39	125.85	118.30
1	CD	143	LEU	CA-CB-CG	8.37	134.54	115.30
1	KE	107	TYR	CB-CG-CD2	-8.37	115.98	121.00
1	ED	128	ARG	NE-CZ-NH1	-8.30	116.15	120.30
2	Nm	222	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	DE	113	ASP	CB-CG-OD1	8.28	125.75	118.30
1	KD	143	LEU	CB-CG-CD2	-8.23	97.02	111.00
1	DD	143	LEU	CB-CG-CD2	-8.12	97.19	111.00
2	Fm	286	LEU	CA-CB-CG	8.03	133.77	115.30
1	ID	120	ILE	CG1-CB-CG2	-7.95	93.90	111.40
2	MM	312	ASP	CB-CG-OD2	7.93	125.44	118.30
2	Bm	286	LEU	CA-CB-CG	7.92	133.53	115.30
1	JB	118	LEU	CA-CB-CG	7.91	133.50	115.30
2	FM	312	ASP	CB-CG-OD2	7.89	125.40	118.30
1	EC	110	ASP	CB-CG-OD2	7.87	125.38	118.30
2	AM	312	ASP	CB-CG-OD2	7.85	125.36	118.30
1	LC	110	ASP	CB-CG-OD2	7.84	125.36	118.30
2	HM	312	ASP	CB-CG-OD2	7.83	125.35	118.30
2	NM	312	ASP	CB-CG-OD2	7.83	125.35	118.30
2	GM	312	ASP	CB-CG-OD2	7.82	125.34	118.30
1	FC	110	ASP	CB-CG-OD2	7.82	125.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	EM	312	ASP	CB-CG-OD2	7.80	125.32	118.30
1	EB	112	LEU	CB-CG-CD2	-7.77	97.79	111.00
2	LM	312	ASP	CB-CG-OD2	7.75	125.28	118.30
2	KM	312	ASP	CB-CG-OD2	7.72	125.25	118.30
1	AE	113	ASP	CB-CG-OD1	7.72	125.25	118.30
2	Hm	286	LEU	CA-CB-CG	7.72	133.05	115.30
2	AM	343	ASP	CB-CG-OD2	7.71	125.24	118.30
1	MC	110	ASP	CB-CG-OD2	7.71	125.23	118.30
2	DM	312	ASP	CB-CG-OD2	7.70	125.23	118.30
1	HE	113	ASP	CB-CG-OD2	7.69	125.22	118.30
5	HX	356	MET	CB-CG-SD	7.65	135.34	112.40
5	KX	356	MET	CB-CG-SD	7.64	135.33	112.40
5	NX	356	MET	CB-CG-SD	7.64	135.32	112.40
5	CX	356	MET	CB-CG-SD	7.64	135.32	112.40
5	GX	356	MET	CB-CG-SD	7.64	135.32	112.40
5	IX	356	MET	CB-CG-SD	7.64	135.32	112.40
5	MX	356	MET	CB-CG-SD	7.64	135.32	112.40
5	FX	356	MET	CB-CG-SD	7.64	135.31	112.40
5	DX	356	MET	CB-CG-SD	7.64	135.31	112.40
5	JX	356	MET	CB-CG-SD	7.63	135.30	112.40
5	AX	356	MET	CB-CG-SD	7.63	135.30	112.40
5	LX	356	MET	CB-CG-SD	7.63	135.30	112.40
5	BX	356	MET	CB-CG-SD	7.63	135.29	112.40
5	EX	356	MET	CB-CG-SD	7.63	135.29	112.40
3	DT	274	ARG	NE-CZ-NH2	-7.62	116.49	120.30
3	CT	274	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	GD	143	LEU	CB-CG-CD2	-7.61	98.06	111.00
1	LD	143	LEU	CA-CB-CG	7.61	132.79	115.30
1	EE	93	ASP	CB-CG-OD2	7.58	125.12	118.30
1	CB	118	LEU	CA-CB-CG	7.55	132.67	115.30
1	BD	81	TYR	CB-CG-CD2	-7.54	116.47	121.00
3	GT	274	ARG	NE-CZ-NH2	-7.54	116.53	120.30
3	IT	274	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	DD	143	LEU	CA-CB-CG	7.54	132.63	115.30
1	FD	81	TYR	CB-CA-C	7.53	125.46	110.40
1	FD	143	LEU	CA-CB-CG	7.53	132.62	115.30
3	HT	274	ARG	NE-CZ-NH2	-7.52	116.54	120.30
3	KT	249	MET	CB-CG-SD	7.51	134.94	112.40
3	DT	249	MET	CB-CG-SD	7.51	134.92	112.40
3	HT	249	MET	CB-CG-SD	7.51	134.92	112.40
3	JT	249	MET	CB-CG-SD	7.50	134.91	112.40
3	BT	249	MET	CB-CG-SD	7.50	134.91	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	IT	249	MET	CB-CG-SD	7.50	134.90	112.40
3	ET	249	MET	CB-CG-SD	7.50	134.90	112.40
3	AT	249	MET	CB-CG-SD	7.50	134.89	112.40
3	CT	249	MET	CB-CG-SD	7.50	134.89	112.40
3	LT	249	MET	CB-CG-SD	7.49	134.88	112.40
3	MT	249	MET	CB-CG-SD	7.49	134.88	112.40
3	NT	249	MET	CB-CG-SD	7.49	134.87	112.40
3	FT	249	MET	CB-CG-SD	7.49	134.86	112.40
3	GT	249	MET	CB-CG-SD	7.49	134.87	112.40
3	KT	274	ARG	NE-CZ-NH2	-7.49	116.56	120.30
3	MT	274	ARG	NE-CZ-NH2	-7.48	116.56	120.30
3	ET	274	ARG	NE-CZ-NH2	-7.47	116.56	120.30
3	JT	274	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	LE	82	ASP	CB-CG-OD1	7.47	125.02	118.30
3	AT	274	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	MD	143	LEU	CA-CB-CG	7.46	132.45	115.30
3	NT	274	ARG	NE-CZ-NH2	-7.45	116.57	120.30
3	LT	274	ARG	NE-CZ-NH2	-7.44	116.58	120.30
6	AY	1780	MET	CG-SD-CE	7.44	112.11	100.20
3	Bt	207	GLU	CA-CB-CG	7.44	129.76	113.40
6	DY	1780	MET	CG-SD-CE	7.43	112.09	100.20
6	JY	1780	MET	CG-SD-CE	7.43	112.09	100.20
6	KY	1780	MET	CG-SD-CE	7.43	112.09	100.20
6	CY	1780	MET	CG-SD-CE	7.43	112.09	100.20
6	FY	1780	MET	CG-SD-CE	7.43	112.09	100.20
6	LY	1780	MET	CG-SD-CE	7.43	112.09	100.20
6	IY	1780	MET	CG-SD-CE	7.43	112.08	100.20
3	BT	274	ARG	NE-CZ-NH2	-7.43	116.59	120.30
3	Dt	207	GLU	CA-CB-CG	7.43	129.74	113.40
2	Lm	286	LEU	CA-CB-CG	7.43	132.38	115.30
2	Mm	286	LEU	CA-CB-CG	7.42	132.37	115.30
6	BY	1780	MET	CG-SD-CE	7.42	112.06	100.20
6	EY	1780	MET	CG-SD-CE	7.42	112.06	100.20
1	FB	136	LEU	CB-CG-CD2	-7.42	98.39	111.00
6	MY	1780	MET	CG-SD-CE	7.42	112.06	100.20
3	Mt	207	GLU	CA-CB-CG	7.42	129.72	113.40
3	At	207	GLU	CA-CB-CG	7.42	129.71	113.40
6	GY	1780	MET	CG-SD-CE	7.42	112.06	100.20
3	Gt	207	GLU	CA-CB-CG	7.42	129.71	113.40
3	Jt	207	GLU	CA-CB-CG	7.42	129.71	113.40
6	NY	1780	MET	CG-SD-CE	7.42	112.06	100.20
3	Et	207	GLU	CA-CB-CG	7.41	129.71	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Ft	207	GLU	CA-CB-CG	7.41	129.71	113.40
3	It	207	GLU	CA-CB-CG	7.41	129.71	113.40
3	Kt	207	GLU	CA-CB-CG	7.41	129.71	113.40
3	Ht	207	GLU	CA-CB-CG	7.41	129.71	113.40
3	Nt	207	GLU	CA-CB-CG	7.41	129.70	113.40
3	FT	274	ARG	NE-CZ-NH2	-7.40	116.60	120.30
3	Lt	207	GLU	CA-CB-CG	7.39	129.67	113.40
3	Ct	207	GLU	CA-CB-CG	7.39	129.66	113.40
6	HY	1780	MET	CG-SD-CE	7.39	112.02	100.20
1	EE	113	ASP	CB-CG-OD2	7.37	124.93	118.30
1	LC	159	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	ED	143	LEU	CA-CB-CG	7.33	132.15	115.30
1	DA	130	MET	CB-CG-SD	7.33	134.38	112.40
1	DC	153	LEU	CB-CG-CD2	7.33	123.45	111.00
1	EA	130	MET	CB-CG-SD	7.33	134.38	112.40
1	GA	130	MET	CB-CG-SD	7.33	134.38	112.40
1	KA	130	MET	CB-CG-SD	7.32	134.37	112.40
1	LA	130	MET	CB-CG-SD	7.32	134.37	112.40
1	NA	130	MET	CB-CG-SD	7.32	134.36	112.40
1	AA	130	MET	CB-CG-SD	7.32	134.35	112.40
1	BA	130	MET	CB-CG-SD	7.32	134.35	112.40
1	HA	130	MET	CB-CG-SD	7.32	134.34	112.40
1	MA	130	MET	CB-CG-SD	7.32	134.34	112.40
1	IA	130	MET	CB-CG-SD	7.31	134.33	112.40
1	CA	130	MET	CB-CG-SD	7.31	134.32	112.40
1	FA	130	MET	CB-CG-SD	7.31	134.32	112.40
1	JA	130	MET	CB-CG-SD	7.30	134.32	112.40
1	EE	109	MET	CB-CG-SD	7.26	134.19	112.40
1	KD	81	TYR	CB-CA-C	7.24	124.88	110.40
1	FE	105	TYR	CA-CB-CG	7.20	127.08	113.40
1	BD	169	GLU	OE1-CD-OE2	-7.16	114.71	123.30
1	JB	121	GLU	CG-CD-OE2	-7.14	104.03	118.30
1	MD	81	TYR	CB-CG-CD2	-7.13	116.72	121.00
1	MB	121	GLU	CG-CD-OE2	-7.11	104.08	118.30
2	Dm	325	LEU	CB-CG-CD1	7.09	123.05	111.00
2	Jm	343	ASP	C-N-CA	7.08	139.41	121.70
1	ME	107	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	LE	107	TYR	CA-CB-CG	6.99	126.68	113.40
2	Dm	286	LEU	CB-CG-CD1	6.96	122.83	111.00
1	KC	153	LEU	CB-CG-CD2	6.95	122.81	111.00
1	KE	107	TYR	CB-CA-C	-6.94	96.53	110.40
1	JE	110	ASP	CB-CG-OD2	6.92	124.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	HD	120	ILE	CG1-CB-CG2	-6.92	96.18	111.40
1	NE	93	ASP	CB-CG-OD2	6.91	124.52	118.30
1	KD	143	LEU	CA-CB-CG	6.91	131.19	115.30
1	FB	121	GLU	CG-CD-OE2	-6.88	104.54	118.30
2	Km	325	LEU	CB-CG-CD1	6.88	122.69	111.00
2	Lm	325	LEU	CB-CG-CD1	6.85	122.65	111.00
1	CB	121	GLU	CG-CD-OE2	-6.84	104.62	118.30
1	GD	143	LEU	CA-CB-CG	6.84	131.03	115.30
2	HM	343	ASP	CB-CG-OD2	6.82	124.44	118.30
5	MX	356	MET	CG-SD-CE	6.81	111.10	100.20
5	BX	356	MET	CG-SD-CE	6.80	111.09	100.20
5	KX	356	MET	CG-SD-CE	6.80	111.09	100.20
5	CX	356	MET	CG-SD-CE	6.80	111.08	100.20
5	JX	356	MET	CG-SD-CE	6.80	111.08	100.20
5	EX	356	MET	CG-SD-CE	6.80	111.08	100.20
5	AX	356	MET	CG-SD-CE	6.80	111.07	100.20
5	LX	356	MET	CG-SD-CE	6.79	111.07	100.20
5	DX	356	MET	CG-SD-CE	6.79	111.07	100.20
5	NX	356	MET	CG-SD-CE	6.79	111.07	100.20
1	DE	128	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	HB	121	GLU	CG-CD-OE2	-6.79	104.72	118.30
2	Fm	222	TYR	CB-CG-CD2	-6.79	116.93	121.00
5	GX	356	MET	CG-SD-CE	6.79	111.06	100.20
5	IX	356	MET	CG-SD-CE	6.79	111.06	100.20
5	HX	356	MET	CG-SD-CE	6.78	111.05	100.20
3	FT	187	ARG	CB-CG-CD	6.77	129.21	111.60
3	AT	187	ARG	CB-CG-CD	6.77	129.21	111.60
1	IE	101	LYS	CD-CE-NZ	-6.77	96.12	111.70
3	KT	187	ARG	CB-CG-CD	6.77	129.20	111.60
2	Lm	341	MET	CG-SD-CE	6.77	111.03	100.20
3	NT	187	ARG	CB-CG-CD	6.77	129.20	111.60
3	DT	187	ARG	CB-CG-CD	6.76	129.19	111.60
5	FX	356	MET	CG-SD-CE	6.76	111.02	100.20
3	BT	187	ARG	CB-CG-CD	6.76	129.17	111.60
3	IT	187	ARG	CB-CG-CD	6.76	129.17	111.60
3	CT	187	ARG	CB-CG-CD	6.75	129.16	111.60
3	ET	187	ARG	CB-CG-CD	6.75	129.16	111.60
3	HT	187	ARG	CB-CG-CD	6.75	129.15	111.60
3	GT	187	ARG	CB-CG-CD	6.75	129.15	111.60
3	JT	187	ARG	CB-CG-CD	6.75	129.15	111.60
6	HY	1780	MET	CB-CG-SD	6.75	132.64	112.40
3	LT	187	ARG	CB-CG-CD	6.75	129.14	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	MT	187	ARG	CB-CG-CD	6.75	129.14	111.60
6	MY	1780	MET	CB-CG-SD	6.74	132.63	112.40
1	GE	156	LEU	CB-CG-CD1	-6.74	99.55	111.00
6	BY	1780	MET	CB-CG-SD	6.74	132.60	112.40
6	CY	1780	MET	CB-CG-SD	6.74	132.61	112.40
6	EY	1780	MET	CB-CG-SD	6.74	132.60	112.40
6	JY	1780	MET	CB-CG-SD	6.74	132.61	112.40
2	FM	282	ASP	CB-CG-OD2	6.73	124.36	118.30
6	KY	1780	MET	CB-CG-SD	6.73	132.60	112.40
6	IY	1780	MET	CB-CG-SD	6.73	132.59	112.40
6	LY	1780	MET	CB-CG-SD	6.73	132.59	112.40
6	EY	1772	LEU	CA-CB-CG	6.72	130.77	115.30
6	FY	1780	MET	CB-CG-SD	6.72	132.57	112.40
6	AY	1780	MET	CB-CG-SD	6.72	132.57	112.40
6	DY	1780	MET	CB-CG-SD	6.72	132.57	112.40
6	DY	1772	LEU	CA-CB-CG	6.72	130.76	115.30
6	GY	1780	MET	CB-CG-SD	6.72	132.56	112.40
6	NY	1780	MET	CB-CG-SD	6.72	132.56	112.40
6	CY	1772	LEU	CA-CB-CG	6.72	130.75	115.30
6	NY	1772	LEU	CA-CB-CG	6.71	130.74	115.30
6	GY	1772	LEU	CA-CB-CG	6.71	130.73	115.30
6	HY	1772	LEU	CA-CB-CG	6.71	130.73	115.30
6	LY	1772	LEU	CA-CB-CG	6.71	130.73	115.30
6	AY	1772	LEU	CA-CB-CG	6.70	130.70	115.30
6	BY	1772	LEU	CA-CB-CG	6.70	130.70	115.30
6	FY	1772	LEU	CA-CB-CG	6.70	130.70	115.30
6	JY	1772	LEU	CA-CB-CG	6.69	130.70	115.30
6	MY	1772	LEU	CA-CB-CG	6.69	130.69	115.30
6	IY	1772	LEU	CA-CB-CG	6.69	130.69	115.30
2	Am	286	LEU	CA-CB-CG	6.69	130.68	115.30
6	KY	1772	LEU	CA-CB-CG	6.69	130.68	115.30
3	Ft	230	TYR	CB-CG-CD2	6.68	125.01	121.00
1	LB	121	GLU	CG-CD-OE2	-6.67	104.95	118.30
2	DM	214	ARG	NE-CZ-NH2	6.67	123.64	120.30
3	It	230	TYR	CB-CG-CD2	6.66	125.00	121.00
1	LD	120	ILE	CG1-CB-CG2	-6.65	96.77	111.40
3	Ct	230	TYR	CB-CG-CD2	6.64	124.98	121.00
3	Jt	230	TYR	CB-CG-CD2	6.63	124.98	121.00
3	Dt	230	TYR	CB-CG-CD2	6.63	124.98	121.00
3	Et	230	TYR	CB-CG-CD2	6.63	124.98	121.00
3	Lt	230	TYR	CB-CG-CD2	6.63	124.98	121.00
3	Ht	230	TYR	CB-CG-CD2	6.62	124.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Mt	230	TYR	CB-CG-CD2	6.60	124.96	121.00
3	Gt	230	TYR	CB-CG-CD2	6.59	124.95	121.00
2	Hm	325	LEU	CB-CG-CD1	6.59	122.20	111.00
1	KE	93	ASP	CB-CG-OD2	6.59	124.23	118.30
3	At	230	TYR	CB-CG-CD2	6.59	124.95	121.00
1	KD	111	LEU	CB-CG-CD1	6.56	122.15	111.00
2	Em	325	LEU	CB-CG-CD1	6.56	122.15	111.00
3	Bt	230	TYR	CB-CG-CD2	6.55	124.93	121.00
3	Kt	230	TYR	CB-CG-CD2	6.55	124.93	121.00
3	Nt	230	TYR	CB-CG-CD2	6.55	124.93	121.00
2	Bm	343	ASP	C-N-CA	6.54	138.06	121.70
1	FB	121	GLU	CB-CA-C	-6.54	97.32	110.40
1	GD	120	ILE	CG1-CB-CG2	-6.54	97.01	111.40
1	LE	93	ASP	CB-CG-OD2	6.53	124.18	118.30
1	DD	120	ILE	CG1-CB-CG2	-6.50	97.09	111.40
1	GE	110	ASP	CB-CG-OD2	6.50	124.15	118.30
2	Am	325	LEU	CB-CG-CD1	6.49	122.04	111.00
5	FX	410	ARG	CG-CD-NE	6.48	125.40	111.80
5	CX	410	ARG	CG-CD-NE	6.47	125.39	111.80
5	DX	410	ARG	CG-CD-NE	6.46	125.38	111.80
5	AX	410	ARG	CG-CD-NE	6.46	125.37	111.80
5	GX	410	ARG	CG-CD-NE	6.46	125.37	111.80
2	Jm	325	LEU	CB-CG-CD1	6.46	121.99	111.00
5	MX	410	ARG	CG-CD-NE	6.46	125.37	111.80
5	IX	410	ARG	CG-CD-NE	6.46	125.37	111.80
5	EX	410	ARG	CG-CD-NE	6.46	125.37	111.80
1	FD	81	TYR	CA-CB-CG	6.46	125.67	113.40
2	FM	214	ARG	NE-CZ-NH2	6.46	123.53	120.30
5	LX	410	ARG	CG-CD-NE	6.46	125.36	111.80
5	HX	410	ARG	CG-CD-NE	6.46	125.36	111.80
1	DE	93	ASP	CB-CG-OD2	6.45	124.11	118.30
5	NX	410	ARG	CG-CD-NE	6.45	125.35	111.80
1	GE	93	ASP	CB-CG-OD2	6.45	124.10	118.30
1	DB	112	LEU	CB-CG-CD1	-6.45	100.04	111.00
1	NC	130	MET	CG-SD-CE	-6.44	89.89	100.20
5	KX	410	ARG	CG-CD-NE	6.44	125.33	111.80
5	BX	410	ARG	CG-CD-NE	6.44	125.32	111.80
1	ID	128	ARG	NE-CZ-NH2	6.44	123.52	120.30
5	JX	410	ARG	CG-CD-NE	6.43	125.31	111.80
2	Im	286	LEU	CA-CB-CG	6.43	130.09	115.30
2	Mm	325	LEU	CB-CG-CD1	6.43	121.93	111.00
2	Nm	325	LEU	CB-CG-CD1	6.42	121.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Hm	343	ASP	C-N-CA	6.42	137.74	121.70
1	AD	111	LEU	CB-CG-CD1	6.40	121.87	111.00
2	Fm	325	LEU	CB-CG-CD1	6.38	121.84	111.00
1	DB	121	GLU	CG-CD-OE2	-6.35	105.60	118.30
2	Am	343	ASP	C-N-CA	6.34	137.55	121.70
5	FX	474	GLU	CA-CB-CG	6.32	127.30	113.40
2	Dm	343	ASP	C-N-CA	6.32	137.49	121.70
1	EA	100	LEU	CA-CB-CG	6.31	129.82	115.30
5	GX	474	GLU	CA-CB-CG	6.31	127.29	113.40
5	JX	474	GLU	CA-CB-CG	6.31	127.28	113.40
5	MX	474	GLU	CA-CB-CG	6.31	127.28	113.40
1	FA	100	LEU	CA-CB-CG	6.30	129.80	115.30
1	DA	100	LEU	CA-CB-CG	6.30	129.79	115.30
5	EX	474	GLU	CA-CB-CG	6.30	127.27	113.40
1	GA	100	LEU	CA-CB-CG	6.30	129.79	115.30
1	KA	100	LEU	CA-CB-CG	6.30	129.79	115.30
5	KX	474	GLU	CA-CB-CG	6.30	127.26	113.40
5	LX	474	GLU	CA-CB-CG	6.30	127.26	113.40
1	IA	100	LEU	CA-CB-CG	6.30	129.79	115.30
5	NX	474	GLU	CA-CB-CG	6.30	127.26	113.40
1	BA	100	LEU	CA-CB-CG	6.30	129.78	115.30
5	BX	474	GLU	CA-CB-CG	6.30	127.25	113.40
5	HX	474	GLU	CA-CB-CG	6.30	127.25	113.40
1	HA	100	LEU	CA-CB-CG	6.29	129.77	115.30
1	MA	100	LEU	CA-CB-CG	6.29	129.77	115.30
5	IX	474	GLU	CA-CB-CG	6.29	127.24	113.40
1	JA	100	LEU	CA-CB-CG	6.29	129.77	115.30
5	AX	474	GLU	CA-CB-CG	6.29	127.23	113.40
5	CX	474	GLU	CA-CB-CG	6.29	127.23	113.40
5	DX	474	GLU	CA-CB-CG	6.29	127.23	113.40
1	LA	100	LEU	CA-CB-CG	6.29	129.76	115.30
1	AA	100	LEU	CA-CB-CG	6.29	129.76	115.30
1	CA	100	LEU	CA-CB-CG	6.29	129.76	115.30
1	NA	100	LEU	CA-CB-CG	6.29	129.76	115.30
1	HB	121	GLU	CB-CA-C	-6.27	97.86	110.40
2	Am	217	LEU	CA-CB-CG	6.26	129.71	115.30
2	Cm	217	LEU	CA-CB-CG	6.26	129.71	115.30
1	ED	120	ILE	CG1-CB-CG2	-6.26	97.62	111.40
2	Gm	286	LEU	CB-CG-CD1	6.26	121.64	111.00
2	Km	343	ASP	C-N-CA	6.26	137.34	121.70
2	Cm	325	LEU	CB-CG-CD1	6.24	121.61	111.00
1	DE	179	LEU	CA-CB-CG	6.23	129.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	FC	165	LEU	CB-CG-CD1	6.23	121.59	111.00
1	KB	121	GLU	CG-CD-OE2	-6.22	105.85	118.30
2	Hm	217	LEU	CA-CB-CG	6.22	129.60	115.30
2	Lm	343	ASP	C-N-CA	6.19	137.18	121.70
2	Mm	343	ASP	C-N-CA	6.19	137.17	121.70
2	Em	343	ASP	C-N-CA	6.17	137.12	121.70
1	LE	106	LEU	CA-CB-CG	6.16	129.46	115.30
2	Em	222	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	MB	121	GLU	CB-CA-C	-6.13	98.14	110.40
3	Gt	257	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	LT	187	ARG	CG-CD-NE	6.12	124.65	111.80
3	Kt	257	ARG	NE-CZ-NH1	6.11	123.36	120.30
2	Gm	343	ASP	C-N-CA	6.11	136.97	121.70
3	JT	187	ARG	CG-CD-NE	6.11	124.63	111.80
3	Jt	257	ARG	NE-CZ-NH1	6.11	123.36	120.30
3	MT	187	ARG	CG-CD-NE	6.11	124.63	111.80
5	CX	378	ASP	CB-CG-OD2	6.11	123.80	118.30
3	FT	187	ARG	CG-CD-NE	6.11	124.62	111.80
3	It	257	ARG	NE-CZ-NH1	6.10	123.35	120.30
3	KT	187	ARG	CG-CD-NE	6.10	124.62	111.80
3	IT	187	ARG	CG-CD-NE	6.10	124.62	111.80
3	JT	187	ARG	NE-CZ-NH1	-6.10	117.25	120.30
3	NT	187	ARG	CG-CD-NE	6.10	124.61	111.80
3	CT	187	ARG	CG-CD-NE	6.10	124.61	111.80
3	ET	187	ARG	CG-CD-NE	6.10	124.61	111.80
5	JX	378	ASP	CB-CG-OD2	6.10	123.79	118.30
3	FT	187	ARG	NE-CZ-NH1	-6.10	117.25	120.30
3	HT	187	ARG	CG-CD-NE	6.10	124.61	111.80
3	DT	187	ARG	CG-CD-NE	6.10	124.60	111.80
3	AT	187	ARG	CG-CD-NE	6.09	124.59	111.80
3	BT	187	ARG	CG-CD-NE	6.09	124.60	111.80
3	GT	187	ARG	CG-CD-NE	6.09	124.58	111.80
2	Cm	343	ASP	C-N-CA	6.08	136.90	121.70
3	KT	187	ARG	NE-CZ-NH1	-6.08	117.26	120.30
3	At	257	ARG	NE-CZ-NH1	6.08	123.34	120.30
5	DX	378	ASP	CB-CG-OD2	6.08	123.77	118.30
