wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 06:15 AM UTC

PDB ID	:	7MUC / pdb_00007muc
EMDB ID	:	EMD-24004
Title	:	Legionella pneumophila Dot/Icm T4SS C1 Reconstruction
Authors	:	Sheedlo, M.J.; Durie, C.L.; Swanson, M.; Lacy, D.B.; Ohi, M.D.
Deposited on	:	2021-05-14
Resolution	:	3.80 Å(reported)

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

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

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

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

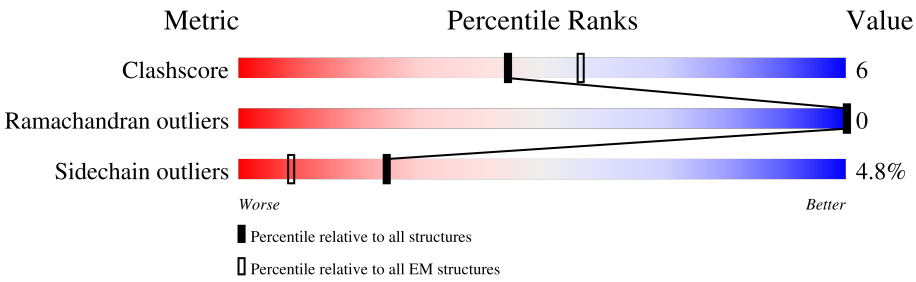
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

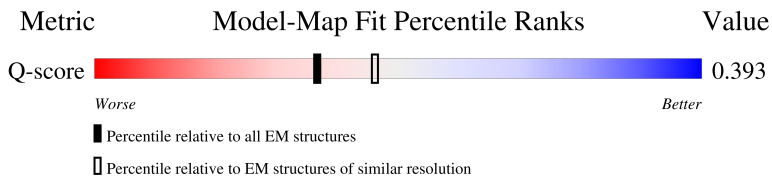
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	AC	303	57% 11% • • 30%
1	BC	303	58% 10% • • 30%
1	CC	303	58% 10% • • 30%
1	DC	303	56% 11% • • 30%

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Mol	Chain	Length	Quality of chain
1	EC	303	58% 10% 30%
1	FC	303	57% 10% 30%
1	GC	303	57% 11% 30%
1	HC	303	57% 11% 30%
1	IC	303	57% 11% 30%
1	JC	303	57% 10% 30%
1	KC	303	56% 11% 30%
1	LC	303	58% 9% 30%
1	MC	303	57% 10% 30%
2	AD	163	75% 10% 14%
2	Ad	163	76% 7% 16%
2	BD	163	77% 7% 14%
2	Bd	163	71% 12% 16%
2	CD	163	69% 16% 14%
2	Cd	163	71% 12% 16%
2	DD	163	72% 13% 14%
2	Dd	163	77% 7% 16%
2	ED	163	74% 11% 14%
2	Ed	163	73% 11% 16%
2	FD	163	78% 7% 14%
2	Fd	163	72% 10% 16%
2	GD	163	75% 10% 14%
2	Gd	163	75% 9% 16%
2	HD	163	74% 12% 14%
2	Hd	163	77% 6% 16%

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Mol	Chain	Length	Quality of chain
2	ID	163	73% 12% 14%
2	Id	163	70% 13% 16%
2	JD	163	75% 10% 14%
2	Jd	163	78% 6% 16%
2	KD	163	72% 12% 14%
2	Kd	163	75% 7% 16%
2	LD	163	75% 10% 14%
2	Ld	163	79% 6% 16%
2	MD	163	75% 10% 14%
2	Md	163	75% 9% 16%
3	AF	269	9% 17% 6% 77%
3	Af	269	19% 78%
3	BF	269	10% 16% 7% 77%
3	Bf	269	19% 78%
3	CF	269	11% 17% 6% 77%
3	Cf	269	19% 78%
3	DF	269	10% 17% 5% 77%
3	Df	269	19% 78%
3	EF	269	12% 17% 6% 77%
3	Ef	269	21% 78%
3	FF	269	11% 16% 7% 77%
3	Ff	269	21% 78%
3	GF	269	10% 16% 7% 77%
3	Gf	269	20% 78%
3	HF	269	11% 17% 6% 77%

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Mol	Chain	Length	Quality of chain
3	Hf	269	17% 78%
3	IF	269	10% 17% 6% 77%
3	If	269	20% 78%
3	JF	269	9% 16% 7% 77%
3	Jf	269	19% 78%
3	KF	269	6% 17% 6% 77%
3	Kf	269	18% 78%
3	LF	269	10% 17% 6% 77%
3	Lf	269	19% 78%
3	MF	269	10% 17% 6% 77%
3	Mf	269	20% 78%
3	VF	269	7% 17% 6% 77%
3	WF	269	10% 16% 6% 77%
3	XF	269	9% 16% 6% 77%
3	YF	269	9% 17% 6% 77%
3	ZF	269	10% 16% 6% 77%
4	AG	1048	97%
4	BG	1048	97%
4	CG	1048	97%
4	DG	1048	97%
4	EG	1048	97%
4	FG	1048	97%
4	GG	1048	97%
4	HG	1048	97%
4	IG	1048	97%

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Mol	Chain	Length	Quality of chain
4	JG	1048	97%
4	KG	1048	97%
4	LG	1048	97%
4	MG	1048	97%
4	VG	1048	97%
4	WG	1048	97%
4	XG	1048	97%
4	YG	1048	97%
4	ZG	1048	97%
5	AH	361	7% 59% 11% 29%
5	BH	361	5% 59% 11% 29%
5	CH	361	5% 58% 12% 29%
5	DH	361	5% 61% 9% 29%
5	EH	361	7% 55% 16% 29%
5	FH	361	7% 61% 9% 29%
5	GH	361	5% 58% 12% 29%
5	HH	361	5% 59% 11% 29%
5	IH	361	6% 58% 12% 29%
5	JH	361	5% 60% 11% 29%
5	KH	361	6% 61% 10% 29%
5	LH	361	7% 58% 11% 29%
5	MH	361	6% 59% 12% 29%
5	VH	361	14% 60% 7% 33%
5	WH	361	27% 55% 11% 33%
5	XH	361	14% 57% 9% 33%

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Mol	Chain	Length	Quality of chain
5	YH	361	20% 59% 8% 33%
5	ZH	361	25% 56% 9% 33%
6	AK	189	69% 8% 20%
6	BK	189	68% 10% 20%
6	CK	189	68% 10% 20%
6	DK	189	68% 9% 20%
6	EK	189	67% 11% 20%
6	FK	189	69% 10% 20%
6	GK	189	69% 9% 20%
6	HK	189	69% 9% 20%
6	IK	189	67% 11% 20%
6	JK	189	68% 10% 20%
6	KK	189	68% 10% 20%
6	LK	189	69% 10% 20%
6	MK	189	69% 10% 20%
7	AL	249	57% 10% 31%
7	BL	249	56% 11% 31%
7	CL	249	56% 11% 31%
7	DL	249	56% 11% 31%
7	EL	249	57% 10% 31%
7	FL	249	56% 10% 31%
7	GL	249	56% 10% 31%
7	HL	249	56% 10% 31%
7	IL	249	56% 10% 31%
7	JL	249	56% 11% 31%

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Mol	Chain	Length	Quality of chain
7	KL	249	56% 10% • 31%
7	LL	249	56% 11% • 31%
7	ML	249	56% 10% • 31%
8	AM	320	25% 71% 18% • 9%
8	BM	320	24% 70% 19% • 9%
8	CM	320	26% 70% 19% • 9%
8	DM	320	25% 70% 19% • 9%
8	EM	320	26% 70% 19% • 9%
8	FM	320	25% 69% 20% • 9%
8	GM	320	27% 72% 17% • 9%
8	HM	320	26% 70% 19% • 9%
8	IM	320	28% 69% 20% • 9%
8	JM	320	27% 71% 18% • 9%
8	KM	320	27% 69% 20% • 9%
8	LM	320	22% 70% 19% • 9%
8	MM	320	22% 70% 19% • 9%
9	AN	124	5% 48% 11% • 37%
9	BN	124	50% 10% • 37%
9	CN	124	7% 52% 8% • 37%
9	DN	124	5% 50% 10% • 37%
9	EN	124	6% 51% 8% • 37%
9	FN	124	7% 48% 11% • 37%
9	GN	124	6% 50% 10% • 37%
9	HN	124	5% 50% 10% • 37%
9	IN	124	6% 52% 7% • 37%

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Mol	Chain	Length	Quality of chain
9	JN	124	5% 51% 9% • 37%
9	KN	124	5% 50% 10% • 37%
9	LN	124	• 51% 10% • 37%
9	MN	124	5% 51% 10% • 37%
10	AU	9	100%
10	BU	9	100%
10	CU	9	100%
10	DU	9	100%
10	EU	9	100%
10	FU	9	100%
10	GU	9	100%
10	HU	9	100%
10	IU	9	100%
10	JU	9	100%
10	KU	9	100%
10	LU	9	100%
10	MU	9	100%
11	AX	48	85% 100%
11	BX	48	88% 100%
11	CX	48	85% 100%
11	DX	48	81% 100%
11	EX	48	79% 100%
11	FX	48	90% 100%
11	GX	48	90% 100%
11	HX	48	85% 100%

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Mol	Chain	Length	Quality of chain
11	IX	48	85% / 100%
11	JX	48	90% / 100%
11	KX	48	75% / 98%
11	LX	48	79% / 100%
11	MX	48	85% / 100%
11	VX	48	81% / 100%
11	WX	48	88% / 100%
11	XX	48	83% / 100%
11	YX	48	83% / 100%
11	ZX	48	83% / 100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 180380 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 DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AC	213	1685	1068	295	316	6	0	0
1	BC	213	1685	1068	295	316	6	0	0
1	CC	213	1685	1068	295	316	6	0	0
1	DC	213	1685	1068	295	316	6	0	0
1	EC	213	1685	1068	295	316	6	0	0
1	FC	213	1685	1068	295	316	6	0	0
1	GC	213	1685	1068	295	316	6	0	0
1	HC	213	1685	1068	295	316	6	0	0
1	IC	213	1685	1068	295	316	6	0	0
1	JC	213	1685	1068	295	316	6	0	0
1	KC	213	1685	1068	295	316	6	0	0
1	LC	213	1685	1068	295	316	6	0	0
1	MC	213	1685	1068	295	316	6	0	0

- Molecule 2 is a protein called DotD.

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

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

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

- Molecule 3 is a protein called DotF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Af	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	BF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Bf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	CF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Cf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	DF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Df	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	EF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Ef	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	FF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Ff	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	GF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Gf	59	449	290	77	81	1	0	0
			Total	C	N	O	S		
3	HF	63	483	308	84	90	1	0	0
			Total	C	N	O	S		
3	Hf	59	449	290	77	81	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	IF	63	483	308	84	90	1	0	0
3	If	59	449	290	77	81	1	0	0
3	JF	63	483	308	84	90	1	0	0
3	Jf	59	449	290	77	81	1	0	0
3	KF	63	483	308	84	90	1	0	0
3	Kf	59	449	290	77	81	1	0	0
3	LF	63	483	308	84	90	1	0	0
3	Lf	59	449	290	77	81	1	0	0
3	MF	63	483	308	84	90	1	0	0
3	Mf	59	449	290	77	81	1	0	0
3	VF	63	483	308	84	90	1	0	0
3	WF	63	483	308	84	90	1	0	0
3	XF	63	483	308	84	90	1	0	0
3	YF	63	483	308	84	90	1	0	0
3	ZF	63	483	308	84	90	1	0	0

- Molecule 4 is a protein called IcmE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AG	34	276	168	47	60	1	0	0
4	BG	34	276	168	47	60	1	0	0
4	CG	34	276	168	47	60	1	0	0
4	DG	34	276	168	47	60	1	0	0

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AH	258	1983	1268	336	371	8	0	0
5	BH	258	1983	1268	336	371	8	0	0
5	CH	258	1983	1268	336	371	8	0	0
5	DH	258	1983	1268	336	371	8	0	0
5	EH	258	1983	1268	336	371	8	0	0

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	ML	173	1388	877	253	253	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AM	292	2320	1467	416	433	4	0	0
8	BM	292	2320	1467	416	433	4	0	0
8	CM	292	2320	1467	416	433	4	0	0
8	DM	292	2320	1467	416	433	4	0	0
8	EM	292	2320	1467	416	433	4	0	0
8	FM	292	2320	1467	416	433	4	0	0
8	GM	292	2320	1467	416	433	4	0	0
8	HM	292	2320	1467	416	433	4	0	0
8	IM	292	2320	1467	416	433	4	0	0
8	JM	292	2320	1467	416	433	4	0	0
8	KM	292	2320	1467	416	433	4	0	0
8	LM	292	2320	1467	416	433	4	0	0
8	MM	292	2320	1467	416	433	4	0	0

- Molecule 9 is a protein called Neurogenic locus notch.

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

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

- Molecule 10 is a protein called Unknown protein fragment.

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	JU	9	45	27	9	9	0	0
10	KU	9	45	27	9	9	0	0
10	LU	9	45	27	9	9	0	0
10	MU	9	45	27	9	9	0	0

- Molecule 11 is a protein called Unknown protein fragment.

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

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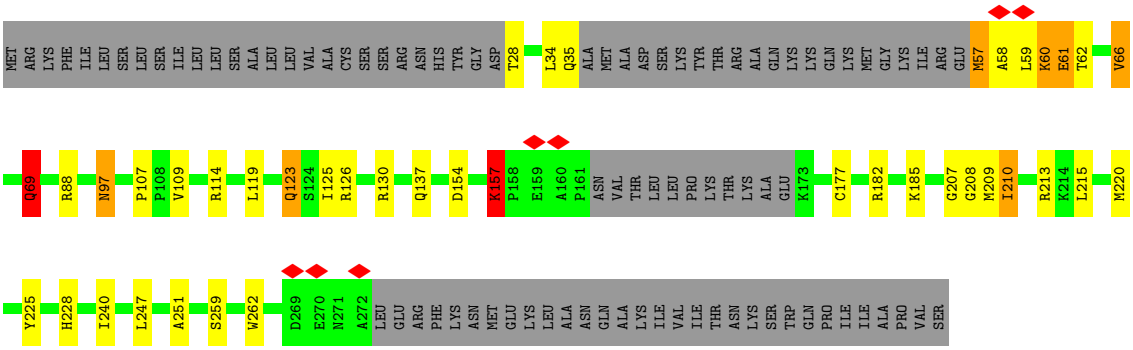
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	XX	48	240	144	48	48	0	0
			Total	C	N	O		
11	YX	48	240	144	48	48	0	0
			Total	C	N	O		
11	ZX	48	240	144	48	48	0	0

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.

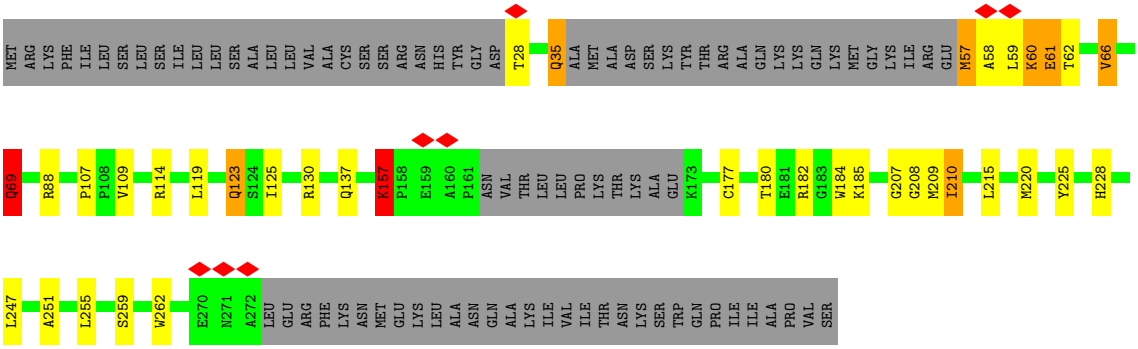
- Molecule 1: DotC

Chain AC:



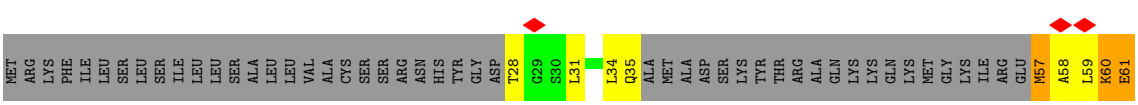
- Molecule 1: DotC

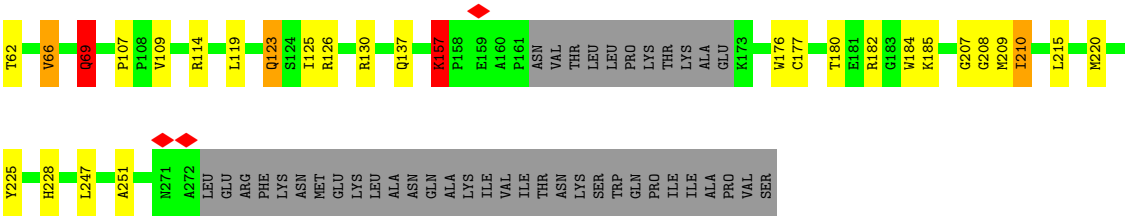
Chain BC:



- Molecule 1: DotC

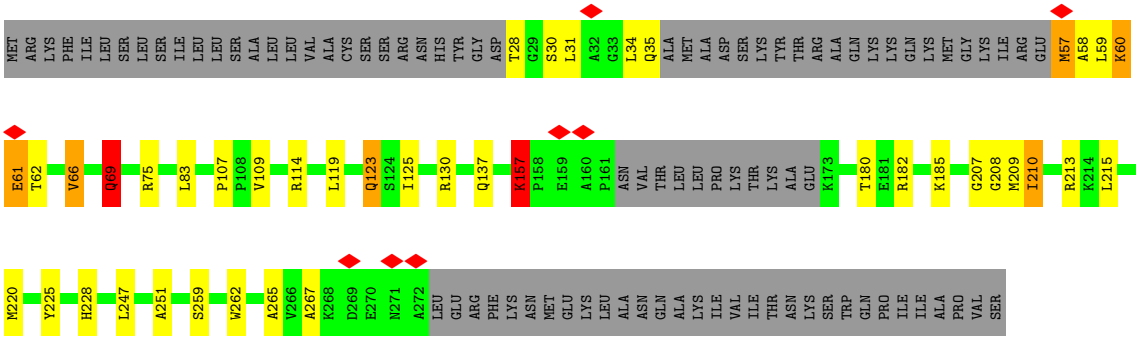
Chain CC:





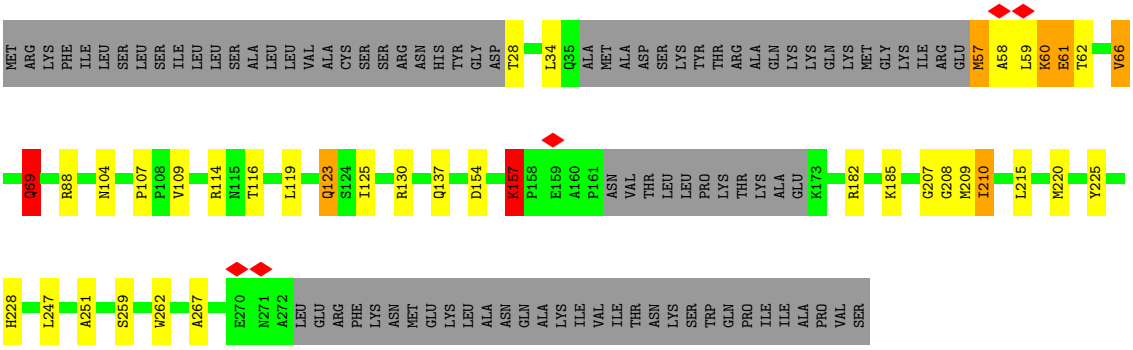
- Molecule 1: DotC

Chain DC:



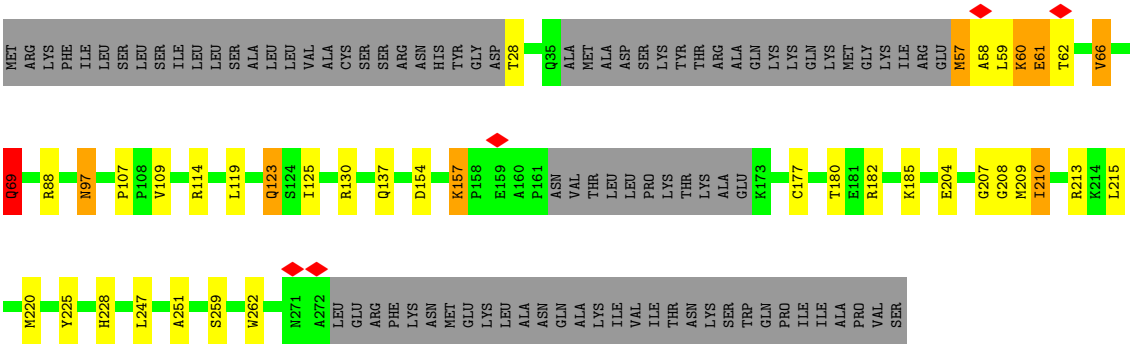
- Molecule 1: DotC

Chain EC:



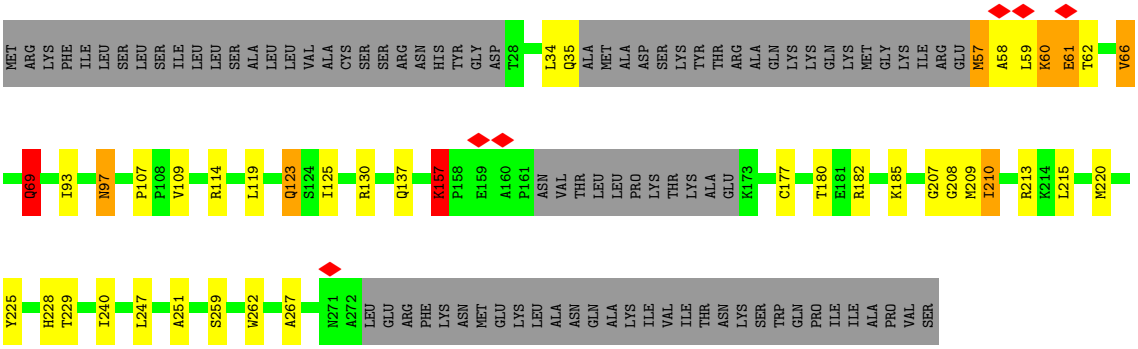
- Molecule 1: DotC

Chain FC:



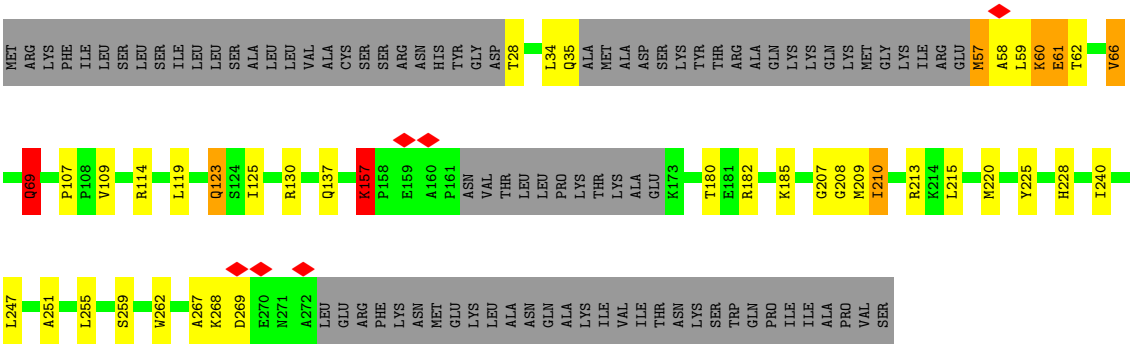
- Molecule 1: DotC

Chain GC:



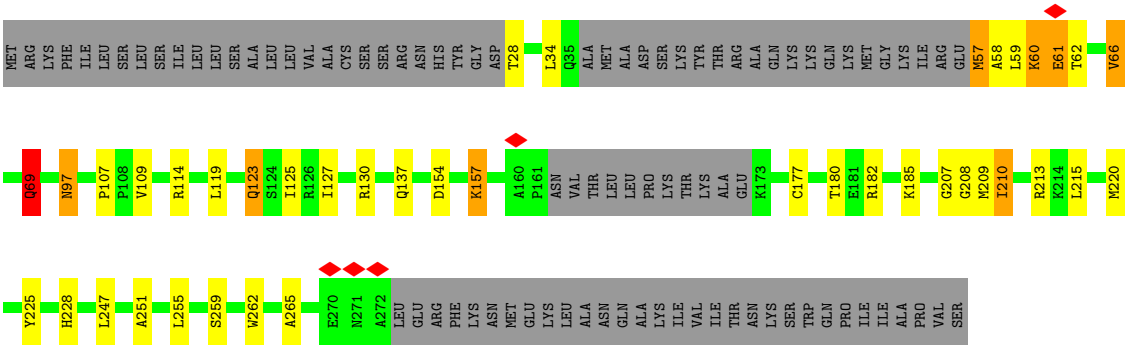
- Molecule 1: DotC

Chain HC:



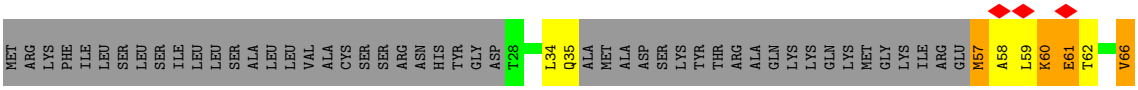
- Molecule 1: DotC

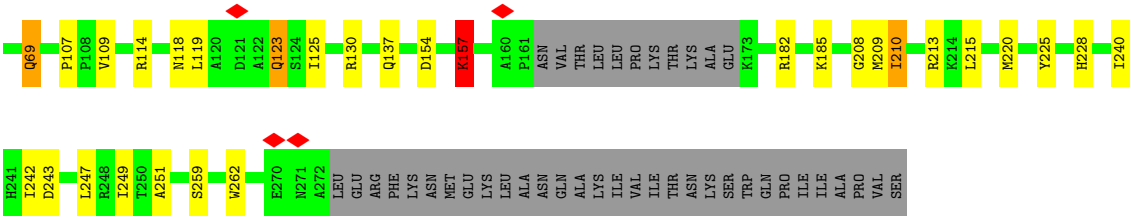
Chain IC:



- Molecule 1: DotC

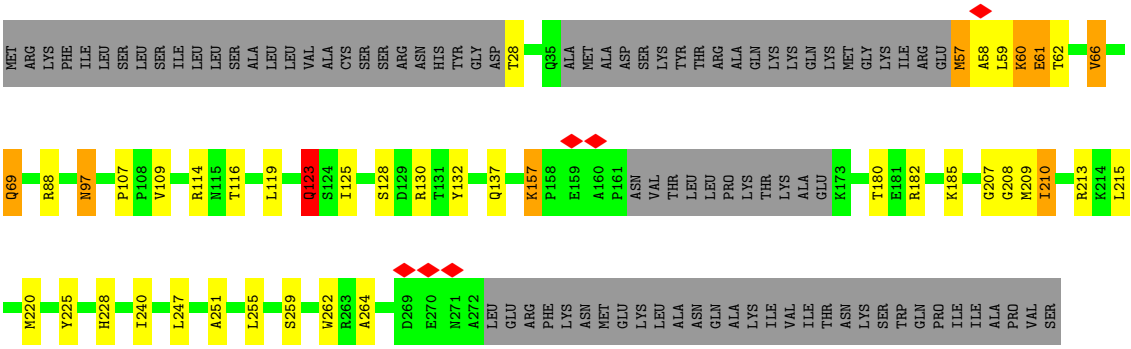
Chain JC:





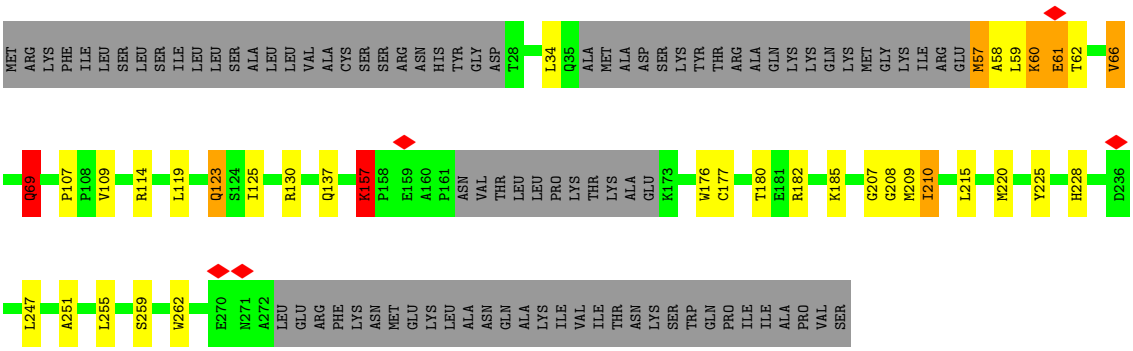
- Molecule 1: DotC

Chain KC:



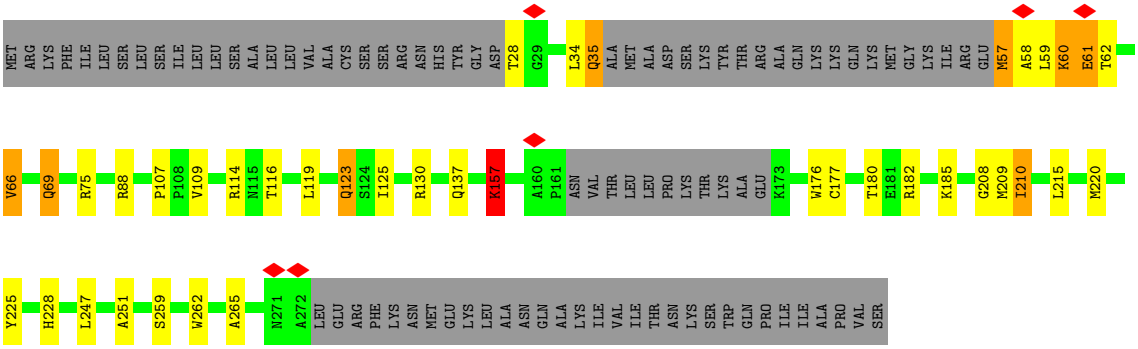
- Molecule 1: DotC

Chain LC:



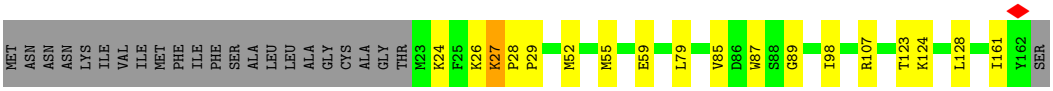
- Molecule 1: DotC

Chain MC:



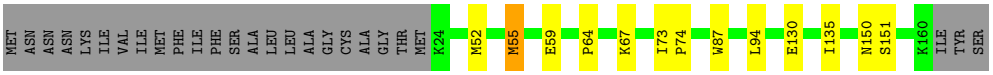
- Molecule 2: DotD

Chain AD:



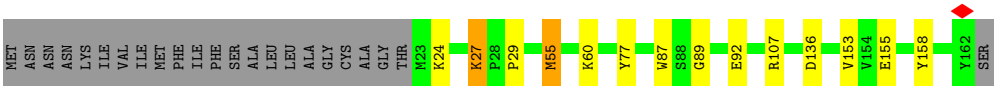
- Molecule 2: DotD

Chain Ad:



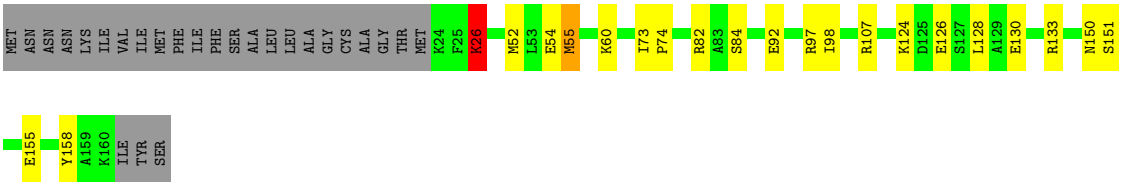
- Molecule 2: DotD

Chain BD:



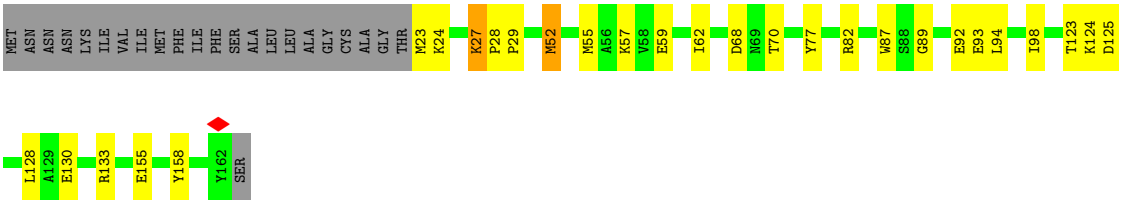
- Molecule 2: DotD

Chain Bd:



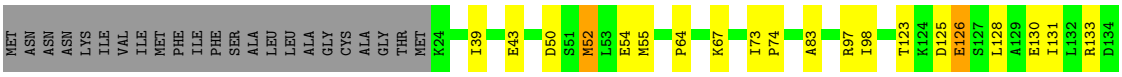
- Molecule 2: DotD

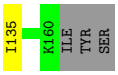
Chain CD:



- Molecule 2: DotD

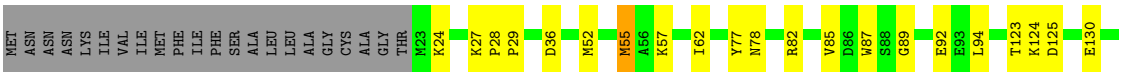
Chain Cd:

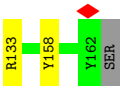




• Molecule 2: DotD

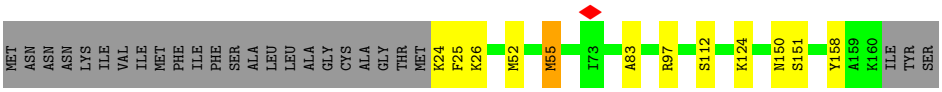
Chain DD:





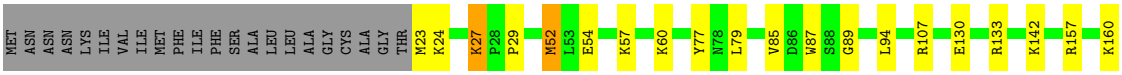
• Molecule 2: DotD

Chain Dd:



• Molecule 2: DotD

Chain ED:

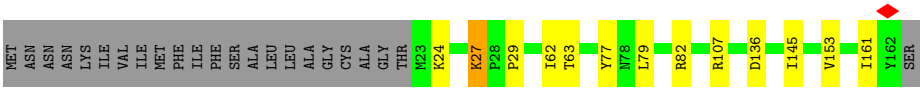


• Molecule 2: DotD

Chain Ed:

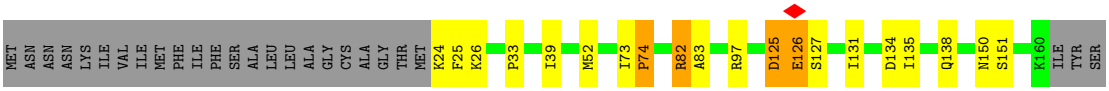
• Molecule 2: DotD

Chain FD:



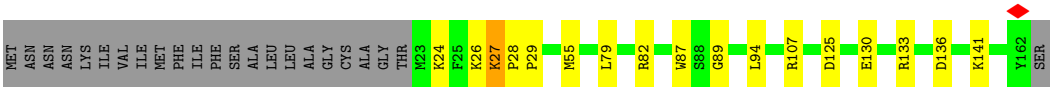
• Molecule 2: DotD

Chain Fd:



• Molecule 2: DotD

Chain GD:

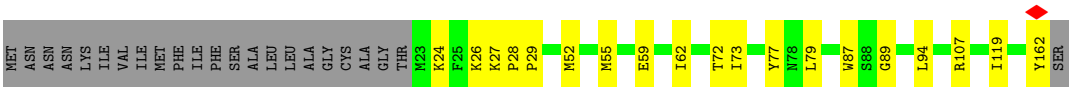


• Molecule 2: DotD

Chain Gd:

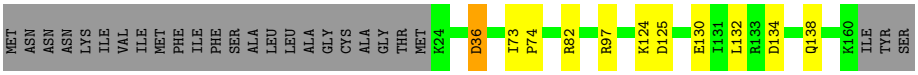
• Molecule 2: DotD

Chain HD:



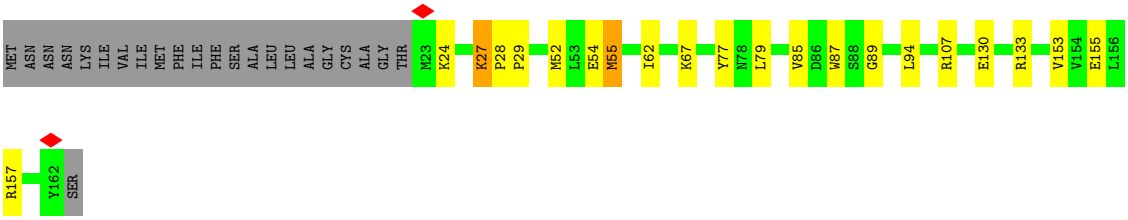
• Molecule 2: DotD

Chain Hd:



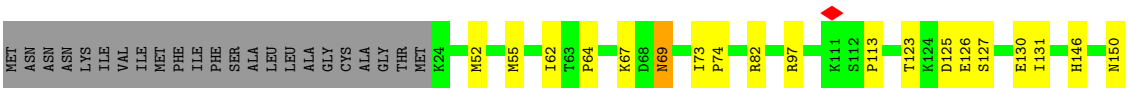
• Molecule 2: DotD

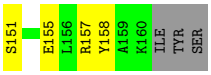
Chain ID:



• Molecule 2: DotD

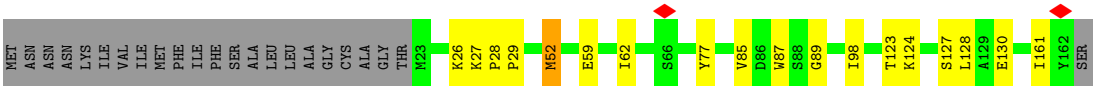
Chain Id:





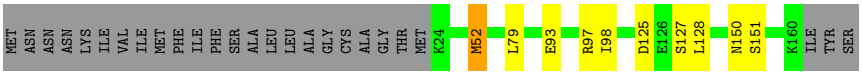
• Molecule 2: DotD

Chain JD:



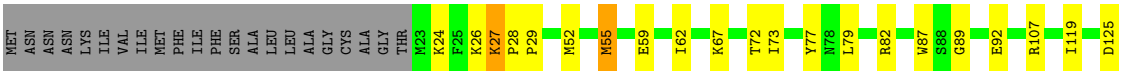
• Molecule 2: DotD

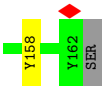
Chain Jd:



• Molecule 2: DotD

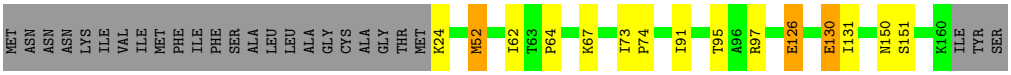
Chain KD:





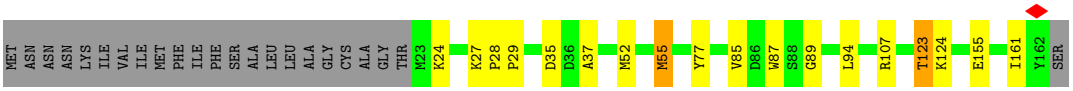
• Molecule 2: DotD

Chain Kd:



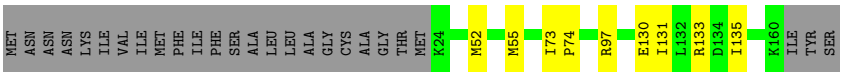
• Molecule 2: DotD

Chain LD:



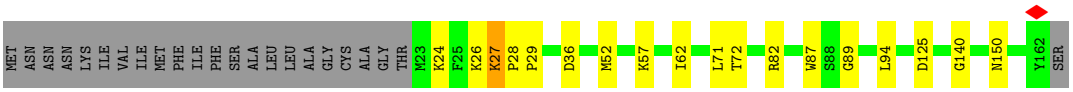
• Molecule 2: DotD

Chain Ld:



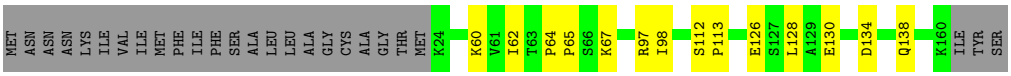
• Molecule 2: DotD

Chain MD:



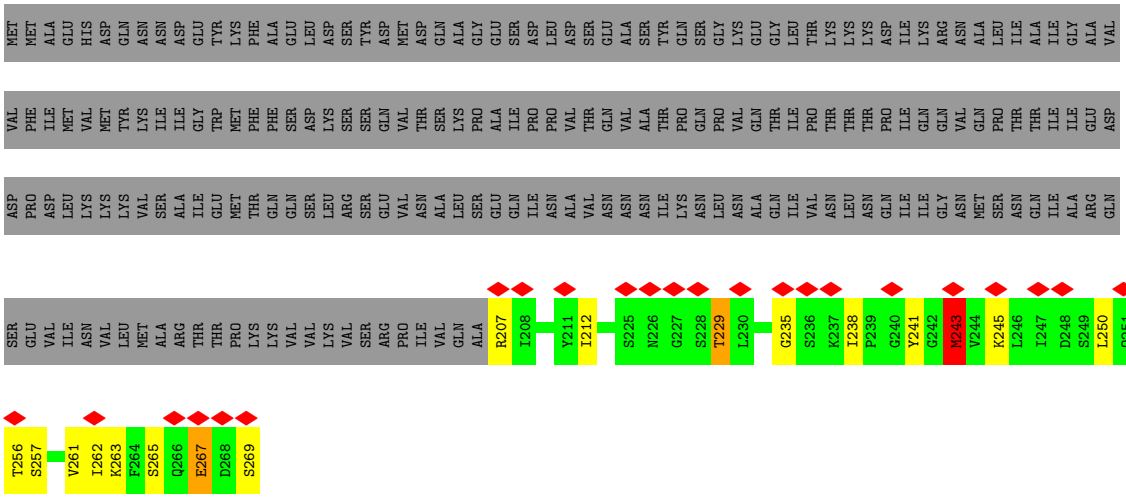
- Molecule 2: DotD

Chain Md:



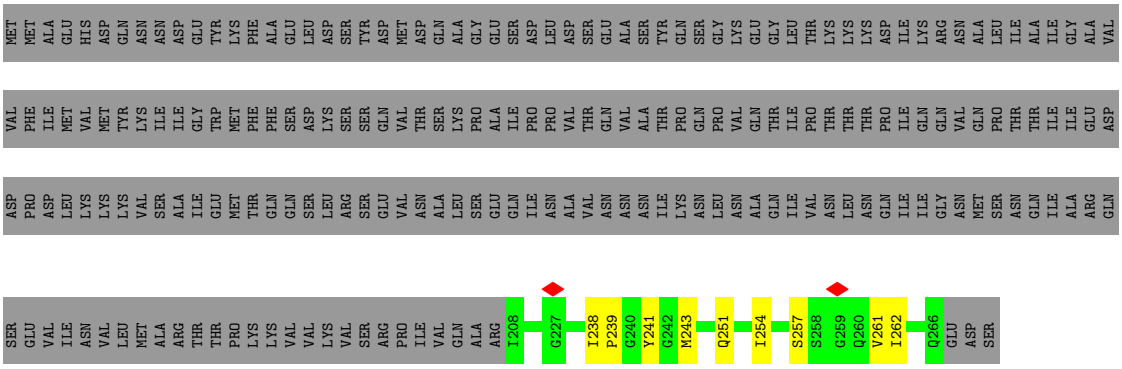
- Molecule 3: DotF

Chain AF:



- Molecule 3: DotF

Chain Af:



- Molecule 3: DotF

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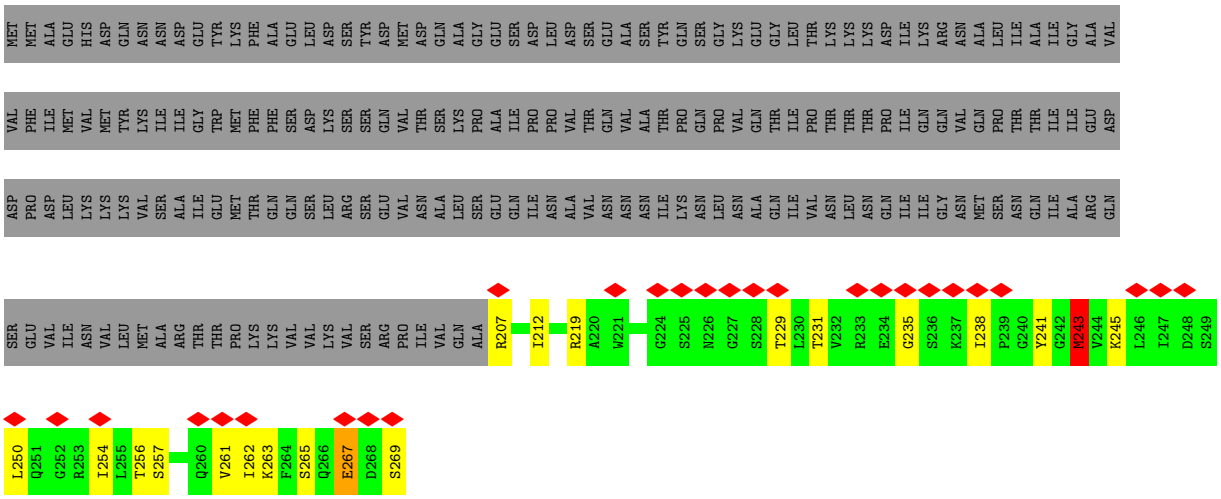
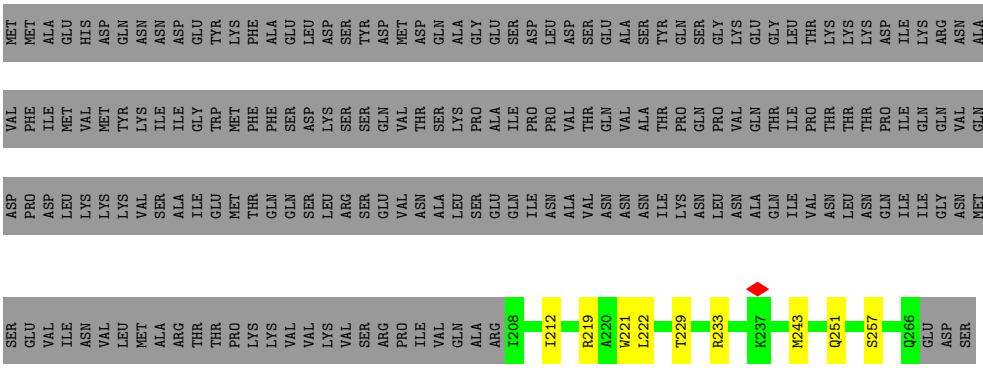


