wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 09:15 AM UTC

PDB ID	:	6X66 / pdb_00006x66
EMDB ID	:	EMD-22071
Title	:	Legionella pneumophila dDot T4SS OMC
Authors	:	Durie, C.L.; Sheedlo, M.J.; Chung, J.M.; Byrne, B.G.; Su, M.; Knight, T.; Swanson, M.S.; Lacy, D.B.; Ohi, M.D.
Deposited on	:	2020-05-27
Resolution	:	4.20 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 ⓘ symbol.

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

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

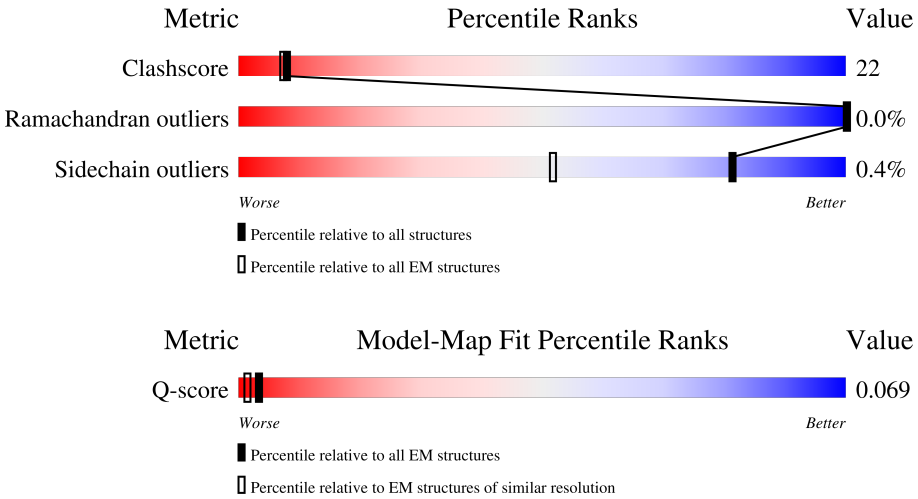
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 4.20 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	5410 (3.70 - 4.70)

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	24% 40% · 34%
1	BC	303	23% 41% · 34%
1	CC	303	23% 41% · 34%
1	DC	303	25% 40% · 34%

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Mol	Chain	Length	Quality of chain
1	EC	303	25% 40% 34%
1	FC	303	23% 42% 34%
1	GC	303	23% 41% 34%
1	HC	303	24% 40% 34%
1	IC	303	25% 40% 34%
1	JC	303	26% 39% 34%
1	KC	303	24% 40% 34%
1	LC	303	22% 42% 34%
1	MC	303	23% 42% 34%
2	AD	163	57% 26% 17%
2	Ad	163	48% 36% 15%
2	BD	163	56% 26% 17%
2	Bd	163	47% 37% 15%
2	CD	163	55% 28% 17%
2	Cd	163	55% 28% 15%
2	DD	163	60% 23% 17%
2	Dd	163	51% 33% 15%
2	ED	163	55% 27% 17%
2	Ed	163	44% 41% 15%
2	FD	163	55% 28% 17%
2	Fd	163	50% 33% 15%
2	GD	163	58% 24% 17%
2	Gd	163	53% 30% 15%
2	HD	163	47% 36% 17%
2	Hd	163	50% 35% 15%

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Mol	Chain	Length	Quality of chain
2	ID	163	56% 26% 17%
2	Id	163	47% 36% 15%
2	JD	163	55% 28% 17%
2	Jd	163	50% 34% 15%
2	KD	163	61% 22% 17%
2	Kd	163	53% 31% 15%
2	LD	163	54% 28% 17%
2	Ld	163	49% 34% 15%
2	MD	163	57% 25% 17%
2	Md	163	53% 32% 15%
3	AH	361	11% 14% 75%
3	BH	361	10% 14% 75%
3	CH	361	10% 15% 75%
3	DH	361	10% 14% 75%
3	EH	361	11% 14% 75%
3	FH	361	10% 15% 75%
3	GH	361	10% 15% 75%
3	HH	361	9% 15% 75%
3	IH	361	9% 15% 75%
3	JH	361	9% 16% 75%
3	KH	361	9% 15% 75%
3	LH	361	10% 15% 75%
3	MH	361	10% 15% 75%
4	AK	189	44% 33% 22%
4	BK	189	45% 32% 22%

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Mol	Chain	Length	Quality of chain
4	CK	189	42% 35% 22%
4	DK	189	44% 33% 22%
4	EK	189	45% 32% 22%
4	FK	189	46% 31% 22%
4	GK	189	43% 34% 22%
4	HK	189	43% 34% 22%
4	IK	189	42% 35% 22%
4	JK	189	45% 33% 22%
4	KK	189	46% 32% 22%
4	LK	189	44% 34% 22%
4	MK	189	43% 34% 22%
5	AX	330	61% 8% 31%
5	AY	330	6% 14% 84%
5	AZ	330	16% 5% 79%
5	BX	330	61% 8% 31%
5	BY	330	5% 14% 84%
5	BZ	330	16% 5% 79%
5	CX	330	61% 8% 31%
5	CY	330	6% 14% 84%
5	CZ	330	16% 5% 79%
5	DX	330	61% 8% 31%
5	DY	330	5% 15% 84%
5	DZ	330	15% 6% 79%
5	EX	330	61% 8% 31%
5	EY	330	5% 14% 84%

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Mol	Chain	Length	Quality of chain
5	EZ	330	16% 5% 79%
5	FX	330	61% 8% 31%
5	FY	330	14% 84%
5	FZ	330	16% 5% 79%
5	GX	330	61% 8% 31%
5	GY	330	5% 14% 84%
5	GZ	330	16% 5% 79%
5	HX	330	61% 8% 31%
5	HY	330	14% 84%
5	HZ	330	15% 6% 79%
5	IX	330	61% 8% 31%
5	IY	330	14% 84%
5	IZ	330	16% 5% 79%
5	JX	330	61% 8% 31%
5	JY	330	5% 14% 84%
5	JZ	330	16% 5% 79%
5	KX	330	61% 8% 31%
5	KY	330	7% 14% 84%
5	KZ	330	15% 6% 79%
5	LX	330	61% 8% 31%
5	LY	330	6% 15% 84%
5	LZ	330	16% 5% 79%
5	MX	330	61% 8% 31%
5	MY	330	6% 15% 84%
5	MZ	330	16% 5% 79%

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Mol	Chain	Length	Quality of chain
6	AA	249	31% 24% 45%
6	BA	249	31% 24% 45%
6	CA	249	31% 24% 45%
6	DA	249	30% 25% 45%
6	EA	249	31% 24% 45%
6	FA	249	30% 24% 45%
6	GA	249	31% 24% 45%
6	HA	249	31% 24% 45%
6	IA	249	30% 24% 45%
6	JA	249	31% 23% 45%
6	KA	249	29% 25% 45%
6	LA	249	31% 24% 45%
6	QA	249	30% 25% 45%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 109070 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
1	AC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	BC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	CC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	DC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	EC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	FC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	GC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	HC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	IC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	JC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	KC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	LC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		
1	MC	200	Total	C	N	O	S	0	0
			1596	1016	280	295	5		

- Molecule 2 is a protein called DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Ad	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Bd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	CD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Cd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	DD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Dd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	ED	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Ed	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	FD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Fd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	GD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Gd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	HD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Hd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	ID	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Id	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	JD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Jd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	KD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Kd	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	LD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ld	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		
2	MD	135	Total	C	N	O	S	0	0
			1040	660	178	200	2		
2	Md	138	Total	C	N	O	S	0	0
			1066	678	183	203	2		

- Molecule 3 is a protein called Type IV secretion protein IcmK.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	BH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	CH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	DH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	EH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	FH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	GH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	HH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	IH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	JH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	KH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	LH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		
3	MH	89	Total	C	N	O	S	0	0
			678	432	119	123	4		

- Molecule 4 is a protein called Inner membrane lipoprotein YiaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	BK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	CK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	DK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	EK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	FK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	GK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	HK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	IK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	JK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	KK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	LK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		
4	MK	148	Total	C	N	O	S	0	0
			1152	731	205	212	4		

- Molecule 5 is a protein called Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	AY	52	Total	C	N	O	0	0
			260	156	52	52		
5	AZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	BX	228	Total	C	N	O	0	0
			1140	684	228	228		
5	BY	52	Total	C	N	O	0	0
			260	156	52	52		
5	BZ	70	Total	C	N	O	0	0
			350	210	70	70		
5	CX	228	Total	C	N	O	0	0
			1140	684	228	228		

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Mol	Chain	Residues	Atoms	AltConf	Trace
5	CY	52	Total C N O 260 156 52 52	0	0
5	CZ	70	Total C N O 350 210 70 70	0	0
5	DX	228	Total C N O 1140 684 228 228	0	0
5	DY	52	Total C N O 260 156 52 52	0	0
5	DZ	70	Total C N O 350 210 70 70	0	0
5	EX	228	Total C N O 1140 684 228 228	0	0
5	EY	52	Total C N O 260 156 52 52	0	0
5	EZ	70	Total C N O 350 210 70 70	0	0
5	FX	228	Total C N O 1140 684 228 228	0	0
5	FY	52	Total C N O 260 156 52 52	0	0
5	FZ	70	Total C N O 350 210 70 70	0	0
5	GX	228	Total C N O 1140 684 228 228	0	0
5	GY	52	Total C N O 260 156 52 52	0	0
5	GZ	70	Total C N O 350 210 70 70	0	0
5	HX	228	Total C N O 1140 684 228 228	0	0
5	HY	52	Total C N O 260 156 52 52	0	0
5	HZ	70	Total C N O 350 210 70 70	0	0
5	IX	228	Total C N O 1140 684 228 228	0	0
5	IY	52	Total C N O 260 156 52 52	0	0
5	IZ	70	Total C N O 350 210 70 70	0	0
5	JX	228	Total C N O 1140 684 228 228	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
5	JY	52	Total C N O 260 156 52 52	0	0
5	JZ	70	Total C N O 350 210 70 70	0	0
5	KX	228	Total C N O 1140 684 228 228	0	0
5	KY	52	Total C N O 260 156 52 52	0	0
5	KZ	70	Total C N O 350 210 70 70	0	0
5	LX	228	Total C N O 1140 684 228 228	0	0
5	LY	52	Total C N O 260 156 52 52	0	0
5	LZ	70	Total C N O 350 210 70 70	0	0
5	MX	228	Total C N O 1140 684 228 228	0	0
5	MY	52	Total C N O 260 156 52 52	0	0
5	MZ	70	Total C N O 350 210 70 70	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
6	AA	136	Total C N O S 1108 701 201 202 4	0	0
6	BA	136	Total C N O S 1108 701 201 202 4	0	0
6	CA	136	Total C N O S 1108 701 201 202 4	0	0
6	DA	136	Total C N O S 1108 701 201 202 4	0	0
6	EA	136	Total C N O S 1108 701 201 202 4	0	0
6	FA	136	Total C N O S 1108 701 201 202 4	0	0
6	GA	136	Total C N O S 1108 701 201 202 4	0	0
6	HA	136	Total C N O S 1108 701 201 202 4	0	0

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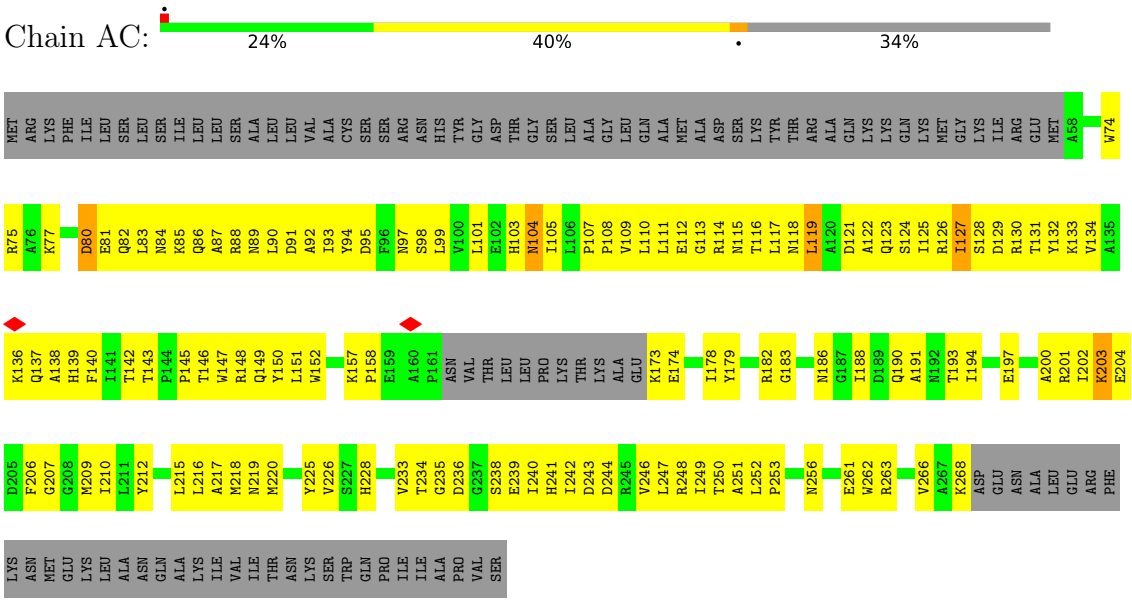
Mol	Chain	Residues	Atoms					AltConf	Trace
6	IA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	JA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	KA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	LA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		
6	QA	136	Total	C	N	O	S	0	0
			1108	701	201	202	4		

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.

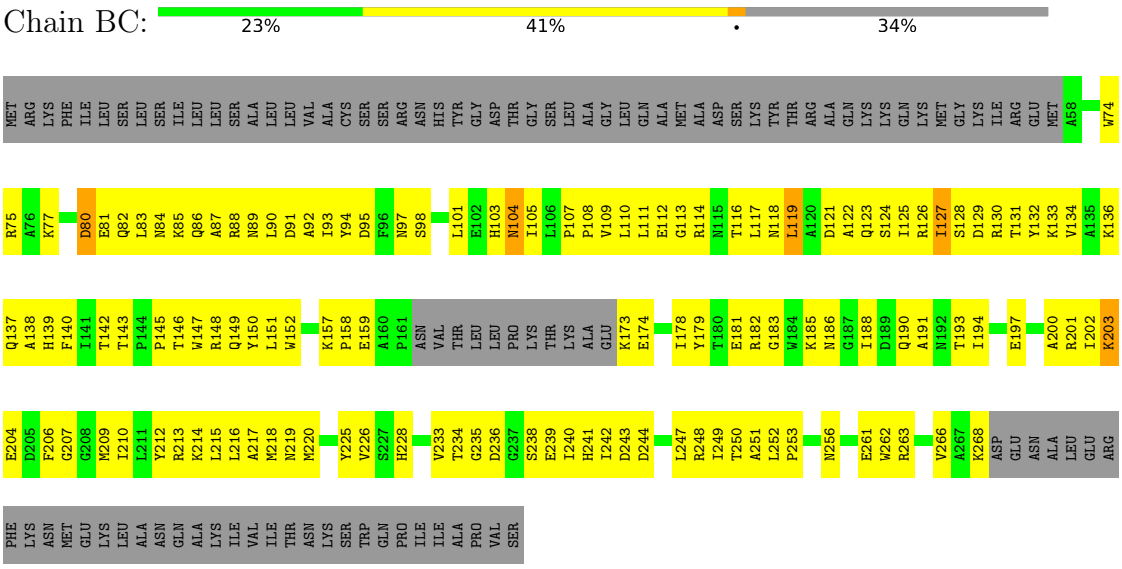
• Molecule 1: DotC

Chain AC:



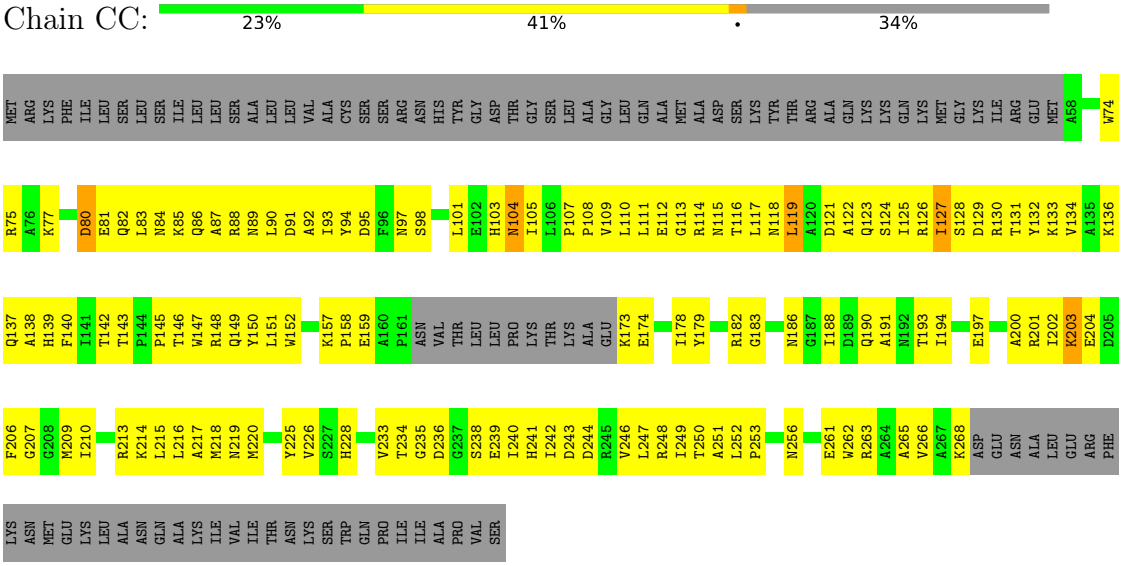
• Molecule 1: DotC

Chain BC:



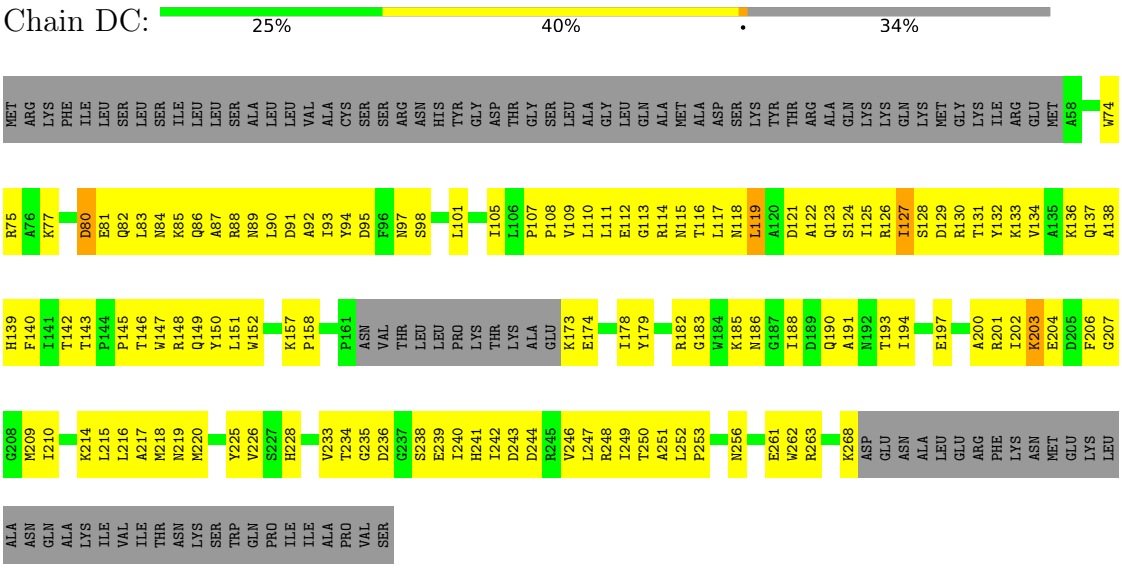
- Molecule 1: DotC

Chain CC:



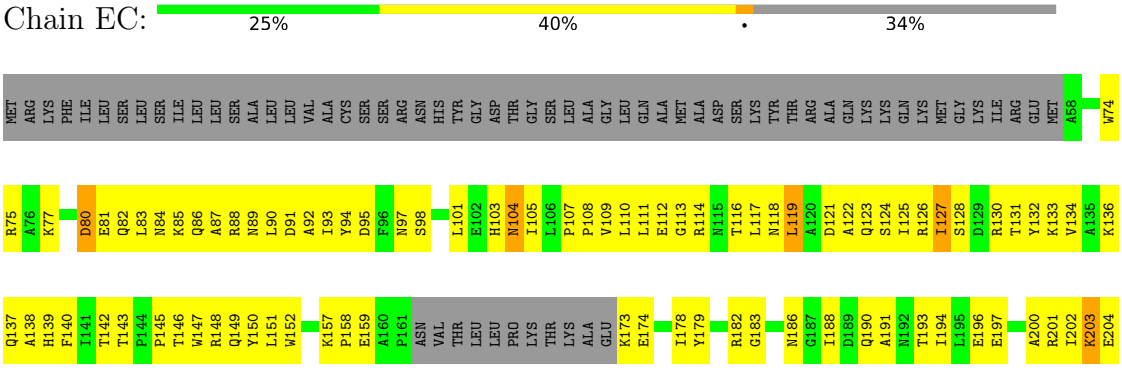
- Molecule 1: DotC

Chain DC:



- Molecule 1: DotC

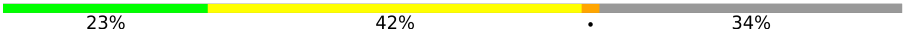
Chain EC:





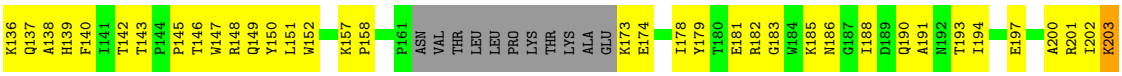
• Molecule 1: DotC

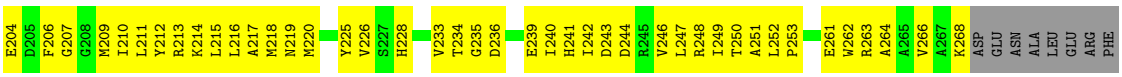
Chain FC:

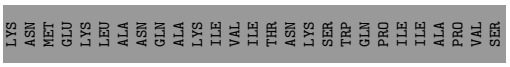












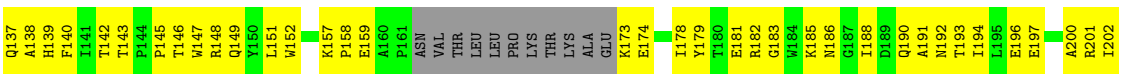
• Molecule 1: DotC

Chain GC:

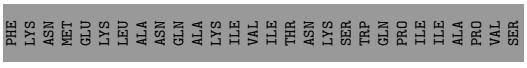










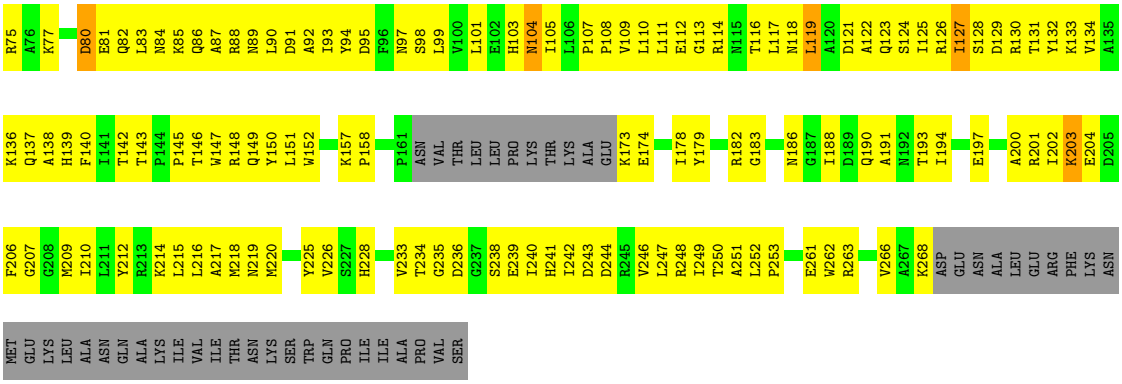


• Molecule 1: DotC

Chain HC:

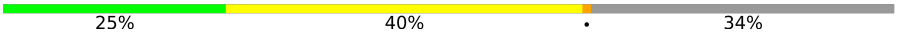


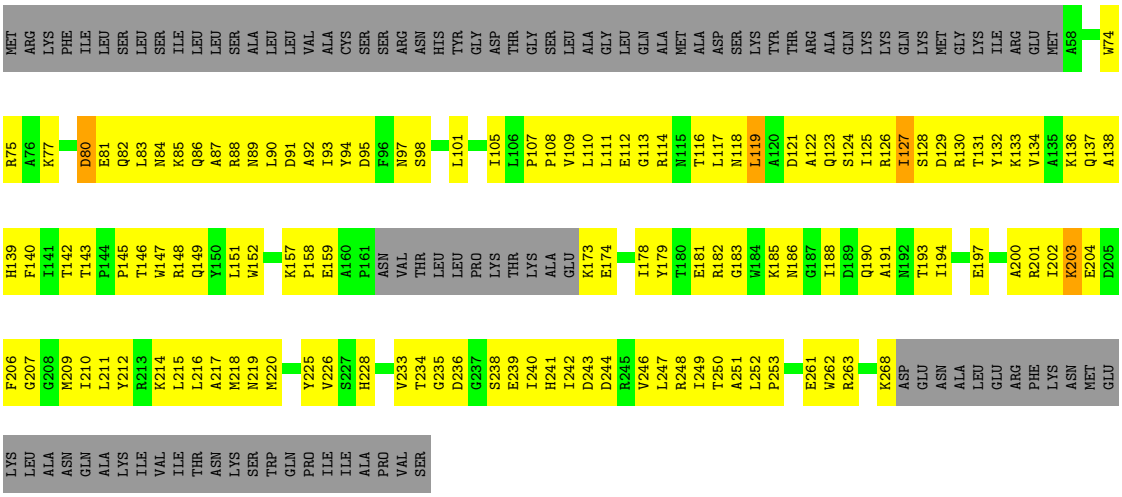




- Molecule 1: DotC

Chain IC:

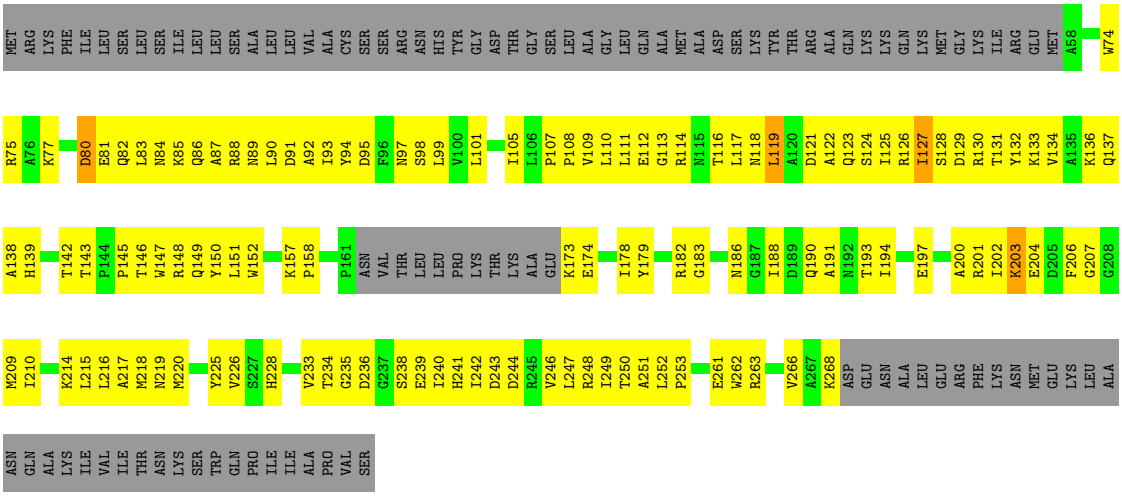




- Molecule 1: DotC

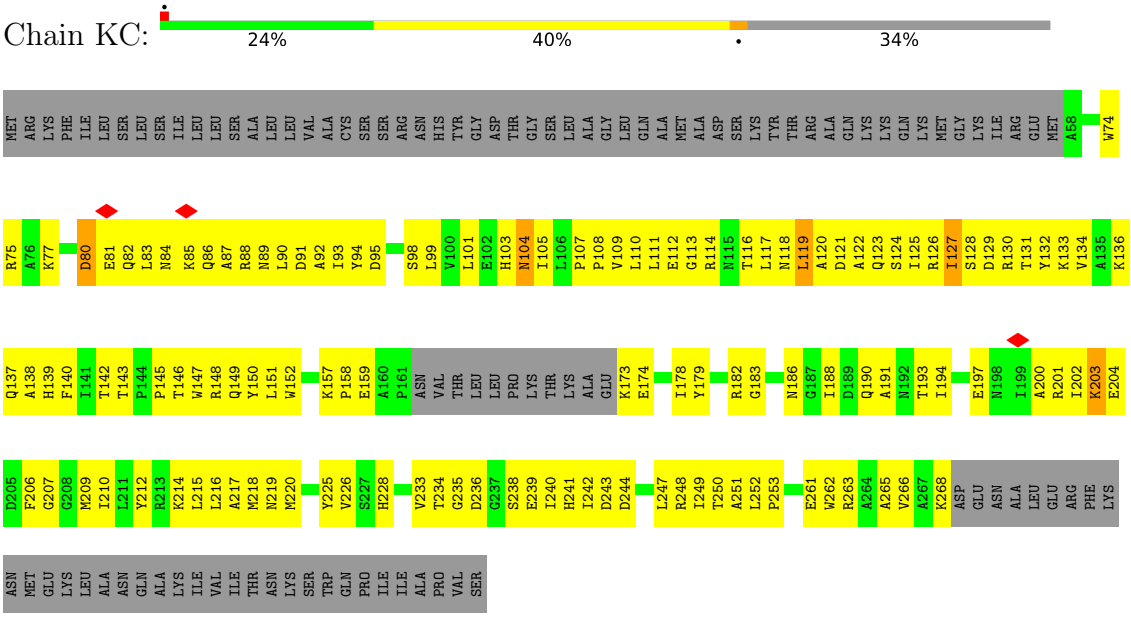
Chain JC:





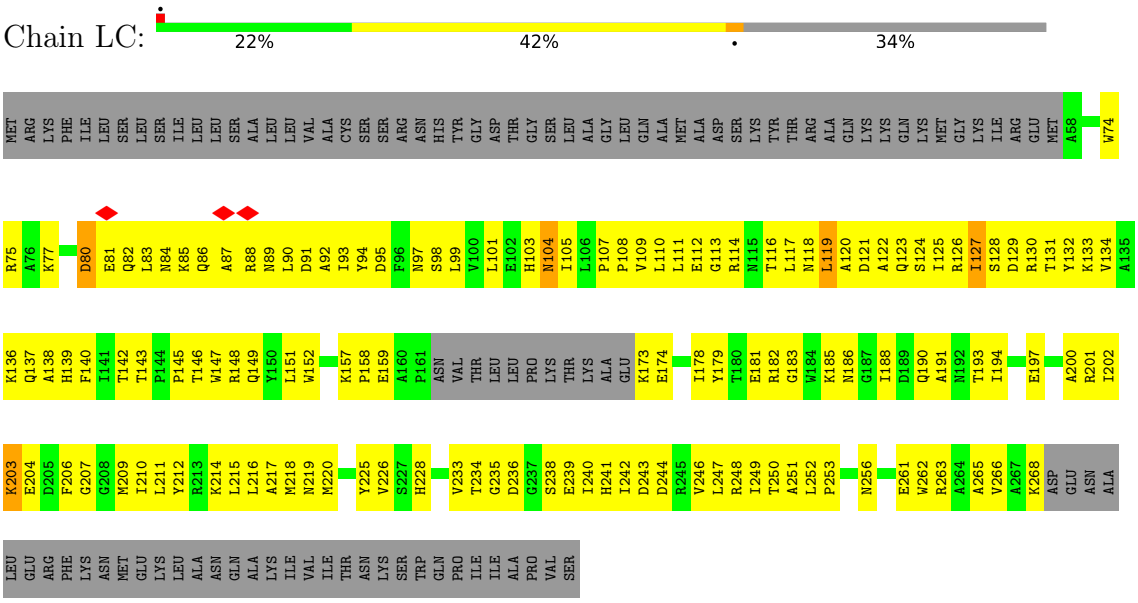
- Molecule 1: DotC

Chain KC:



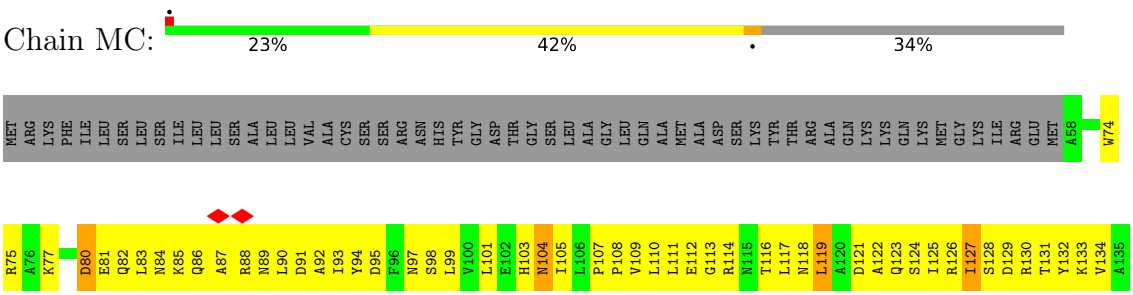
• Molecule 1: DotC

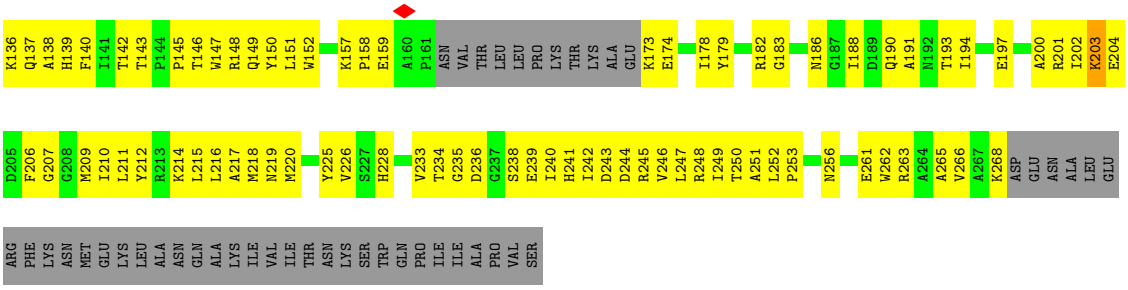
Chain LC:



• Molecule 1: DotC

Chain MC:

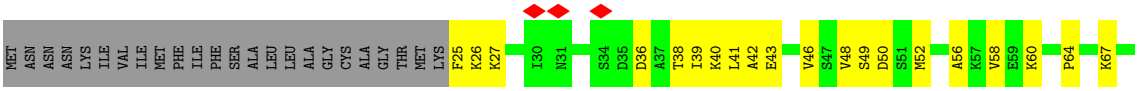




• Molecule 2: DotD

Chain AD:



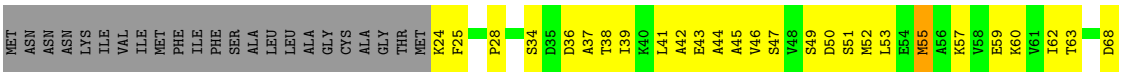


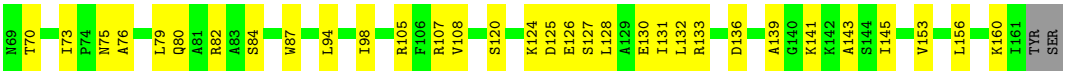


• Molecule 2: DotD

Chain Ad:



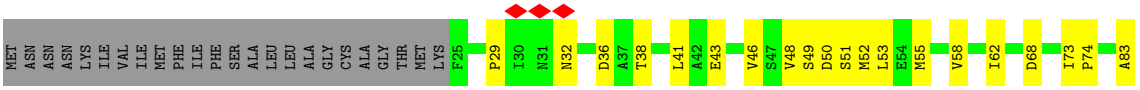


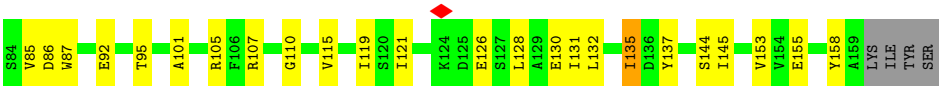


• Molecule 2: DotD

Chain BD:

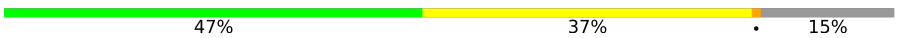


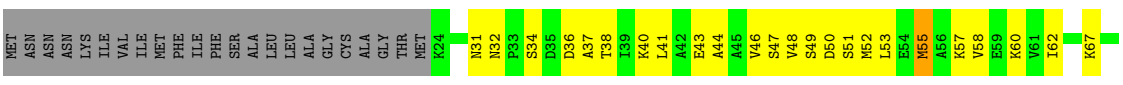




• Molecule 2: DotD

Chain Bd:



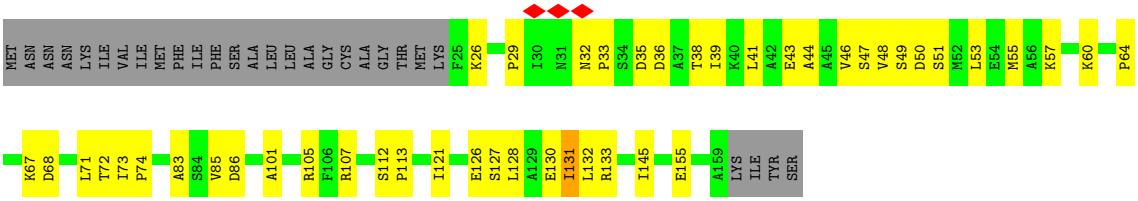




• Molecule 2: DotD

Chain CD:

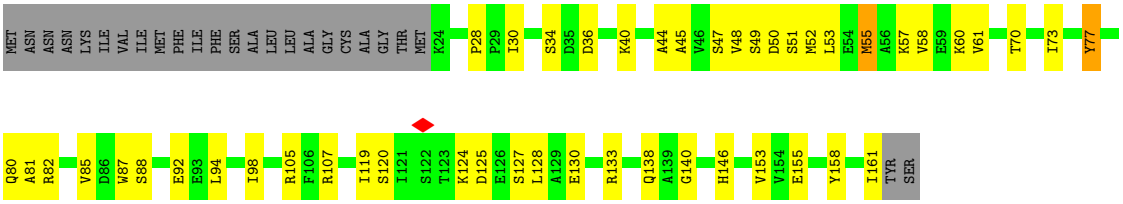




• Molecule 2: DotD

Chain Cd:

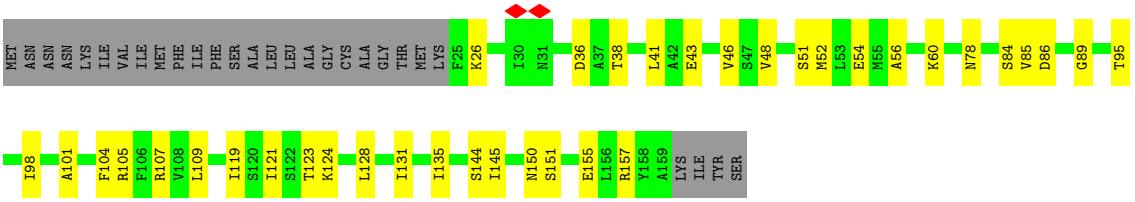




• Molecule 2: DotD

Chain DD:

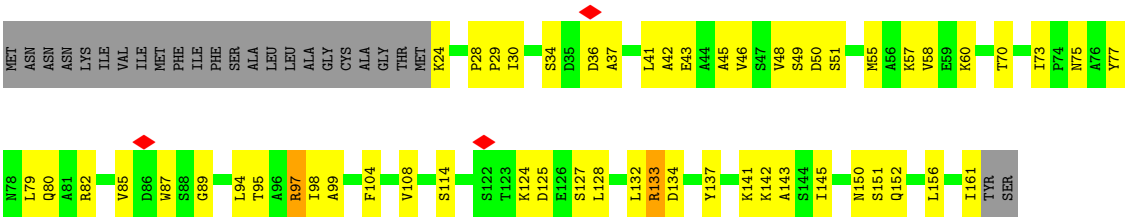




• Molecule 2: DotD

Chain Dd:

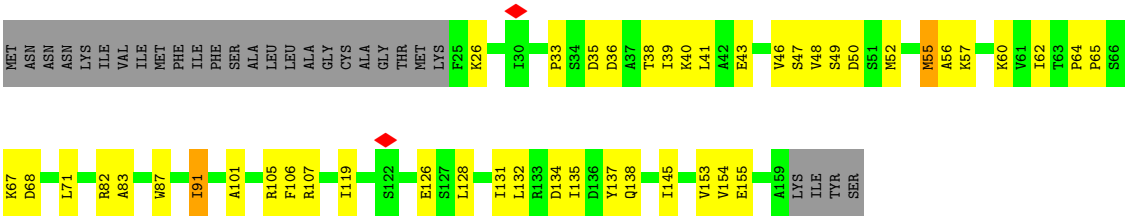




• Molecule 2: DotD

Chain ED:

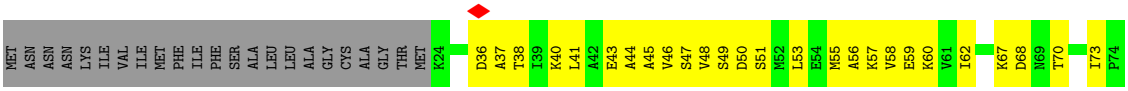


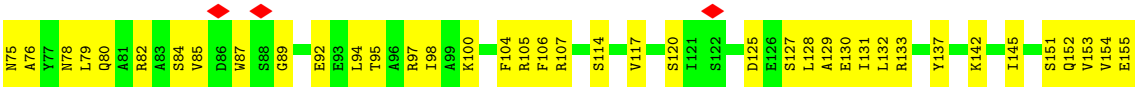


• Molecule 2: DotD

Chain Ed:





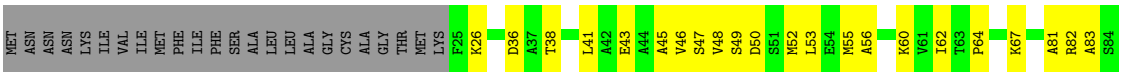


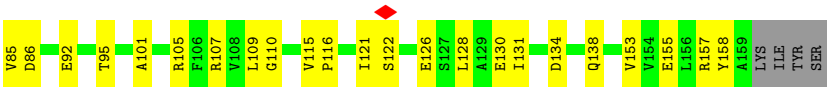


• Molecule 2: DotD

Chain FD:



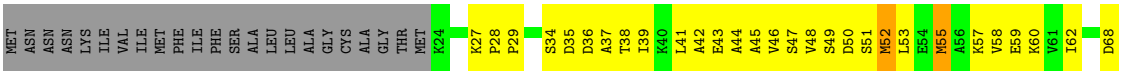


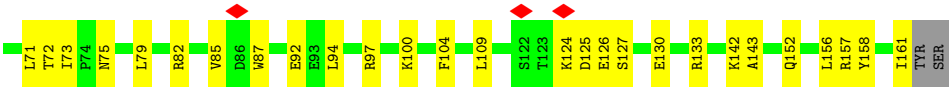


• Molecule 2: DotD

Chain Fd:



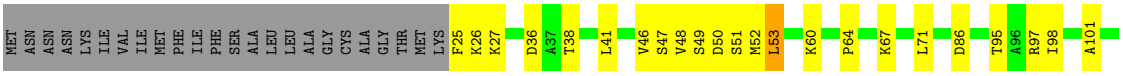




• Molecule 2: DotD

Chain GD:





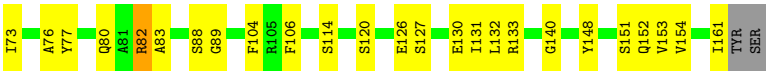


• Molecule 2: DotD

Chain Gd:

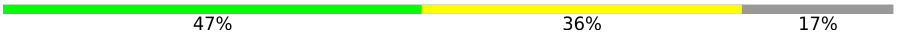


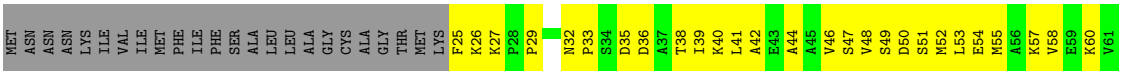




• Molecule 2: DotD

Chain HD:



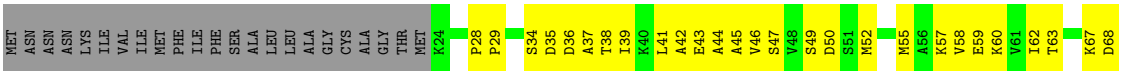




• Molecule 2: DotD

Chain Hd:



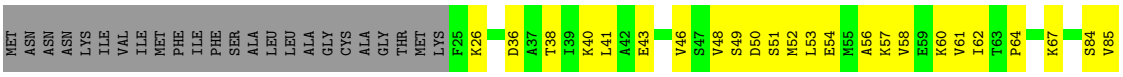




• Molecule 2: DotD

Chain ID:

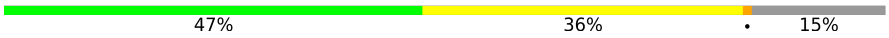


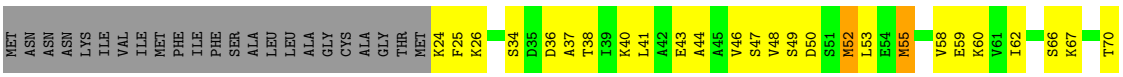


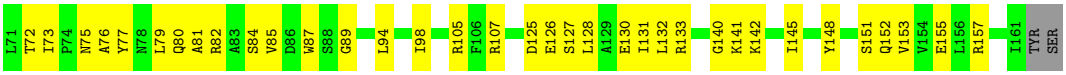


• Molecule 2: DotD

Chain Id:



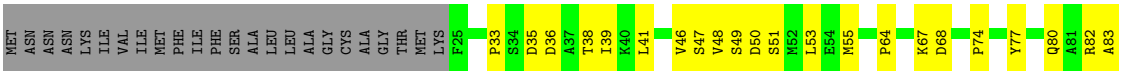




• Molecule 2: DotD

Chain JD:



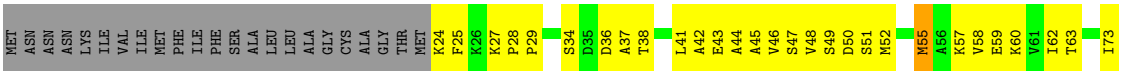


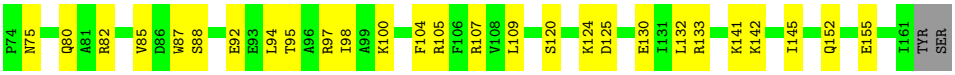


• Molecule 2: DotD

Chain Jd:



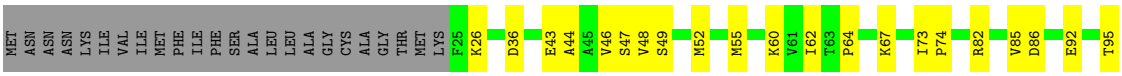




• Molecule 2: DotD

Chain KD:



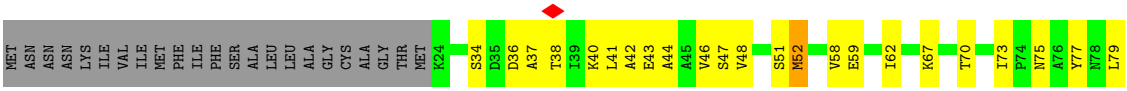




• Molecule 2: DotD

Chain Kd:



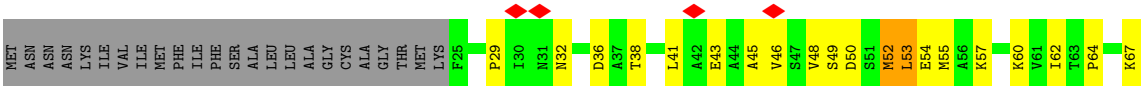




• Molecule 2: DotD

Chain LD:



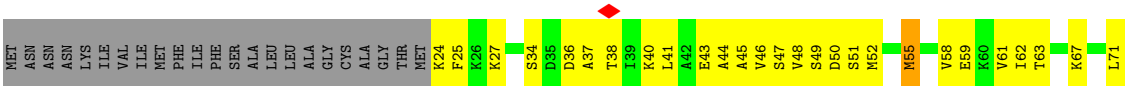




• Molecule 2: DotD

Chain Ld:



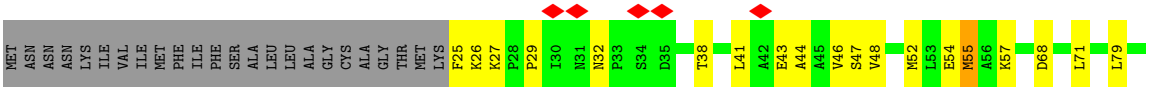


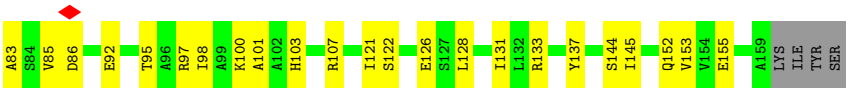


• Molecule 2: DotD

Chain MD:







• Molecule 2: DotD

Chain Md:



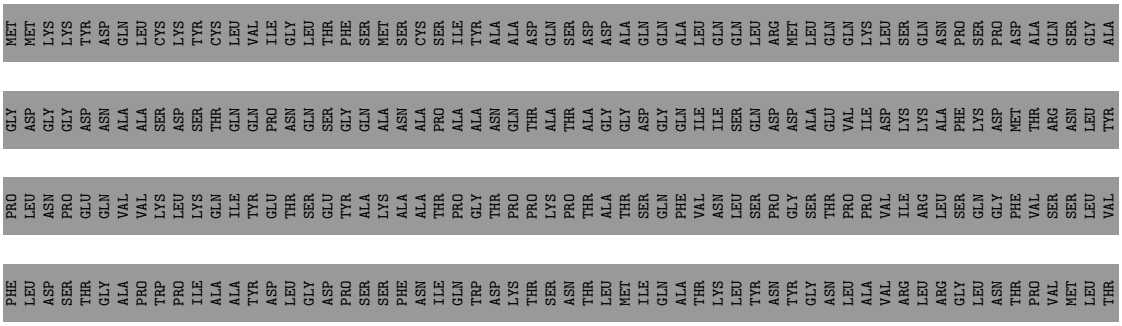




• Molecule 3: Type IV secretion protein IcmK

Chain AH:



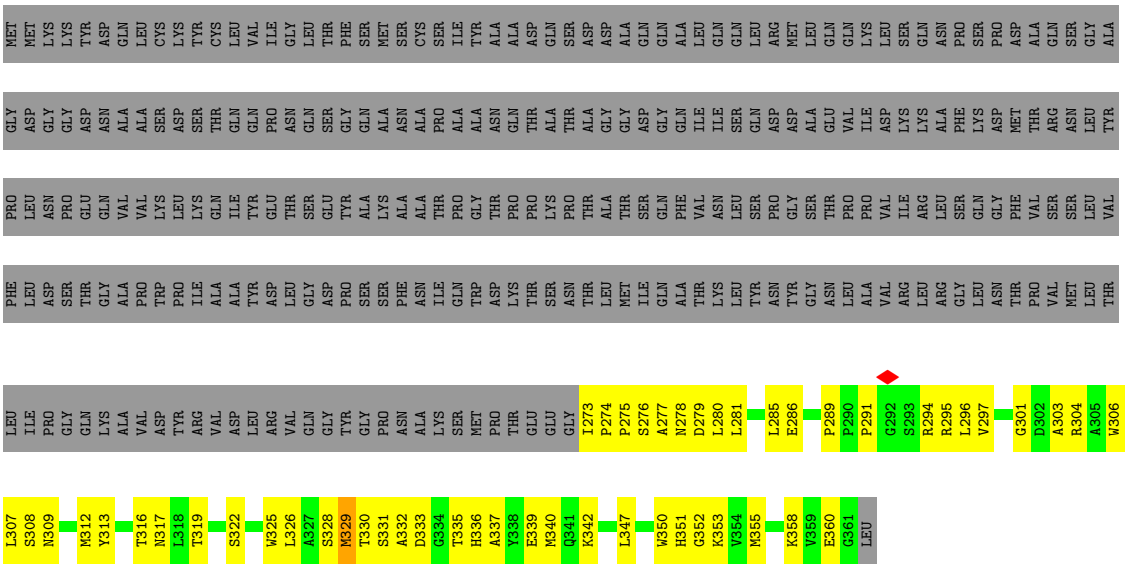




• Molecule 3: Type IV secretion protein IcmK

Chain BH:

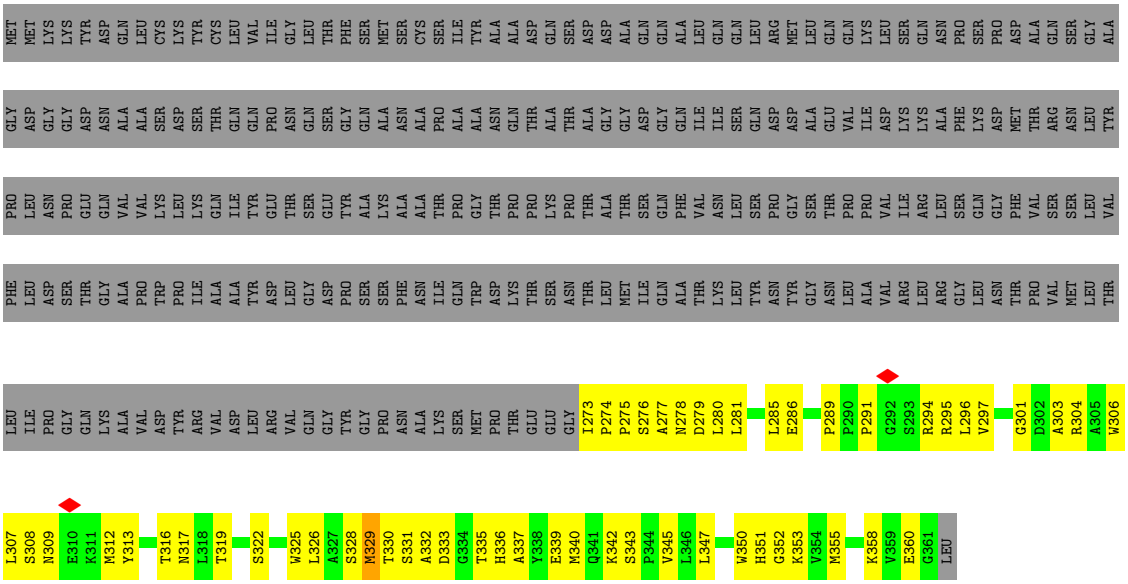




• Molecule 3: Type IV secretion protein IcmK

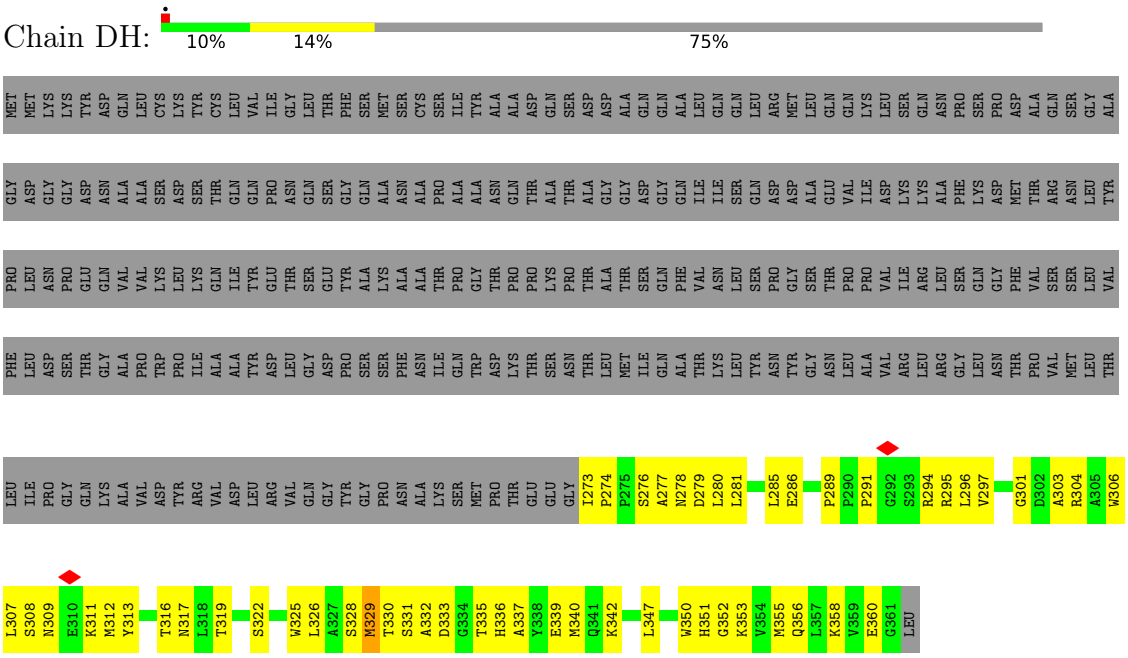
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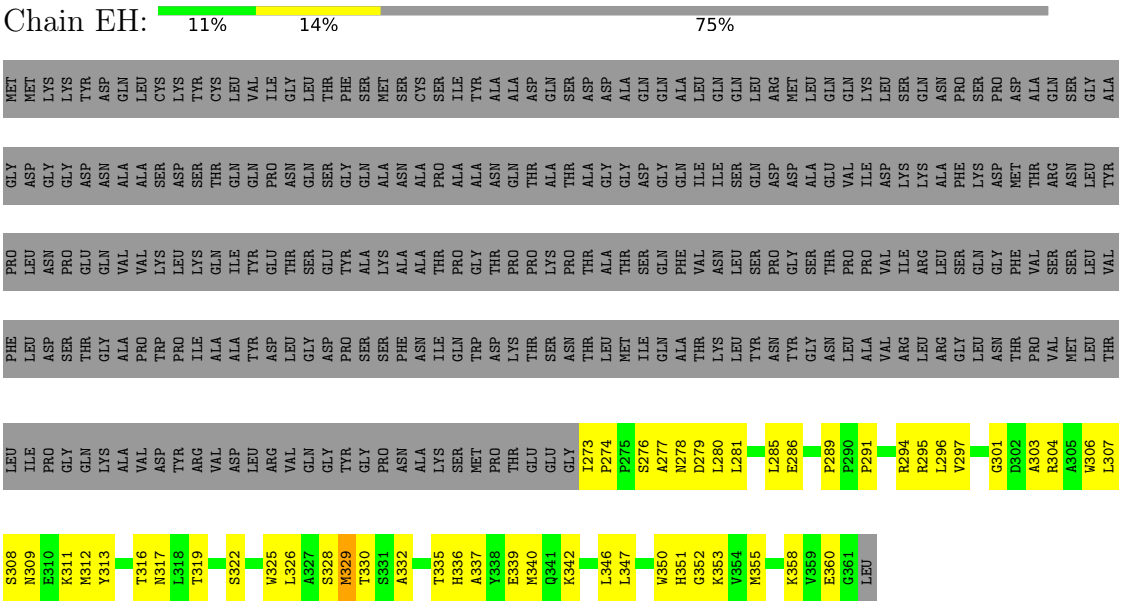
• Molecule 3: Type IV secretion protein IcmK