5	IX	378	ASP	CB-CG-OD2	6.08	123.77	118.30
3	Nt	257	ARG	NE-CZ-NH1	6.07	123.33	120.30
3	Et	257	ARG	NE-CZ-NH1	6.06	123.33	120.30
5	EX	378	ASP	CB-CG-OD2	6.06	123.75	118.30
2	Nm	217	LEU	CA-CB-CG	6.06	129.24	115.30
3	Lt	257	ARG	NE-CZ-NH1	6.06	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	EB	136	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	JB	118	LEU	CB-CG-CD2	6.05	121.29	111.00
3	Mt	257	ARG	NE-CZ-NH1	6.05	123.33	120.30
3	Dt	257	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	HE	135	ASP	CB-CG-OD1	6.05	123.75	118.30
1	BE	93	ASP	CB-CG-OD1	6.05	123.74	118.30
3	Ft	257	ARG	NE-CZ-NH1	6.05	123.32	120.30
3	IT	187	ARG	NE-CZ-NH1	-6.04	117.28	120.30
5	KX	378	ASP	CB-CG-OD2	6.04	123.74	118.30
2	GM	214	ARG	NE-CZ-NH1	6.04	123.32	120.30
3	Ct	257	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	EE	106	LEU	CA-CB-CG	6.04	129.19	115.30
5	HX	378	ASP	CB-CG-OD2	6.04	123.73	118.30
3	AT	187	ARG	NE-CZ-NH1	-6.03	117.28	120.30
2	Em	217	LEU	CA-CB-CG	6.03	129.18	115.30
5	NX	378	ASP	CB-CG-OD2	6.03	123.73	118.30
5	AX	378	ASP	CB-CG-OD2	6.03	123.73	118.30
5	FX	378	ASP	CB-CG-OD2	6.03	123.73	118.30
1	KE	110	ASP	CB-CG-OD2	6.03	123.73	118.30
5	GX	378	ASP	CB-CG-OD2	6.03	123.72	118.30
2	Fm	343	ASP	C-N-CA	6.03	136.76	121.70
1	JB	121	GLU	CB-CA-C	-6.03	98.35	110.40
2	Bm	222	TYR	CB-CG-CD2	-6.02	117.39	121.00
2	Gm	325	LEU	CB-CG-CD1	6.02	121.23	111.00
2	Im	343	ASP	C-N-CA	6.02	136.75	121.70
3	Bt	257	ARG	NE-CZ-NH1	6.02	123.31	120.30
5	LX	378	ASP	CB-CG-OD2	6.01	123.71	118.30
3	LT	187	ARG	NE-CZ-NH1	-6.01	117.29	120.30
5	BX	378	ASP	CB-CG-OD2	6.01	123.71	118.30
3	GT	187	ARG	NE-CZ-NH1	-6.01	117.30	120.30
2	Bm	217	LEU	CA-CB-CG	6.01	129.12	115.30
5	MX	378	ASP	CB-CG-OD2	6.01	123.71	118.30
1	KE	107	TYR	CE1-CZ-OH	6.00	136.31	120.10
2	Lm	217	LEU	CA-CB-CG	6.00	129.10	115.30
3	ET	187	ARG	NE-CZ-NH1	-6.00	117.30	120.30
3	GT	249	MET	CG-SD-CE	6.00	109.79	100.20
3	MT	187	ARG	NE-CZ-NH1	-5.99	117.30	120.30
3	LT	249	MET	CG-SD-CE	5.99	109.79	100.20
3	NT	187	ARG	NE-CZ-NH1	-5.99	117.30	120.30
3	NT	249	MET	CG-SD-CE	5.99	109.78	100.20
3	HT	187	ARG	NE-CZ-NH1	-5.99	117.31	120.30
3	MT	249	MET	CG-SD-CE	5.99	109.78	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BT	249	MET	CG-SD-CE	5.98	109.77	100.20
2	Mm	217	LEU	CA-CB-CG	5.98	129.05	115.30
3	AT	249	MET	CG-SD-CE	5.98	109.77	100.20
2	Im	217	LEU	CA-CB-CG	5.98	129.05	115.30
3	FT	249	MET	CG-SD-CE	5.98	109.76	100.20
3	JT	249	MET	CG-SD-CE	5.98	109.76	100.20
3	ET	249	MET	CG-SD-CE	5.98	109.76	100.20
3	CT	249	MET	CG-SD-CE	5.97	109.76	100.20
3	CT	187	ARG	NE-CZ-NH1	-5.97	117.31	120.30
3	DT	249	MET	CG-SD-CE	5.97	109.75	100.20
3	HT	249	MET	CG-SD-CE	5.97	109.75	100.20
2	Gm	217	LEU	CA-CB-CG	5.96	129.02	115.30
3	DT	187	ARG	NE-CZ-NH1	-5.96	117.32	120.30
3	IT	249	MET	CG-SD-CE	5.96	109.74	100.20
3	Ht	257	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	KT	249	MET	CG-SD-CE	5.96	109.73	100.20
1	DA	288	GLU	CA-CB-CG	5.93	126.45	113.40
2	Fm	217	LEU	CA-CB-CG	5.93	128.94	115.30
1	LA	288	GLU	CA-CB-CG	5.92	126.43	113.40
2	Nm	343	ASP	C-N-CA	5.92	136.50	121.70
1	IA	288	GLU	CA-CB-CG	5.92	126.41	113.40
1	BA	288	GLU	CA-CB-CG	5.91	126.41	113.40
3	BT	187	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	IE	93	ASP	CB-CG-OD1	5.91	123.62	118.30
1	NA	288	GLU	CA-CB-CG	5.91	126.40	113.40
1	AA	288	GLU	CA-CB-CG	5.91	126.39	113.40
1	CA	288	GLU	CA-CB-CG	5.91	126.39	113.40
1	FA	288	GLU	CA-CB-CG	5.91	126.40	113.40
1	EA	288	GLU	CA-CB-CG	5.91	126.39	113.40
1	GA	288	GLU	CA-CB-CG	5.90	126.39	113.40
1	KA	288	GLU	CA-CB-CG	5.90	126.39	113.40
1	HA	288	GLU	CA-CB-CG	5.90	126.38	113.40
1	JA	288	GLU	CA-CB-CG	5.90	126.37	113.40
1	MA	288	GLU	CA-CB-CG	5.90	126.38	113.40
1	BC	106	LEU	CA-CB-CG	5.90	128.86	115.30
2	KM	257	MET	CA-CB-CG	5.90	123.32	113.30
1	CB	121	GLU	CB-CA-C	-5.89	98.61	110.40
2	Nm	286	LEU	CA-CB-CG	5.89	128.85	115.30
1	KC	118	LEU	CB-CG-CD2	-5.89	100.99	111.00
1	JE	93	ASP	CB-CG-OD1	5.87	123.58	118.30
2	Jm	217	LEU	CA-CB-CG	5.87	128.79	115.30
1	GE	135	ASP	CB-CG-OD1	5.85	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AE	135	ASP	CB-CG-OD1	5.84	123.56	118.30
1	IB	112	LEU	CB-CG-CD2	-5.84	101.07	111.00
5	KX	410	ARG	CD-NE-CZ	5.84	131.78	123.60
2	FM	195	LEU	CA-CB-CG	5.83	128.72	115.30
1	LC	159	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	FE	124	ILE	CG1-CB-CG2	-5.83	98.59	111.40
5	DX	410	ARG	CD-NE-CZ	5.82	131.74	123.60
5	AX	410	ARG	CD-NE-CZ	5.81	131.74	123.60
5	IX	410	ARG	CD-NE-CZ	5.81	131.74	123.60
1	EB	121	GLU	CA-CB-CG	-5.81	100.63	113.40
5	GX	410	ARG	CD-NE-CZ	5.81	131.73	123.60
1	JD	136	LEU	CB-CG-CD2	5.81	120.87	111.00
5	BX	410	ARG	CD-NE-CZ	5.80	131.72	123.60
5	EX	410	ARG	CD-NE-CZ	5.80	131.72	123.60
5	JX	410	ARG	CD-NE-CZ	5.80	131.72	123.60
5	CX	410	ARG	CD-NE-CZ	5.80	131.72	123.60
5	NX	410	ARG	CD-NE-CZ	5.80	131.72	123.60
5	FX	410	ARG	CD-NE-CZ	5.79	131.70	123.60
5	LX	410	ARG	CD-NE-CZ	5.79	131.70	123.60
2	Km	217	LEU	CA-CB-CG	5.78	128.60	115.30
5	MX	410	ARG	CD-NE-CZ	5.77	131.68	123.60
5	HX	410	ARG	CD-NE-CZ	5.77	131.68	123.60
2	NM	221	ASP	CB-CG-OD2	5.76	123.49	118.30
1	HE	118	LEU	CB-CG-CD2	5.76	120.80	111.00
1	DD	94	TRP	CA-CB-CG	5.75	124.63	113.70
2	AM	195	LEU	CA-CB-CG	5.75	128.53	115.30
1	CB	118	LEU	CB-CG-CD2	5.73	120.74	111.00
1	MC	151	ASN	N-CA-CB	-5.71	100.32	110.60
1	HB	118	LEU	CA-CB-CG	5.70	128.40	115.30
1	GE	109	MET	CA-CB-CG	5.69	122.98	113.30
1	BC	110	ASP	CB-CG-OD2	5.69	123.42	118.30
1	CD	120	ILE	CG1-CB-CG2	-5.67	98.92	111.40
1	ED	175	GLN	CA-CB-CG	5.66	125.86	113.40
1	ED	179	LEU	CA-CB-CG	5.66	128.31	115.30
1	HE	93	ASP	CB-CG-OD1	5.65	123.39	118.30
1	BE	135	ASP	CB-CG-OD1	5.64	123.38	118.30
2	Im	341	MET	CG-SD-CE	5.64	109.22	100.20
2	Jm	341	MET	CA-CB-CG	5.60	122.82	113.30
1	DB	156	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	JD	180	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	GC	137	ILE	CG1-CB-CG2	-5.58	99.13	111.40
1	NB	136	LEU	CB-CG-CD1	-5.57	101.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	ME	93	ASP	CB-CG-OD1	5.56	123.31	118.30
1	DC	106	LEU	CA-CB-CG	5.56	128.08	115.30
2	Lm	222	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	KE	105	TYR	CA-CB-CG	5.55	123.95	113.40
1	DB	121	GLU	CB-CA-C	-5.55	99.30	110.40
1	LD	130	MET	CB-CG-SD	-5.54	95.77	112.40
1	FE	135	ASP	CB-CG-OD1	5.54	123.29	118.30
1	KD	81	TYR	OH-CZ-CE2	5.54	135.06	120.10
1	KB	121	GLU	CB-CA-C	-5.54	99.33	110.40
2	NM	195	LEU	CA-CB-CG	5.53	128.02	115.30
1	AD	158	LYS	CD-CE-NZ	-5.53	98.98	111.70
1	NE	135	ASP	CB-CG-OD1	5.53	123.28	118.30
1	DE	81	TYR	C-N-CA	5.52	135.50	121.70
2	GM	195	LEU	CA-CB-CG	5.51	127.98	115.30
1	LB	121	GLU	CB-CA-C	-5.51	99.37	110.40
1	AE	93	ASP	CB-CG-OD1	5.51	123.26	118.30
1	ND	106	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	NA	210	MET	CB-CA-C	5.50	121.41	110.40
1	ID	81	TYR	CB-CA-C	5.49	121.38	110.40
1	FE	179	LEU	CA-CB-CG	5.49	127.92	115.30
1	GA	210	MET	CB-CA-C	5.49	121.37	110.40
1	CA	210	MET	CB-CA-C	5.48	121.37	110.40
1	FA	210	MET	CB-CA-C	5.48	121.36	110.40
1	IE	135	ASP	CB-CG-OD1	5.48	123.23	118.30
1	JA	210	MET	CB-CA-C	5.48	121.37	110.40
1	IA	210	MET	CB-CA-C	5.48	121.36	110.40
1	MA	210	MET	CB-CA-C	5.48	121.35	110.40
1	NB	156	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	JD	130	MET	CA-CB-CG	-5.47	103.99	113.30
1	AA	210	MET	CB-CA-C	5.47	121.34	110.40
1	LA	210	MET	CB-CA-C	5.47	121.34	110.40
1	EA	210	MET	CB-CA-C	5.47	121.34	110.40
1	KA	210	MET	CB-CA-C	5.47	121.33	110.40
1	HD	130	MET	CA-CB-CG	-5.46	104.02	113.30
1	HA	210	MET	CB-CA-C	5.45	121.31	110.40
1	FD	79	ASP	CB-CG-OD2	5.45	123.20	118.30
1	DA	210	MET	CB-CA-C	5.45	121.29	110.40
2	IM	195	LEU	CA-CB-CG	5.44	127.82	115.30
1	DC	130	MET	CA-CB-CG	-5.44	104.05	113.30
2	Gm	222	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	BA	210	MET	CB-CA-C	5.44	121.28	110.40
2	CM	199	GLN	N-CA-CB	5.42	120.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DE	135	ASP	CB-CG-OD1	5.42	123.18	118.30
1	HE	110	ASP	CB-CG-OD2	5.42	123.18	118.30
2	Dm	217	LEU	CA-CB-CG	5.42	127.76	115.30
1	JE	135	ASP	CB-CG-OD1	5.39	123.15	118.30
1	NE	109	MET	CB-CG-SD	5.39	128.57	112.40
1	LC	126	LYS	CD-CE-NZ	-5.38	99.32	111.70
2	AM	199	GLN	N-CA-CB	5.38	120.28	110.60
1	FC	146	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	FE	93	ASP	CB-CG-OD1	5.38	123.14	118.30
1	DE	82	ASP	CB-CG-OD2	-5.38	113.46	118.30
2	IM	199	GLN	N-CA-CB	5.37	120.27	110.60
2	Hm	298	LEU	CA-CB-CG	5.37	127.65	115.30
2	MM	195	LEU	CA-CB-CG	5.36	127.62	115.30
1	EC	159	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	GC	166	LYS	CD-CE-NZ	-5.35	99.39	111.70
2	MM	199	GLN	N-CA-CB	5.35	120.23	110.60
1	CE	156	LEU	CA-CB-CG	5.35	127.60	115.30
1	JD	120	ILE	CG1-CB-CG2	-5.35	99.64	111.40
2	EM	343	ASP	CB-CG-OD2	5.34	123.11	118.30
2	CM	270	TYR	CB-CA-C	5.33	121.07	110.40
1	ND	120	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	EE	135	ASP	CB-CG-OD1	5.33	123.10	118.30
1	ME	135	ASP	CB-CG-OD1	5.33	123.10	118.30
1	HE	107	TYR	CA-CB-CG	5.31	123.49	113.40
2	Hm	222	TYR	CB-CG-CD1	5.30	124.18	121.00
1	AB	118	LEU	CB-CG-CD2	5.30	120.01	111.00
1	CC	153	LEU	CB-CG-CD2	5.29	120.00	111.00
1	LC	184	ARG	CA-CB-CG	5.27	125.00	113.40
3	MT	249	MET	CA-CB-CG	5.27	122.26	113.30
3	NT	249	MET	CA-CB-CG	5.27	122.26	113.30
3	ET	249	MET	CA-CB-CG	5.27	122.25	113.30
3	JT	249	MET	CA-CB-CG	5.27	122.25	113.30
1	CE	135	ASP	CB-CG-OD1	5.26	123.04	118.30
1	KC	137	ILE	CG1-CB-CG2	-5.26	99.82	111.40
3	AT	249	MET	CA-CB-CG	5.26	122.25	113.30
3	LT	249	MET	CA-CB-CG	5.26	122.25	113.30
1	BD	81	TYR	CA-CB-CG	5.26	123.39	113.40
1	HD	180	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	ME	110	ASP	CB-CG-OD2	5.26	123.03	118.30
3	BT	249	MET	CA-CB-CG	5.25	122.23	113.30
3	IT	249	MET	CA-CB-CG	5.25	122.23	113.30
3	FT	249	MET	CA-CB-CG	5.25	122.23	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CT	249	MET	CA-CB-CG	5.25	122.22	113.30
3	DT	249	MET	CA-CB-CG	5.25	122.22	113.30
3	GT	249	MET	CA-CB-CG	5.25	122.22	113.30
1	ND	126	LYS	CD-CE-NZ	-5.25	99.63	111.70
3	HT	249	MET	CA-CB-CG	5.24	122.21	113.30
1	FB	121	GLU	N-CA-CB	5.24	120.03	110.60
1	KE	135	ASP	CB-CG-OD1	5.24	123.01	118.30
1	ED	81	TYR	CB-CA-C	5.23	120.86	110.40
3	KT	249	MET	CA-CB-CG	5.23	122.19	113.30
2	Em	325	LEU	CA-CB-CG	5.21	127.29	115.30
2	KM	232	ASP	CB-CG-OD1	5.21	122.99	118.30
1	EB	121	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	LE	135	ASP	CB-CG-OD1	5.21	122.99	118.30
2	Im	298	LEU	CA-CB-CG	5.21	127.27	115.30
3	BT	274	ARG	CD-NE-CZ	5.20	130.88	123.60
3	NT	274	ARG	CD-NE-CZ	5.19	130.87	123.60
3	FT	274	ARG	CD-NE-CZ	5.19	130.87	123.60
2	Hm	224	LEU	CA-CB-CG	5.19	127.24	115.30
1	JE	105	TYR	CA-CB-CG	5.19	123.26	113.40
3	AT	274	ARG	CD-NE-CZ	5.19	130.87	123.60
3	IT	274	ARG	CD-NE-CZ	5.18	130.85	123.60
3	Ct	76	ASP	CB-CG-OD2	5.17	122.95	118.30
2	CM	195	LEU	CA-CB-CG	5.17	127.19	115.30
2	GM	214	ARG	NE-CZ-NH2	-5.17	117.72	120.30
3	MT	274	ARG	CD-NE-CZ	5.17	130.83	123.60
5	GX	456	ASP	CB-CG-OD1	5.16	122.95	118.30
1	ME	179	LEU	CA-CB-CG	5.16	127.18	115.30
5	MX	456	ASP	CB-CG-OD1	5.16	122.94	118.30
3	ET	274	ARG	CD-NE-CZ	5.16	130.82	123.60
3	JT	274	ARG	CD-NE-CZ	5.16	130.82	123.60
3	Lt	76	ASP	CB-CG-OD2	5.16	122.94	118.30
5	AX	456	ASP	CB-CG-OD1	5.15	122.94	118.30
5	IX	456	ASP	CB-CG-OD1	5.15	122.93	118.30
1	DE	105	TYR	CA-CB-CG	5.15	123.18	113.40
5	CX	456	ASP	CB-CG-OD1	5.14	122.93	118.30
3	Ft	76	ASP	CB-CG-OD2	5.14	122.93	118.30
3	GT	274	ARG	CD-NE-CZ	5.14	130.80	123.60
1	NC	110	ASP	CB-CG-OD2	5.14	122.93	118.30
3	DT	274	ARG	CD-NE-CZ	5.14	130.80	123.60
3	KT	274	ARG	CD-NE-CZ	5.14	130.80	123.60
5	KX	456	ASP	CB-CG-OD1	5.14	122.93	118.30
3	LT	274	ARG	CD-NE-CZ	5.14	130.79	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	FC	153	LEU	CB-CG-CD2	5.13	119.73	111.00
3	IT	152	ASP	CB-CG-OD1	5.13	122.92	118.30
3	HT	274	ARG	CD-NE-CZ	5.13	130.79	123.60
5	NX	456	ASP	CB-CG-OD1	5.13	122.92	118.30
3	AT	152	ASP	CB-CG-OD1	5.13	122.92	118.30
3	CT	274	ARG	CD-NE-CZ	5.13	130.78	123.60
3	JT	152	ASP	CB-CG-OD1	5.13	122.92	118.30
3	Nt	76	ASP	CB-CG-OD2	5.13	122.92	118.30
3	Ft	230	TYR	CB-CG-CD1	-5.12	117.93	121.00
5	HX	456	ASP	CB-CG-OD1	5.12	122.91	118.30
3	It	76	ASP	CB-CG-OD2	5.12	122.91	118.30
5	BX	456	ASP	CB-CG-OD1	5.12	122.91	118.30
3	Bt	76	ASP	CB-CG-OD2	5.12	122.90	118.30
5	EX	456	ASP	CB-CG-OD1	5.11	122.90	118.30
5	LX	456	ASP	CB-CG-OD1	5.11	122.90	118.30
3	Gt	76	ASP	CB-CG-OD2	5.11	122.90	118.30
3	DT	152	ASP	CB-CG-OD1	5.11	122.90	118.30
5	FX	456	ASP	CB-CG-OD1	5.10	122.89	118.30
3	Jt	76	ASP	CB-CG-OD2	5.10	122.89	118.30
1	BB	118	LEU	CA-CB-CG	5.10	127.02	115.30
3	Kt	76	ASP	CB-CG-OD2	5.10	122.89	118.30
3	Et	230	TYR	CB-CG-CD1	-5.09	117.94	121.00
3	Lt	230	TYR	CB-CG-CD1	-5.09	117.94	121.00
5	JX	456	ASP	CB-CG-OD1	5.09	122.88	118.30
1	KE	82	ASP	CB-CG-OD1	5.09	122.88	118.30
2	NM	199	GLN	N-CA-CB	5.09	119.76	110.60
3	At	76	ASP	CB-CG-OD2	5.08	122.88	118.30
3	Dt	230	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	Et	76	ASP	CB-CG-OD2	5.08	122.88	118.30
1	MB	118	LEU	CA-CB-CG	5.08	126.99	115.30
2	Dm	340	MET	CA-CB-CG	5.08	121.94	113.30
3	Dt	76	ASP	CB-CG-OD2	5.08	122.87	118.30
3	ET	152	ASP	CB-CG-OD1	5.08	122.87	118.30
1	KC	110	ASP	CB-CG-OD2	5.08	122.87	118.30
3	Ct	230	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	BD	81	TYR	CB-CA-C	5.07	120.55	110.40
3	FT	152	ASP	CB-CG-OD1	5.07	122.86	118.30
1	ID	81	TYR	CA-CB-CG	5.07	123.03	113.40
3	Nt	230	TYR	CB-CG-CD1	-5.07	117.96	121.00
3	It	260	LEU	CA-CB-CG	5.07	126.95	115.30
2	GM	199	GLN	N-CA-CB	5.07	119.72	110.60
1	LE	101	LYS	CA-CB-CG	5.07	124.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	At	260	LEU	CA-CB-CG	5.06	126.95	115.30
5	DX	456	ASP	CB-CG-OD1	5.06	122.86	118.30
3	Bt	260	LEU	CA-CB-CG	5.06	126.94	115.30
3	Ht	76	ASP	CB-CG-OD2	5.06	122.86	118.30
1	ID	77	LEU	CA-CB-CG	5.06	126.94	115.30
3	Ht	260	LEU	CA-CB-CG	5.06	126.94	115.30
3	CT	152	ASP	CB-CG-OD1	5.06	122.85	118.30
3	Dt	260	LEU	CA-CB-CG	5.06	126.94	115.30
3	KT	152	ASP	CB-CG-OD1	5.06	122.85	118.30
3	NT	152	ASP	CB-CG-OD1	5.06	122.85	118.30
1	AB	118	LEU	CA-CB-CG	5.06	126.93	115.30
3	GT	152	ASP	CB-CG-OD1	5.06	122.85	118.30
3	It	230	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	BD	77	LEU	CA-CB-CG	5.05	126.92	115.30
2	FM	199	GLN	N-CA-CB	5.05	119.69	110.60
3	Ct	260	LEU	CA-CB-CG	5.05	126.91	115.30
3	LT	152	ASP	CB-CG-OD1	5.05	122.84	118.30
3	Mt	76	ASP	CB-CG-OD2	5.05	122.84	118.30
3	Et	260	LEU	CA-CB-CG	5.05	126.91	115.30
3	Ft	260	LEU	CA-CB-CG	5.05	126.91	115.30
3	Gt	260	LEU	CA-CB-CG	5.05	126.91	115.30
3	Ht	230	TYR	CB-CG-CD1	-5.05	117.97	121.00
3	Kt	230	TYR	CB-CG-CD1	-5.05	117.97	121.00
3	MT	152	ASP	CB-CG-OD1	5.05	122.84	118.30
3	Mt	230	TYR	CB-CG-CD1	-5.05	117.97	121.00
3	HT	152	ASP	CB-CG-OD1	5.04	122.84	118.30
2	BM	341	MET	CA-CB-CG	5.04	121.87	113.30
3	Bt	230	TYR	CB-CG-CD1	-5.04	117.98	121.00
3	Kt	260	LEU	CA-CB-CG	5.04	126.89	115.30
3	Jt	230	TYR	CB-CG-CD1	-5.04	117.98	121.00
3	Mt	260	LEU	CA-CB-CG	5.04	126.89	115.30
3	Lt	260	LEU	CA-CB-CG	5.04	126.88	115.30
1	AC	118	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	FC	151	ASN	N-CA-CB	-5.03	101.54	110.60
3	Nt	260	LEU	CA-CB-CG	5.03	126.88	115.30
2	Lm	341	MET	CA-CB-CG	5.03	121.85	113.30
1	CD	180	ARG	NE-CZ-NH2	-5.02	117.79	120.30
3	Jt	260	LEU	CA-CB-CG	5.02	126.85	115.30
1	ND	128	ARG	NE-CZ-NH2	5.02	122.81	120.30
2	Cm	224	LEU	CA-CB-CG	5.02	126.84	115.30
1	KE	107	TYR	OH-CZ-CE2	-5.01	106.56	120.10
3	BT	152	ASP	CB-CG-OD1	5.01	122.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	JC	137	ILE	CG1-CB-CG2	-5.01	100.38	111.40
1	GD	158	LYS	CD-CE-NZ	-5.01	100.19	111.70
2	LM	341	MET	CG-SD-CE	5.00	108.20	100.20