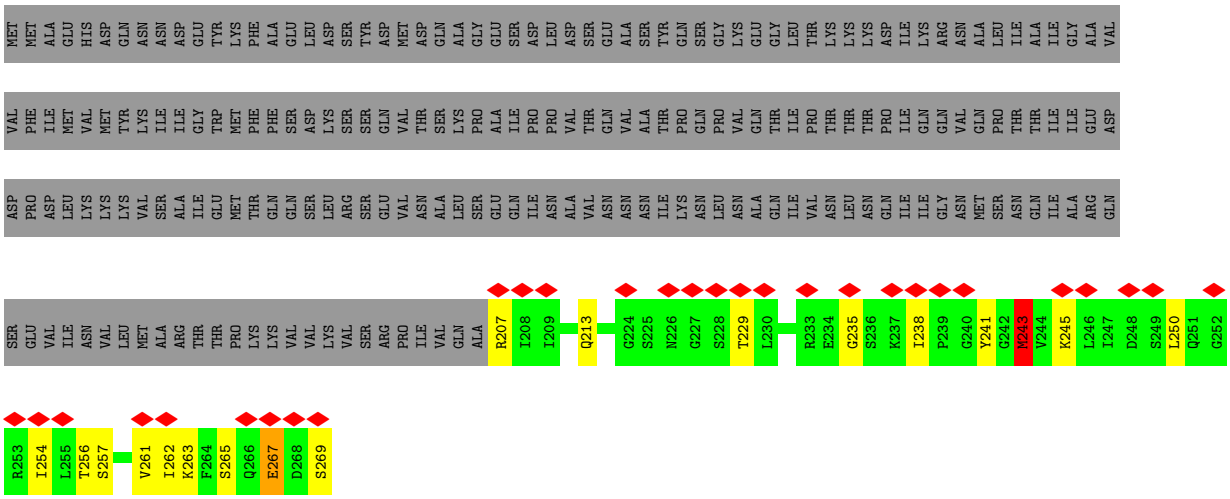
- Molecule 3: DotF

Chain Bf:



- Molecule 3: DotF

Chain CF:



- Molecule 3: DotF

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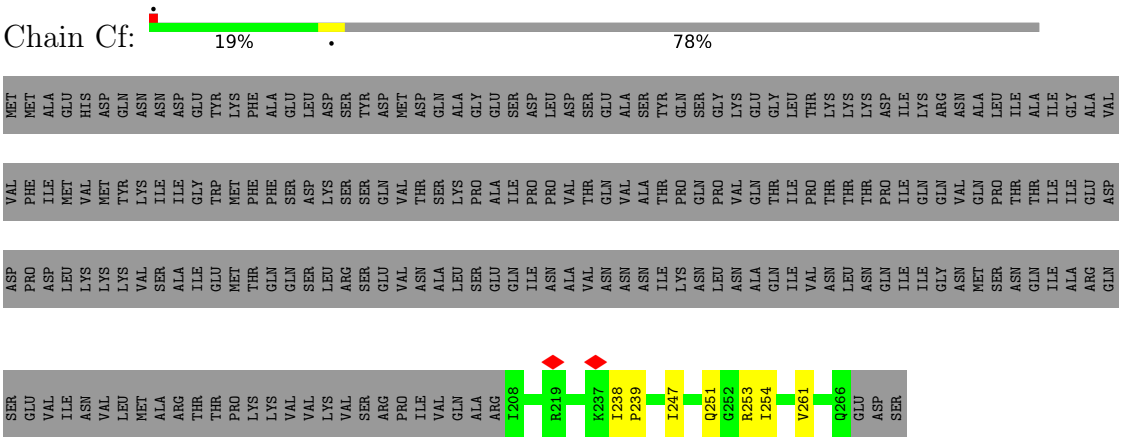

- Molecule 3: DotF

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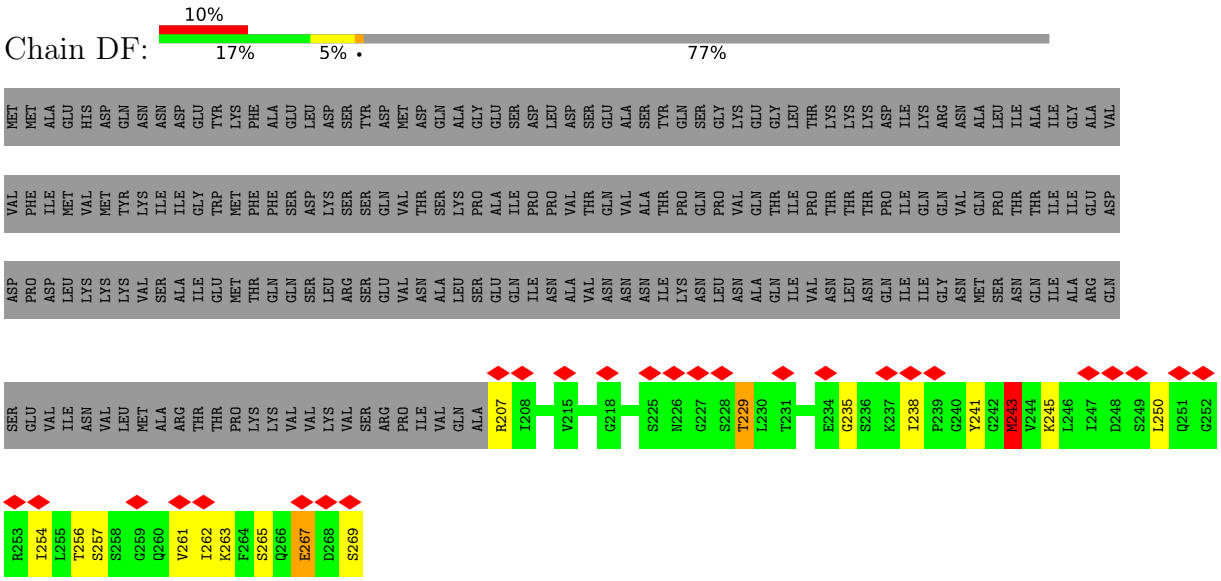

- Molecule 3: DotF

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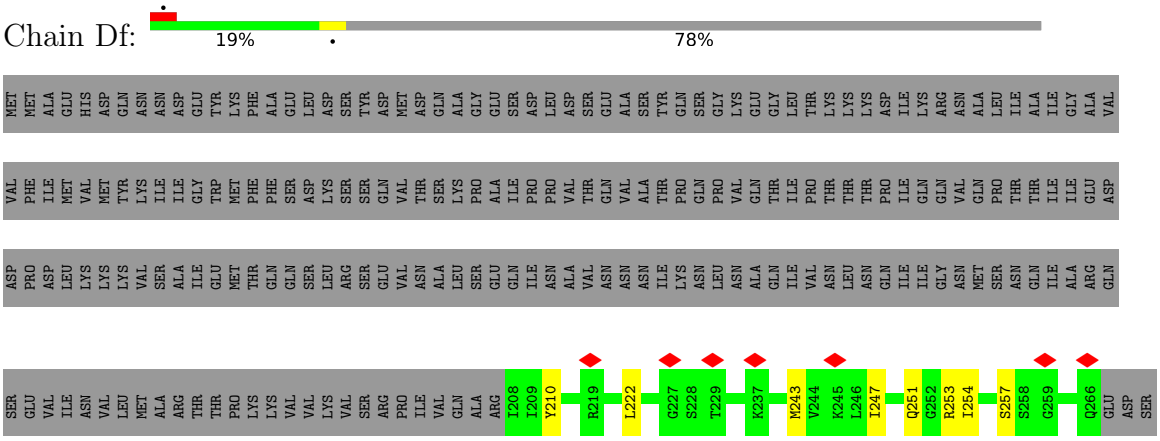
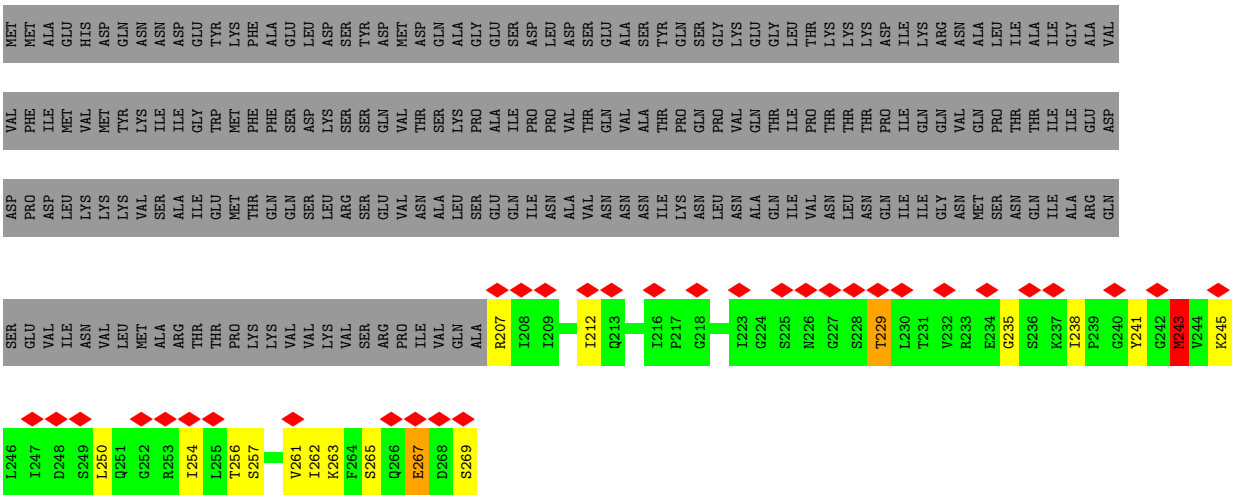


- Molecule 3: DotF

Chain EF:



- Molecule 3: DotF

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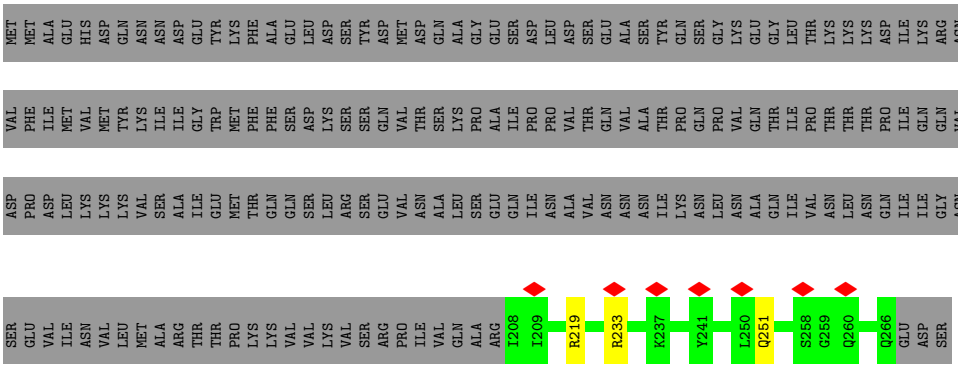

- Molecule 3: DotF

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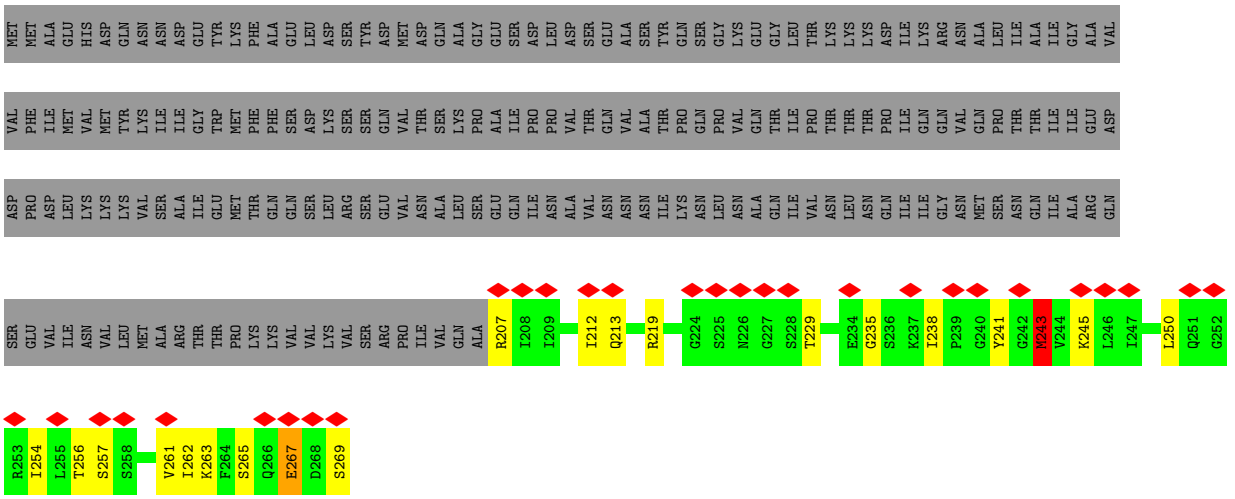

- Molecule 3: DotF

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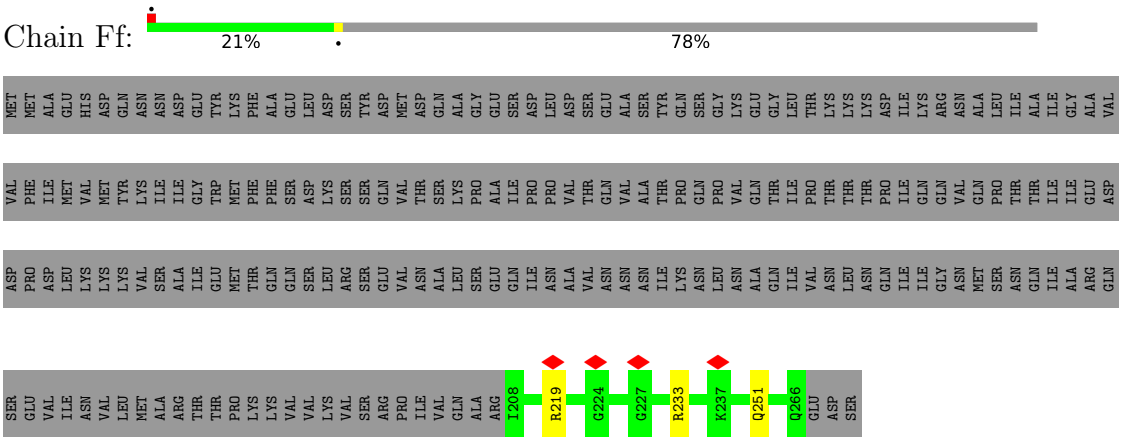
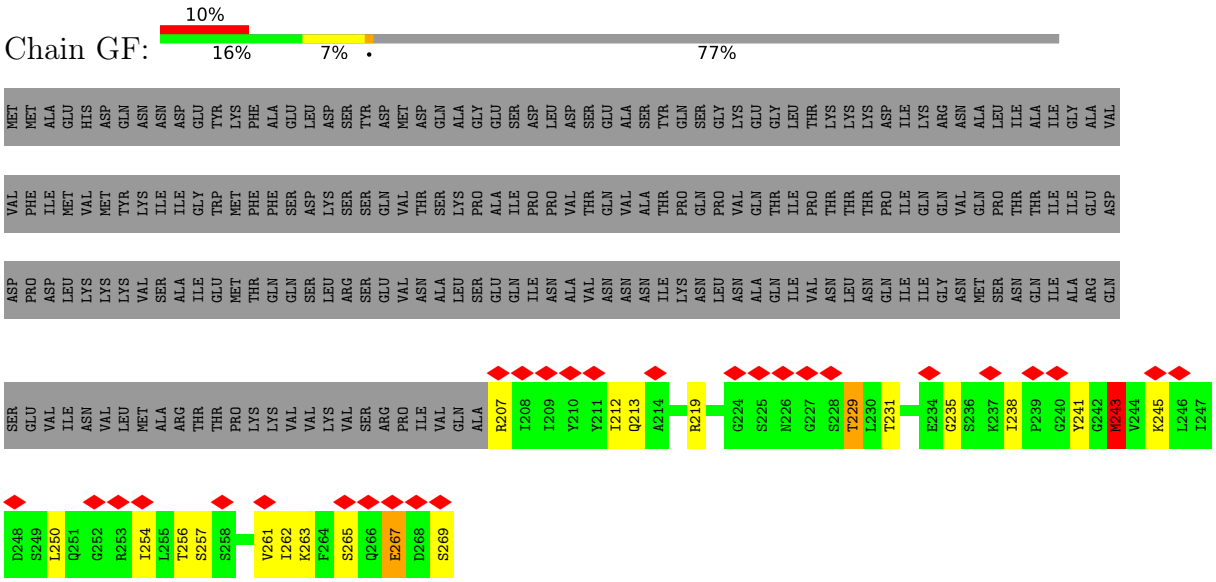


- Molecule 3: DotF

Chain GF:



- Molecule 3: DotF

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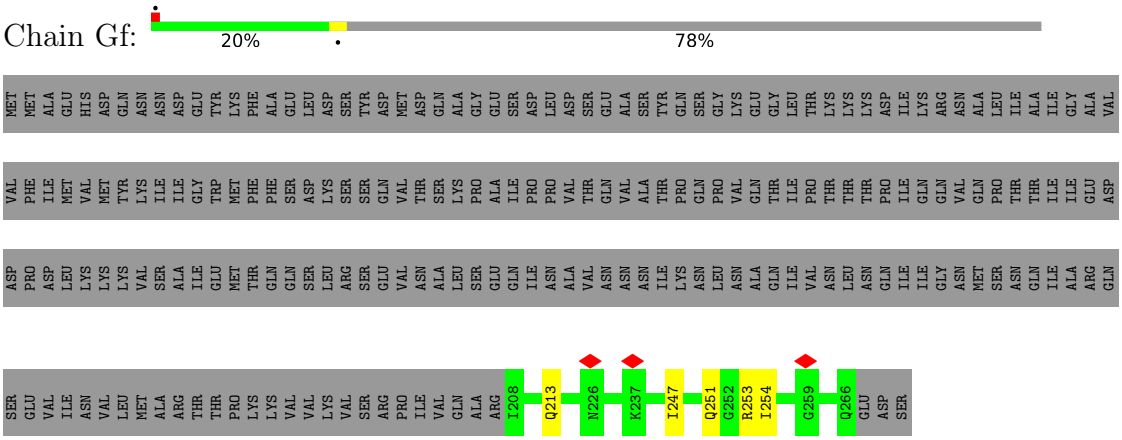

- Molecule 3: DotF

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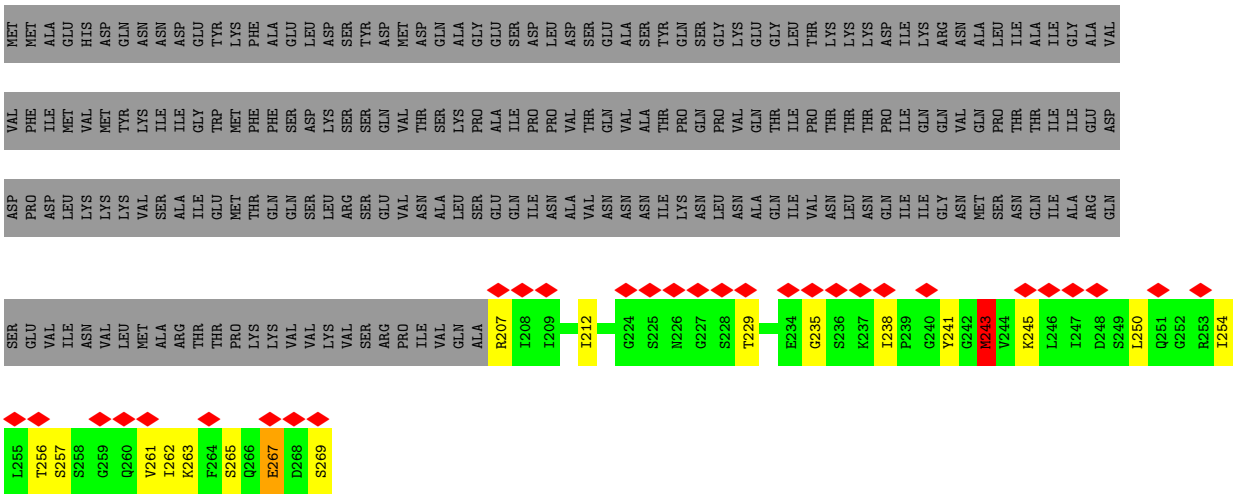
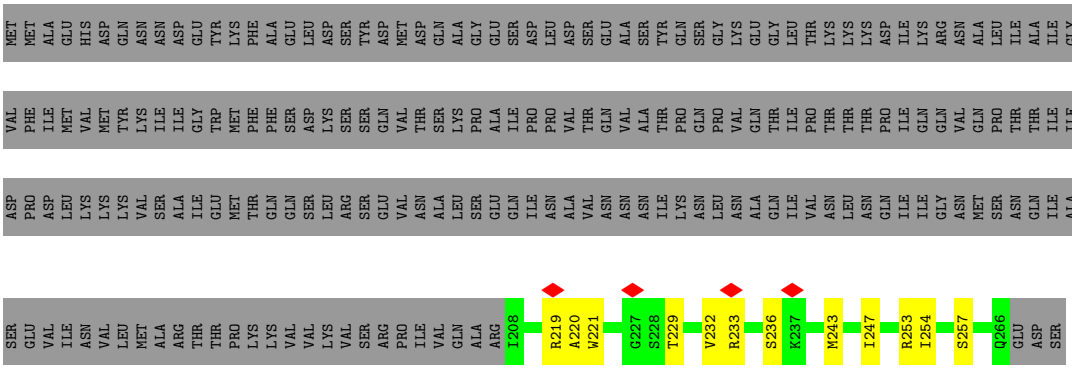


- Molecule 3: DotF

Chain Hf:



- Molecule 3: DotF

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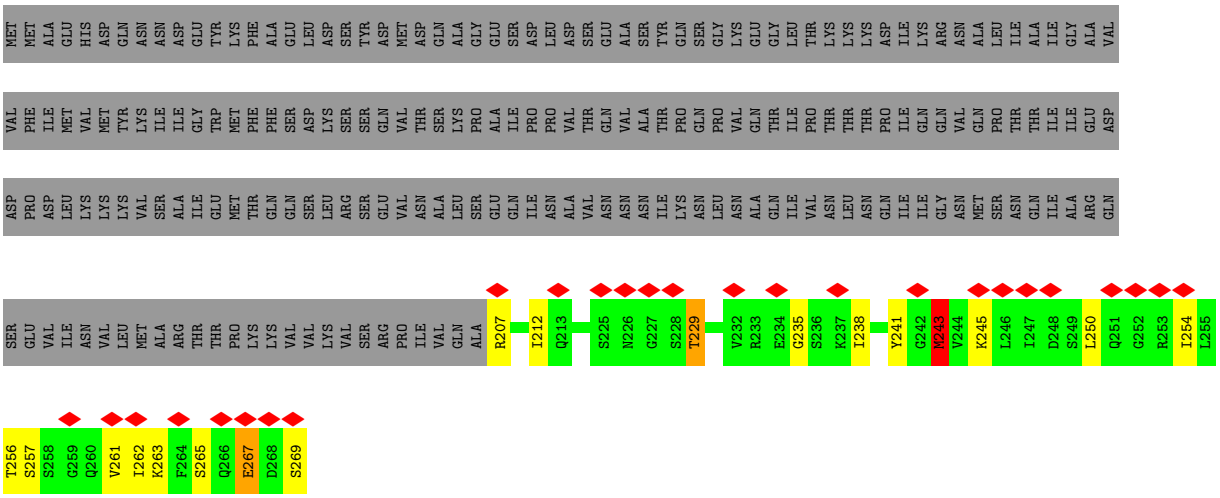
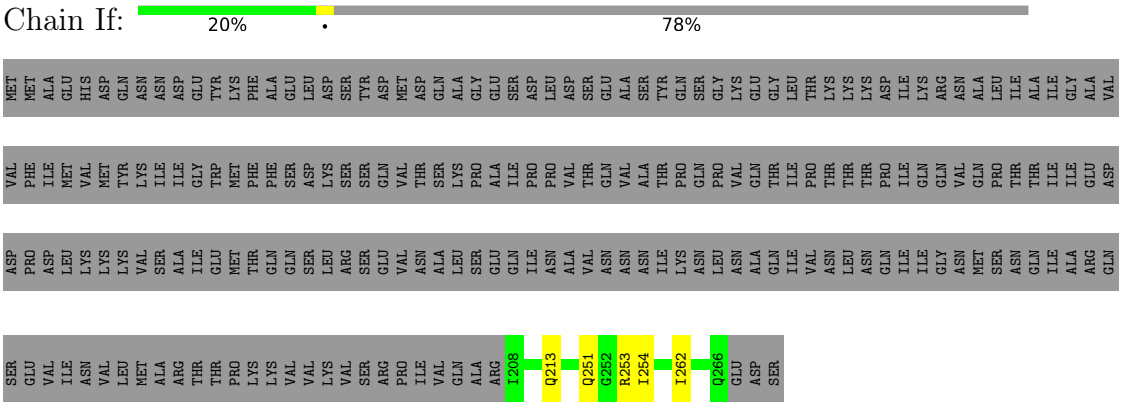


- Molecule 3: DotF

Chain If:



- Molecule 3: DotF

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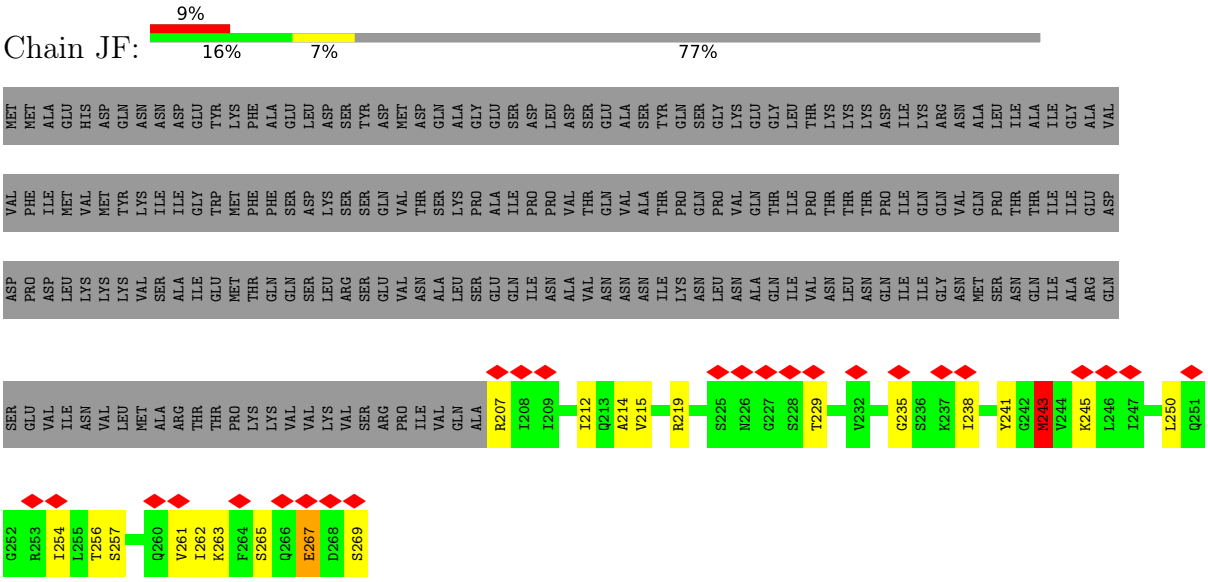

- Molecule 3: DotF

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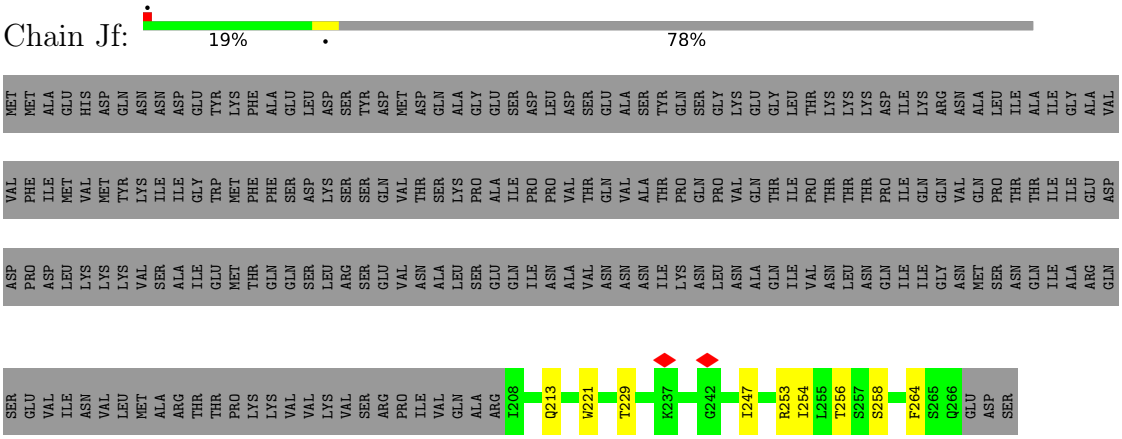
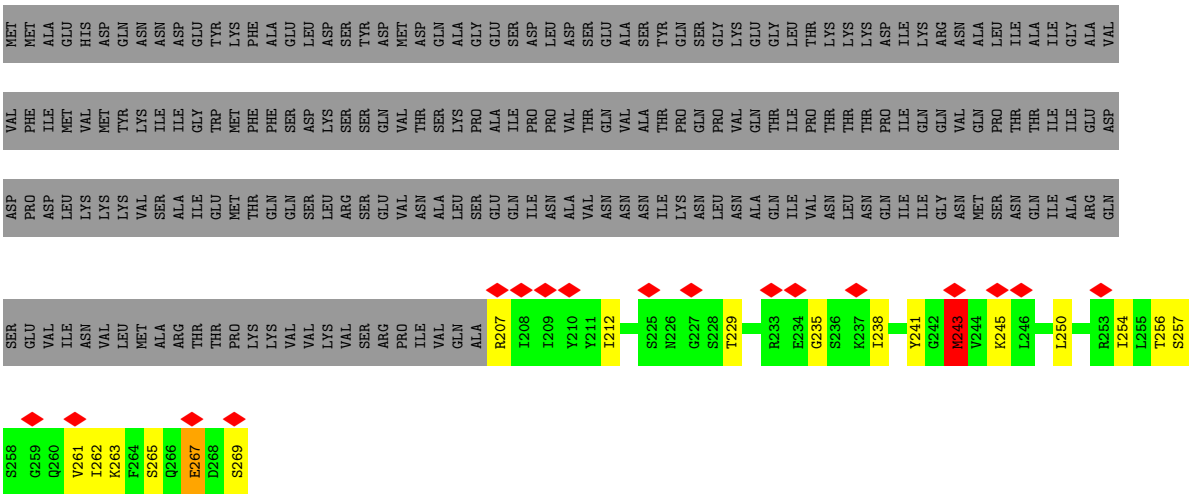


- Molecule 3: DotF

Chain KF:



- Molecule 3: DotF

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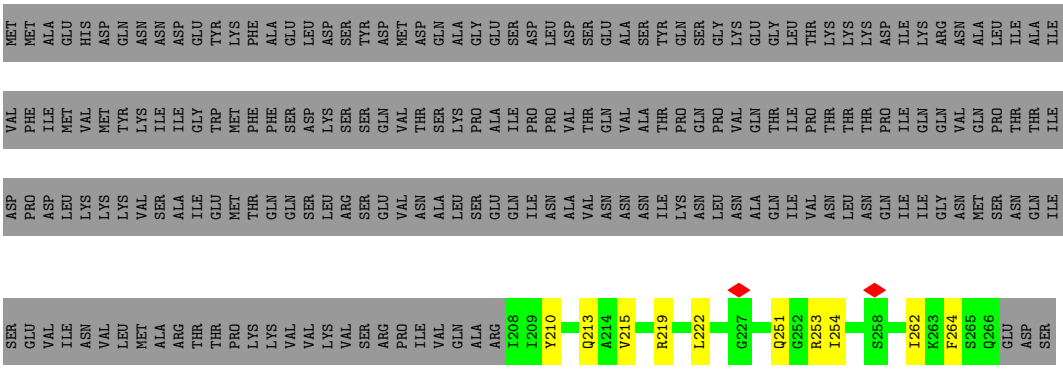
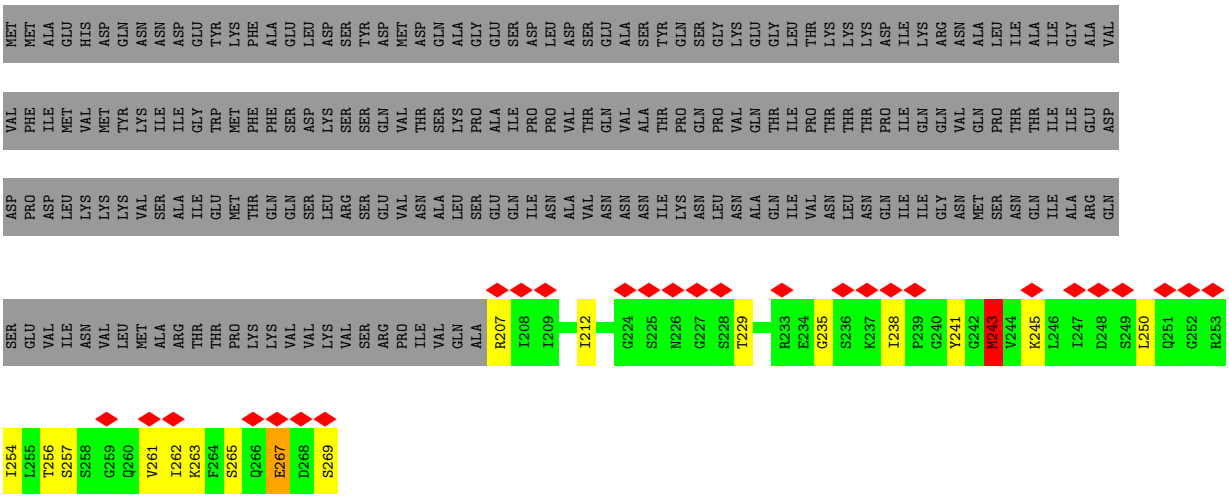


- Molecule 3: DotF

Chain LF:



- Molecule 3: DotF

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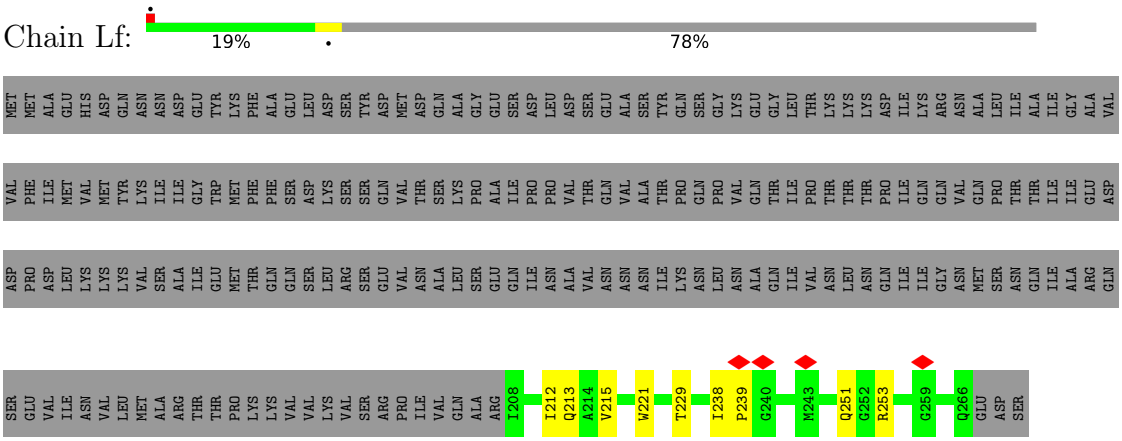

- Molecule 3: DotF

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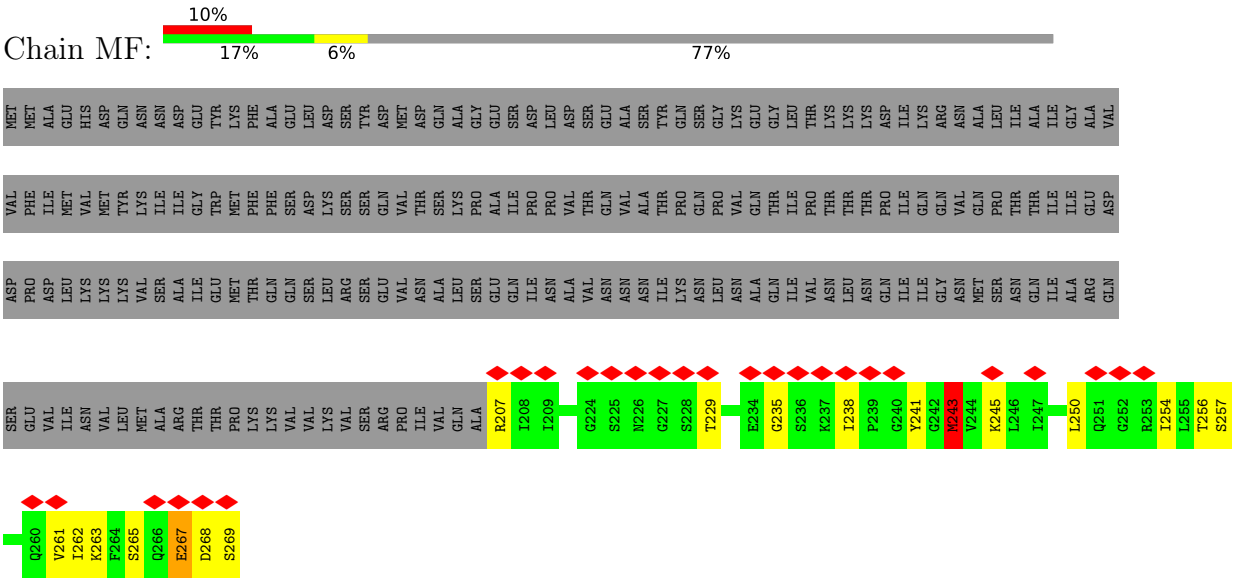
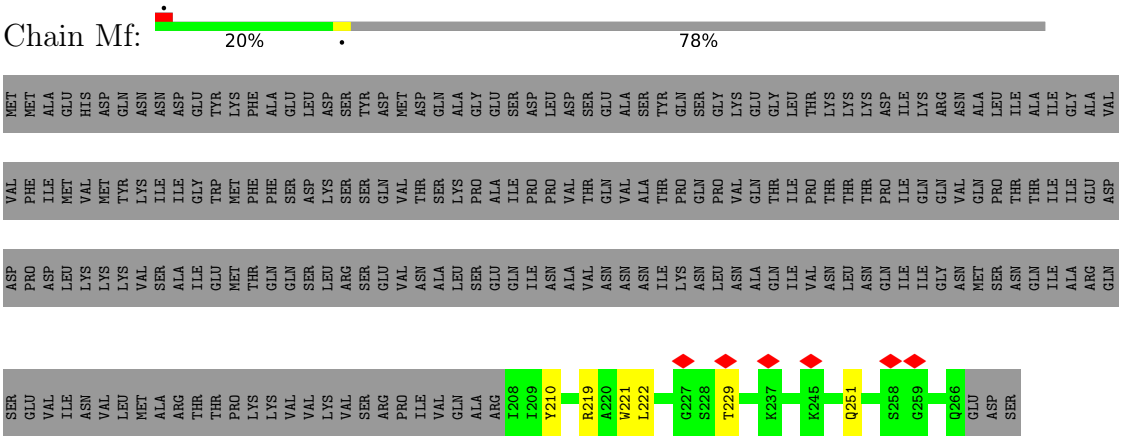


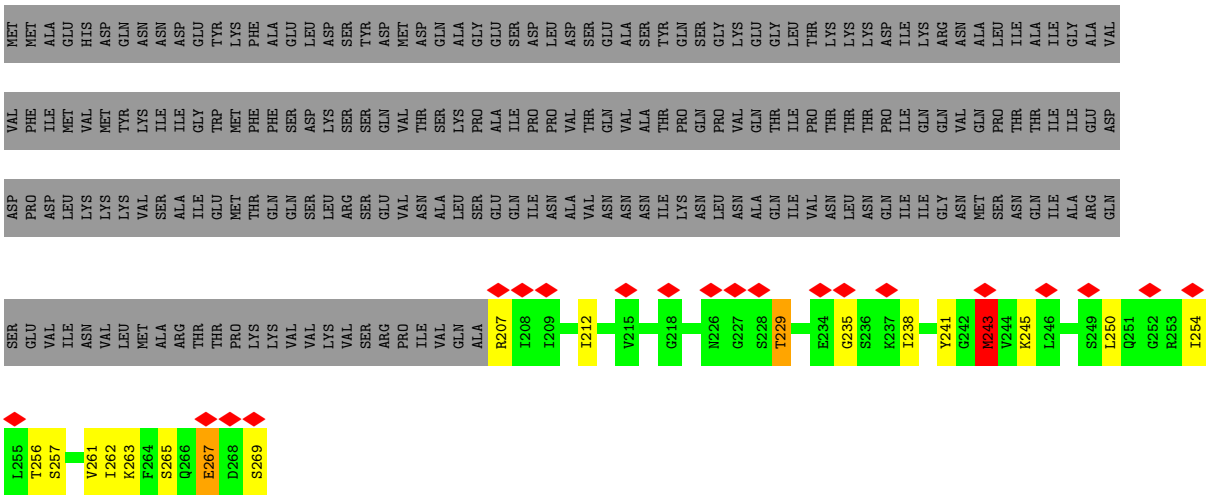
- Molecule 3: DotF

Chain Mf:



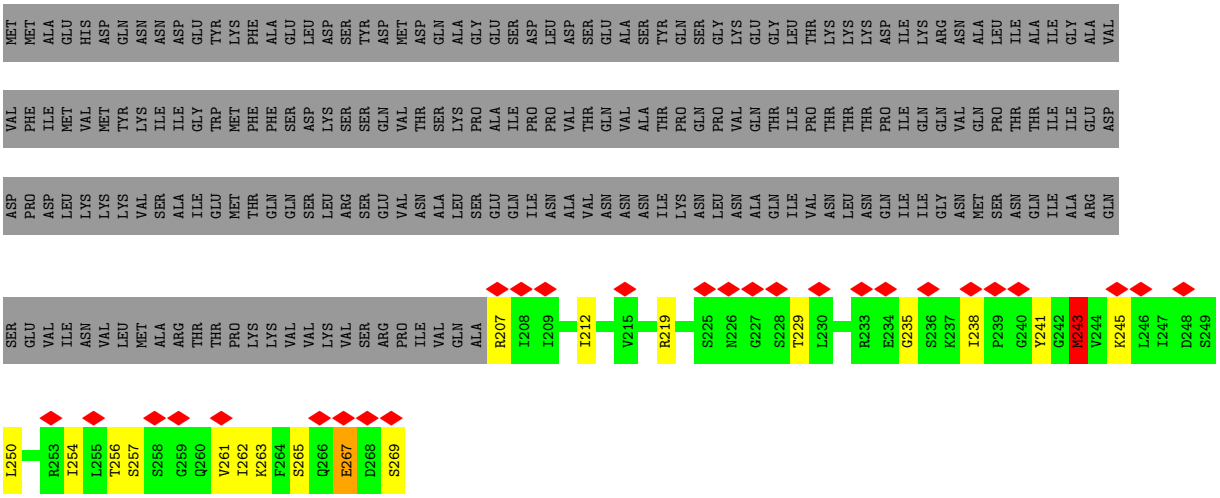
- Molecule 3: DotF

Chain VF:



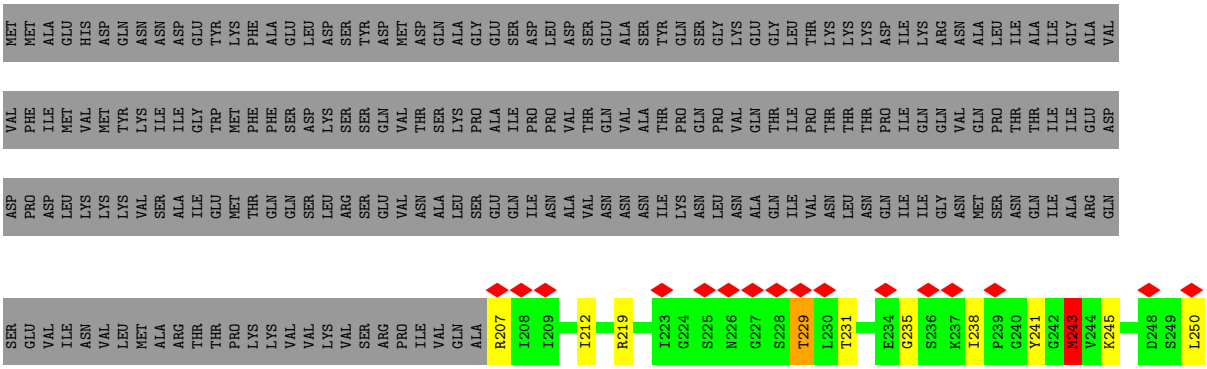
• Molecule 3: DotF

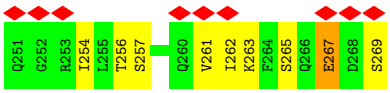
Chain WF: 10% 16% 6% 77%



• Molecule 3: DotF

Chain XF: 9% 16% 6% • 77%





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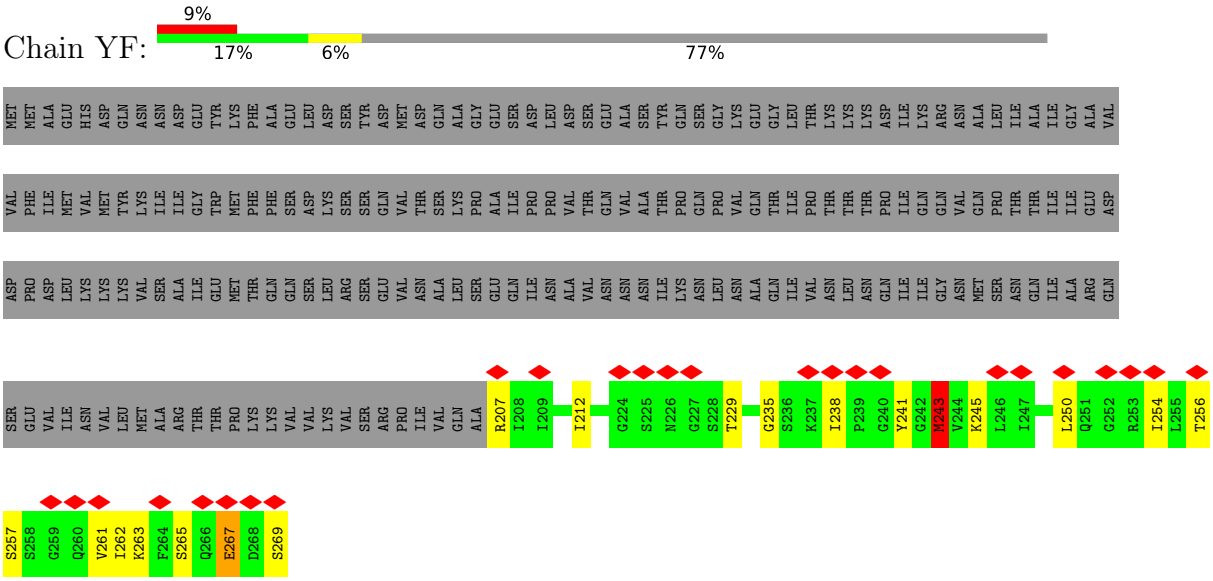
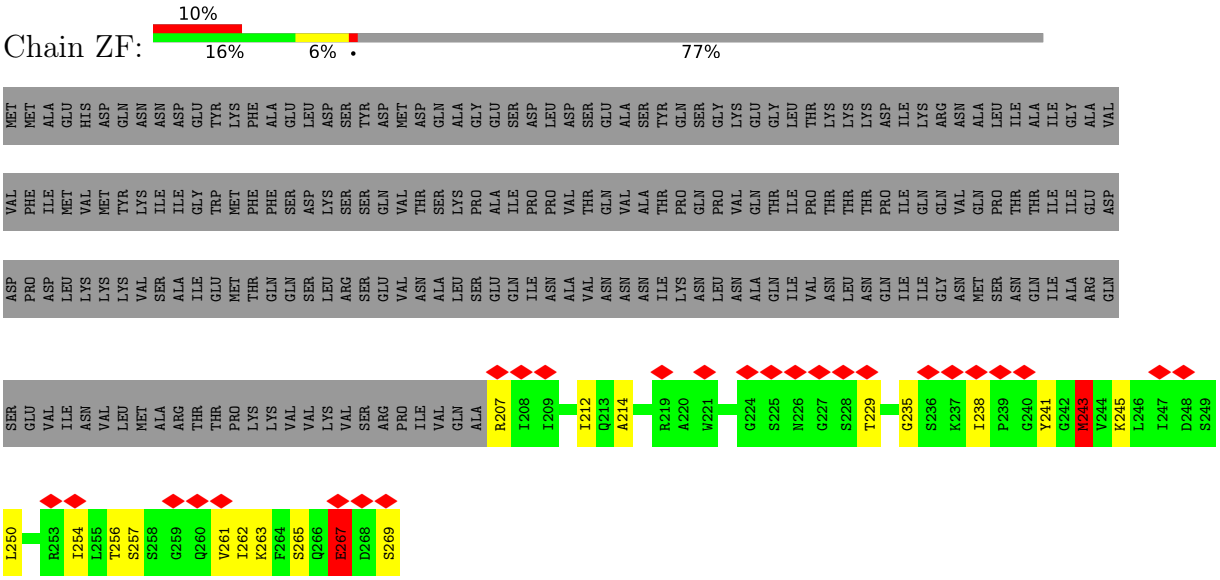
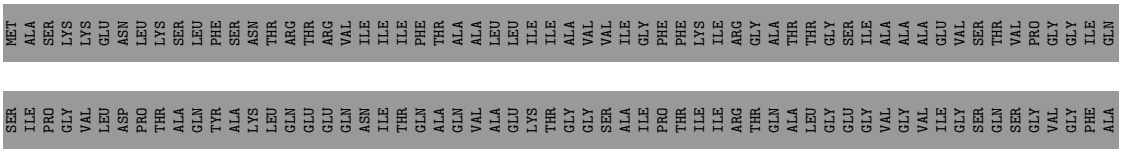
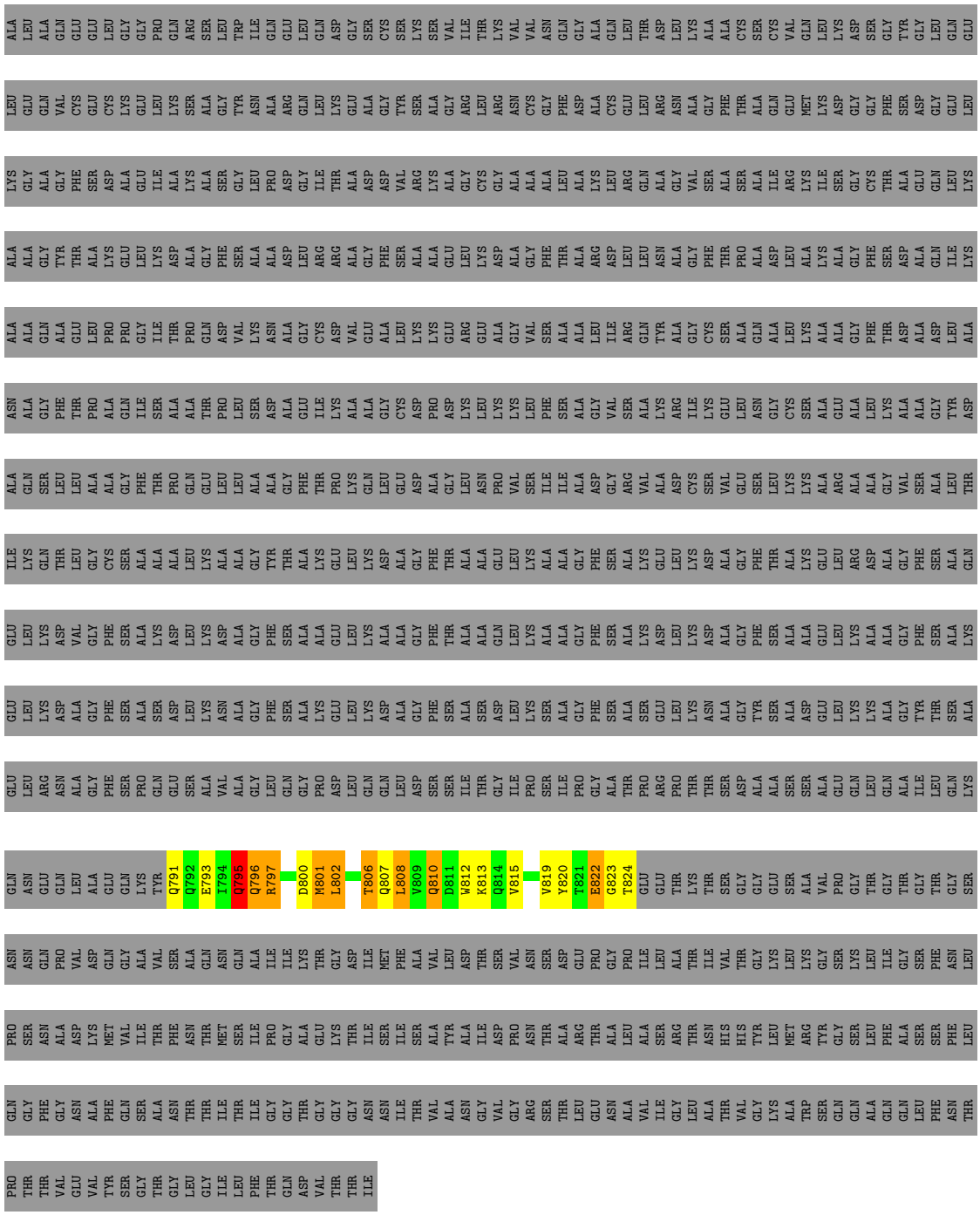