Chain DH:



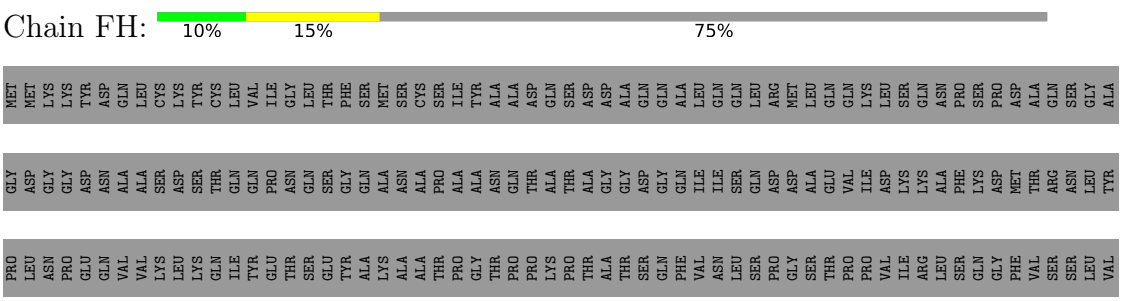
• Molecule 3: Type IV secretion protein IcmK

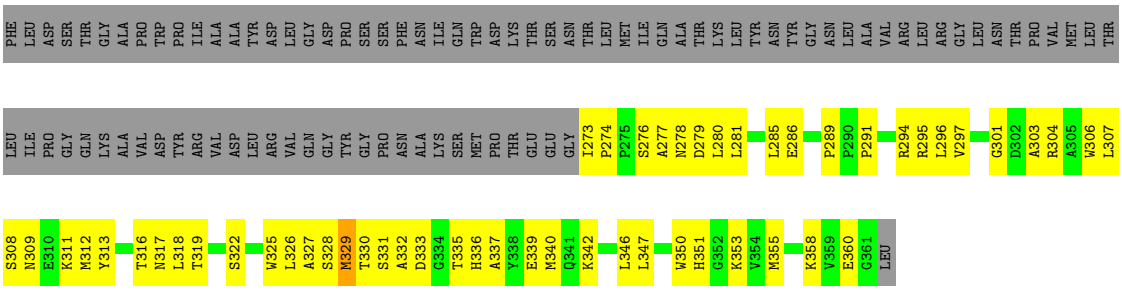
Chain EH:



• Molecule 3: Type IV secretion protein IcmK

Chain FH:

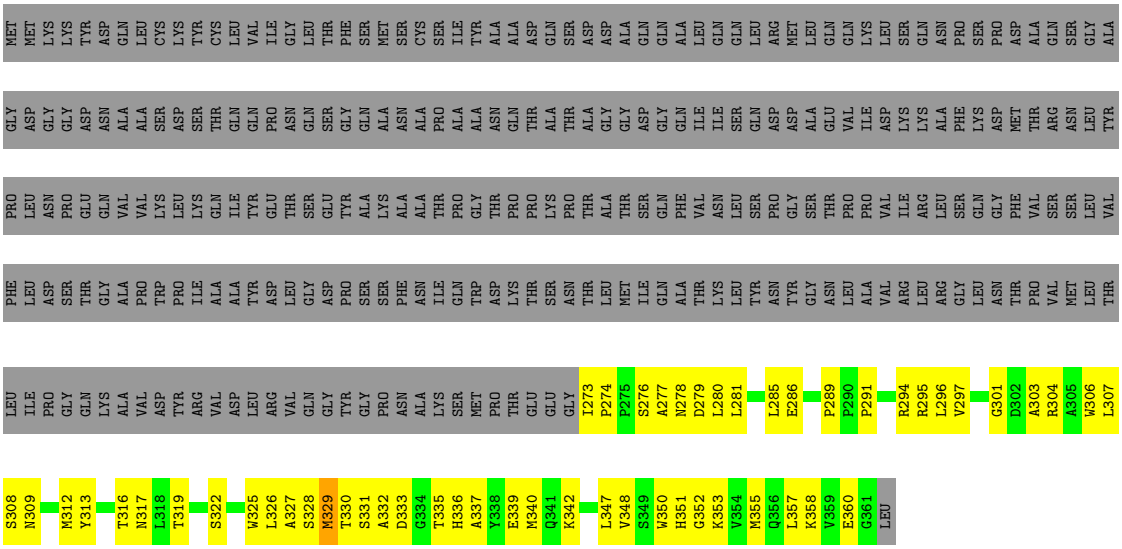




• Molecule 3: Type IV secretion protein IcmK

Chain GH:

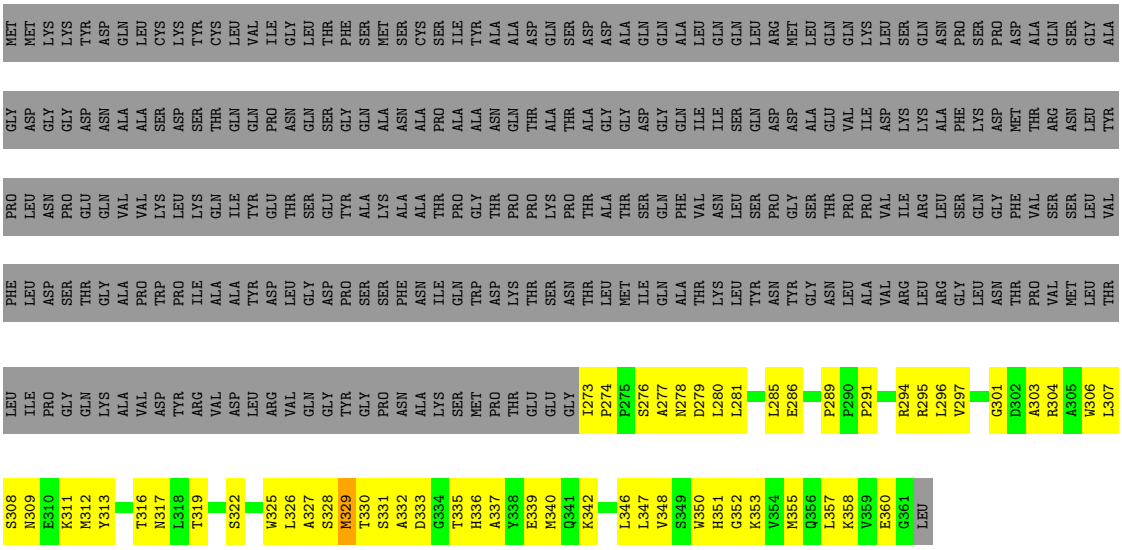




• Molecule 3: Type IV secretion protein IcmK

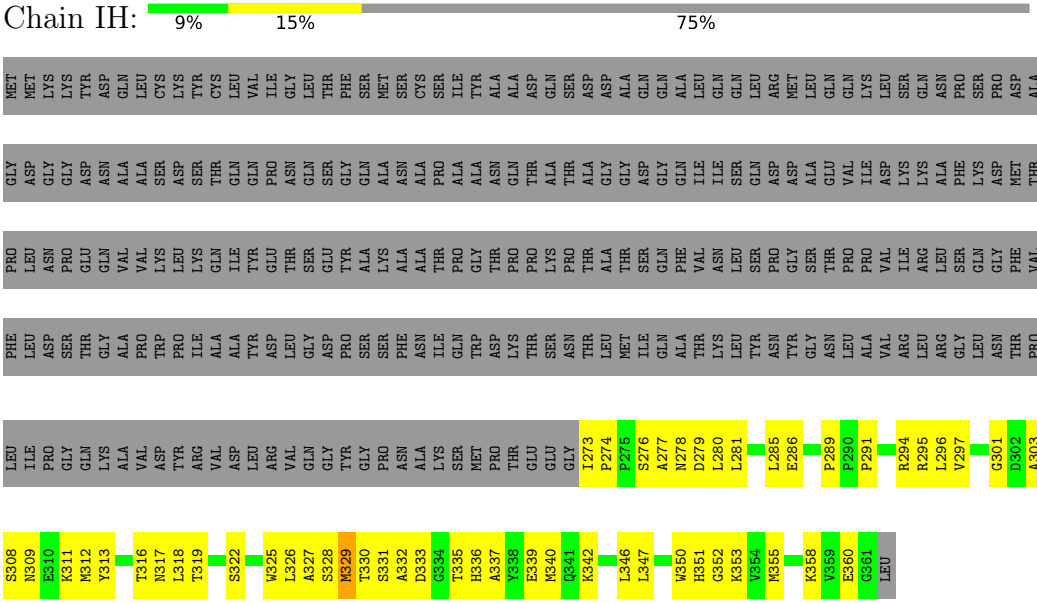
Chain HH:





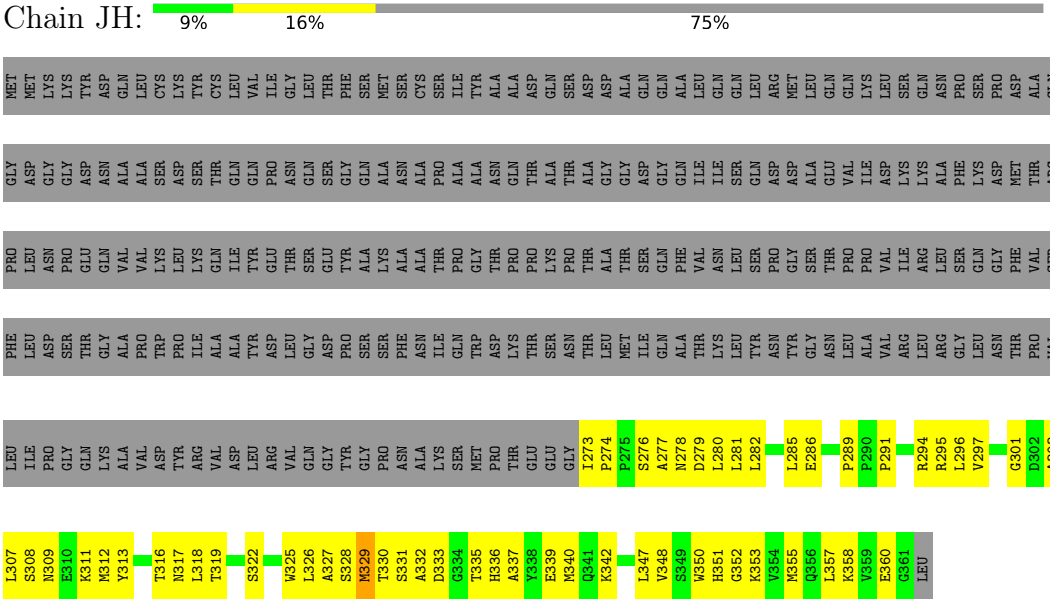
• Molecule 3: Type IV secretion protein IcmK

Chain IH:



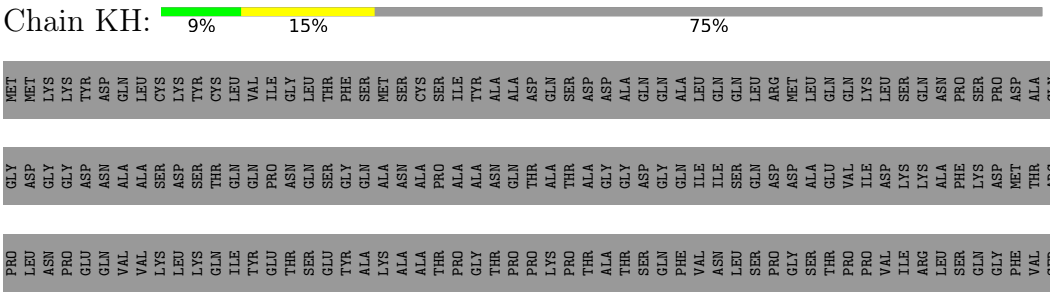
• Molecule 3: Type IV secretion protein IcmK

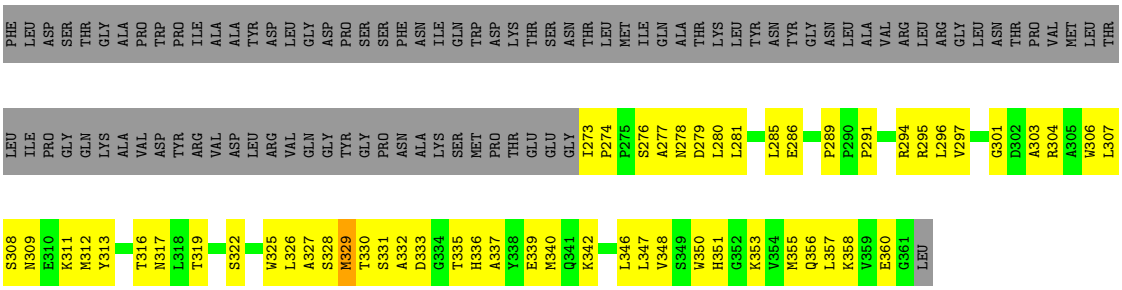
Chain JH:



• Molecule 3: Type IV secretion protein IcmK

Chain KH:

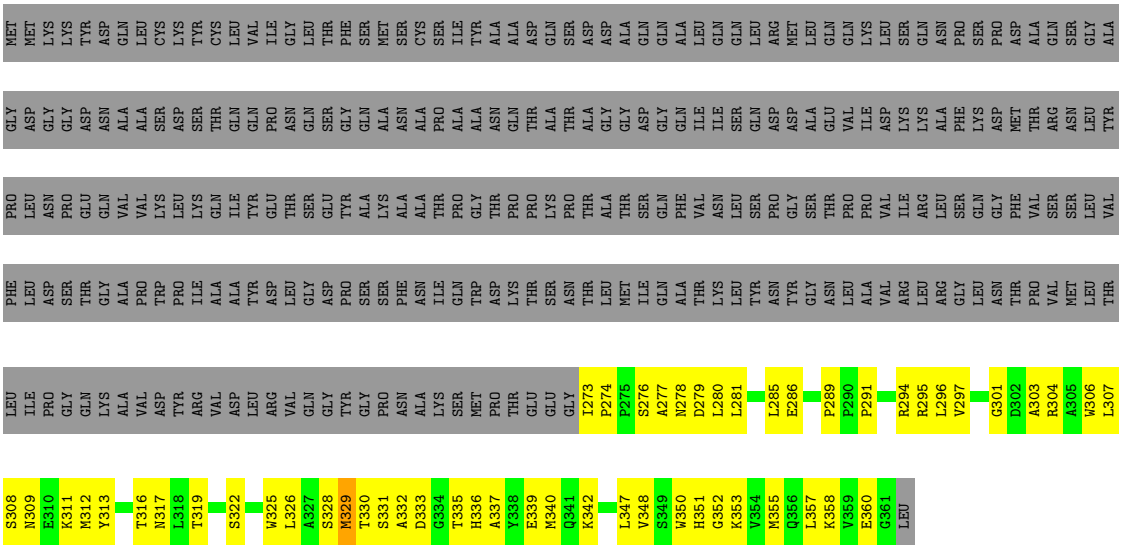




• Molecule 3: Type IV secretion protein IcmK

Chain LH:

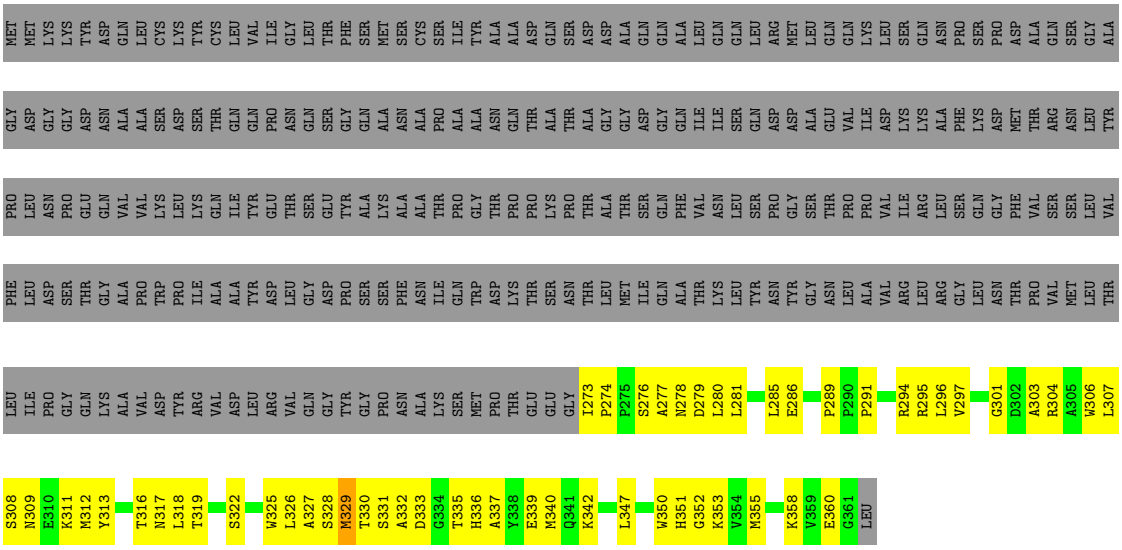




• Molecule 3: Type IV secretion protein IcmK

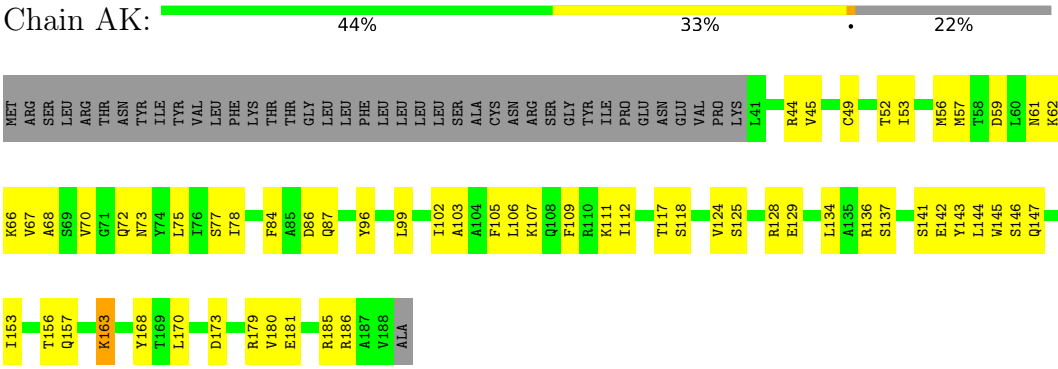
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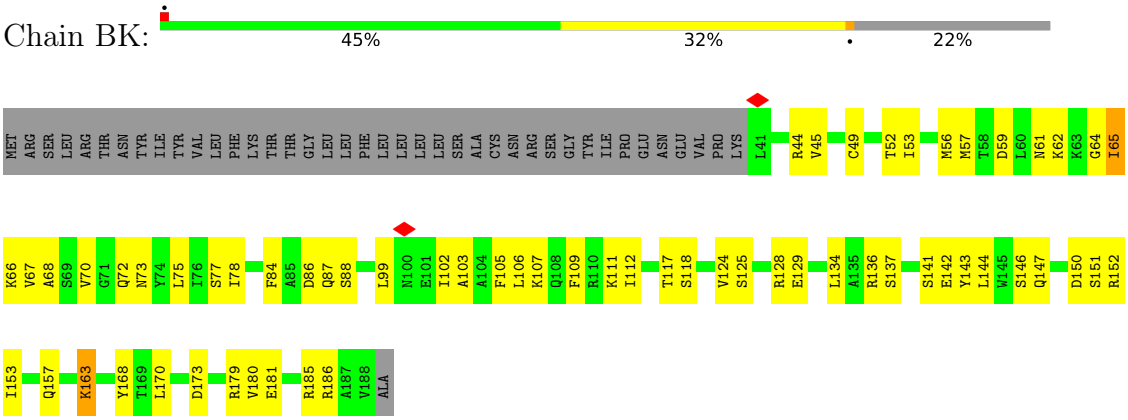
• Molecule 4: Inner membrane lipoprotein YiaD

Chain AK:



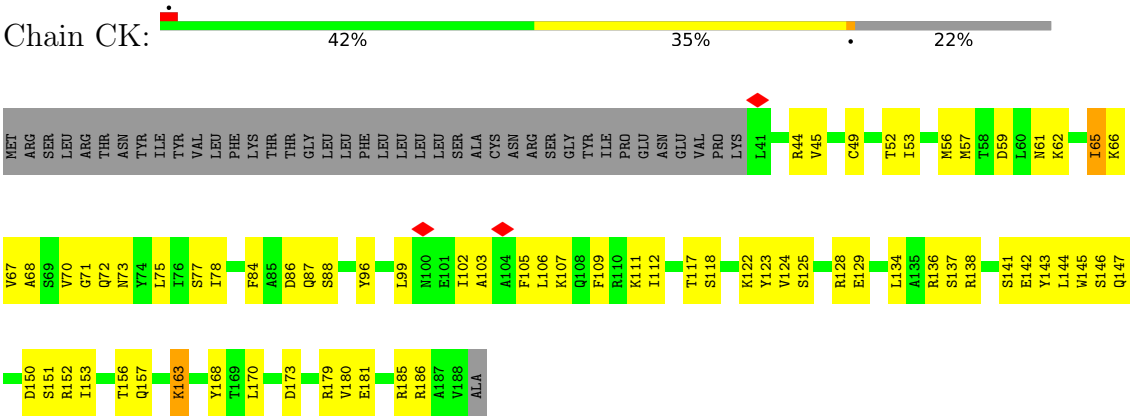
• Molecule 4: Inner membrane lipoprotein YiaD

Chain BK:



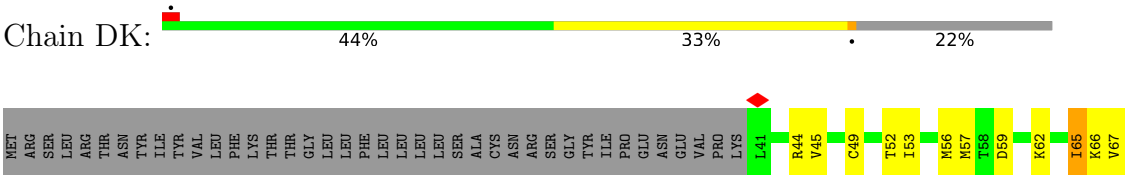
• Molecule 4: Inner membrane lipoprotein YiaD

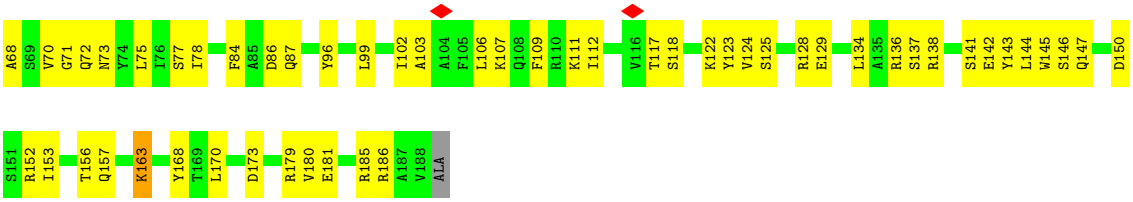
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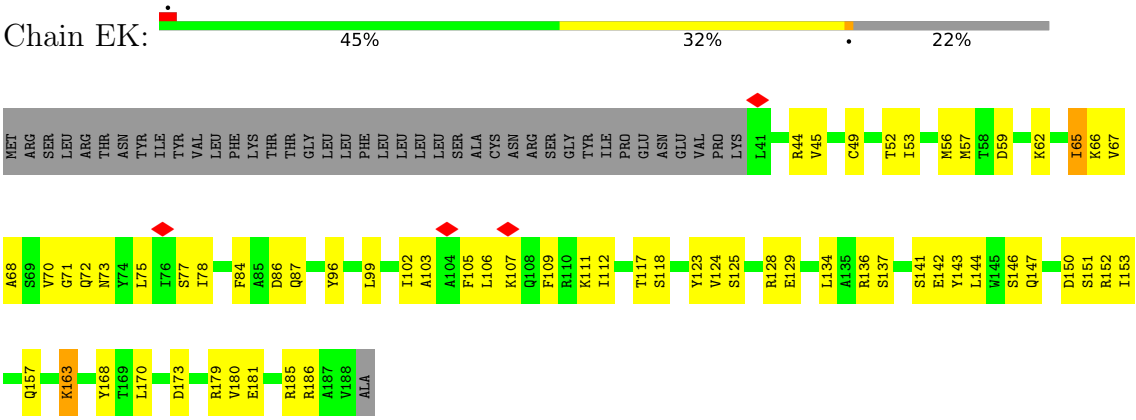
• Molecule 4: Inner membrane lipoprotein YiaD

Chain DK:

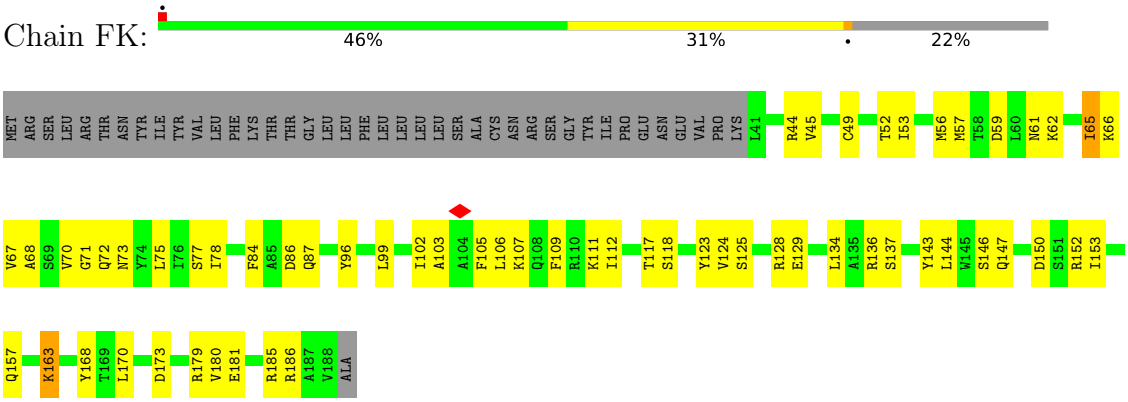




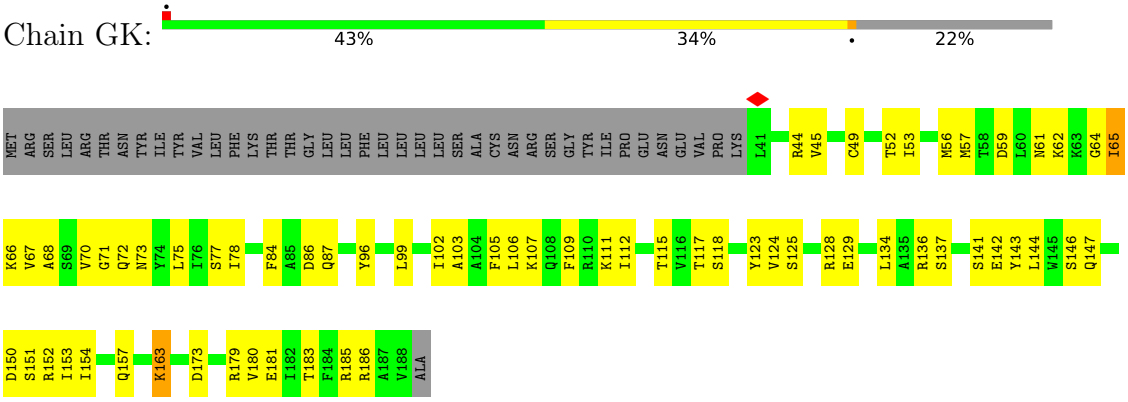
• Molecule 4: Inner membrane lipoprotein YiaD