There are no chirality outliers.

All (107) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	253	TYR	Peptide
1	AA	275	ALA	Peptide
1	AA	304	LYS	Peptide
1	AD	131	GLY	Peptide
1	AD	94	TRP	Peptide
1	AE	104	THR	Peptide
5	AX	498	THR	Peptide
2	Am	343	ASP	Peptide
1	BA	253	TYR	Peptide
1	BA	275	ALA	Peptide
1	BA	304	LYS	Peptide
1	BD	169	GLU	Sidechain
1	BD	81	TYR	Sidechain
5	BX	498	THR	Peptide
2	Bm	342	SER	Peptide
2	Bm	343	ASP	Peptide
1	CA	253	TYR	Peptide
1	CA	275	ALA	Peptide
1	CA	304	LYS	Peptide
1	CB	121	GLU	Sidechain
1	CD	131	GLY	Peptide
5	CX	498	THR	Peptide
2	Cm	343	ASP	Peptide
1	DA	253	TYR	Peptide
1	DA	275	ALA	Peptide
1	DA	304	LYS	Peptide
1	DB	121	GLU	Sidechain
5	DX	498	THR	Peptide
2	Dm	343	ASP	Peptide
1	EA	253	TYR	Peptide
1	EA	275	ALA	Peptide
1	EA	304	LYS	Peptide
1	ED	131	GLY	Peptide
1	EE	108	ALA	Peptide

