Full wwPDB EM Validation Report ⓘ

Feb 25, 2024 – 09:18 AM EST

PDB ID	:	6X65
EMDB ID	:	EMD-22070
Title	:	Legionella pneumophila Dot/Icm T4SS
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	:	3.70 Å(reported)

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

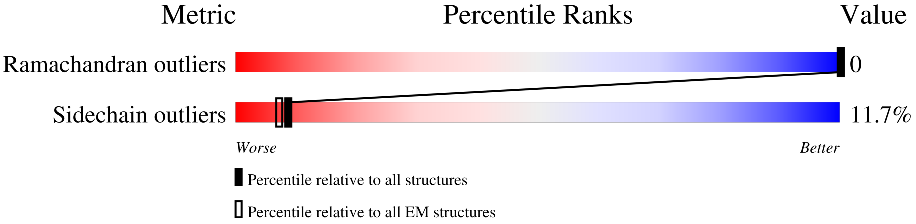
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

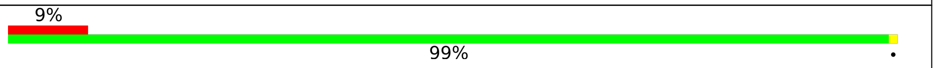
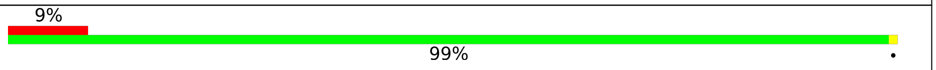
The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AV	228	
1	AW	228	
1	AX	228	
1	AY	228	
1	AZ	228	
1	BV	228	
1	BW	228	
1	BX	228	
1	BY	228	

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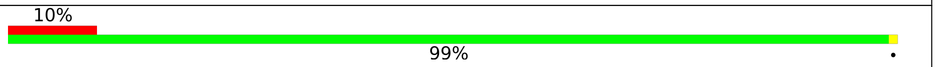
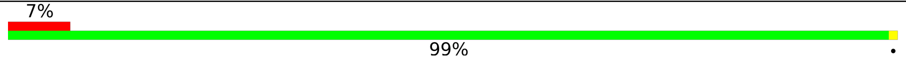
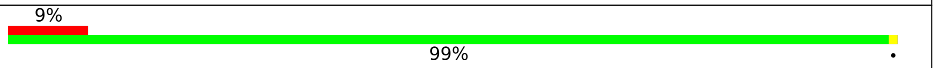
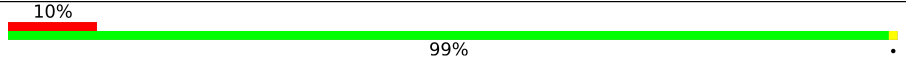
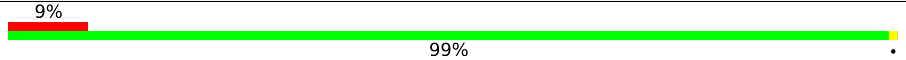
Mol	Chain	Length	Quality of chain
1	BZ	228	
1	CV	228	
1	CW	228	
1	CX	228	
1	CY	228	
1	CZ	228	
1	DV	228	
1	DW	228	
1	DX	228	
1	DY	228	
1	DZ	228	
1	EV	228	
1	EW	228	
1	EX	228	
1	EY	228	
1	EZ	228	
1	FV	228	
1	FW	228	
1	FX	228	
1	FY	228	
1	FZ	228	
1	GV	228	
1	GW	228	
1	GX	228	
1	GY	228	

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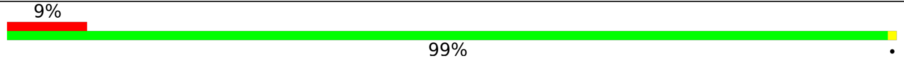
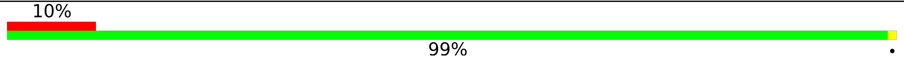
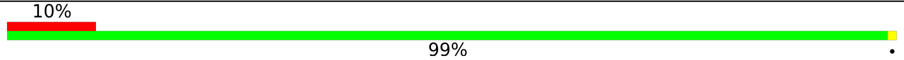
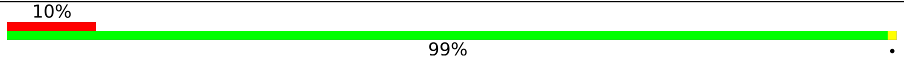
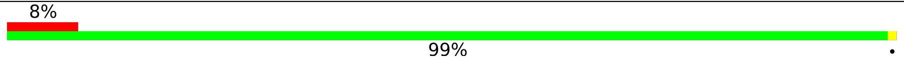
Mol	Chain	Length	Quality of chain
1	GZ	228	
1	HV	228	
1	HW	228	
1	HX	228	
1	HY	228	
1	HZ	228	
1	IV	228	
1	IW	228	
1	IX	228	
1	IY	228	
1	IZ	228	
1	JV	228	
1	JW	228	
1	JX	228	
1	JY	228	
1	JZ	228	
1	KV	228	
1	KW	228	
1	KX	228	
1	KY	228	
1	KZ	228	
1	LV	228	
1	LW	228	
1	LX	228	
1	LY	228	

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Mol	Chain	Length	Quality of chain
1	LZ	228	30% 69%
1	MV	228	63% 37%
1	MW	228	14% 86%
1	MX	228	9% 99%
1	MY	228	23% 77%
1	MZ	228	30% 69%
1	NV	228	63% 37%
1	NW	228	14% 86%
1	OV	228	62% 37%
1	OW	228	14% 86%
1	PV	228	63% 37%
1	PW	228	14% 86%
1	QV	228	63% 37%
1	QW	228	14% 86%
1	RV	228	63% 37%
1	RW	228	14% 86%
2	AC	303	62% 34%
2	BC	303	60% 6% 34%
2	CC	303	60% 6% 34%
2	DC	303	59% 7% 34%
2	EC	303	60% 6% 34%
2	FC	303	61% 5% 34%
2	GC	303	60% 6% 34%
2	HC	303	61% 5% 34%
2	IC	303	60% 6% 34%

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Mol	Chain	Length	Quality of chain
2	JC	303	
2	KC	303	
2	LC	303	
2	MC	303	
3	AD	163	
3	Ad	163	
3	BD	163	
3	Bd	163	
3	CD	163	
3	Cd	163	
3	DD	163	
3	Dd	163	
3	ED	163	
3	Ed	163	
3	FD	163	
3	Fd	163	
3	GD	163	
3	Gd	163	
3	HD	163	
3	Hd	163	
3	ID	163	
3	Id	163	
3	JD	163	
3	Jd	163	
3	KD	163	

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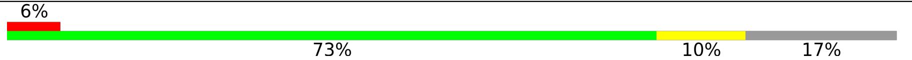
Mol	Chain	Length	Quality of chain
3	Kd	163	 • 72% 12% • 15%
3	LD	163	 • 72% 11% 17%
3	Ld	163	 • 74% 10% • 15%
3	MD	163	 6% 73% 10% 17%
3	Md	163	 • 71% 12% • 15%
4	AH	361	 22% • 75%
4	BH	361	 21% • 75%
4	CH	361	 • 22% • 75%
4	DH	361	 21% • 75%
4	EH	361	 22% • 75%
4	FH	361	 • 23% • 75%
4	GH	361	 21% • 75%
4	HH	361	 • 23% • 75%
4	IH	361	 22% • 75%
4	JH	361	 • 21% • 75%
4	KH	361	 • 22% • 75%
4	LH	361	 21% • 75%
4	MH	361	 22% • 75%
5	AK	189	 • 69% 10% 22%
5	BK	189	 • 68% 10% • 22%
5	CK	189	 • 66% 12% • 22%
5	DK	189	 • 69% 10% 22%
5	EK	189	 • 69% 9% 22%
5	FK	189	 • 66% 13% 22%
5	GK	189	 • 68% 11% 22%

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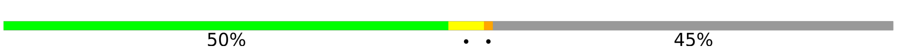
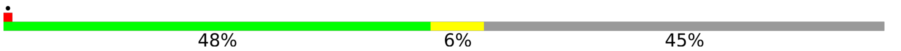
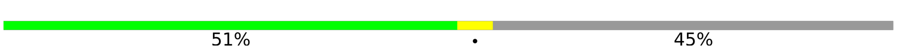
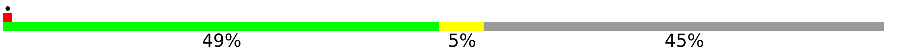
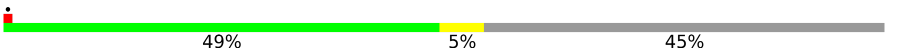
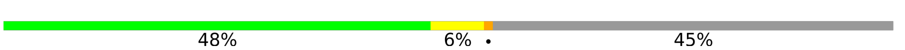
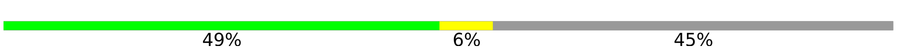
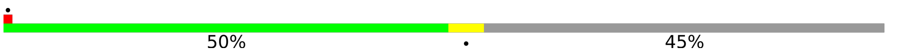
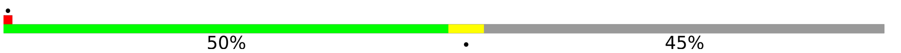
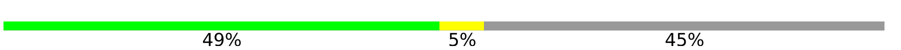
Mol	Chain	Length	Quality of chain
5	HK	189	
5	IK	189	
5	JK	189	
5	KK	189	
5	LK	189	
5	MK	189	
6	N	249	
6	O	249	
6	P	249	
6	Q	249	
6	R	249	
6	S	249	
6	T	249	
6	U	249	
6	V	249	
6	W	249	
6	X	249	
6	Y	249	
6	Z	249	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 124910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Type IV secretion system unknown protein fragment.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	AV	144	Total C N O 720 432 144 144	0	0
1	AW	32	Total C N O 160 96 32 32	0	0
1	BV	144	Total C N O 720 432 144 144	0	0
1	BW	32	Total C N O 160 96 32 32	0	0
1	CV	144	Total C N O 720 432 144 144	0	0
1	CW	32	Total C N O 160 96 32 32	0	0
1	DV	144	Total C N O 720 432 144 144	0	0
1	DW	32	Total C N O 160 96 32 32	0	0
1	EV	144	Total C N O 720 432 144 144	0	0
1	EW	32	Total C N O 160 96 32 32	0	0
1	FV	144	Total C N O 720 432 144 144	0	0
1	FW	32	Total C N O 160 96 32 32	0	0
1	GV	144	Total C N O 720 432 144 144	0	0
1	GW	32	Total C N O 160 96 32 32	0	0
1	HV	144	Total C N O 720 432 144 144	0	0
1	HW	32	Total C N O 160 96 32 32	0	0
1	IV	144	Total C N O 720 432 144 144	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	IW	32	Total C N O 160 96 32 32	0	0
1	JV	144	Total C N O 720 432 144 144	0	0
1	JW	32	Total C N O 160 96 32 32	0	0
1	KV	144	Total C N O 720 432 144 144	0	0
1	KW	32	Total C N O 160 96 32 32	0	0
1	LV	144	Total C N O 720 432 144 144	0	0
1	LW	32	Total C N O 160 96 32 32	0	0
1	MV	144	Total C N O 720 432 144 144	0	0
1	MW	32	Total C N O 160 96 32 32	0	0
1	NV	144	Total C N O 720 432 144 144	0	0
1	NW	32	Total C N O 160 96 32 32	0	0
1	OV	144	Total C N O 720 432 144 144	0	0
1	OW	32	Total C N O 160 96 32 32	0	0
1	PV	144	Total C N O 720 432 144 144	0	0
1	PW	32	Total C N O 160 96 32 32	0	0
1	QV	144	Total C N O 720 432 144 144	0	0
1	QW	32	Total C N O 160 96 32 32	0	0
1	RV	144	Total C N O 720 432 144 144	0	0
1	RW	32	Total C N O 160 96 32 32	0	0
1	AX	228	Total C N O 1140 684 228 228	0	0
1	AY	52	Total C N O 260 156 52 52	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
1	AZ	70	Total C N O 350 210 70 70	0	0
1	BX	228	Total C N O 1140 684 228 228	0	0
1	BY	52	Total C N O 260 156 52 52	0	0
1	BZ	70	Total C N O 350 210 70 70	0	0
1	CX	228	Total C N O 1140 684 228 228	0	0
1	CY	52	Total C N O 260 156 52 52	0	0
1	CZ	70	Total C N O 350 210 70 70	0	0
1	DX	228	Total C N O 1140 684 228 228	0	0
1	DY	52	Total C N O 260 156 52 52	0	0
1	DZ	70	Total C N O 350 210 70 70	0	0
1	EX	228	Total C N O 1140 684 228 228	0	0
1	EY	52	Total C N O 260 156 52 52	0	0
1	EZ	70	Total C N O 350 210 70 70	0	0
1	FX	228	Total C N O 1140 684 228 228	0	0
1	FY	52	Total C N O 260 156 52 52	0	0
1	FZ	70	Total C N O 350 210 70 70	0	0
1	GX	228	Total C N O 1140 684 228 228	0	0
1	GY	52	Total C N O 260 156 52 52	0	0
1	GZ	70	Total C N O 350 210 70 70	0	0
1	HX	228	Total C N O 1140 684 228 228	0	0
1	HY	52	Total C N O 260 156 52 52	0	0

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

- Molecule 2 is a protein called DotC.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	AC	200	Total C N O S 1596 1016 280 295 5	0	0
2	BC	200	Total C N O S 1596 1016 280 295 5	0	0
2	CC	200	Total C N O S 1596 1016 280 295 5	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
2	DC	200	Total C N O S 1596 1016 280 295 5	0	0
2	EC	200	Total C N O S 1596 1016 280 295 5	0	0
2	FC	200	Total C N O S 1596 1016 280 295 5	0	0
2	GC	200	Total C N O S 1596 1016 280 295 5	0	0
2	HC	200	Total C N O S 1596 1016 280 295 5	0	0
2	IC	200	Total C N O S 1596 1016 280 295 5	0	0
2	JC	200	Total C N O S 1596 1016 280 295 5	0	0
2	KC	200	Total C N O S 1596 1016 280 295 5	0	0
2	LC	200	Total C N O S 1596 1016 280 295 5	0	0
2	MC	200	Total C N O S 1596 1016 280 295 5	0	0