- Molecule 3: DotF



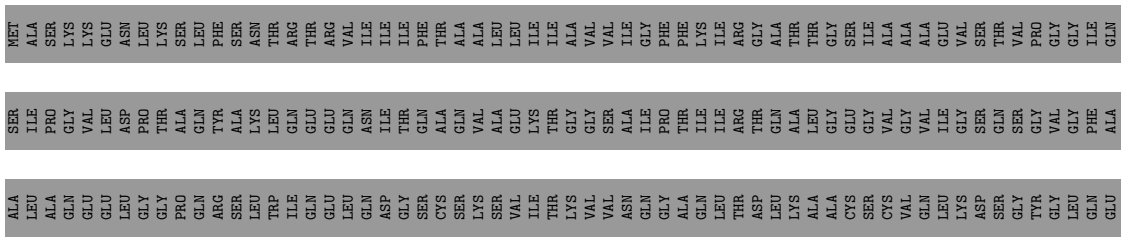
- Molecule 4: IcmE protein

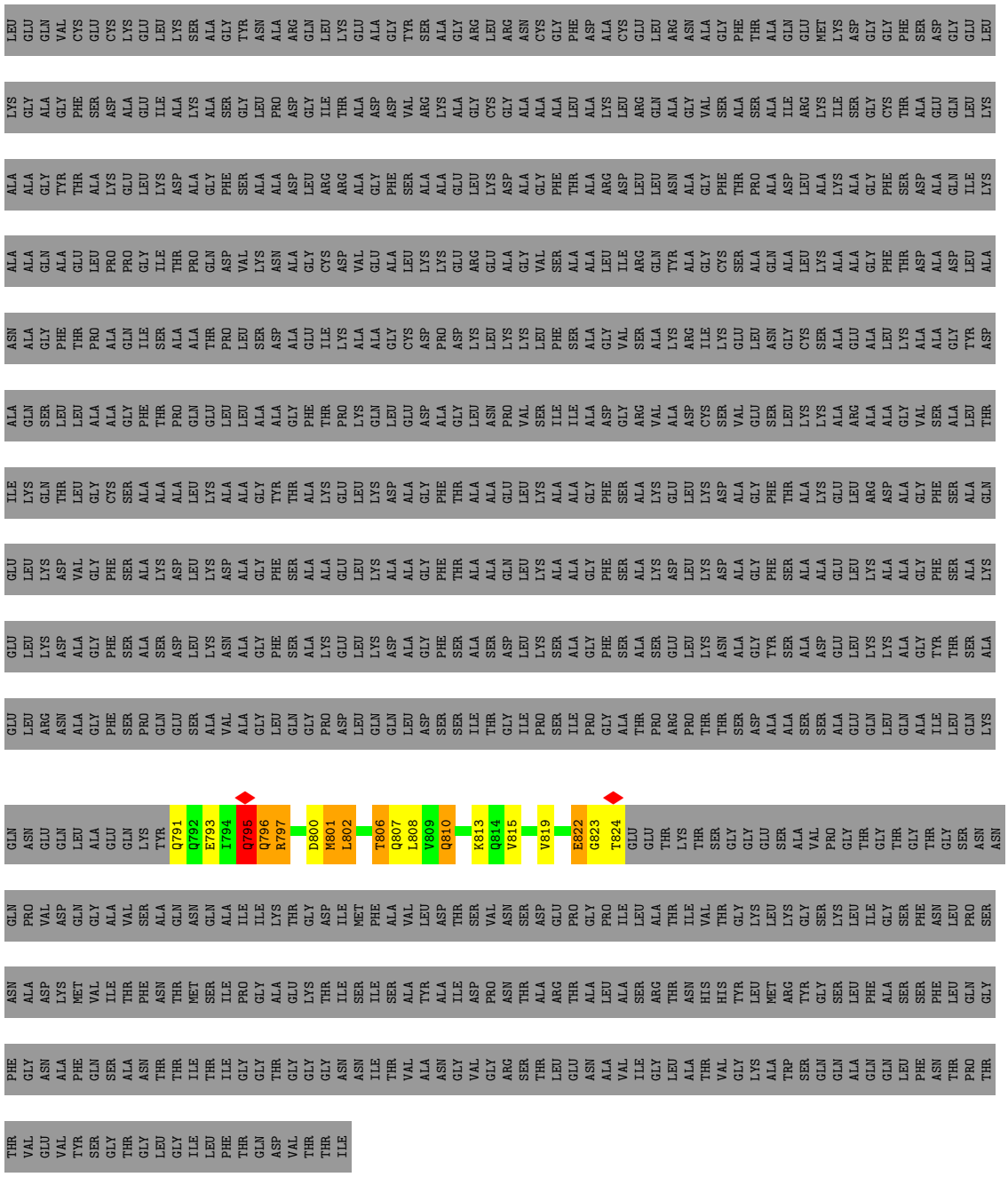




- Molecule 4: IcmE protein

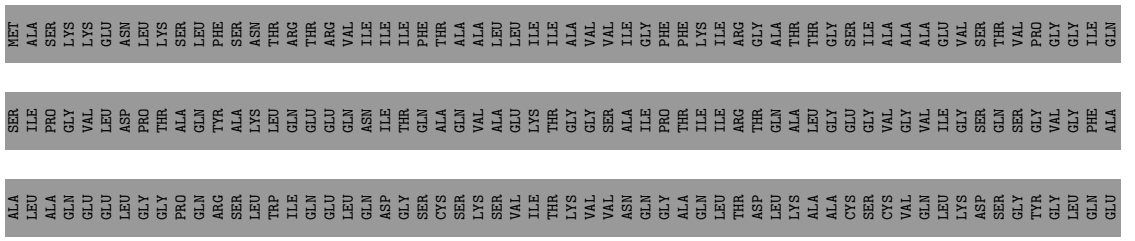
Chain BG: ••• 97%

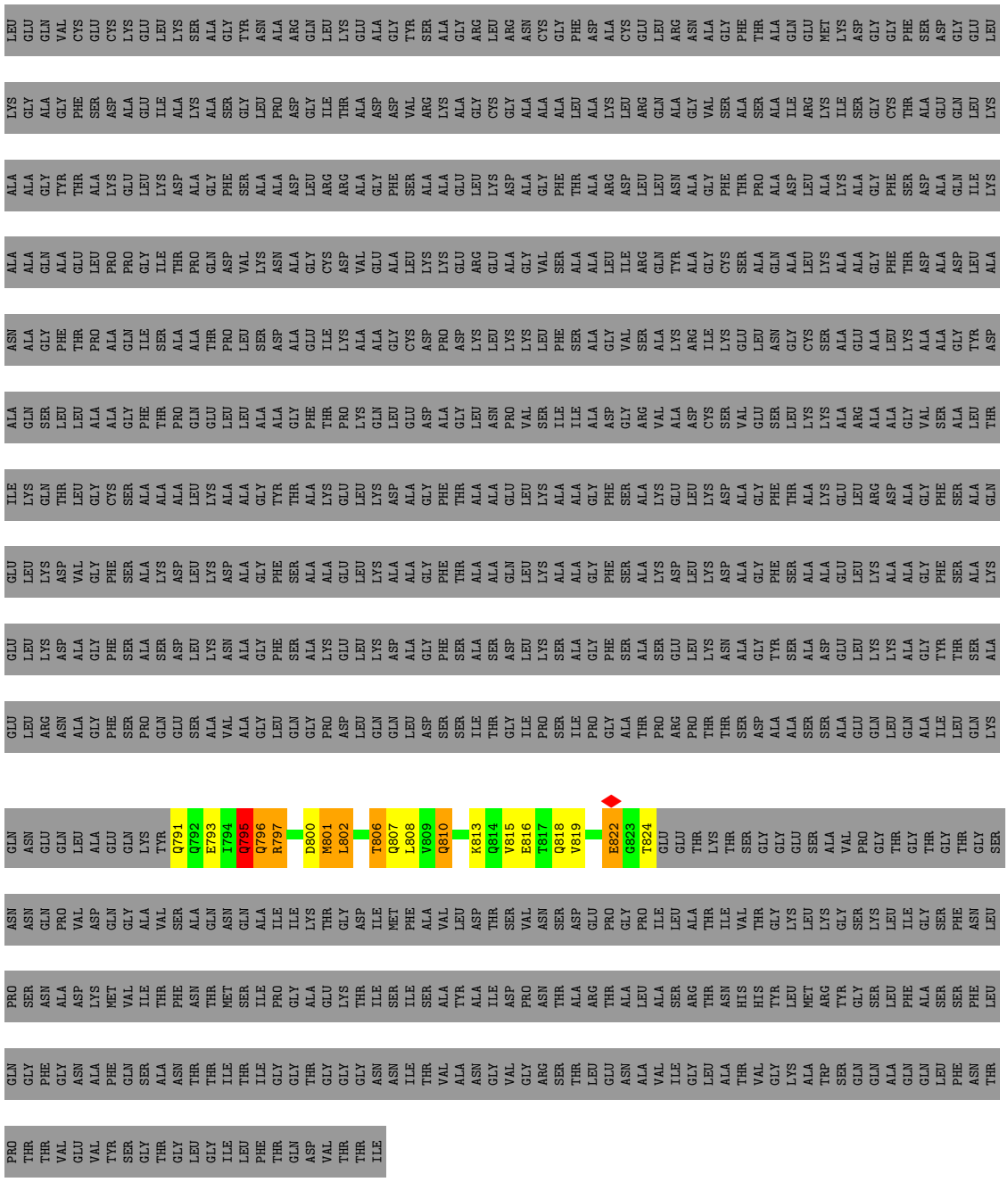




- Molecule 4: IcmE protein

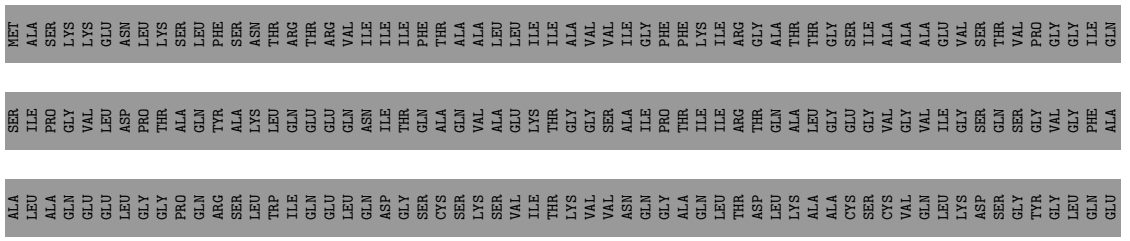
Chain CG: ... 97%

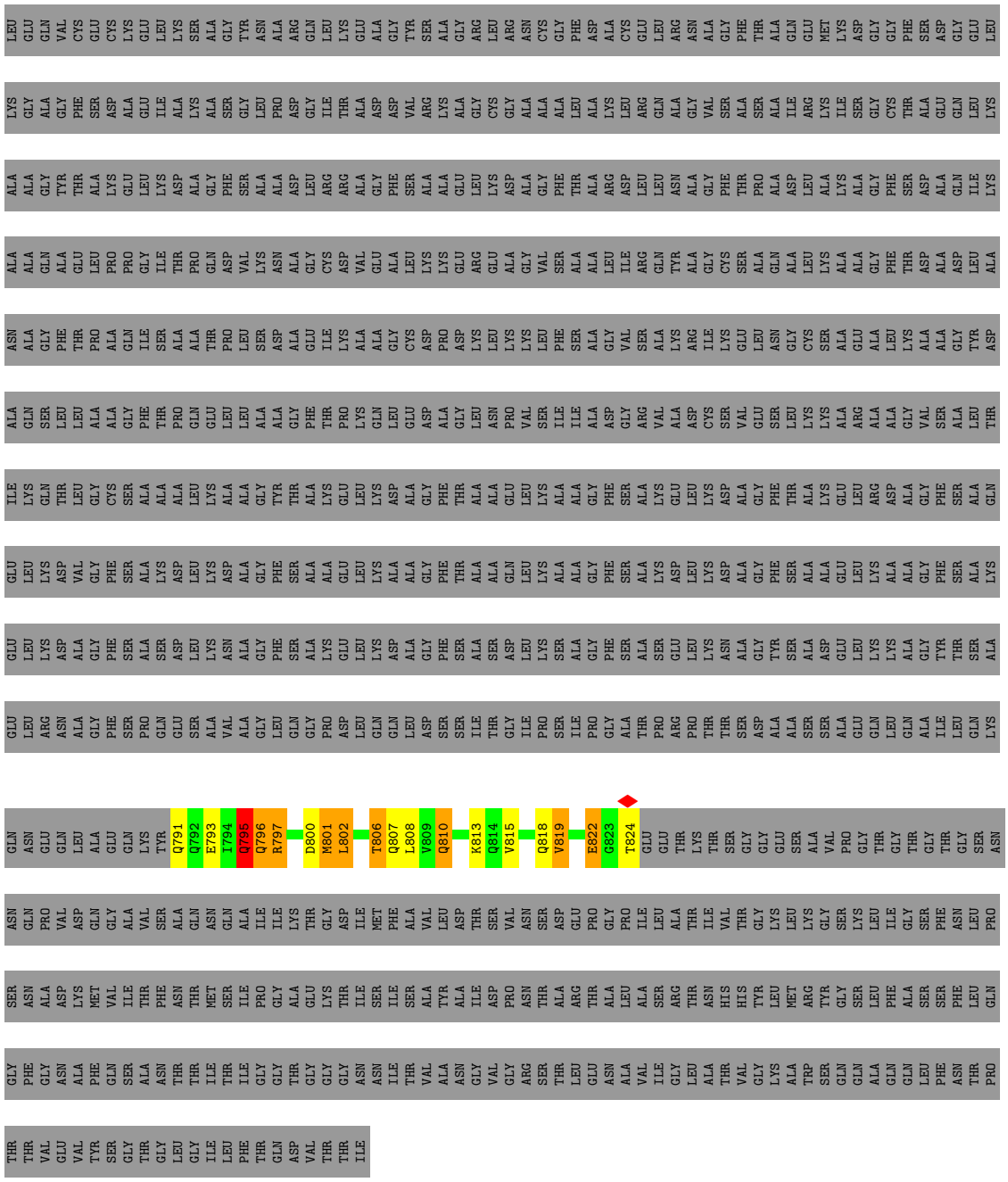




• Molecule 4: IcmE protein

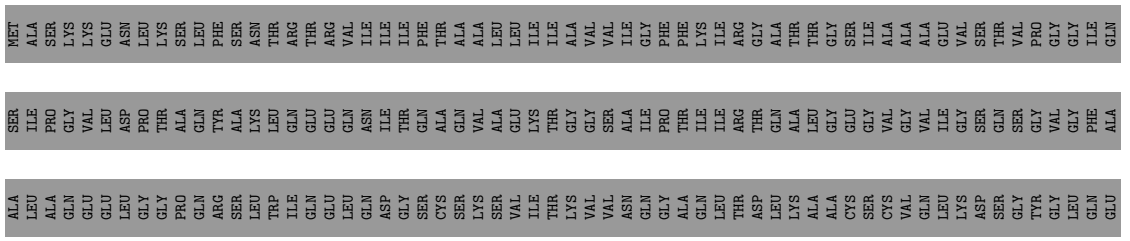
Chain DG: 97%

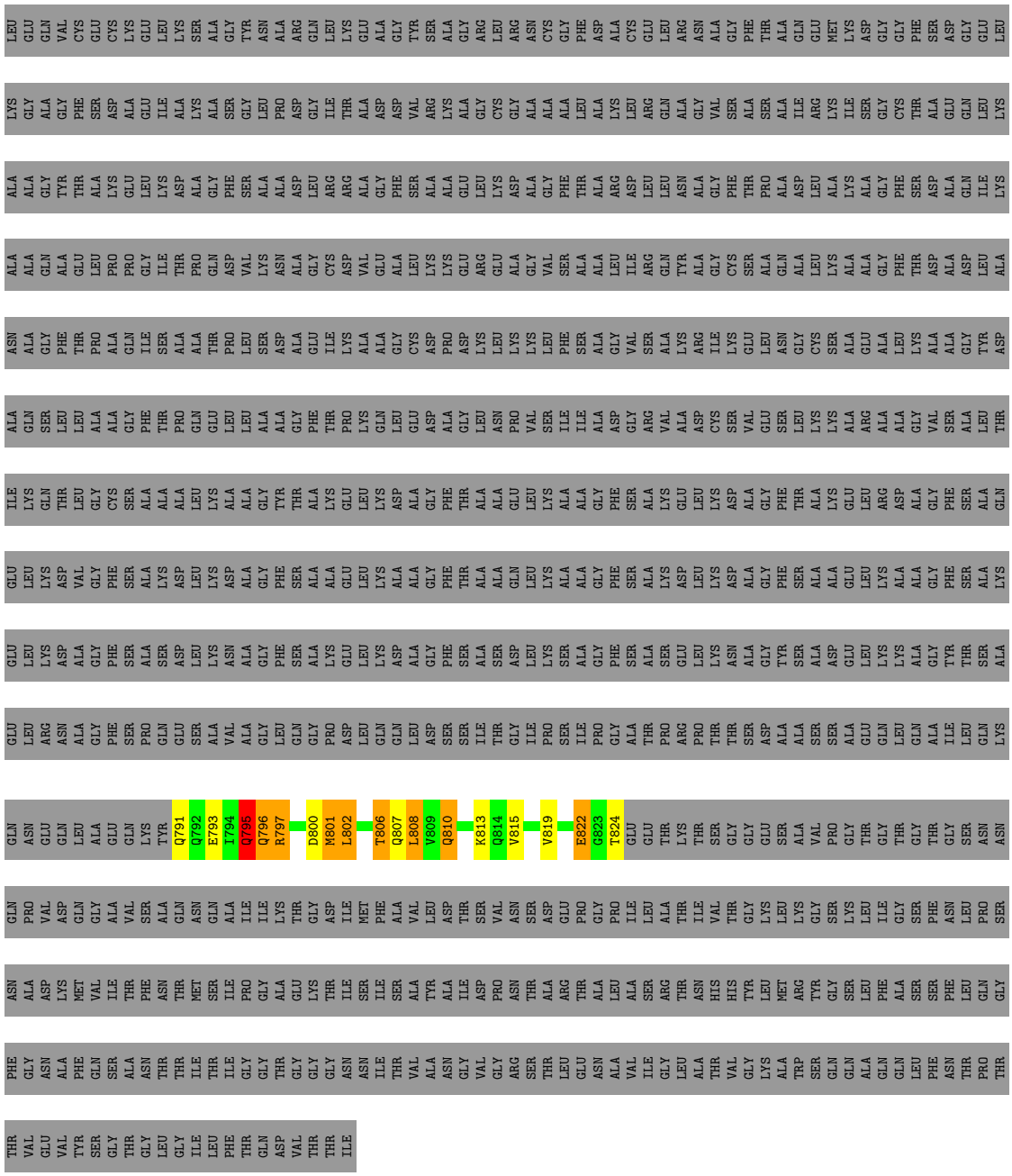




• Molecule 4: IcmE protein

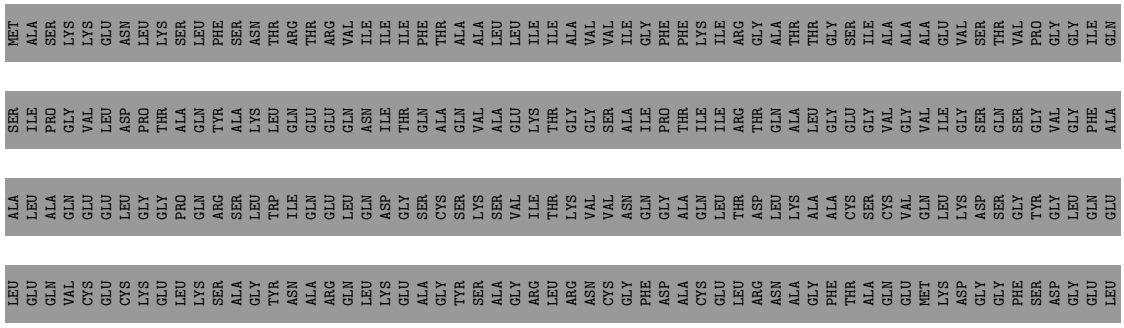
Chain EG: ••• 97%

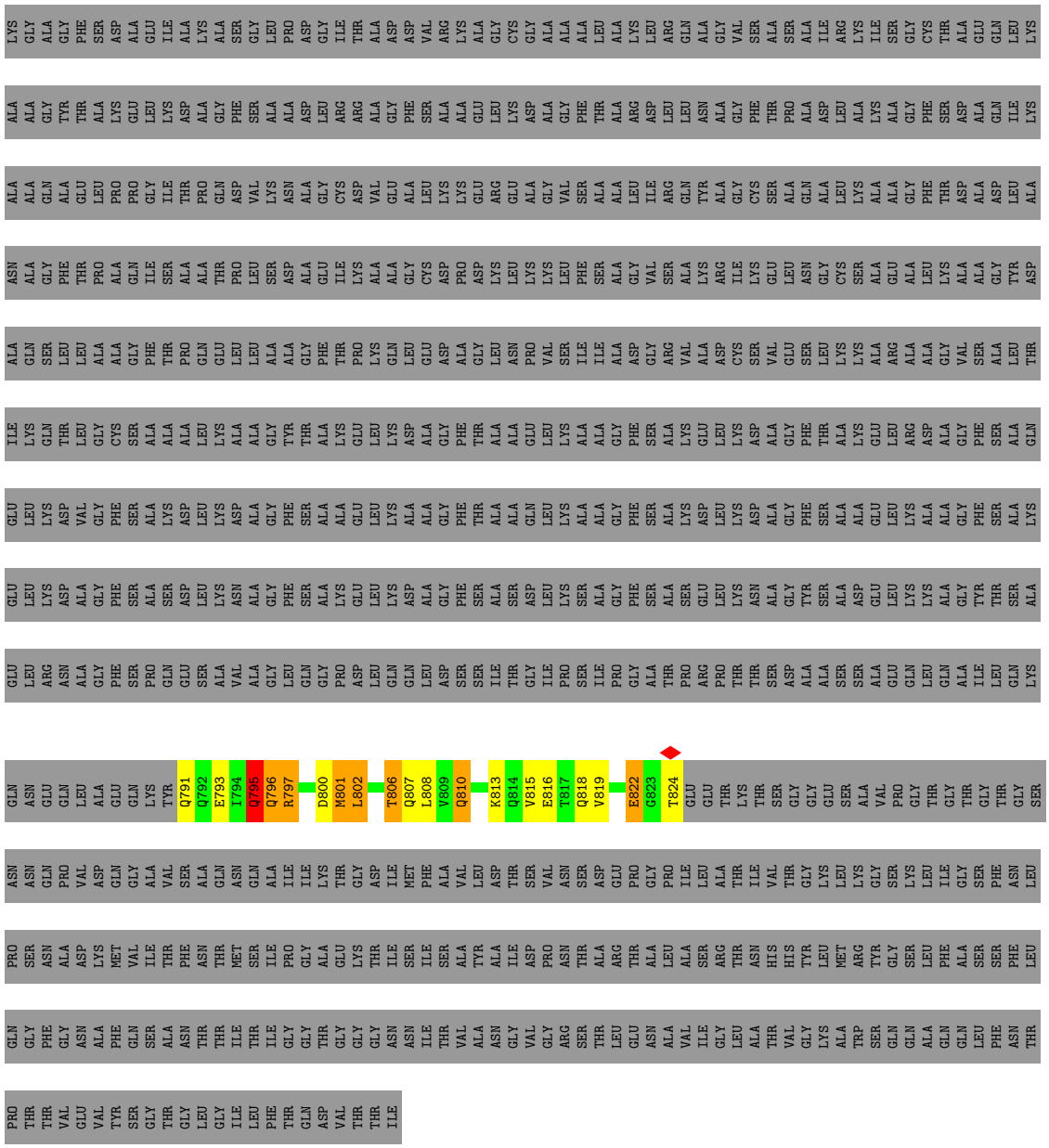




- Molecule 4: IcmE protein

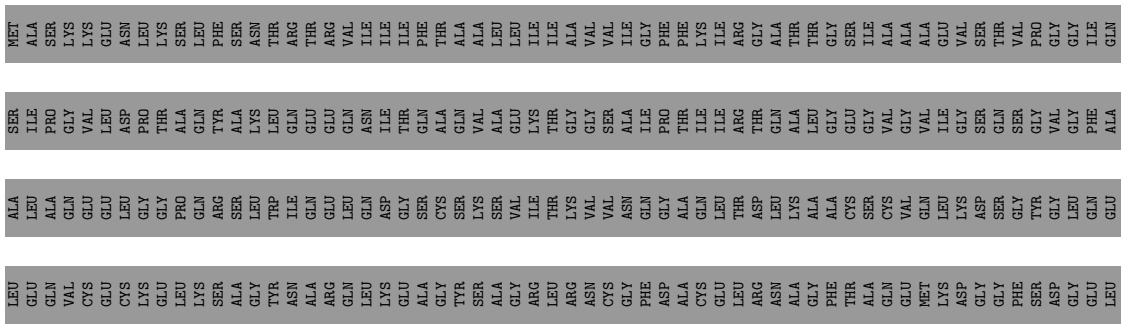
Chain FG: ... 97%

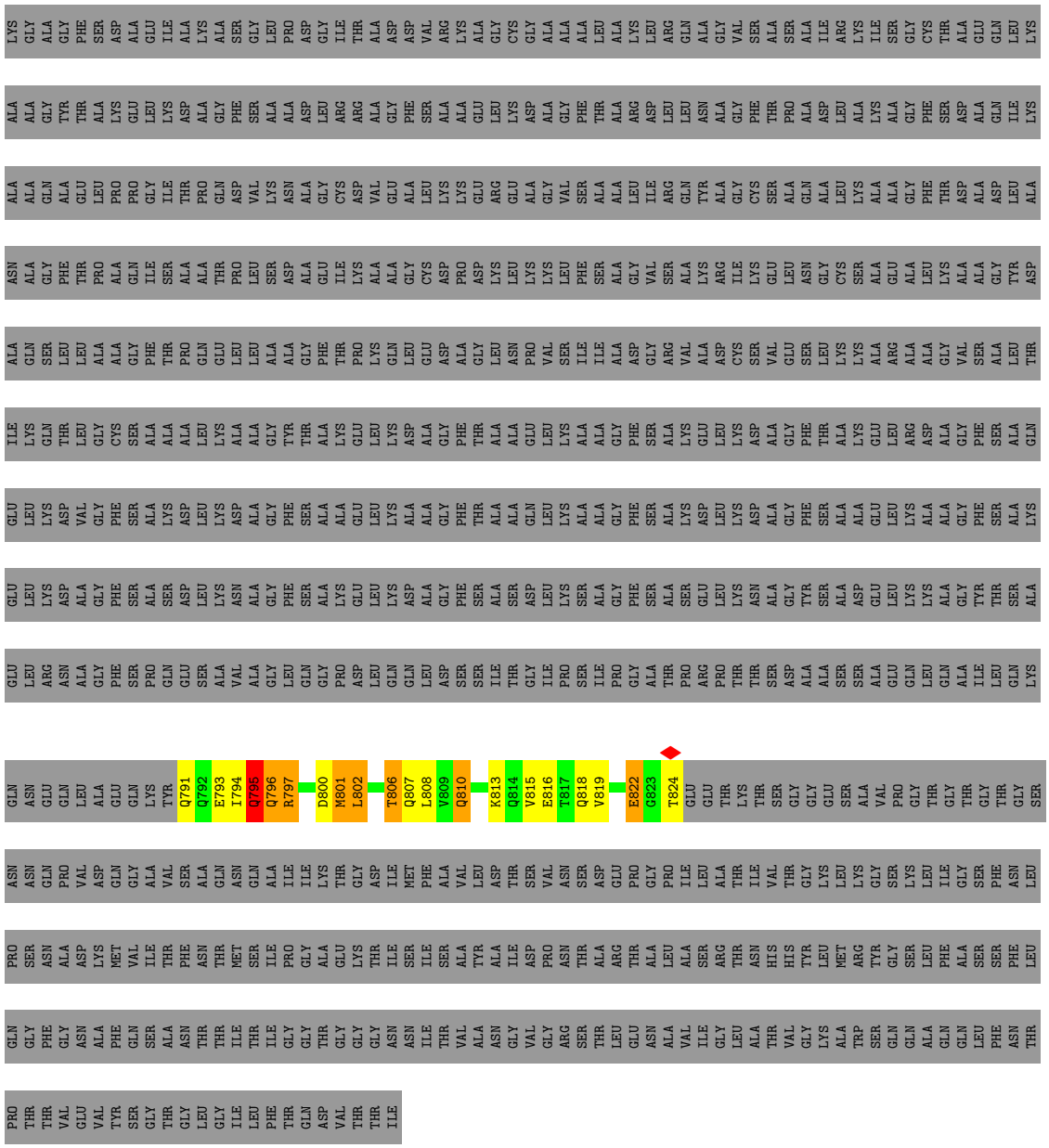




- Molecule 4: IcmE protein

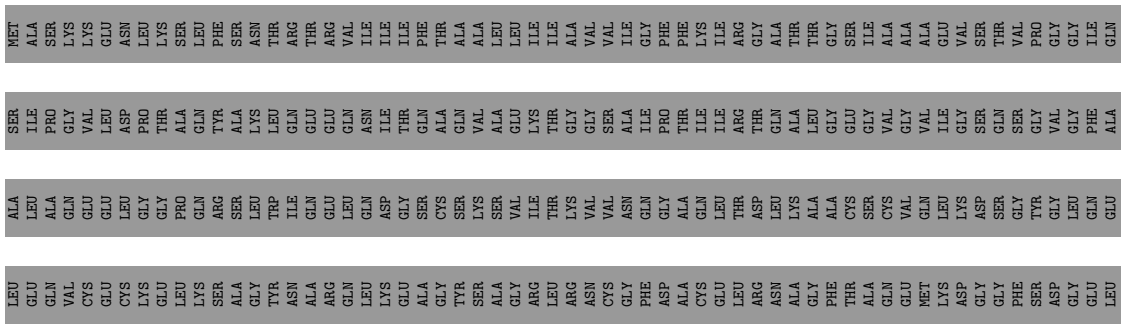
Chain GG: 97%

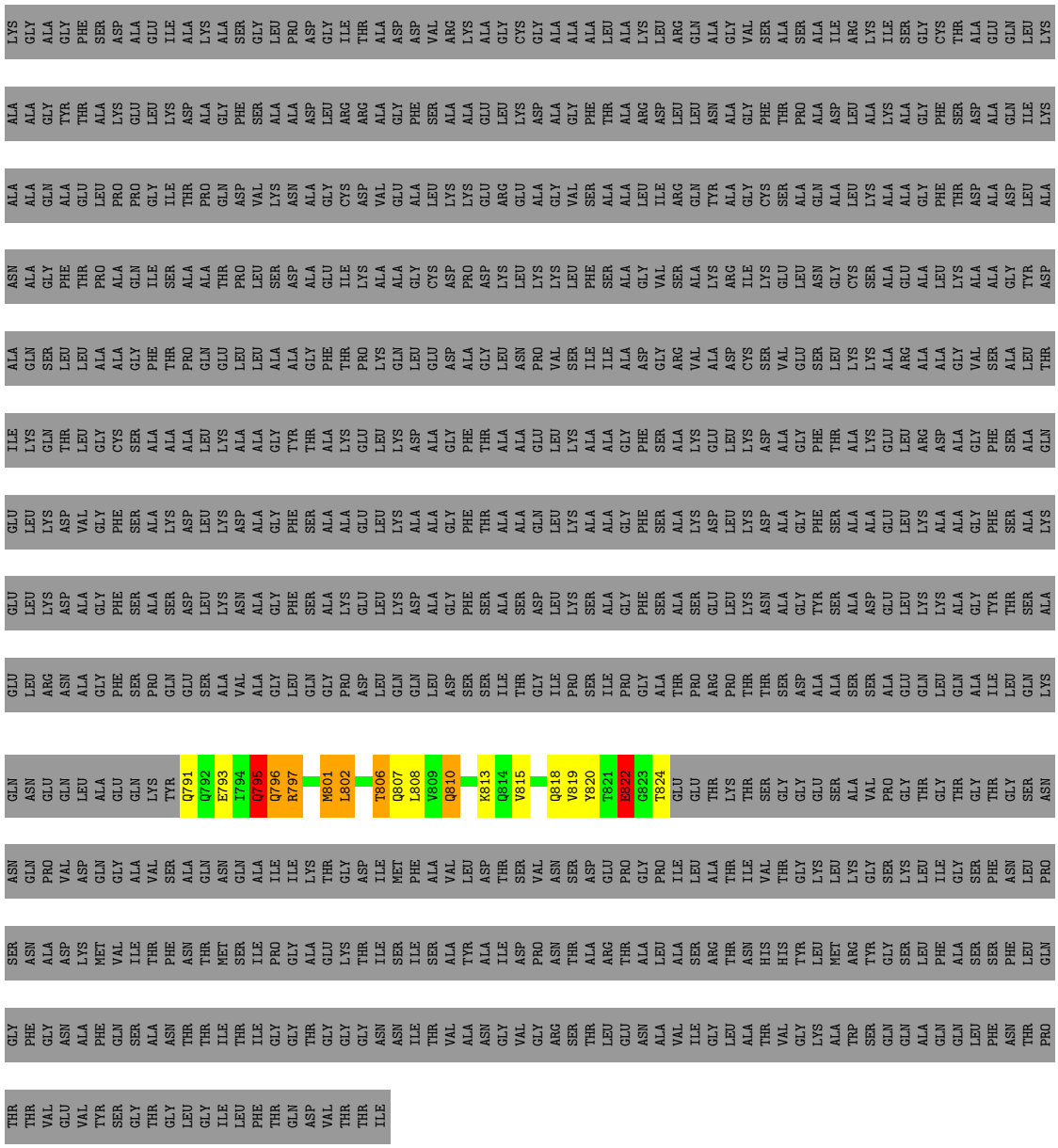




- Molecule 4: IcmE protein

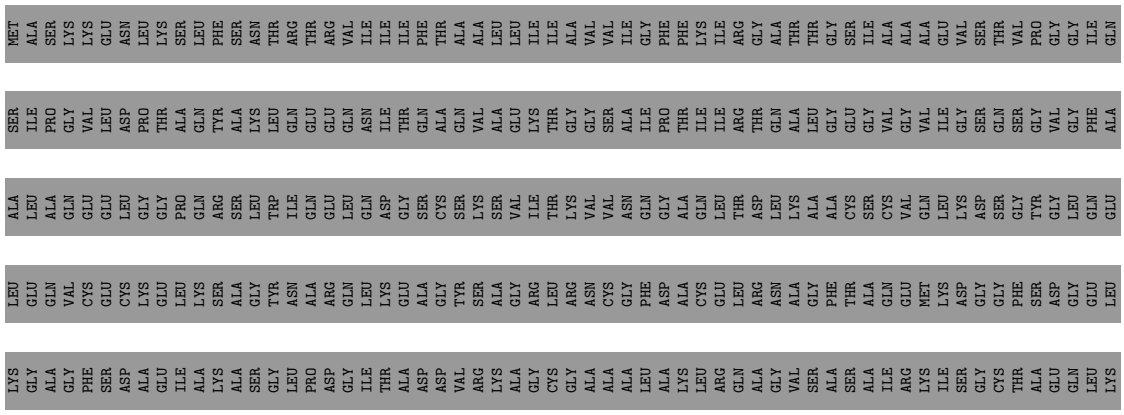
Chain HG: 97%

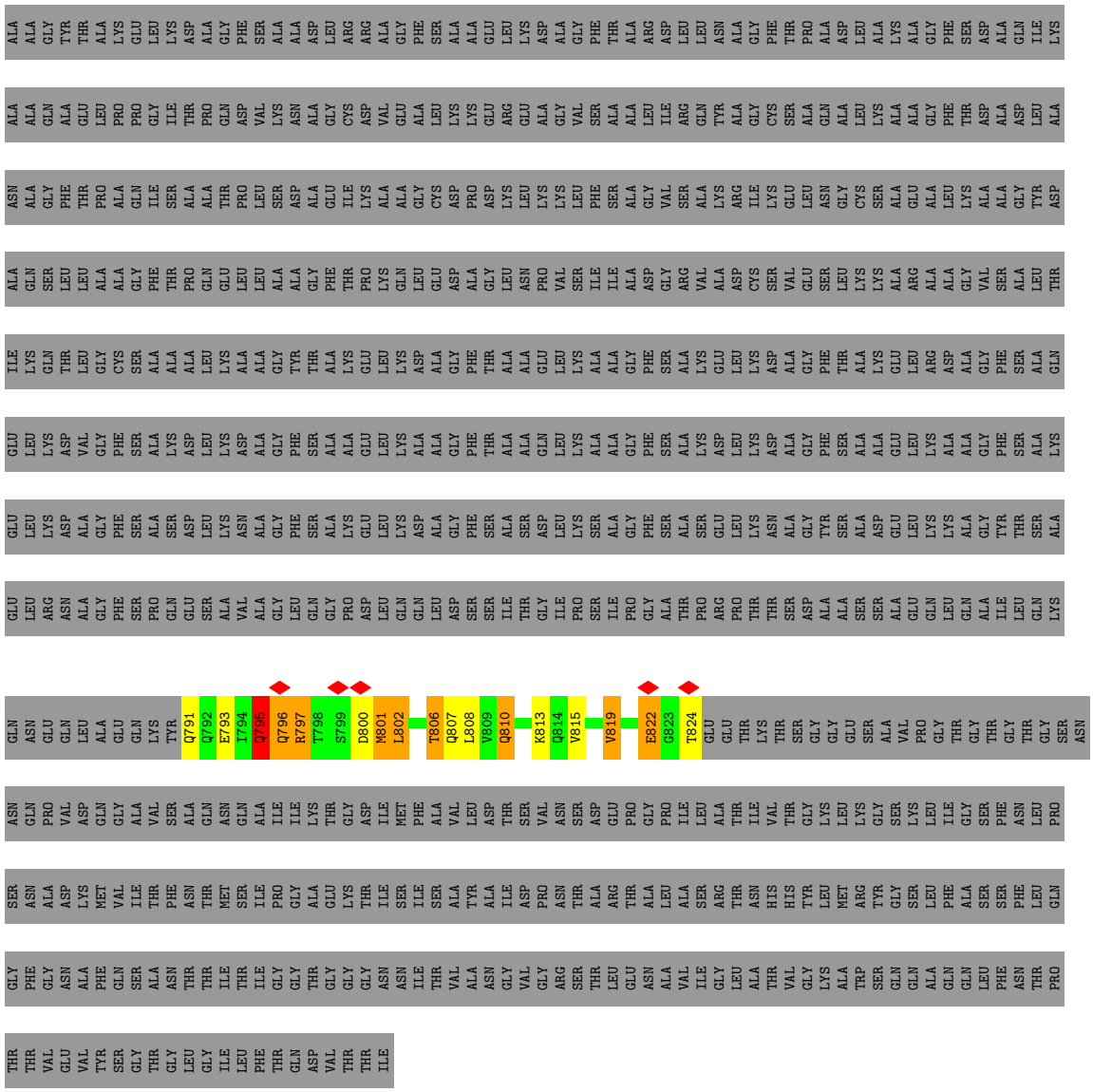




- Molecule 4: IcmE protein

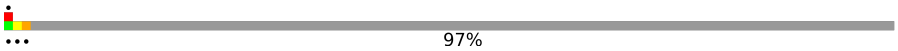
Chain IG: 97%

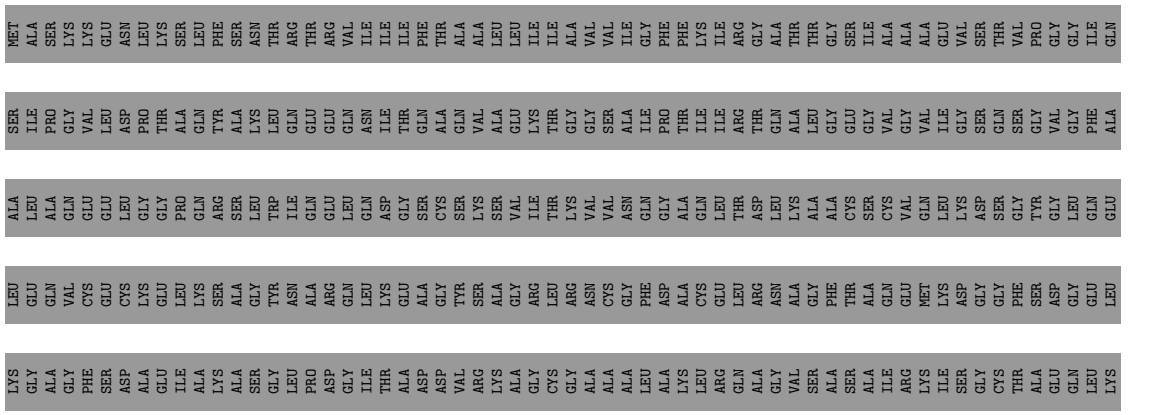


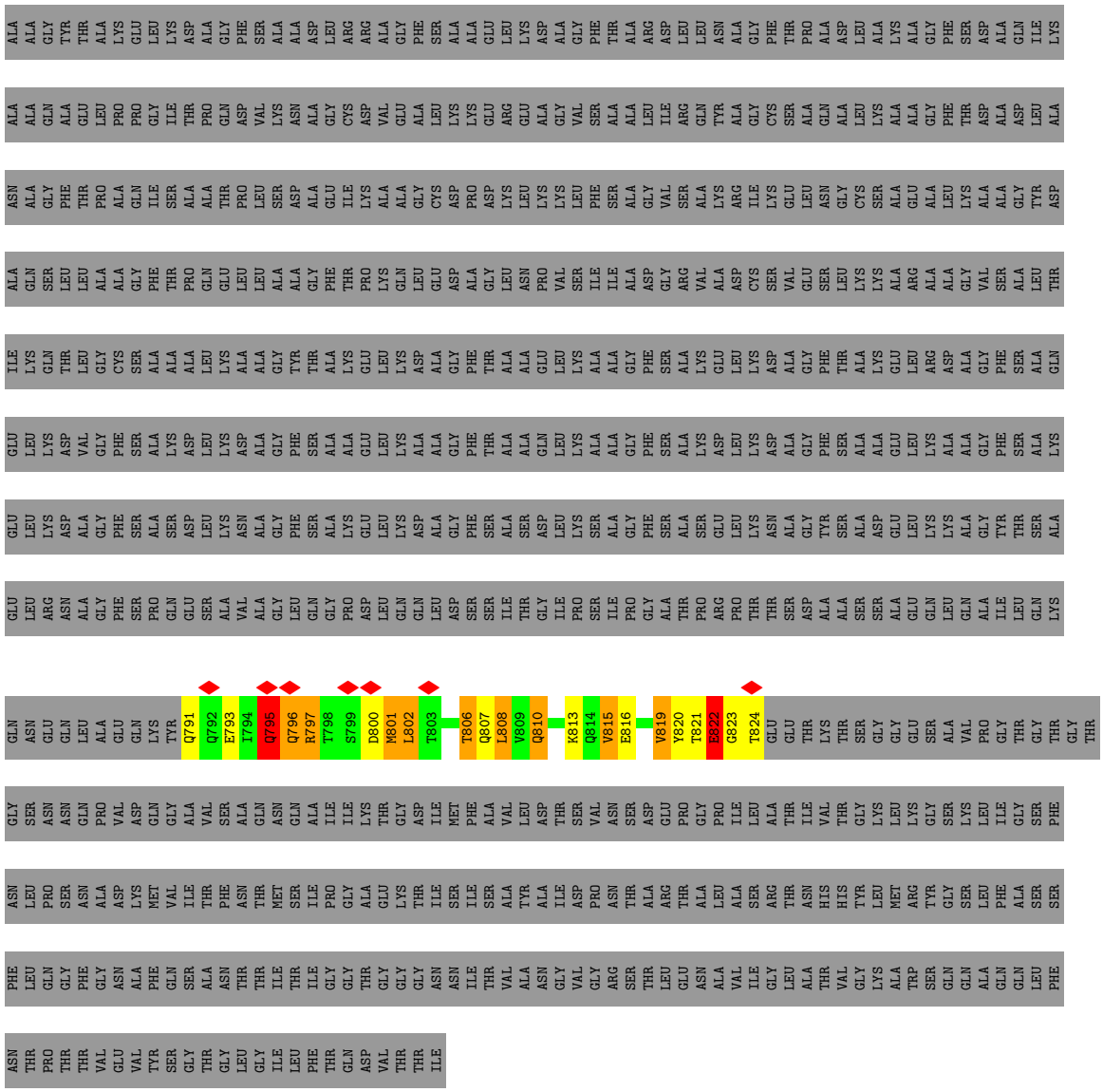


- Molecule 4: IcmE protein

Chain JG:

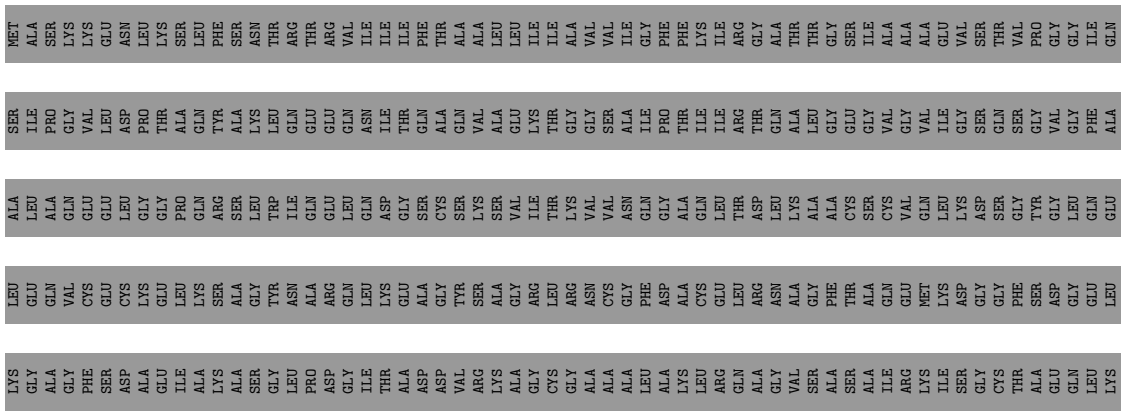


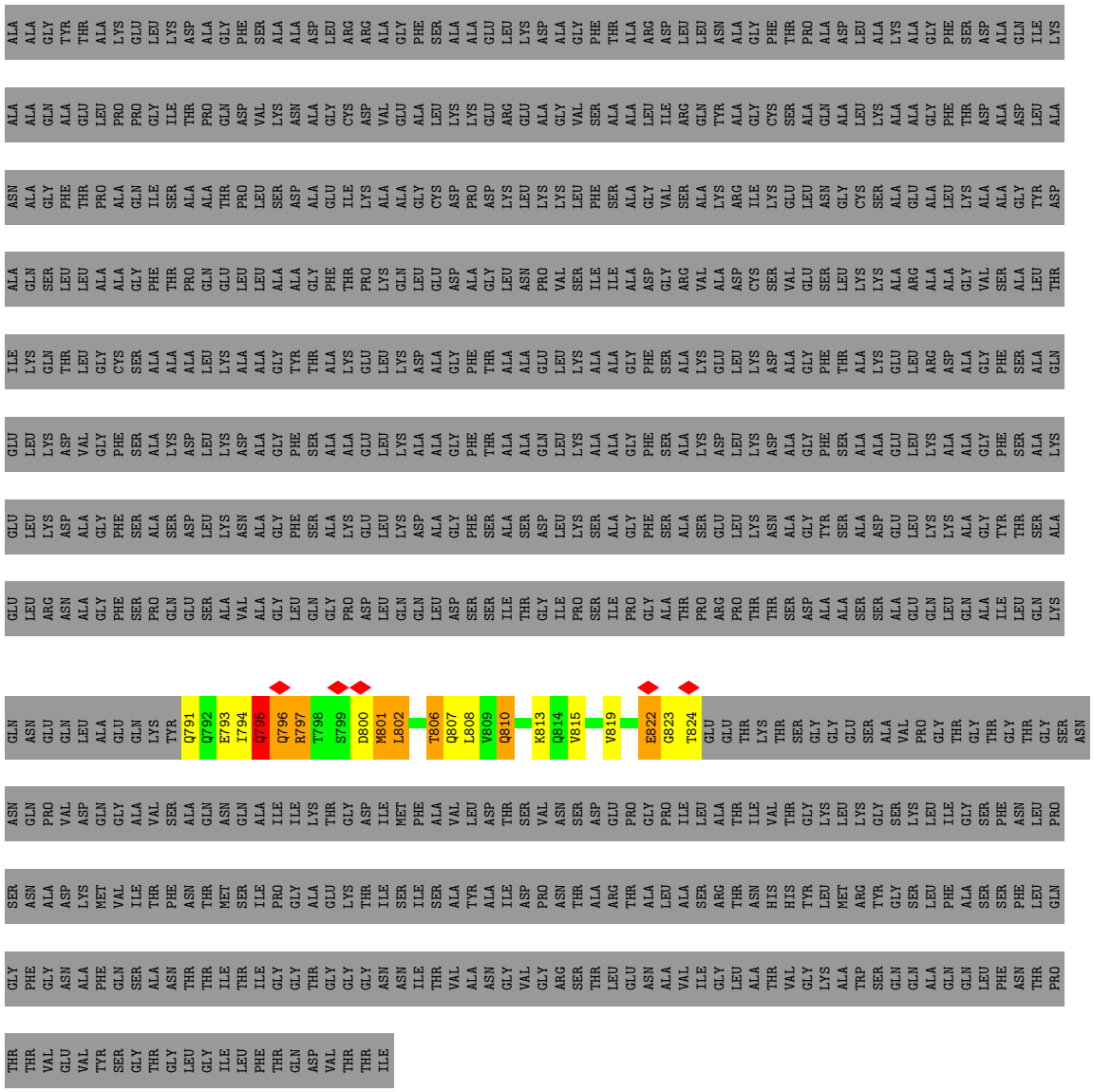




• Molecule 4: IcmE protein

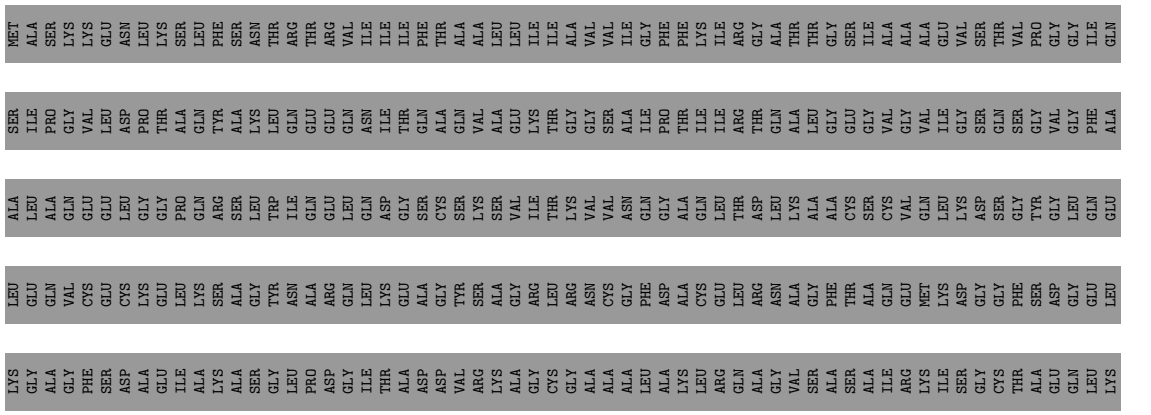
Chain KG: ... 97%

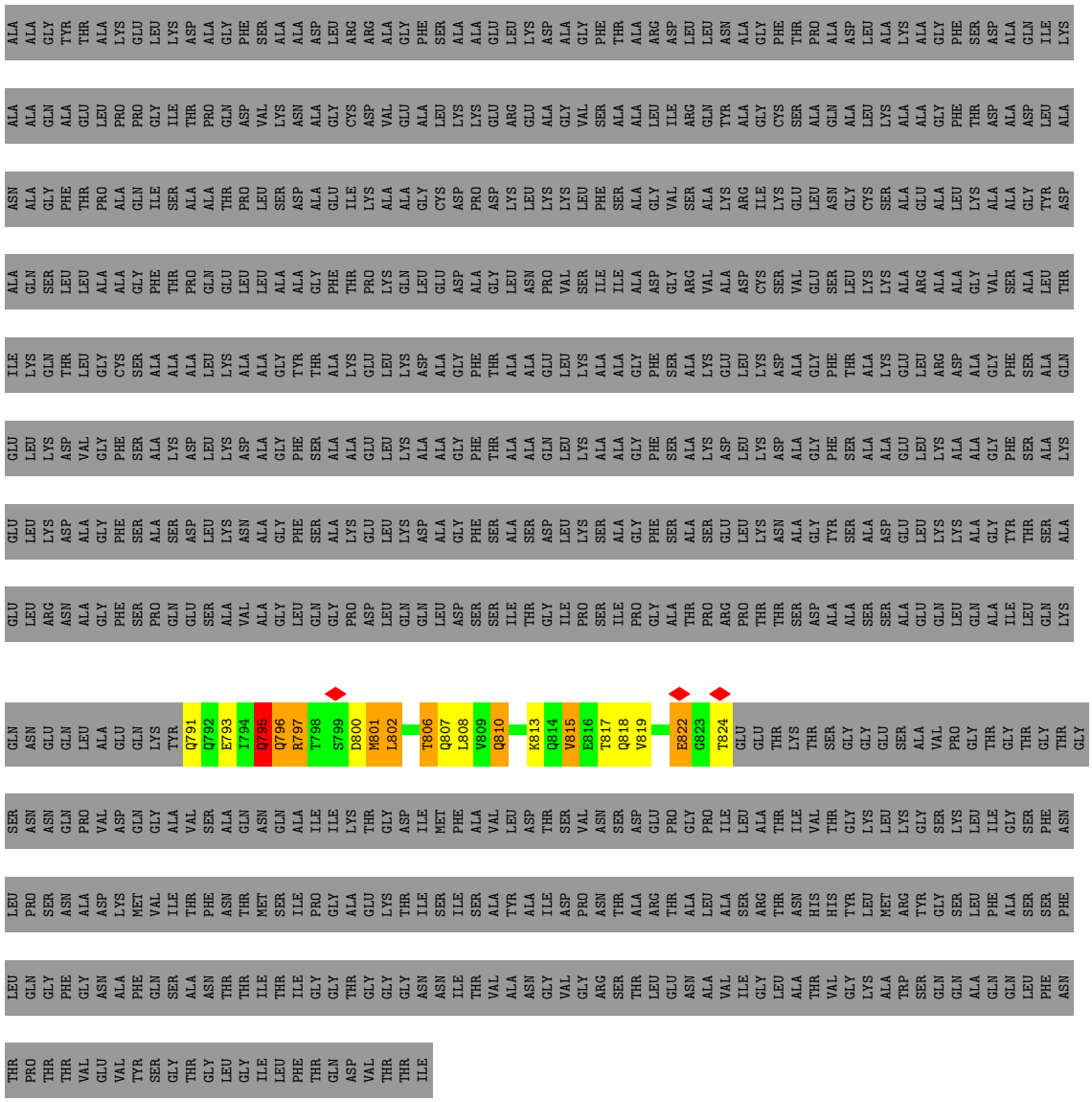




- Molecule 4: IcmE protein

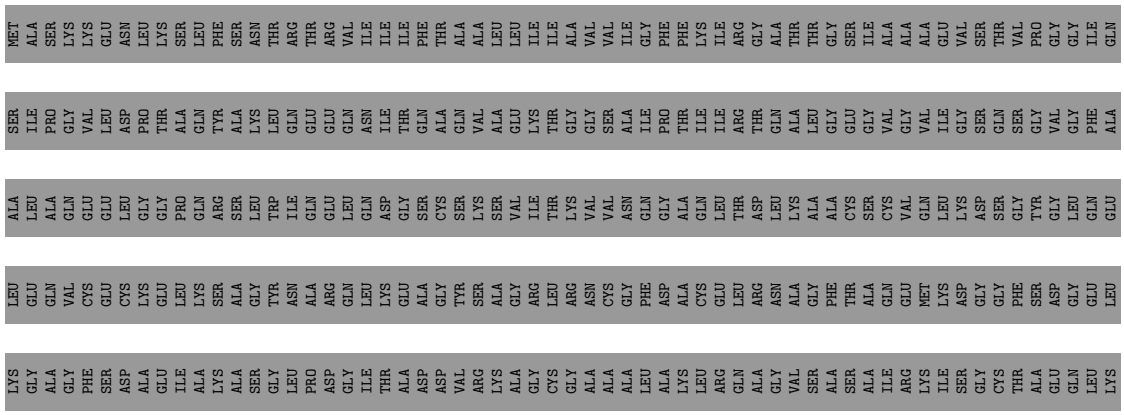
Chain LG: 97%

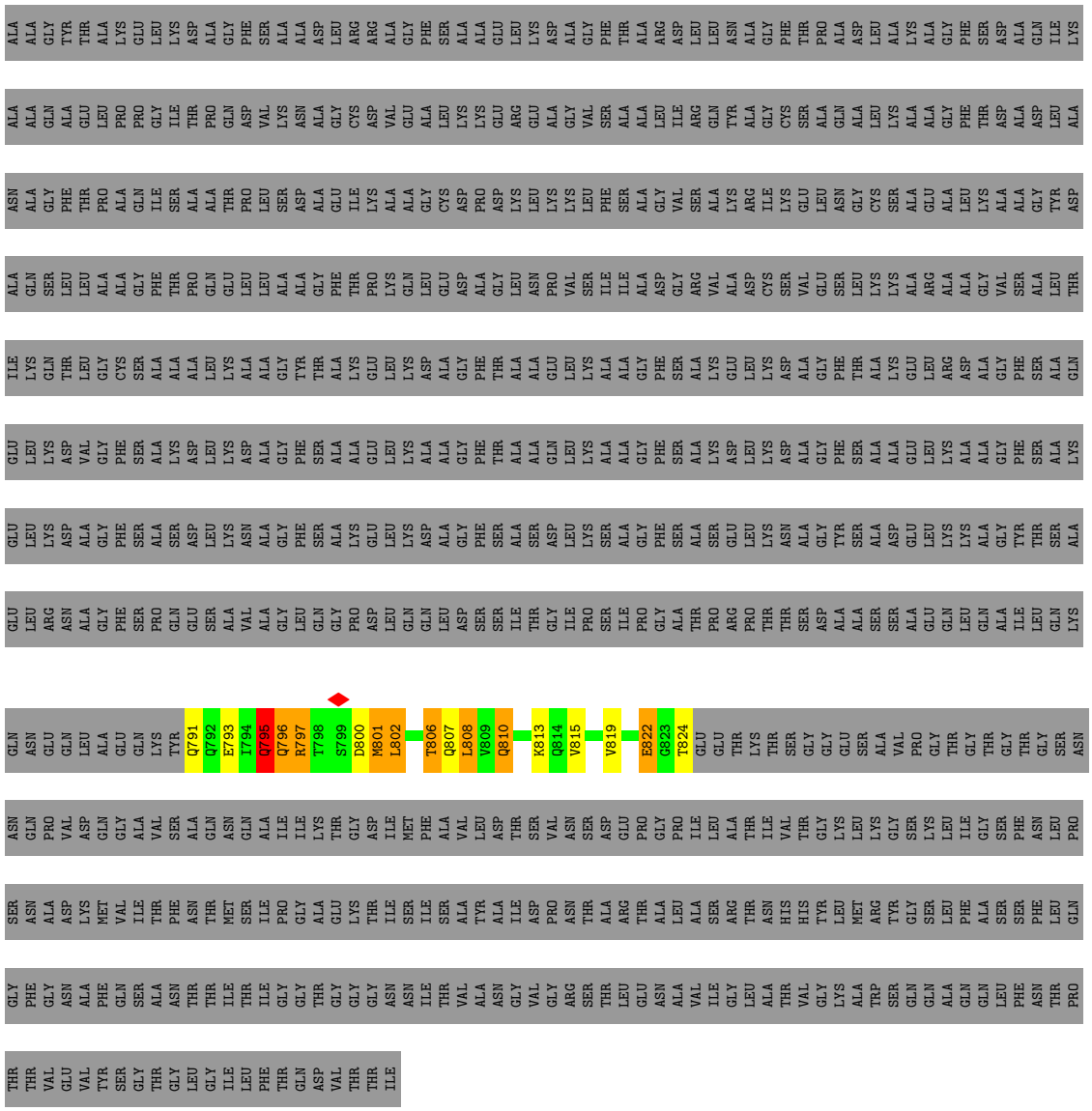




• Molecule 4: IcmE protein

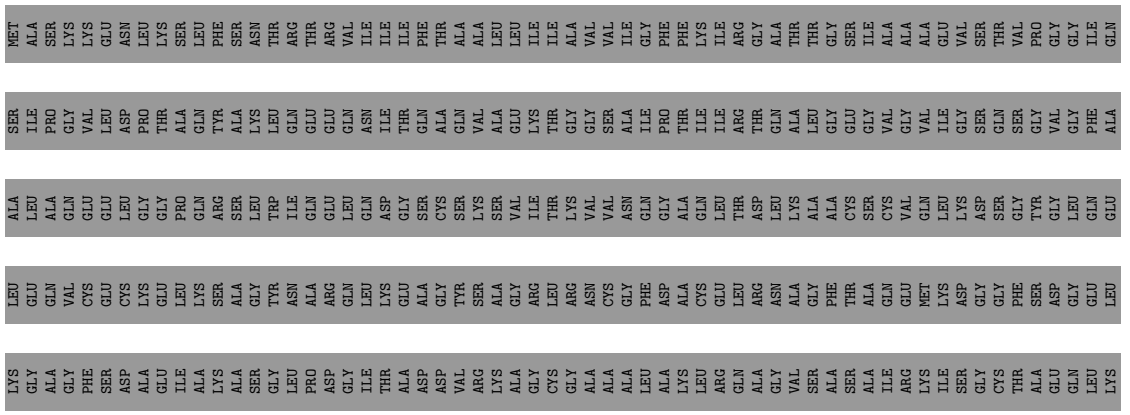
Chain MG: ... 97%

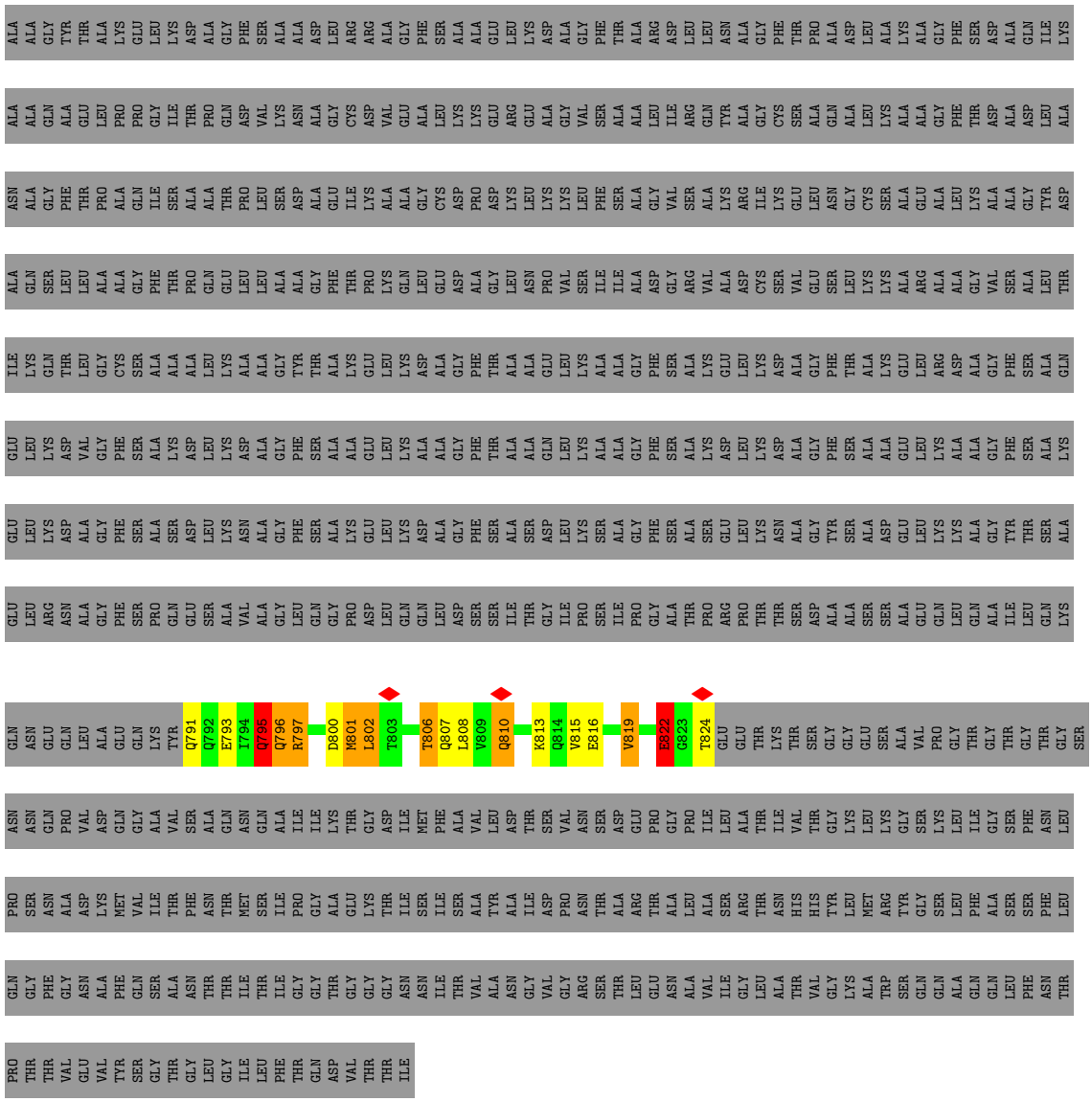




- Molecule 4: IcmE protein

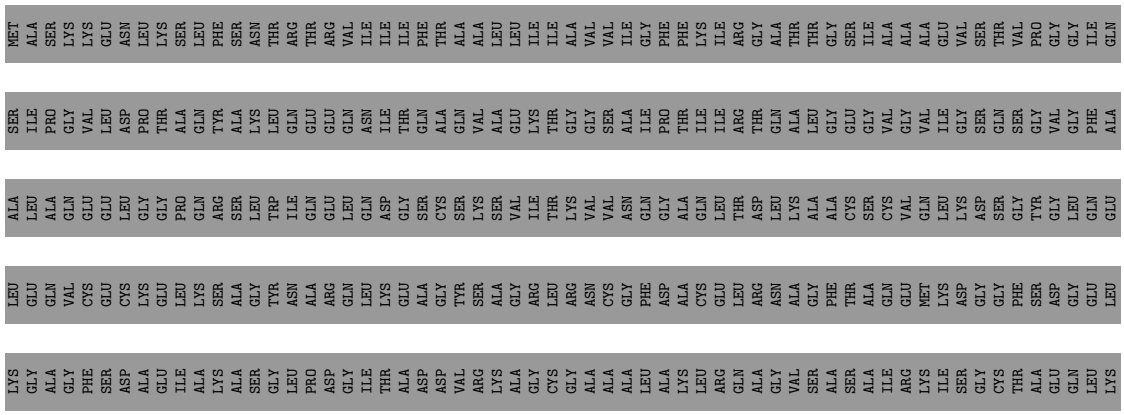
Chain VG: 97%

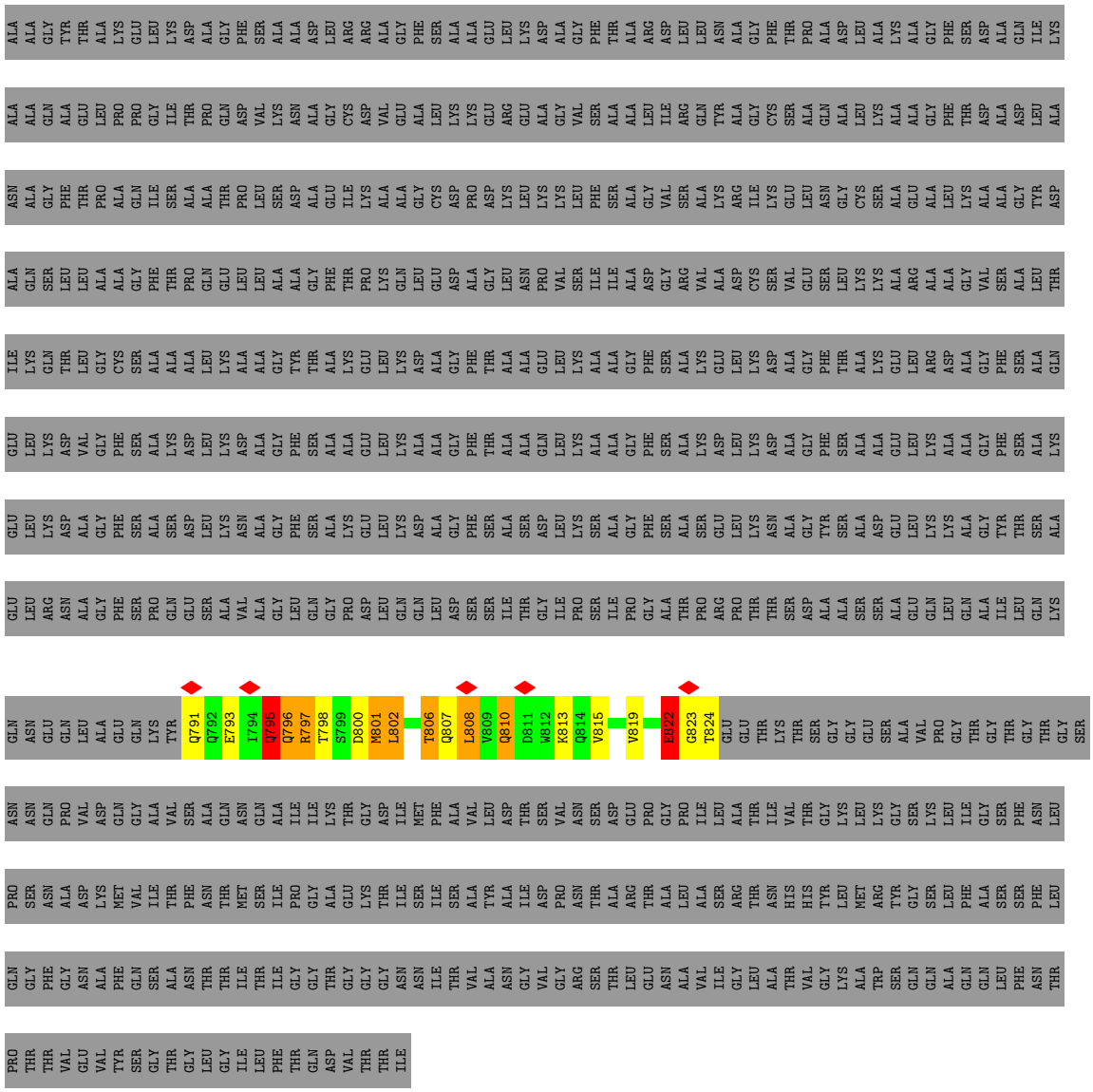




- Molecule 4: IcmE protein

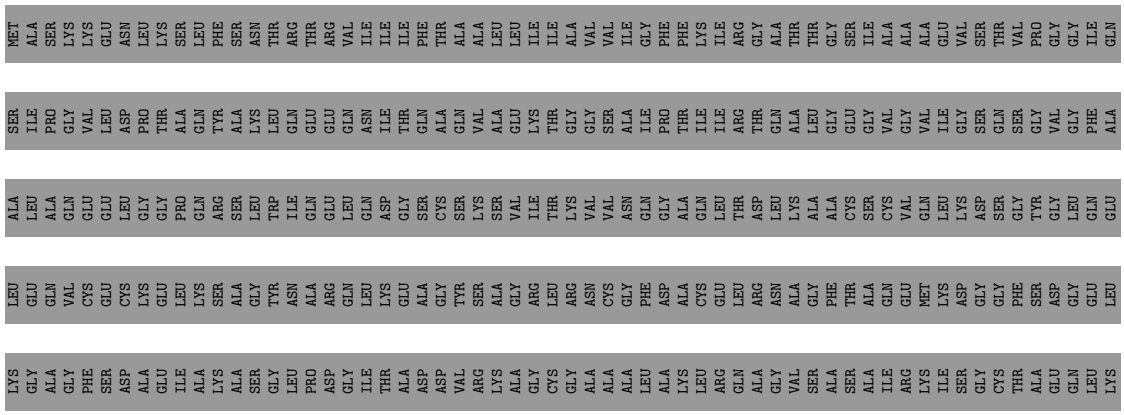
Chain WG: ... 97%

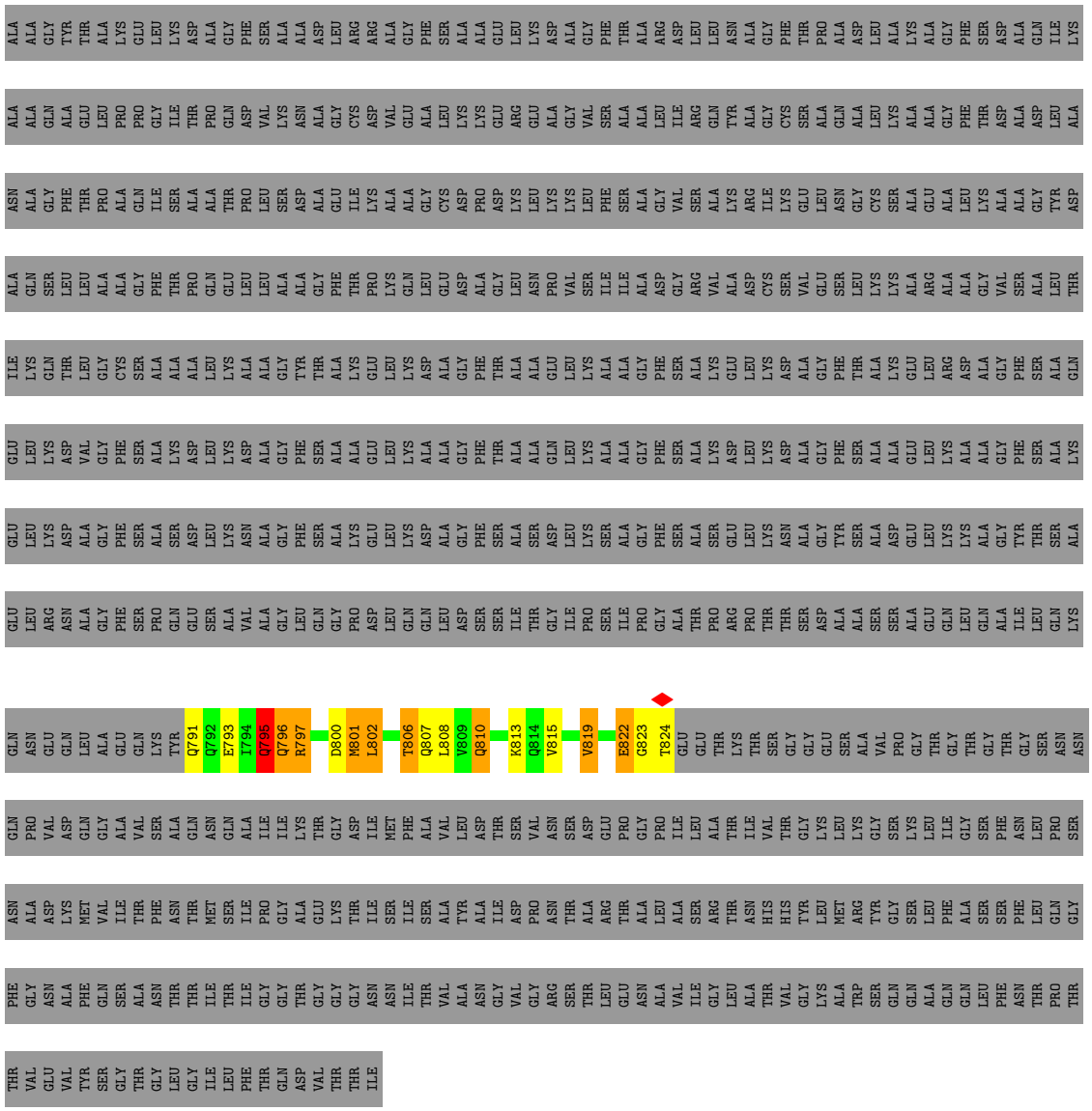




• Molecule 4: IcmE protein

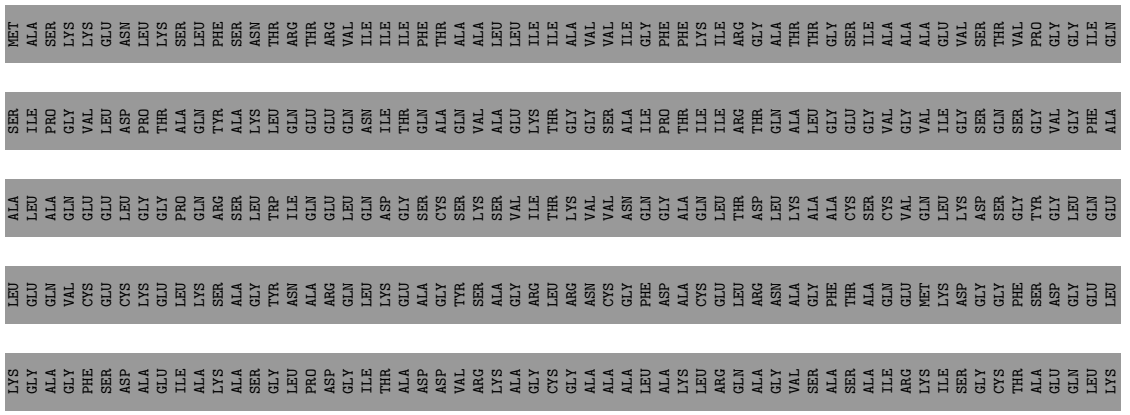
Chain XG: 97%

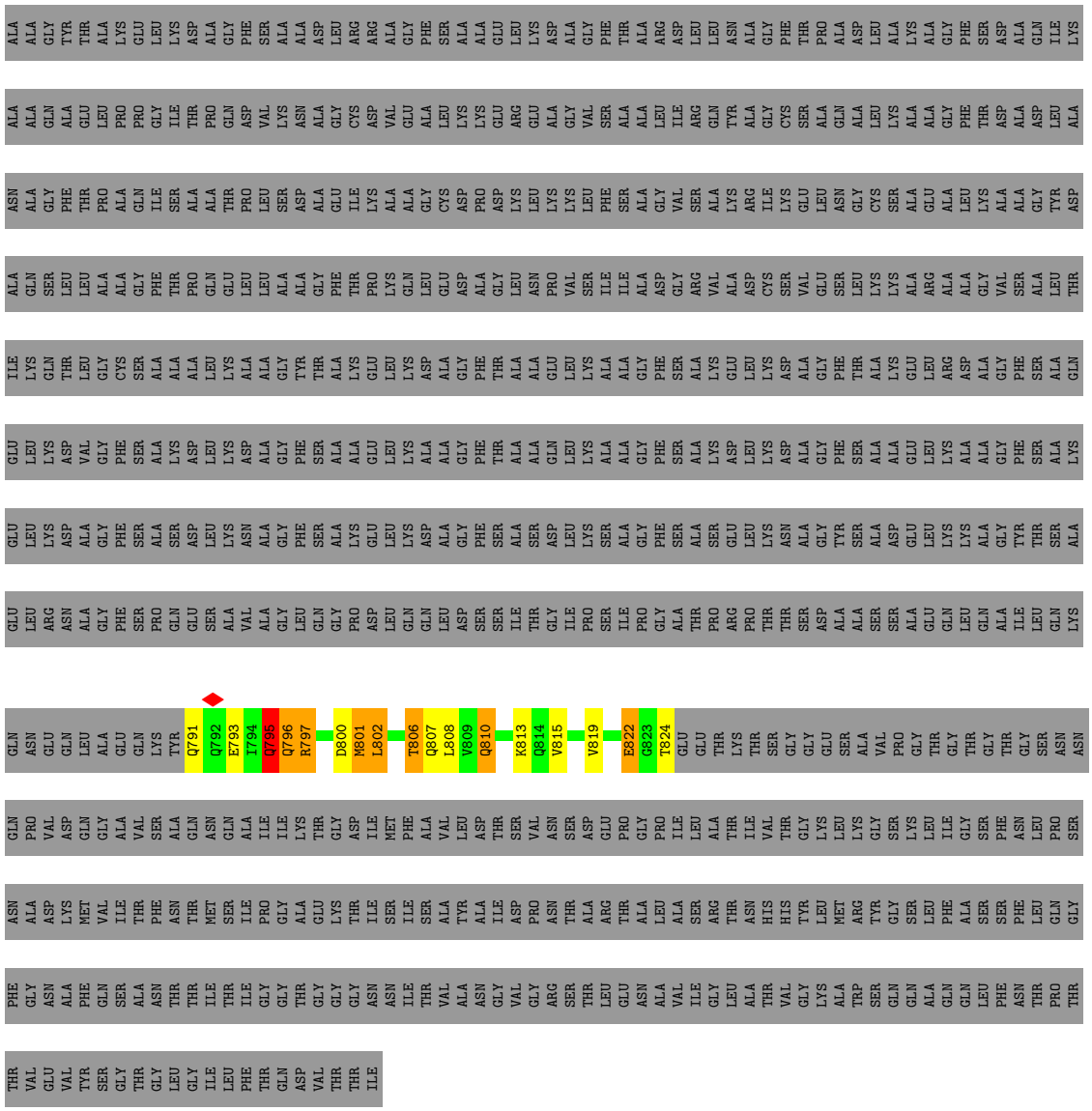




- Molecule 4: IcmE protein

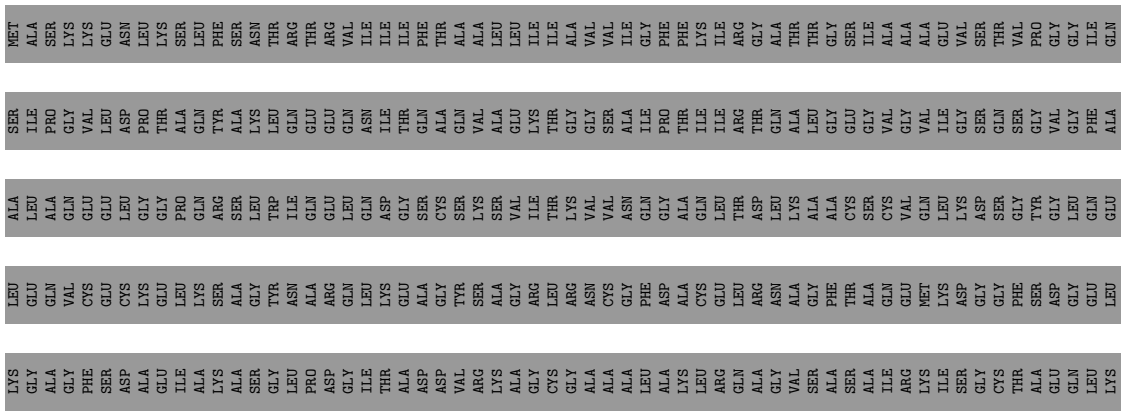
Chain YG: 97%

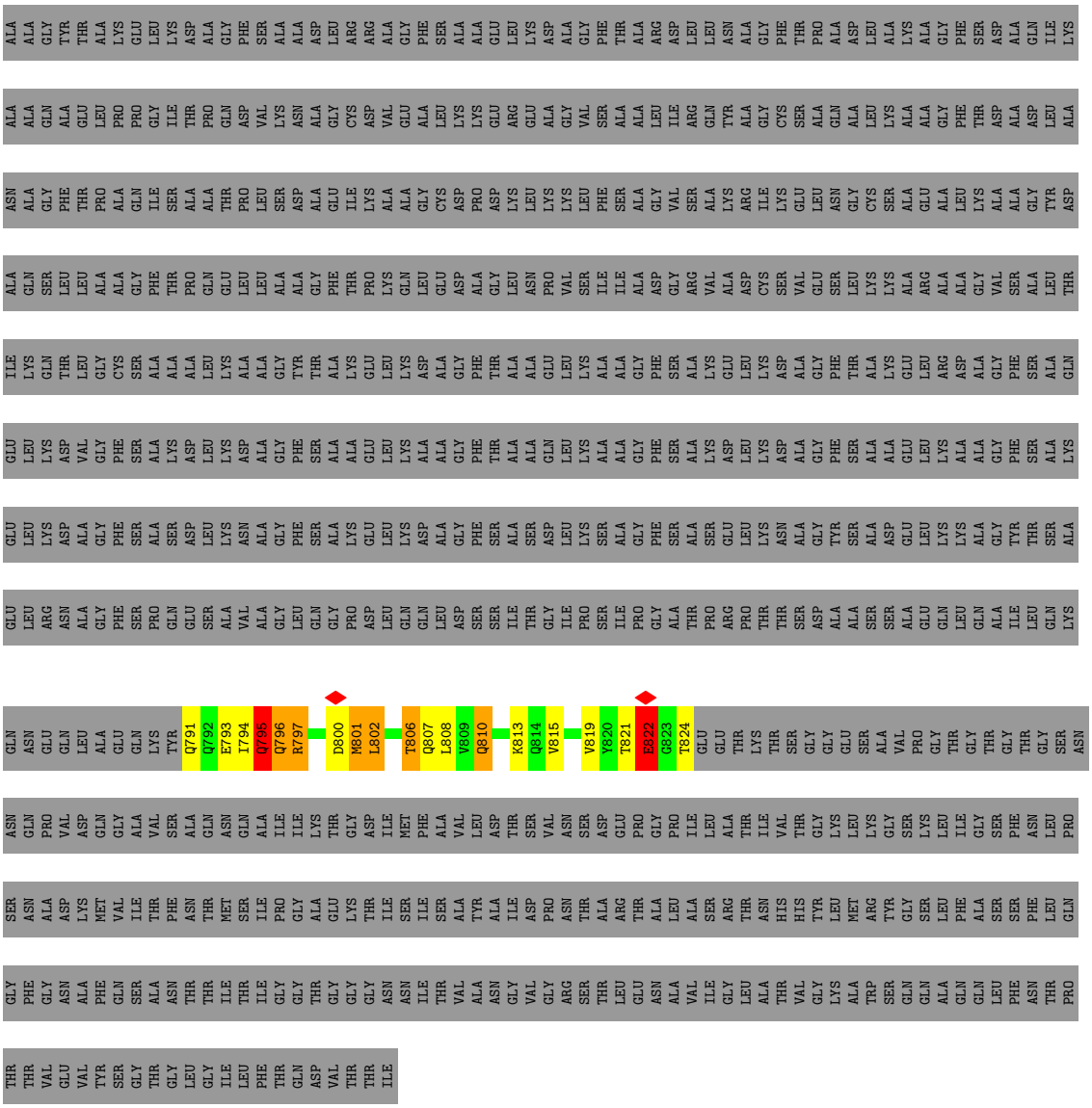




- Molecule 4: IcmE protein

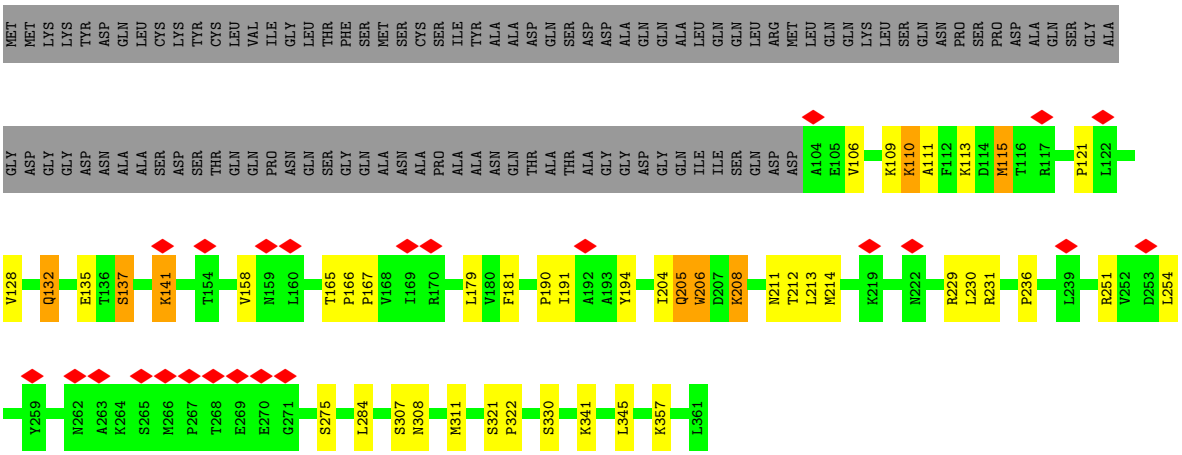
Chain ZG: ... 97%





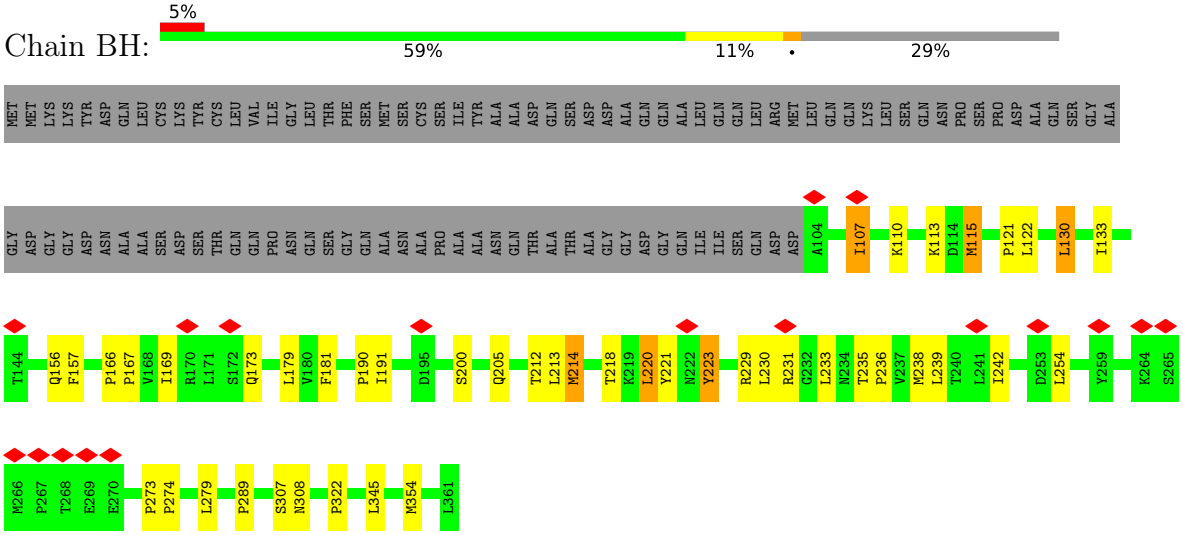
• Molecule 5: Type IV secretion protein IcmK

Chain AH:



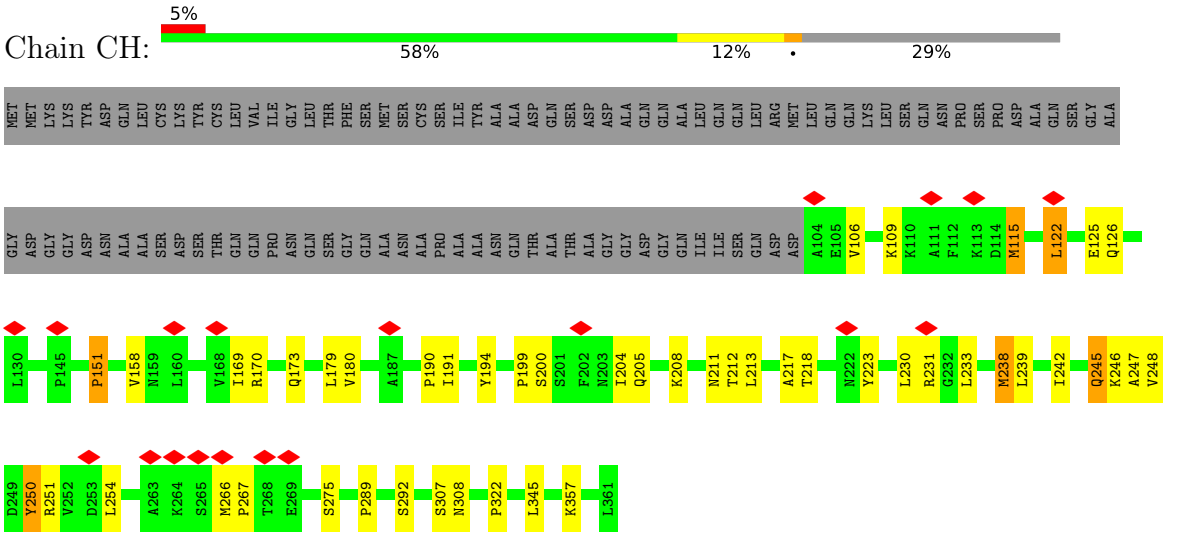
• Molecule 5: Type IV secretion protein IcmK

Chain BH:



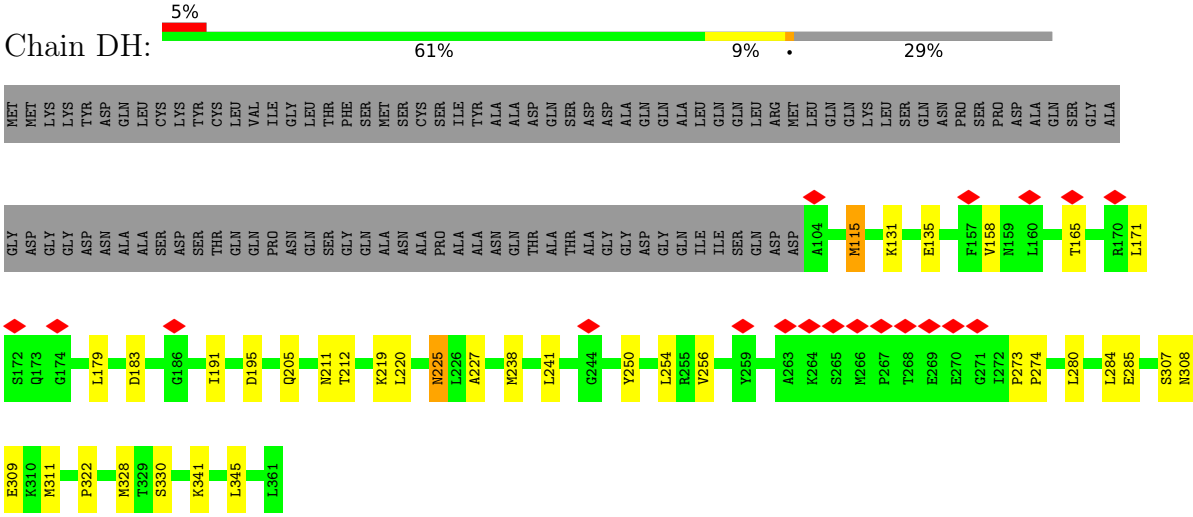
• Molecule 5: Type IV secretion protein IcmK

Chain CH:



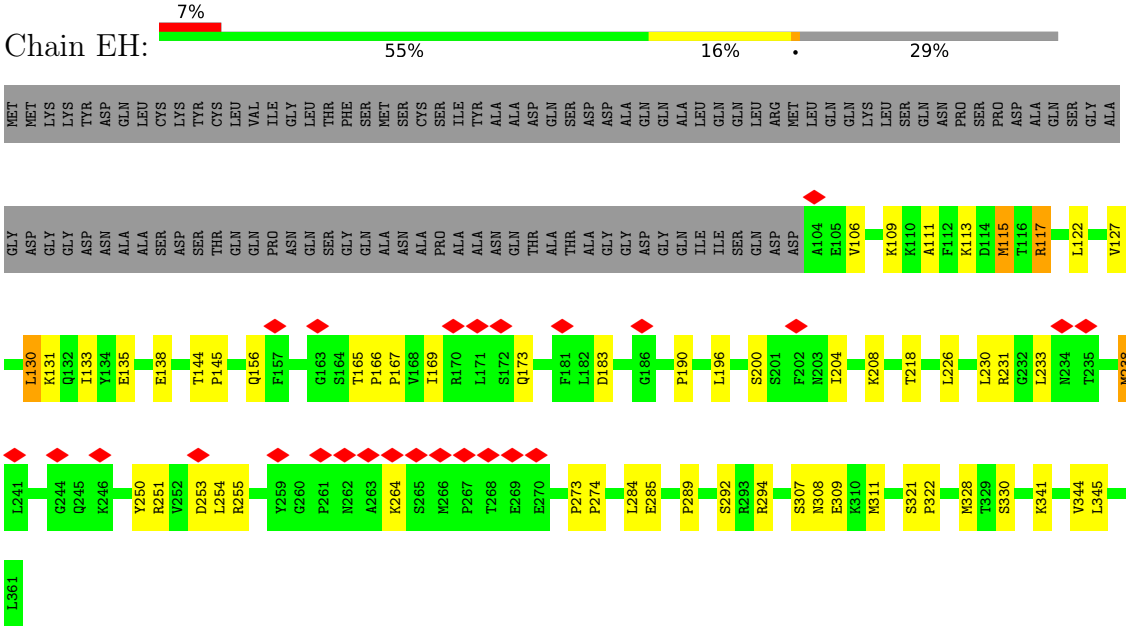
• Molecule 5: Type IV secretion protein IcmK

Chain DH:



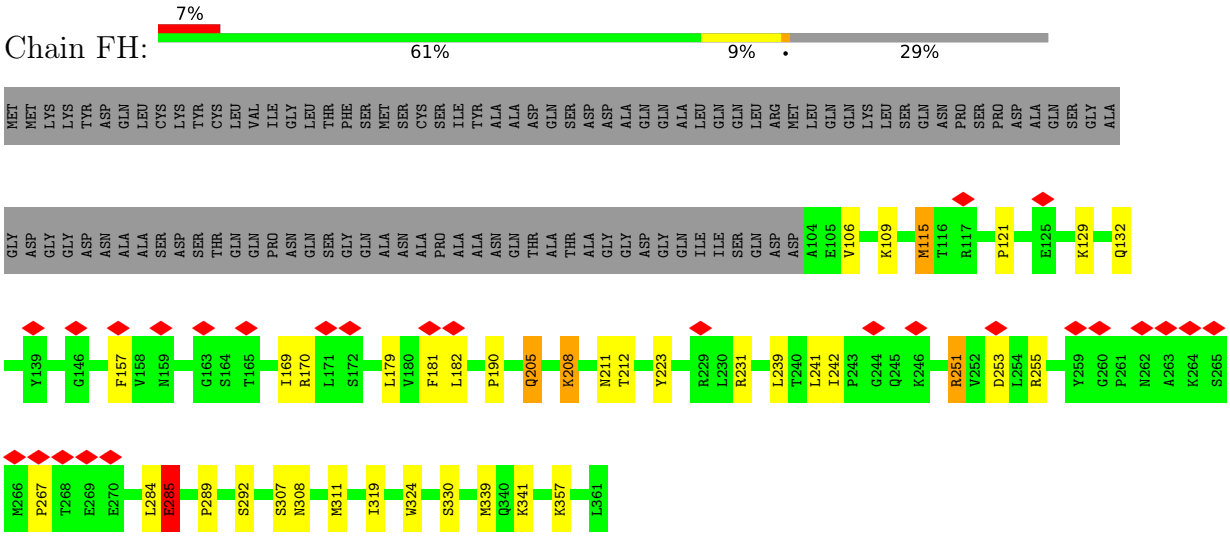
• Molecule 5: Type IV secretion protein IcmK

Chain EH:



• Molecule 5: Type IV secretion protein IcmK

Chain FH:



• Molecule 5: Type IV secretion protein IcmK

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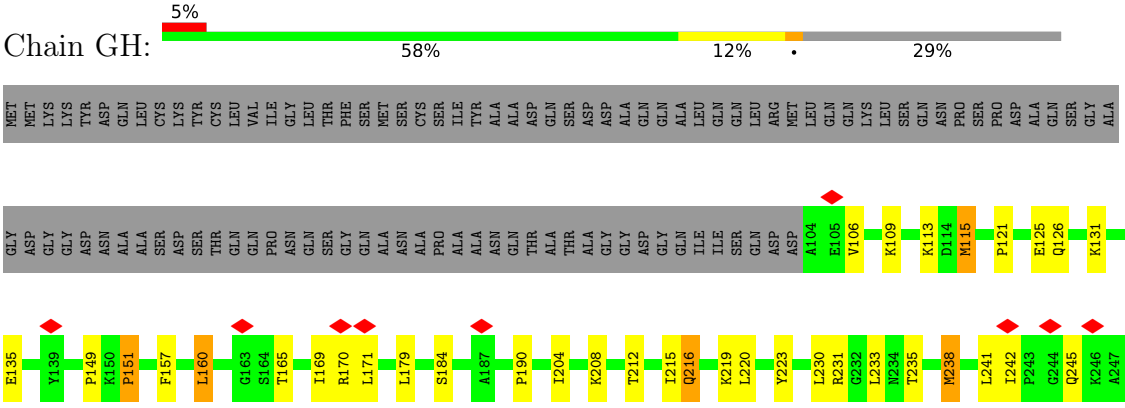
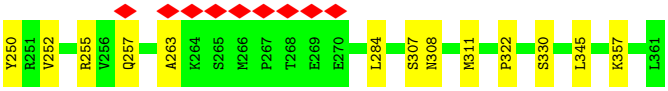
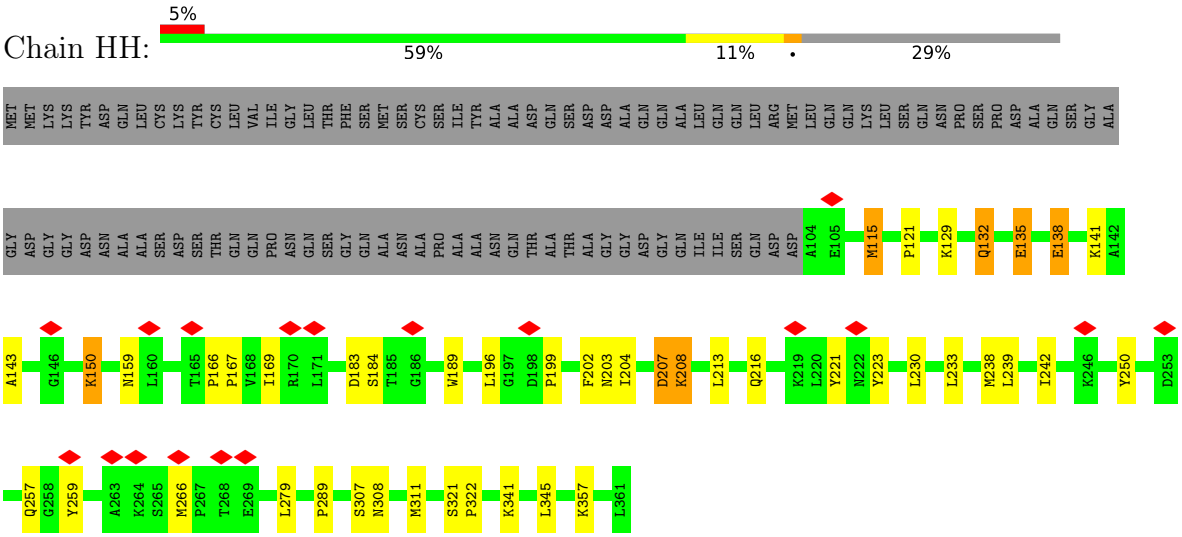
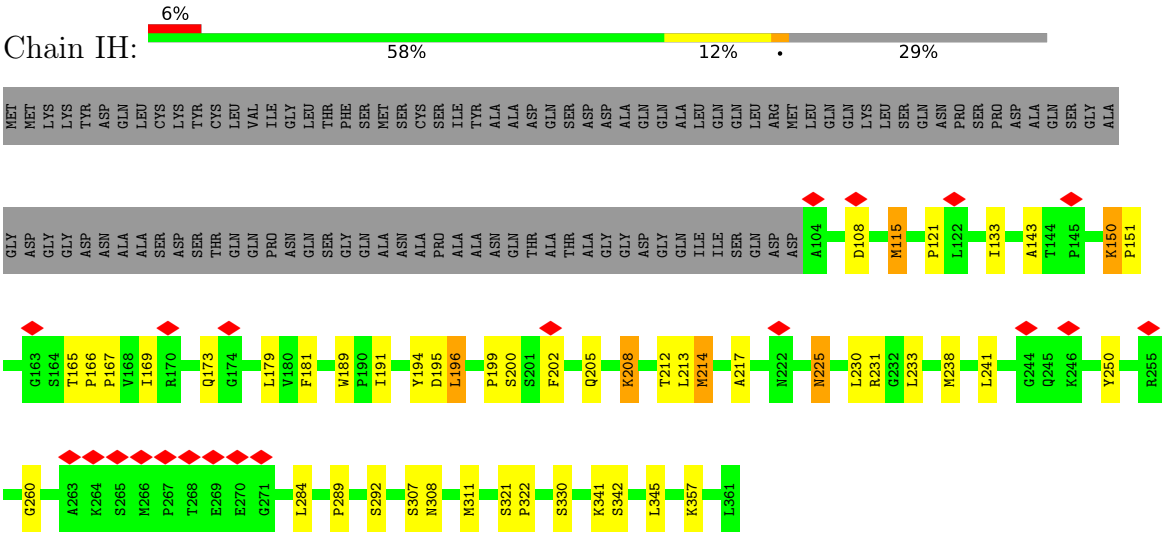




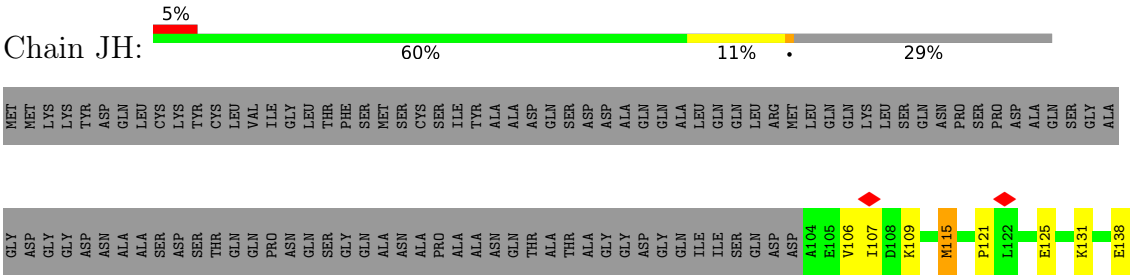
• Molecule 5: Type IV secretion protein IcmK

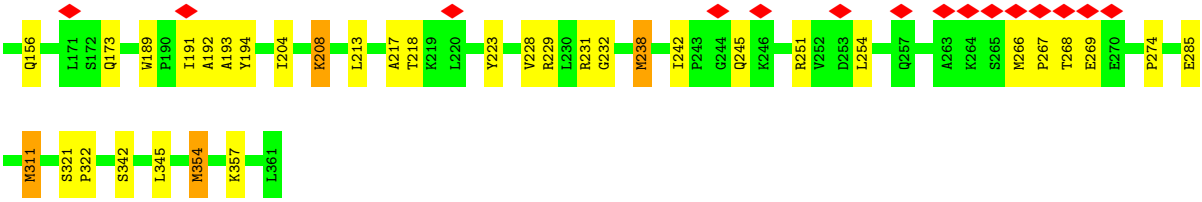


• Molecule 5: Type IV secretion protein IcmK

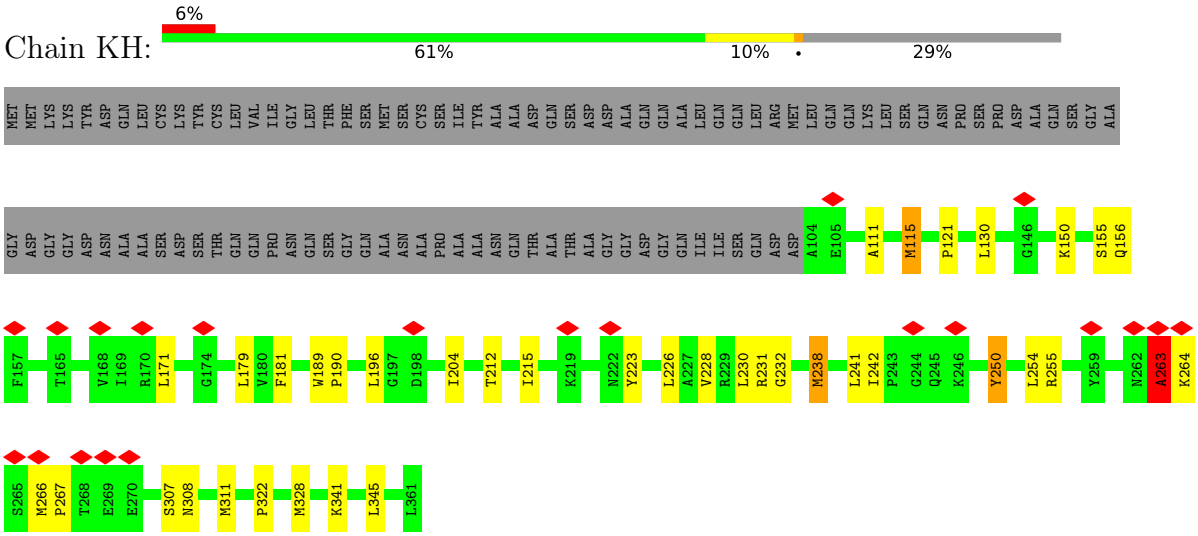


• Molecule 5: Type IV secretion protein IcmK

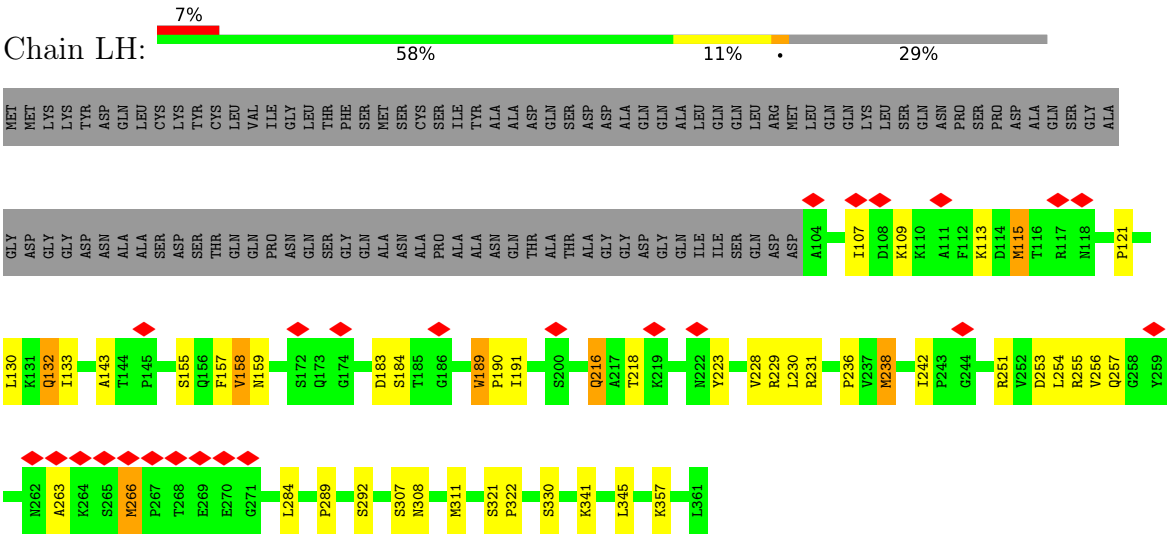




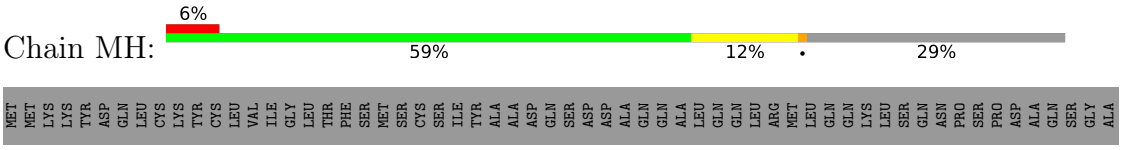
• Molecule 5: Type IV secretion protein IcmK

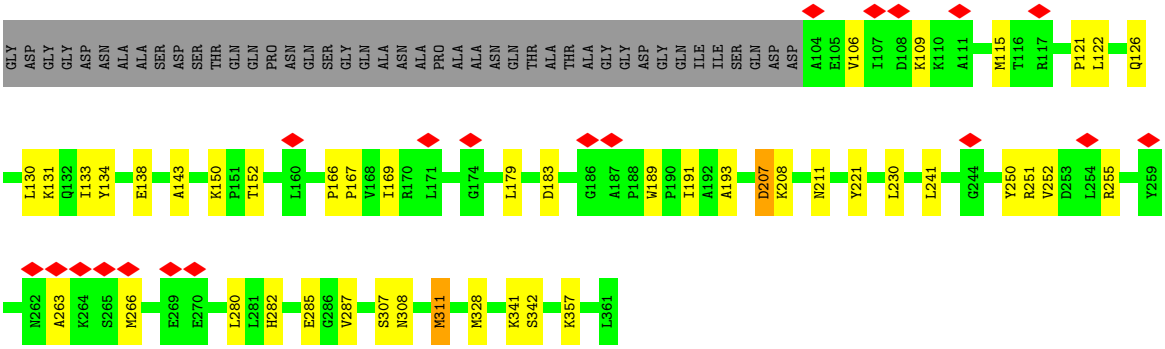


• Molecule 5: Type IV secretion protein IcmK



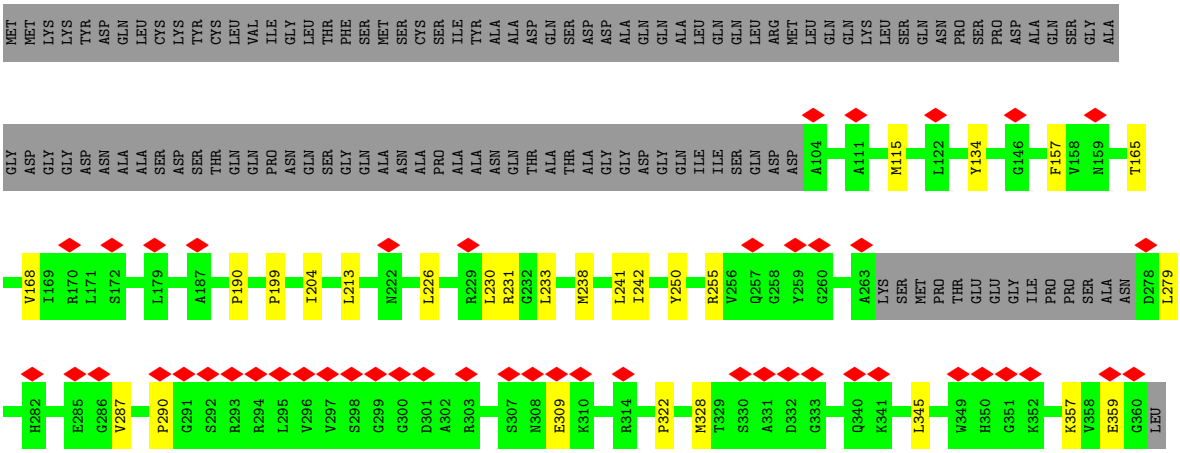
• Molecule 5: Type IV secretion protein IcmK





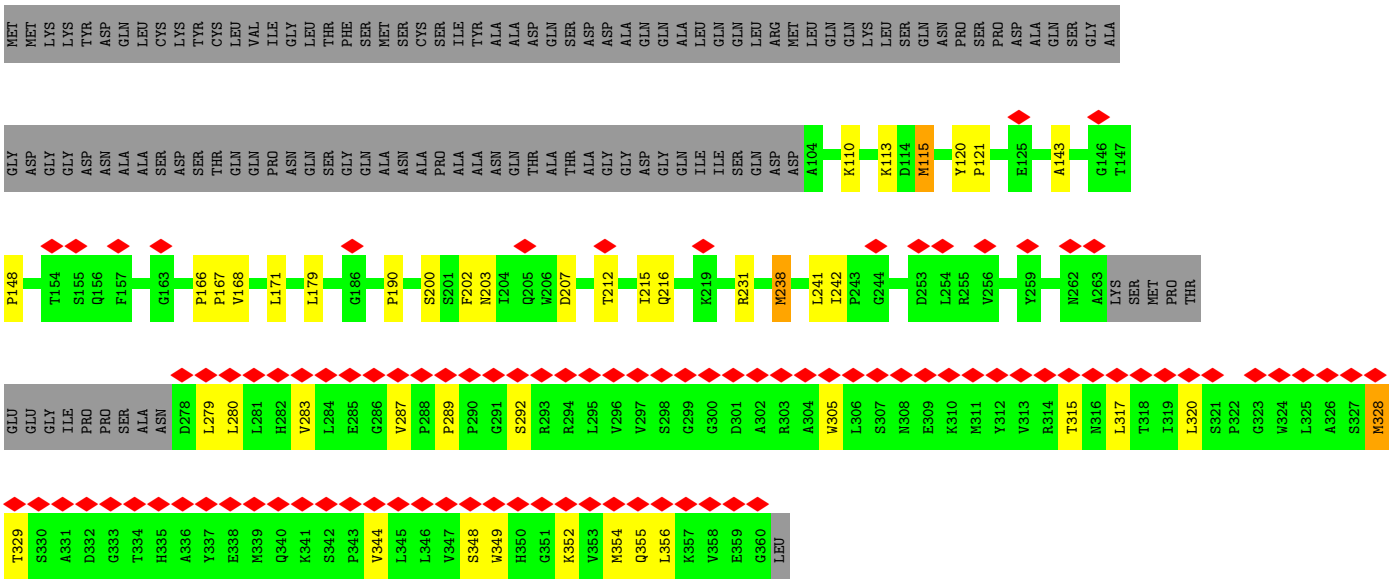
• Molecule 5: Type IV secretion protein IcmK

Chain VH:



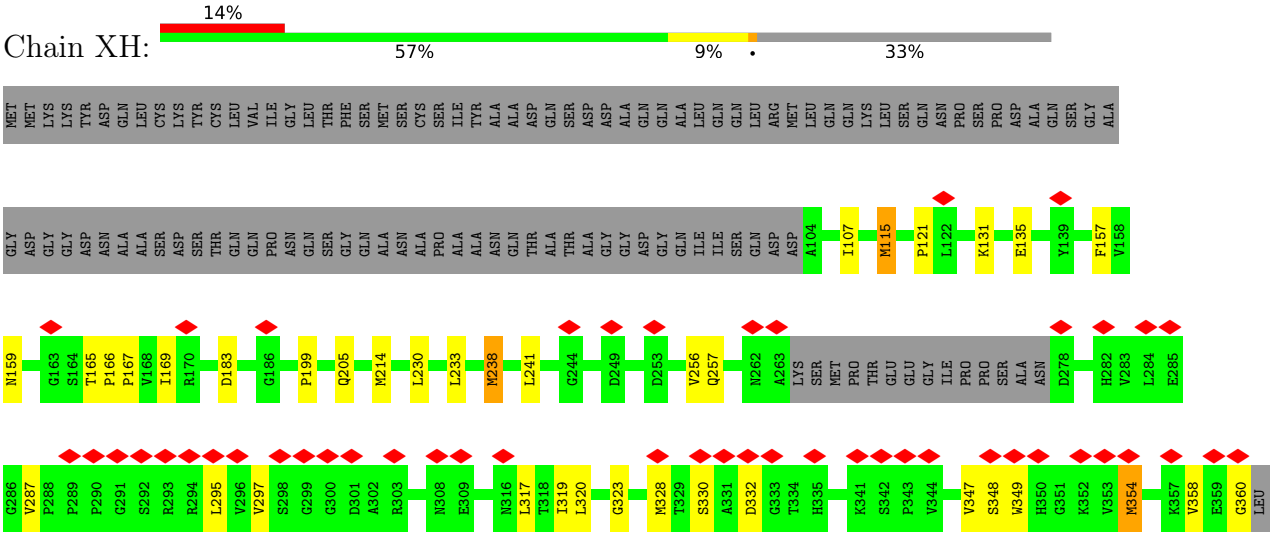
• Molecule 5: Type IV secretion protein IcmK

Chain WH:



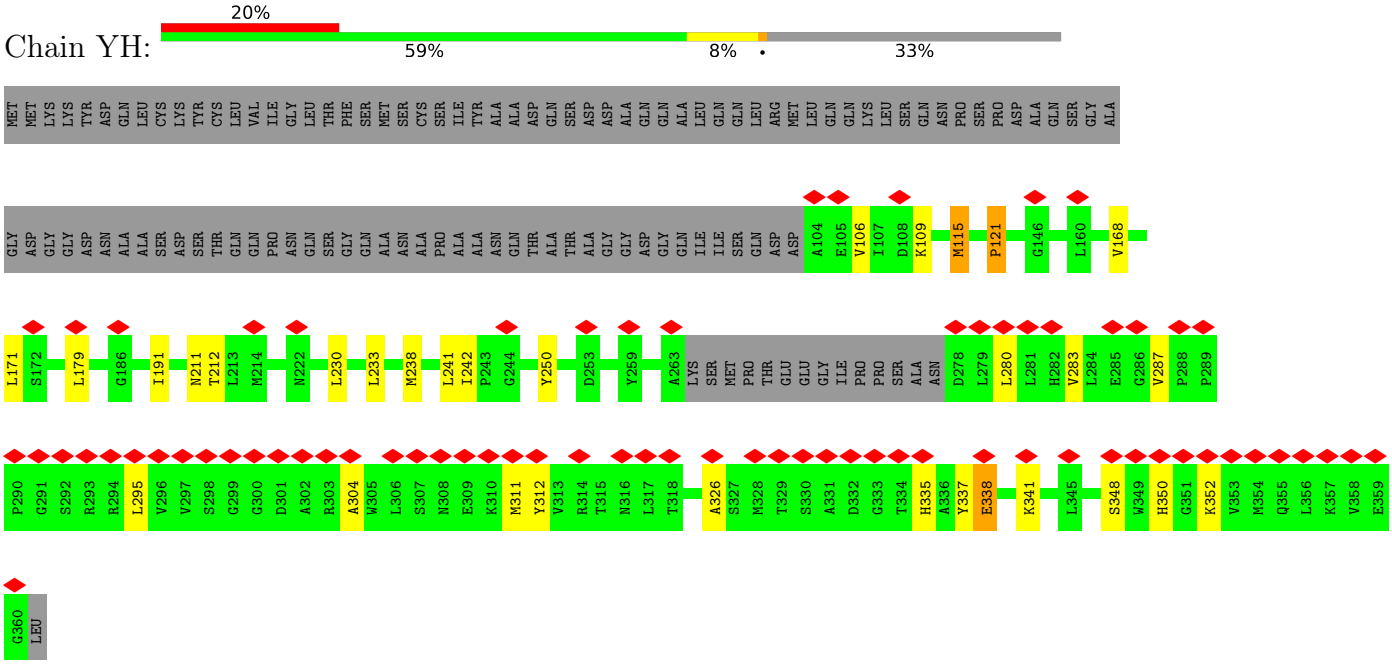
• Molecule 5: Type IV secretion protein IcmK

Chain XH:



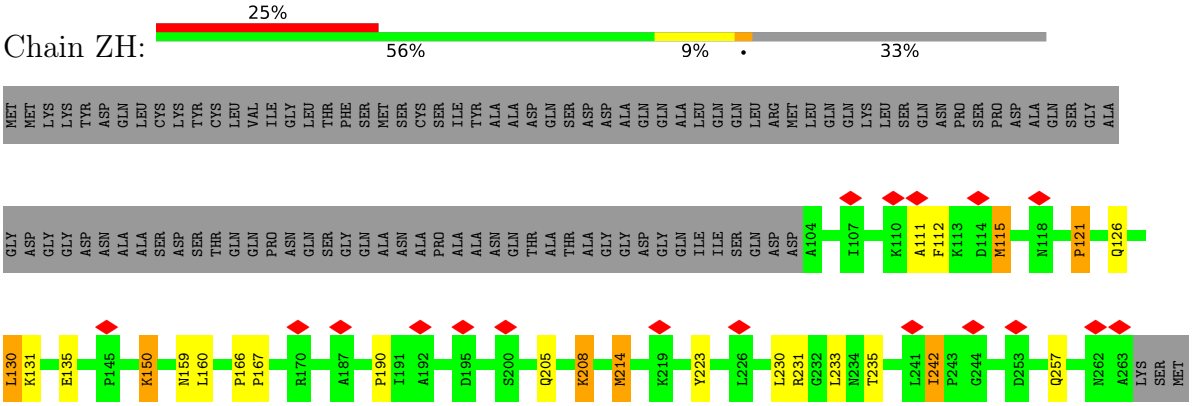
- Molecule 5: Type IV secretion protein IcmK

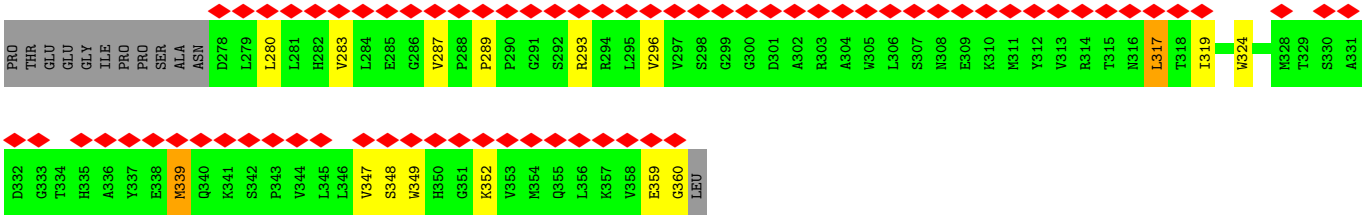
Chain YH:



- Molecule 5: Type IV secretion protein IcmK

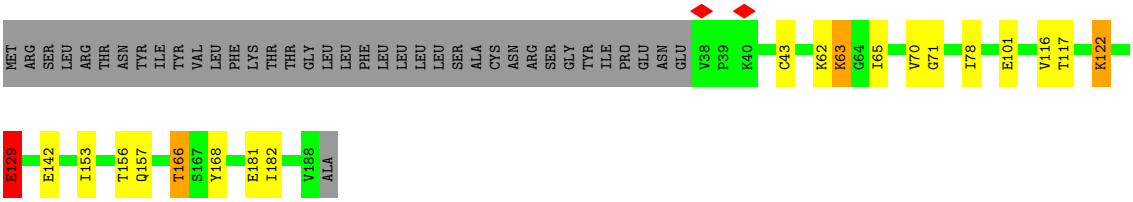
Chain ZH:





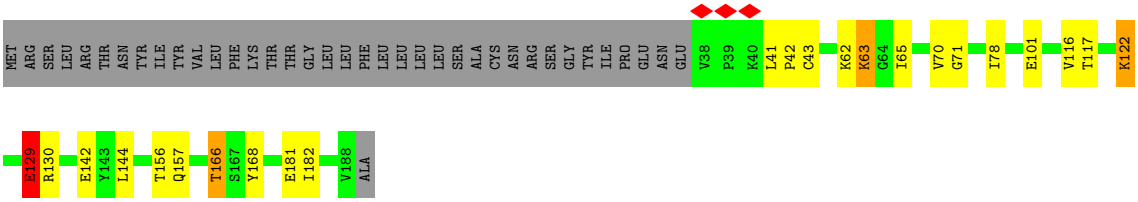
• Molecule 6: Inner membrane lipoprotein YiaD

Chain AK:



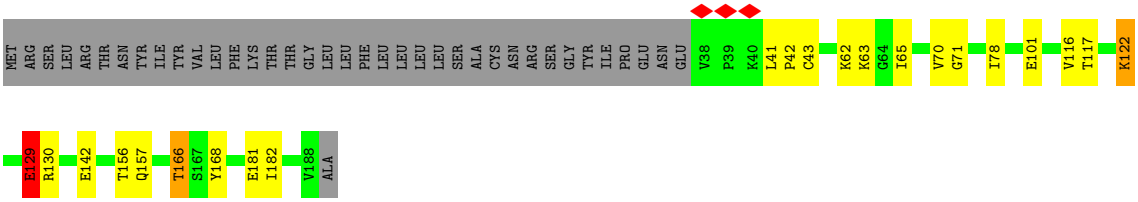
• Molecule 6: Inner membrane lipoprotein YiaD

Chain BK:



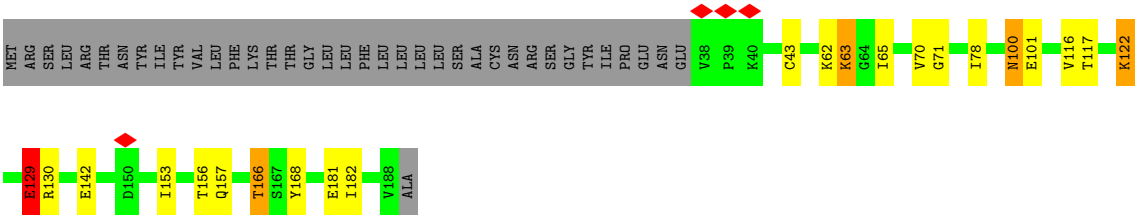
• Molecule 6: Inner membrane lipoprotein YiaD