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Mol	Chain	Res	Type	Group
5	EX	498	THR	Peptide
2	Em	343	ASP	Peptide
1	FA	253	TYR	Peptide
1	FA	275	ALA	Peptide
1	FA	304	LYS	Peptide
1	FB	121	GLU	Sidechain
1	FE	107	TYR	Sidechain
5	FX	498	THR	Peptide
2	Fm	343	ASP	Peptide
1	GA	253	TYR	Peptide
1	GA	275	ALA	Peptide
1	GA	304	LYS	Peptide
1	GC	179	LEU	Peptide
1	GD	131	GLY	Peptide
1	GD	94	TRP	Peptide
1	GE	149	TYR	Sidechain
5	GX	498	THR	Peptide
2	Gm	343	ASP	Peptide
1	HA	253	TYR	Peptide
1	HA	275	ALA	Peptide
1	HA	304	LYS	Peptide
1	HB	121	GLU	Sidechain
1	HD	131	GLY	Peptide
1	HD	179	LEU	Peptide
5	HX	498	THR	Peptide
2	Hm	343	ASP	Peptide
1	IA	253	TYR	Peptide
1	IA	275	ALA	Peptide
1	IA	304	LYS	Peptide
5	IX	498	THR	Peptide
2	Im	343	ASP	Peptide
1	JA	253	TYR	Peptide
1	JA	275	ALA	Peptide
1	JA	304	LYS	Peptide
1	JB	121	GLU	Sidechain
1	JD	130	MET	Peptide
1	JD	131	GLY	Peptide
5	JX	498	THR	Peptide
2	Jm	342	SER	Peptide
1	KA	253	TYR	Peptide
1	KA	275	ALA	Peptide
1	KA	304	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	KB	121	GLU	Sidechain
1	KD	142	SER	Peptide
1	KD	81	TYR	Sidechain
1	KE	105	TYR	Sidechain
1	KE	107	TYR	Sidechain
5	KX	498	THR	Peptide
2	Km	343	ASP	Peptide
1	LA	253	TYR	Peptide
1	LA	275	ALA	Peptide
1	LA	304	LYS	Peptide
1	LB	121	GLU	Sidechain
1	LD	131	GLY	Peptide
2	LM	344	LYS	Peptide
5	LX	498	THR	Peptide
2	Lm	343	ASP	Peptide
1	MA	253	TYR	Peptide
1	MA	275	ALA	Peptide
1	MA	304	LYS	Peptide
1	MB	121	GLU	Sidechain
1	MD	81	TYR	Sidechain
1	ME	107	TYR	Sidechain
5	MX	498	THR	Peptide
2	Mm	343	ASP	Peptide
1	NA	253	TYR	Peptide
1	NA	275	ALA	Peptide
1	NA	304	LYS	Peptide
1	NC	179	LEU	Peptide
1	ND	131	GLY	Peptide
1	NE	149	TYR	Sidechain
5	NX	498	THR	Peptide
2	Nm	343	ASP	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	AB	88/481 (18%)	81 (92%)	7 (8%)	0	100	100
1	AC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	AD	91/481 (19%)	80 (88%)	11 (12%)	0	100	100
1	AE	102/481 (21%)	97 (95%)	5 (5%)	0	100	100
1	BA	246/481 (51%)	217 (88%)	29 (12%)	0	100	100
1	BB	88/481 (18%)	84 (96%)	4 (4%)	0	100	100
1	BC	90/481 (19%)	84 (93%)	6 (7%)	0	100	100
1	BD	91/481 (19%)	79 (87%)	11 (12%)	1 (1%)	14	44
1	BE	102/481 (21%)	96 (94%)	6 (6%)	0	100	100
1	CA	246/481 (51%)	217 (88%)	29 (12%)	0	100	100
1	CB	88/481 (18%)	83 (94%)	5 (6%)	0	100	100
1	CC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	CD	91/481 (19%)	77 (85%)	14 (15%)	0	100	100
1	CE	102/481 (21%)	99 (97%)	3 (3%)	0	100	100
1	DA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	DB	88/481 (18%)	81 (92%)	7 (8%)	0	100	100
1	DC	90/481 (19%)	86 (96%)	4 (4%)	0	100	100
1	DD	91/481 (19%)	76 (84%)	15 (16%)	0	100	100
1	DE	102/481 (21%)	94 (92%)	8 (8%)	0	100	100
1	EA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	EB	88/481 (18%)	81 (92%)	7 (8%)	0	100	100
1	EC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	ED	91/481 (19%)	78 (86%)	13 (14%)	0	100	100
1	EE	102/481 (21%)	98 (96%)	4 (4%)	0	100	100
1	FA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	FB	88/481 (18%)	82 (93%)	6 (7%)	0	100	100
1	FC	90/481 (19%)	84 (93%)	6 (7%)	0	100	100
1	FD	91/481 (19%)	77 (85%)	14 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FE	102/481 (21%)	96 (94%)	6 (6%)	0	100	100
1	GA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	GB	88/481 (18%)	84 (96%)	4 (4%)	0	100	100
1	GC	90/481 (19%)	84 (93%)	6 (7%)	0	100	100
1	GD	91/481 (19%)	79 (87%)	12 (13%)	0	100	100
1	GE	102/481 (21%)	95 (93%)	7 (7%)	0	100	100
1	HA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	HB	88/481 (18%)	83 (94%)	5 (6%)	0	100	100
1	HC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	HD	91/481 (19%)	77 (85%)	14 (15%)	0	100	100
1	HE	102/481 (21%)	96 (94%)	6 (6%)	0	100	100
1	IA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	IB	88/481 (18%)	84 (96%)	4 (4%)	0	100	100
1	IC	90/481 (19%)	86 (96%)	4 (4%)	0	100	100
1	ID	91/481 (19%)	78 (86%)	12 (13%)	1 (1%)	14	44
1	IE	102/481 (21%)	96 (94%)	6 (6%)	0	100	100
1	JA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	JB	88/481 (18%)	83 (94%)	5 (6%)	0	100	100
1	JC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	JD	91/481 (19%)	79 (87%)	12 (13%)	0	100	100
1	JE	102/481 (21%)	97 (95%)	5 (5%)	0	100	100
1	KA	246/481 (51%)	217 (88%)	29 (12%)	0	100	100
1	KB	88/481 (18%)	81 (92%)	7 (8%)	0	100	100
1	KC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	KD	91/481 (19%)	80 (88%)	11 (12%)	0	100	100
1	KE	102/481 (21%)	96 (94%)	6 (6%)	0	100	100
1	LA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	LB	88/481 (18%)	79 (90%)	9 (10%)	0	100	100
1	LC	90/481 (19%)	84 (93%)	6 (7%)	0	100	100
1	LD	91/481 (19%)	76 (84%)	15 (16%)	0	100	100
1	LE	102/481 (21%)	96 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	MA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	MB	88/481 (18%)	84 (96%)	4 (4%)	0	100	100
1	MC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	MD	91/481 (19%)	79 (87%)	12 (13%)	0	100	100
1	ME	102/481 (21%)	97 (95%)	5 (5%)	0	100	100
1	NA	246/481 (51%)	216 (88%)	30 (12%)	0	100	100
1	NB	88/481 (18%)	81 (92%)	7 (8%)	0	100	100
1	NC	90/481 (19%)	85 (94%)	5 (6%)	0	100	100
1	ND	91/481 (19%)	80 (88%)	11 (12%)	0	100	100
1	NE	102/481 (21%)	97 (95%)	5 (5%)	0	100	100
2	AM	178/376 (47%)	170 (96%)	8 (4%)	0	100	100
2	Am	177/376 (47%)	167 (94%)	10 (6%)	0	100	100
2	BM	178/376 (47%)	170 (96%)	8 (4%)	0	100	100
2	Bm	177/376 (47%)	169 (96%)	8 (4%)	0	100	100
2	CM	178/376 (47%)	170 (96%)	8 (4%)	0	100	100
2	Cm	177/376 (47%)	166 (94%)	11 (6%)	0	100	100
2	DM	178/376 (47%)	172 (97%)	6 (3%)	0	100	100
2	Dm	177/376 (47%)	168 (95%)	9 (5%)	0	100	100
2	EM	178/376 (47%)	169 (95%)	9 (5%)	0	100	100
2	Em	177/376 (47%)	169 (96%)	8 (4%)	0	100	100
2	FM	178/376 (47%)	171 (96%)	7 (4%)	0	100	100
2	Fm	177/376 (47%)	166 (94%)	11 (6%)	0	100	100
2	GM	178/376 (47%)	167 (94%)	11 (6%)	0	100	100
2	Gm	177/376 (47%)	167 (94%)	10 (6%)	0	100	100
2	HM	178/376 (47%)	169 (95%)	9 (5%)	0	100	100
2	Hm	177/376 (47%)	167 (94%)	10 (6%)	0	100	100
2	IM	178/376 (47%)	171 (96%)	7 (4%)	0	100	100
2	Im	177/376 (47%)	168 (95%)	9 (5%)	0	100	100
2	JM	178/376 (47%)	170 (96%)	8 (4%)	0	100	100
2	Jm	177/376 (47%)	168 (95%)	9 (5%)	0	100	100
2	KM	178/376 (47%)	172 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Km	177/376 (47%)	169 (96%)	8 (4%)	0	100	100
2	LM	178/376 (47%)	168 (94%)	10 (6%)	0	100	100
2	Lm	177/376 (47%)	170 (96%)	7 (4%)	0	100	100
2	MM	178/376 (47%)	170 (96%)	8 (4%)	0	100	100
2	Mm	177/376 (47%)	168 (95%)	9 (5%)	0	100	100
2	NM	178/376 (47%)	169 (95%)	9 (5%)	0	100	100
2	Nm	177/376 (47%)	168 (95%)	9 (5%)	0	100	100
3	AT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	At	186/280 (66%)	179 (96%)	7 (4%)	0	100	100
3	BT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Bt	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	CT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Ct	186/280 (66%)	179 (96%)	7 (4%)	0	100	100
3	DT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Dt	186/280 (66%)	179 (96%)	7 (4%)	0	100	100
3	ET	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Et	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	FT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Ft	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	GT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Gt	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	HT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Ht	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	IT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	It	186/280 (66%)	179 (96%)	7 (4%)	0	100	100
3	JT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Jt	186/280 (66%)	179 (96%)	7 (4%)	0	100	100
3	KT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Kt	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	LT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Lt	186/280 (66%)	178 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	MT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Mt	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
3	NT	251/280 (90%)	242 (96%)	9 (4%)	0	100	100
3	Nt	186/280 (66%)	178 (96%)	8 (4%)	0	100	100
5	AX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	BX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	CX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	DX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	EX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	FX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	GX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	HX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	IX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	JX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	KX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	LX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	MX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
5	NX	164/522 (31%)	156 (95%)	8 (5%)	0	100	100
6	AY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	BY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	CY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	DY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	EY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	FY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	GY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	HY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	IY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	JY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	KY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	LY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
6	MY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	NY	199/1927 (10%)	190 (96%)	9 (4%)	0	100	100
All	All	24808/86324 (29%)	23268 (94%)	1538 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	ID	160	ASN
1	BD	160	ASN