• Molecule 4: Inner membrane lipoprotein YiaD

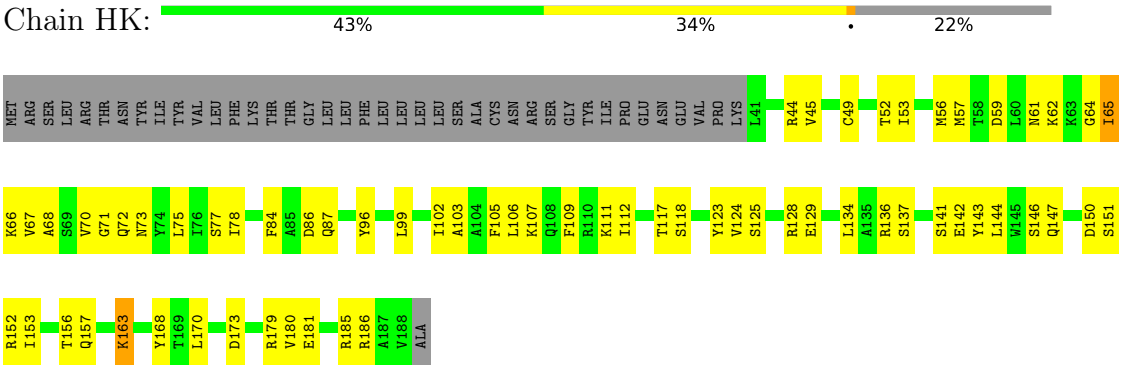


• Molecule 4: Inner membrane lipoprotein YiaD



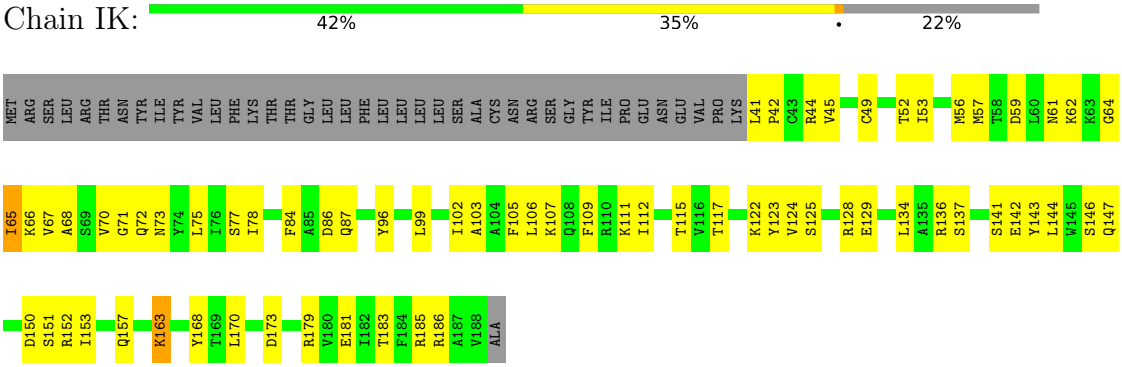
• Molecule 4: Inner membrane lipoprotein YiaD

Chain HK:



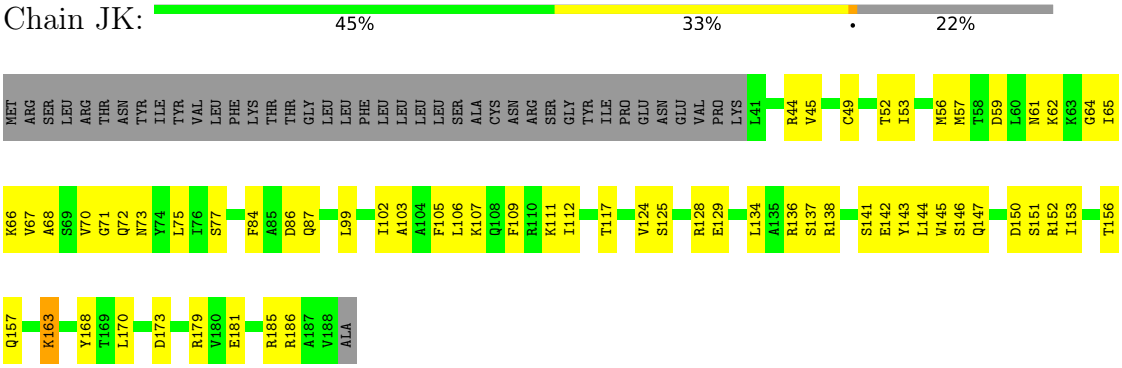
• Molecule 4: Inner membrane lipoprotein YiaD

Chain IK:



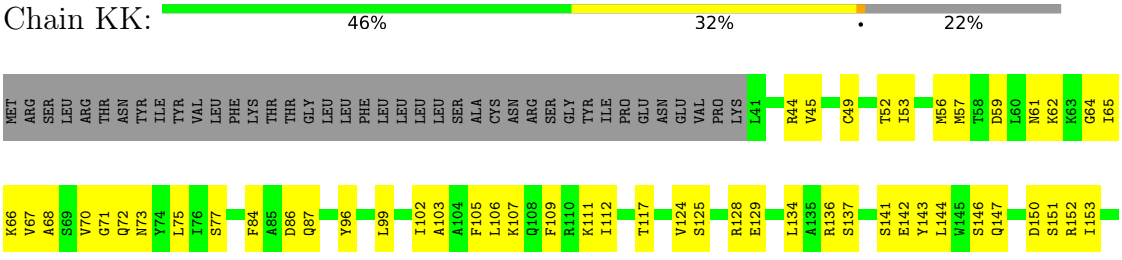
• Molecule 4: Inner membrane lipoprotein YiaD

Chain JK:



• Molecule 4: Inner membrane lipoprotein YiaD

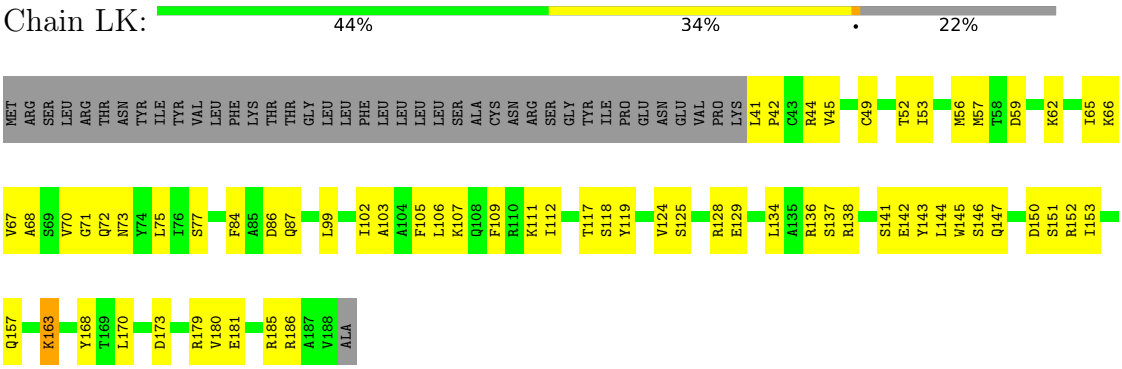
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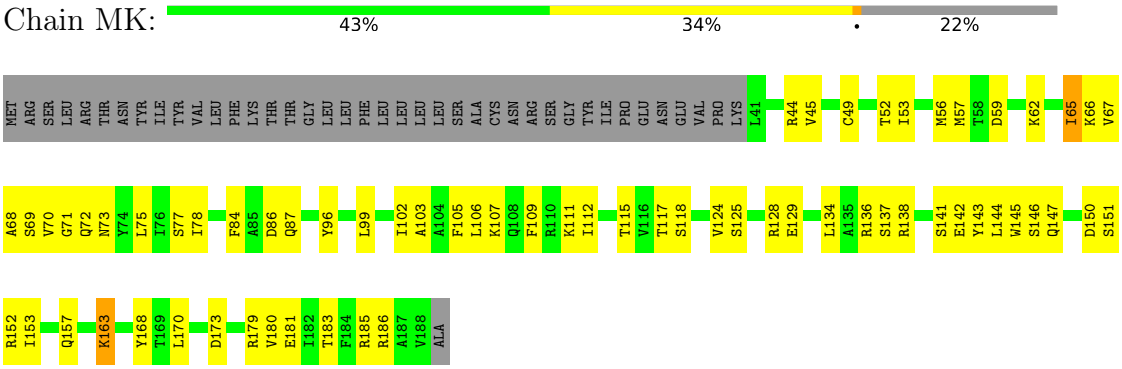
• Molecule 4: Inner membrane lipoprotein YiaD

Chain LK:



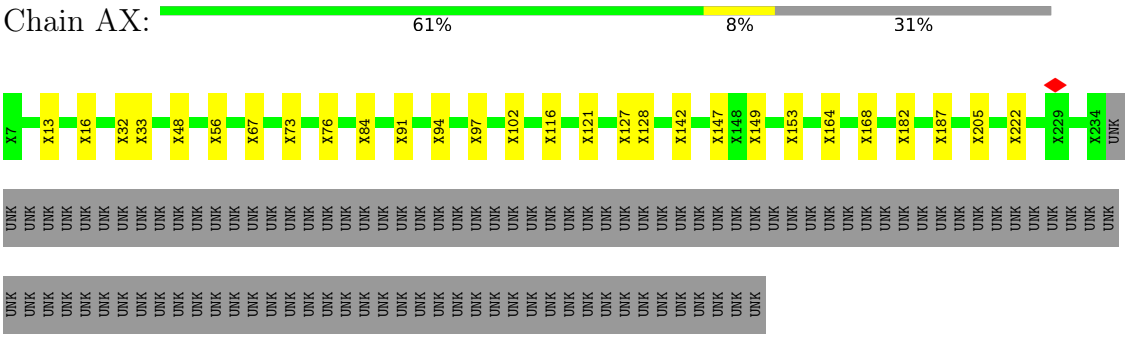
• Molecule 4: Inner membrane lipoprotein YiaD

Chain MK:



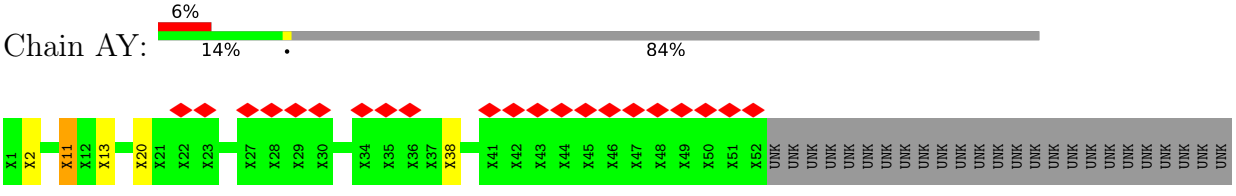
• Molecule 5: Type IV secretion system unknown protein fragment

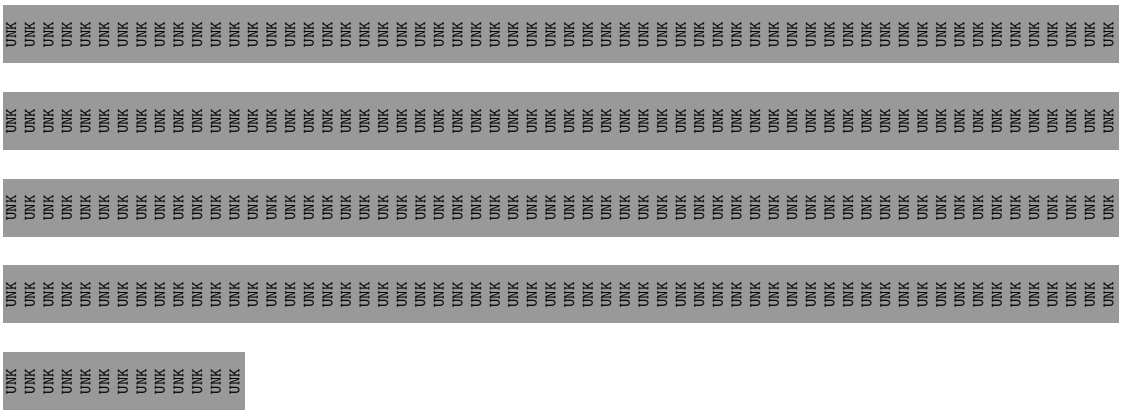
Chain AX:



• Molecule 5: Type IV secretion system unknown protein fragment

Chain AY:

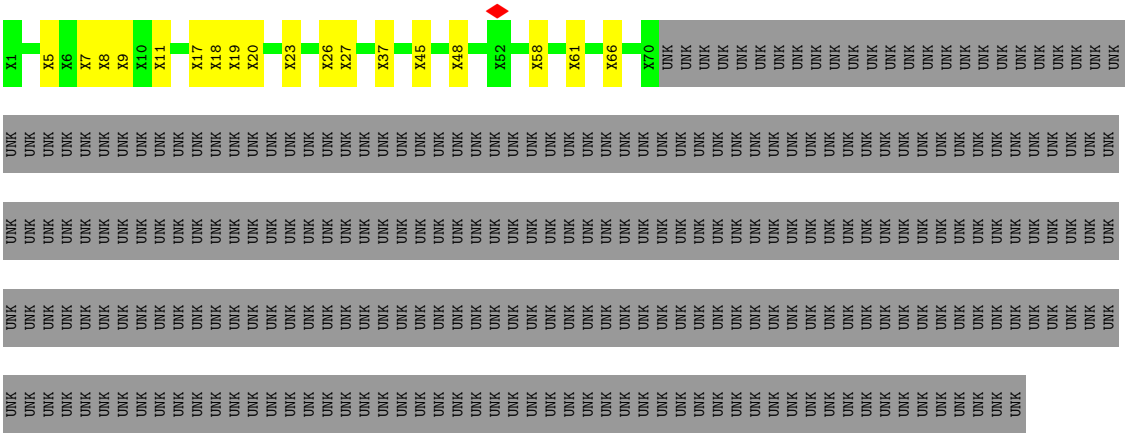




• Molecule 5: Type IV secretion system unknown protein fragment

Chain AZ:

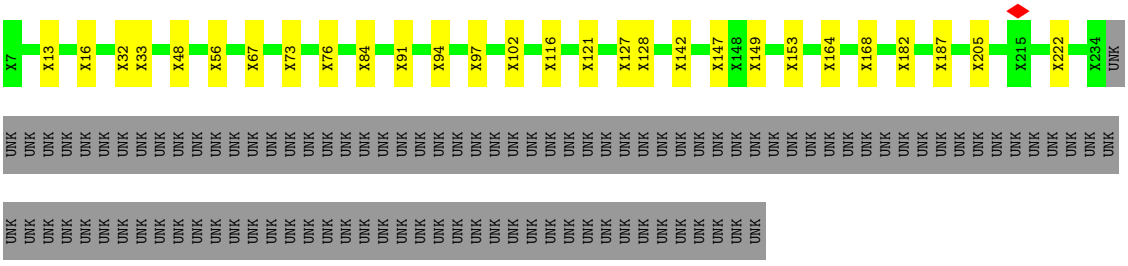




• Molecule 5: Type IV secretion system unknown protein fragment

Chain BX:

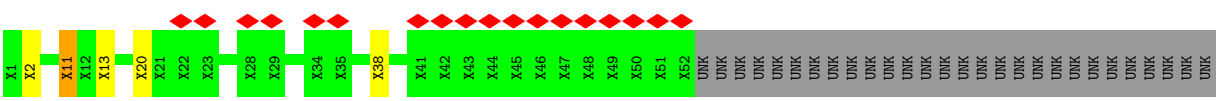


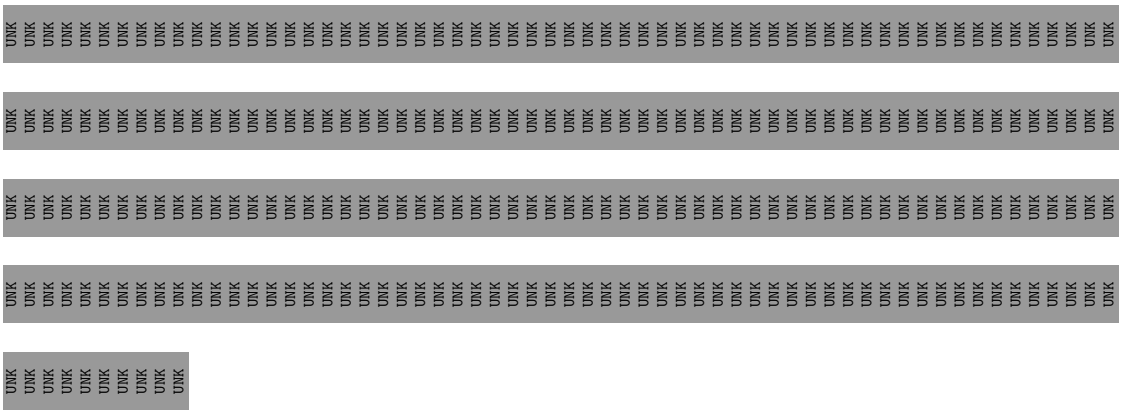


• Molecule 5: Type IV secretion system unknown protein fragment

Chain BY:

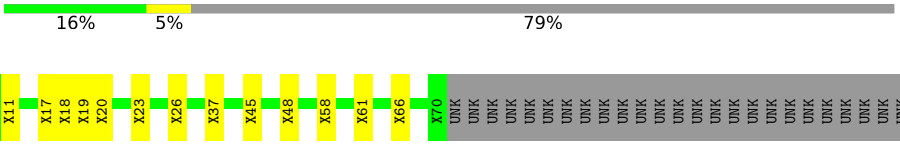






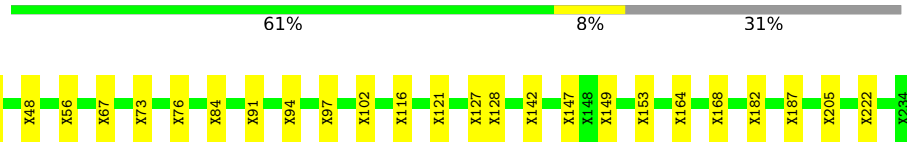
• Molecule 5: Type IV secretion system unknown protein fragment

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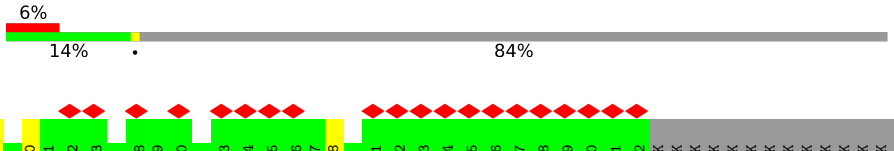
• Molecule 5: Type IV secretion system unknown protein fragment

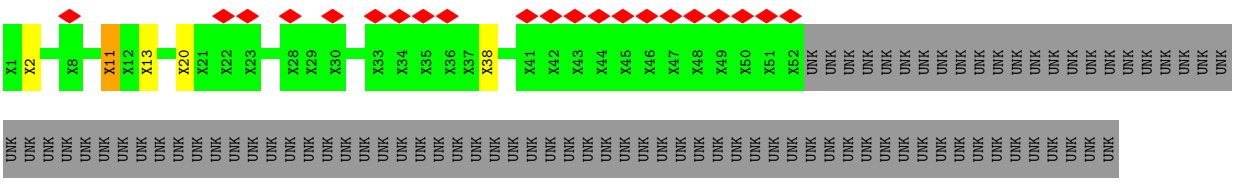
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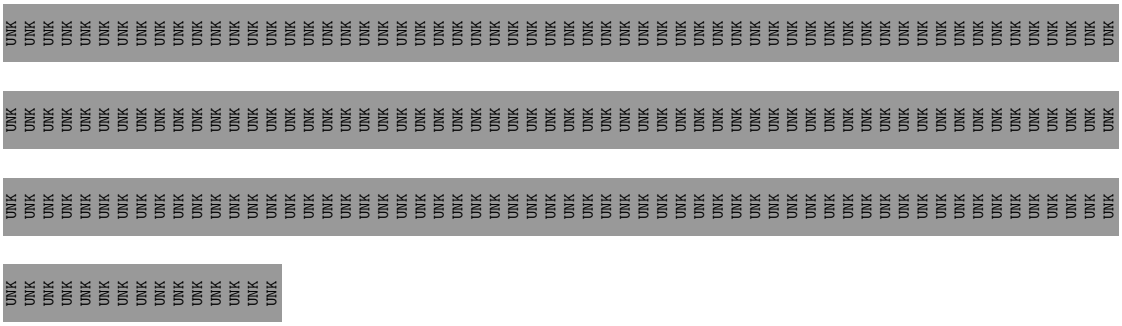


• Molecule 5: Type IV secretion system unknown protein fragment

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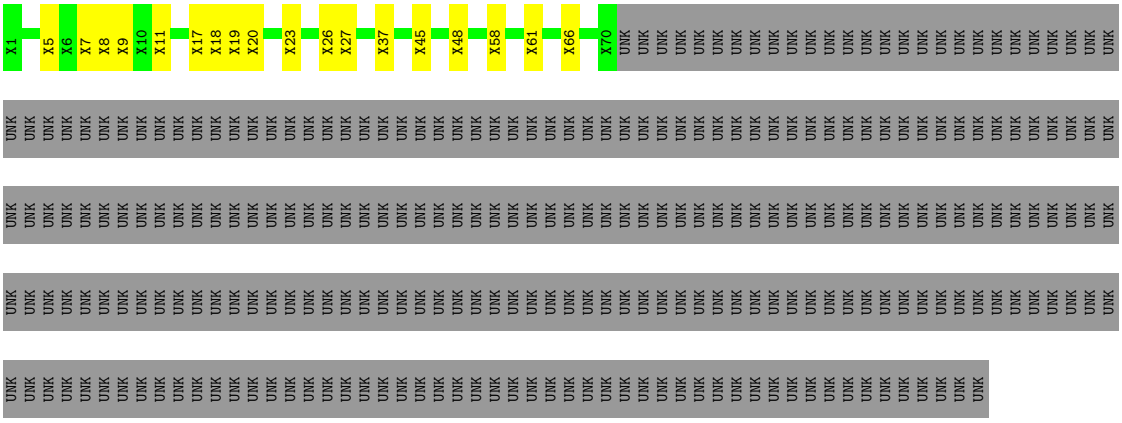




• Molecule 5: Type IV secretion system unknown protein fragment

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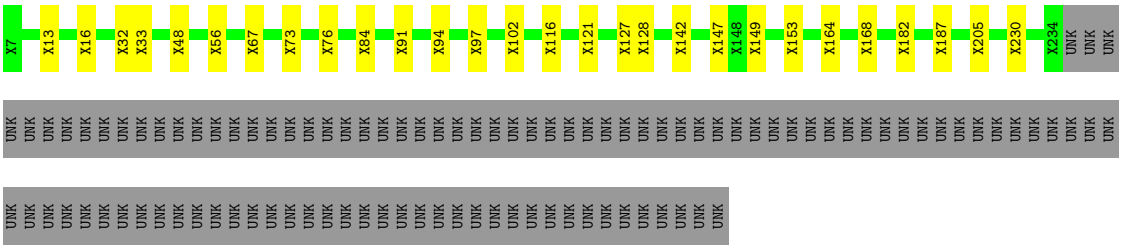




• Molecule 5: Type IV secretion system unknown protein fragment

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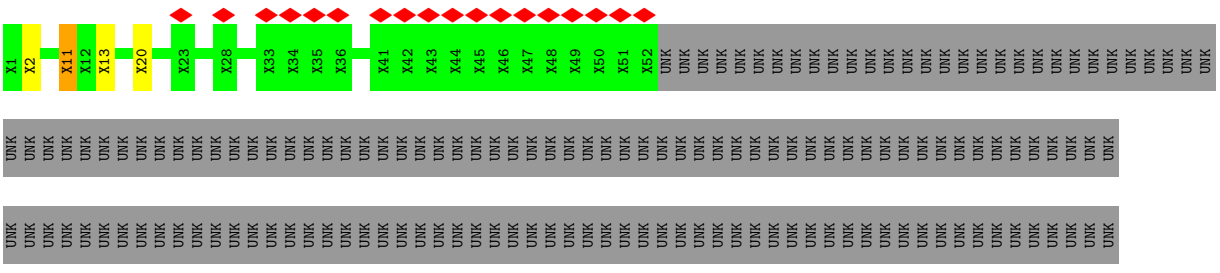


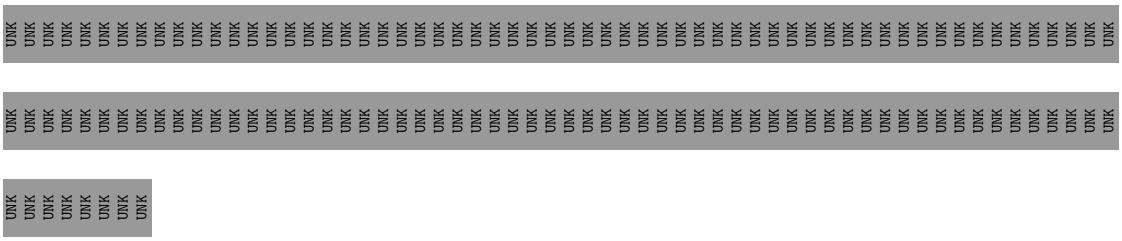


• Molecule 5: Type IV secretion system unknown protein fragment

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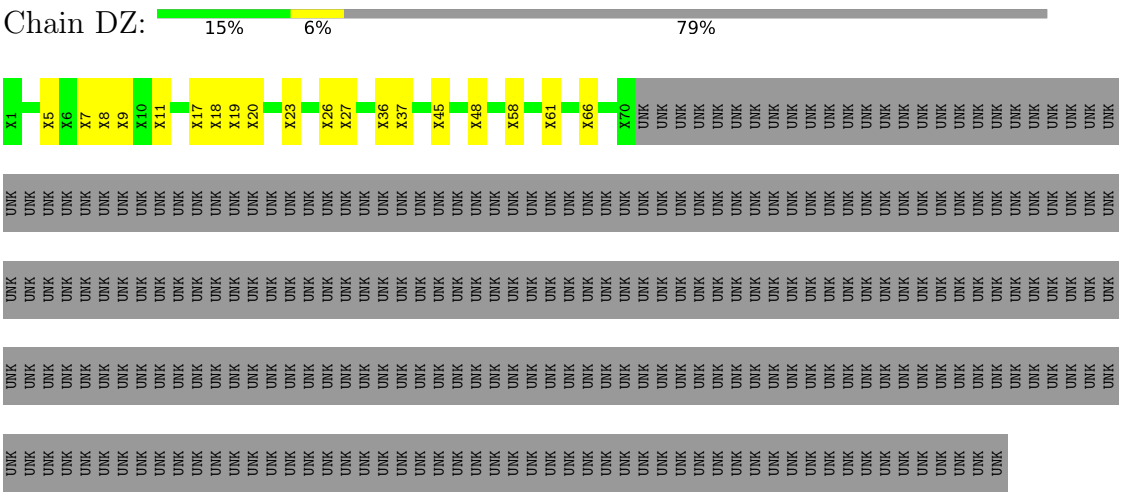






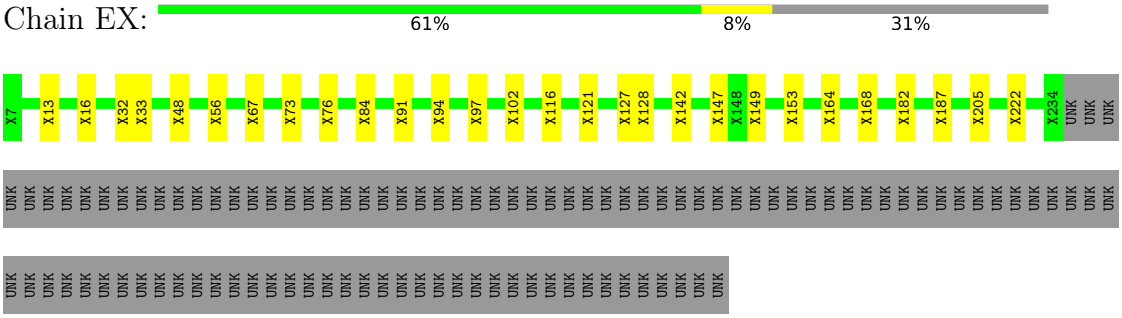
• Molecule 5: Type IV secretion system unknown protein fragment