Chain CK:



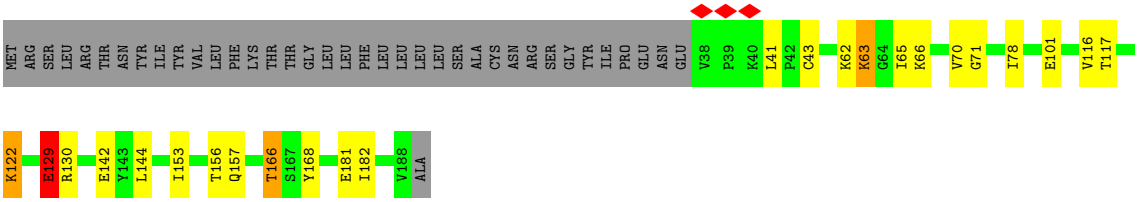
• Molecule 6: Inner membrane lipoprotein YiaD

Chain DK:



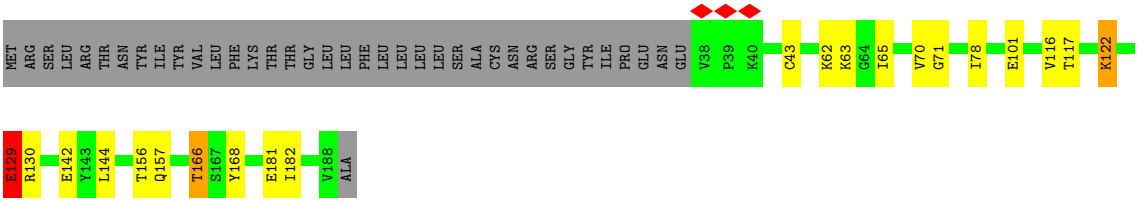
- Molecule 6: Inner membrane lipoprotein YiaD

Chain EK:



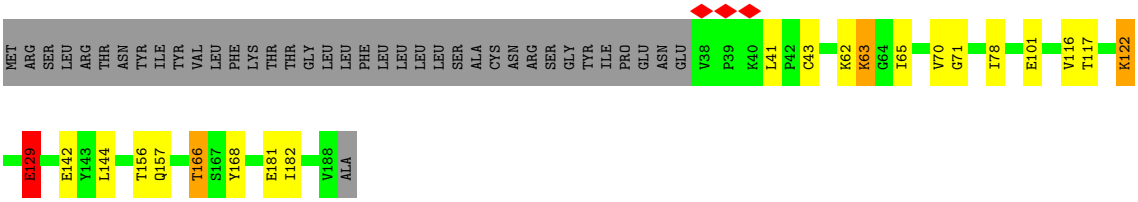
- Molecule 6: Inner membrane lipoprotein YiaD

Chain FK:



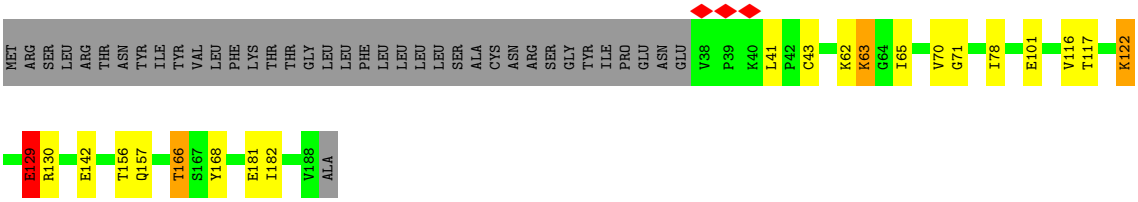
- Molecule 6: Inner membrane lipoprotein YiaD

Chain GK:



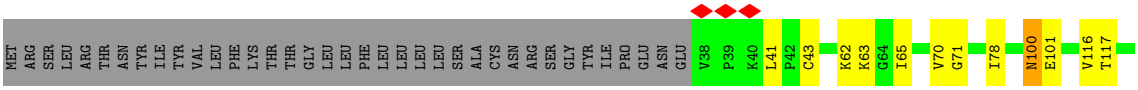
- Molecule 6: Inner membrane lipoprotein YiaD

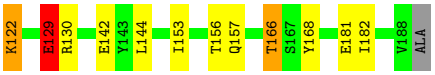
Chain HK:



- Molecule 6: Inner membrane lipoprotein YiaD

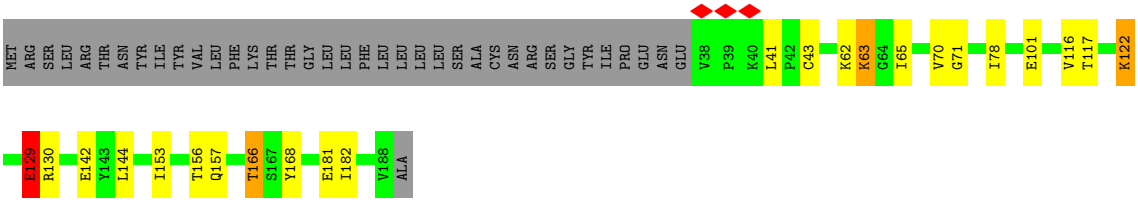
Chain IK:





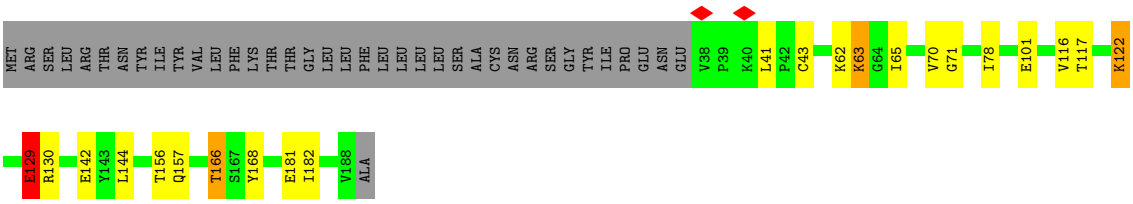
• Molecule 6: Inner membrane lipoprotein YiaD

Chain JK:



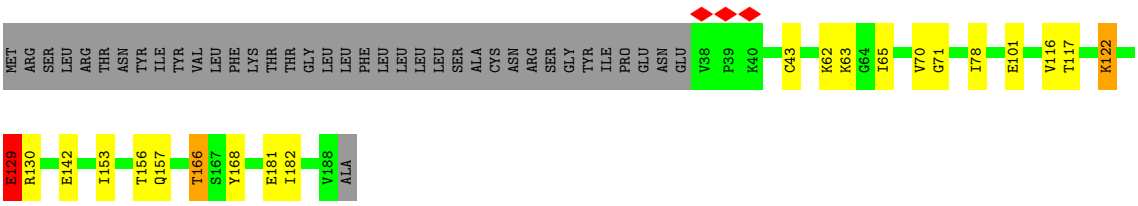
• Molecule 6: Inner membrane lipoprotein YiaD

Chain KK:



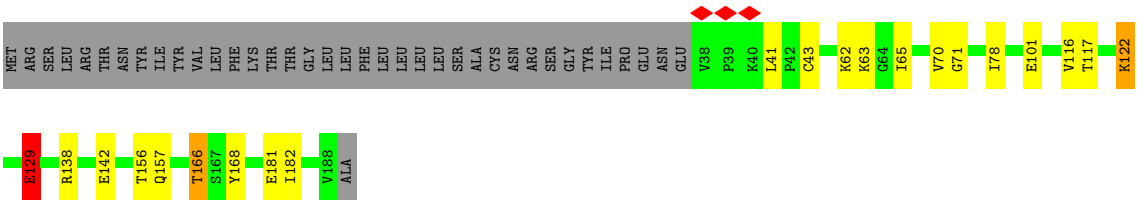
• Molecule 6: Inner membrane lipoprotein YiaD

Chain LK:



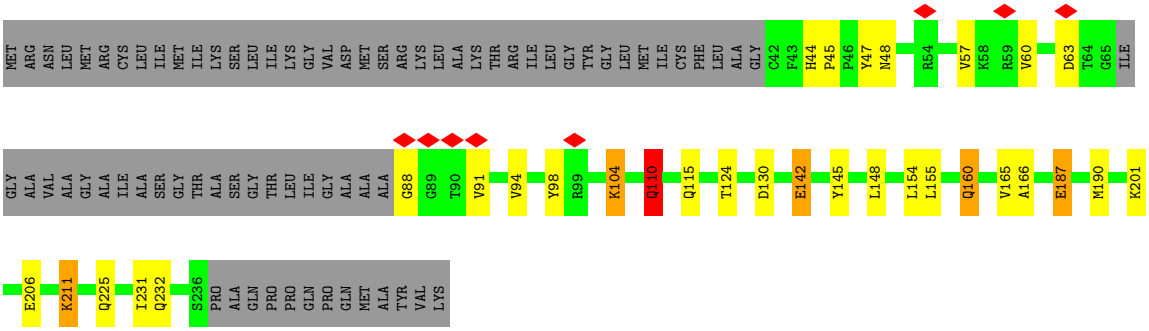
• Molecule 6: Inner membrane lipoprotein YiaD

Chain MK:



• Molecule 7: Outer membrane protein, OmpA family protein

Chain AL:



• Molecule 7: Outer membrane protein, OmpA family protein

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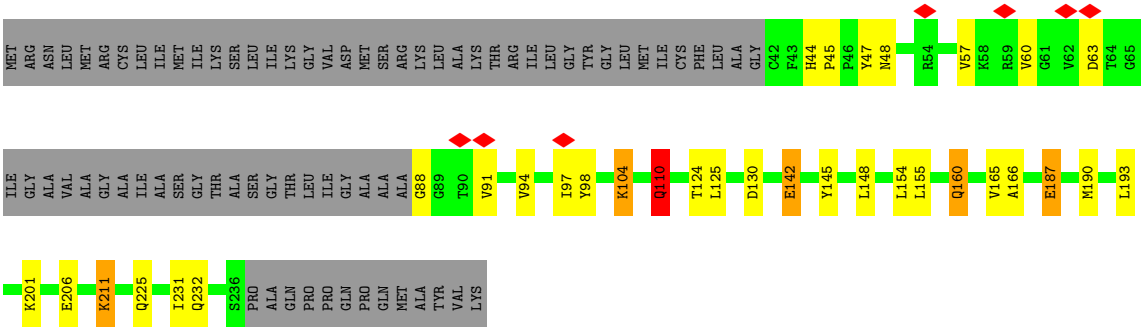
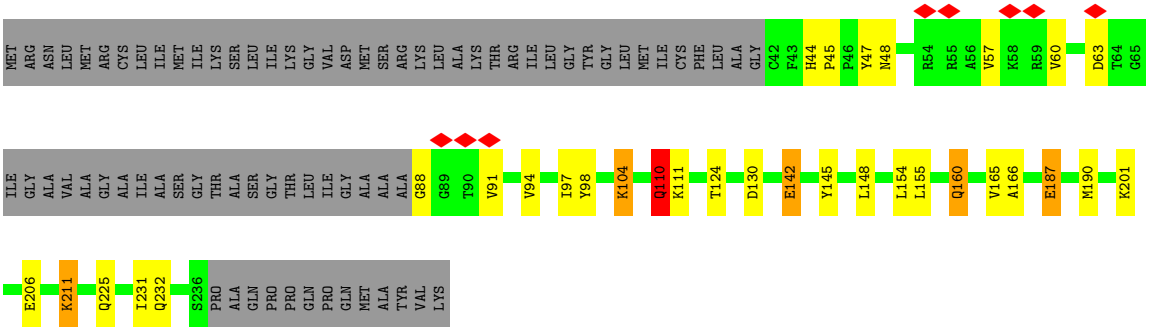


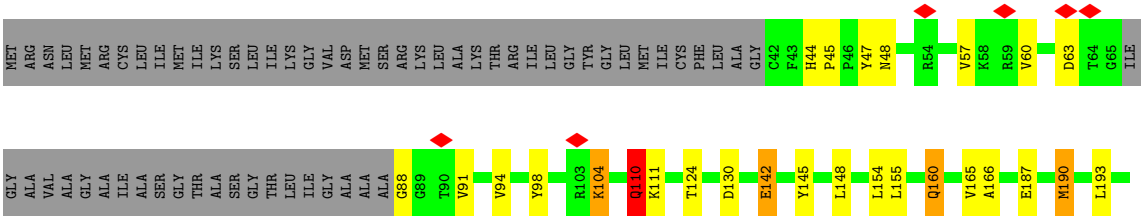
• Molecule 7: Outer membrane protein, OmpA family protein

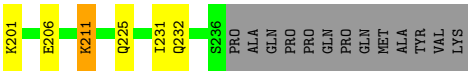
Chain CL:



• Molecule 7: Outer membrane protein, OmpA family protein

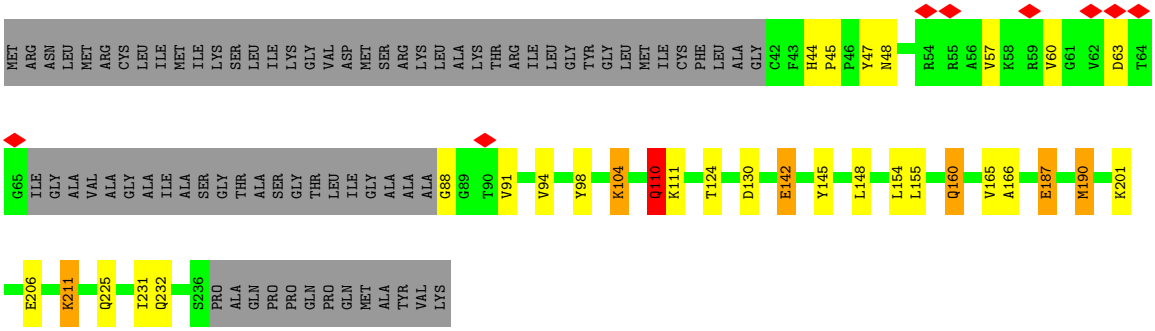
Chain DL:





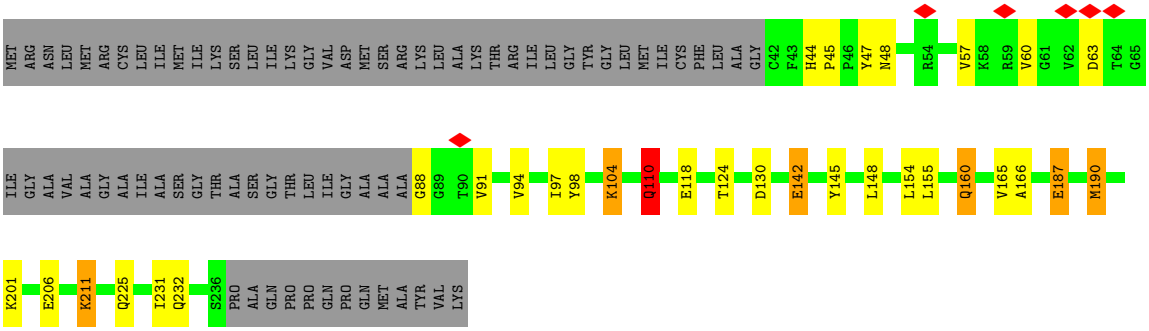
• Molecule 7: Outer membrane protein, OmpA family protein

Chain EL:



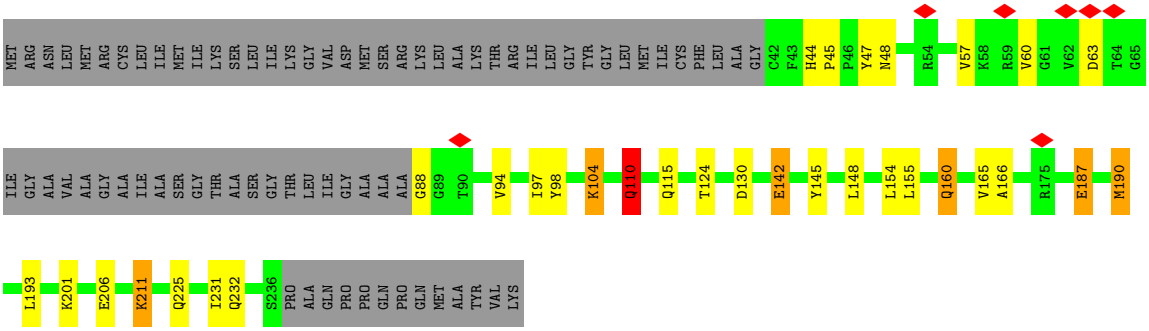
• Molecule 7: Outer membrane protein, OmpA family protein

Chain FL:



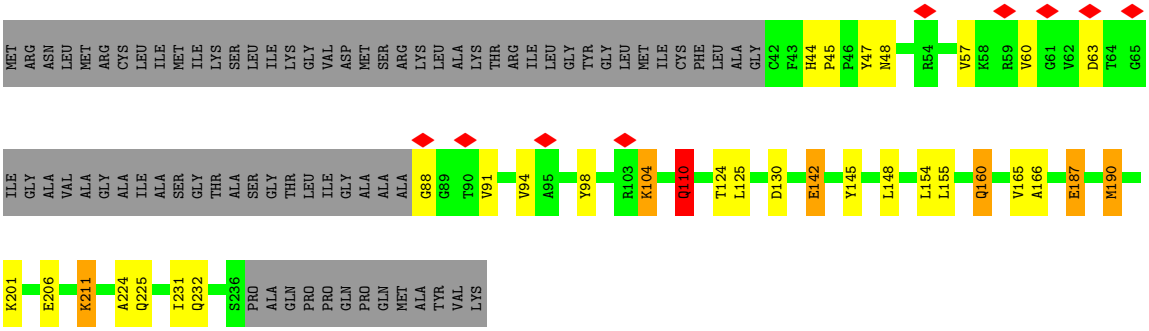
• Molecule 7: Outer membrane protein, OmpA family protein

Chain GL:



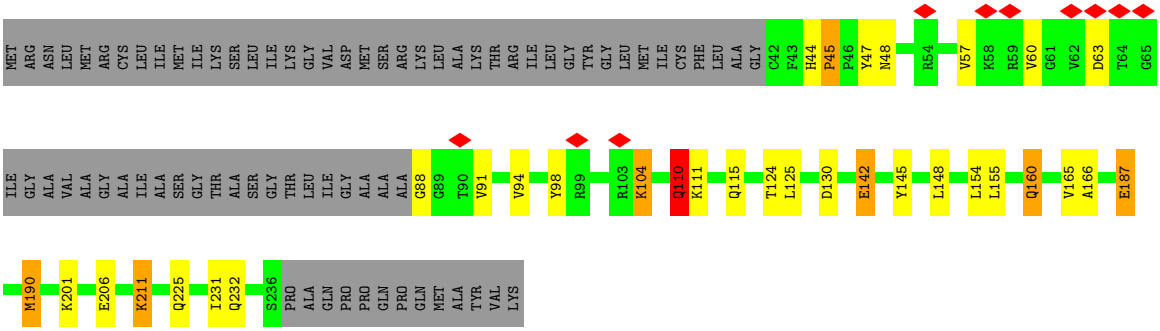
• Molecule 7: Outer membrane protein, OmpA family protein

Chain HL:



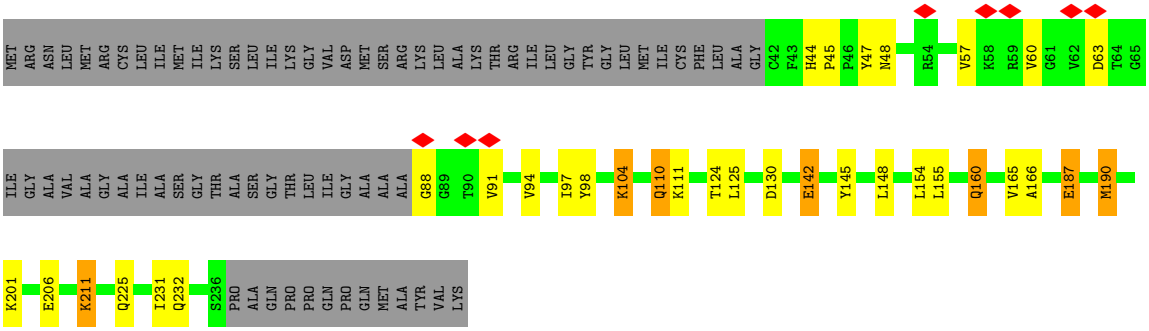
• Molecule 7: Outer membrane protein, OmpA family protein

Chain IL:



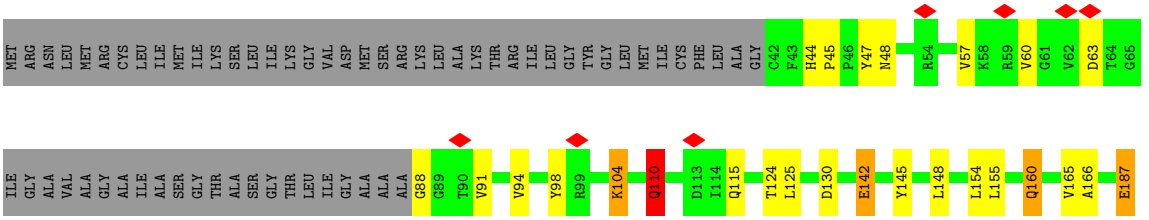
• Molecule 7: Outer membrane protein, OmpA family protein

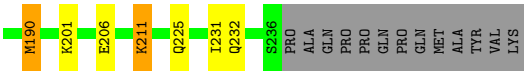
Chain JL:



• Molecule 7: Outer membrane protein, OmpA family protein

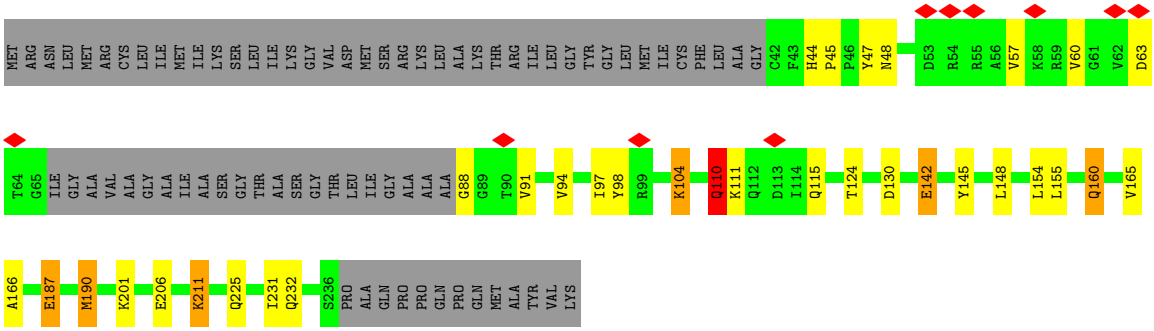
Chain KL:





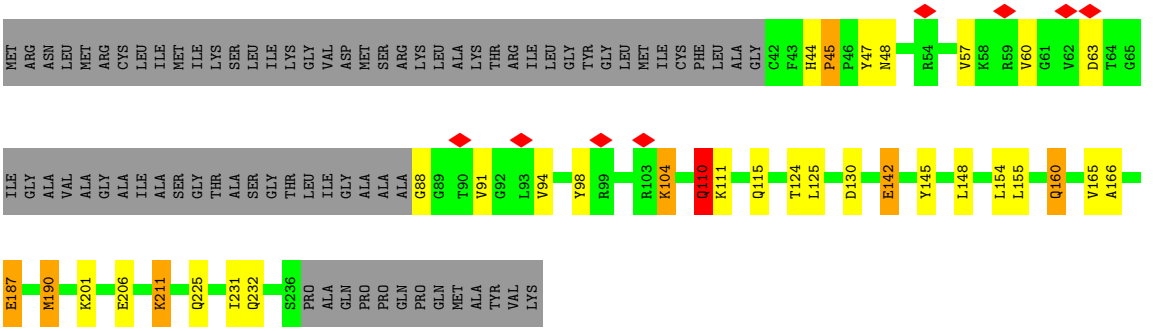
• Molecule 7: Outer membrane protein, OmpA family protein

Chain LL:



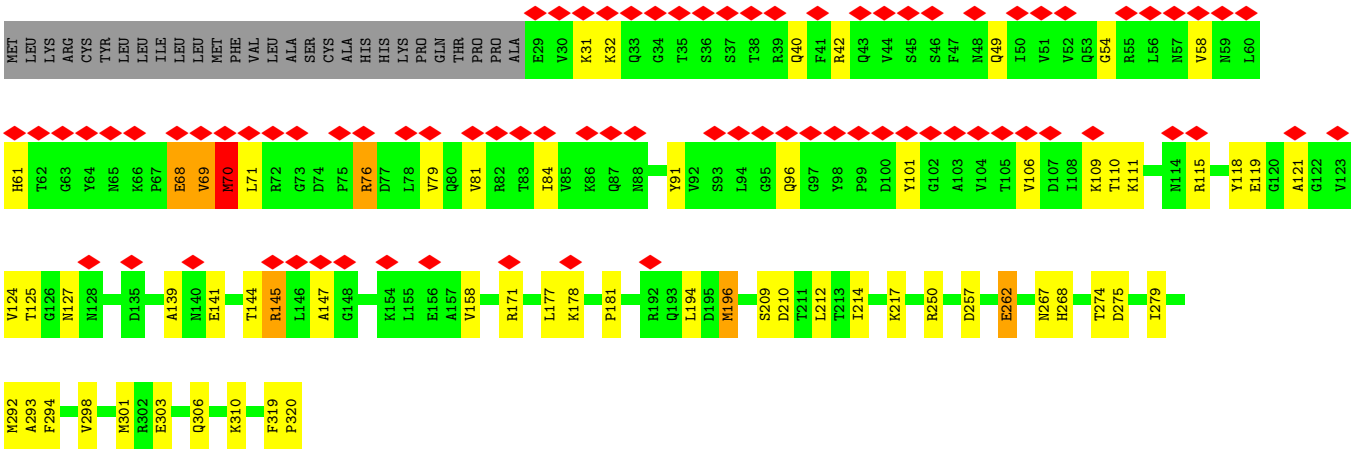
• Molecule 7: Outer membrane protein, OmpA family protein

Chain ML:



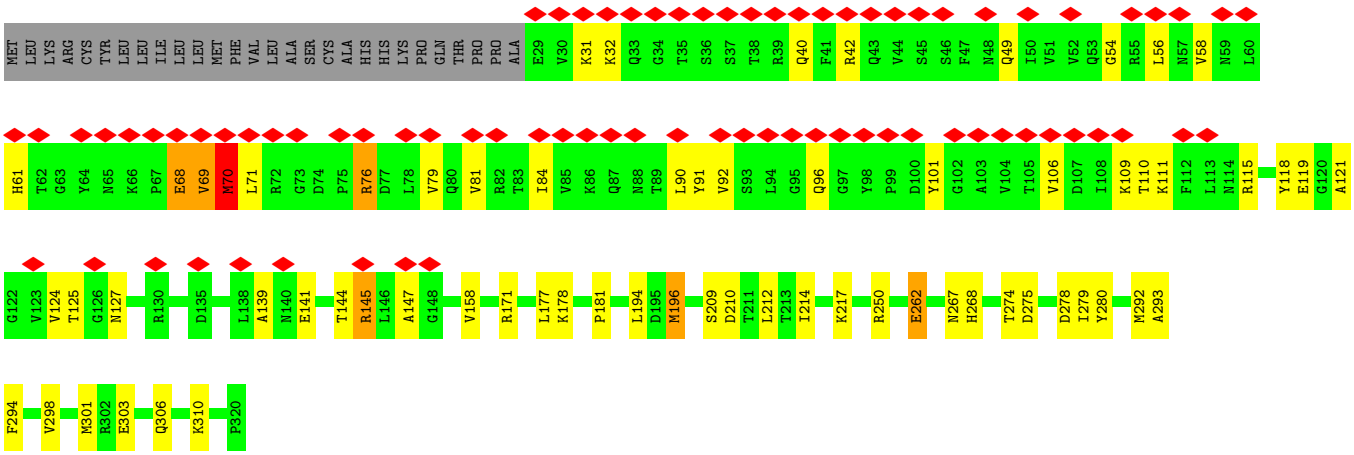
• Molecule 8: DUF2807 domain-containing protein

Chain AM:



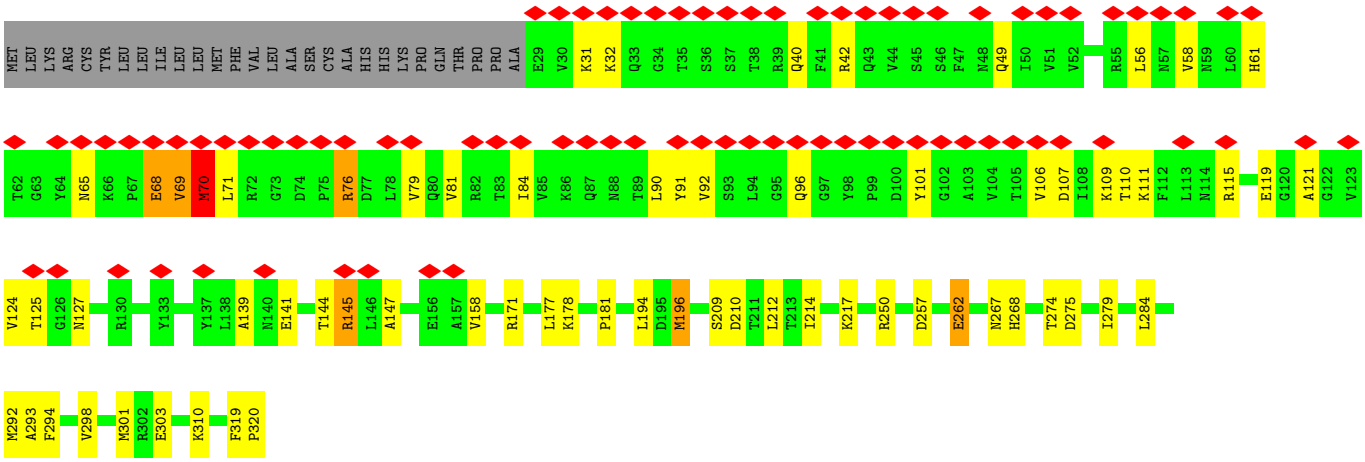
• Molecule 8: DUF2807 domain-containing protein

Chain BM:



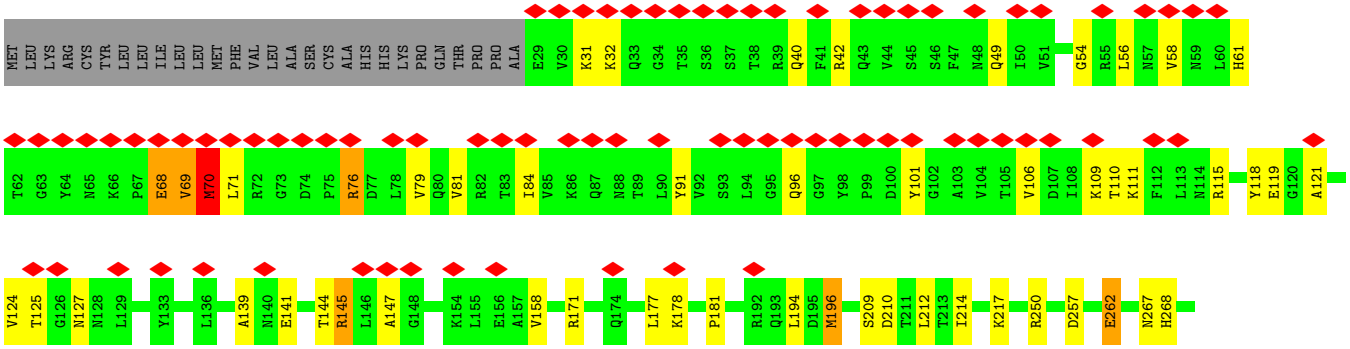
- Molecule 8: DUF2807 domain-containing protein

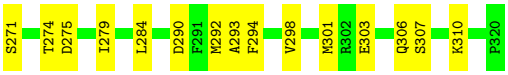
Chain CM:



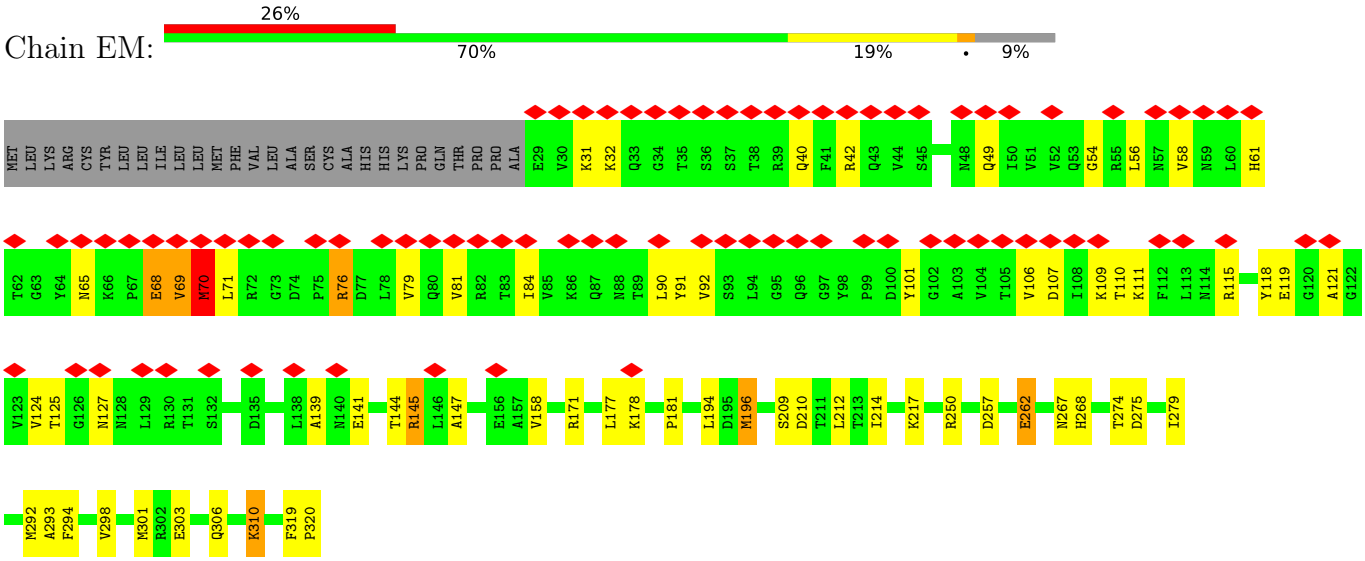
- Molecule 8: DUF2807 domain-containing protein

Chain DM:

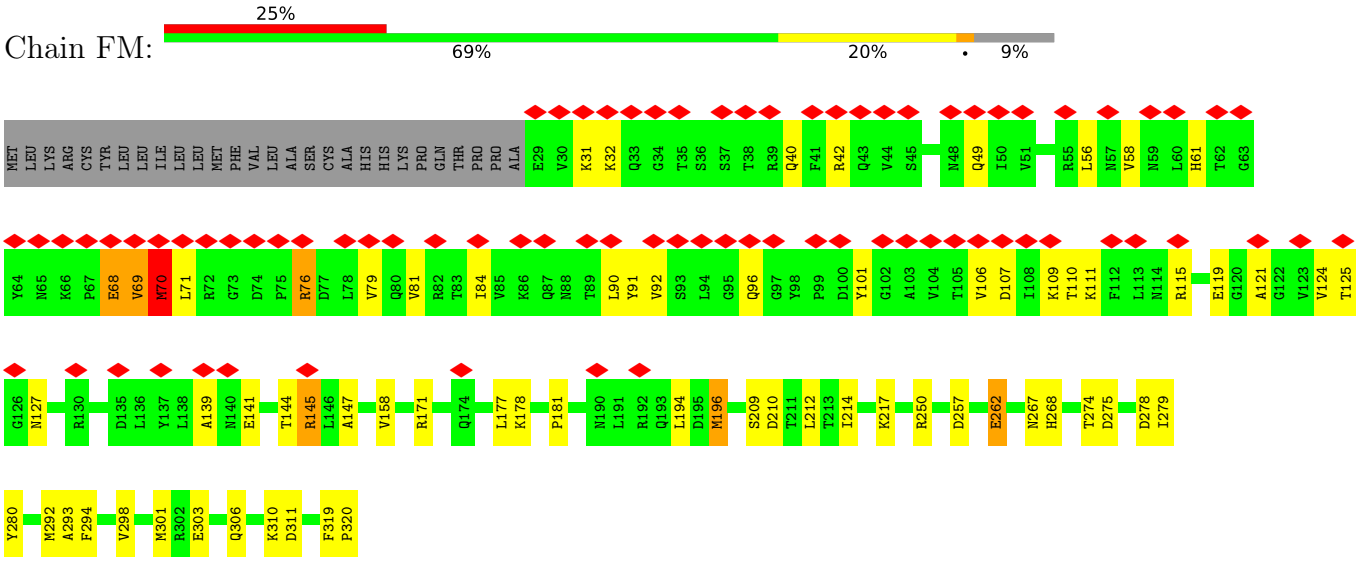




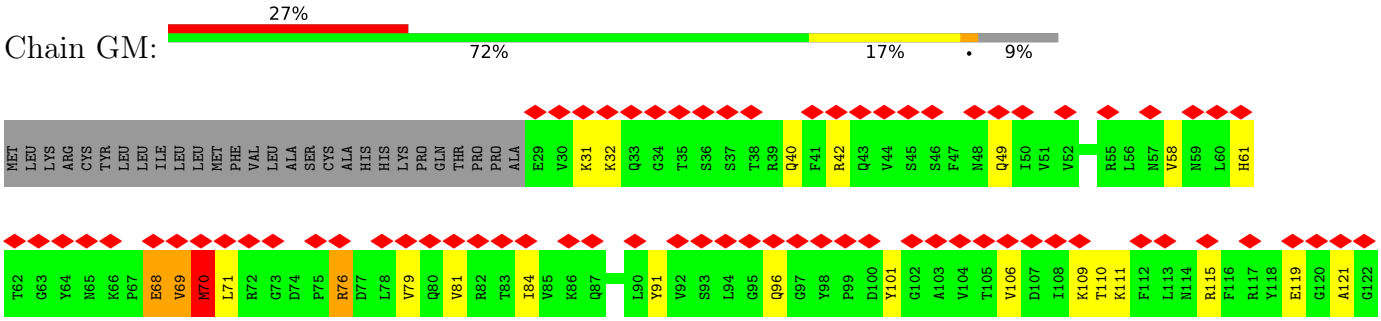
• Molecule 8: DUF2807 domain-containing protein

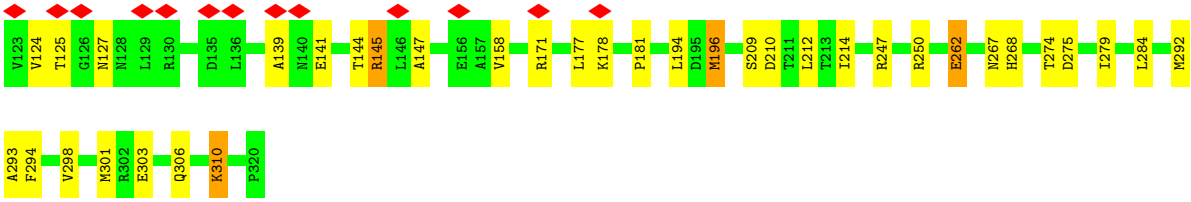


• Molecule 8: DUF2807 domain-containing protein



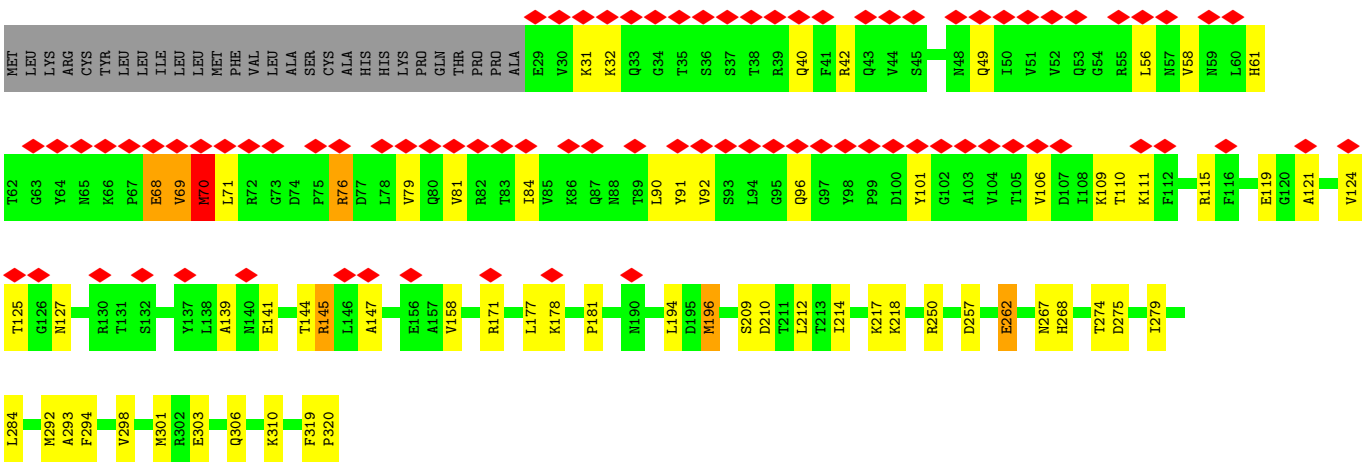
• Molecule 8: DUF2807 domain-containing protein





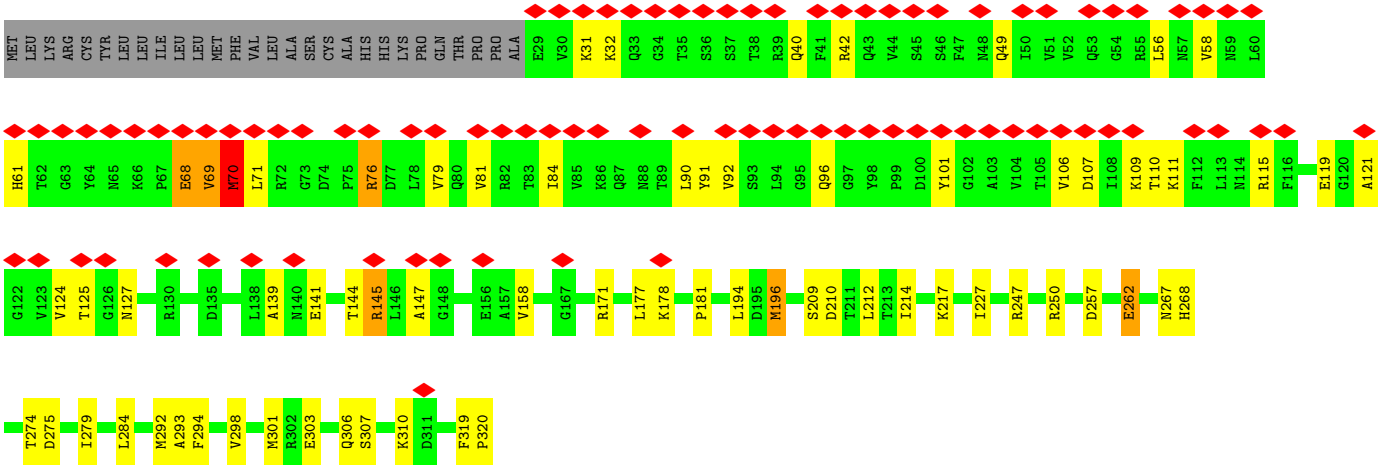
• Molecule 8: DUF2807 domain-containing protein

Chain HM:



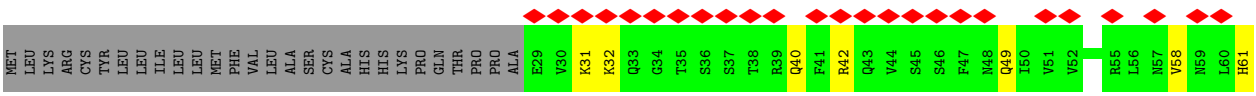
• Molecule 8: DUF2807 domain-containing protein

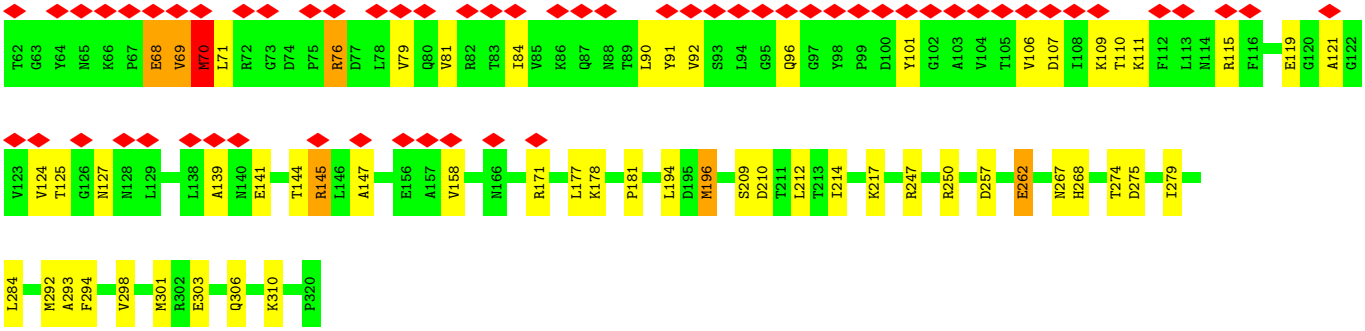
Chain IM:



• Molecule 8: DUF2807 domain-containing protein

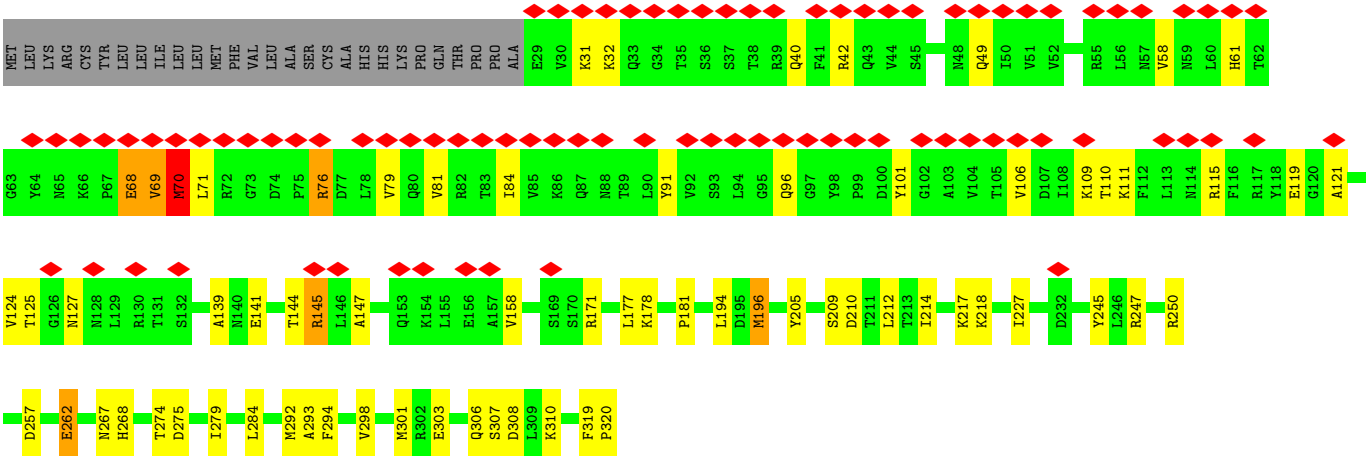
Chain JM:





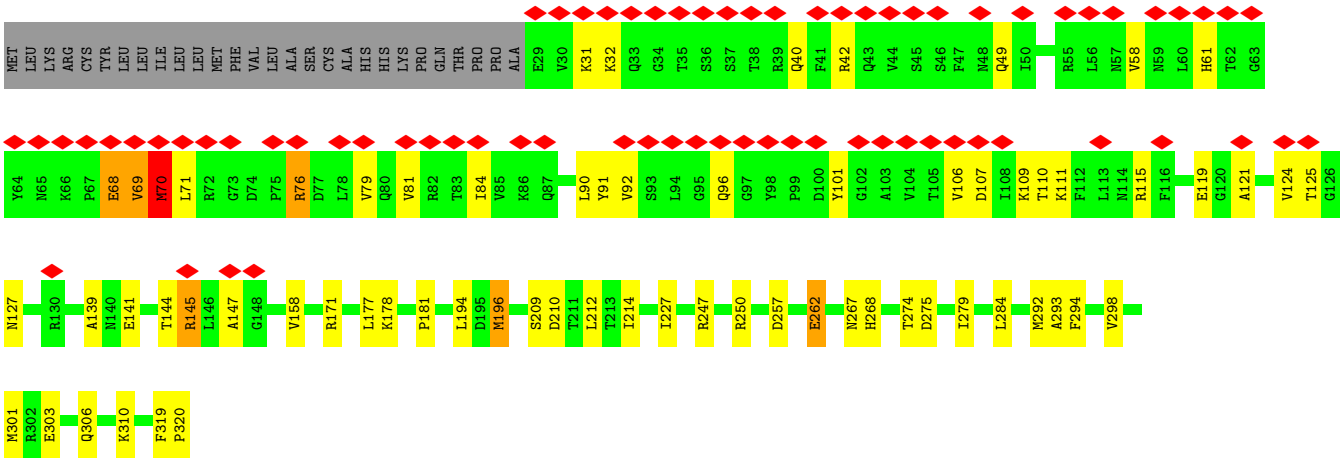
• Molecule 8: DUF2807 domain-containing protein

Chain KM:



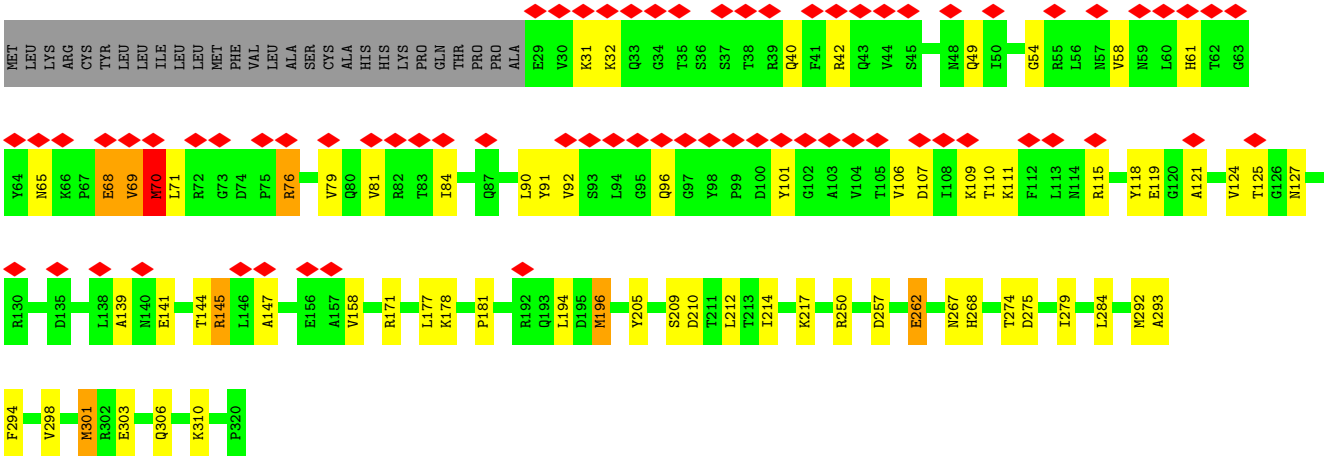
• Molecule 8: DUF2807 domain-containing protein

Chain LM:



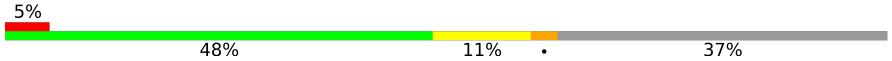
• Molecule 8: DUF2807 domain-containing protein

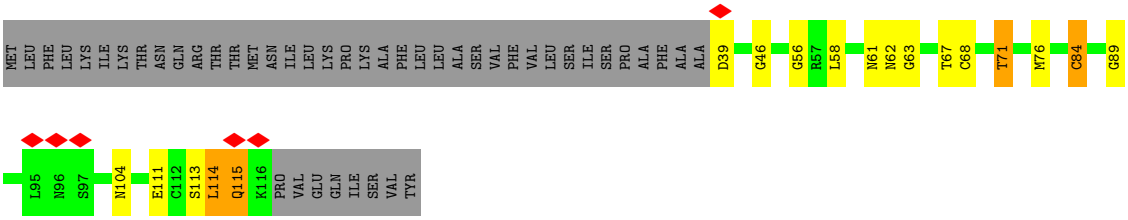
Chain MM:



- Molecule 9: Neurogenic locus notch

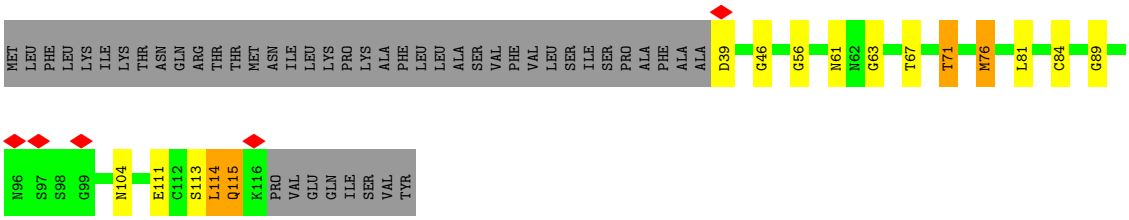
Chain AN:





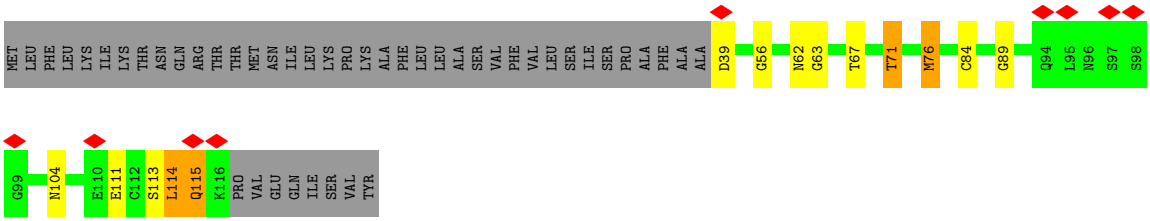
- Molecule 9: Neurogenic locus notch

Chain BN:



- Molecule 9: Neurogenic locus notch

Chain CN:



- Molecule 9: Neurogenic locus notch

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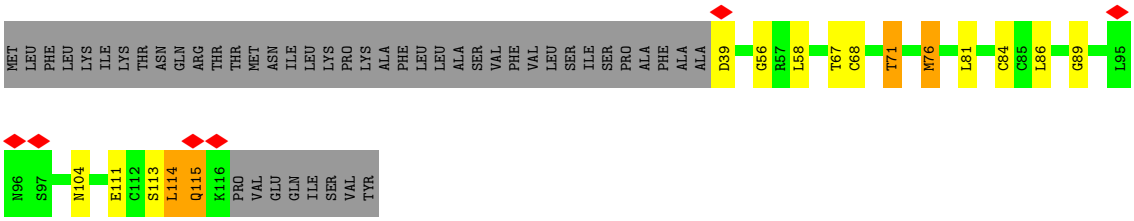
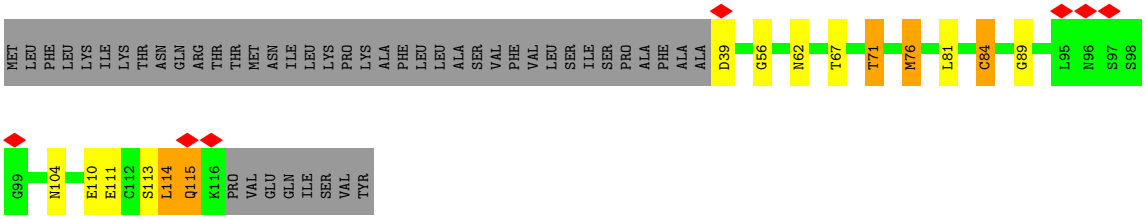


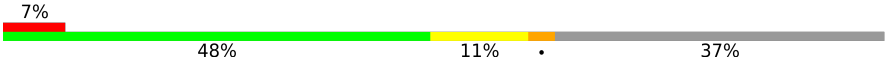
- Molecule 9: Neurogenic locus notch

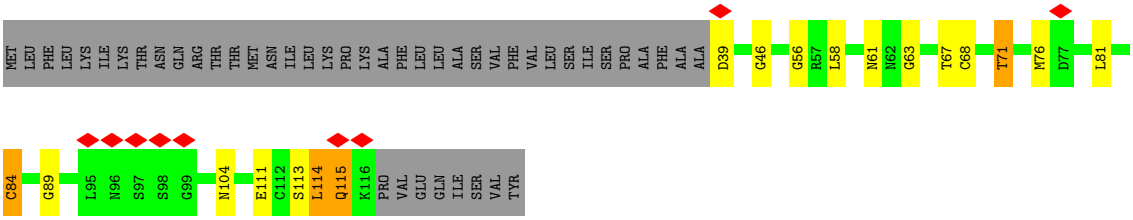
Chain EN:



- Molecule 9: Neurogenic locus notch

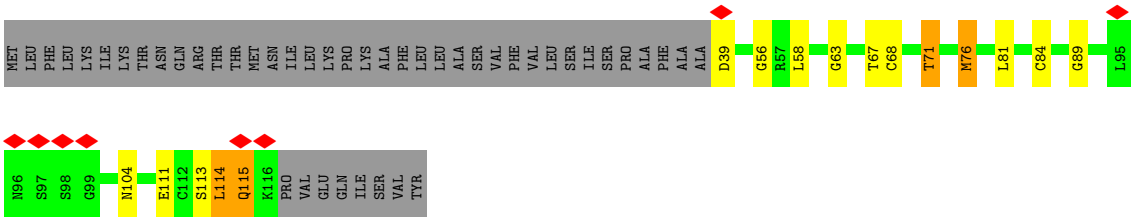
Chain FN:





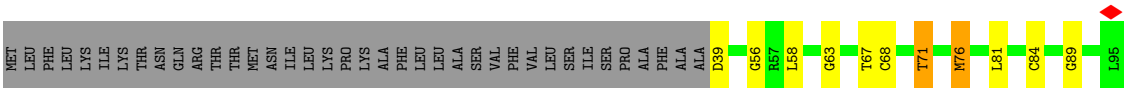
- Molecule 9: Neurogenic locus notch

Chain GN:



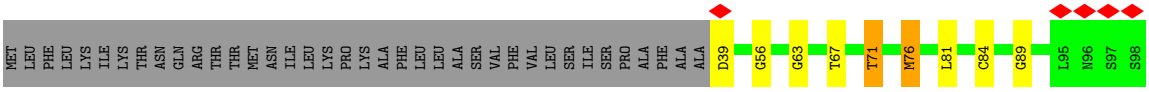
- Molecule 9: Neurogenic locus notch

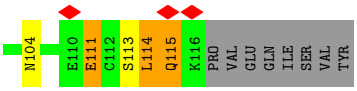
Chain HN:



• Molecule 9: Neurogenic locus notch

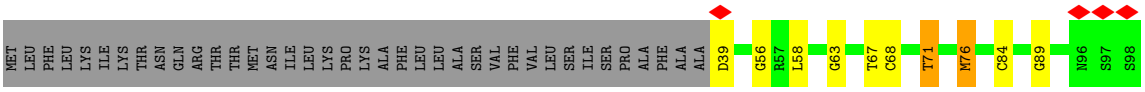
Chain IN:

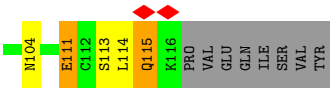




• Molecule 9: Neurogenic locus notch

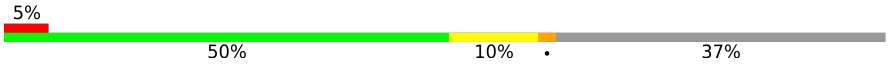
Chain JN:

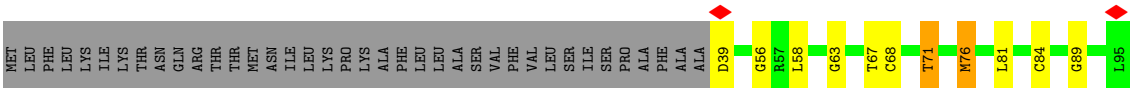




• Molecule 9: Neurogenic locus notch

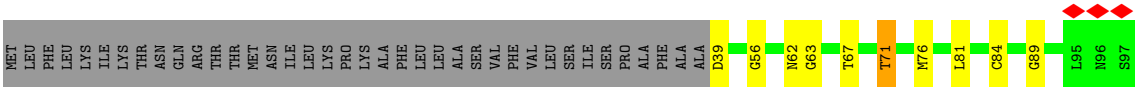
Chain KN:

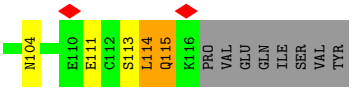




• Molecule 9: Neurogenic locus notch

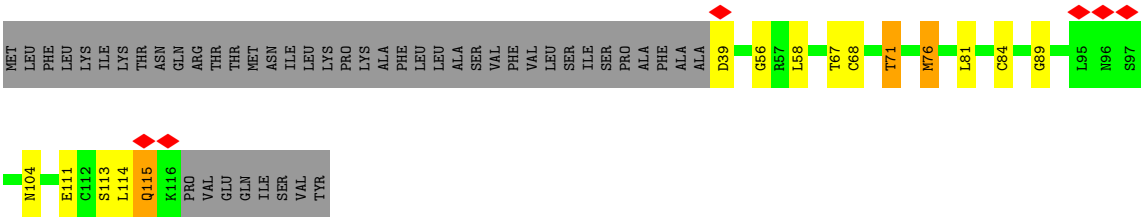
Chain LN:



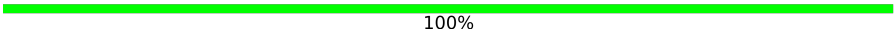


• Molecule 9: Neurogenic locus notch

Chain MN:

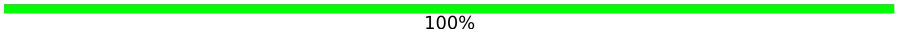


- Molecule 10: Unknown protein fragment

Chain AU: 

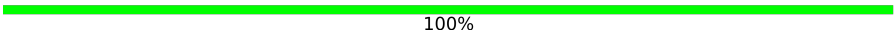
There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain BU: 

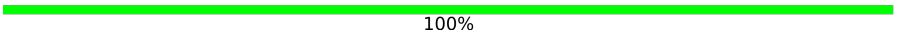
There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain CU: 

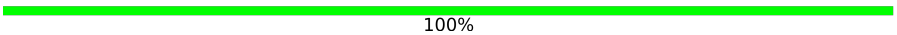
There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain DU: 

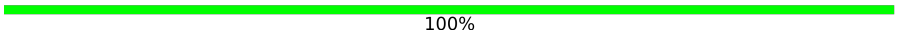
There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain EU: 

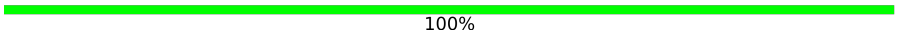
There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain FU: 

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain GU: 

There are no outlier residues recorded for this chain.

- Molecule 10: Unknown protein fragment

Chain HU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain IU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain JU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain KU: 100%

There are no outlier residues recorded for this chain.

• Molecule 10: Unknown protein fragment

Chain LU: 100%

There are no outlier residues recorded for this chain.

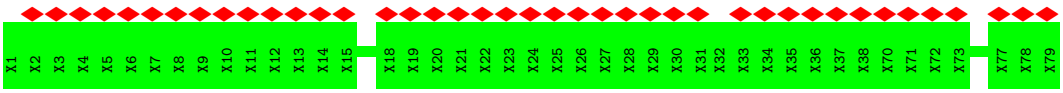
• Molecule 10: Unknown protein fragment

Chain MU: 100%

There are no outlier residues recorded for this chain.

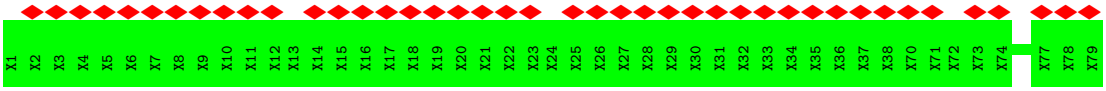
• Molecule 11: Unknown protein fragment

Chain AX: 85% 100%



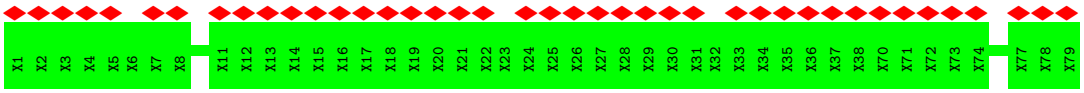
• Molecule 11: Unknown protein fragment

Chain BX: 88% 100%



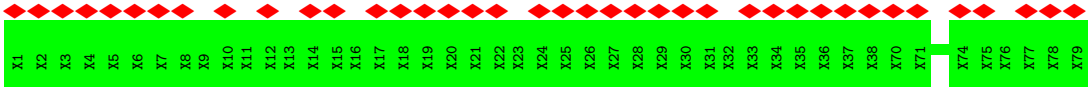
• Molecule 11: Unknown protein fragment

Chain CX: 85% 100%



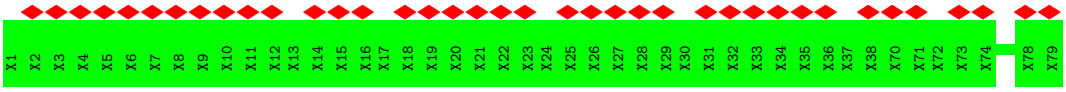
• Molecule 11: Unknown protein fragment

Chain DX:



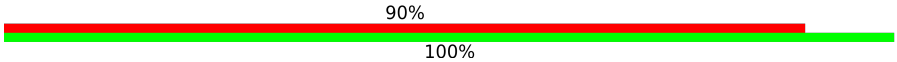
• Molecule 11: Unknown protein fragment

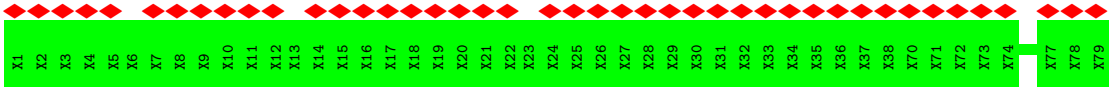
Chain EX:



• Molecule 11: Unknown protein fragment

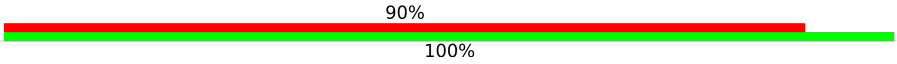
Chain FX:

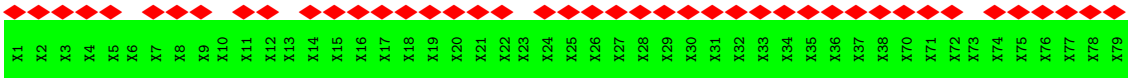




• Molecule 11: Unknown protein fragment

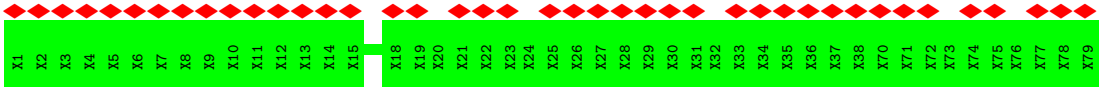
Chain GX:





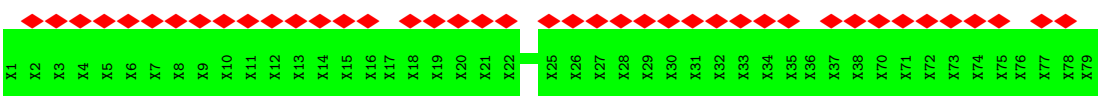
• Molecule 11: Unknown protein fragment

Chain HX:



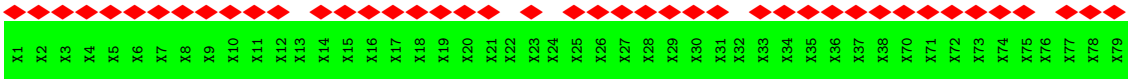
• Molecule 11: Unknown protein fragment

Chain IX:



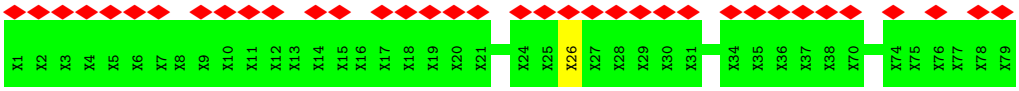
• Molecule 11: Unknown protein fragment

Chain JX: 90% 100%



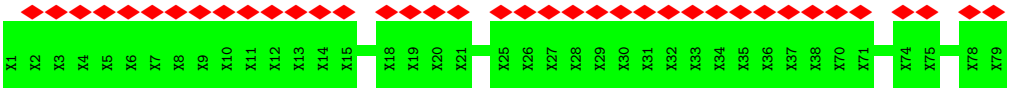
• Molecule 11: Unknown protein fragment

Chain KX: 75% 98%



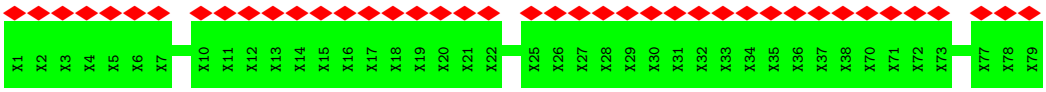
• Molecule 11: Unknown protein fragment

Chain LX: 79% 100%



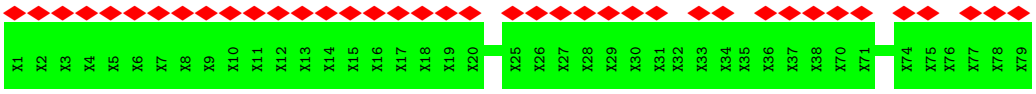
• Molecule 11: Unknown protein fragment

Chain MX: 85% 100%



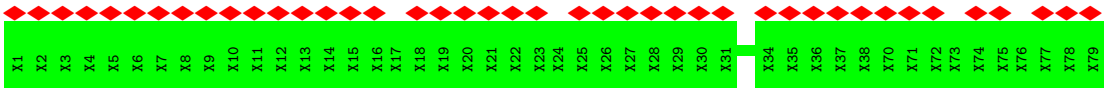
• Molecule 11: Unknown protein fragment

Chain VX: 81% 100%



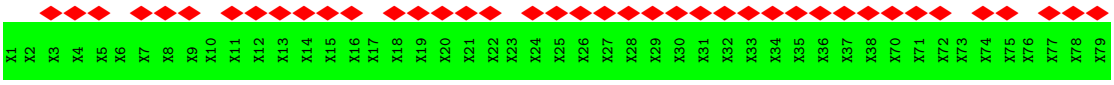
• Molecule 11: Unknown protein fragment

Chain WX: 88% 100%



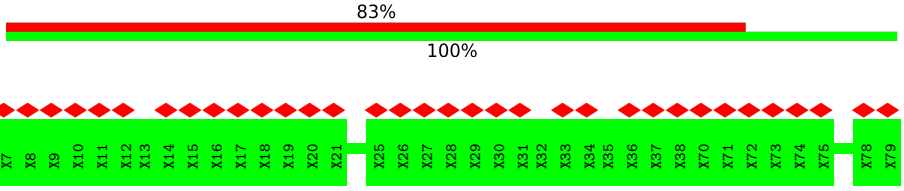
• Molecule 11: Unknown protein fragment

Chain XX: 83% 100%



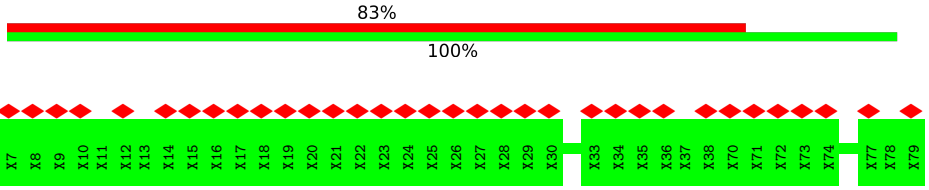
- Molecule 11: Unknown protein fragment

Chain YX:



- Molecule 11: Unknown protein fragment

Chain ZX:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136818	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.337	Depositor
Minimum map value	-1.017	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	561.0, 561.0, 561.0	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	AC	0.46	0/1717	0.90	8/2331 (0.3%)
1	BC	0.47	0/1717	0.90	8/2331 (0.3%)
1	CC	0.47	0/1717	0.90	8/2331 (0.3%)
1	DC	0.47	0/1717	0.91	8/2331 (0.3%)
1	EC	0.47	0/1717	0.90	8/2331 (0.3%)
1	FC	0.47	0/1717	0.90	8/2331 (0.3%)
1	GC	0.46	0/1717	0.90	8/2331 (0.3%)
1	HC	0.46	0/1717	0.90	8/2331 (0.3%)
1	IC	0.46	0/1717	0.90	8/2331 (0.3%)
1	JC	0.46	0/1717	0.90	8/2331 (0.3%)
1	KC	0.46	0/1717	0.90	8/2331 (0.3%)
1	LC	0.46	0/1717	0.90	8/2331 (0.3%)
1	MC	0.47	0/1717	0.90	8/2331 (0.3%)
2	AD	0.59	1/1107 (0.1%)	0.91	1/1502 (0.1%)
2	Ad	0.53	0/1078	0.93	2/1463 (0.1%)
2	BD	0.57	1/1107 (0.1%)	0.89	1/1502 (0.1%)
2	Bd	0.58	0/1078	0.90	3/1463 (0.2%)
2	CD	0.56	0/1107	0.86	3/1502 (0.2%)
2	Cd	0.61	1/1078 (0.1%)	1.04	5/1463 (0.3%)
2	DD	0.59	2/1107 (0.2%)	0.89	3/1502 (0.2%)
2	Dd	0.54	1/1078 (0.1%)	0.92	2/1463 (0.1%)
2	ED	0.60	0/1107	1.00	5/1502 (0.3%)
2	Ed	0.51	0/1078	0.87	0/1463
2	FD	0.50	0/1107	0.80	0/1502
2	Fd	1.03	8/1078 (0.7%)	1.13	13/1463 (0.9%)
2	GD	0.58	1/1107 (0.1%)	0.92	1/1502 (0.1%)
2	Gd	0.58	1/1078 (0.1%)	0.98	3/1463 (0.2%)
2	HD	0.61	1/1107 (0.1%)	0.93	2/1502 (0.1%)
2	Hd	0.56	1/1078 (0.1%)	0.84	0/1463
2	ID	0.54	0/1107	0.88	3/1502 (0.2%)
2	Id	0.53	0/1078	0.91	2/1463 (0.1%)
2	JD	0.52	1/1107 (0.1%)	0.88	1/1502 (0.1%)
2	Jd	0.54	0/1078	0.90	5/1463 (0.3%)
2	KD	0.57	2/1107 (0.2%)	0.88	3/1502 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Kd	0.54	0/1078	0.91	3/1463 (0.2%)
2	LD	0.60	1/1107 (0.1%)	0.94	5/1502 (0.3%)
2	Ld	0.55	0/1078	0.95	4/1463 (0.3%)
2	MD	0.57	1/1107 (0.1%)	0.84	0/1502
2	Md	0.59	0/1078	0.85	0/1463
3	AF	0.32	0/490	1.07	2/660 (0.3%)
3	Af	0.18	0/456	0.53	0/615
3	BF	0.32	0/490	1.07	2/660 (0.3%)
3	Bf	0.22	0/456	0.57	0/615
3	CF	0.32	0/490	1.07	2/660 (0.3%)
3	Cf	0.17	0/456	0.49	0/615
3	DF	0.31	0/490	1.07	2/660 (0.3%)
3	Df	0.18	0/456	0.53	0/615
3	EF	0.32	0/490	1.07	2/660 (0.3%)
3	Ef	0.19	0/456	0.54	0/615
3	FF	0.32	0/490	1.07	2/660 (0.3%)
3	Ff	0.20	0/456	0.52	0/615
3	GF	0.32	0/490	1.07	2/660 (0.3%)
3	Gf	0.16	0/456	0.38	0/615
3	HF	0.32	0/490	1.07	2/660 (0.3%)
3	Hf	0.19	0/456	0.58	0/615
3	IF	0.32	0/490	1.07	2/660 (0.3%)
3	If	0.20	0/456	0.57	0/615
3	JF	0.32	0/490	1.07	2/660 (0.3%)
3	Jf	0.17	0/456	0.51	0/615
3	KF	0.32	0/490	1.07	2/660 (0.3%)
3	Kf	0.20	0/456	0.49	0/615
3	LF	0.32	0/490	1.07	2/660 (0.3%)
3	Lf	0.17	0/456	0.43	0/615
3	MF	0.31	0/490	1.07	2/660 (0.3%)
3	Mf	0.18	0/456	0.55	0/615
3	VF	0.32	0/490	1.07	2/660 (0.3%)
3	WF	0.31	0/490	1.07	2/660 (0.3%)
3	XF	0.32	0/490	1.07	2/660 (0.3%)
3	YF	0.32	0/490	1.07	2/660 (0.3%)
3	ZF	0.31	0/490	1.07	2/660 (0.3%)
4	AG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	BG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	CG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	DG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	EG	0.81	1/278 (0.4%)	1.82	9/377 (2.4%)
4	FG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	GG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	HG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	IG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	JG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	KG	0.81	1/278 (0.4%)	1.82	9/377 (2.4%)
4	LG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	MG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	VG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
4	WG	0.81	1/278 (0.4%)	1.82	9/377 (2.4%)
4	XG	0.81	1/278 (0.4%)	1.82	9/377 (2.4%)
4	YG	0.81	1/278 (0.4%)	1.82	9/377 (2.4%)
4	ZG	0.82	1/278 (0.4%)	1.82	9/377 (2.4%)
5	AH	0.75	5/2033 (0.2%)	0.95	13/2775 (0.5%)
5	BH	0.56	3/2033 (0.1%)	0.92	10/2775 (0.4%)
5	CH	0.65	4/2033 (0.2%)	0.99	5/2775 (0.2%)
5	DH	0.66	4/2033 (0.2%)	0.94	5/2775 (0.2%)
5	EH	0.69	5/2033 (0.2%)	1.04	16/2775 (0.6%)
5	FH	0.66	3/2033 (0.1%)	0.96	10/2775 (0.4%)
5	GH	0.65	3/2033 (0.1%)	0.98	10/2775 (0.4%)
5	HH	0.67	5/2033 (0.2%)	1.00	12/2775 (0.4%)
5	IH	0.65	3/2033 (0.1%)	1.06	14/2775 (0.5%)
5	JH	0.58	2/2033 (0.1%)	0.99	11/2775 (0.4%)
5	KH	0.51	0/2033	0.92	6/2775 (0.2%)
5	LH	0.66	3/2033 (0.1%)	0.97	8/2775 (0.3%)
5	MH	0.59	0/2033	0.95	7/2775 (0.3%)
5	VH	0.45	1/1921 (0.1%)	0.92	6/2620 (0.2%)
5	WH	0.51	3/1921 (0.2%)	0.90	7/2620 (0.3%)
5	XH	0.53	4/1921 (0.2%)	0.97	6/2620 (0.2%)
5	YH	0.60	2/1921 (0.1%)	0.98	4/2620 (0.2%)
5	ZH	0.62	5/1921 (0.3%)	1.03	11/2620 (0.4%)
6	AK	0.48	0/1195	0.89	4/1616 (0.2%)
6	BK	0.48	0/1195	0.89	4/1616 (0.2%)
6	CK	0.48	0/1195	0.89	4/1616 (0.2%)
6	DK	0.48	0/1195	0.89	4/1616 (0.2%)
6	EK	0.48	0/1195	0.89	4/1616 (0.2%)
6	FK	0.48	0/1195	0.89	4/1616 (0.2%)
6	GK	0.48	0/1195	0.89	4/1616 (0.2%)
6	HK	0.48	0/1195	0.89	4/1616 (0.2%)
6	IK	0.48	0/1195	0.89	4/1616 (0.2%)
6	JK	0.48	0/1195	0.89	4/1616 (0.2%)
6	KK	0.48	0/1195	0.89	4/1616 (0.2%)
6	LK	0.48	0/1195	0.89	4/1616 (0.2%)
6	MK	0.48	0/1195	0.89	4/1616 (0.2%)
7	AL	0.48	0/1417	1.19	12/1912 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	BL	0.47	0/1417	1.19	12/1912 (0.6%)
7	CL	0.47	0/1417	1.19	11/1912 (0.6%)
7	DL	0.48	0/1417	1.19	11/1912 (0.6%)
7	EL	0.47	0/1417	1.19	11/1912 (0.6%)
7	FL	0.47	0/1417	1.19	11/1912 (0.6%)
7	GL	0.47	0/1417	1.19	11/1912 (0.6%)
7	HL	0.48	0/1417	1.19	12/1912 (0.6%)
7	IL	0.48	0/1417	1.19	11/1912 (0.6%)
7	JL	0.47	0/1417	1.19	12/1912 (0.6%)
7	KL	0.47	0/1417	1.19	12/1912 (0.6%)
7	LL	0.48	0/1417	1.19	12/1912 (0.6%)
7	ML	0.47	0/1417	1.19	12/1912 (0.6%)
8	AM	0.42	0/2359	0.93	11/3183 (0.3%)
8	BM	0.42	0/2359	0.93	11/3183 (0.3%)
8	CM	0.42	0/2359	0.93	10/3183 (0.3%)
8	DM	0.42	0/2359	0.93	11/3183 (0.3%)
8	EM	0.42	0/2359	0.93	8/3183 (0.3%)
8	FM	0.42	0/2359	0.93	11/3183 (0.3%)
8	GM	0.42	0/2359	0.93	10/3183 (0.3%)
8	HM	0.42	0/2359	0.93	11/3183 (0.3%)
8	IM	0.42	0/2359	0.93	11/3183 (0.3%)
8	JM	0.42	0/2359	0.93	11/3183 (0.3%)
8	KM	0.42	0/2359	0.93	10/3183 (0.3%)
8	LM	0.42	0/2359	0.93	11/3183 (0.3%)
8	MM	0.42	0/2359	0.93	11/3183 (0.3%)
9	AN	0.45	0/593	1.00	3/799 (0.4%)
9	BN	0.45	0/593	1.01	3/799 (0.4%)
9	CN	0.45	0/593	1.01	3/799 (0.4%)
9	DN	0.45	0/593	1.00	3/799 (0.4%)
9	EN	0.45	0/593	1.01	3/799 (0.4%)
9	FN	0.45	0/593	1.00	3/799 (0.4%)
9	GN	0.46	0/593	1.00	3/799 (0.4%)
9	HN	0.45	0/593	1.00	3/799 (0.4%)
9	IN	0.45	0/593	1.00	3/799 (0.4%)
9	JN	0.45	0/593	1.00	3/799 (0.4%)
9	KN	0.45	0/593	1.01	3/799 (0.4%)
9	LN	0.45	0/593	1.00	3/799 (0.4%)
9	MN	0.45	0/593	1.00	3/799 (0.4%)
All	All	0.52	96/178844 (0.1%)	0.99	911/242314 (0.4%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AD	0	1
2	BD	0	1
2	Bd	0	1
2	CD	0	1
2	Cd	0	1
2	DD	0	1
2	ED	0	1
2	FD	0	1
2	Fd	0	1
2	GD	0	1
2	ID	0	1
2	KD	0	1
2	MD	0	1
5	AH	0	2
5	BH	0	1
5	DH	0	1
5	EH	0	1
5	FH	0	2
5	GH	0	2
5	HH	0	1
5	IH	0	1
5	JH	0	3
5	KH	0	2
5	LH	0	1
5	MH	0	1
5	VH	0	1
5	WH	0	1
5	XH	0	1
5	YH	0	2
5	ZH	0	1
8	AM	0	1
8	BM	0	1
8	CM	0	1
8	DM	0	1
8	EM	0	1
8	FM	0	1
8	GM	0	1
8	HM	0	1
8	IM	0	1
8	JM	0	1
8	KM	0	1
8	LM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	MM	0	1
9	AN	0	1
9	BN	0	1
9	CN	0	1
9	DN	0	1
9	EN	0	1
9	FN	0	1
9	GN	0	1
9	HN	0	1
9	IN	0	1
9	JN	0	1
9	KN	0	1
9	LN	0	1
9	MN	0	1
All	All	0	63

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AH	205	GLN	CG-CD	-16.68	1.10	1.52
2	Fd	82	ARG	CB-CG	13.11	1.91	1.52
5	IH	115	MET	CB-CG	-12.40	1.15	1.52
5	HH	115	MET	CB-CG	-11.80	1.17	1.52
5	DH	115	MET	CB-CG	-11.62	1.17	1.52

The worst 5 of 911 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	EL	187	GLU	CG-CD-OE2	20.68	165.97	118.40
7	BL	187	GLU	CG-CD-OE2	20.67	165.95	118.40
7	HL	187	GLU	CG-CD-OE2	20.67	165.94	118.40
7	AL	187	GLU	CG-CD-OE2	20.66	165.92	118.40
7	GL	187	GLU	CG-CD-OE2	20.65	165.89	118.40

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AD	27	LYS	Peptide
5	AH	121	PRO	Mainchain
5	AH	137	SER	Mainchain

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Mol	Chain	Res	Type	Group
8	AM	68	GLU	Sidechain
9	AN	115	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	1685	0	1684	32	0
1	BC	1685	0	1684	41	0
1	CC	1685	0	1684	46	0
1	DC	1685	0	1684	42	0
1	EC	1685	0	1684	31	0
1	FC	1685	0	1684	24	0
1	GC	1685	0	1684	36	0
1	HC	1685	0	1684	36	0
1	IC	1685	0	1684	30	0
1	JC	1685	0	1684	30	0
1	KC	1685	0	1684	32	0
1	LC	1685	0	1684	25	0
1	MC	1685	0	1684	33	0
2	AD	1086	0	1121	15	0
2	Ad	1058	0	1092	8	0
2	BD	1086	0	1121	14	0
2	Bd	1058	0	1092	16	0
2	CD	1086	0	1121	20	0
2	Cd	1058	0	1092	12	0
2	DD	1086	0	1121	17	0
2	Dd	1058	0	1092	8	0
2	ED	1086	0	1119	18	0
2	Ed	1058	0	1092	12	0
2	FD	1086	0	1121	10	0
2	Fd	1058	0	1092	22	0
2	GD	1086	0	1121	13	0
2	Gd	1058	0	1092	12	0
2	HD	1086	0	1121	14	0
2	Hd	1058	0	1092	8	0
2	ID	1086	0	1121	18	0
2	Id	1058	0	1092	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	JD	1086	0	1121	13	0
2	Jd	1058	0	1092	6	0
2	KD	1086	0	1121	17	0
2	Kd	1058	0	1092	10	0
2	LD	1086	0	1121	16	0
2	Ld	1058	0	1092	4	0
2	MD	1086	0	1121	18	0
2	Md	1058	0	1092	10	0
3	AF	483	0	502	8	0
3	Af	449	0	474	6	0
3	BF	483	0	502	9	0
3	Bf	449	0	474	5	0
3	CF	483	0	502	8	0
3	Cf	449	0	474	4	0
3	DF	483	0	502	7	0
3	Df	449	0	474	5	0
3	EF	483	0	502	8	0
3	Ef	449	0	474	3	0
3	FF	483	0	502	9	0
3	Ff	449	0	474	5	0
3	GF	483	0	502	15	0
3	Gf	449	0	474	4	0
3	HF	483	0	502	8	0
3	Hf	449	0	474	15	0
3	IF	483	0	502	8	0
3	If	449	0	474	5	0
3	JF	483	0	502	10	0
3	Jf	449	0	474	6	0
3	KF	483	0	502	7	0
3	Kf	449	0	474	15	0
3	LF	483	0	502	7	0
3	Lf	449	0	474	7	0
3	MF	483	0	502	7	0
3	Mf	449	0	474	4	0
3	VF	483	0	502	8	0
3	WF	483	0	502	8	0
3	XF	483	0	502	15	0
3	YF	483	0	502	7	0
3	ZF	483	0	502	10	0
4	AG	276	0	263	17	0
4	BG	276	0	263	8	0
4	CG	276	0	263	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DG	276	0	263	15	0
4	EG	276	0	263	9	0
4	FG	276	0	263	9	0
4	GG	276	0	263	14	0
4	HG	276	0	263	12	0
4	IG	276	0	263	8	0
4	JG	276	0	263	16	0
4	KG	276	0	263	13	0
4	LG	276	0	263	11	0
4	MG	276	0	263	9	0
4	VG	276	0	263	10	0
4	WG	276	0	263	11	0
4	XG	276	0	263	9	0
4	YG	276	0	263	6	0
4	ZG	276	0	263	14	0
5	AH	1983	0	2009	35	0
5	BH	1983	0	2009	32	0
5	CH	1983	0	2009	44	0
5	DH	1983	0	2009	23	0
5	EH	1983	0	2009	41	0
5	FH	1983	0	2009	28	0
5	GH	1983	0	2009	43	0
5	HH	1983	0	2009	33	0
5	IH	1983	0	2009	43	0
5	JH	1983	0	2009	31	0
5	KH	1983	0	2009	24	0
5	LH	1983	0	2009	36	0
5	MH	1983	0	2009	30	0
5	VH	1875	0	1900	14	0
5	WH	1875	0	1900	26	0
5	XH	1875	0	1900	27	0
5	YH	1875	0	1900	20	0
5	ZH	1875	0	1900	31	0
6	AK	1175	0	1221	9	0
6	BK	1175	0	1221	13	0
6	CK	1175	0	1221	11	0
6	DK	1175	0	1221	11	0
6	EK	1175	0	1221	13	0
6	FK	1175	0	1221	9	0
6	GK	1175	0	1221	10	0
6	HK	1175	0	1221	10	0
6	IK	1175	0	1221	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	JK	1175	0	1221	12	0
6	KK	1175	0	1221	11	0
6	LK	1175	0	1221	9	0
6	MK	1175	0	1221	9	0
7	AL	1388	0	1378	15	0
7	BL	1388	0	1378	17	0
7	CL	1388	0	1378	16	0
7	DL	1388	0	1378	16	0
7	EL	1388	0	1378	16	0
7	FL	1388	0	1378	17	0
7	GL	1388	0	1378	17	0
7	HL	1388	0	1378	17	0
7	IL	1388	0	1378	19	0
7	JL	1388	0	1378	17	0
7	KL	1388	0	1378	17	0
7	LL	1388	0	1378	18	0
7	ML	1388	0	1378	19	0
8	AM	2320	0	2343	36	0
8	BM	2320	0	2343	37	0
8	CM	2320	0	2343	39	0
8	DM	2320	0	2343	37	0
8	EM	2320	0	2343	41	0
8	FM	2320	0	2343	43	0
8	GM	2320	0	2343	36	0
8	HM	2320	0	2343	46	0
8	IM	2320	0	2343	41	0
8	JM	2320	0	2343	38	0
8	KM	2320	0	2343	47	0
8	LM	2320	0	2343	38	0
8	MM	2320	0	2343	40	0
9	AN	582	0	530	8	0
9	BN	582	0	530	9	0
9	CN	582	0	530	8	0
9	DN	582	0	530	7	0
9	EN	582	0	530	9	0
9	FN	582	0	530	8	0
9	GN	582	0	530	7	0
9	HN	582	0	530	7	0
9	IN	582	0	530	7	0
9	JN	582	0	530	6	0
9	KN	582	0	530	6	0
9	LN	582	0	530	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	MN	582	0	530	6	0
10	AU	45	0	12	0	0
10	BU	45	0	12	0	0
10	CU	45	0	12	0	0
10	DU	45	0	12	0	0
10	EU	45	0	12	0	0
10	FU	45	0	12	0	0
10	GU	45	0	12	0	0
10	HU	45	0	12	0	0
10	IU	45	0	12	0	0
10	JU	45	0	12	0	0
10	KU	45	0	12	0	0
10	LU	45	0	12	0	0
10	MU	45	0	12	0	0
11	AX	240	0	54	0	0
11	BX	240	0	54	0	0
11	CX	240	0	54	0	0
11	DX	240	0	54	0	0
11	EX	240	0	54	0	0
11	FX	240	0	54	0	0
11	GX	240	0	54	0	0
11	HX	240	0	54	0	0
11	IX	240	0	54	0	0
11	JX	240	0	54	0	0
11	KX	240	0	54	1	0
11	LX	240	0	54	0	0
11	MX	240	0	54	0	0
11	VX	240	0	54	0	0
11	WX	240	0	54	0	0
11	XX	240	0	54	0	0
11	YX	240	0	54	0	0
11	ZX	240	0	54	0	0
All	All	180380	0	178472	2286	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2286 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Fd:82:ARG:CB	2:Fd:82:ARG:CG	1.91	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:GH:115:MET:SD	5:GH:115:MET:CE	2.04	1.46
1:BC:177:CYS:HB2	1:CC:35:GLN:NE2	1.38	1.39
5:GH:115:MET:CE	5:GH:115:MET:HB2	1.71	1.21
1:BC:177:CYS:CB	1:CC:35:GLN:NE2	2.04	1.18