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	AA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	AB	79/433 (18%)	79 (100%)	0	100	100
1	AC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	AD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	AE	91/433 (21%)	91 (100%)	0	100	100
1	BA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	BB	79/433 (18%)	79 (100%)	0	100	100
1	BC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	BD	83/433 (19%)	80 (96%)	3 (4%)	35	63
1	BE	91/433 (21%)	91 (100%)	0	100	100
1	CA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	CB	79/433 (18%)	79 (100%)	0	100	100
1	CC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	CD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	CE	91/433 (21%)	91 (100%)	0	100	100
1	DA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	DB	79/433 (18%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	DD	83/433 (19%)	81 (98%)	2 (2%)	49	74
1	DE	91/433 (21%)	91 (100%)	0	100	100
1	EA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	EB	79/433 (18%)	79 (100%)	0	100	100
1	EC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	ED	83/433 (19%)	81 (98%)	2 (2%)	49	74
1	EE	91/433 (21%)	91 (100%)	0	100	100
1	FA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	FB	79/433 (18%)	79 (100%)	0	100	100
1	FC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	FD	83/433 (19%)	81 (98%)	2 (2%)	49	74
1	FE	91/433 (21%)	91 (100%)	0	100	100
1	GA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	GB	79/433 (18%)	79 (100%)	0	100	100
1	GC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	GD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	GE	91/433 (21%)	91 (100%)	0	100	100
1	HA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	HB	79/433 (18%)	79 (100%)	0	100	100
1	HC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	HD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	HE	91/433 (21%)	91 (100%)	0	100	100
1	IA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	IB	79/433 (18%)	79 (100%)	0	100	100
1	IC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	ID	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	IE	91/433 (21%)	91 (100%)	0	100	100
1	JA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	JB	79/433 (18%)	79 (100%)	0	100	100
1	JC	80/433 (18%)	79 (99%)	1 (1%)	69	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	JE	91/433 (21%)	91 (100%)	0	100	100
1	KA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	KB	79/433 (18%)	79 (100%)	0	100	100
1	KC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	KD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	KE	91/433 (21%)	90 (99%)	1 (1%)	73	86
1	LA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	LB	79/433 (18%)	79 (100%)	0	100	100
1	LC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	LD	83/433 (19%)	81 (98%)	2 (2%)	49	74
1	LE	91/433 (21%)	91 (100%)	0	100	100
1	MA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	MB	79/433 (18%)	79 (100%)	0	100	100
1	MC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	MD	83/433 (19%)	82 (99%)	1 (1%)	71	85
1	ME	91/433 (21%)	91 (100%)	0	100	100
1	NA	220/433 (51%)	214 (97%)	6 (3%)	44	70
1	NB	79/433 (18%)	79 (100%)	0	100	100
1	NC	80/433 (18%)	79 (99%)	1 (1%)	69	84
1	ND	83/433 (19%)	81 (98%)	2 (2%)	49	74
1	NE	91/433 (21%)	91 (100%)	0	100	100
2	AM	168/342 (49%)	168 (100%)	0	100	100
2	Am	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	BM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Bm	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	CM	168/342 (49%)	166 (99%)	2 (1%)	71	85
2	Cm	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	DM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Dm	167/342 (49%)	165 (99%)	2 (1%)	71	85
2	EM	168/342 (49%)	167 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Em	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	FM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Fm	167/342 (49%)	167 (100%)	0	100	100
2	GM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Gm	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	HM	168/342 (49%)	168 (100%)	0	100	100
2	Hm	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	IM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Im	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	JM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Jm	167/342 (49%)	167 (100%)	0	100	100
2	KM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Km	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	LM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Lm	167/342 (49%)	166 (99%)	1 (1%)	86	94
2	MM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Mm	167/342 (49%)	167 (100%)	0	100	100
2	NM	168/342 (49%)	167 (99%)	1 (1%)	86	94
2	Nm	167/342 (49%)	166 (99%)	1 (1%)	86	94
3	AT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	At	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	BT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Bt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	CT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Ct	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	DT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Dt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	ET	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Et	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	FT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Ft	181/255 (71%)	175 (97%)	6 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	GT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Gt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	HT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Ht	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	IT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	It	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	JT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Jt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	KT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Kt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	LT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Lt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	MT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Mt	181/255 (71%)	175 (97%)	6 (3%)	38	66
3	NT	234/255 (92%)	227 (97%)	7 (3%)	41	68
3	Nt	181/255 (71%)	175 (97%)	6 (3%)	38	66
5	AX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	BX	148/470 (32%)	138 (93%)	10 (7%)	16	45
5	CX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	DX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	EX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	FX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	GX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	HX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	IX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	JX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	KX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	LX	148/470 (32%)	138 (93%)	10 (7%)	16	45
5	MX	148/470 (32%)	139 (94%)	9 (6%)	18	48
5	NX	148/470 (32%)	139 (94%)	9 (6%)	18	48
6	AY	171/1724 (10%)	163 (95%)	8 (5%)	26	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	CY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	DY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	EY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	FY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	GY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	HY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	IY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	JY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	KY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	LY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	MY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
6	NY	171/1724 (10%)	163 (95%)	8 (5%)	26	57
All	All	22708/77742 (29%)	22141 (98%)	567 (2%)	50	72

All (567) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	130	MET
1	AA	159	ARG
1	AA	184	ARG
1	AA	210	MET
1	AA	225	GLU
1	AA	302	ARG
1	AC	180	ARG
1	AD	159	ARG
3	AT	45	GLU
3	AT	103	LEU
3	AT	187	ARG
3	AT	249	MET
3	AT	259	LYS
3	AT	267	GLU
3	AT	274	ARG
5	AX	356	MET
5	AX	365	LYS
5	AX	384	GLU
5	AX	393	LYS

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Mol	Chain	Res	Type
5	AX	408	GLU
5	AX	410	ARG
5	AX	418	GLU
5	AX	474	GLU
5	AX	484	LEU
6	AY	1691	VAL
6	AY	1739	TYR
6	AY	1752	MET
6	AY	1780	MET
6	AY	1783	GLU
6	AY	1789	TYR
6	AY	1894	LYS
6	AY	1907	GLN
2	Am	326	LYS
3	At	37	THR
3	At	207	GLU
3	At	213	ARG
3	At	223	THR
3	At	230	TYR
3	At	233	ARG
1	BA	130	MET
1	BA	159	ARG
1	BA	184	ARG
1	BA	210	MET
1	BA	225	GLU
1	BA	302	ARG
1	BC	180	ARG
1	BD	157	ASN
1	BD	159	ARG
1	BD	180	ARG
2	BM	268	ARG
3	BT	45	GLU
3	BT	103	LEU
3	BT	187	ARG
3	BT	249	MET
3	BT	259	LYS
3	BT	267	GLU
3	BT	274	ARG
5	BX	356	MET
5	BX	365	LYS
5	BX	379	GLN
5	BX	384	GLU

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Mol	Chain	Res	Type
5	BX	393	LYS
5	BX	408	GLU
5	BX	410	ARG
5	BX	418	GLU
5	BX	474	GLU
5	BX	484	LEU
6	BY	1691	VAL
6	BY	1739	TYR
6	BY	1752	MET
6	BY	1780	MET
6	BY	1783	GLU
6	BY	1789	TYR
6	BY	1894	LYS
6	BY	1907	GLN
2	Bm	326	LYS
3	Bt	37	THR
3	Bt	207	GLU
3	Bt	213	ARG
3	Bt	223	THR
3	Bt	230	TYR
3	Bt	233	ARG
1	CA	130	MET
1	CA	159	ARG
1	CA	184	ARG
1	CA	210	MET
1	CA	225	GLU
1	CA	302	ARG
1	CC	180	ARG
1	CD	159	ARG
2	CM	268	ARG
2	CM	291	LYS
3	CT	45	GLU
3	CT	103	LEU
3	CT	187	ARG
3	CT	249	MET
3	CT	259	LYS
3	CT	267	GLU
3	CT	274	ARG
5	CX	356	MET
5	CX	365	LYS
5	CX	384	GLU
5	CX	393	LYS

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Mol	Chain	Res	Type
5	CX	408	GLU
5	CX	410	ARG
5	CX	418	GLU
5	CX	474	GLU
5	CX	484	LEU
6	CY	1691	VAL
6	CY	1739	TYR
6	CY	1752	MET
6	CY	1780	MET
6	CY	1783	GLU
6	CY	1789	TYR
6	CY	1894	LYS
6	CY	1907	GLN
2	Cm	199	GLN
3	Ct	37	THR
3	Ct	207	GLU
3	Ct	213	ARG
3	Ct	223	THR
3	Ct	230	TYR
3	Ct	233	ARG
1	DA	130	MET
1	DA	159	ARG
1	DA	184	ARG
1	DA	210	MET
1	DA	225	GLU
1	DA	302	ARG
1	DC	180	ARG
1	DD	159	ARG
1	DD	180	ARG
2	DM	268	ARG
3	DT	45	GLU
3	DT	103	LEU
3	DT	187	ARG
3	DT	249	MET
3	DT	259	LYS
3	DT	267	GLU
3	DT	274	ARG
5	DX	356	MET
5	DX	365	LYS
5	DX	384	GLU
5	DX	393	LYS
5	DX	408	GLU

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Mol	Chain	Res	Type
5	DX	410	ARG
5	DX	418	GLU
5	DX	474	GLU
5	DX	484	LEU
6	DY	1691	VAL
6	DY	1739	TYR
6	DY	1752	MET
6	DY	1780	MET
6	DY	1783	GLU
6	DY	1789	TYR
6	DY	1894	LYS
6	DY	1907	GLN
2	Dm	326	LYS
2	Dm	340	MET
3	Dt	37	THR
3	Dt	207	GLU
3	Dt	213	ARG
3	Dt	223	THR
3	Dt	230	TYR
3	Dt	233	ARG
1	EA	130	MET
1	EA	159	ARG
1	EA	184	ARG
1	EA	210	MET
1	EA	225	GLU
1	EA	302	ARG
1	EC	180	ARG
1	ED	159	ARG
1	ED	180	ARG
2	EM	268	ARG
3	ET	45	GLU
3	ET	103	LEU
3	ET	187	ARG
3	ET	249	MET
3	ET	259	LYS
3	ET	267	GLU
3	ET	274	ARG
5	EX	356	MET
5	EX	365	LYS
5	EX	384	GLU
5	EX	393	LYS
5	EX	408	GLU

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Mol	Chain	Res	Type
5	EX	410	ARG
5	EX	418	GLU
5	EX	474	GLU
5	EX	484	LEU
6	EY	1691	VAL
6	EY	1739	TYR
6	EY	1752	MET
6	EY	1780	MET
6	EY	1783	GLU
6	EY	1789	TYR
6	EY	1894	LYS
6	EY	1907	GLN
2	Em	326	LYS
3	Et	37	THR
3	Et	207	GLU
3	Et	213	ARG
3	Et	223	THR
3	Et	230	TYR
3	Et	233	ARG
1	FA	130	MET
1	FA	159	ARG
1	FA	184	ARG
1	FA	210	MET
1	FA	225	GLU
1	FA	302	ARG
1	FC	180	ARG
1	FD	157	ASN
1	FD	159	ARG
2	FM	268	ARG
3	FT	45	GLU
3	FT	103	LEU
3	FT	187	ARG
3	FT	249	MET
3	FT	259	LYS
3	FT	267	GLU
3	FT	274	ARG
5	FX	356	MET
5	FX	365	LYS
5	FX	384	GLU
5	FX	393	LYS
5	FX	408	GLU
5	FX	410	ARG

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Mol	Chain	Res	Type
5	FX	418	GLU
5	FX	474	GLU
5	FX	484	LEU
6	FY	1691	VAL
6	FY	1739	TYR
6	FY	1752	MET
6	FY	1780	MET
6	FY	1783	GLU
6	FY	1789	TYR
6	FY	1894	LYS
6	FY	1907	GLN
3	Ft	37	THR
3	Ft	207	GLU
3	Ft	213	ARG
3	Ft	223	THR
3	Ft	230	TYR
3	Ft	233	ARG
1	GA	130	MET
1	GA	159	ARG
1	GA	184	ARG
1	GA	210	MET
1	GA	225	GLU
1	GA	302	ARG
1	GC	180	ARG
1	GD	159	ARG
2	GM	268	ARG
3	GT	45	GLU
3	GT	103	LEU
3	GT	187	ARG
3	GT	249	MET
3	GT	259	LYS
3	GT	267	GLU
3	GT	274	ARG
5	GX	356	MET
5	GX	365	LYS
5	GX	384	GLU
5	GX	393	LYS
5	GX	408	GLU
5	GX	410	ARG
5	GX	418	GLU
5	GX	474	GLU
5	GX	484	LEU

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Mol	Chain	Res	Type
6	GY	1691	VAL
6	GY	1739	TYR
6	GY	1752	MET
6	GY	1780	MET
6	GY	1783	GLU
6	GY	1789	TYR
6	GY	1894	LYS
6	GY	1907	GLN
2	Gm	326	LYS
3	Gt	37	THR
3	Gt	207	GLU
3	Gt	213	ARG
3	Gt	223	THR
3	Gt	230	TYR
3	Gt	233	ARG
1	HA	130	MET
1	HA	159	ARG
1	HA	184	ARG
1	HA	210	MET
1	HA	225	GLU
1	HA	302	ARG
1	HC	180	ARG
1	HD	159	ARG
3	HT	45	GLU
3	HT	103	LEU
3	HT	187	ARG
3	HT	249	MET
3	HT	259	LYS
3	HT	267	GLU
3	HT	274	ARG
5	HX	356	MET
5	HX	365	LYS
5	HX	384	GLU
5	HX	393	LYS
5	HX	408	GLU
5	HX	410	ARG
5	HX	418	GLU
5	HX	474	GLU
5	HX	484	LEU
6	HY	1691	VAL
6	HY	1739	TYR
6	HY	1752	MET

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Mol	Chain	Res	Type
6	HY	1780	MET
6	HY	1783	GLU
6	HY	1789	TYR
6	HY	1894	LYS
6	HY	1907	GLN
2	Hm	326	LYS
3	Ht	37	THR
3	Ht	207	GLU
3	Ht	213	ARG
3	Ht	223	THR
3	Ht	230	TYR
3	Ht	233	ARG
1	IA	130	MET
1	IA	159	ARG
1	IA	184	ARG
1	IA	210	MET
1	IA	225	GLU
1	IA	302	ARG
1	IC	180	ARG
1	ID	159	ARG
2	IM	268	ARG
3	IT	45	GLU
3	IT	103	LEU
3	IT	187	ARG
3	IT	249	MET
3	IT	259	LYS
3	IT	267	GLU
3	IT	274	ARG
5	IX	356	MET
5	IX	365	LYS
5	IX	384	GLU
5	IX	393	LYS
5	IX	408	GLU
5	IX	410	ARG
5	IX	418	GLU
5	IX	474	GLU
5	IX	484	LEU
6	IY	1691	VAL
6	IY	1739	TYR
6	IY	1752	MET
6	IY	1780	MET
6	IY	1783	GLU

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Mol	Chain	Res	Type
6	IY	1789	TYR
6	IY	1894	LYS
6	IY	1907	GLN
2	Im	326	LYS
3	It	37	THR
3	It	207	GLU
3	It	213	ARG
3	It	223	THR
3	It	230	TYR
3	It	233	ARG
1	JA	130	MET
1	JA	159	ARG
1	JA	184	ARG
1	JA	210	MET
1	JA	225	GLU
1	JA	302	ARG
1	JC	180	ARG
1	JD	159	ARG
2	JM	268	ARG
3	JT	45	GLU
3	JT	103	LEU
3	JT	187	ARG
3	JT	249	MET
3	JT	259	LYS
3	JT	267	GLU
3	JT	274	ARG
5	JX	356	MET
5	JX	365	LYS
5	JX	384	GLU
5	JX	393	LYS
5	JX	408	GLU
5	JX	410	ARG
5	JX	418	GLU
5	JX	474	GLU
5	JX	484	LEU
6	JY	1691	VAL
6	JY	1739	TYR
6	JY	1752	MET
6	JY	1780	MET
6	JY	1783	GLU
6	JY	1789	TYR
6	JY	1894	LYS

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Mol	Chain	Res	Type
6	JY	1907	GLN
3	Jt	37	THR
3	Jt	207	GLU
3	Jt	213	ARG
3	Jt	223	THR
3	Jt	230	TYR
3	Jt	233	ARG
1	KA	130	MET
1	KA	159	ARG
1	KA	184	ARG
1	KA	210	MET
1	KA	225	GLU
1	KA	302	ARG
1	KC	180	ARG
1	KD	159	ARG
1	KE	175	GLN
2	KM	268	ARG
3	KT	45	GLU
3	KT	103	LEU
3	KT	187	ARG
3	KT	249	MET
3	KT	259	LYS
3	KT	267	GLU
3	KT	274	ARG
5	KX	356	MET
5	KX	365	LYS
5	KX	384	GLU
5	KX	393	LYS
5	KX	408	GLU
5	KX	410	ARG
5	KX	418	GLU
5	KX	474	GLU
5	KX	484	LEU
6	KY	1691	VAL
6	KY	1739	TYR
6	KY	1752	MET
6	KY	1780	MET
6	KY	1783	GLU
6	KY	1789	TYR
6	KY	1894	LYS
6	KY	1907	GLN
2	Km	326	LYS