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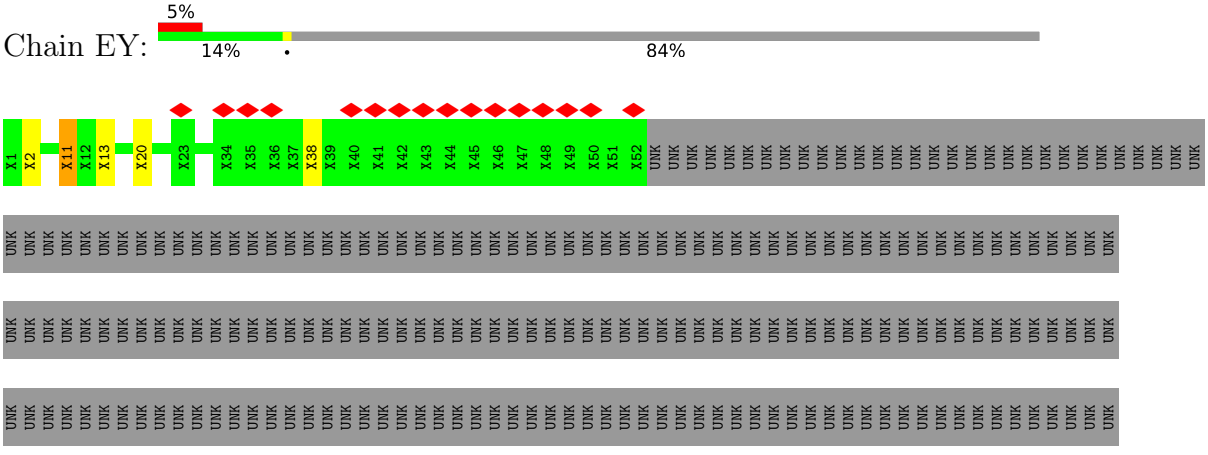
• Molecule 5: Type IV secretion system unknown protein fragment

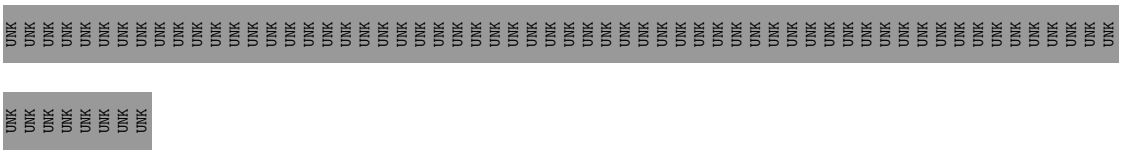
Chain EX:



• Molecule 5: Type IV secretion system unknown protein fragment

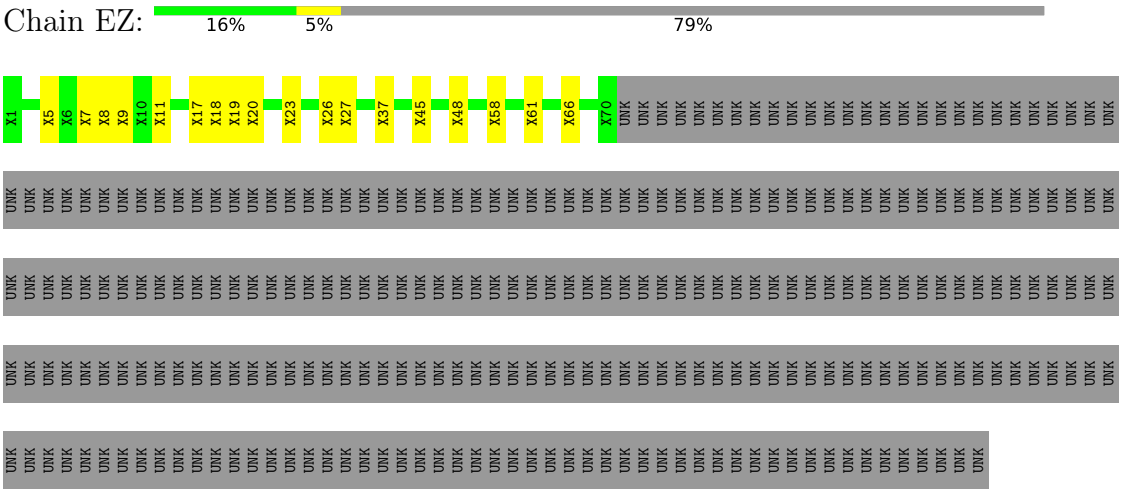
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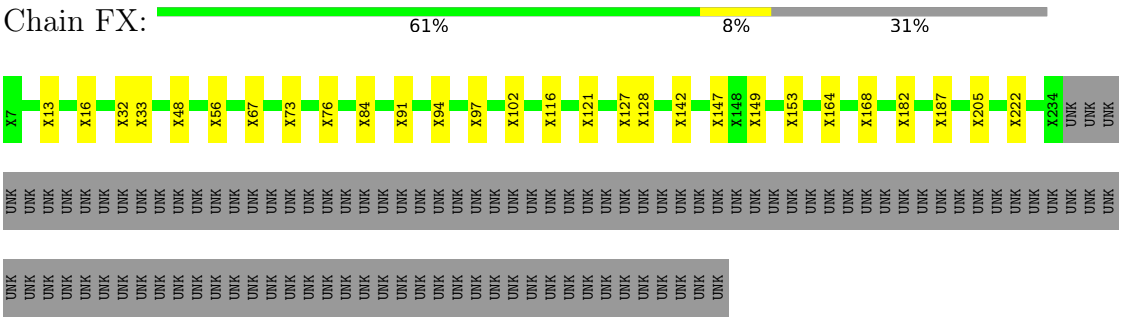
• Molecule 5: Type IV secretion system unknown protein fragment

Chain EZ:



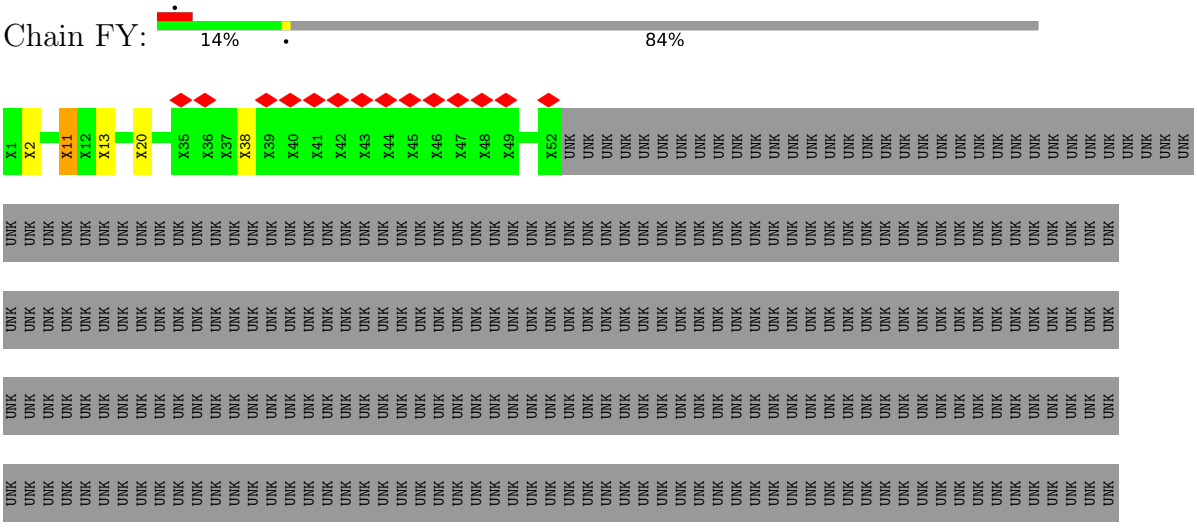
• Molecule 5: Type IV secretion system unknown protein fragment

Chain FX:



• Molecule 5: Type IV secretion system unknown protein fragment

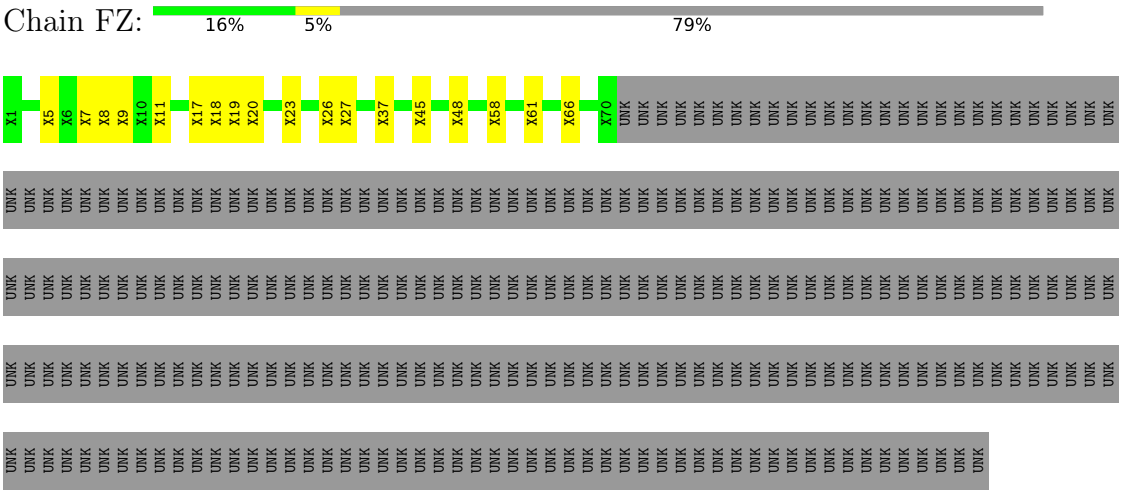
Chain FY:





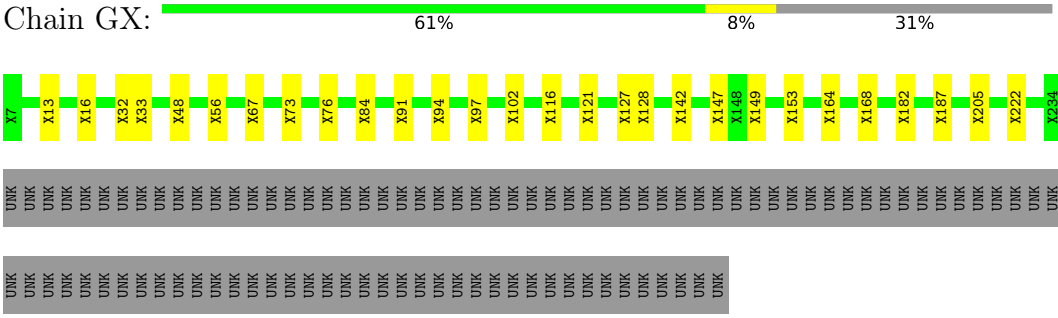
• Molecule 5: Type IV secretion system unknown protein fragment

Chain FZ:



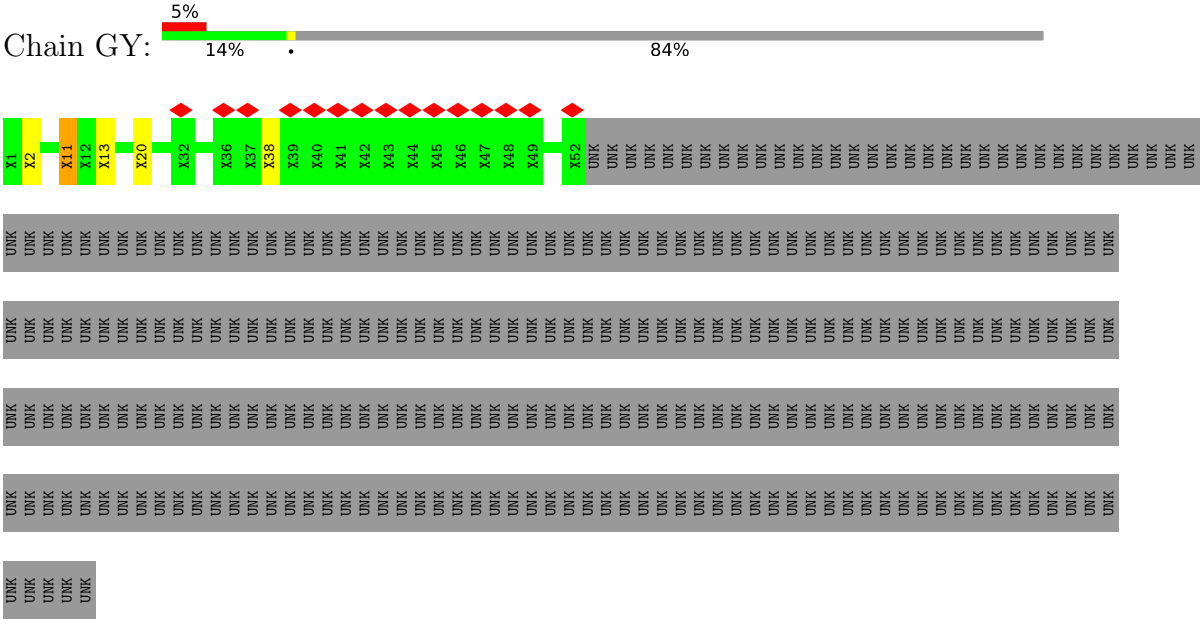
• Molecule 5: Type IV secretion system unknown protein fragment

Chain GX:



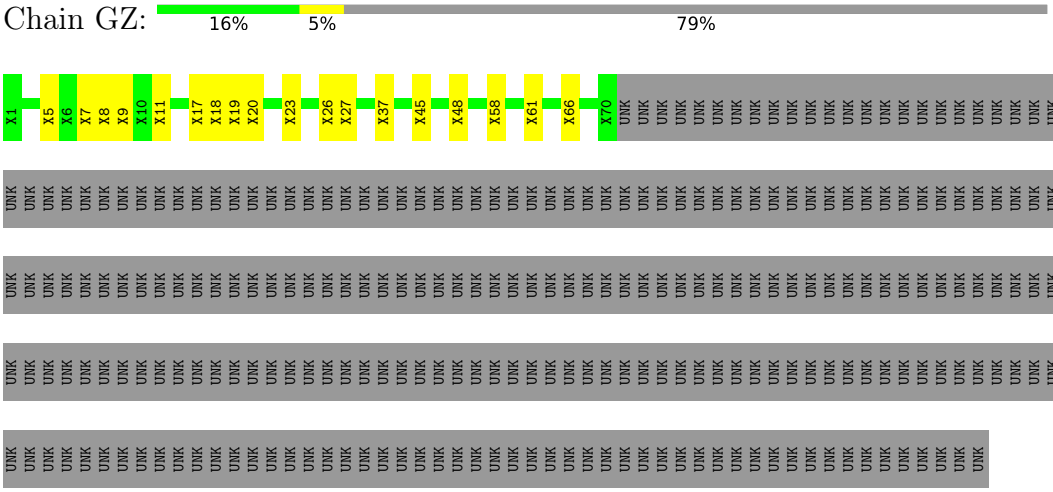
• Molecule 5: Type IV secretion system unknown protein fragment

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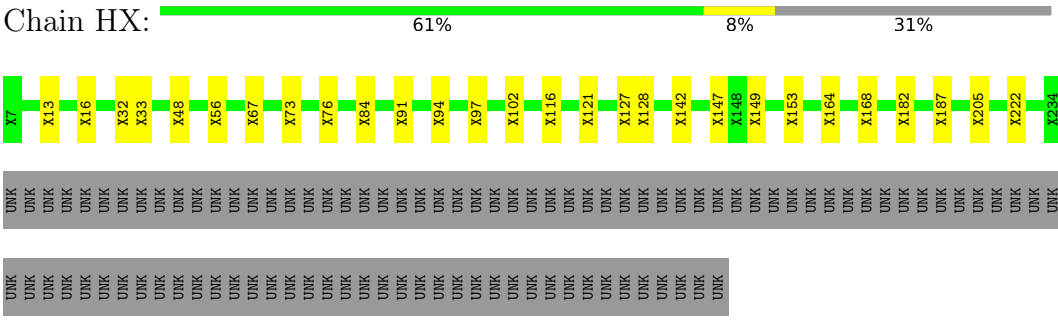
• Molecule 5: Type IV secretion system unknown protein fragment

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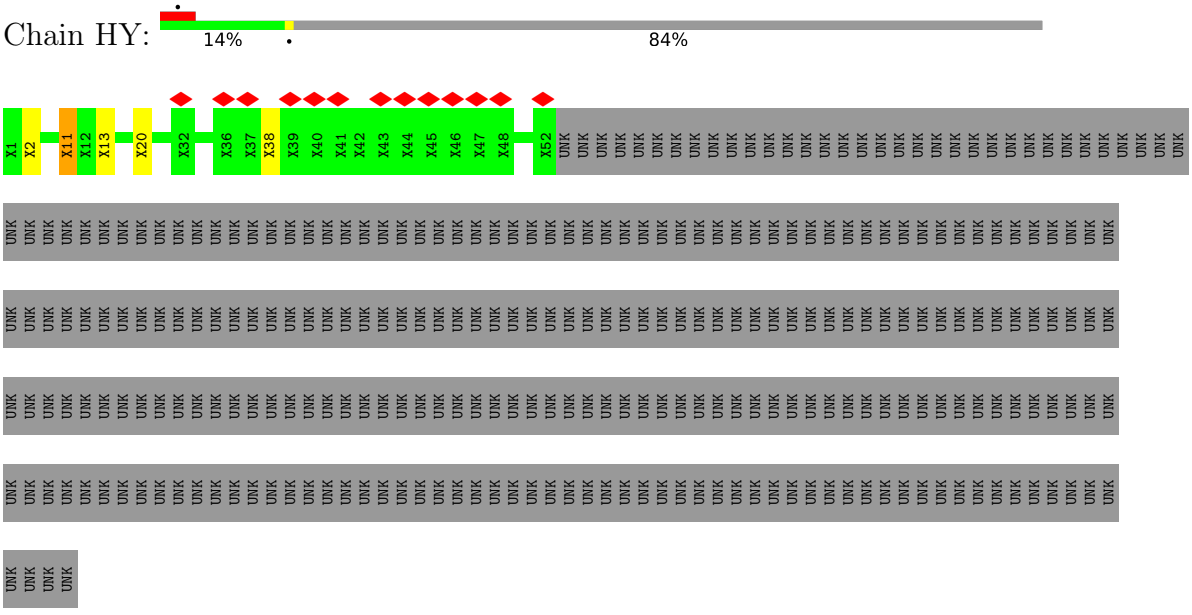
• Molecule 5: Type IV secretion system unknown protein fragment

Chain HX:



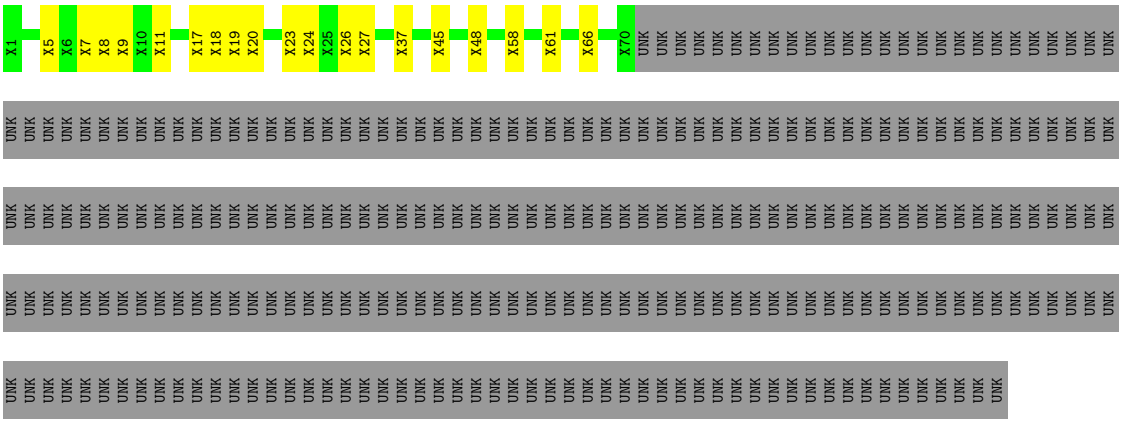
• Molecule 5: Type IV secretion system unknown protein fragment

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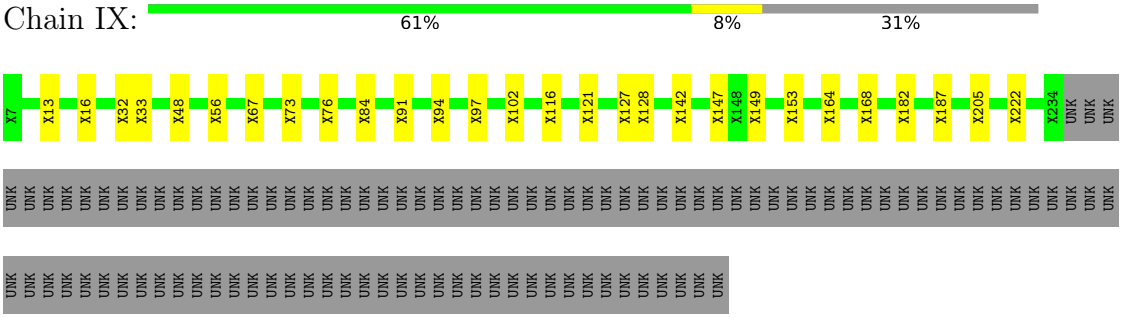
• Molecule 5: Type IV secretion system unknown protein fragment

Chain HZ:



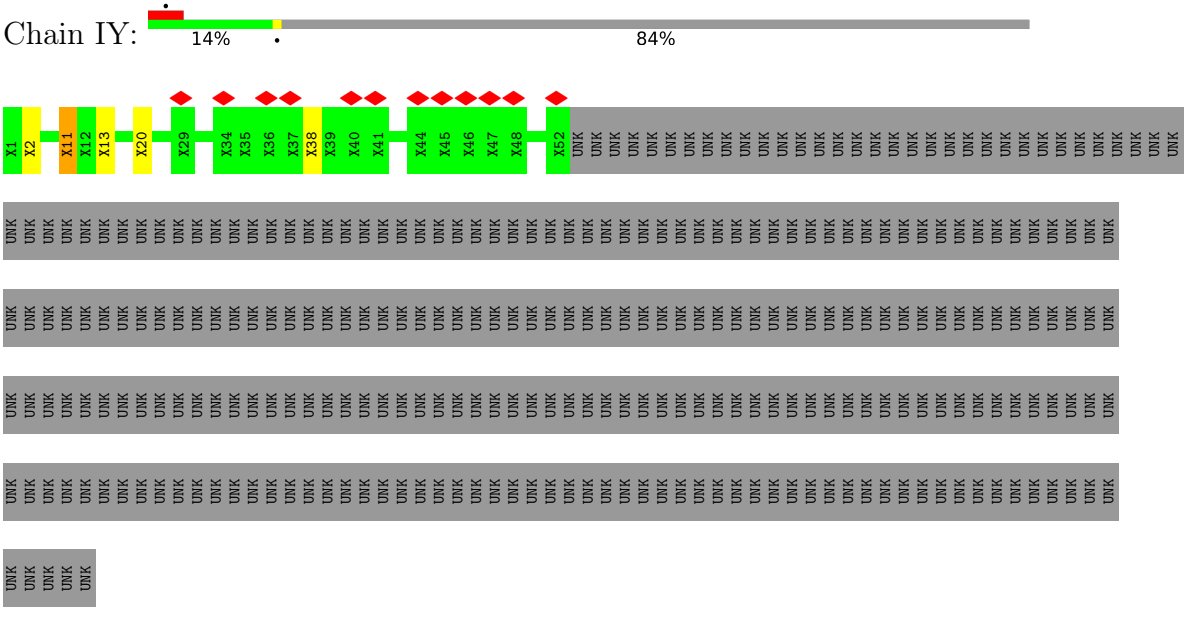
• Molecule 5: Type IV secretion system unknown protein fragment

Chain IX:



• Molecule 5: Type IV secretion system unknown protein fragment

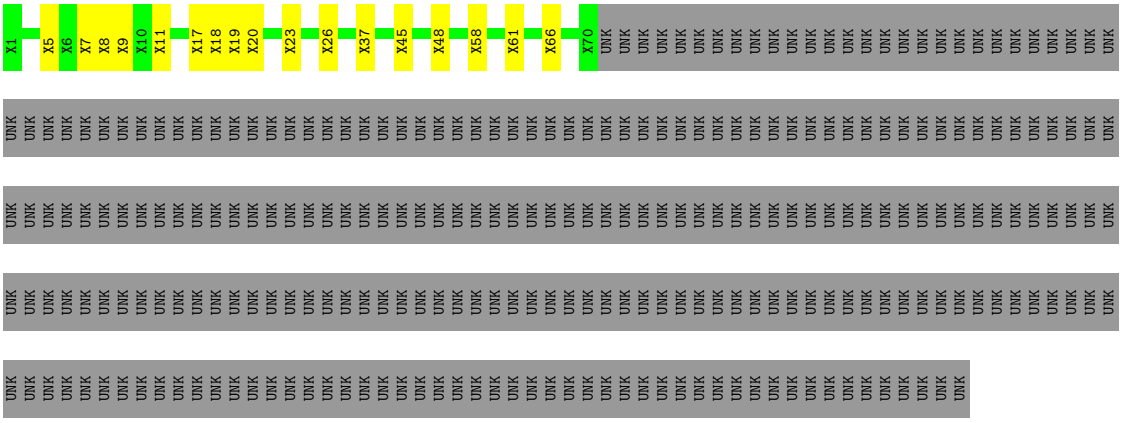
Chain IY:



• Molecule 5: Type IV secretion system unknown protein fragment

Chain IZ:

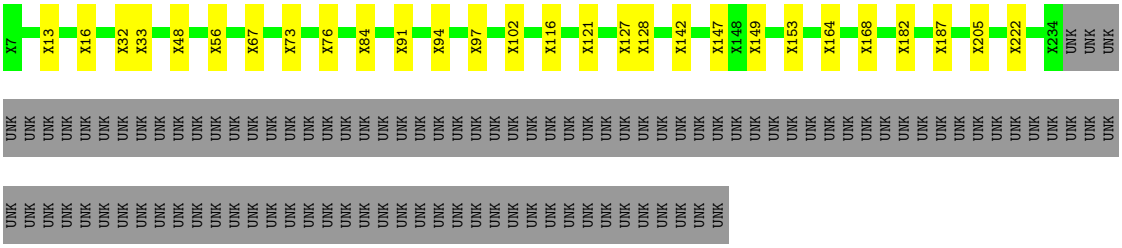




• Molecule 5: Type IV secretion system unknown protein fragment

Chain JX:

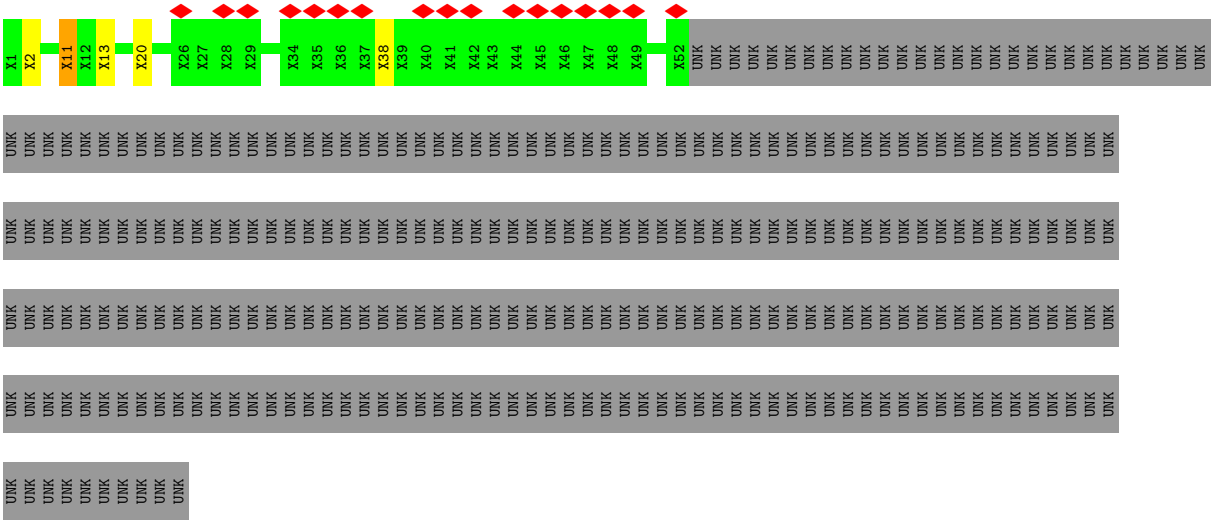




• Molecule 5: Type IV secretion system unknown protein fragment

Chain JY:

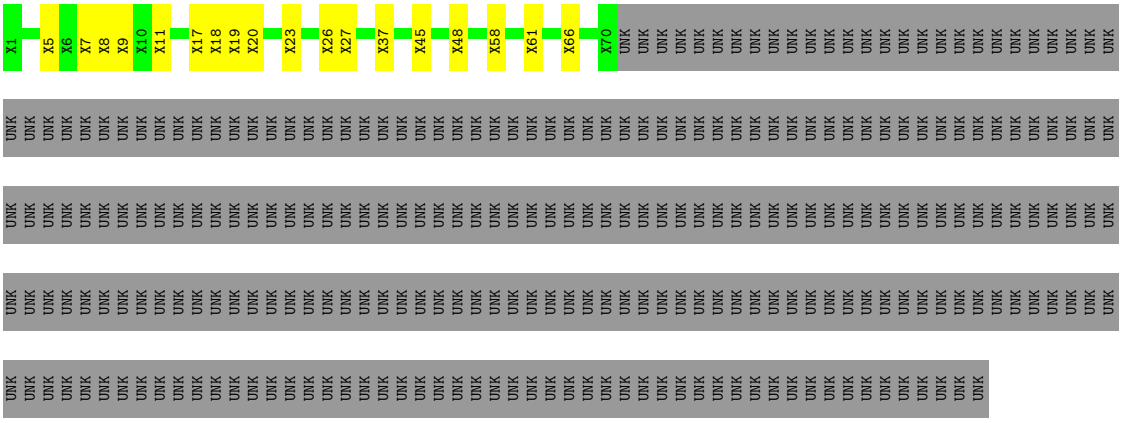




• Molecule 5: Type IV secretion system unknown protein fragment

Chain JZ:

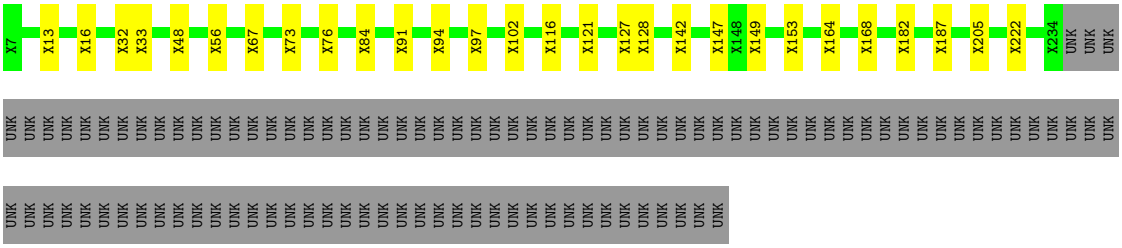




• Molecule 5: Type IV secretion system unknown protein fragment

Chain KX:

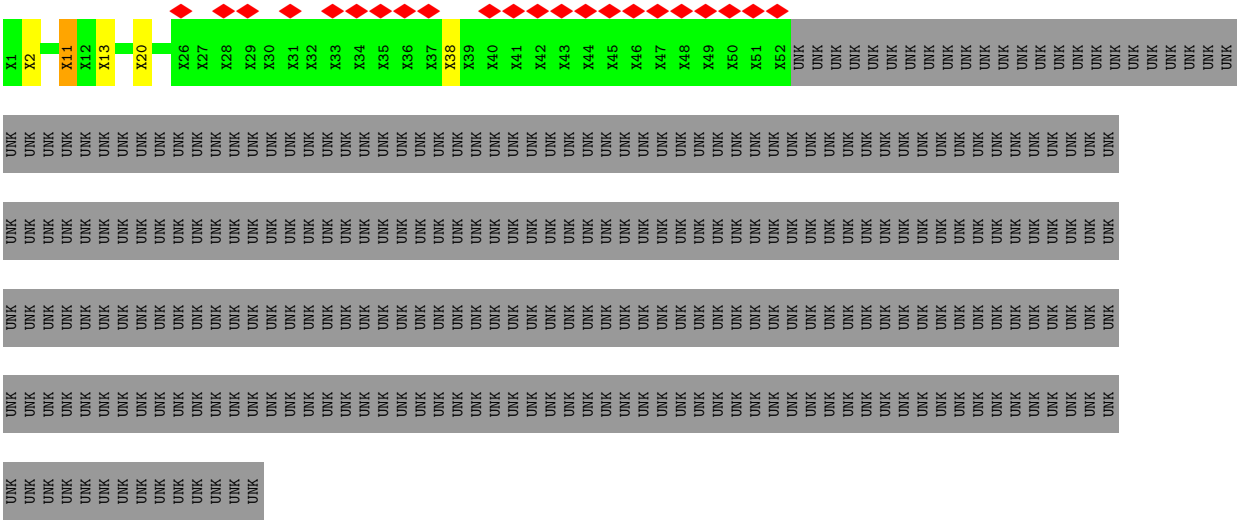




• Molecule 5: Type IV secretion system unknown protein fragment

Chain KY:

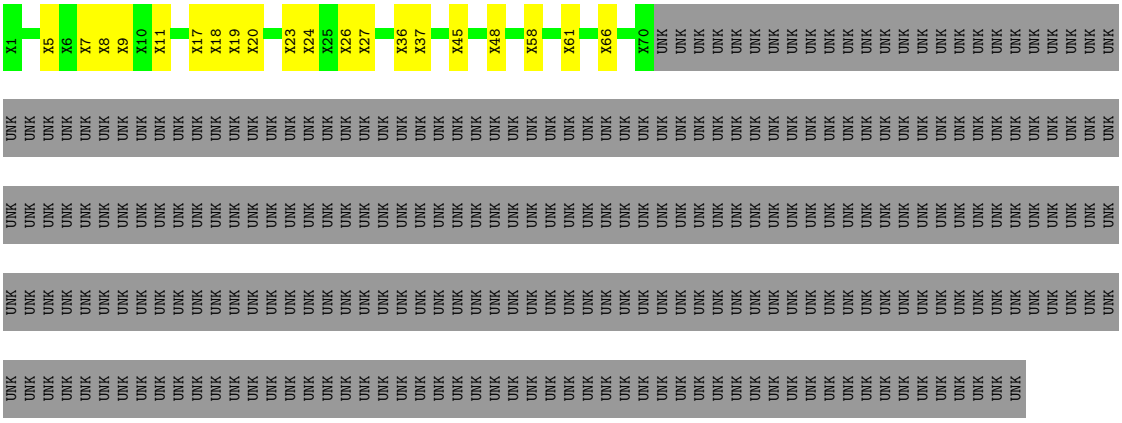




• Molecule 5: Type IV secretion system unknown protein fragment

Chain KZ:

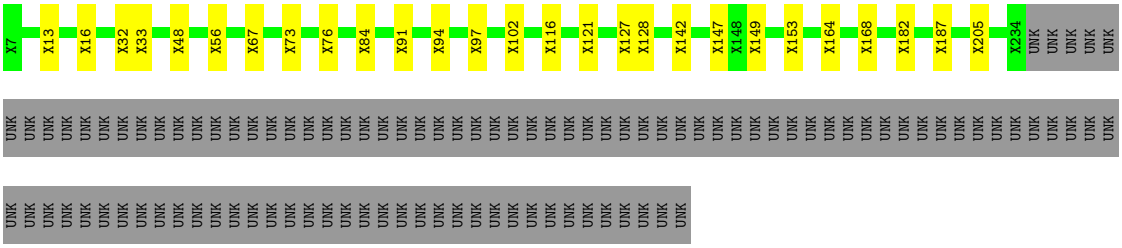




• Molecule 5: Type IV secretion system unknown protein fragment

Chain LX:

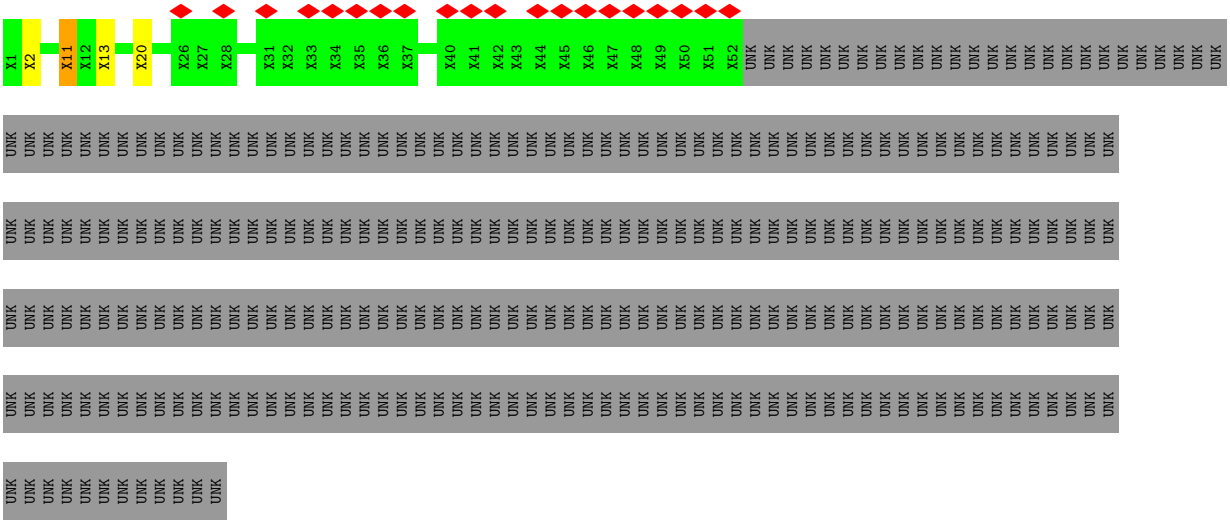




• Molecule 5: Type IV secretion system unknown protein fragment

Chain LY:

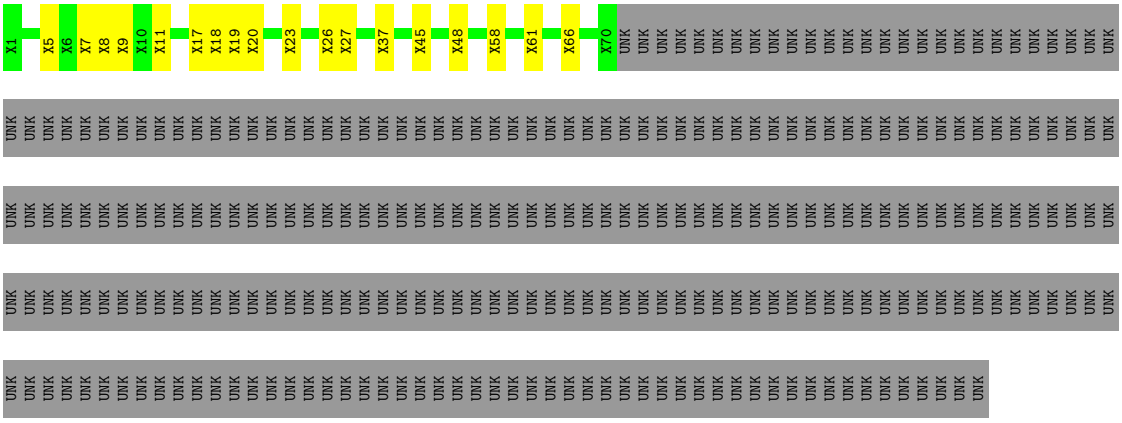




• Molecule 5: Type IV secretion system unknown protein fragment

Chain LZ:

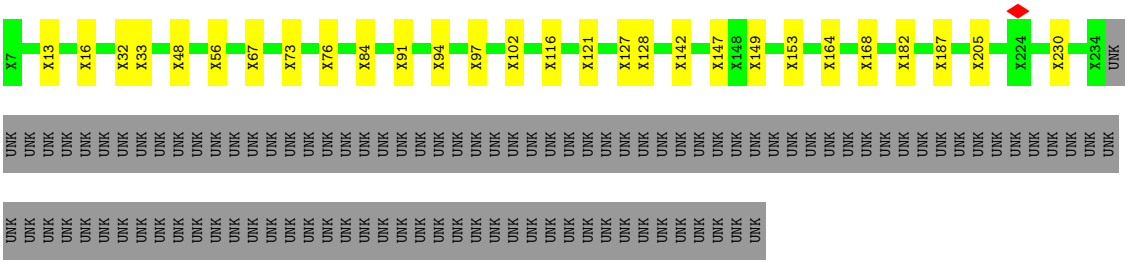




• Molecule 5: Type IV secretion system unknown protein fragment

Chain MX:

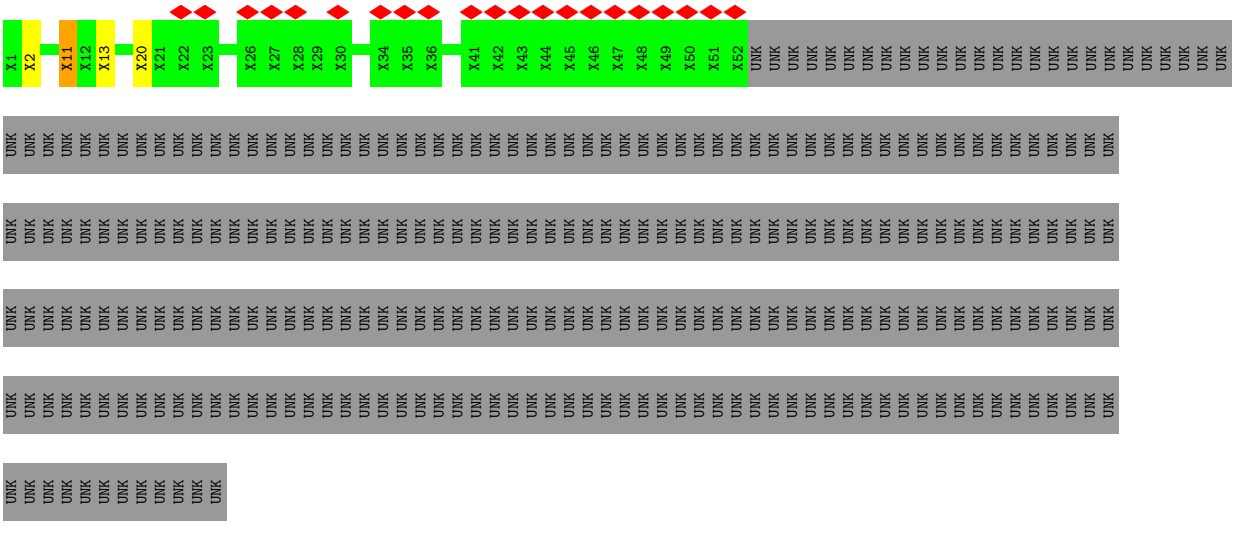




• Molecule 5: Type IV secretion system unknown protein fragment

Chain MY:

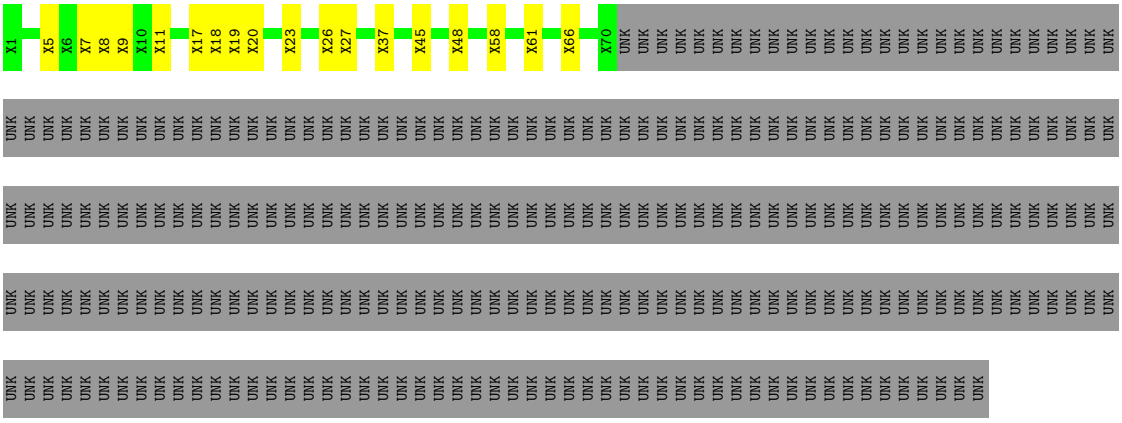




• Molecule 5: Type IV secretion system unknown protein fragment

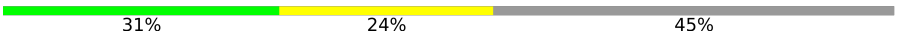
Chain MZ:





• Molecule 6: Outer membrane protein, OmpA family protein

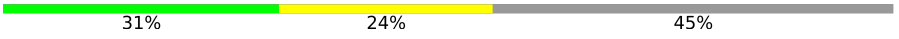
Chain AA:

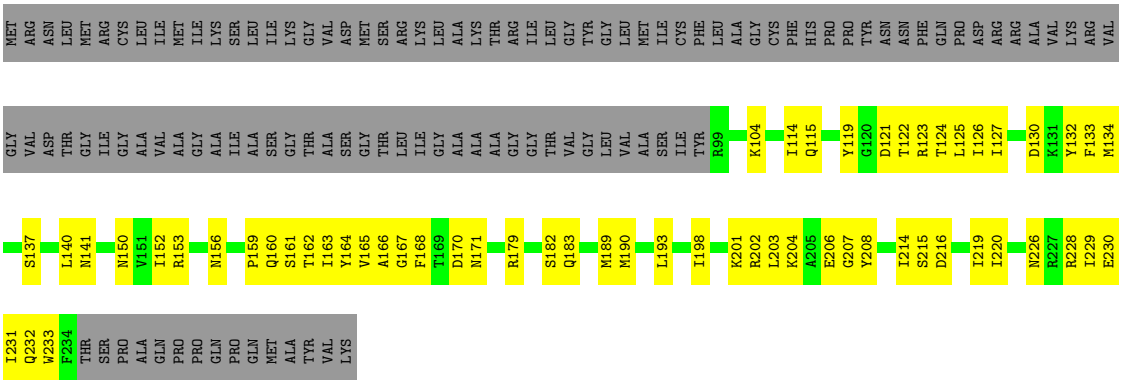




• Molecule 6: Outer membrane protein, OmpA family protein

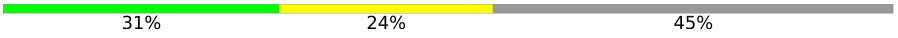
Chain BA:



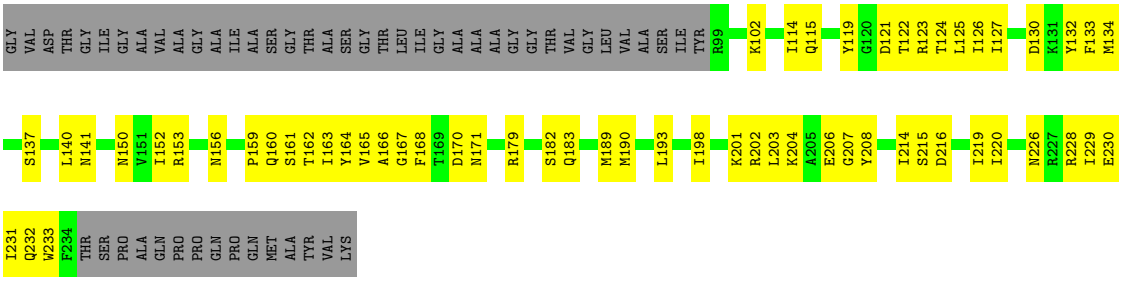


• Molecule 6: Outer membrane protein, OmpA family protein

Chain CA:

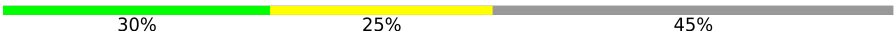






• Molecule 6: Outer membrane protein, OmpA family protein

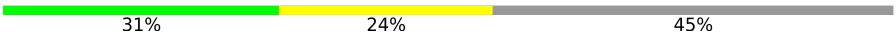
Chain DA:

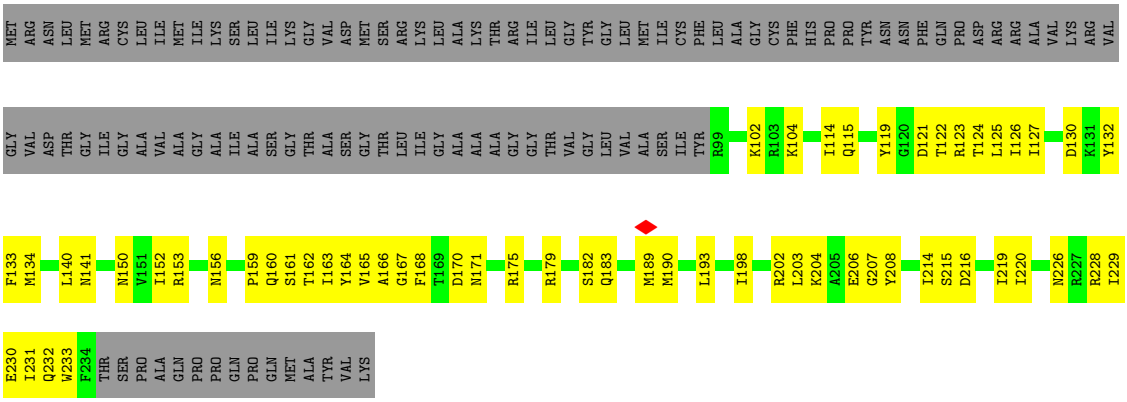




• Molecule 6: Outer membrane protein, OmpA family protein

Chain EA:

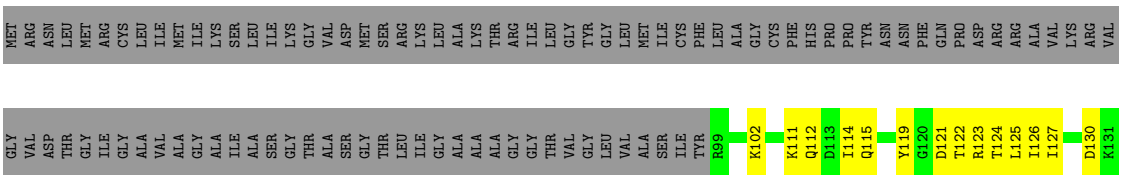


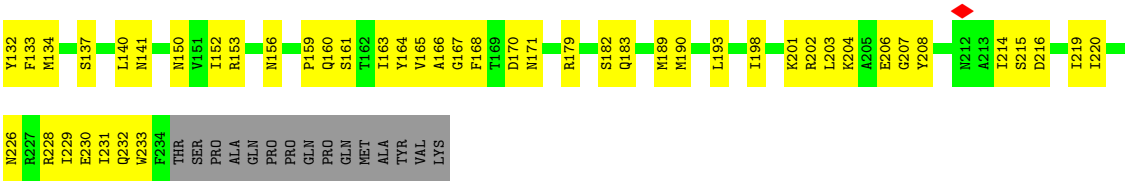


• Molecule 6: Outer membrane protein, OmpA family protein

Chain FA:



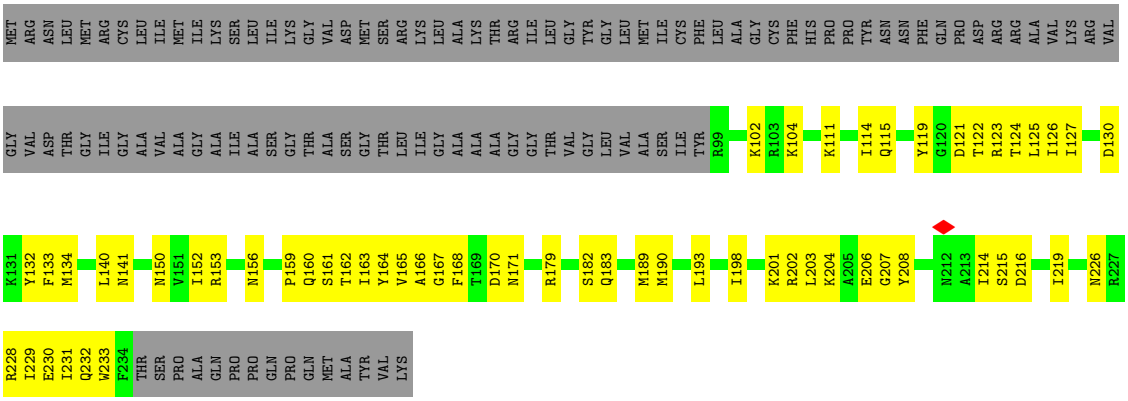




• Molecule 6: Outer membrane protein, OmpA family protein

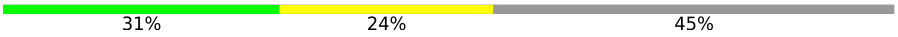
Chain GA:

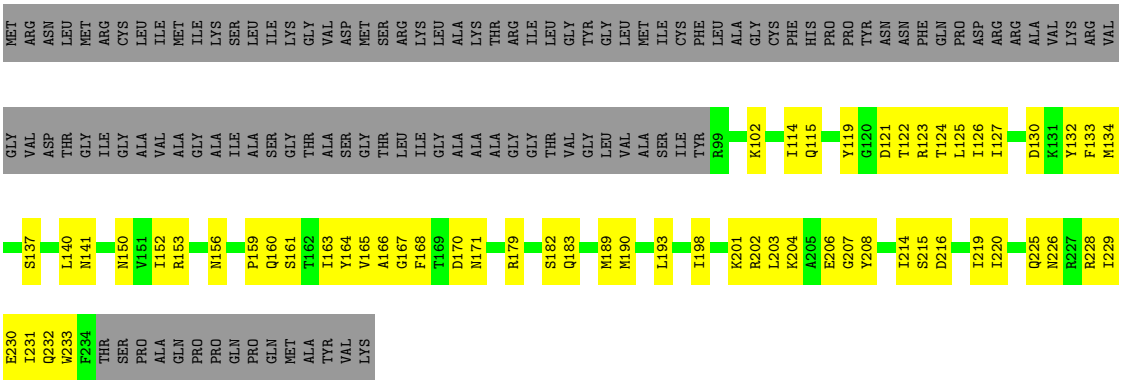




• Molecule 6: Outer membrane protein, OmpA family protein

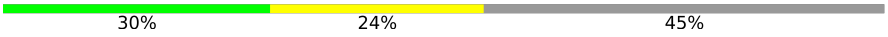
Chain HA:

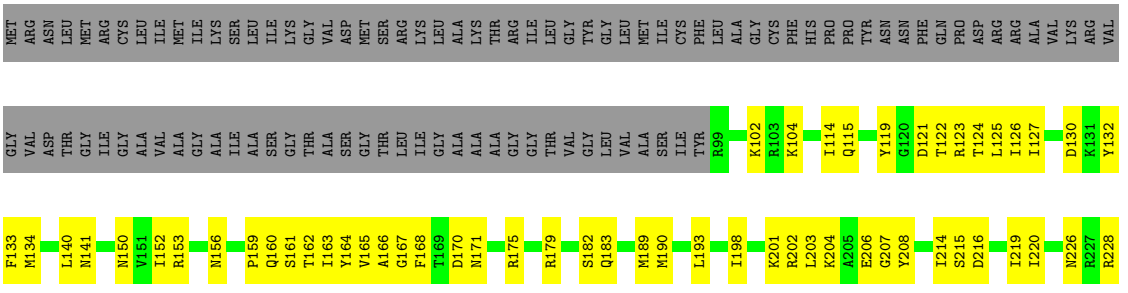


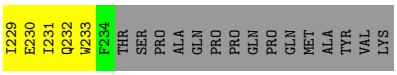


• Molecule 6: Outer membrane protein, OmpA family protein

Chain IA:

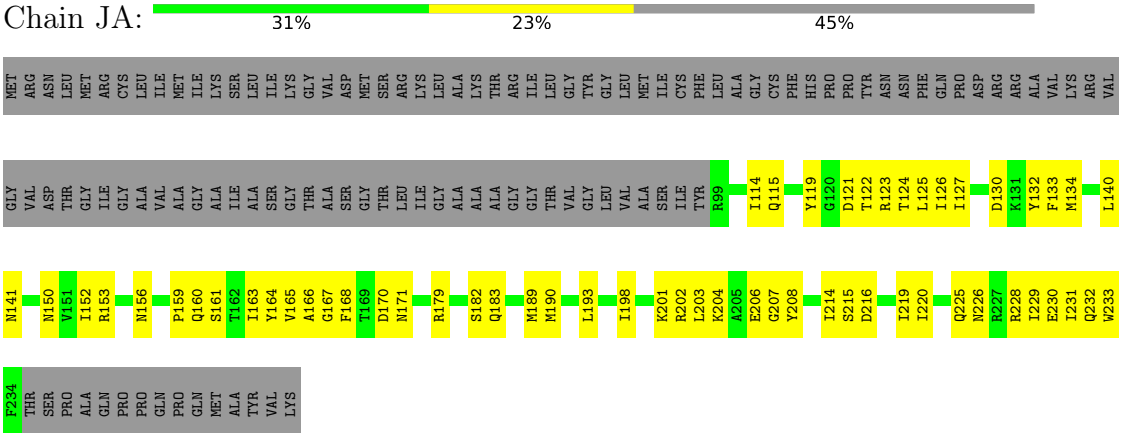






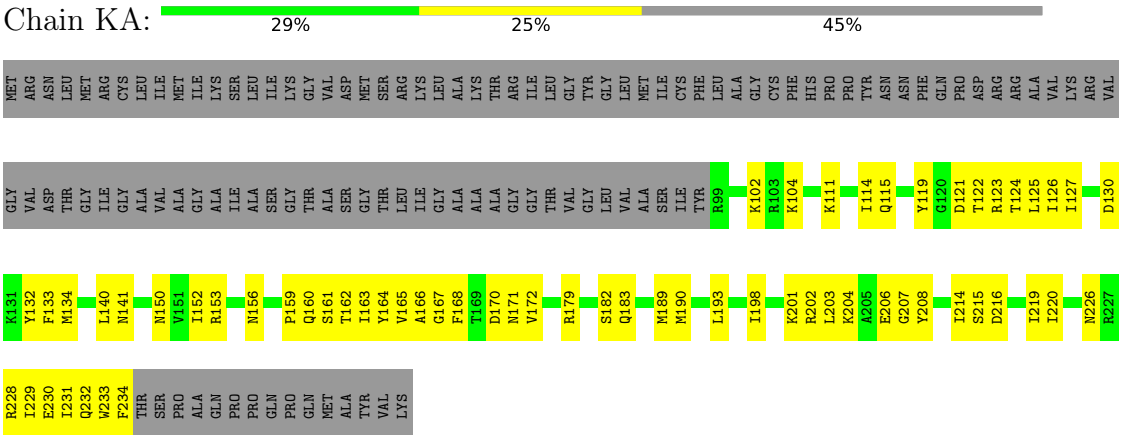
• Molecule 6: Outer membrane protein, OmpA family protein

Chain JA:



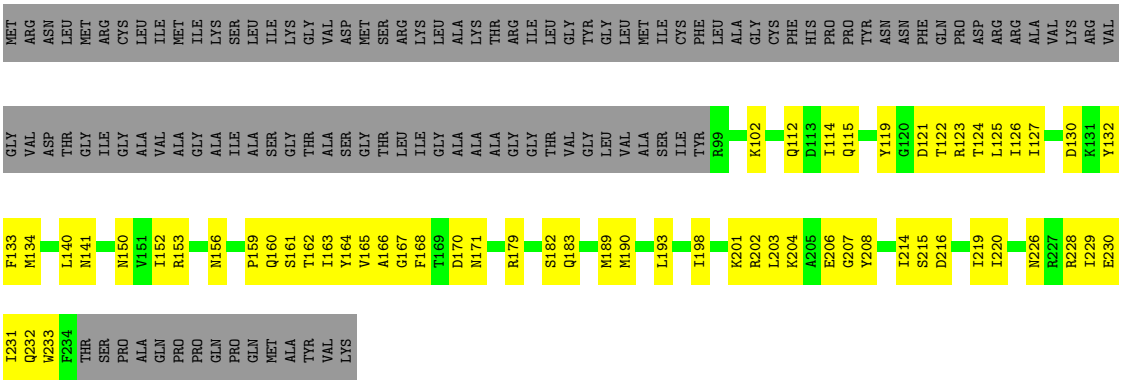
• Molecule 6: Outer membrane protein, OmpA family protein

Chain KA:



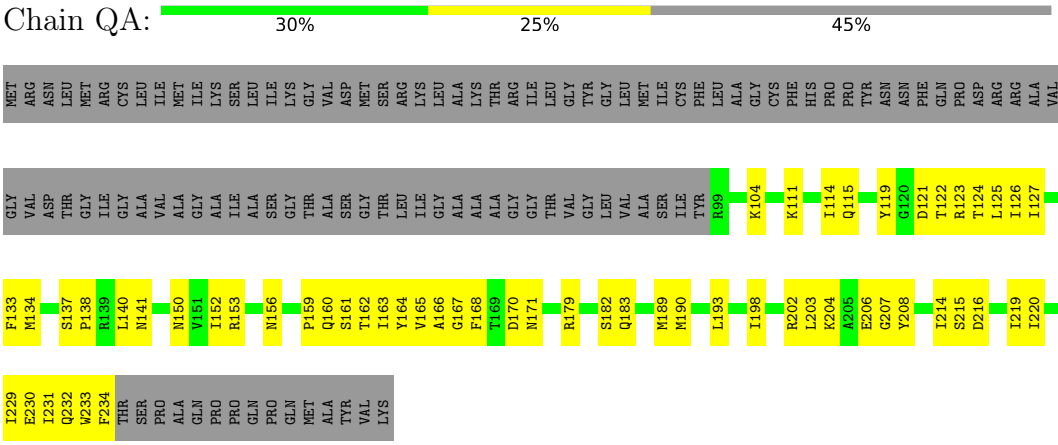
• Molecule 6: Outer membrane protein, OmpA family protein

Chain LA:



• Molecule 6: Outer membrane protein, OmpA family protein

Chain QA:


30%
25%
45%
MET ARG ASN LEU MET ARG CYS LEU ILE MET ILE LYS SER LEU ILE LYS GLY VAL ASP MET SER ARG LYS LEU ALA LYS THR ARG ILE LEU GLY TYR GLY LEU MET ILE CYS PHE LEU ALA GLY CYS PHE HIS PRO PRO TYR ASN ASN PHE GLN PRO ASP ARG ARG ALA VAL LYS ARG VAL
GLY VAL ASP THR GLY ILE GLY ALA VAL ALA ALA GLY ALA ILE ALA SER GLY THR ALA SER GLY THR LEU ILE GLY ALA ALA ALA GLY GLY THR VAL GLY LEU VAL ALA SER ILE TYR R99 K104 K111 I114 Q115 Y119 G120 D121 T122 R123 T124 L125 I126 I127 D130 K131 Y132
F133 M134 S137 P138 R139 L140 N141 N150 V151 I152 R153 N156 P159 Q160 S161 T162 I163 Y164 V165 A166 G167 F168 T169 D170 N171 R179 S182 Q183 M189 M190 L193 I198 R202 L203 K204 A205 E206 G207 Y208 I214 S215 D216 I219 I220 N226 R227 R228
I229 E230 I231 Q232 W233 F234 THR SER PRO ALA GLN PRO PRO GLN PRO GLN MET ALA TYR VAL LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6342	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 ($e^-/Å^2$)	65.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.955	Depositor
Minimum map value	-0.292	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	688.5, 688.5, 688.5	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AC	0.97	0/1629	1.17	8/2214 (0.4%)
1	BC	0.97	0/1629	1.17	8/2214 (0.4%)
1	CC	0.97	0/1629	1.17	7/2214 (0.3%)
1	DC	0.97	0/1629	1.17	7/2214 (0.3%)
1	EC	0.97	0/1629	1.17	7/2214 (0.3%)
1	FC	0.97	0/1629	1.17	7/2214 (0.3%)
1	GC	0.97	0/1629	1.17	7/2214 (0.3%)
1	HC	0.97	0/1629	1.17	7/2214 (0.3%)
1	IC	0.97	0/1629	1.17	8/2214 (0.4%)
1	JC	0.97	0/1629	1.17	7/2214 (0.3%)
1	KC	0.97	0/1629	1.17	7/2214 (0.3%)
1	LC	0.97	0/1629	1.17	7/2214 (0.3%)
1	MC	0.97	0/1629	1.17	7/2214 (0.3%)
2	AD	0.82	0/1060	0.99	0/1441
2	Ad	0.93	1/1086 (0.1%)	1.08	3/1474 (0.2%)
2	BD	0.84	0/1060	1.05	2/1441 (0.1%)
2	Bd	0.92	0/1086	1.07	3/1474 (0.2%)
2	CD	0.82	0/1060	0.95	1/1441 (0.1%)
2	Cd	0.91	0/1086	1.08	5/1474 (0.3%)
2	DD	0.82	0/1060	0.95	0/1441
2	Dd	0.94	0/1086	1.12	9/1474 (0.6%)
2	ED	0.82	0/1060	1.05	3/1441 (0.2%)
2	Ed	0.92	0/1086	1.06	0/1474
2	FD	0.81	0/1060	0.99	2/1441 (0.1%)
2	Fd	0.95	0/1086	1.11	6/1474 (0.4%)
2	GD	0.81	0/1060	0.95	4/1441 (0.3%)
2	Gd	0.93	2/1086 (0.2%)	1.11	5/1474 (0.3%)
2	HD	0.82	0/1060	0.96	0/1441
2	Hd	0.92	0/1086	1.06	2/1474 (0.1%)
2	ID	0.88	1/1060 (0.1%)	1.00	0/1441
2	Id	0.91	0/1086	1.08	6/1474 (0.4%)
2	JD	0.85	0/1060	0.99	2/1441 (0.1%)
2	Jd	0.93	0/1086	1.08	4/1474 (0.3%)
2	KD	0.81	0/1060	0.95	0/1441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Kd	0.90	0/1086	1.06	8/1474 (0.5%)
2	LD	0.81	0/1060	1.04	3/1441 (0.2%)
2	Ld	0.89	0/1086	0.97	3/1474 (0.2%)
2	MD	0.80	0/1060	0.96	1/1441 (0.1%)
2	Md	0.90	0/1086	1.03	2/1474 (0.1%)
3	AH	1.02	0/695	1.25	6/947 (0.6%)
3	BH	1.02	0/695	1.25	4/947 (0.4%)
3	CH	1.02	0/695	1.25	4/947 (0.4%)
3	DH	1.02	0/695	1.25	6/947 (0.6%)
3	EH	1.02	0/695	1.25	6/947 (0.6%)
3	FH	1.02	0/695	1.25	6/947 (0.6%)
3	GH	1.02	0/695	1.25	4/947 (0.4%)
3	HH	1.02	0/695	1.25	6/947 (0.6%)
3	IH	1.02	0/695	1.25	6/947 (0.6%)
3	JH	1.02	0/695	1.25	6/947 (0.6%)
3	KH	1.02	0/695	1.25	6/947 (0.6%)
3	LH	1.02	0/695	1.25	6/947 (0.6%)
3	MH	1.02	0/695	1.25	6/947 (0.6%)
4	AK	0.84	0/1171	1.12	4/1583 (0.3%)
4	BK	0.84	0/1171	1.12	4/1583 (0.3%)
4	CK	0.84	0/1171	1.12	4/1583 (0.3%)
4	DK	0.84	0/1171	1.12	4/1583 (0.3%)
4	EK	0.84	0/1171	1.12	4/1583 (0.3%)
4	FK	0.84	0/1171	1.12	4/1583 (0.3%)
4	GK	0.85	0/1171	1.12	4/1583 (0.3%)
4	HK	0.84	0/1171	1.12	4/1583 (0.3%)
4	IK	0.84	0/1171	1.12	4/1583 (0.3%)
4	JK	0.84	0/1171	1.12	4/1583 (0.3%)
4	KK	0.84	0/1171	1.12	4/1583 (0.3%)
4	LK	0.84	0/1171	1.12	4/1583 (0.3%)
4	MK	0.84	0/1171	1.12	4/1583 (0.3%)
6	AA	0.88	0/1130	1.07	0/1522
6	BA	0.88	0/1130	1.07	0/1522
6	CA	0.88	0/1130	1.07	0/1522
6	DA	0.88	0/1130	1.07	0/1522
6	EA	0.88	0/1130	1.06	0/1522
6	FA	0.89	0/1130	1.07	2/1522 (0.1%)
6	GA	0.88	0/1130	1.07	0/1522
6	HA	0.88	0/1130	1.07	0/1522
6	IA	0.88	0/1130	1.07	0/1522
6	JA	0.88	0/1130	1.07	0/1522
6	KA	0.88	0/1130	1.07	0/1522
6	LA	0.88	0/1130	1.07	2/1522 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
6	QA	0.88	0/1130	1.07	0/1522
All	All	0.91	4/88023 (0.0%)	1.11	296/119353 (0.2%)

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	Bd	0	1
2	Cd	0	1
2	Dd	0	1
2	Ed	0	2
2	Fd	0	1
2	Hd	0	1
2	Id	0	1
2	Jd	0	1
2	Ld	0	2
2	Md	0	1
4	AK	0	1
4	BK	0	1
4	CK	0	1
4	DK	0	1
4	EK	0	1
4	FK	0	1
4	GK	0	1
4	HK	0	1
4	IK	0	1
4	JK	0	1
4	KK	0	1
4	LK	0	1
4	MK	0	1
5	AX	0	2
5	AY	0	1
5	AZ	0	2
5	BX	0	2
5	BY	0	1
5	BZ	0	2
5	CX	0	2
5	CY	0	1
5	CZ	0	2
5	DX	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	DY	0	1
5	DZ	0	2
5	EX	0	2
5	EY	0	1
5	EZ	0	2
5	FX	0	2
5	FY	0	1
5	FZ	0	2
5	GX	0	2
5	GY	0	1
5	GZ	0	2
5	HX	0	2
5	HY	0	1
5	HZ	0	2
5	IX	0	2
5	IY	0	1
5	IZ	0	2
5	JX	0	2
5	JY	0	1
5	JZ	0	2
5	KX	0	2
5	KY	0	1
5	KZ	0	2
5	LX	0	2
5	LY	0	1
5	LZ	0	2
5	MX	0	2
5	MY	0	1
5	MZ	0	2
6	AA	0	1
6	BA	0	1
6	CA	0	1
6	DA	0	1
6	EA	0	1
6	FA	0	1
6	GA	0	1
6	HA	0	1
6	IA	0	1
6	JA	0	1
6	KA	0	1
6	LA	0	1
6	QA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	103

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Ad	55	MET	CA-C	-5.66	1.45	1.52
2	Gd	82	ARG	CZ-NH1	-5.58	1.25	1.32
2	ID	87	TRP	CB-CG	-5.54	1.33	1.50
2	Gd	55	MET	CB-CG	-5.48	1.36	1.52

The worst 5 of 296 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Kd	52	MET	CG-SD-CE	7.62	117.67	100.90
4	MK	56	MET	CB-CA-C	-7.46	99.47	110.96
4	GK	56	MET	CB-CA-C	-7.45	99.49	110.96
4	CK	56	MET	CB-CA-C	-7.44	99.50	110.96
4	FK	56	MET	CB-CA-C	-7.44	99.50	110.96

There are no chirality outliers.

5 of 103 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AK	65	ILE	Peptide
5	AX	142	UNK	Peptide
5	AX	153	UNK	Peptide
5	AY	11	UNK	Peptide
5	AZ	5	UNK	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	1596	0	1602	139	0
1	BC	1596	0	1602	139	0
1	CC	1596	0	1602	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DC	1596	0	1602	139	0
1	EC	1596	0	1602	134	0
1	FC	1596	0	1602	143	0
1	GC	1596	0	1602	140	0
1	HC	1596	0	1602	137	0
1	IC	1596	0	1602	138	0
1	JC	1596	0	1602	129	0
1	KC	1596	0	1602	134	0
1	LC	1596	0	1602	143	0
1	MC	1596	0	1602	141	0
2	AD	1040	0	1066	32	0
2	Ad	1066	0	1103	47	0
2	BD	1040	0	1066	32	0
2	Bd	1066	0	1103	44	0
2	CD	1040	0	1066	34	0
2	Cd	1066	0	1103	41	0
2	DD	1040	0	1066	28	0
2	Dd	1066	0	1103	37	0
2	ED	1040	0	1066	37	0
2	Ed	1066	0	1103	54	0
2	FD	1040	0	1066	33	0
2	Fd	1066	0	1103	42	0
2	GD	1040	0	1066	32	0
2	Gd	1066	0	1103	48	0
2	HD	1040	0	1066	43	0
2	Hd	1066	0	1103	41	0
2	ID	1040	0	1066	32	0
2	Id	1066	0	1103	47	0
2	JD	1040	0	1066	33	0
2	Jd	1066	0	1103	43	0
2	KD	1040	0	1066	26	0
2	Kd	1066	0	1103	32	0
2	LD	1040	0	1066	35	0
2	Ld	1066	0	1103	45	0
2	MD	1040	0	1066	29	0
2	Md	1066	0	1103	39	0
3	AH	678	0	689	45	0
3	BH	678	0	689	47	0
3	CH	678	0	689	44	0
3	DH	678	0	689	50	0
3	EH	678	0	689	45	0
3	FH	678	0	689	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	GH	678	0	689	50	0
3	HH	678	0	689	49	0
3	IH	678	0	689	48	0
3	JH	678	0	689	51	0
3	KH	678	0	689	51	0
3	LH	678	0	689	48	0
3	MH	678	0	689	48	0
4	AK	1152	0	1192	51	0
4	BK	1152	0	1192	48	0
4	CK	1152	0	1192	59	0
4	DK	1152	0	1192	54	0
4	EK	1152	0	1192	51	0
4	FK	1152	0	1192	51	0
4	GK	1152	0	1192	52	0
4	HK	1152	0	1192	54	0
4	IK	1152	0	1192	52	0
4	JK	1152	0	1192	50	0
4	KK	1152	0	1192	51	0
4	LK	1152	0	1192	52	0
4	MK	1152	0	1192	54	0
5	AX	1140	0	259	16	0
5	AY	260	0	57	3	0
5	AZ	350	0	78	10	0
5	BX	1140	0	259	16	0
5	BY	260	0	57	3	0
5	BZ	350	0	78	9	0
5	CX	1140	0	259	16	0
5	CY	260	0	57	3	0
5	CZ	350	0	78	10	0
5	DX	1140	0	259	16	0
5	DY	260	0	57	2	0
5	DZ	350	0	78	12	0
5	EX	1140	0	259	16	0
5	EY	260	0	57	3	0
5	EZ	350	0	78	10	0
5	FX	1140	0	259	16	0
5	FY	260	0	57	3	0
5	FZ	350	0	78	10	0
5	GX	1140	0	259	17	0
5	GY	260	0	57	3	0
5	GZ	350	0	78	10	0
5	HX	1140	0	259	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	HY	260	0	57	3	0
5	HZ	350	0	78	12	0
5	IX	1140	0	259	16	0
5	IY	260	0	57	3	0
5	IZ	350	0	78	9	0
5	JX	1140	0	259	17	0
5	JY	260	0	57	3	0
5	JZ	350	0	78	10	0
5	KX	1140	0	259	16	0
5	KY	260	0	57	3	0
5	KZ	350	0	78	14	0
5	LX	1140	0	259	16	0
5	LY	260	0	57	2	0
5	LZ	350	0	78	10	0
5	MX	1140	0	259	16	0
5	MY	260	0	57	2	0
5	MZ	350	0	78	10	0
6	AA	1108	0	1107	50	0
6	BA	1108	0	1107	51	0
6	CA	1108	0	1107	50	0
6	DA	1108	0	1107	54	0
6	EA	1108	0	1107	50	0
6	FA	1108	0	1107	50	0
6	GA	1108	0	1107	49	0
6	HA	1108	0	1107	53	0
6	IA	1108	0	1107	54	0
6	JA	1108	0	1107	50	0
6	KA	1108	0	1107	53	0
6	LA	1108	0	1107	50	0
6	QA	1108	0	1107	54	0
All	All	109070	0	92989	4513	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 22.

The worst 5 of 4513 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)
4:GK:154:ILE:O	2:Gd:83:ALA:HA	1.55	1.04
6:AA:124:THR:HA	6:AA:231:ILE:O	1.62	1.00
6:BA:124:THR:HA	6:BA:231:ILE:O	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:QA:124:THR:HA	6:QA:231:ILE:O	1.62	1.00
6:KA:124:THR:HA	6:KA:231:ILE:O	1.62	0.99

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	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	BC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	CC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	DC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	EC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	FC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	GC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	HC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	IC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	JC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	KC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	LC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
1	MC	196/303 (65%)	179 (91%)	17 (9%)	0	100	100
2	AD	133/163 (82%)	131 (98%)	2 (2%)	0	100	100
2	Ad	136/163 (83%)	129 (95%)	6 (4%)	1 (1%)	18	54
2	BD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Bd	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
2	CD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Cd	136/163 (83%)	121 (89%)	15 (11%)	0	100	100
2	DD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
2	Dd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
2	ED	133/163 (82%)	124 (93%)	9 (7%)	0	100	100
2	Ed	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
2	FD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
2	Fd	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
2	GD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Gd	136/163 (83%)	122 (90%)	13 (10%)	1 (1%)	18	54
2	HD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Hd	136/163 (83%)	121 (89%)	15 (11%)	0	100	100
2	ID	133/163 (82%)	131 (98%)	2 (2%)	0	100	100
2	Id	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
2	JD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
2	Jd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
2	KD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
2	Kd	136/163 (83%)	122 (90%)	14 (10%)	0	100	100
2	LD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
2	Ld	136/163 (83%)	124 (91%)	12 (9%)	0	100	100
2	MD	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
2	Md	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
3	AH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	BH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	CH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	DH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	EH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	FH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	GH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	HH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	IH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	JH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	KH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	LH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
3	MH	87/361 (24%)	74 (85%)	13 (15%)	0	100	100
4	AK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	BK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	CK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	DK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	EK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	FK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	GK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	HK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	IK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	JK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	KK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	LK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
4	MK	146/189 (77%)	132 (90%)	14 (10%)	0	100	100
6	AA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	BA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	CA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	DA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	EA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	FA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	GA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	HA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	IA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	JA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	KA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	LA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
6	QA	134/249 (54%)	119 (89%)	15 (11%)	0	100	100
All	All	10816/18564 (58%)	9831 (91%)	983 (9%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Ad	28	PRO
2	Gd	28	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	BC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	CC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	DC	169/257 (66%)	169 (100%)	0	100	100
1	EC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	FC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	GC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	HC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	IC	169/257 (66%)	169 (100%)	0	100	100
1	JC	169/257 (66%)	169 (100%)	0	100	100
1	KC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	LC	169/257 (66%)	168 (99%)	1 (1%)	78	80
1	MC	169/257 (66%)	168 (99%)	1 (1%)	78	80
2	AD	116/139 (84%)	116 (100%)	0	100	100
2	Ad	119/139 (86%)	119 (100%)	0	100	100
2	BD	116/139 (84%)	116 (100%)	0	100	100
2	Bd	119/139 (86%)	119 (100%)	0	100	100
2	CD	116/139 (84%)	116 (100%)	0	100	100
2	Cd	119/139 (86%)	119 (100%)	0	100	100
2	DD	116/139 (84%)	116 (100%)	0	100	100
2	Dd	119/139 (86%)	119 (100%)	0	100	100
2	ED	116/139 (84%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ed	119/139 (86%)	119 (100%)	0	100	100
2	FD	116/139 (84%)	116 (100%)	0	100	100
2	Fd	119/139 (86%)	119 (100%)	0	100	100
2	GD	116/139 (84%)	116 (100%)	0	100	100
2	Gd	119/139 (86%)	119 (100%)	0	100	100
2	HD	116/139 (84%)	116 (100%)	0	100	100
2	Hd	119/139 (86%)	119 (100%)	0	100	100
2	ID	116/139 (84%)	116 (100%)	0	100	100
2	Id	119/139 (86%)	119 (100%)	0	100	100
2	JD	116/139 (84%)	116 (100%)	0	100	100
2	Jd	119/139 (86%)	119 (100%)	0	100	100
2	KD	116/139 (84%)	116 (100%)	0	100	100
2	Kd	119/139 (86%)	119 (100%)	0	100	100
2	LD	116/139 (84%)	116 (100%)	0	100	100
2	Ld	119/139 (86%)	119 (100%)	0	100	100
2	MD	116/139 (84%)	116 (100%)	0	100	100
2	Md	119/139 (86%)	119 (100%)	0	100	100
3	AH	75/300 (25%)	75 (100%)	0	100	100
3	BH	75/300 (25%)	75 (100%)	0	100	100
3	CH	75/300 (25%)	75 (100%)	0	100	100
3	DH	75/300 (25%)	75 (100%)	0	100	100
3	EH	75/300 (25%)	75 (100%)	0	100	100
3	FH	75/300 (25%)	75 (100%)	0	100	100
3	GH	75/300 (25%)	75 (100%)	0	100	100
3	HH	75/300 (25%)	75 (100%)	0	100	100
3	IH	75/300 (25%)	75 (100%)	0	100	100
3	JH	75/300 (25%)	75 (100%)	0	100	100
3	KH	75/300 (25%)	75 (100%)	0	100	100
3	LH	75/300 (25%)	75 (100%)	0	100	100
3	MH	75/300 (25%)	75 (100%)	0	100	100
4	AK	126/163 (77%)	125 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	CK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	DK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	EK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	FK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	GK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	HK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	IK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	JK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	KK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	LK	126/163 (77%)	125 (99%)	1 (1%)	73	77
4	MK	126/163 (77%)	125 (99%)	1 (1%)	73	77
6	AA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	BA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	CA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	DA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	EA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	FA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	GA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	HA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	IA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	JA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	KA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	LA	118/203 (58%)	117 (99%)	1 (1%)	73	77
6	QA	118/203 (58%)	117 (99%)	1 (1%)	73	77
All	All	9399/15613 (60%)	9363 (100%)	36 (0%)	81	82

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	FA	119	TYR
6	QA	119	TYR
6	GA	119	TYR

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Mol	Chain	Res	Type
6	JA	119	TYR
4	GK	163	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	HC	104	ASN
1	JC	149	GLN
6	GA	156	ASN
1	HC	149	GLN
3	IH	356	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)

There are no chain breaks in this entry.

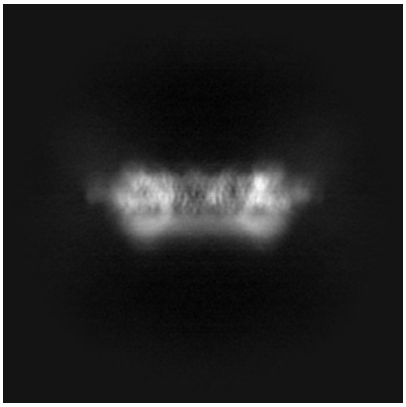
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22071. These allow visual inspection of the internal detail of the map and identification of artifacts.

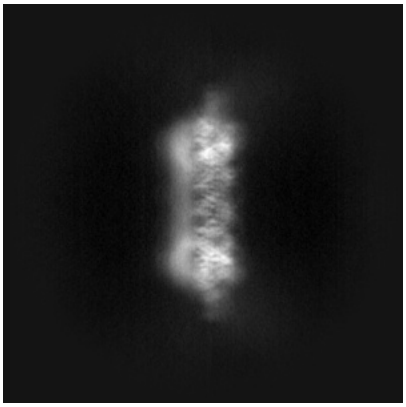
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

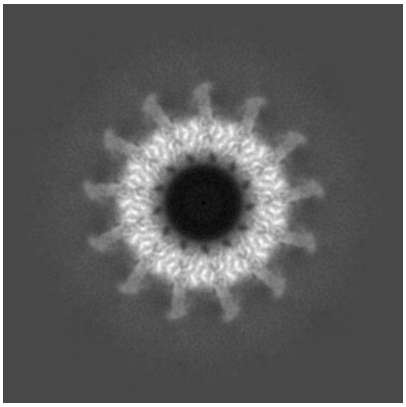
6.1.1 Primary map



X



Y

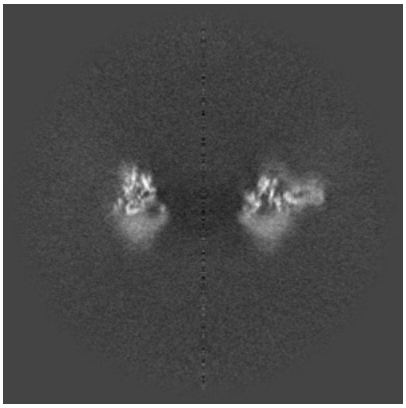


Z

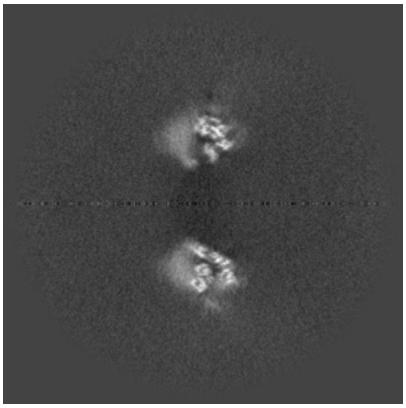
The images above show the map projected in three orthogonal directions.