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	BC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	CC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	DC	207/303 (68%)	201 (97%)	6 (3%)	0	100	100
1	EC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	FC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	GC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	HC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	IC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	JC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	KC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	LC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
1	MC	207/303 (68%)	202 (98%)	5 (2%)	0	100	100
2	AD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Ad	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	BD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	CD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Cd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	DD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Dd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ED	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Ed	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	FD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Fd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	GD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Gd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	HD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Hd	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	ID	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Id	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	JD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Jd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	KD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Kd	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
2	LD	138/163 (85%)	133 (96%)	5 (4%)	0	100	100
2	Ld	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
2	MD	138/163 (85%)	134 (97%)	4 (3%)	0	100	100
2	Md	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
3	AF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Af	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	BF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Bf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	CF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Cf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	DF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Df	57/269 (21%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Ef	57/269 (21%)	52 (91%)	5 (9%)	0	100	100
3	FF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Ff	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	GF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Gf	57/269 (21%)	56 (98%)	1 (2%)	0	100	100
3	HF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Hf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	IF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	If	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	JF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Jf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	KF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Kf	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
3	LF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Lf	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
3	MF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	Mf	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
3	VF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	WF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	XF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	YF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
3	ZF	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
4	AG	32/1048 (3%)	32 (100%)	0	0	100	100
4	BG	32/1048 (3%)	32 (100%)	0	0	100	100
4	CG	32/1048 (3%)	32 (100%)	0	0	100	100
4	DG	32/1048 (3%)	32 (100%)	0	0	100	100
4	EG	32/1048 (3%)	32 (100%)	0	0	100	100
4	FG	32/1048 (3%)	32 (100%)	0	0	100	100
4	GG	32/1048 (3%)	32 (100%)	0	0	100	100
4	HG	32/1048 (3%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	IG	32/1048 (3%)	32 (100%)	0	0	100	100
4	JG	32/1048 (3%)	32 (100%)	0	0	100	100
4	KG	32/1048 (3%)	32 (100%)	0	0	100	100
4	LG	32/1048 (3%)	32 (100%)	0	0	100	100
4	MG	32/1048 (3%)	32 (100%)	0	0	100	100
4	VG	32/1048 (3%)	32 (100%)	0	0	100	100
4	WG	32/1048 (3%)	32 (100%)	0	0	100	100
4	XG	32/1048 (3%)	32 (100%)	0	0	100	100
4	YG	32/1048 (3%)	32 (100%)	0	0	100	100
4	ZG	32/1048 (3%)	32 (100%)	0	0	100	100
5	AH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	BH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	CH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	DH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	EH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	FH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	GH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100
5	HH	256/361 (71%)	245 (96%)	11 (4%)	0	100	100
5	IH	256/361 (71%)	240 (94%)	16 (6%)	0	100	100
5	JH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	KH	256/361 (71%)	242 (94%)	14 (6%)	0	100	100
5	LH	256/361 (71%)	241 (94%)	15 (6%)	0	100	100
5	MH	256/361 (71%)	243 (95%)	13 (5%)	0	100	100
5	VH	239/361 (66%)	231 (97%)	8 (3%)	0	100	100
5	WH	239/361 (66%)	231 (97%)	8 (3%)	0	100	100
5	XH	239/361 (66%)	230 (96%)	9 (4%)	0	100	100
5	YH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
5	ZH	239/361 (66%)	232 (97%)	7 (3%)	0	100	100
6	AK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	BK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	CK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	DK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	EK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	FK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	GK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	HK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	IK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	JK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	KK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	LK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
6	MK	149/189 (79%)	144 (97%)	5 (3%)	0	100	100
7	AL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	BL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	CL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	DL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	EL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	FL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	GL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	HL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	IL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	JL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	KL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	LL	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
7	ML	169/249 (68%)	159 (94%)	10 (6%)	0	100	100
8	AM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	BM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	CM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	DM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	EM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	FM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	GM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	HM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	IM	290/320 (91%)	266 (92%)	24 (8%)	0	100	100
8	JM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	KM	290/320 (91%)	266 (92%)	24 (8%)	0	100	100
8	LM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
8	MM	290/320 (91%)	265 (91%)	25 (9%)	0	100	100
9	AN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	BN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	CN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	DN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	EN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	FN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	GN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	HN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	IN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	JN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	KN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	LN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
9	MN	76/124 (61%)	68 (90%)	8 (10%)	0	100	100
All	All	22070/53344 (41%)	20933 (95%)	1137 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	178/257 (69%)	166 (93%)	12 (7%)	15	41
1	BC	178/257 (69%)	166 (93%)	12 (7%)	15	41
1	CC	178/257 (69%)	167 (94%)	11 (6%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DC	178/257 (69%)	167 (94%)	11 (6%)	16	42
1	EC	178/257 (69%)	167 (94%)	11 (6%)	16	42
1	FC	178/257 (69%)	166 (93%)	12 (7%)	15	41
1	GC	178/257 (69%)	166 (93%)	12 (7%)	15	41
1	HC	178/257 (69%)	167 (94%)	11 (6%)	16	42
1	IC	178/257 (69%)	166 (93%)	12 (7%)	15	41
1	JC	178/257 (69%)	167 (94%)	11 (6%)	16	42
1	KC	178/257 (69%)	166 (93%)	12 (7%)	15	41
1	LC	178/257 (69%)	167 (94%)	11 (6%)	16	42
1	MC	178/257 (69%)	166 (93%)	12 (7%)	15	41
2	AD	121/139 (87%)	121 (100%)	0	100	100
2	Ad	118/139 (85%)	118 (100%)	0	100	100
2	BD	121/139 (87%)	121 (100%)	0	100	100
2	Bd	118/139 (85%)	118 (100%)	0	100	100
2	CD	121/139 (87%)	121 (100%)	0	100	100
2	Cd	118/139 (85%)	118 (100%)	0	100	100
2	DD	121/139 (87%)	121 (100%)	0	100	100
2	Dd	118/139 (85%)	118 (100%)	0	100	100
2	ED	121/139 (87%)	121 (100%)	0	100	100
2	Ed	118/139 (85%)	118 (100%)	0	100	100
2	FD	121/139 (87%)	121 (100%)	0	100	100
2	Fd	118/139 (85%)	118 (100%)	0	100	100
2	GD	121/139 (87%)	121 (100%)	0	100	100
2	Gd	118/139 (85%)	118 (100%)	0	100	100
2	HD	121/139 (87%)	121 (100%)	0	100	100
2	Hd	118/139 (85%)	118 (100%)	0	100	100
2	ID	121/139 (87%)	121 (100%)	0	100	100
2	Id	118/139 (85%)	117 (99%)	1 (1%)	73	76
2	JD	121/139 (87%)	121 (100%)	0	100	100
2	Jd	118/139 (85%)	118 (100%)	0	100	100
2	KD	121/139 (87%)	121 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Kd	118/139 (85%)	118 (100%)	0	100	100
2	LD	121/139 (87%)	121 (100%)	0	100	100
2	Ld	118/139 (85%)	118 (100%)	0	100	100
2	MD	121/139 (87%)	121 (100%)	0	100	100
2	Md	118/139 (85%)	118 (100%)	0	100	100
3	AF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Af	49/237 (21%)	49 (100%)	0	100	100
3	BF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Bf	49/237 (21%)	49 (100%)	0	100	100
3	CF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Cf	49/237 (21%)	49 (100%)	0	100	100
3	DF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Df	49/237 (21%)	49 (100%)	0	100	100
3	EF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Ef	49/237 (21%)	49 (100%)	0	100	100
3	FF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Ff	49/237 (21%)	49 (100%)	0	100	100
3	GF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Gf	49/237 (21%)	49 (100%)	0	100	100
3	HF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Hf	49/237 (21%)	49 (100%)	0	100	100
3	IF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	If	49/237 (21%)	49 (100%)	0	100	100
3	JF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Jf	49/237 (21%)	49 (100%)	0	100	100
3	KF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Kf	49/237 (21%)	49 (100%)	0	100	100
3	LF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Lf	49/237 (21%)	49 (100%)	0	100	100
3	MF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	Mf	49/237 (21%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	VF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	WF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	XF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	YF	53/237 (22%)	46 (87%)	7 (13%)	4	19
3	ZF	53/237 (22%)	46 (87%)	7 (13%)	4	19
4	AG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	BG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	CG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	DG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	EG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	FG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	GG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	HG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	IG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	JG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	KG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	LG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	MG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	VG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	WG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	XG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	YG	31/765 (4%)	21 (68%)	10 (32%)	0	1
4	ZG	31/765 (4%)	21 (68%)	10 (32%)	0	1
5	AH	220/300 (73%)	220 (100%)	0	100	100
5	BH	220/300 (73%)	220 (100%)	0	100	100
5	CH	220/300 (73%)	219 (100%)	1 (0%)	81	81
5	DH	220/300 (73%)	219 (100%)	1 (0%)	81	81
5	EH	220/300 (73%)	220 (100%)	0	100	100
5	FH	220/300 (73%)	220 (100%)	0	100	100
5	GH	220/300 (73%)	220 (100%)	0	100	100
5	HH	220/300 (73%)	220 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	IH	220/300 (73%)	219 (100%)	1 (0%)	81	81
5	JH	220/300 (73%)	220 (100%)	0	100	100
5	KH	220/300 (73%)	220 (100%)	0	100	100
5	LH	220/300 (73%)	220 (100%)	0	100	100
5	MH	220/300 (73%)	220 (100%)	0	100	100
5	VH	207/300 (69%)	207 (100%)	0	100	100
5	WH	207/300 (69%)	207 (100%)	0	100	100
5	XH	207/300 (69%)	207 (100%)	0	100	100
5	YH	207/300 (69%)	207 (100%)	0	100	100
5	ZH	207/300 (69%)	207 (100%)	0	100	100
6	AK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	BK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	CK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	DK	129/163 (79%)	118 (92%)	11 (8%)	10	33
6	EK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	FK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	GK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	HK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	IK	129/163 (79%)	118 (92%)	11 (8%)	10	33
6	JK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	KK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	LK	129/163 (79%)	119 (92%)	10 (8%)	11	36
6	MK	129/163 (79%)	119 (92%)	10 (8%)	11	36
7	AL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	BL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	CL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	DL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	EL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	FL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	GL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	HL	148/203 (73%)	139 (94%)	9 (6%)	17	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	IL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	JL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	KL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	LL	148/203 (73%)	139 (94%)	9 (6%)	17	43
7	ML	148/203 (73%)	139 (94%)	9 (6%)	17	43
8	AM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	BM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	CM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	DM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	EM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	FM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	GM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	HM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	IM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	JM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	KM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	LM	251/276 (91%)	241 (96%)	10 (4%)	28	52
8	MM	251/276 (91%)	241 (96%)	10 (4%)	28	52
9	AN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	BN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	CN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	DN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	EN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	FN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	GN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	HN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	IN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	JN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	KN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	LN	66/107 (62%)	60 (91%)	6 (9%)	9	32
9	MN	66/107 (62%)	60 (91%)	6 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	19187/43209 (44%)	18270 (95%)	917 (5%)	24 47

5 of 917 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	HF	250	LEU
3	YF	243	MET
9	IN	71	THR
4	XG	808	LEU
6	MK	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 181 such sidechains are listed below:

Mol	Chain	Res	Type
8	IM	164	GLN
8	KM	88	ASN
2	JD	32	ASN
3	Jf	266	GLN
6	LK	147	GLN

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 oligosaccharides 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
11	AX	1
11	BX	1
11	CX	1
11	DX	1
11	EX	1
11	FX	1
11	GX	1
11	HX	1
11	IX	1
11	JX	1
11	KX	1
11	LX	1
11	MX	1
11	VX	1
11	WX	1
11	XX	1
11	YX	1
11	ZX	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AX	38:UNK	C	70:UNK	N	24.20
1	BX	38:UNK	C	70:UNK	N	24.20
1	CX	38:UNK	C	70:UNK	N	24.20
1	DX	38:UNK	C	70:UNK	N	24.20
1	EX	38:UNK	C	70:UNK	N	24.20

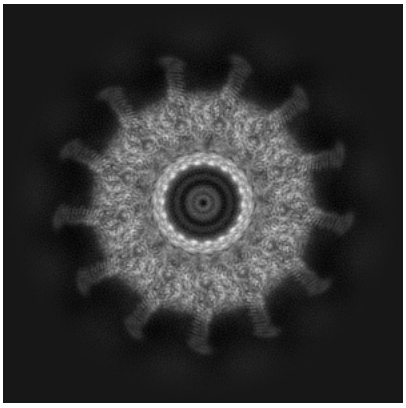
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24004. These allow visual inspection of the internal detail of the map and identification of artifacts.

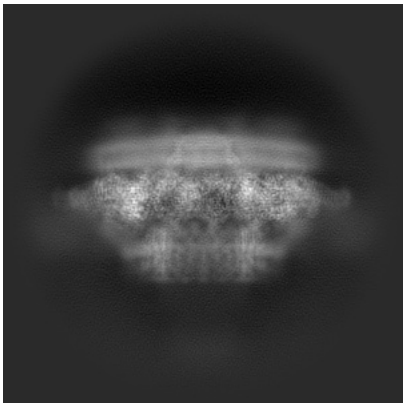
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

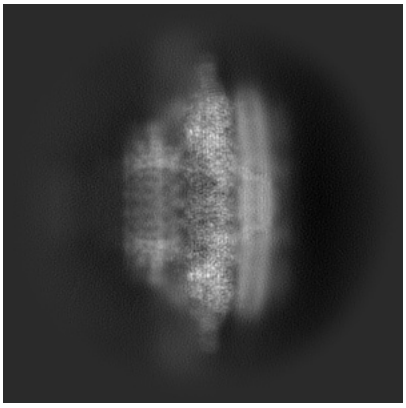
6.1.1 Primary map



X



Y

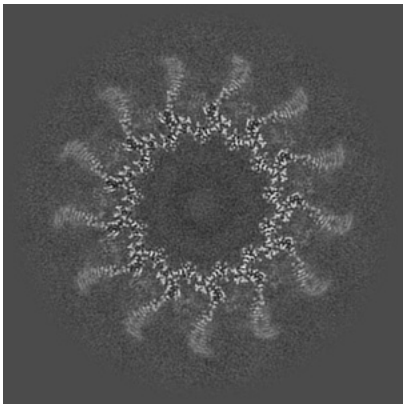


Z

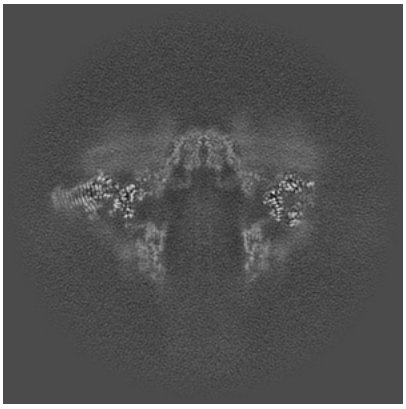
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

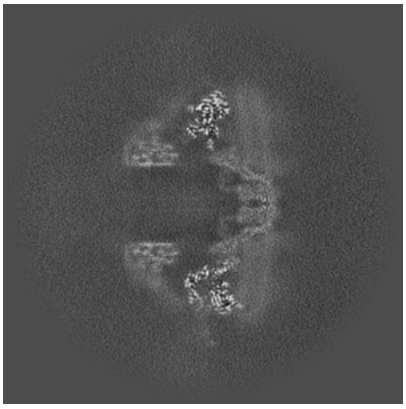
6.2.1 Primary map



X Index: 255



Y Index: 255

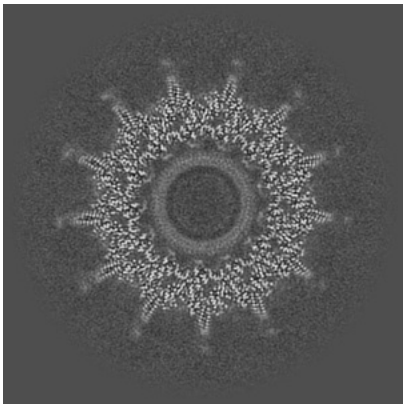


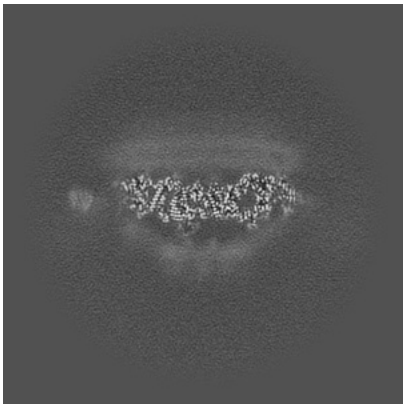
Z Index: 255

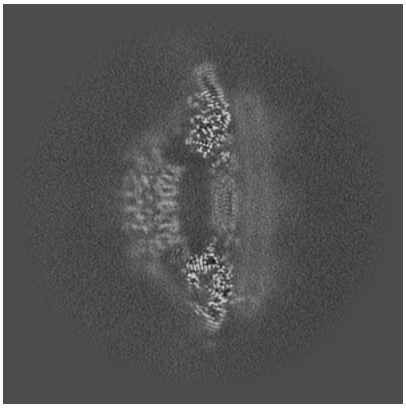
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 274


Y Index: 164

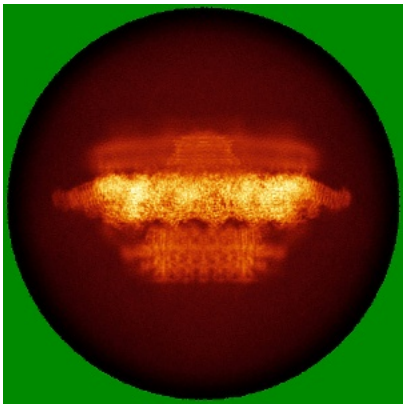

Z Index: 309

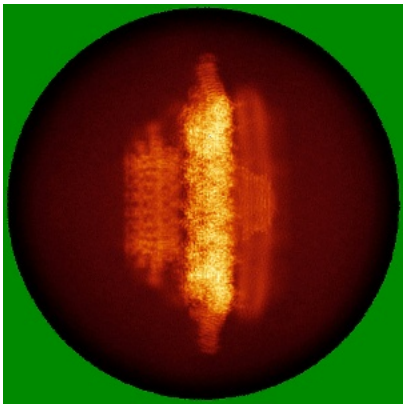
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

X

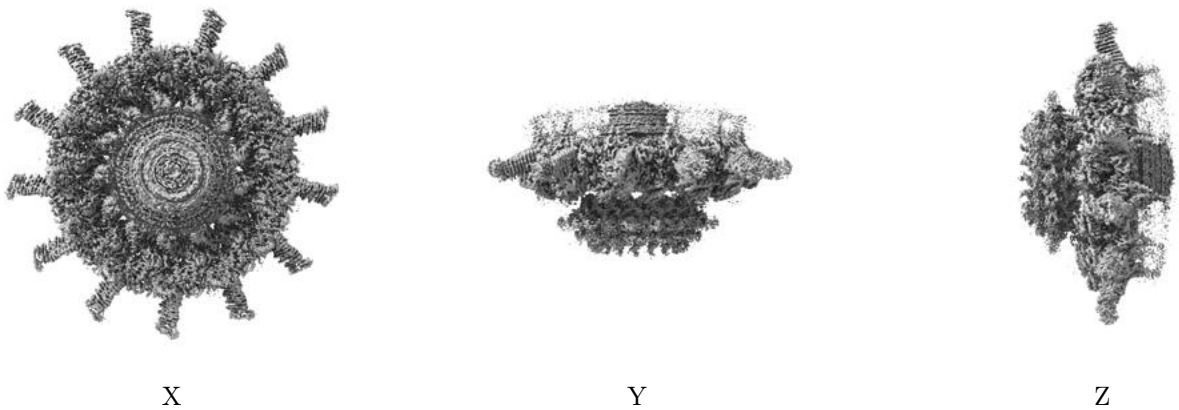

Y


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



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

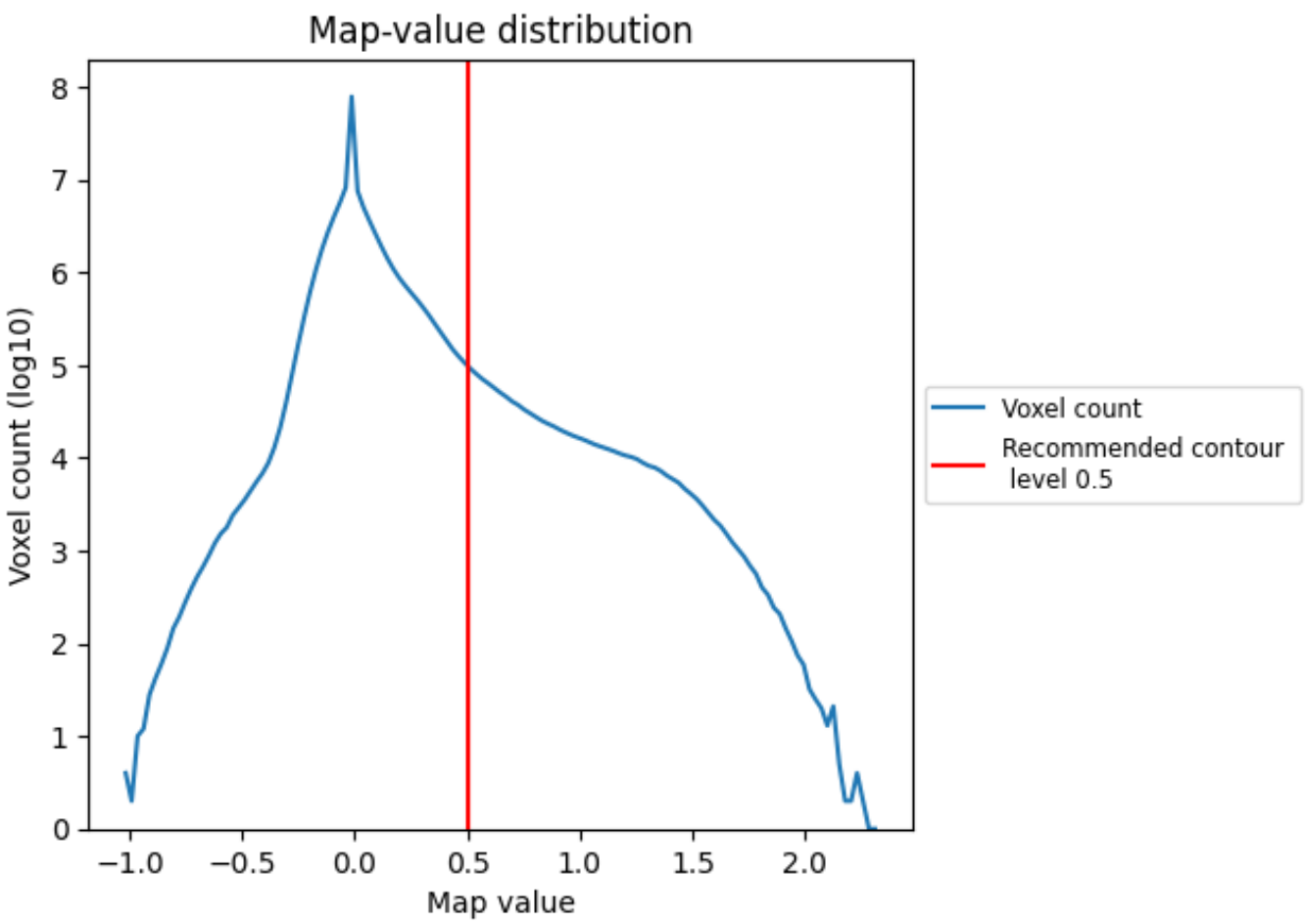
6.6 Mask visualisation (i)

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

7 Map analysis (i)

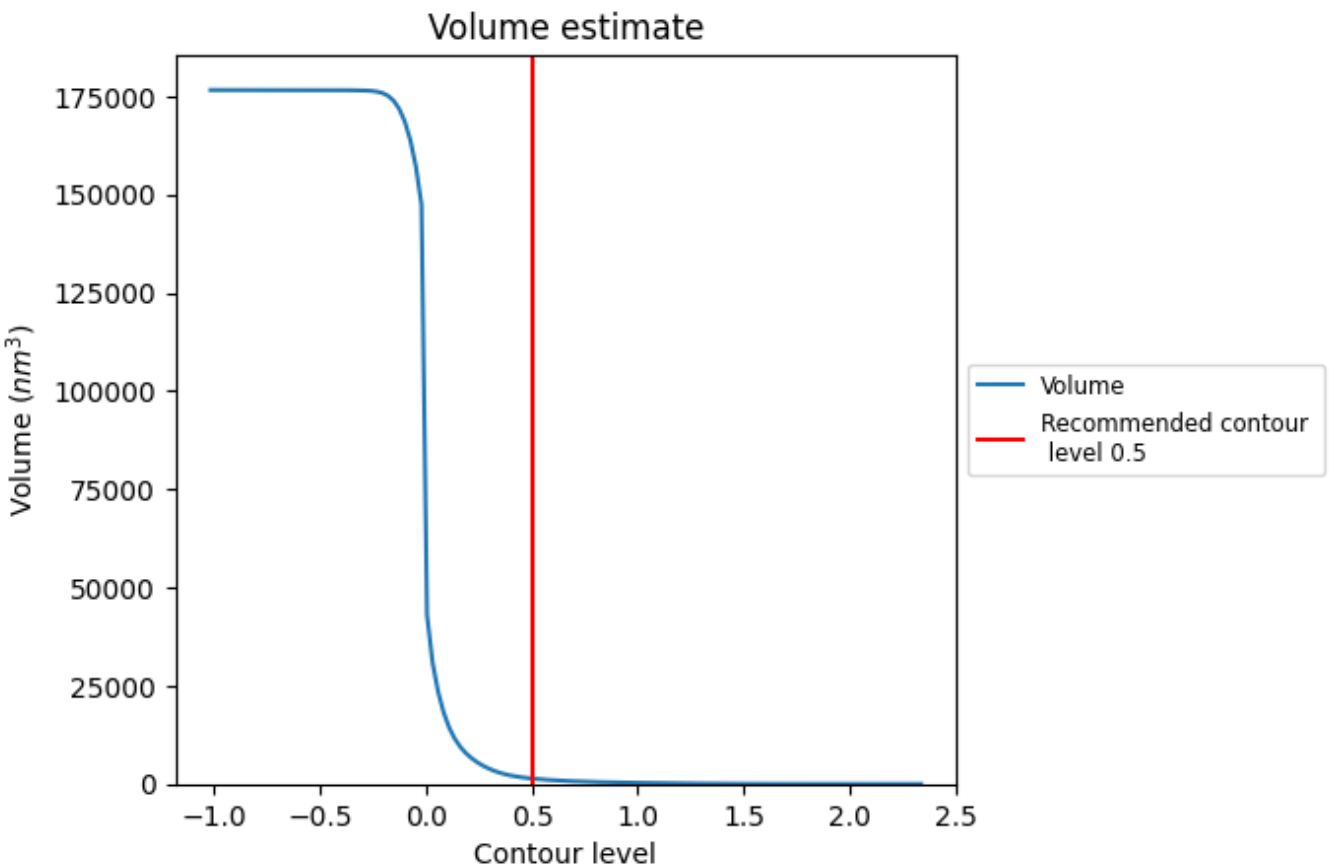
This section contains the results of statistical analysis of the map.

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.

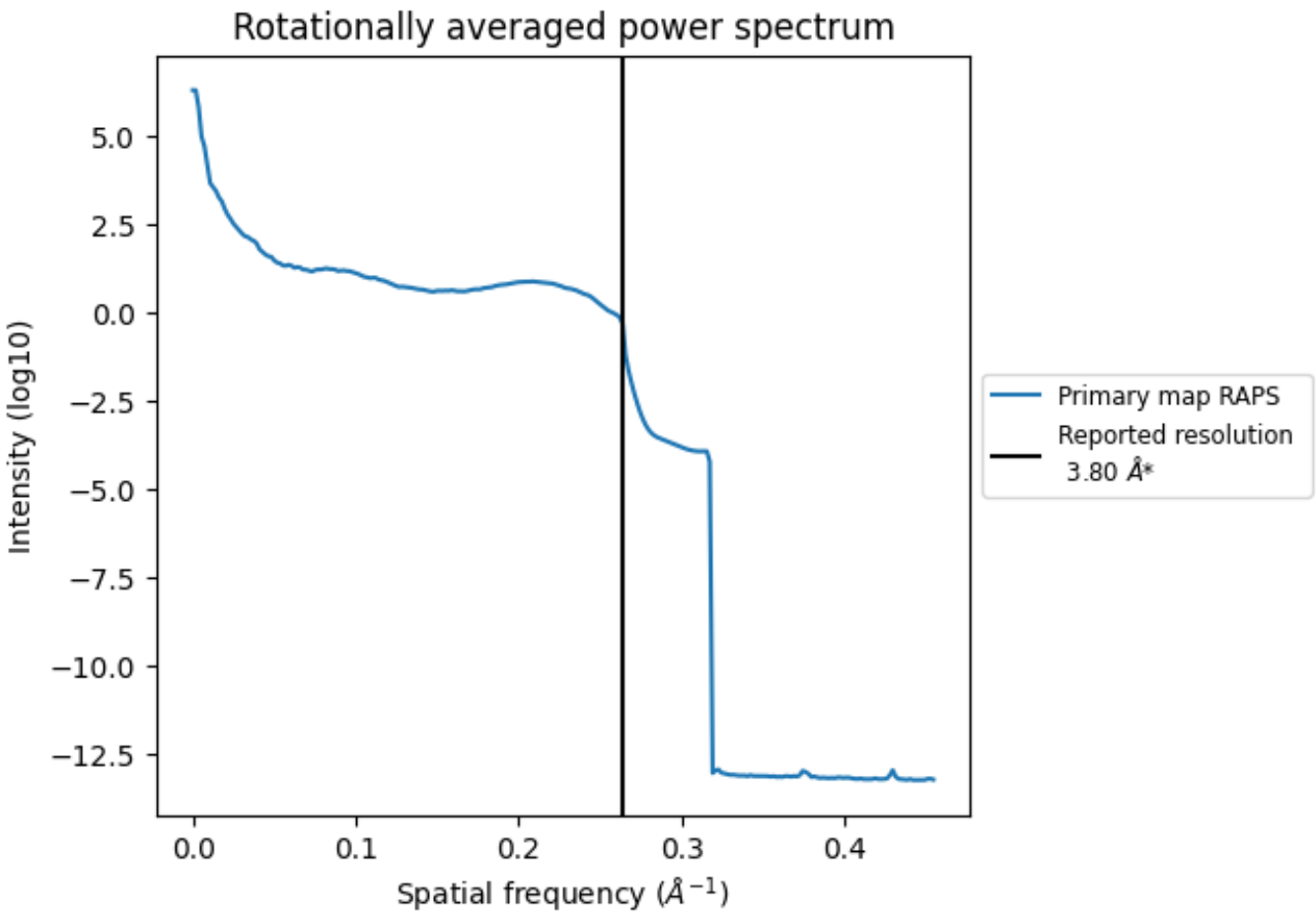
7.2 Volume estimate (i)



The volume at the recommended contour level is 1376 nm^3; this corresponds to an approximate mass of 1243 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 0.263 Å^{-1}

8 Fourier-Shell correlation (i)

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

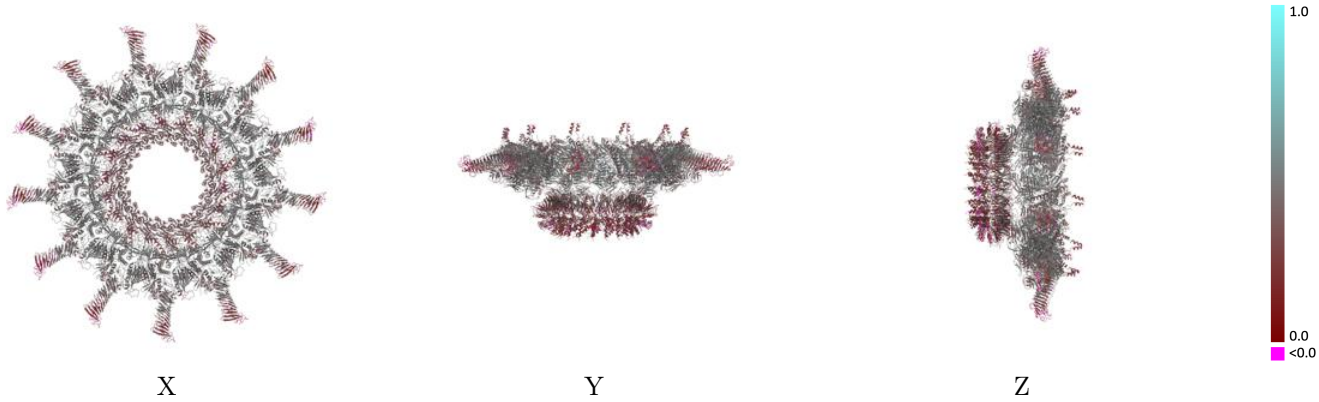
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24004 and PDB model 7MUC. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay (i)

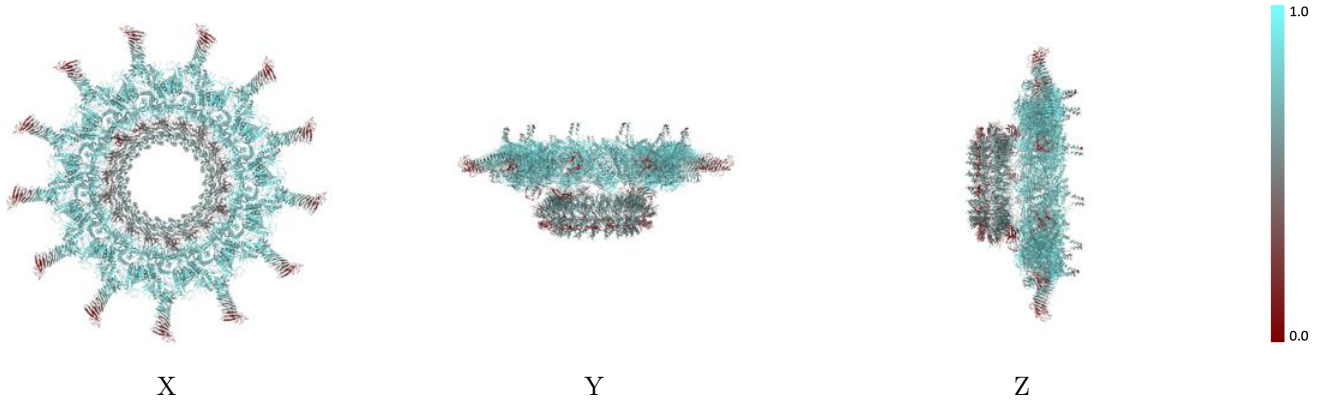
This section was not generated.

9.2 Q-score mapped to coordinate model (i)



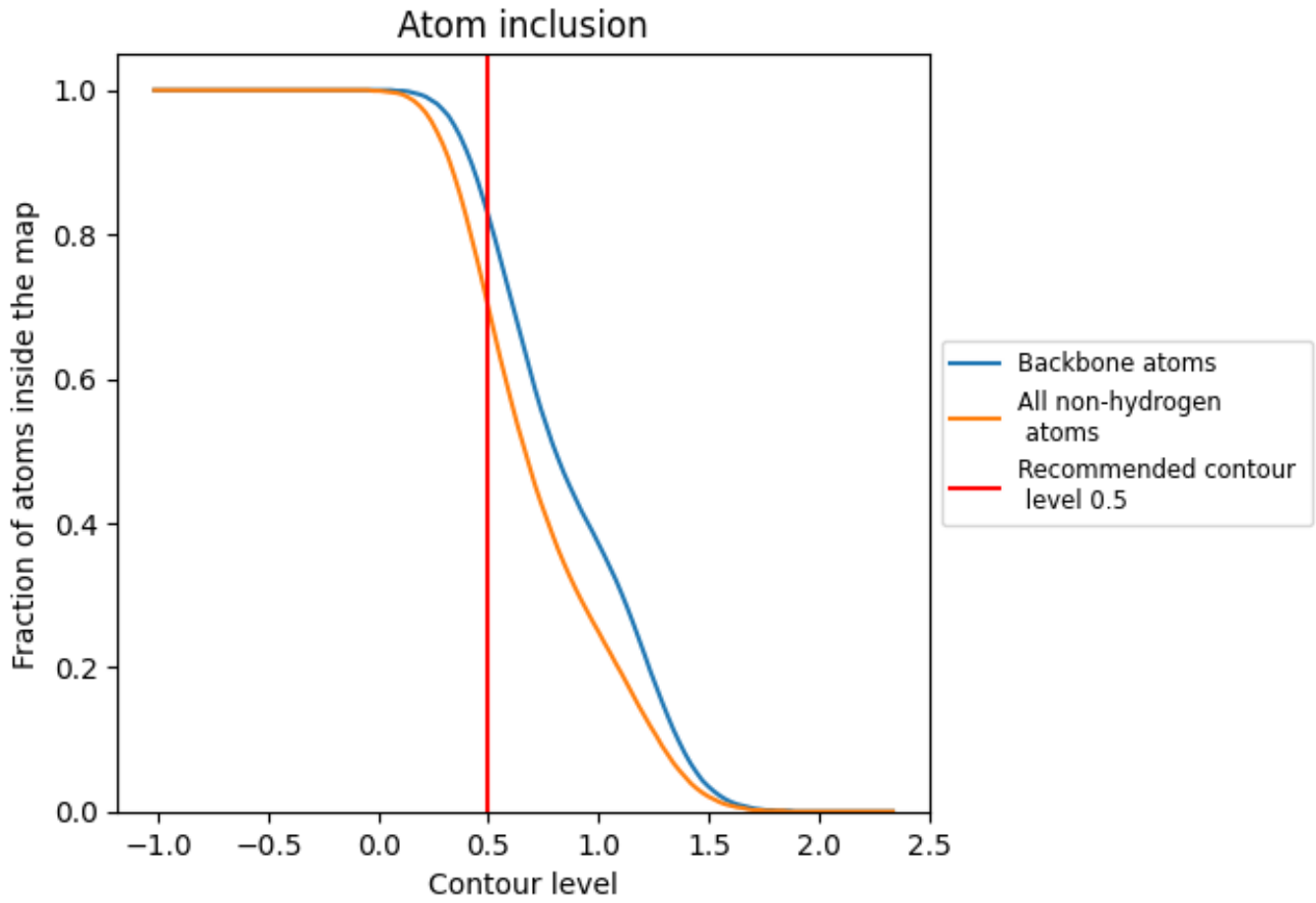
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.3930
AC	0.8190	0.4550
AD	0.8240	0.4650
AF	0.4500	0.1820
AG	0.6250	0.2810
AH	0.7010	0.3920
AK	0.8420	0.4630
AL	0.8060	0.4360
AM	0.5890	0.3380
AN	0.7550	0.4370
AU	0.9780	0.5100
AX	0.2000	0.1820
Ad	0.8210	0.4560
Af	0.6810	0.3970
BC	0.8200	0.4520
BD	0.8260	0.4700
BF	0.4500	0.2010
BG	0.5960	0.2570
BH	0.7030	0.3960
BK	0.8310	0.4620
BL	0.8020	0.4370
BM	0.5840	0.3440
BN	0.7740	0.4500
BU	0.9780	0.4820
BX	0.2460	0.1950
Bd	0.8180	0.4450
Bf	0.6950	0.4160
CC	0.8130	0.4560
CD	0.8070	0.4570
CF	0.4630	0.2440
CG	0.6140	0.2620
CH	0.7140	0.3900
CK	0.8270	0.4540
CL	0.7960	0.4250
CM	0.5760	0.3460

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Chain	Atom inclusion	Q-score
CN	0.7760	0.4520
CU	0.9560	0.4740
CX	0.2290	0.2120
Cd	0.8120	0.4340
Cf	0.6990	0.4220
DC	0.8190	0.4540
DD	0.8100	0.4530
DF	0.4500	0.2320
DG	0.6210	0.2840
DH	0.6940	0.3890
DK	0.8180	0.4550
DL	0.7780	0.4060
DM	0.5820	0.3490
DN	0.7660	0.4460
DU	0.9780	0.4920
DX	0.1880	0.1930
Dd	0.7940	0.4430
Df	0.6400	0.3980
EC	0.8050	0.4460
ED	0.8070	0.4580
EF	0.4250	0.2200
EG	0.6360	0.2780
EH	0.6890	0.3750
EK	0.8260	0.4550
EL	0.7920	0.4160
EM	0.5730	0.3520
EN	0.7640	0.4370
EU	0.9330	0.4800
EX	0.2420	0.2010
Ed	0.8130	0.4420
Ef	0.6700	0.4050
FC	0.8140	0.4510
FD	0.8170	0.4560
FF	0.4220	0.2120
FG	0.6210	0.2620
FH	0.6860	0.3820
FK	0.8230	0.4560
FL	0.7870	0.4180
FM	0.5760	0.3380
FN	0.7520	0.4420
FU	0.9780	0.4960
FX	0.1750	0.1330

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Chain	Atom inclusion	Q-score
Fd	0.8020	0.4400
Ff	0.6670	0.4050
GC	0.8220	0.4500
GD	0.8070	0.4550
GF	0.4290	0.2140
GG	0.6030	0.2800
GH	0.6920	0.3900
GK	0.8220	0.4580
GL	0.8030	0.4330
GM	0.5740	0.3360
GN	0.7660	0.4420
GU	1.0000	0.4930
GX	0.1380	0.1290
Gd	0.8120	0.4500
Gf	0.6720	0.4280
HC	0.8160	0.4510
HD	0.8140	0.4590
HF	0.4460	0.2430
HG	0.6030	0.2610
HH	0.7010	0.3910
HK	0.8270	0.4580
HL	0.8200	0.4290
HM	0.5780	0.3400
HN	0.7730	0.4470
HU	0.9780	0.4860
HX	0.2460	0.1990
Hd	0.7990	0.4530
Hf	0.6540	0.4050
IC	0.8060	0.4400
ID	0.8010	0.4520
IF	0.4690	0.2400
IG	0.5880	0.2820
IH	0.6970	0.3920
IK	0.8150	0.4440
IL	0.8020	0.4310
IM	0.5610	0.3410
IN	0.7600	0.4540
IU	0.9330	0.4920
IX	0.2080	0.1450
Id	0.7900	0.4370
If	0.6900	0.4050
JC	0.8020	0.4300

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Chain	Atom inclusion	Q-score
JD	0.8080	0.4530
JF	0.4610	0.2370
JG	0.5440	0.2460
JH	0.7090	0.3910
JK	0.8150	0.4500
JL	0.8010	0.4270
JM	0.5790	0.3450
JN	0.7660	0.4470
JU	0.9780	0.5140
JX	0.1960	0.2150
Jd	0.8140	0.4430
Jf	0.6720	0.4180
KC	0.8100	0.4390
KD	0.8160	0.4540
KF	0.5010	0.2500
KG	0.5810	0.2350
KH	0.6990	0.3820
KK	0.8210	0.4490
KL	0.8070	0.4250
KM	0.5820	0.3400
KN	0.7710	0.4510
KU	0.9330	0.5000
KX	0.2710	0.2290
Kd	0.8030	0.4480
Kf	0.6930	0.4170
LC	0.8160	0.4490
LD	0.8170	0.4600
LF	0.4780	0.2500
LG	0.5920	0.2450
LH	0.6940	0.3830
LK	0.8320	0.4530
LL	0.8080	0.4230
LM	0.6000	0.3570
LN	0.7810	0.4580
LU	0.8890	0.4570
LX	0.2120	0.2290
Ld	0.8210	0.4480
Lf	0.6970	0.4160
MC	0.8250	0.4510
MD	0.8140	0.4600
MF	0.4670	0.2240
MG	0.6030	0.2910

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Chain	Atom inclusion	Q-score
MH	0.7230	0.4020
MK	0.8300	0.4590
ML	0.8120	0.4330
MM	0.6080	0.3410
MN	0.7730	0.4500
MU	0.9560	0.4940
MX	0.2250	0.2070
Md	0.8130	0.4450
Mf	0.6810	0.4110
VF	0.4710	0.2340
VG	0.5920	0.2670
VH	0.5600	0.3600
VX	0.2630	0.2330
WF	0.4120	0.1920
WG	0.6100	0.2230
WH	0.4280	0.3360
WX	0.1750	0.1610
XF	0.4520	0.2420
XG	0.6100	0.2740
XH	0.5640	0.3700
XX	0.1960	0.1580
YF	0.4800	0.2430
YG	0.6180	0.2900
YH	0.5060	0.3500
YX	0.2290	0.2210
ZF	0.4310	0.2010
ZG	0.5880	0.2450
ZH	0.4770	0.3490
ZX	0.2170	0.2010