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Mol	Chain	Res	Type
3	Kt	37	THR
3	Kt	207	GLU
3	Kt	213	ARG
3	Kt	223	THR
3	Kt	230	TYR
3	Kt	233	ARG
1	LA	130	MET
1	LA	159	ARG
1	LA	184	ARG
1	LA	210	MET
1	LA	225	GLU
1	LA	302	ARG
1	LC	180	ARG
1	LD	128	ARG
1	LD	159	ARG
2	LM	268	ARG
3	LT	45	GLU
3	LT	103	LEU
3	LT	187	ARG
3	LT	249	MET
3	LT	259	LYS
3	LT	267	GLU
3	LT	274	ARG
5	LX	356	MET
5	LX	365	LYS
5	LX	379	GLN
5	LX	384	GLU
5	LX	393	LYS
5	LX	408	GLU
5	LX	410	ARG
5	LX	418	GLU
5	LX	474	GLU
5	LX	484	LEU
6	LY	1691	VAL
6	LY	1739	TYR
6	LY	1752	MET
6	LY	1780	MET
6	LY	1783	GLU
6	LY	1789	TYR
6	LY	1894	LYS
6	LY	1907	GLN
2	Lm	326	LYS

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Mol	Chain	Res	Type
3	Lt	37	THR
3	Lt	207	GLU
3	Lt	213	ARG
3	Lt	223	THR
3	Lt	230	TYR
3	Lt	233	ARG
1	MA	130	MET
1	MA	159	ARG
1	MA	184	ARG
1	MA	210	MET
1	MA	225	GLU
1	MA	302	ARG
1	MC	180	ARG
1	MD	159	ARG
2	MM	268	ARG
3	MT	45	GLU
3	MT	103	LEU
3	MT	187	ARG
3	MT	249	MET
3	MT	259	LYS
3	MT	267	GLU
3	MT	274	ARG
5	MX	356	MET
5	MX	365	LYS
5	MX	384	GLU
5	MX	393	LYS
5	MX	408	GLU
5	MX	410	ARG
5	MX	418	GLU
5	MX	474	GLU
5	MX	484	LEU
6	MY	1691	VAL
6	MY	1739	TYR
6	MY	1752	MET
6	MY	1780	MET
6	MY	1783	GLU
6	MY	1789	TYR
6	MY	1894	LYS
6	MY	1907	GLN
3	Mt	37	THR
3	Mt	207	GLU
3	Mt	213	ARG

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Mol	Chain	Res	Type
3	Mt	223	THR
3	Mt	230	TYR
3	Mt	233	ARG
1	NA	130	MET
1	NA	159	ARG
1	NA	184	ARG
1	NA	210	MET
1	NA	225	GLU
1	NA	302	ARG
1	NC	180	ARG
1	ND	126	LYS
1	ND	159	ARG
2	NM	268	ARG
3	NT	45	GLU
3	NT	103	LEU
3	NT	187	ARG
3	NT	249	MET
3	NT	259	LYS
3	NT	267	GLU
3	NT	274	ARG
5	NX	356	MET
5	NX	365	LYS
5	NX	384	GLU
5	NX	393	LYS
5	NX	408	GLU
5	NX	410	ARG
5	NX	418	GLU
5	NX	474	GLU
5	NX	484	LEU
6	NY	1691	VAL
6	NY	1739	TYR
6	NY	1752	MET
6	NY	1780	MET
6	NY	1783	GLU
6	NY	1789	TYR
6	NY	1894	LYS
6	NY	1907	GLN
2	Nm	326	LYS
3	Nt	37	THR
3	Nt	207	GLU
3	Nt	213	ARG
3	Nt	223	THR

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Mol	Chain	Res	Type
3	Nt	230	TYR
3	Nt	233	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	147	ASN
1	AE	87	ASN
1	AE	157	ASN
2	AM	244	ASN
5	AX	379	GLN
2	Am	207	ASN
1	BE	87	ASN
1	BE	157	ASN
2	BM	244	ASN
2	Bm	207	ASN
1	CE	87	ASN
1	CE	157	ASN
2	CM	244	ASN
5	CX	379	GLN
2	Cm	207	ASN
2	Cm	229	ASN
1	DE	87	ASN
1	DE	157	ASN
2	DM	244	ASN
3	DT	231	GLN
5	DX	379	GLN
2	Dm	207	ASN
2	Dm	229	ASN
1	EE	87	ASN
2	EM	244	ASN
3	ET	231	GLN
5	EX	379	GLN
2	Em	207	ASN
1	FC	157	ASN
1	FE	87	ASN
1	FE	157	ASN
2	FM	244	ASN
2	Fm	207	ASN
1	GE	87	ASN
1	GE	157	ASN
2	GM	244	ASN

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Mol	Chain	Res	Type
2	Gm	207	ASN
1	HE	87	ASN
2	HM	244	ASN
2	Hm	207	ASN
1	IC	175	GLN
1	ID	157	ASN
1	IE	87	ASN
1	IE	157	ASN
2	IM	244	ASN
2	Im	207	ASN
1	JE	87	ASN
2	JM	244	ASN
5	JX	379	GLN
2	Jm	207	ASN
1	KE	87	ASN
1	KE	175	GLN
2	KM	244	ASN
5	KX	379	GLN
2	Km	207	ASN
1	LC	175	GLN
1	LE	87	ASN
2	LM	244	ASN
3	LT	231	GLN
2	Lm	207	ASN
1	ME	87	ASN
1	ME	145	GLN
1	ME	157	ASN
2	MM	244	ASN
5	MX	379	GLN
2	Mm	207	ASN
1	NE	87	ASN
1	NE	157	ASN
2	NM	244	ASN
5	NX	379	GLN
2	Nm	207	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	AU	8
4	BU	8
4	CU	8
4	DU	8
4	EU	8
4	FU	8
4	GU	8
4	HU	8
4	IU	8
4	JU	8
4	KU	8
4	LU	8
4	MU	8
4	NU	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AU	723:UNK	C	801:UNK	N	98.58
1	BU	723:UNK	C	801:UNK	N	98.58
1	CU	723:UNK	C	801:UNK	N	98.58

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DU	723:UNK	C	801:UNK	N	98.58
1	EU	723:UNK	C	801:UNK	N	98.58
1	FU	723:UNK	C	801:UNK	N	98.58
1	GU	723:UNK	C	801:UNK	N	98.58
1	HU	723:UNK	C	801:UNK	N	98.58
1	IU	723:UNK	C	801:UNK	N	98.58
1	JU	723:UNK	C	801:UNK	N	98.58
1	KU	723:UNK	C	801:UNK	N	98.58
1	LU	723:UNK	C	801:UNK	N	98.58
1	MU	723:UNK	C	801:UNK	N	98.58
1	NU	723:UNK	C	801:UNK	N	98.58
1	AU	523:UNK	C	601:UNK	N	87.28
1	BU	523:UNK	C	601:UNK	N	87.28
1	CU	523:UNK	C	601:UNK	N	87.28
1	DU	523:UNK	C	601:UNK	N	87.28
1	EU	523:UNK	C	601:UNK	N	87.28
1	FU	523:UNK	C	601:UNK	N	87.28
1	GU	523:UNK	C	601:UNK	N	87.28
1	HU	523:UNK	C	601:UNK	N	87.28
1	IU	523:UNK	C	601:UNK	N	87.28
1	JU	523:UNK	C	601:UNK	N	87.28
1	KU	523:UNK	C	601:UNK	N	87.28
1	LU	523:UNK	C	601:UNK	N	87.28
1	MU	523:UNK	C	601:UNK	N	87.28
1	NU	523:UNK	C	601:UNK	N	87.28
1	AU	422:UNK	C	501:UNK	N	75.39
1	BU	422:UNK	C	501:UNK	N	75.39
1	CU	422:UNK	C	501:UNK	N	75.39
1	DU	422:UNK	C	501:UNK	N	75.39
1	EU	422:UNK	C	501:UNK	N	75.39
1	FU	422:UNK	C	501:UNK	N	75.39
1	GU	422:UNK	C	501:UNK	N	75.39
1	HU	422:UNK	C	501:UNK	N	75.39
1	IU	422:UNK	C	501:UNK	N	75.39
1	JU	422:UNK	C	501:UNK	N	75.39
1	KU	422:UNK	C	501:UNK	N	75.39
1	LU	422:UNK	C	501:UNK	N	75.39
1	MU	422:UNK	C	501:UNK	N	75.39
1	NU	422:UNK	C	501:UNK	N	75.39
1	AU	620:UNK	C	701:UNK	N	74.33
1	BU	620:UNK	C	701:UNK	N	74.33
1	CU	620:UNK	C	701:UNK	N	74.33

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DU	620:UNK	C	701:UNK	N	74.33
1	EU	620:UNK	C	701:UNK	N	74.33
1	FU	620:UNK	C	701:UNK	N	74.33
1	GU	620:UNK	C	701:UNK	N	74.33
1	HU	620:UNK	C	701:UNK	N	74.33
1	IU	620:UNK	C	701:UNK	N	74.33
1	JU	620:UNK	C	701:UNK	N	74.33
1	KU	620:UNK	C	701:UNK	N	74.33
1	LU	620:UNK	C	701:UNK	N	74.33
1	MU	620:UNK	C	701:UNK	N	74.33
1	NU	620:UNK	C	701:UNK	N	74.33
1	AU	10:UNK	C	101:UNK	N	40.07
1	BU	10:UNK	C	101:UNK	N	40.07
1	CU	10:UNK	C	101:UNK	N	40.07
1	DU	10:UNK	C	101:UNK	N	40.07
1	EU	10:UNK	C	101:UNK	N	40.07
1	FU	10:UNK	C	101:UNK	N	40.07
1	GU	10:UNK	C	101:UNK	N	40.07
1	HU	10:UNK	C	101:UNK	N	40.07
1	IU	10:UNK	C	101:UNK	N	40.07
1	JU	10:UNK	C	101:UNK	N	40.07
1	KU	10:UNK	C	101:UNK	N	40.07
1	LU	10:UNK	C	101:UNK	N	40.07
1	MU	10:UNK	C	101:UNK	N	40.07
1	NU	10:UNK	C	101:UNK	N	40.07
1	AU	217:UNK	C	301:UNK	N	29.34
1	BU	217:UNK	C	301:UNK	N	29.34
1	CU	217:UNK	C	301:UNK	N	29.34
1	DU	217:UNK	C	301:UNK	N	29.34
1	EU	217:UNK	C	301:UNK	N	29.34
1	FU	217:UNK	C	301:UNK	N	29.34
1	GU	217:UNK	C	301:UNK	N	29.34
1	HU	217:UNK	C	301:UNK	N	29.34
1	IU	217:UNK	C	301:UNK	N	29.34
1	JU	217:UNK	C	301:UNK	N	29.34
1	KU	217:UNK	C	301:UNK	N	29.34
1	LU	217:UNK	C	301:UNK	N	29.34
1	MU	217:UNK	C	301:UNK	N	29.34
1	NU	217:UNK	C	301:UNK	N	29.34
1	AU	120:UNK	C	201:UNK	N	28.69
1	BU	120:UNK	C	201:UNK	N	28.69
1	CU	120:UNK	C	201:UNK	N	28.69

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DU	120:UNK	C	201:UNK	N	28.69
1	EU	120:UNK	C	201:UNK	N	28.69
1	FU	120:UNK	C	201:UNK	N	28.69
1	GU	120:UNK	C	201:UNK	N	28.69
1	HU	120:UNK	C	201:UNK	N	28.69
1	IU	120:UNK	C	201:UNK	N	28.69
1	JU	120:UNK	C	201:UNK	N	28.69
1	KU	120:UNK	C	201:UNK	N	28.69
1	LU	120:UNK	C	201:UNK	N	28.69
1	MU	120:UNK	C	201:UNK	N	28.69
1	NU	120:UNK	C	201:UNK	N	28.69
1	AU	314:UNK	C	401:UNK	N	17.39
1	BU	314:UNK	C	401:UNK	N	17.39
1	CU	314:UNK	C	401:UNK	N	17.39
1	DU	314:UNK	C	401:UNK	N	17.39
1	EU	314:UNK	C	401:UNK	N	17.39
1	FU	314:UNK	C	401:UNK	N	17.39
1	GU	314:UNK	C	401:UNK	N	17.39
1	HU	314:UNK	C	401:UNK	N	17.39
1	IU	314:UNK	C	401:UNK	N	17.39
1	JU	314:UNK	C	401:UNK	N	17.39
1	KU	314:UNK	C	401:UNK	N	17.39
1	LU	314:UNK	C	401:UNK	N	17.39
1	MU	314:UNK	C	401:UNK	N	17.39
1	NU	314:UNK	C	401:UNK	N	17.39

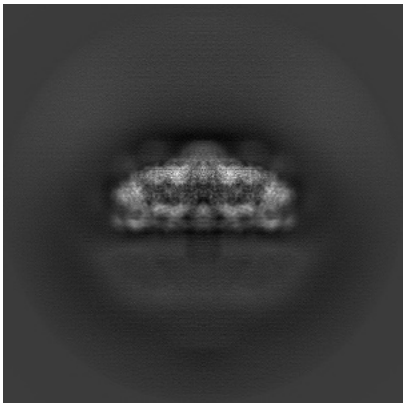
6 Map visualisation (i)

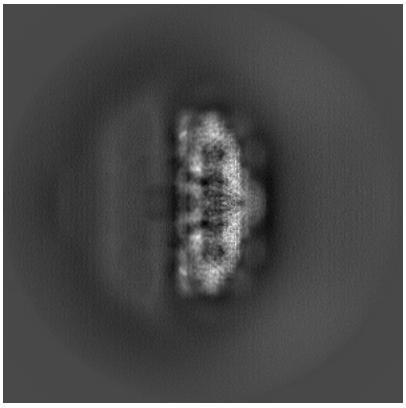
This section contains visualisations of the EMDB entry EMD-22081. These allow visual inspection of the internal detail of the map and identification of artifacts.

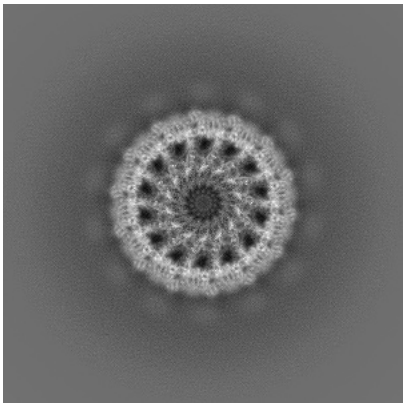
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

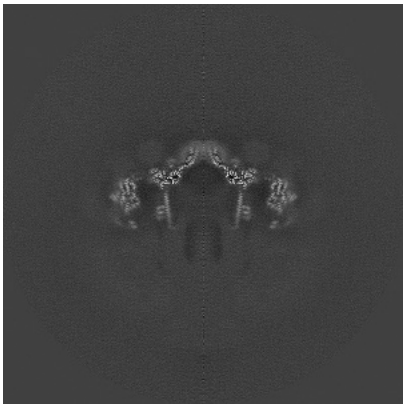

Y

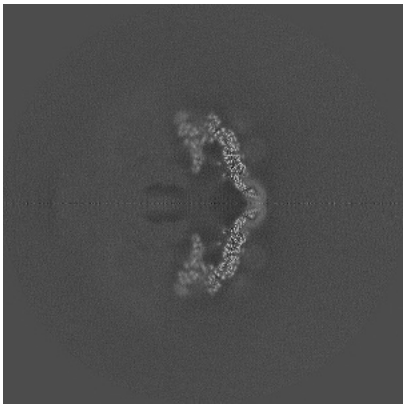

Z

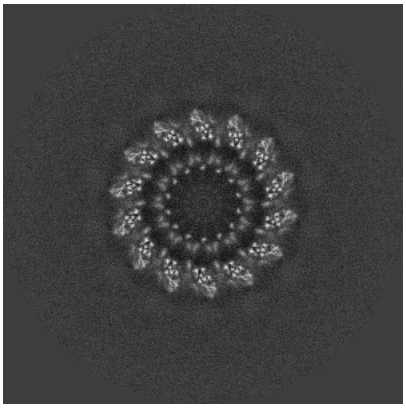
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 255