6.2 Central slices

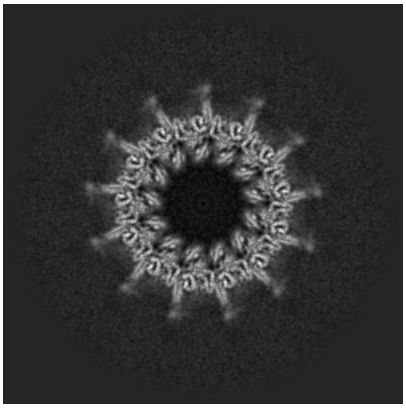
6.2.1 Primary map



X Index: 255



Y Index: 255

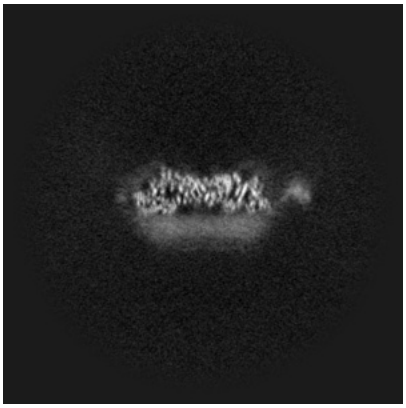


Z Index: 255

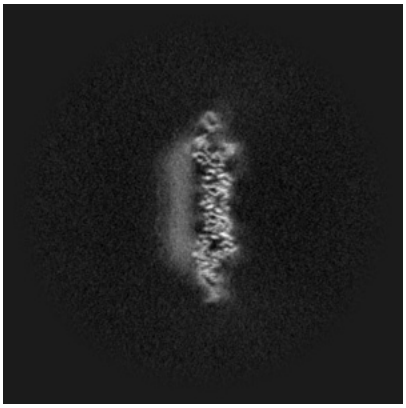
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

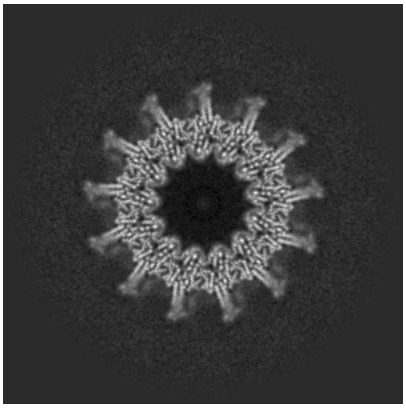
6.3.1 Primary map



X Index: 184



Y Index: 326

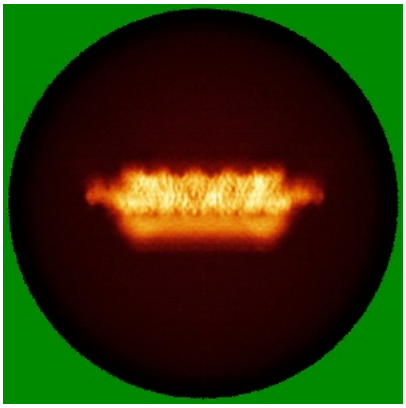


Z Index: 258

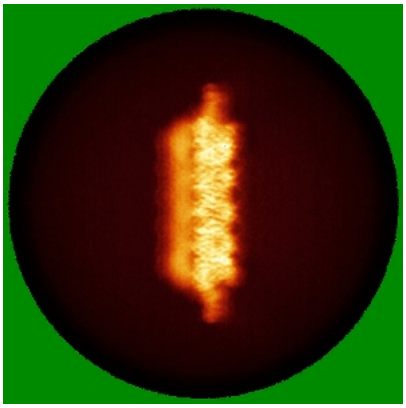
The images above show the largest variance slices of the map in three orthogonal directions.

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

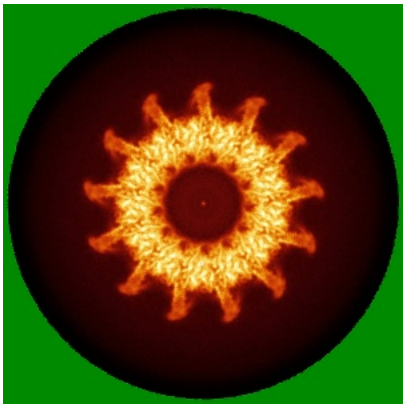
6.4.1 Primary map



X



Y

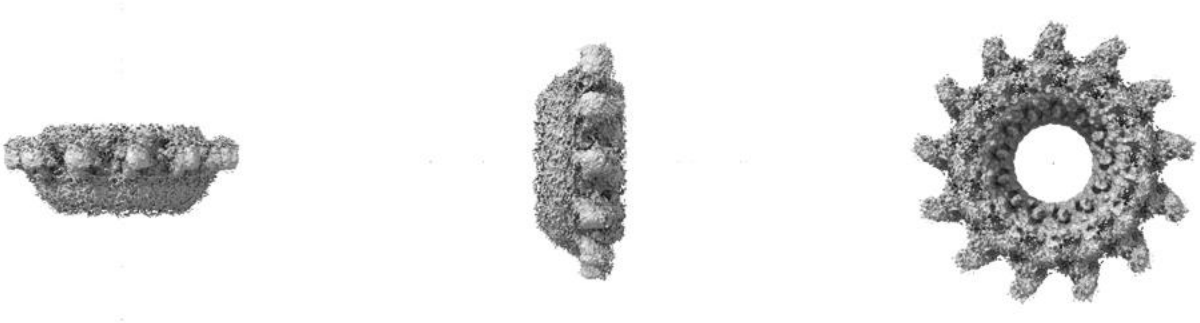


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

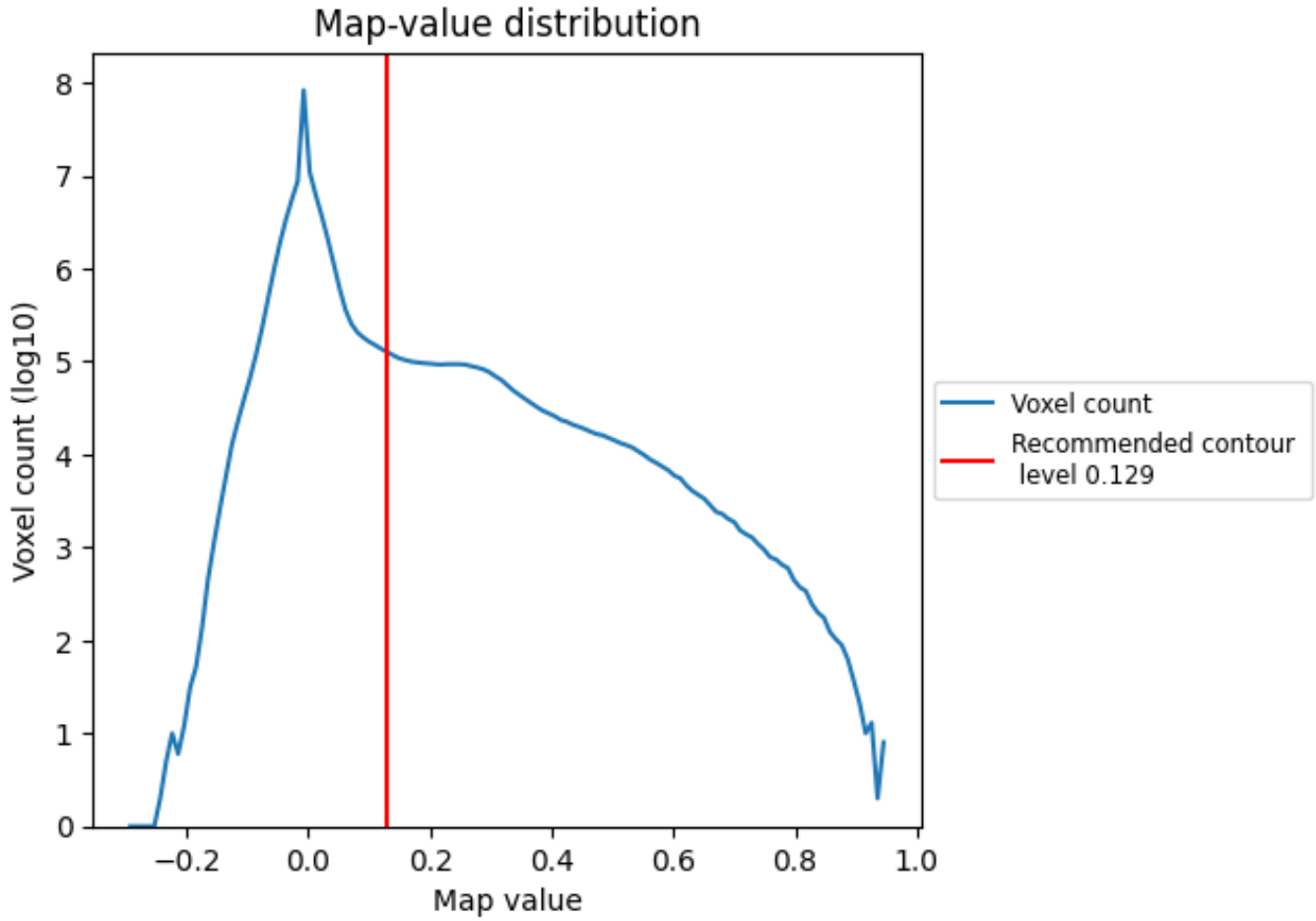
6.6 Mask visualisation (i)

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

7 Map analysis

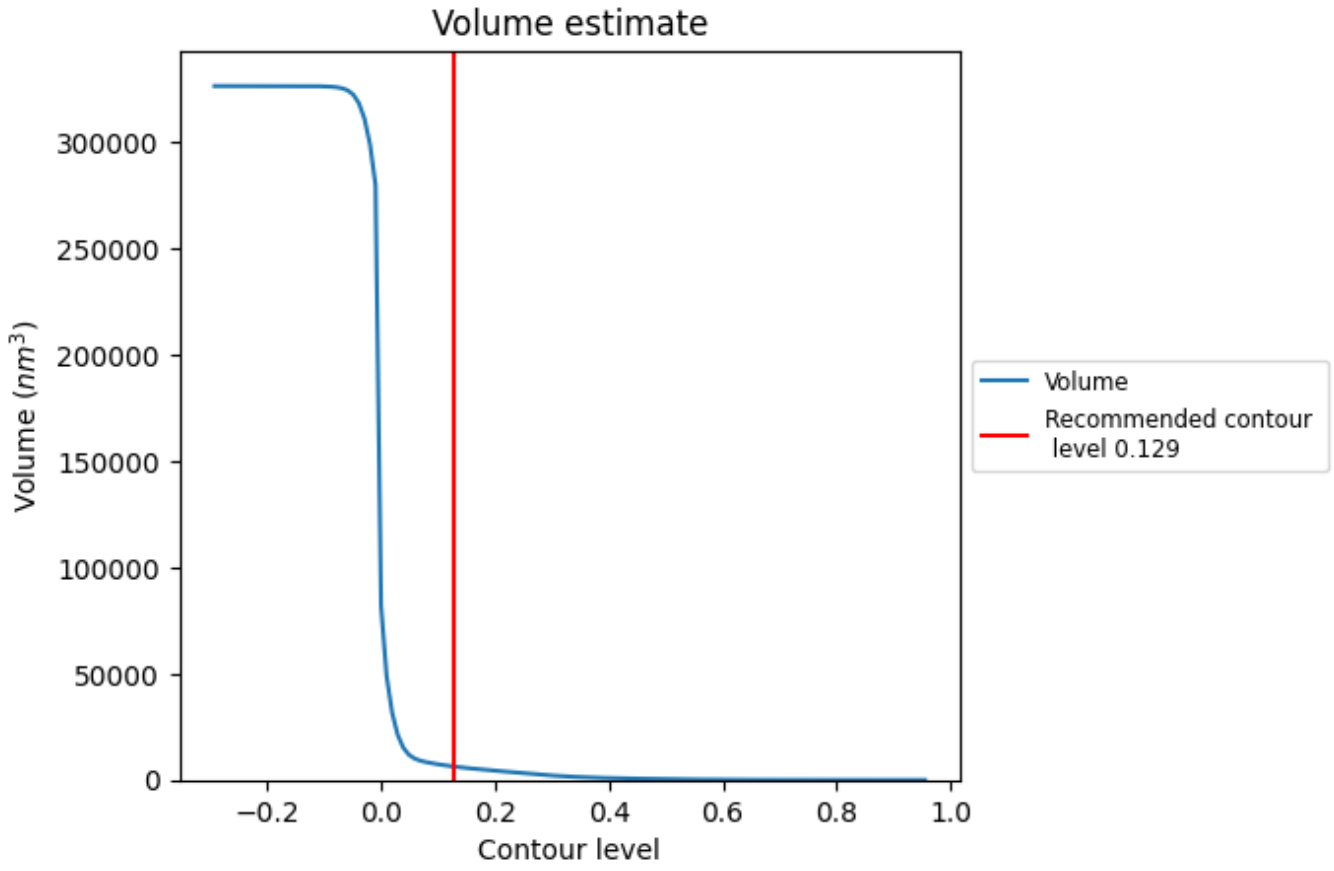
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

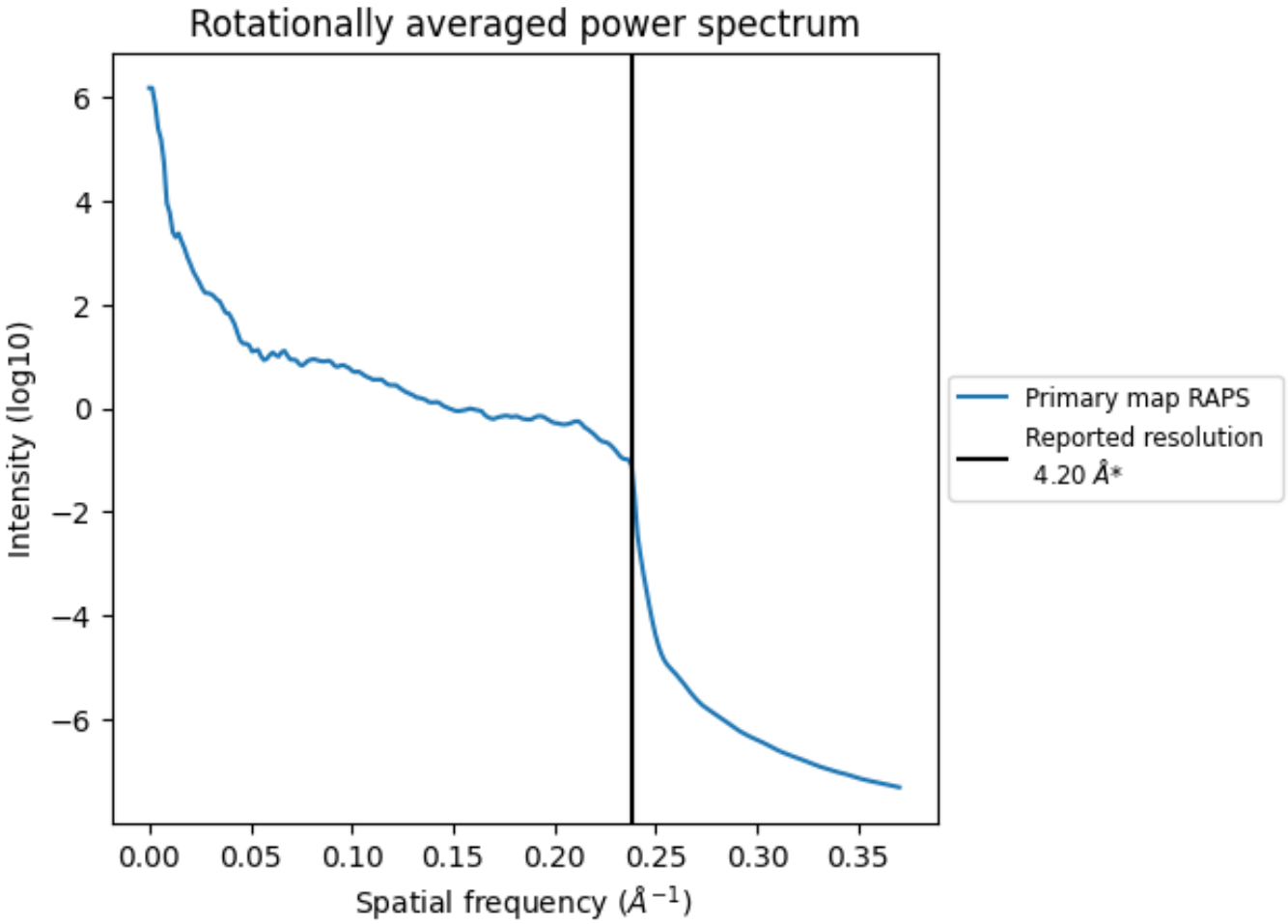
7.2 Volume estimate (i)



The volume at the recommended contour level is 6278 nm^3; this corresponds to an approximate mass of 5671 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 0.238 Å^{-1}

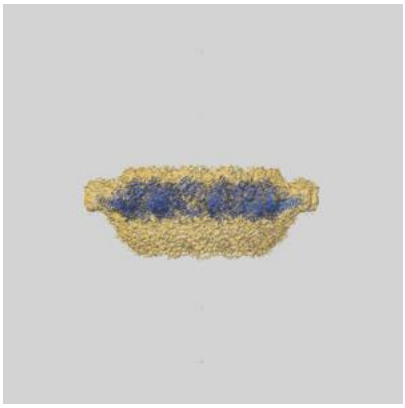
8 Fourier-Shell correlation

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

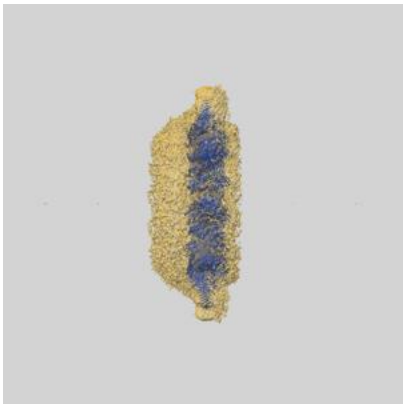
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22071 and PDB model 6X66. Per-residue inclusion information can be found in section 3 on page 15.

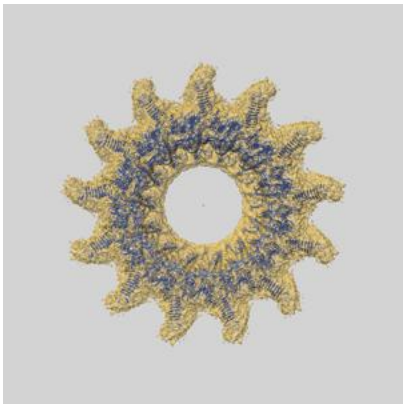
9.1 Map-model overlay



X



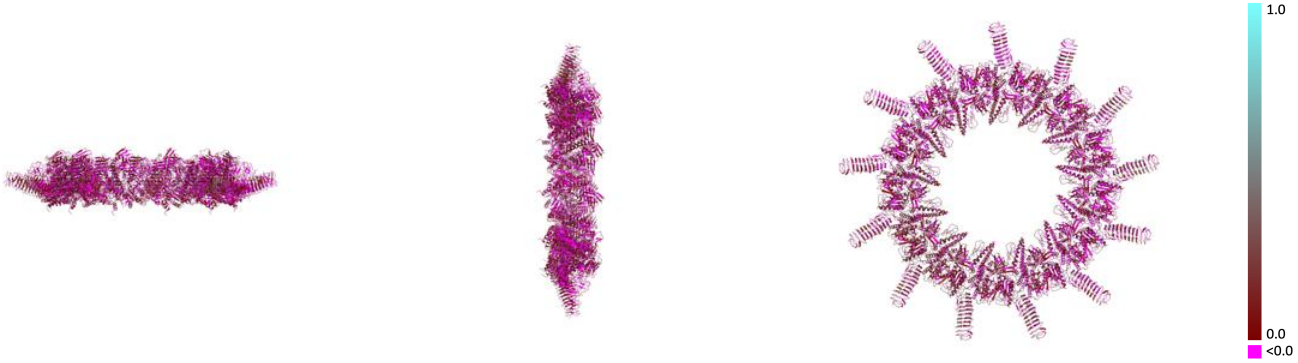
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

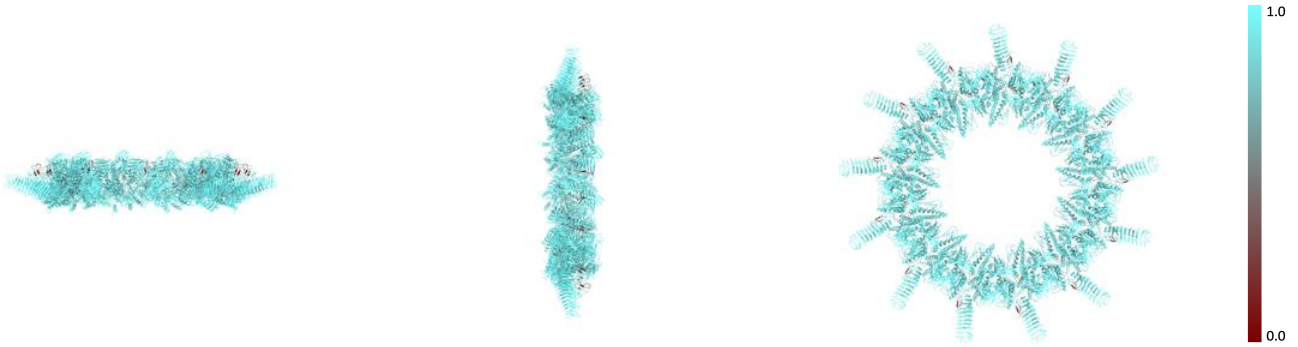
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

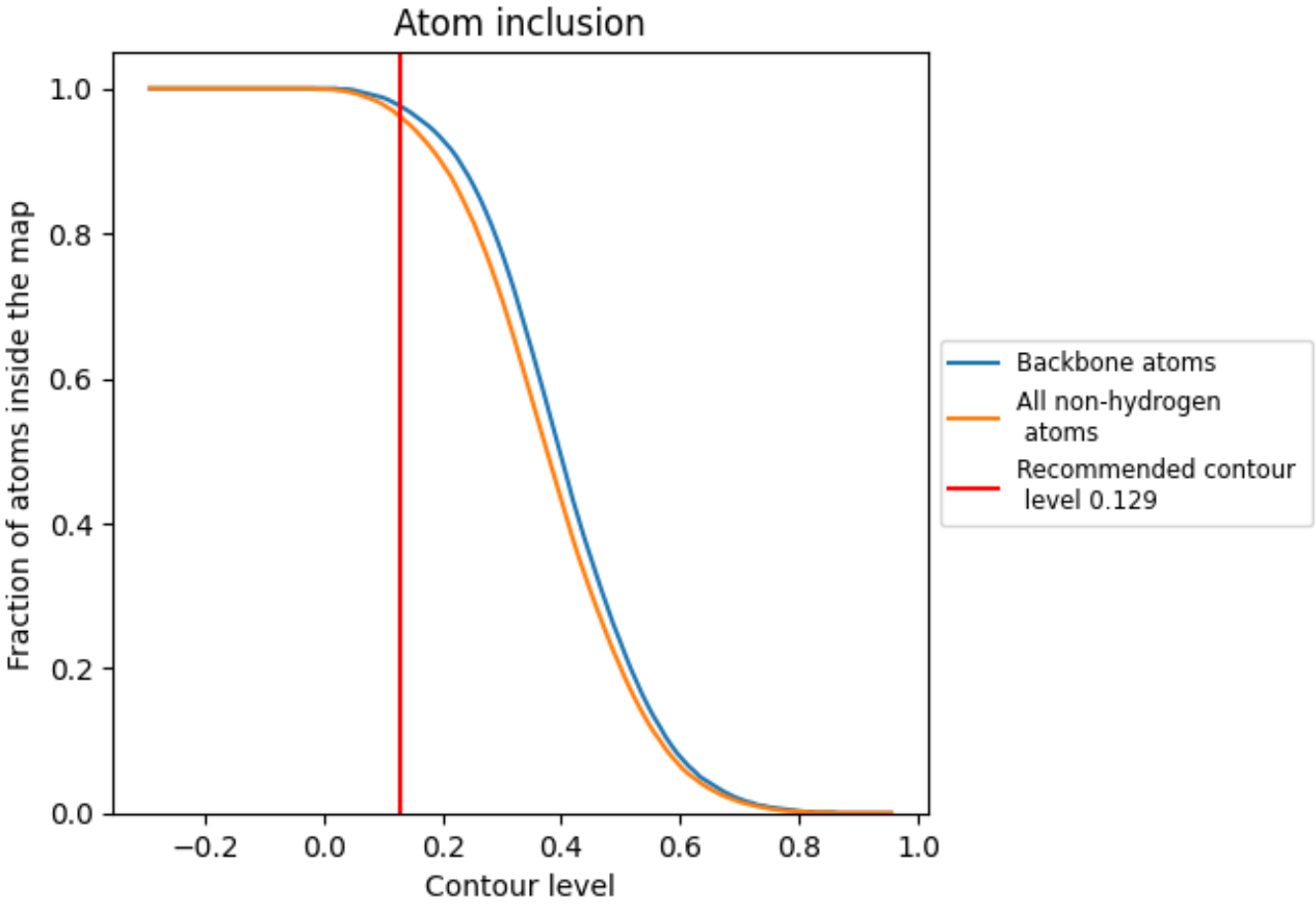
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.129).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.0690
AA	0.9770	0.0470
AC	0.9780	0.0500
AD	0.9400	0.0030
AH	0.9550	0.0500
AK	0.9710	0.0520
AX	0.9920	0.1080
AY	0.6120	0.0340
AZ	0.9510	0.1000
Ad	0.9510	0.0310
BA	0.9750	0.0560
BC	0.9800	0.0670
BD	0.9410	0.0240
BH	0.9530	0.0670
BK	0.9650	0.0620
BX	0.9920	0.1080
BY	0.6270	-0.0210
BZ	0.9660	0.1110
Bd	0.9550	0.0370
CA	0.9690	0.0540
CC	0.9790	0.0720
CD	0.9580	0.0580
CH	0.9430	0.0610
CK	0.9520	0.0490
CX	0.9950	0.0350
CY	0.6000	-0.0600
CZ	0.9710	0.1010
Cd	0.9660	0.0470
DA	0.9680	0.0420
DC	0.9760	0.0650
DD	0.9600	0.0780
DH	0.9320	0.0470
DK	0.9430	0.0320
DX	0.9900	-0.0110
DY	0.6380	-0.0340



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Chain	Atom inclusion	Q-score
DZ	0.9830	0.1030
Dd	0.9430	0.0460
EA	0.9710	0.0300
EC	0.9750	0.0570
ED	0.9640	0.0750
EH	0.9490	0.0420
EK	0.9460	0.0200
EX	0.9880	0.0320
EY	0.6920	-0.0170
EZ	0.9970	0.1040
Ed	0.9290	0.0380
FA	0.9710	0.0450
FC	0.9660	0.0660
FD	0.9710	0.0670
FH	0.9520	0.0360
FK	0.9580	0.0340
FX	0.9930	0.0520
FY	0.7230	-0.0370
FZ	0.9910	0.0780
Fd	0.9280	0.0400
GA	0.9880	0.0830
GC	0.9670	0.0870
GD	0.9690	0.0760
GH	0.9610	0.0440
GK	0.9700	0.0810
GX	0.9960	0.0550
GY	0.7230	-0.0310
GZ	0.9890	0.0780
Gd	0.9330	0.0540
HA	0.9940	0.1260
HC	0.9670	0.1100
HD	0.9690	0.0920
HH	0.9680	0.0780
HK	0.9840	0.1240
HX	0.9990	0.0940
HY	0.7390	-0.0200
HZ	0.9890	0.0990
Hd	0.9580	0.0870
IA	0.9860	0.1260
IC	0.9760	0.1140
ID	0.9820	0.1250
IH	0.9700	0.1150

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Chain	Atom inclusion	Q-score
IK	0.9890	0.1330
IX	1.0000	0.1570
IY	0.7190	-0.0220
IZ	0.9890	0.1280
Id	0.9850	0.1270
JA	0.9780	0.0840
JC	0.9800	0.0990
JD	0.9800	0.1420
JH	0.9740	0.1160
JK	0.9850	0.1070
JX	1.0000	0.1980
JY	0.6730	-0.0200
JZ	0.9940	0.1360
Jd	0.9820	0.1100
KA	0.9790	0.0560
KC	0.9700	0.0750
KD	0.9740	0.1220
KH	0.9620	0.0850
KK	0.9800	0.0760
KX	0.9990	0.1460
KY	0.6000	-0.0060
KZ	1.0000	0.1190
Kd	0.9690	0.0700
LA	0.9750	0.0430
LC	0.9660	0.0570
LD	0.9550	0.0730
LH	0.9580	0.0570
LK	0.9780	0.0560
LX	0.9960	0.0440
LY	0.6310	0.0210
LZ	0.9800	0.0890
Ld	0.9540	0.0490
MC	0.9720	0.0470
MD	0.9370	0.0150
MH	0.9580	0.0440
MK	0.9710	0.0510
MX	0.9930	0.0460
MY	0.6080	0.0550
MZ	0.9660	0.0800
Md	0.9400	0.0440
QA	0.9730	0.0410