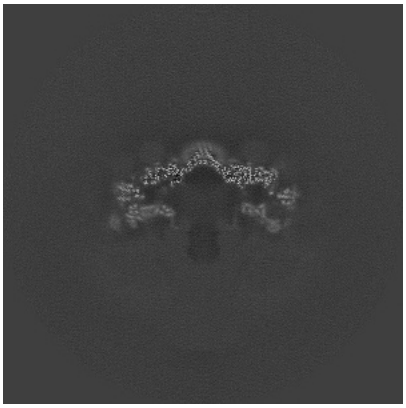

Y Index: 255

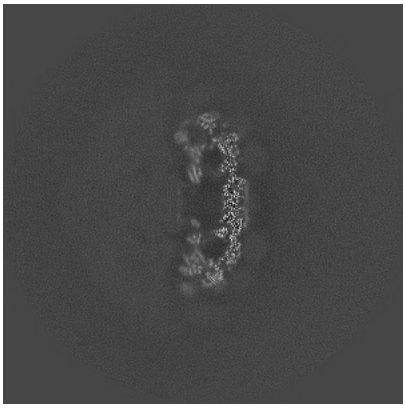

Z Index: 255

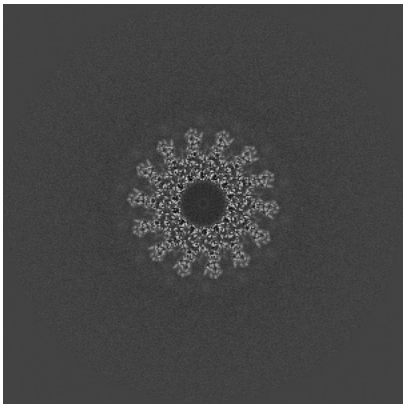
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 241

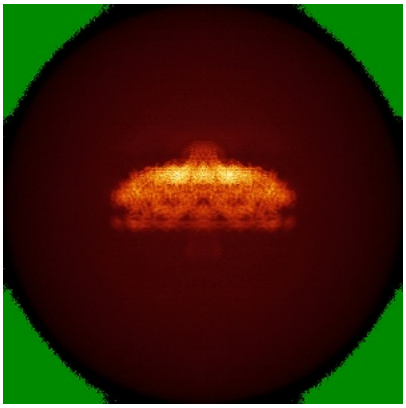

Y Index: 289

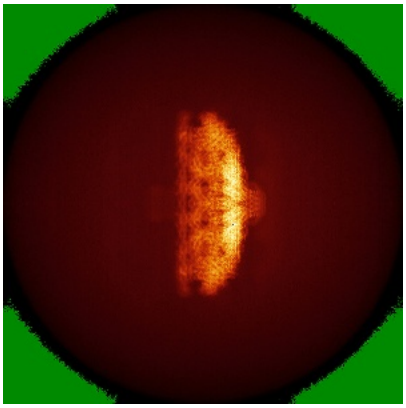

Z Index: 291

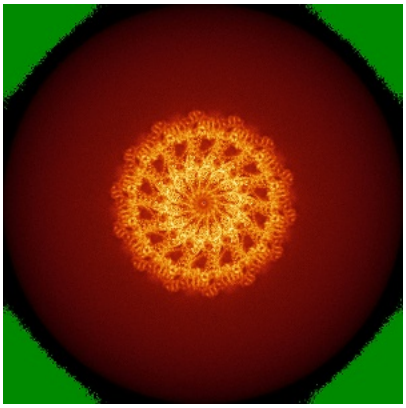
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

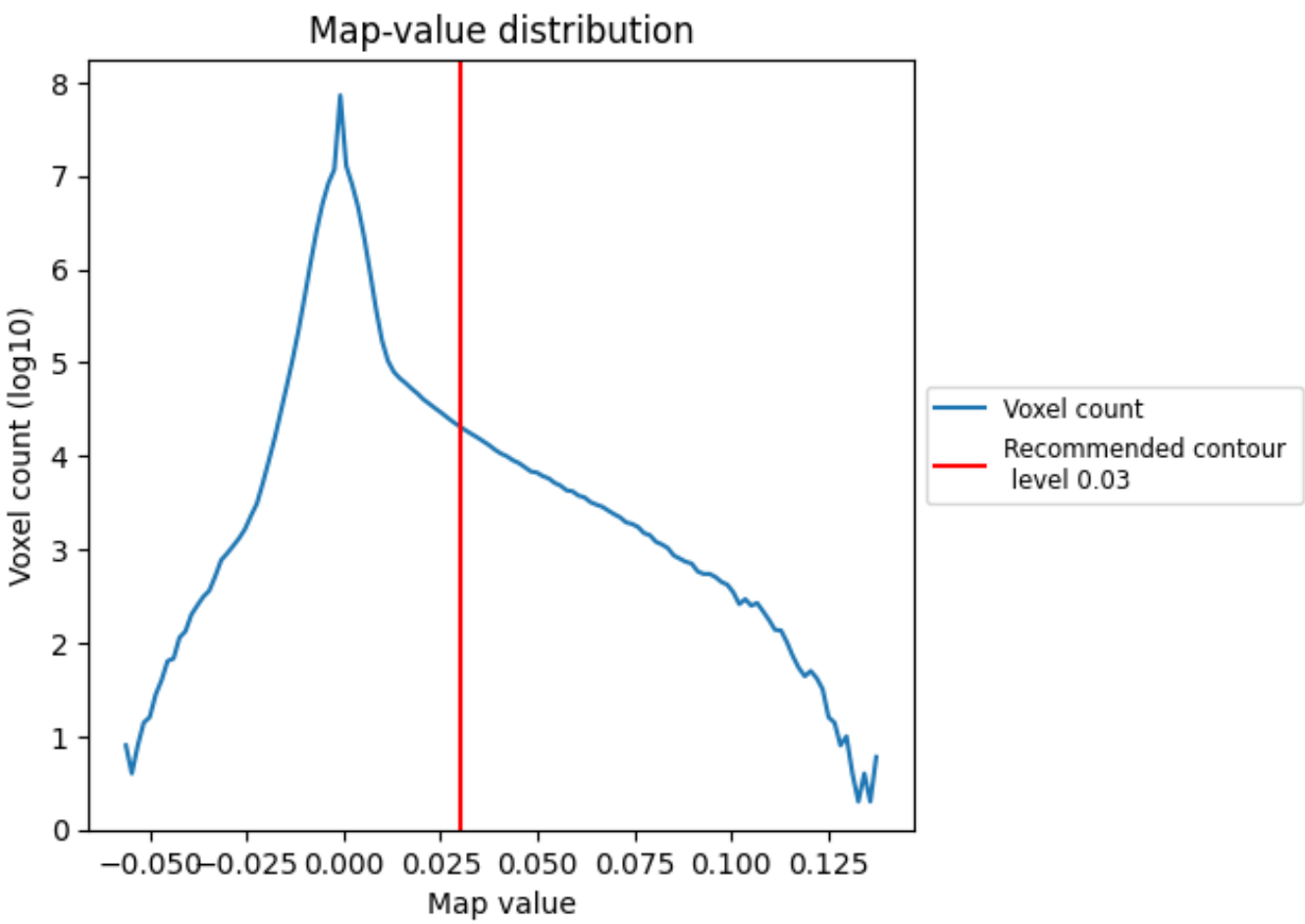
6.6 Mask visualisation (i)

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

7 Map analysis (i)

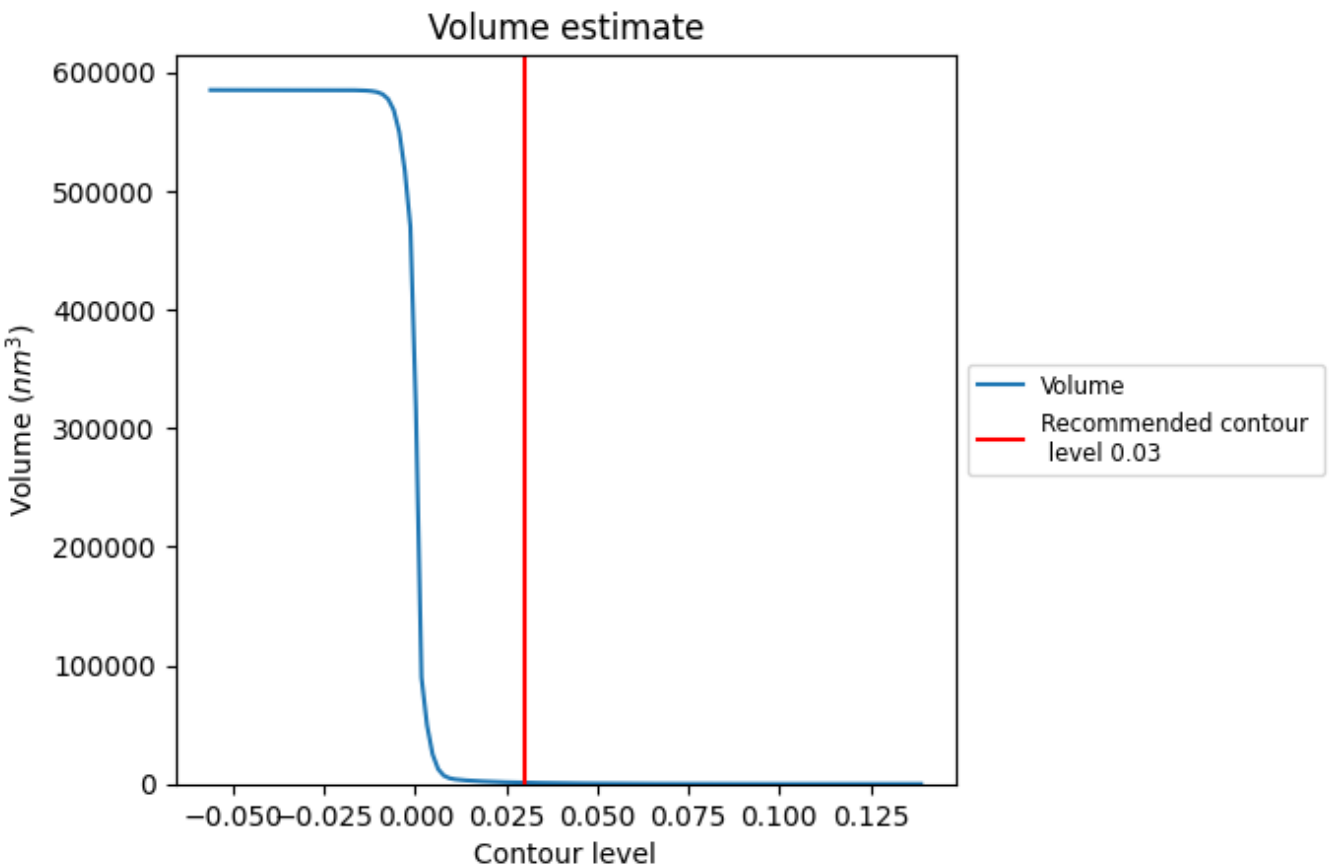
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

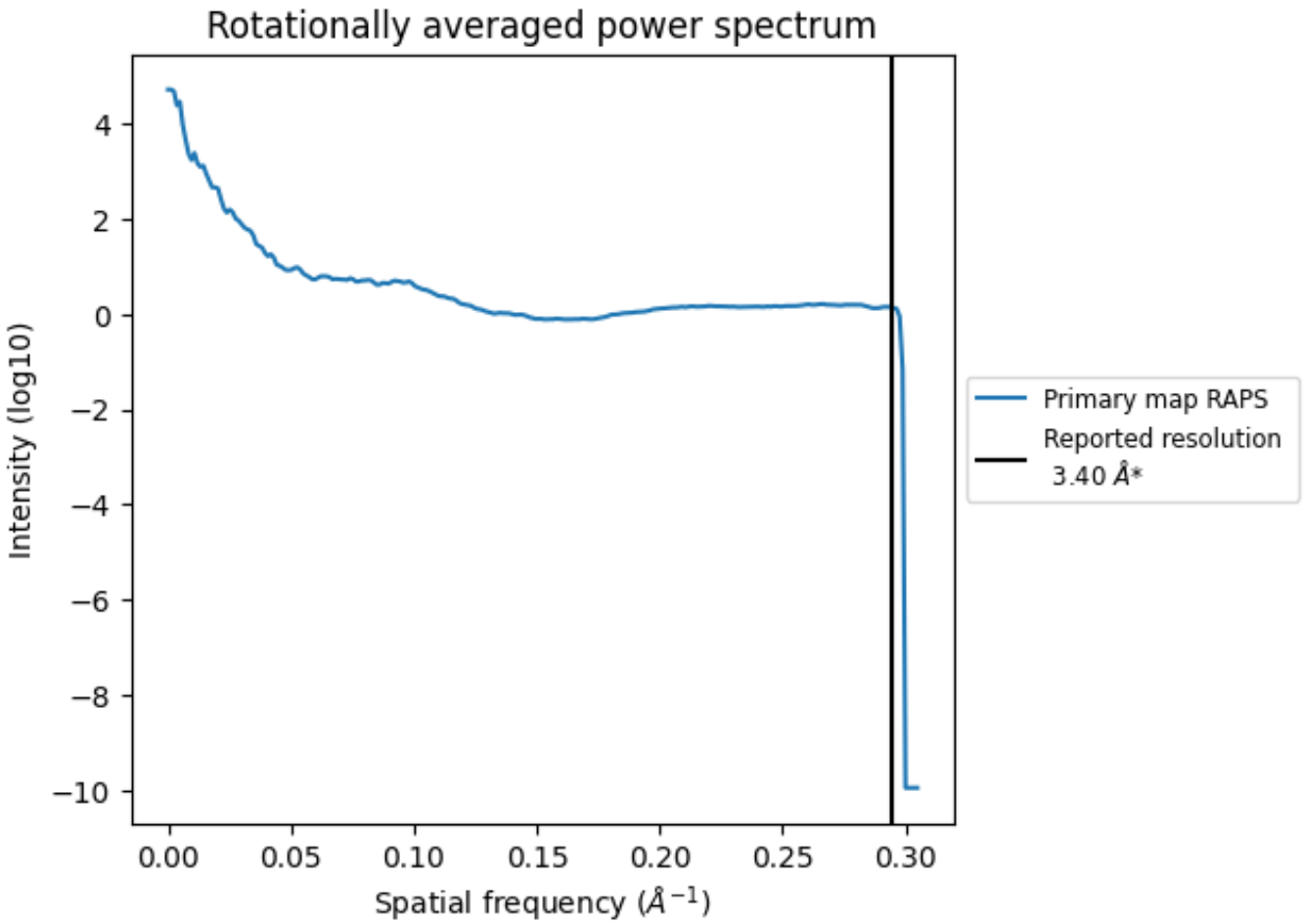
7.2 Volume estimate (i)



The volume at the recommended contour level is 1078 nm^3; this corresponds to an approximate mass of 974 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)

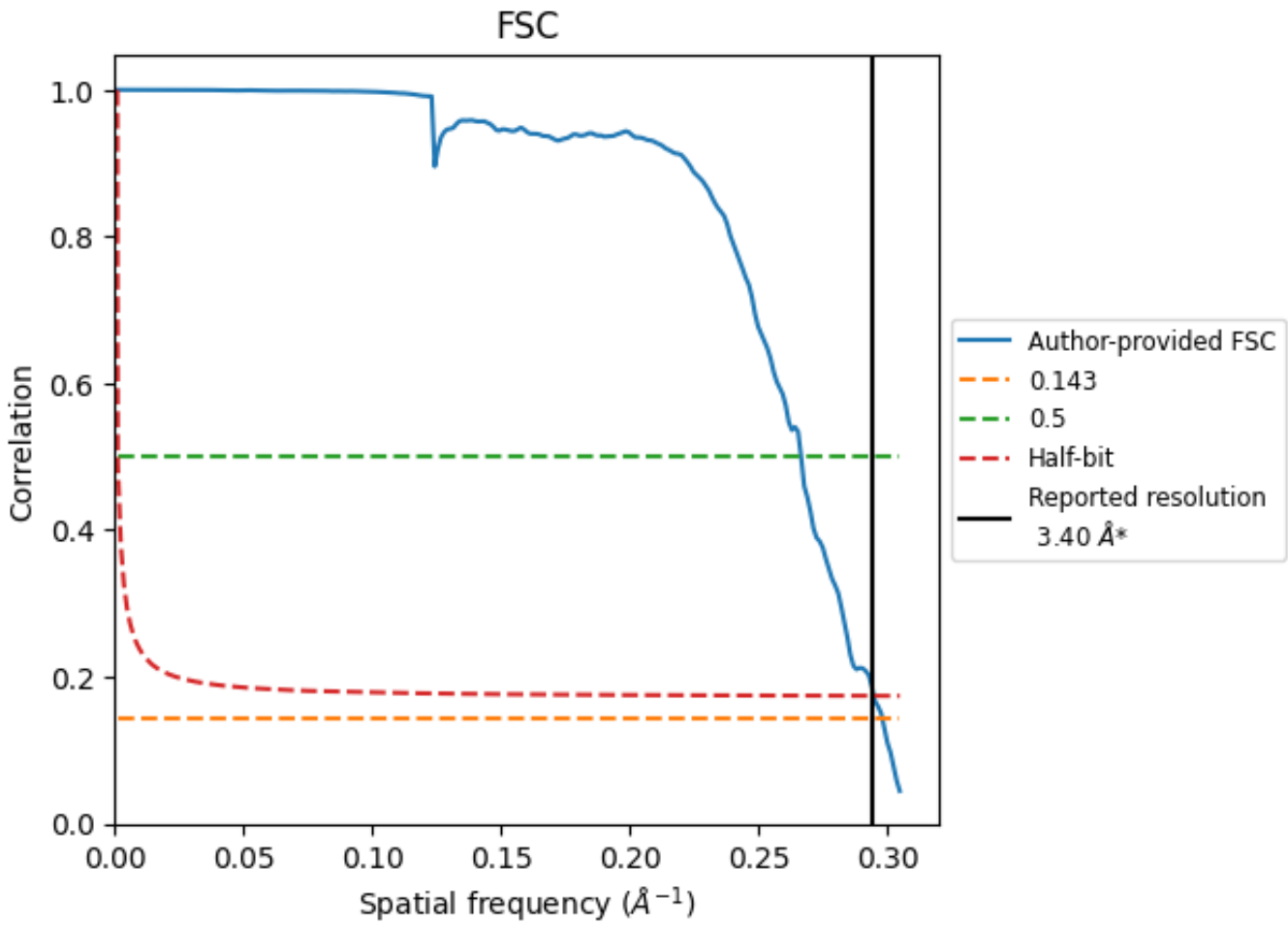


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

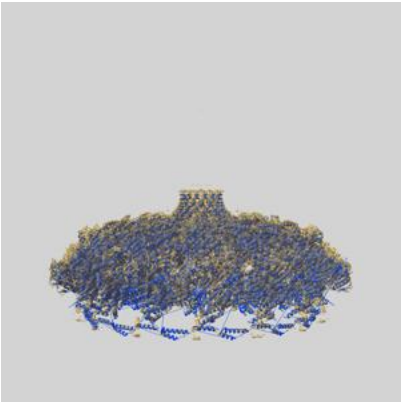
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.35	3.75	3.39
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

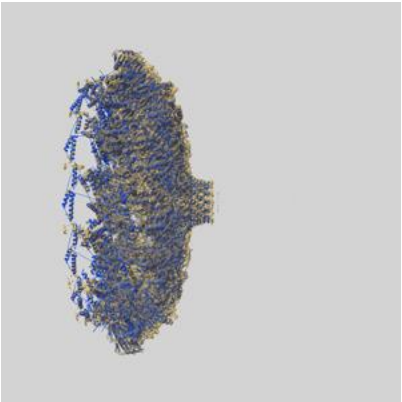
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22081 and PDB model 6X6S. Per-residue inclusion information can be found in section 3 on page 21.

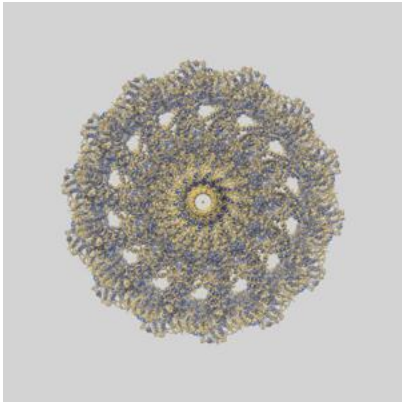
9.1 Map-model overlay (i)



X



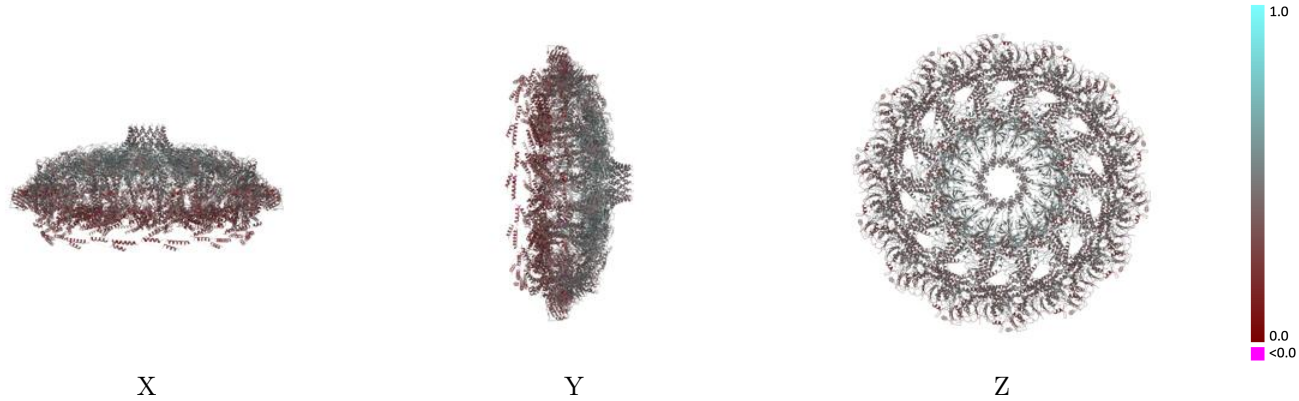
Y



Z

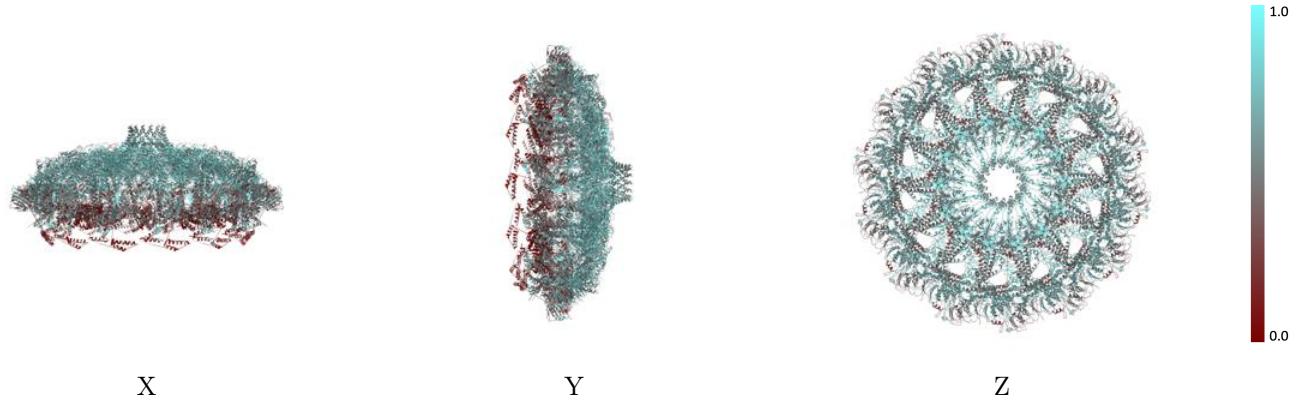
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



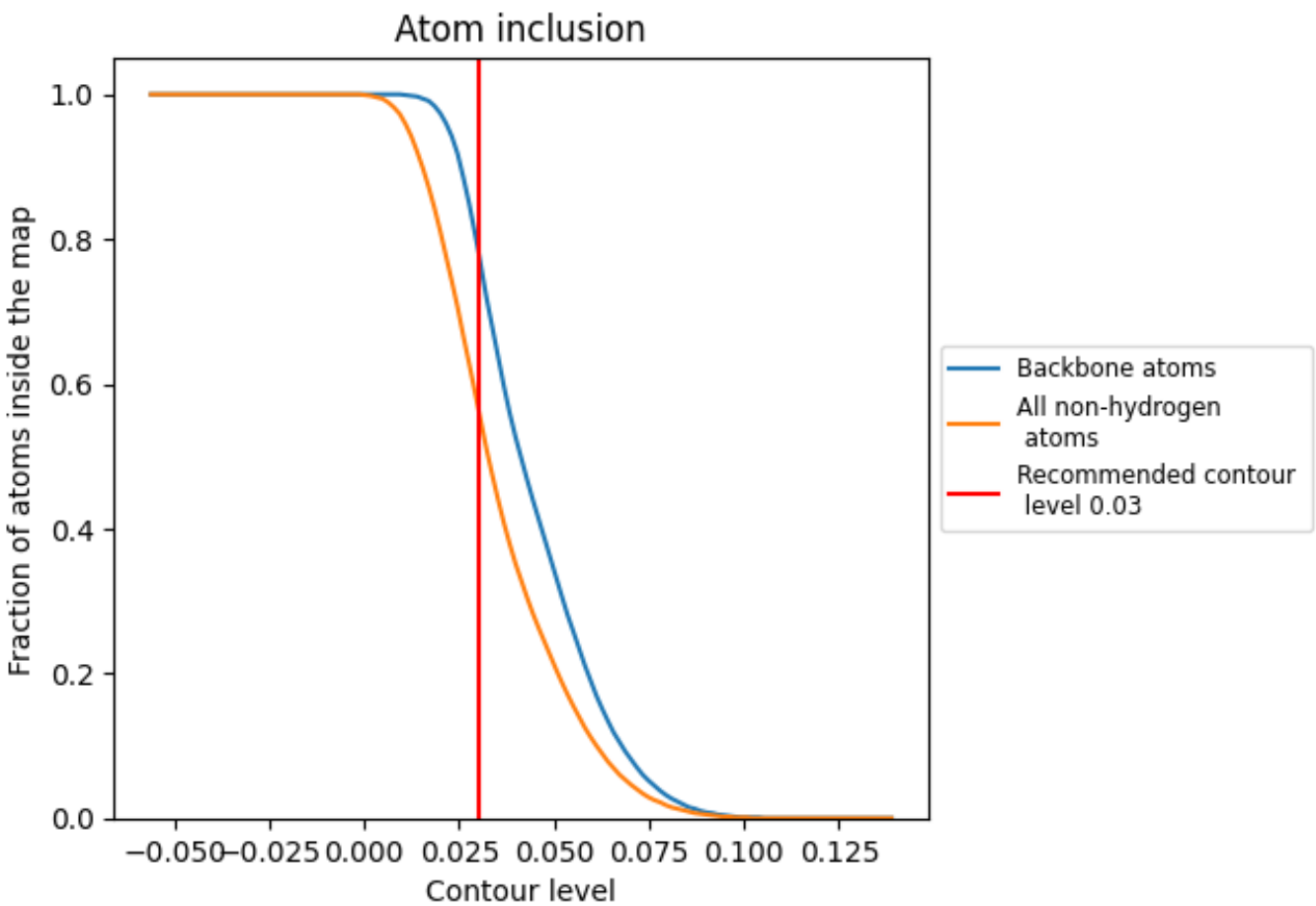
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5680	0.4030
AA	0.5830	0.4110
AB	0.6710	0.4540
AC	0.6500	0.4320
AD	0.4750	0.3500
AE	0.4190	0.3380
AM	0.5260	0.3640
AT	0.6750	0.4620
AU	0.4120	0.3410
AX	0.7080	0.4760
AY	0.7460	0.5050
Am	0.2610	0.2510
At	0.5610	0.4120
BA	0.5780	0.4100
BB	0.6740	0.4410
BC	0.6360	0.4250
BD	0.4840	0.3550
BE	0.4220	0.3390
BM	0.5250	0.3670
BT	0.6780	0.4630
BU	0.4110	0.3360
BX	0.7080	0.4750
BY	0.7390	0.5020
Bm	0.2600	0.2460
Bt	0.5670	0.4100
CA	0.5820	0.4110
CB	0.6660	0.4380
CC	0.6370	0.4250
CD	0.4650	0.3530
CE	0.4260	0.3360
CM	0.5210	0.3620
CT	0.6750	0.4620
CU	0.4170	0.3380
CX	0.7070	0.4750
CY	0.7480	0.5020

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Chain	Atom inclusion	Q-score
Cm	0.2610	0.2470
Ct	0.5660	0.4090
DA	0.5840	0.4090
DB	0.6590	0.4340
DC	0.6410	0.4330
DD	0.4790	0.3550
DE	0.4300	0.3380
DM	0.5150	0.3640
DT	0.6770	0.4600
DU	0.4120	0.3350
DX	0.7100	0.4760
DY	0.7420	0.5020
Dm	0.2570	0.2480
Dt	0.5650	0.4100
EA	0.5780	0.4050
EB	0.6600	0.4390
EC	0.6500	0.4230
ED	0.4720	0.3520
EE	0.4220	0.3280
EM	0.5190	0.3620
ET	0.6810	0.4620
EU	0.4140	0.3370
EX	0.7000	0.4730
EY	0.7410	0.5030
Em	0.2600	0.2470
Et	0.5740	0.4100
FA	0.5790	0.4050
FB	0.6740	0.4380
FC	0.6430	0.4240
FD	0.4840	0.3660
FE	0.4260	0.3340
FM	0.5220	0.3640
FT	0.6830	0.4610
FU	0.4040	0.3350
FX	0.7060	0.4730
FY	0.7390	0.4990
Fm	0.2650	0.2470
Ft	0.5700	0.4110
GA	0.5770	0.4050
GB	0.6640	0.4380
GC	0.6440	0.4280
GD	0.4710	0.3550

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Chain	Atom inclusion	Q-score
GE	0.4240	0.3330
GM	0.5190	0.3660
GT	0.6810	0.4620
GU	0.4110	0.3310
GX	0.7080	0.4750
GY	0.7440	0.4980
Gm	0.2620	0.2470
Gt	0.5700	0.4140
HA	0.5830	0.4120
HB	0.6740	0.4520
HC	0.6510	0.4250
HD	0.4740	0.3540
HE	0.4200	0.3390
HM	0.5260	0.3650
HT	0.6750	0.4610
HU	0.4030	0.3370
HX	0.7050	0.4760
HY	0.7480	0.5030
Hm	0.2570	0.2480
Ht	0.5620	0.4100
IA	0.5780	0.4090
IB	0.6680	0.4390
IC	0.6410	0.4290
ID	0.4790	0.3520
IE	0.4220	0.3440
IM	0.5240	0.3650
IT	0.6770	0.4640
IU	0.4110	0.3360
IX	0.7040	0.4770
IY	0.7390	0.5000
Im	0.2610	0.2450
It	0.5640	0.4050
JA	0.5830	0.4130
JB	0.6700	0.4380
JC	0.6450	0.4210
JD	0.4690	0.3580
JE	0.4210	0.3330
JM	0.5200	0.3610
JT	0.6750	0.4620
JU	0.4220	0.3370
JX	0.7080	0.4750
JY	0.7470	0.5010

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Chain	Atom inclusion	Q-score
Jm	0.2630	0.2460
Jt	0.5670	0.4080
KA	0.5820	0.4100
KB	0.6610	0.4390
KC	0.6480	0.4310
KD	0.4750	0.3550
KE	0.4270	0.3370
KM	0.5120	0.3630
KT	0.6780	0.4600
KU	0.4070	0.3370
KX	0.7170	0.4770
KY	0.7420	0.5020
Km	0.2580	0.2480
Kt	0.5670	0.4090
LA	0.5770	0.4090
LB	0.6660	0.4440
LC	0.6540	0.4280
LD	0.4740	0.3490
LE	0.4210	0.3410
LM	0.5200	0.3600
LT	0.6800	0.4640
LU	0.4070	0.3330
LX	0.7080	0.4750
LY	0.7370	0.5050
Lm	0.2580	0.2450
Lt	0.5720	0.4110
MA	0.5810	0.4080
MB	0.6670	0.4320
MC	0.6400	0.4310
MD	0.4820	0.3650
ME	0.4250	0.3410
MM	0.5200	0.3620
MT	0.6810	0.4630
MU	0.3990	0.3380
MX	0.7080	0.4720
MY	0.7390	0.5000
Mm	0.2630	0.2500
Mt	0.5690	0.4120
NA	0.5810	0.4120
NB	0.6700	0.4380
NC	0.6470	0.4280
ND	0.4820	0.3560

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Chain	Atom inclusion	Q-score
NE	0.4250	0.3380
NM	0.5190	0.3630
NT	0.6750	0.4620
NU	0.4170	0.3350
NX	0.7080	0.4750
NY	0.7420	0.5010
Nm	0.2630	0.2460
Nt	0.5710	0.4130