- Molecule 3 is a protein called DotD.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	AD	135	Total C N O S 1040 660 178 200 2	0	0
3	Ad	138	Total C N O S 1066 678 183 203 2	0	0
3	BD	135	Total C N O S 1040 660 178 200 2	0	0
3	Bd	138	Total C N O S 1066 678 183 203 2	0	0
3	CD	135	Total C N O S 1040 660 178 200 2	0	0
3	Cd	138	Total C N O S 1066 678 183 203 2	0	0
3	DD	135	Total C N O S 1040 660 178 200 2	0	0
3	Dd	138	Total C N O S 1066 678 183 203 2	0	0
3	ED	135	Total C N O S 1040 660 178 200 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ed	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	FD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Fd	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	GD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Gd	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	HD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Hd	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	ID	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Id	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	JD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Jd	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	KD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Kd	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	LD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Ld	138	Total 1066	C 678	N 183	O 203	S 2	0	0
3	MD	135	Total 1040	C 660	N 178	O 200	S 2	0	0
3	Md	138	Total 1066	C 678	N 183	O 203	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AH	89	Total 678	C 432	N 119	O 123	S 4	0	0
4	BH	89	Total 678	C 432	N 119	O 123	S 4	0	0

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AK	148	1152	731	205	212	4	0	0
5	BK	148	1152	731	205	212	4	0	0
5	CK	148	1152	731	205	212	4	0	0
5	DK	148	1152	731	205	212	4	0	0
5	EK	148	1152	731	205	212	4	0	0
5	FK	148	1152	731	205	212	4	0	0
5	GK	148	1152	731	205	212	4	0	0
5	HK	148	1152	731	205	212	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	IK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	JK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	KK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	LK	148	Total 1152	C 731	N 205	O 212	S 4	0	0
5	MK	148	Total 1152	C 731	N 205	O 212	S 4	0	0

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

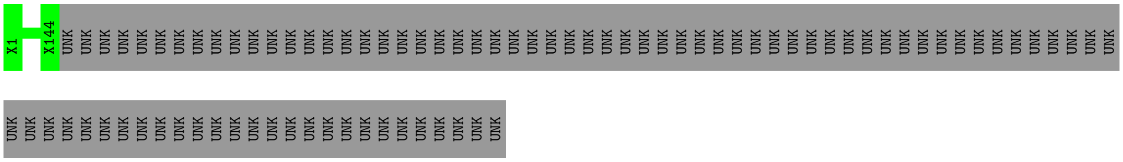
Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	O	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	P	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	Q	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	R	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	S	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	T	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	U	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	V	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	W	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	X	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	Y	136	Total 1108	C 701	N 201	O 202	S 4	0	0
6	Z	136	Total 1108	C 701	N 201	O 202	S 4	0	0

3 Residue-property plots ⓘ

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

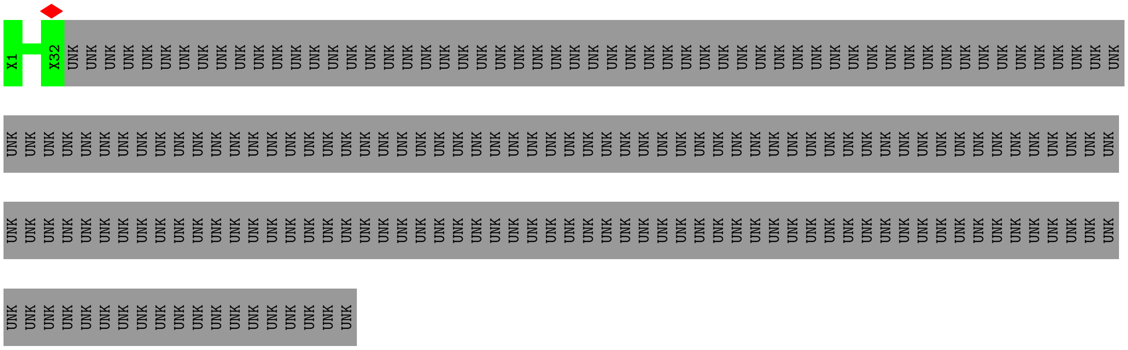
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AV:



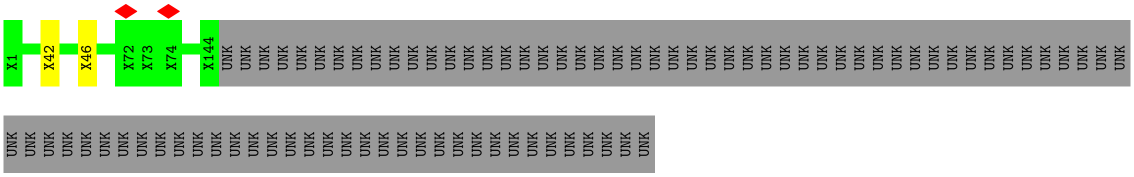
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AW:



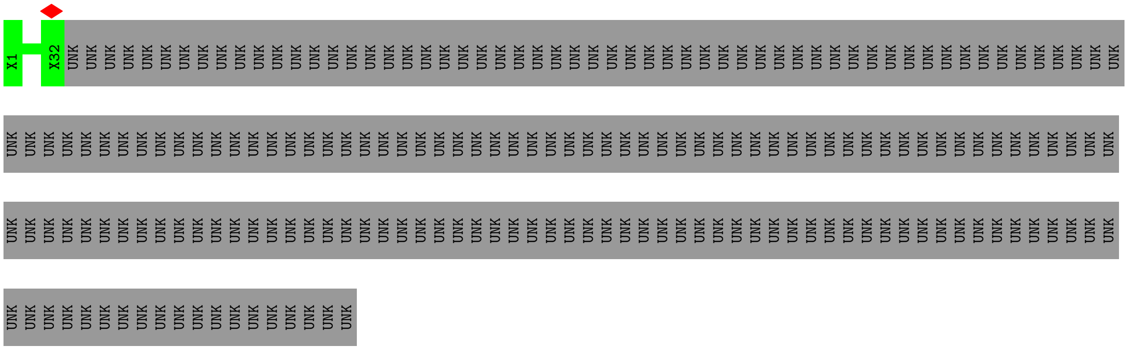
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BV:



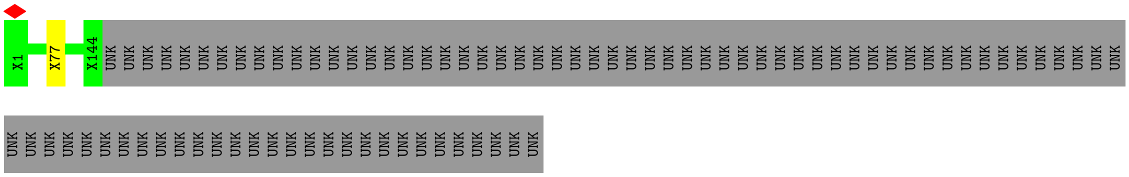
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BW:



- Molecule 1: Type IV secretion system unknown protein fragment

Chain CV:

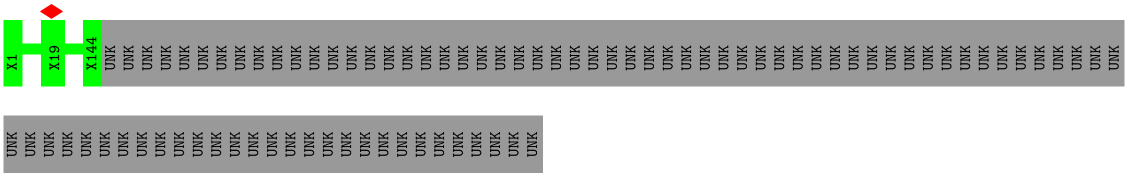


- Molecule 1: Type IV secretion system unknown protein fragment

Chain CW:

- Molecule 1: Type IV secretion system unknown protein fragment

Chain DV:

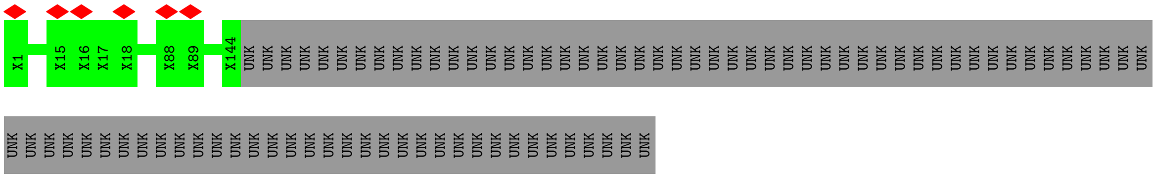


- Molecule 1: Type IV secretion system unknown protein fragment

Chain DW:

- Molecule 1: Type IV secretion system unknown protein fragment

Chain EV:

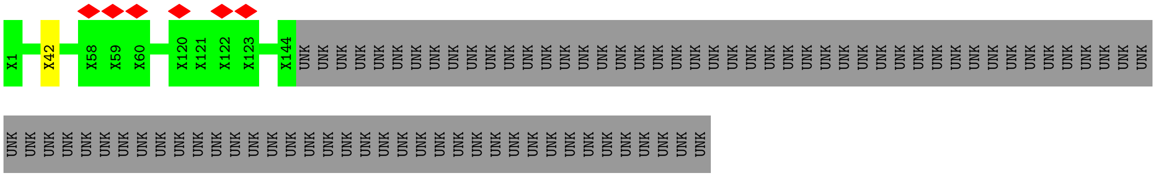


- Molecule 1: Type IV secretion system unknown protein fragment

Chain EW:

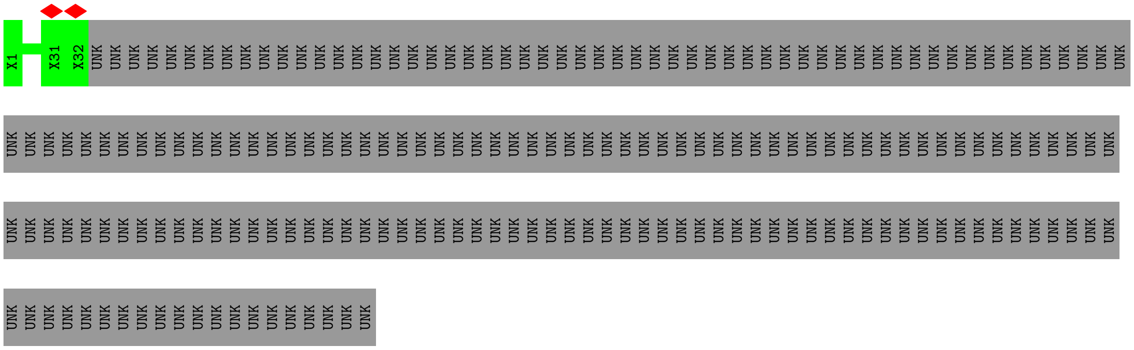
- Molecule 1: Type IV secretion system unknown protein fragment

Chain FV:



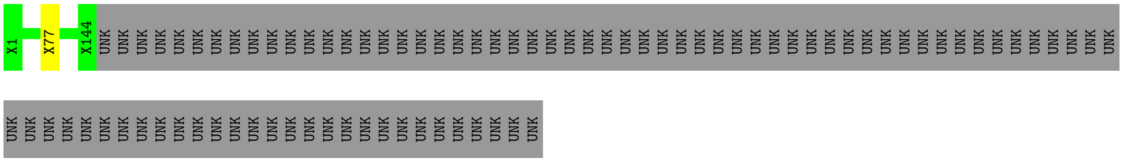
- Molecule 1: Type IV secretion system unknown protein fragment

Chain FW:



- Molecule 1: Type IV secretion system unknown protein fragment

Chain GV:

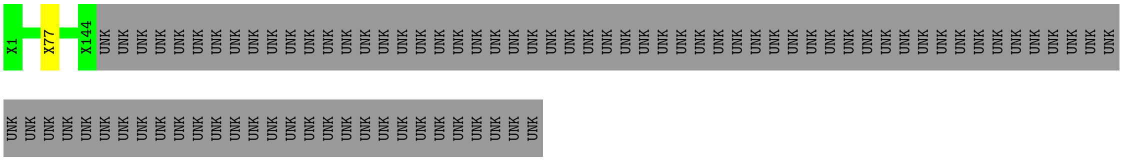



- Molecule 1: Type IV secretion system unknown protein fragment

Chain GW:


- Molecule 1: Type IV secretion system unknown protein fragment

Chain HV:

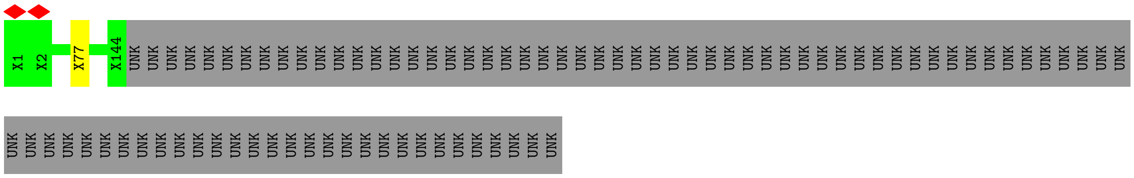



- Molecule 1: Type IV secretion system unknown protein fragment

Chain HW:


- Molecule 1: Type IV secretion system unknown protein fragment

Chain IV:

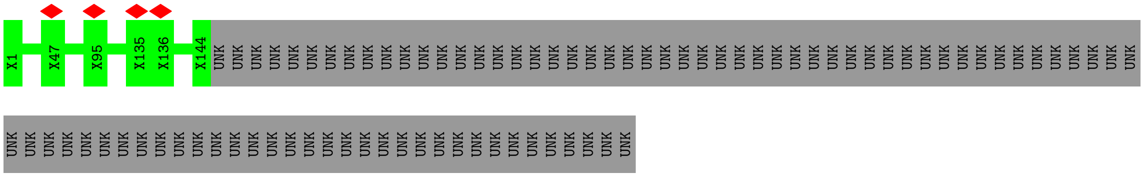


- Molecule 1: Type IV secretion system unknown protein fragment

Chain IW:

- Molecule 1: Type IV secretion system unknown protein fragment

Chain JV:

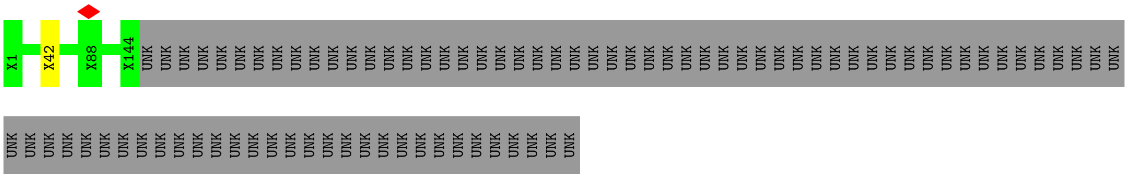


- Molecule 1: Type IV secretion system unknown protein fragment

Chain JW:

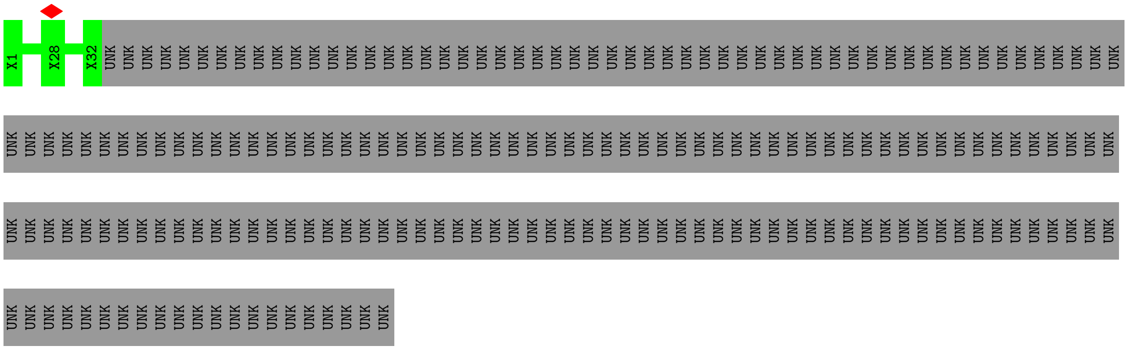
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KV:

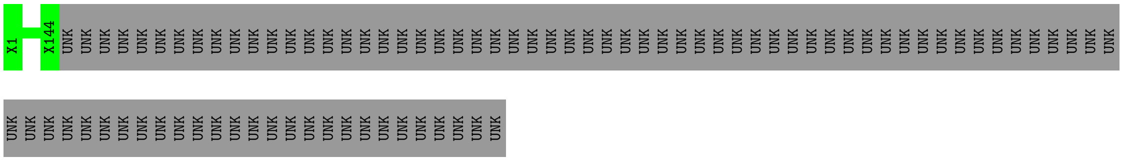
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KW:

- Molecule 1: Type IV secretion system unknown protein fragment

Chain LV:

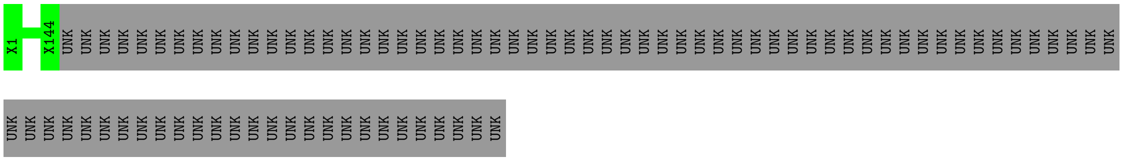



- Molecule 1: Type IV secretion system unknown protein fragment

Chain LW:


- Molecule 1: Type IV secretion system unknown protein fragment

Chain MV:

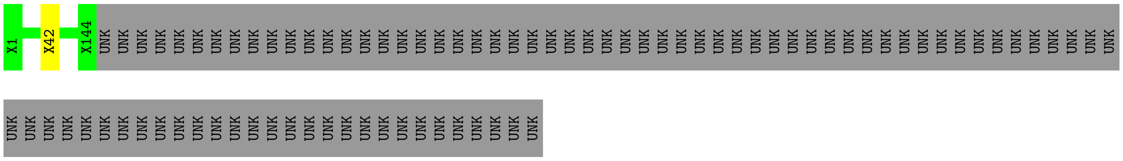


- Molecule 1: Type IV secretion system unknown protein fragment

Chain MW:

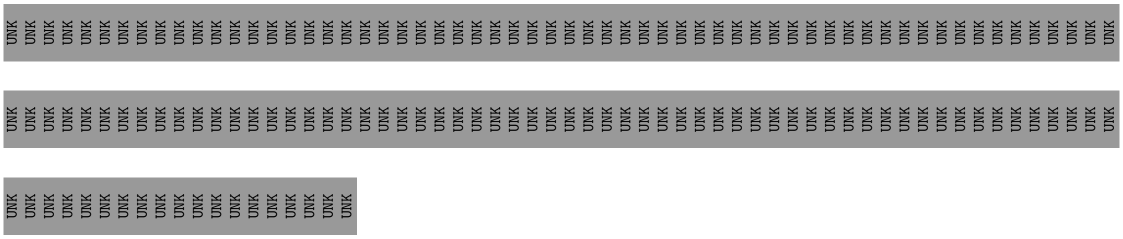
- Molecule 1: Type IV secretion system unknown protein fragment

Chain NV:



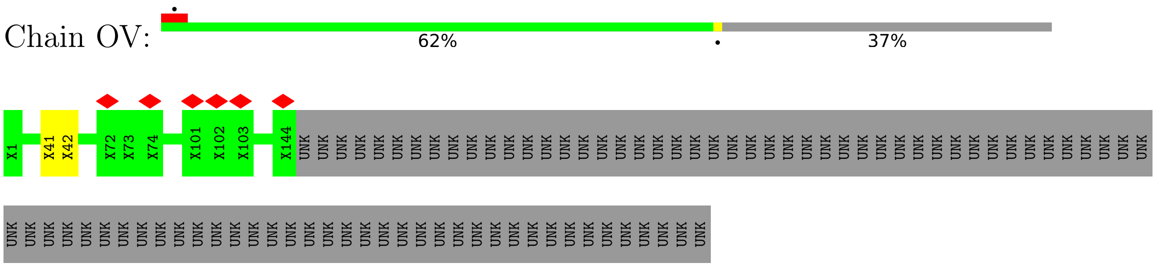
- Molecule 1: Type IV secretion system unknown protein fragment

Chain NW:



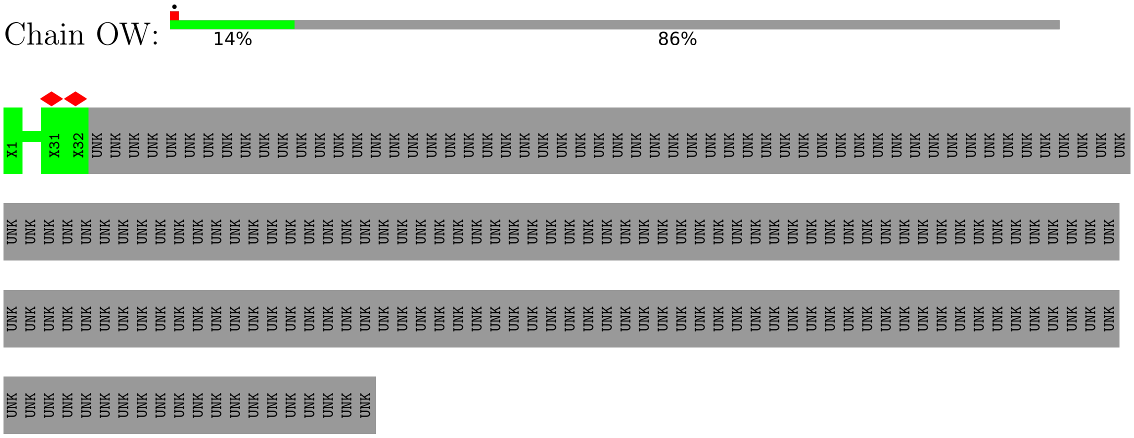
- Molecule 1: Type IV secretion system unknown protein fragment

Chain OV:



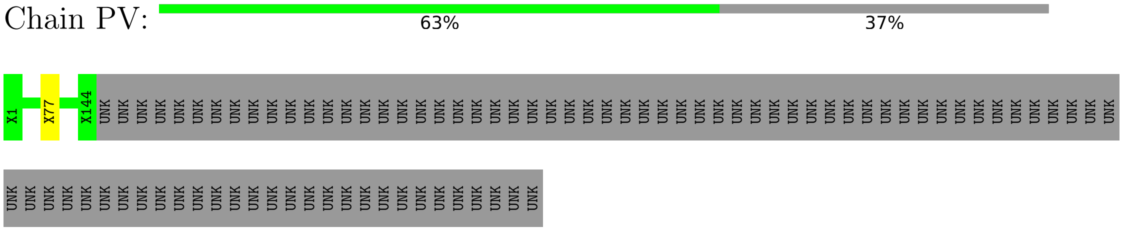
- Molecule 1: Type IV secretion system unknown protein fragment

Chain OW:



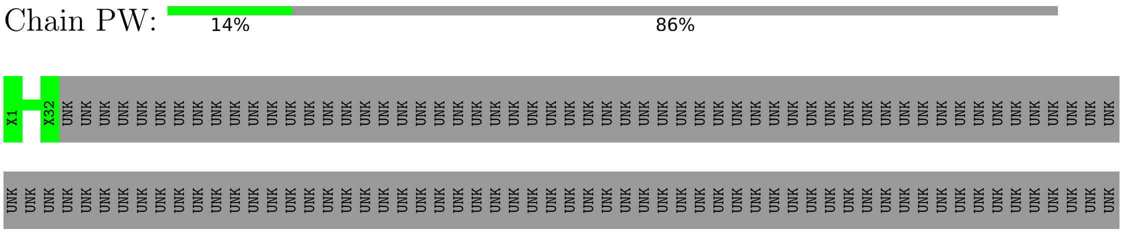
- Molecule 1: Type IV secretion system unknown protein fragment

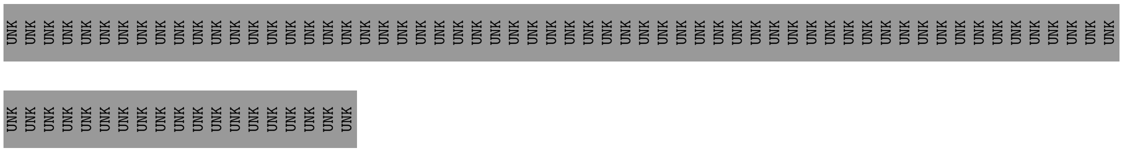
Chain PV:



- Molecule 1: Type IV secretion system unknown protein fragment

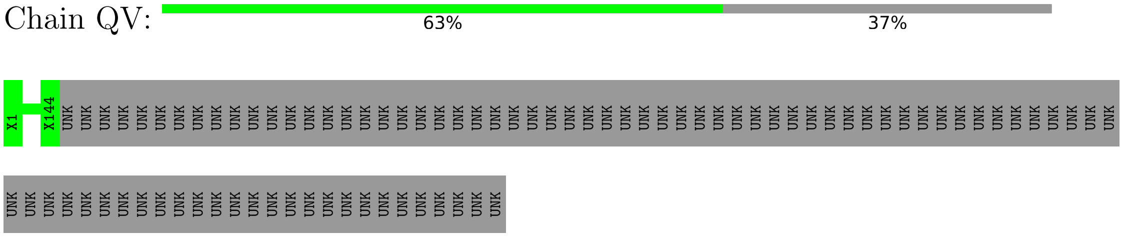
Chain PW:





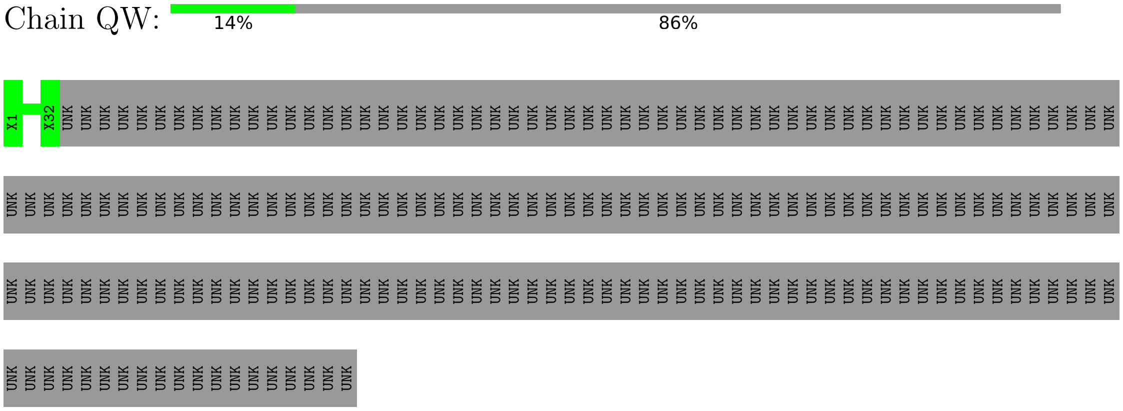
- Molecule 1: Type IV secretion system unknown protein fragment

Chain QV:



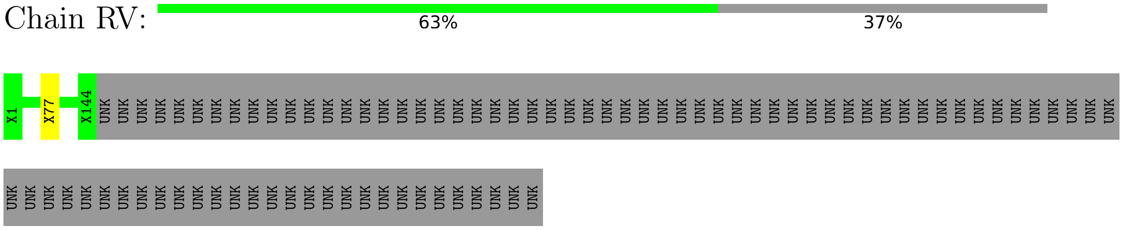
- Molecule 1: Type IV secretion system unknown protein fragment

Chain QW:



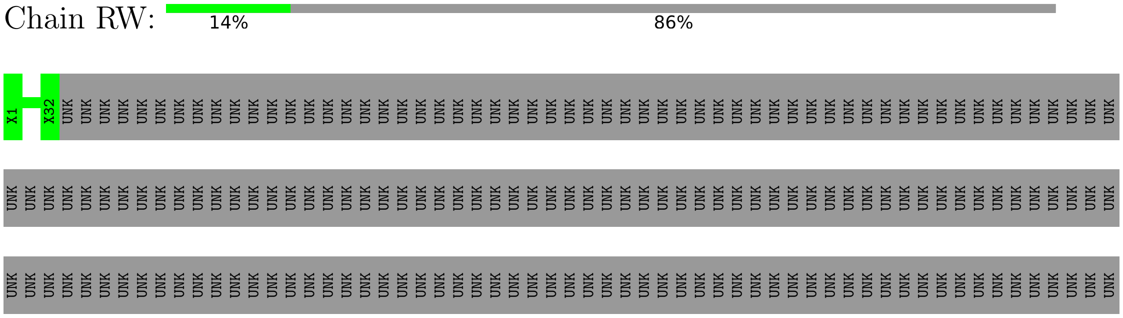
- Molecule 1: Type IV secretion system unknown protein fragment

Chain RV:



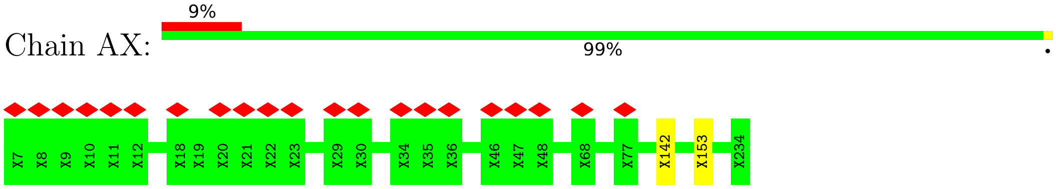
- Molecule 1: Type IV secretion system unknown protein fragment

Chain RW:



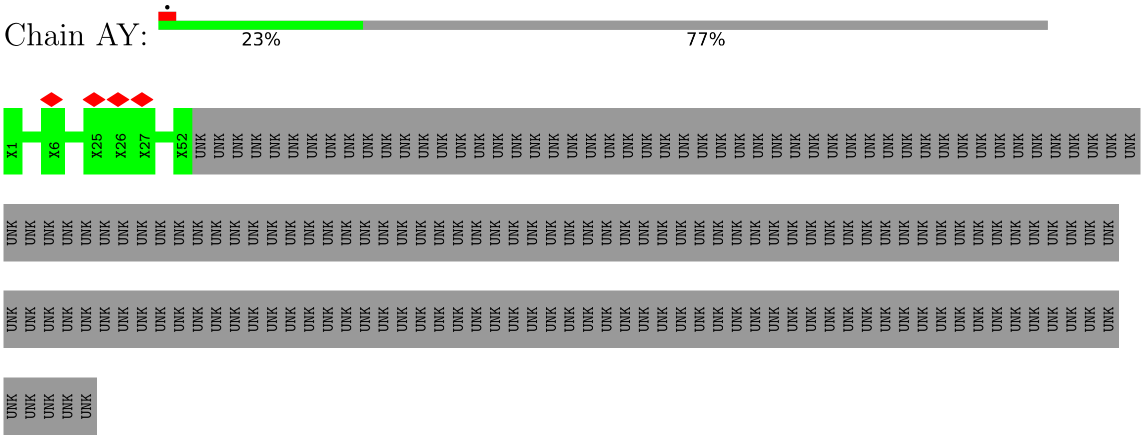
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AX:



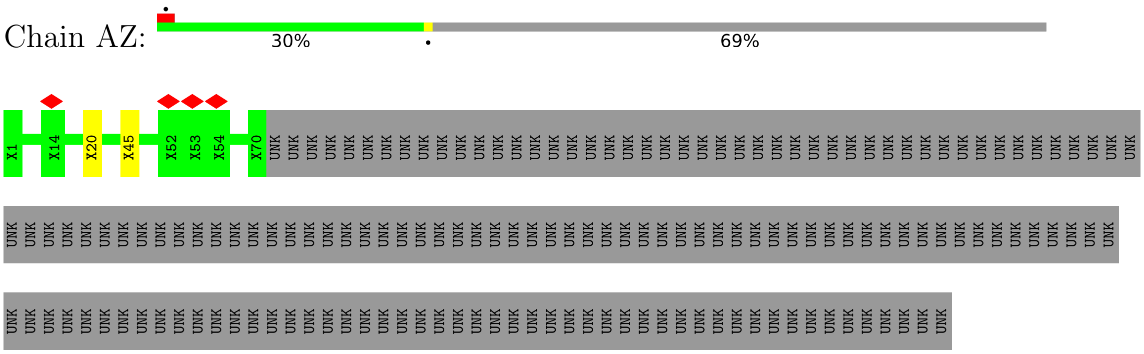
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AY:



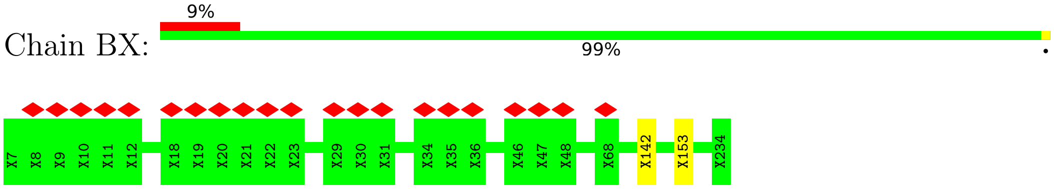
- Molecule 1: Type IV secretion system unknown protein fragment

Chain AZ:



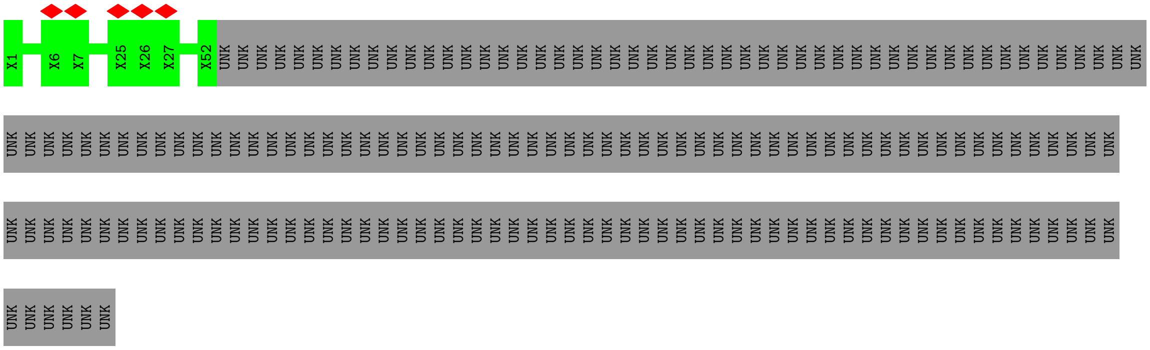
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BX:



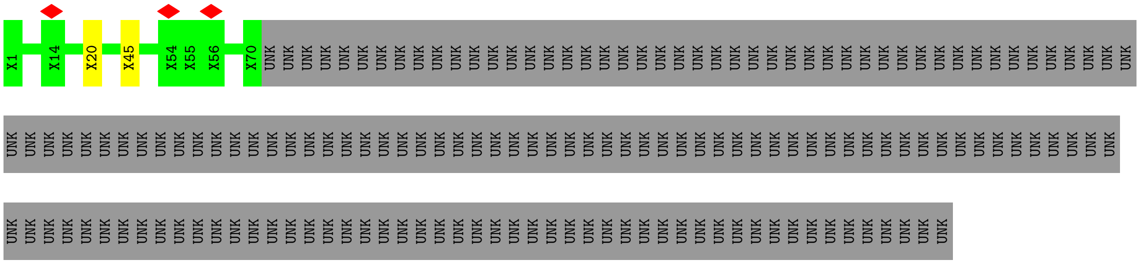
- Molecule 1: Type IV secretion system unknown protein fragment

Chain BY:



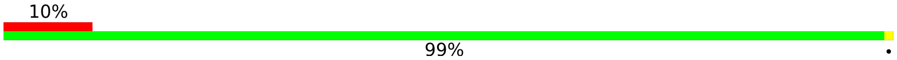
- Molecule 1: Type IV secretion system unknown protein fragment

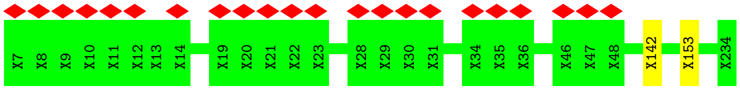
Chain BZ:



- Molecule 1: Type IV secretion system unknown protein fragment

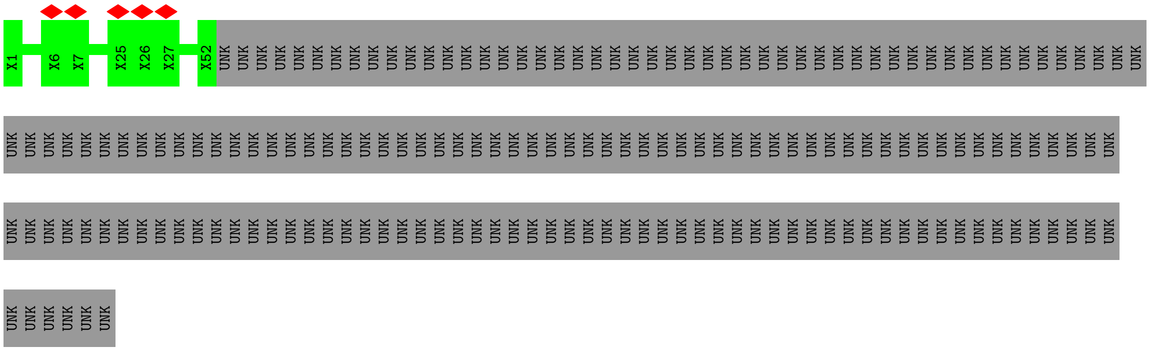
Chain CX:





- Molecule 1: Type IV secretion system unknown protein fragment

Chain CY:

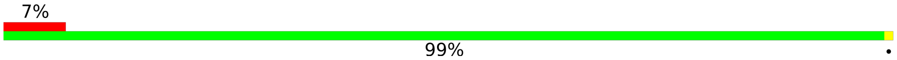


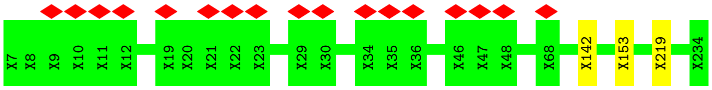
- Molecule 1: Type IV secretion system unknown protein fragment

Chain CZ:

• Molecule 1: Type IV secretion system unknown protein fragment

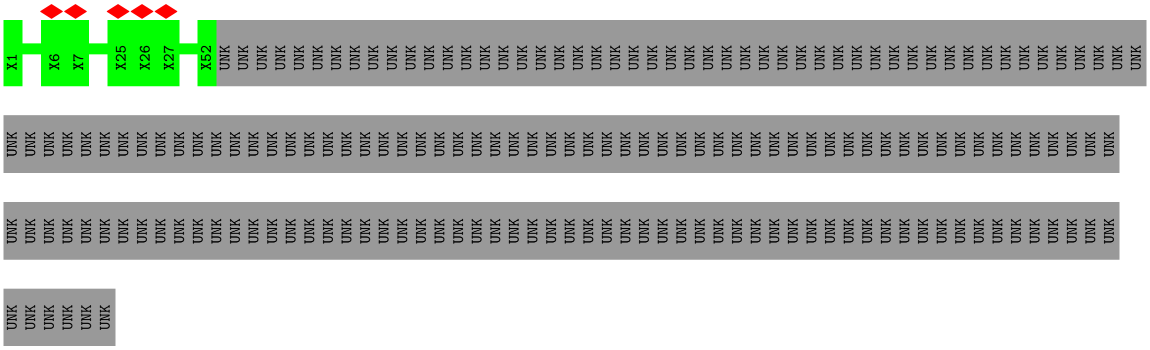
Chain DX:





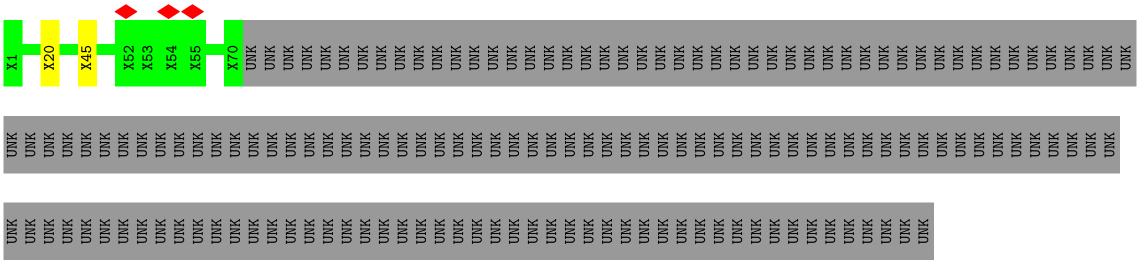
• Molecule 1: Type IV secretion system unknown protein fragment

Chain DY:



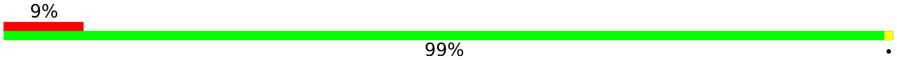
• Molecule 1: Type IV secretion system unknown protein fragment

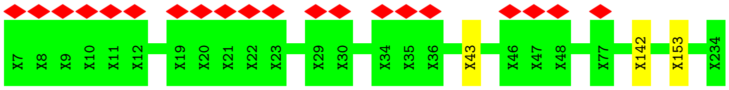
Chain DZ:



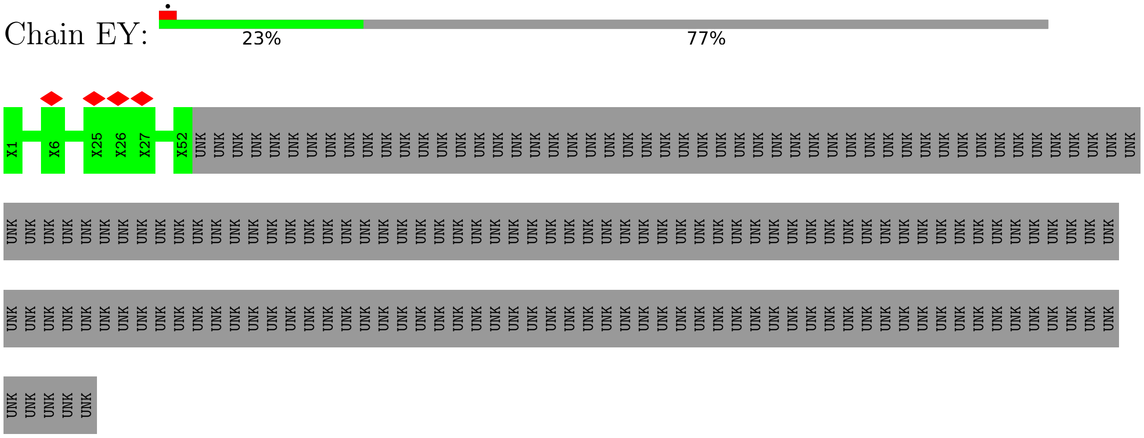
• Molecule 1: Type IV secretion system unknown protein fragment

Chain EX:

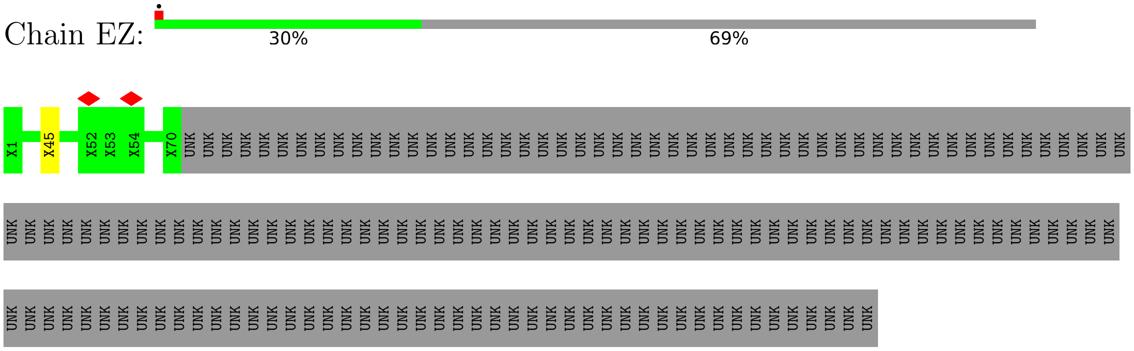




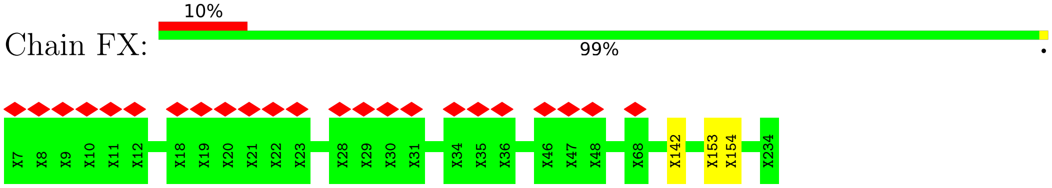
- Molecule 1: Type IV secretion system unknown protein fragment



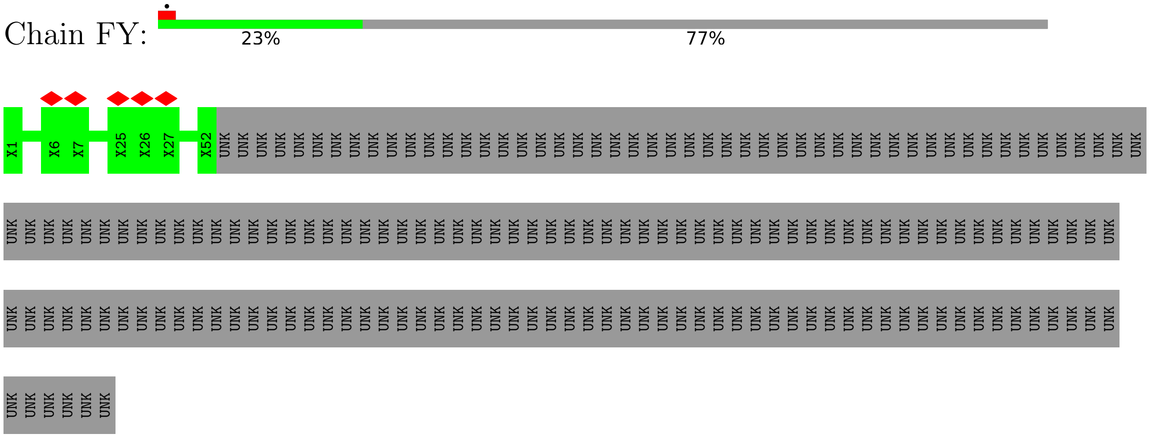
- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment



- Molecule 1: Type IV secretion system unknown protein fragment

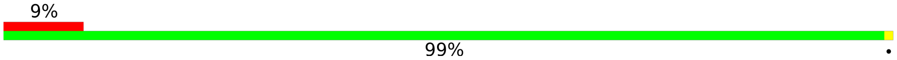


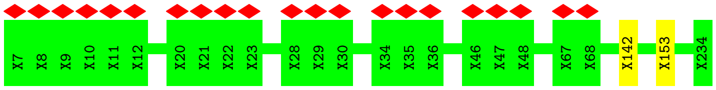
- Molecule 1: Type IV secretion system unknown protein fragment

Chain FZ:

- Molecule 1: Type IV secretion system unknown protein fragment

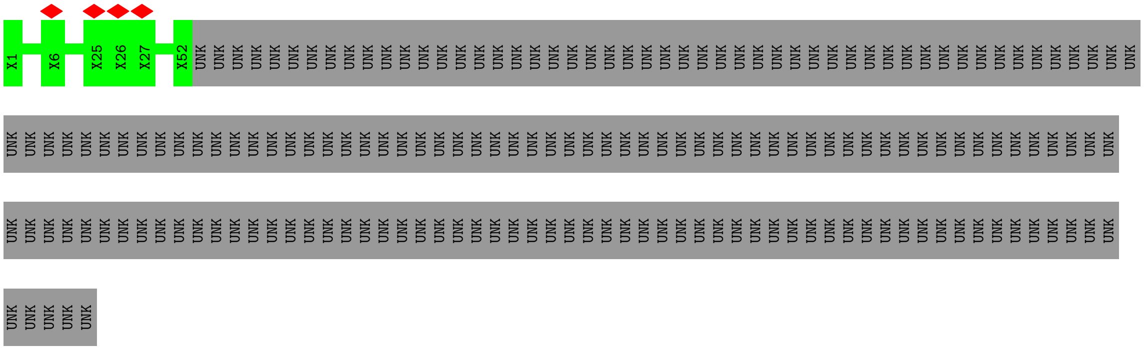
Chain GX:





- Molecule 1: Type IV secretion system unknown protein fragment

Chain GY:

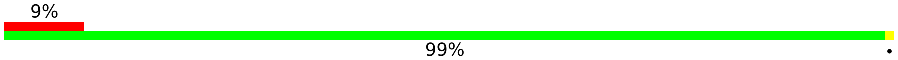


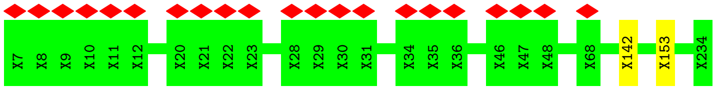
- Molecule 1: Type IV secretion system unknown protein fragment

Chain GZ:

- Molecule 1: Type IV secretion system unknown protein fragment

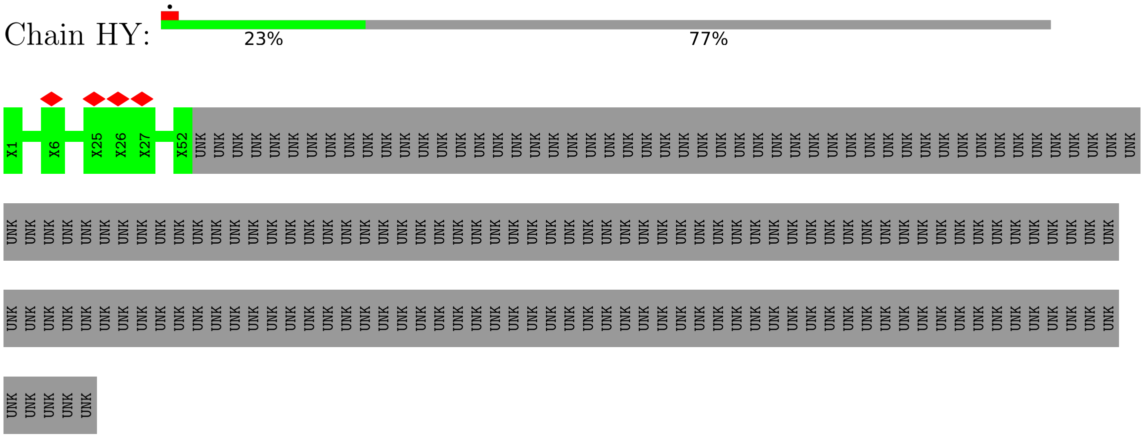
Chain HX:





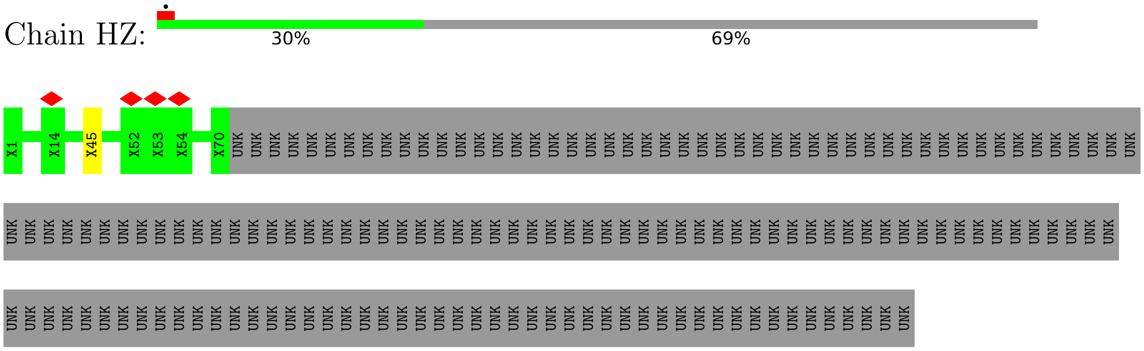
- Molecule 1: Type IV secretion system unknown protein fragment

Chain HY:



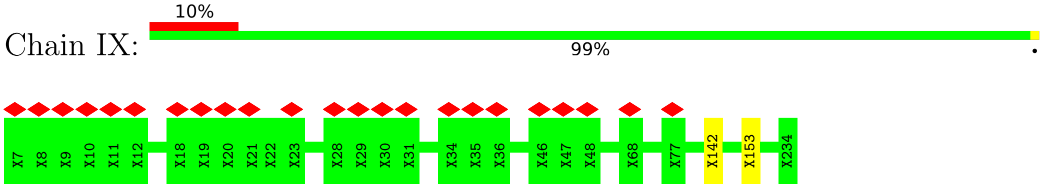
- Molecule 1: Type IV secretion system unknown protein fragment

Chain HZ:



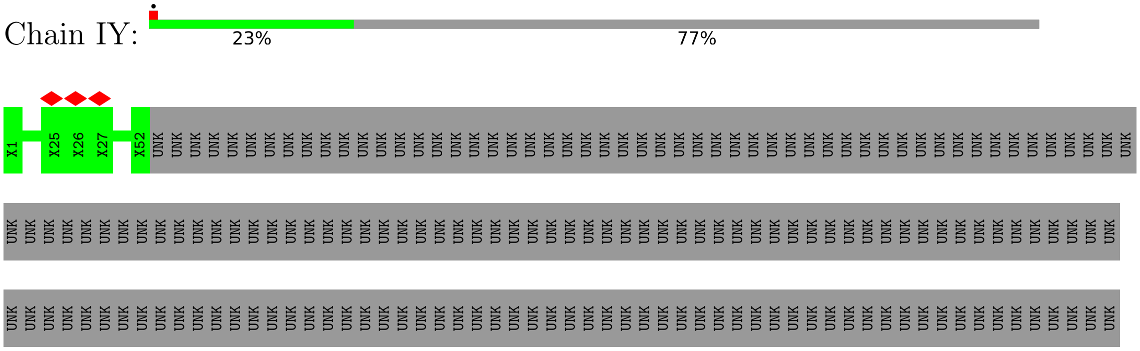
- Molecule 1: Type IV secretion system unknown protein fragment

Chain IX:



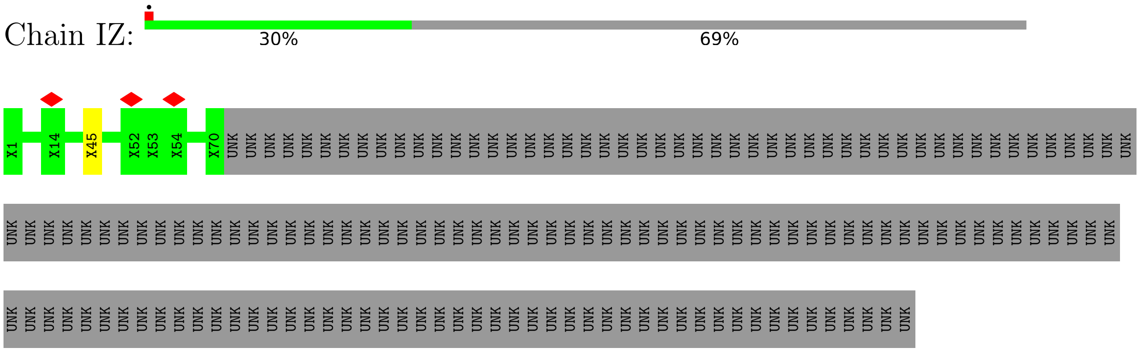
- Molecule 1: Type IV secretion system unknown protein fragment

Chain IY:



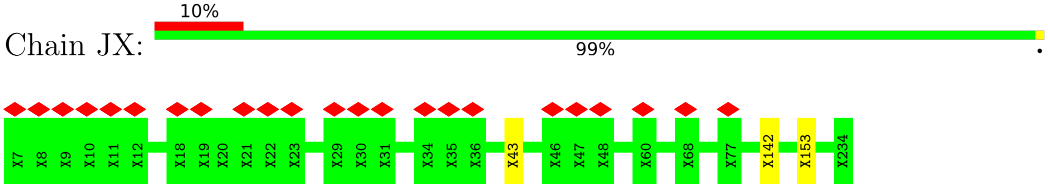
- Molecule 1: Type IV secretion system unknown protein fragment

Chain IZ:



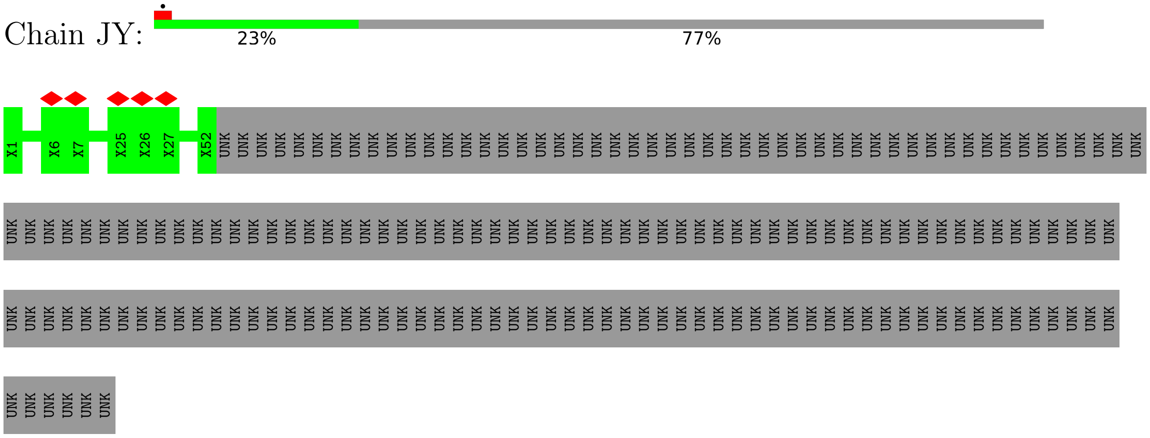
- Molecule 1: Type IV secretion system unknown protein fragment

Chain JX:



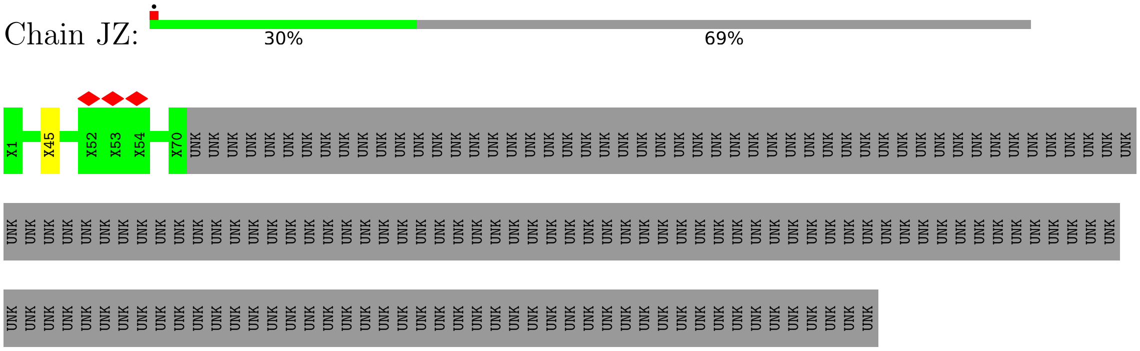
- Molecule 1: Type IV secretion system unknown protein fragment

Chain JY:



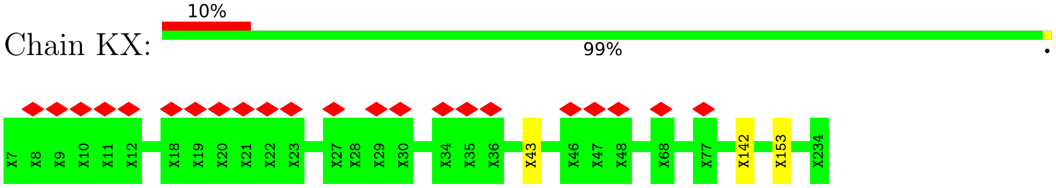
- Molecule 1: Type IV secretion system unknown protein fragment

Chain JZ:



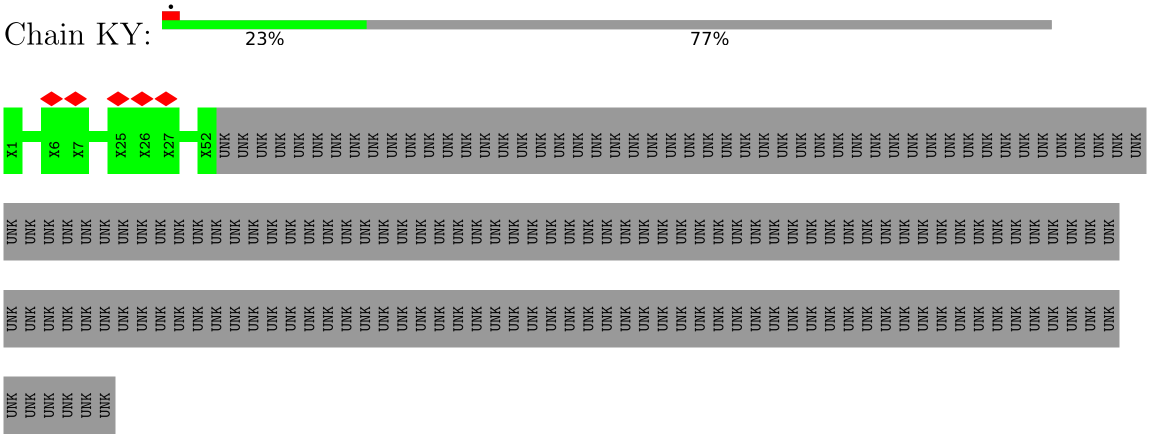
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KX:



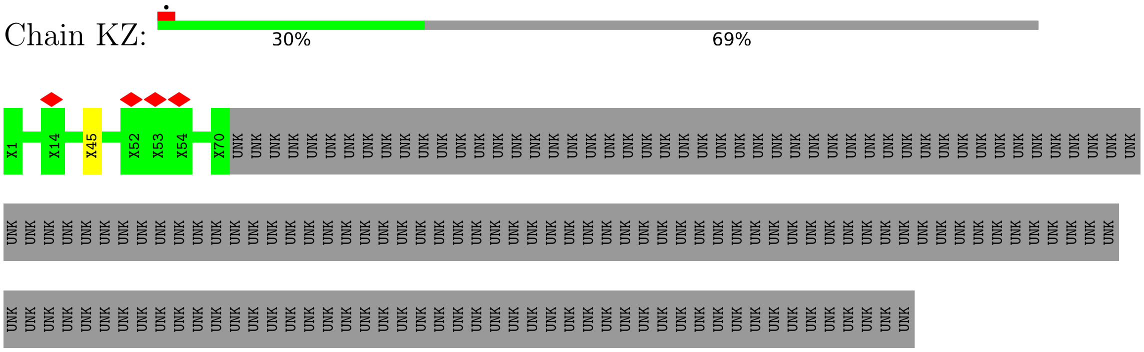
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KY:



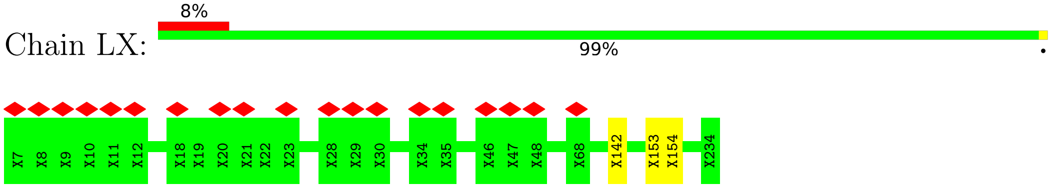
- Molecule 1: Type IV secretion system unknown protein fragment

Chain KZ:



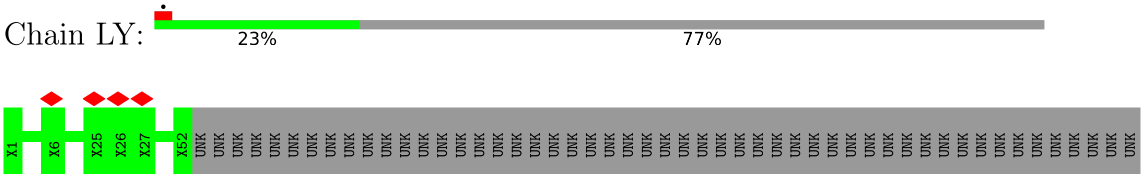
- Molecule 1: Type IV secretion system unknown protein fragment

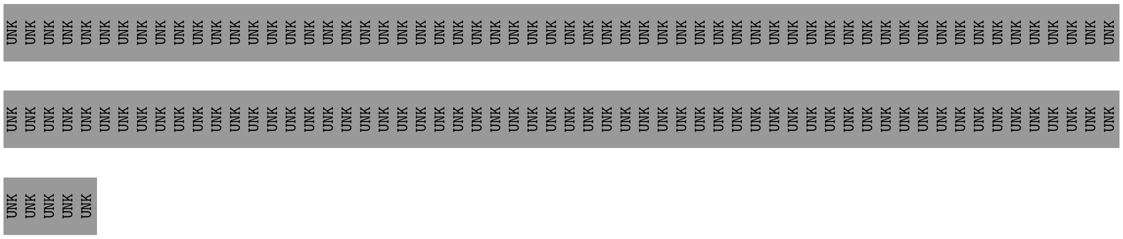
Chain LX:



- Molecule 1: Type IV secretion system unknown protein fragment

Chain LY:



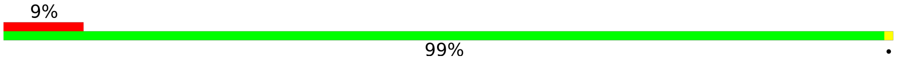


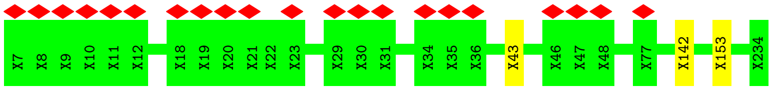
- Molecule 1: Type IV secretion system unknown protein fragment

Chain LZ:

- Molecule 1: Type IV secretion system unknown protein fragment

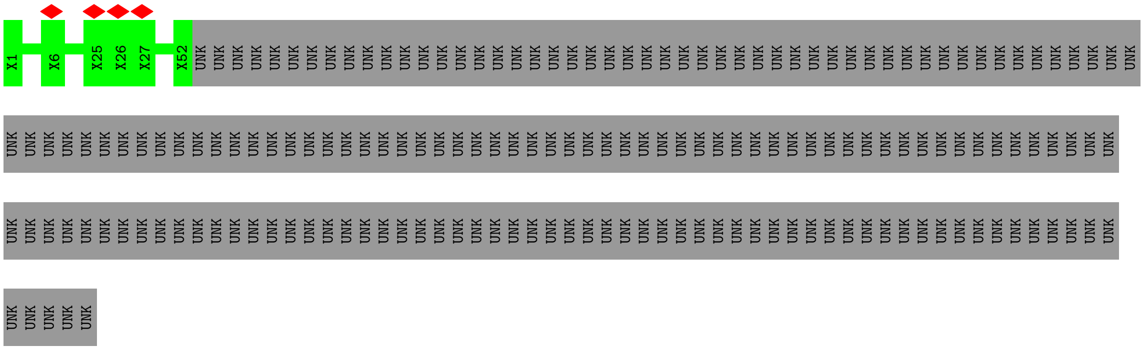
Chain MX:





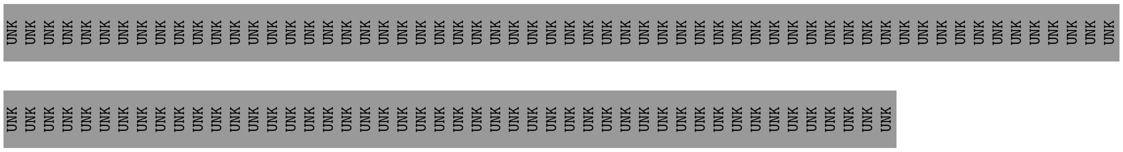
- Molecule 1: Type IV secretion system unknown protein fragment

Chain MY:



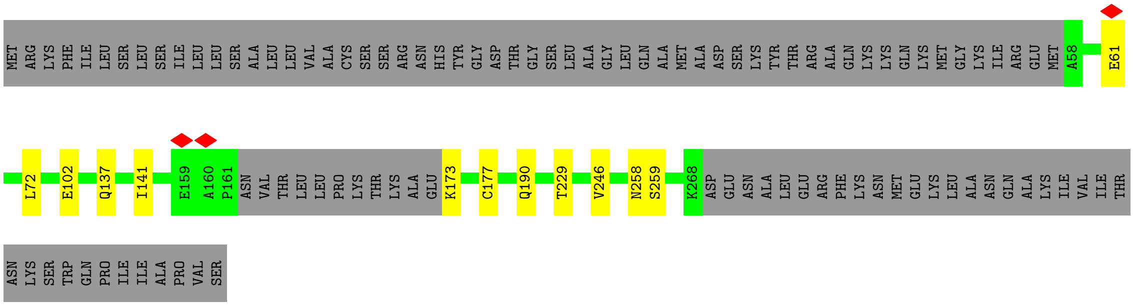
- Molecule 1: Type IV secretion system unknown protein fragment

Chain MZ:



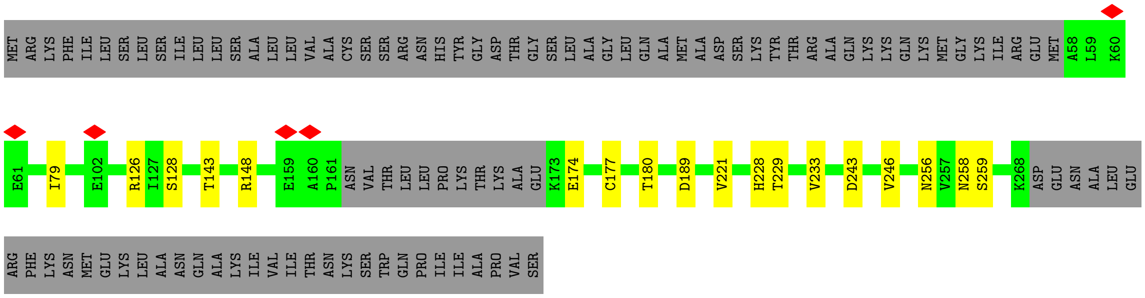
- Molecule 2: DotC

Chain AC:



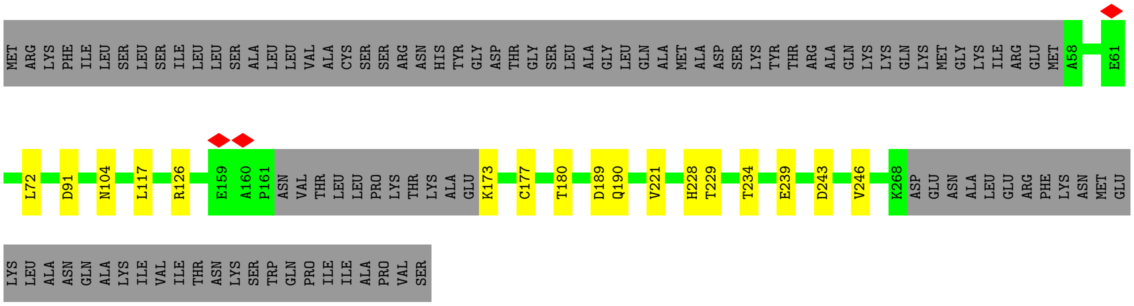
- Molecule 2: DotC

Chain BC:



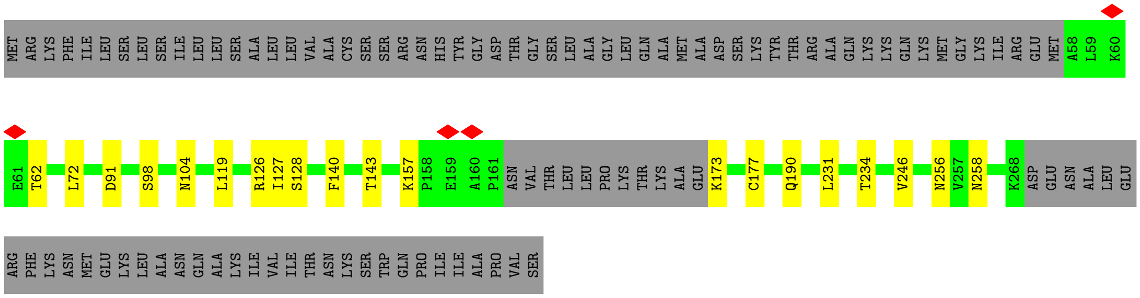
- Molecule 2: DotC

Chain CC:



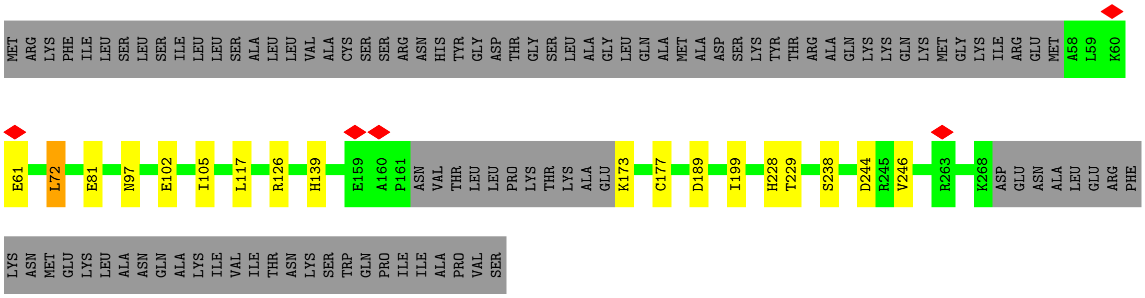
- Molecule 2: DotC

Chain DC:



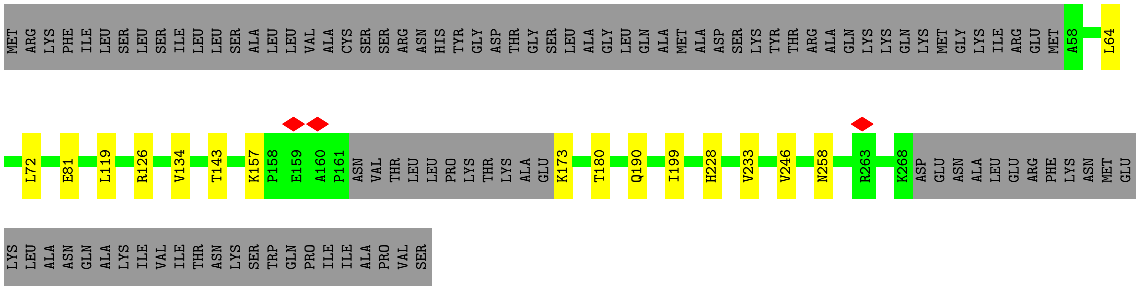
- Molecule 2: DotC

Chain EC:



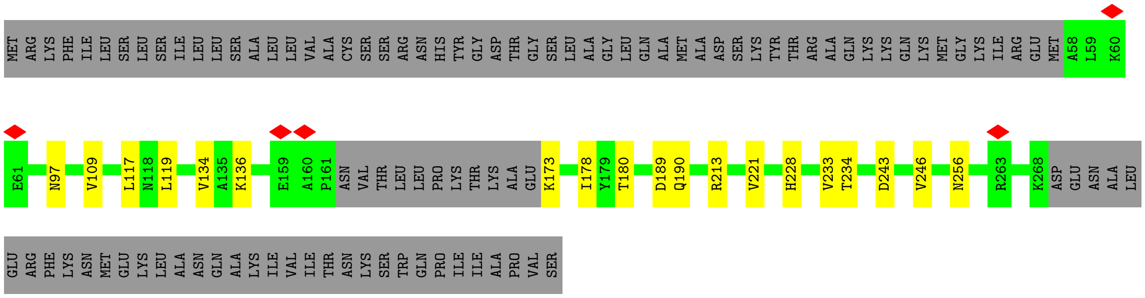
- Molecule 2: DotC

Chain FC:

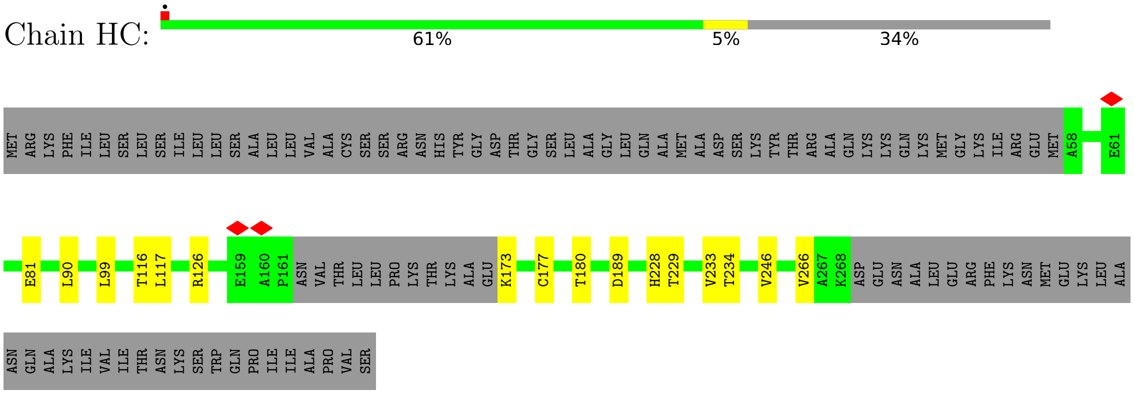


- Molecule 2: DotC

Chain GC:



- Molecule 2: DotC



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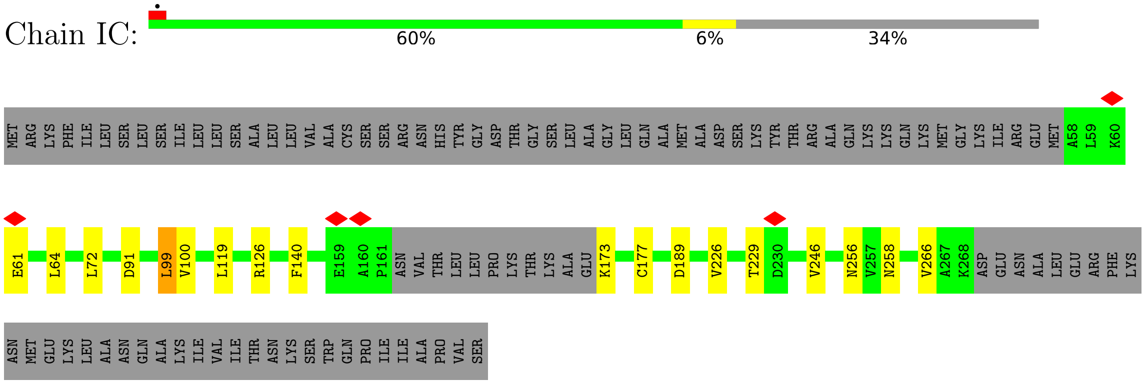

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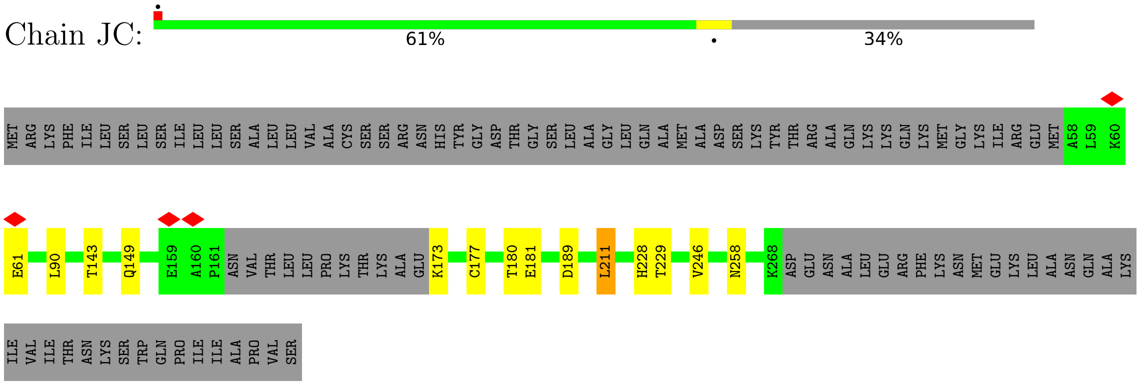

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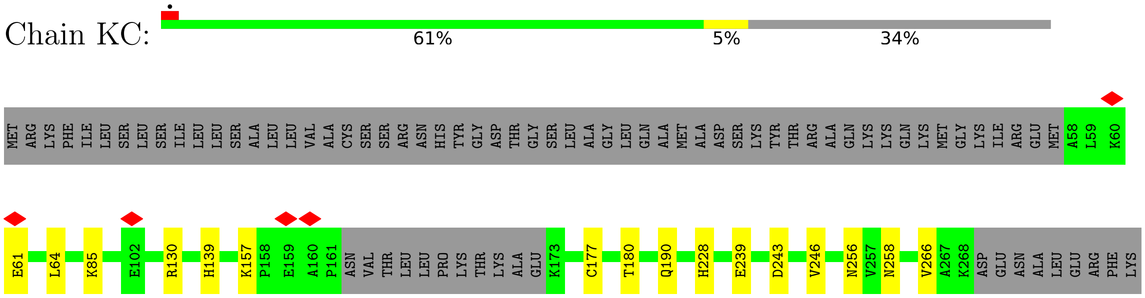
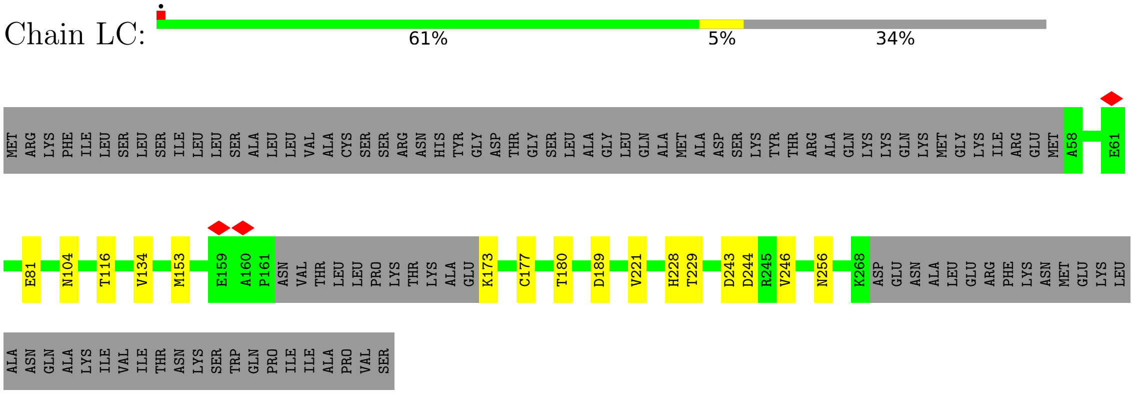


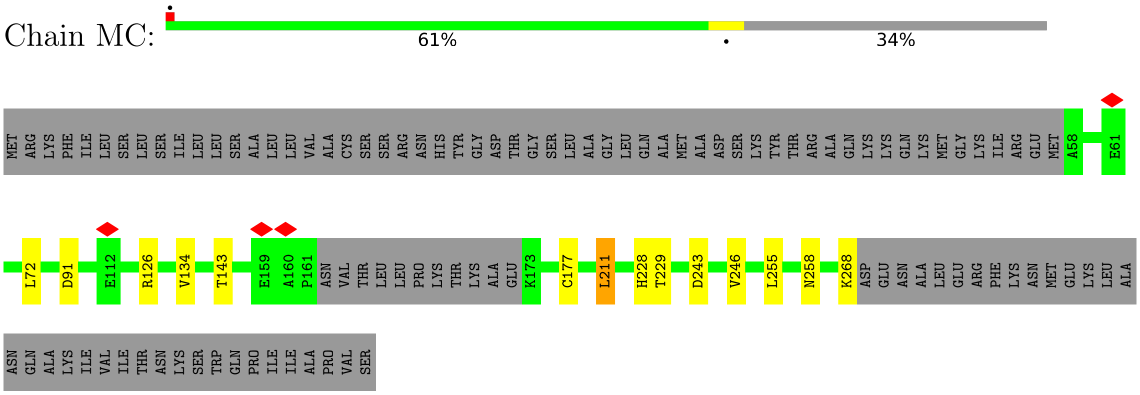
- Molecule 2: DotC

Chain LC:



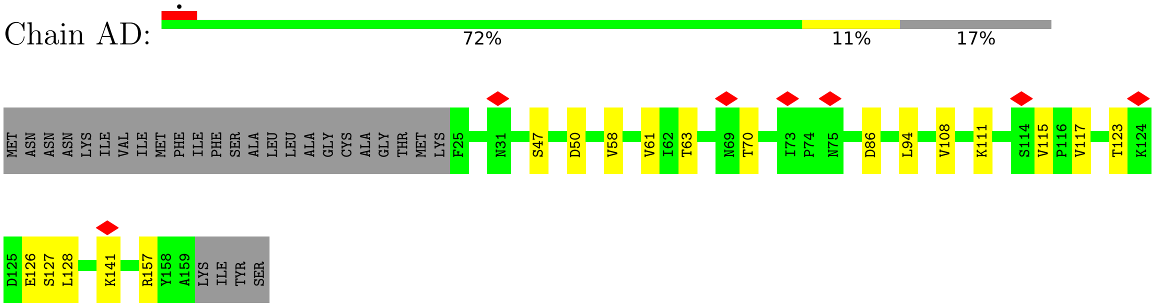
- Molecule 2: DotC

Chain MC:



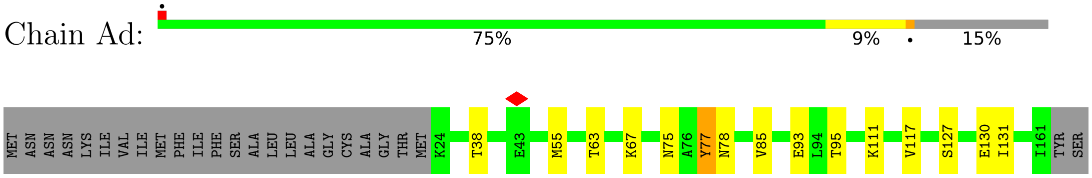
- Molecule 3: DotD

Chain AD:



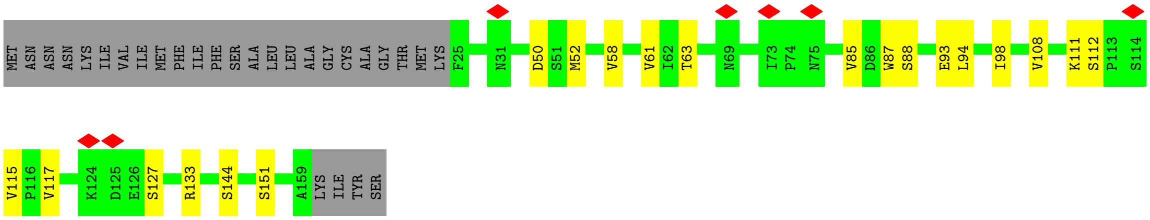
- Molecule 3: DotD

Chain Ad:



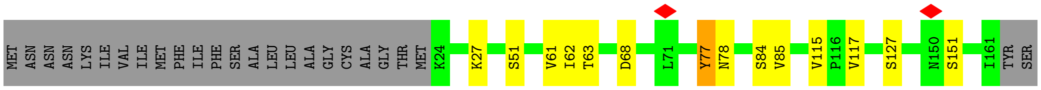
- Molecule 3: DotD

Chain BD:



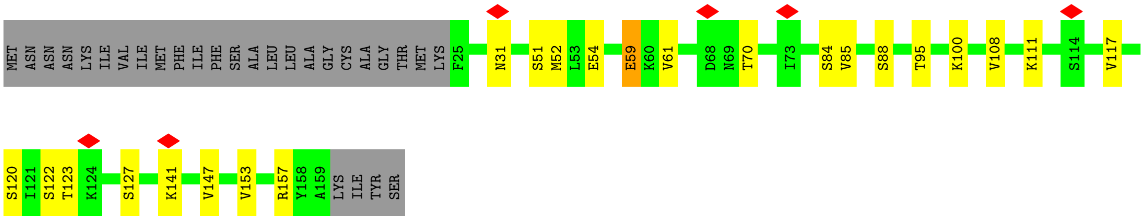
• Molecule 3: DotD

Chain Bd:



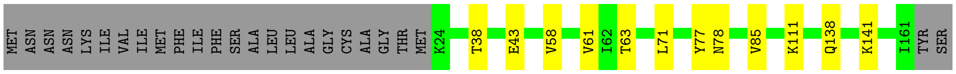
• Molecule 3: DotD

Chain CD:



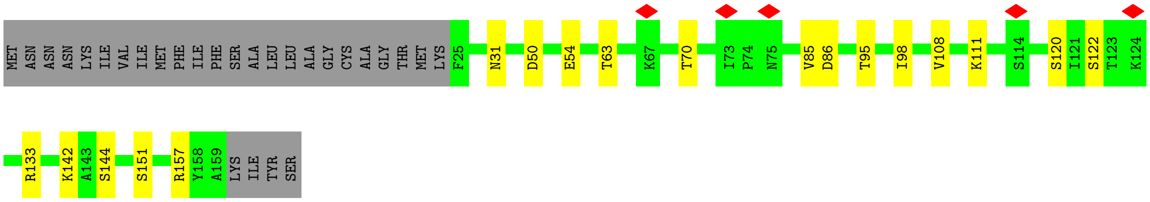
• Molecule 3: DotD

Chain Cd:



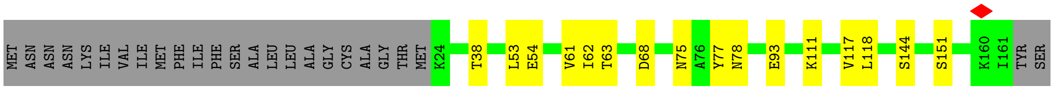
• Molecule 3: DotD

Chain DD:



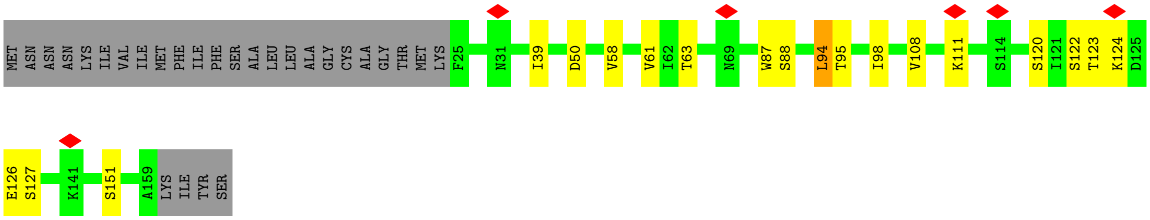
• Molecule 3: DotD

Chain Dd:



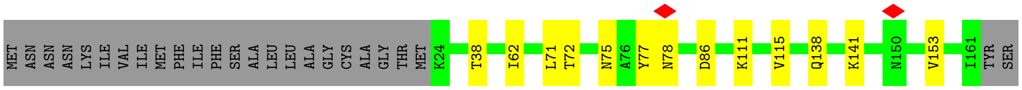
- Molecule 3: DotD

Chain ED:



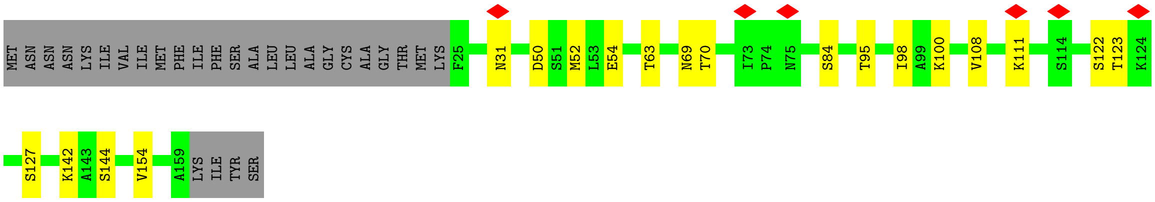
- Molecule 3: DotD

Chain Ed:



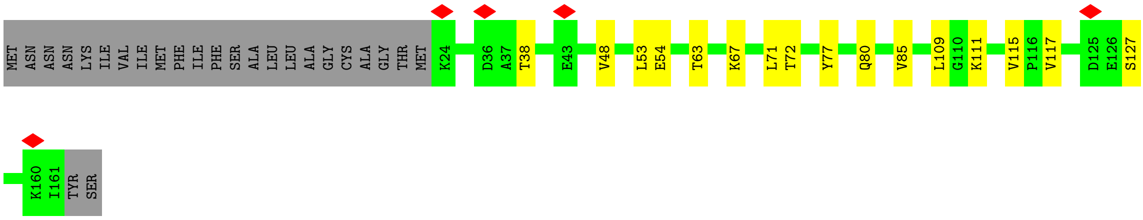
- Molecule 3: DotD

Chain FD:



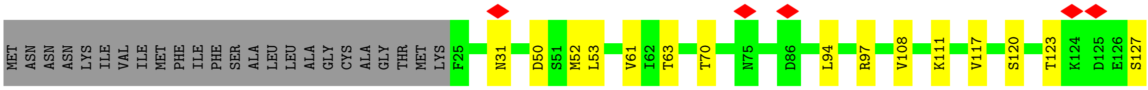
- Molecule 3: DotD

Chain Fd:



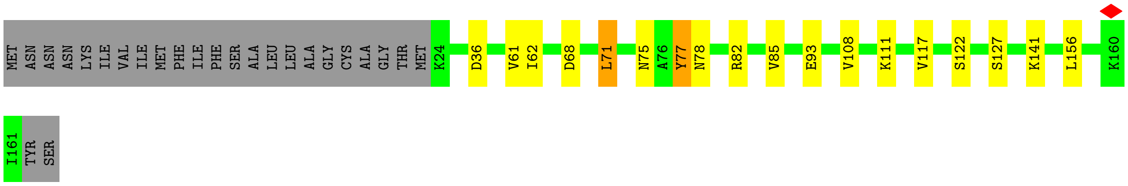
- Molecule 3: DotD

Chain GD:



- Molecule 3: DotD

Chain Gd:



- Molecule 3: DotD

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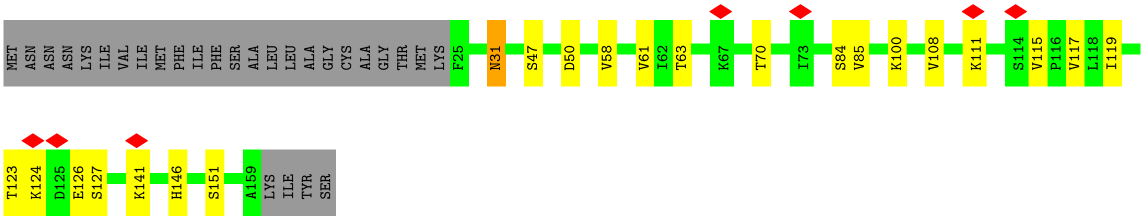
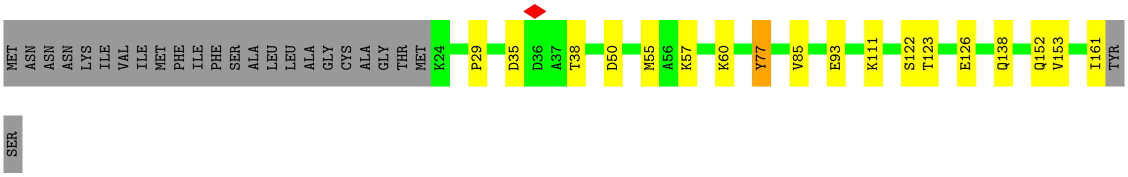


- Molecule 3: DotD

Chain Hd:



- Molecule 3: DotD

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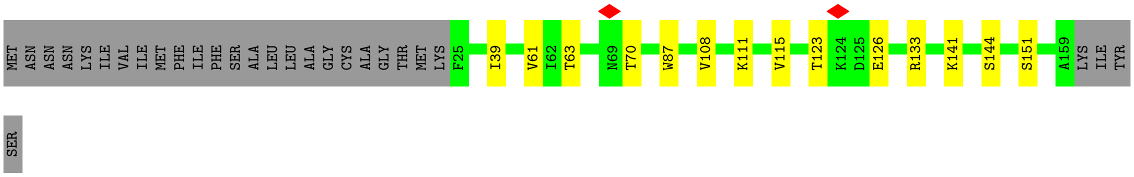

- Molecule 3: DotD

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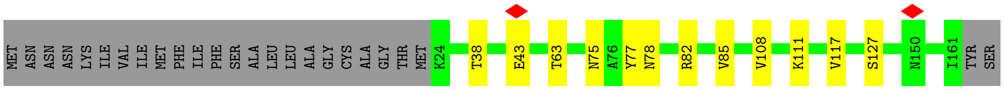

- Molecule 3: DotD

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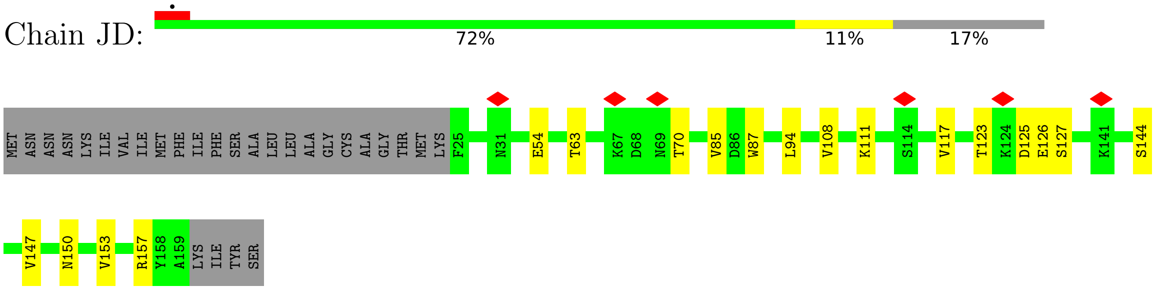
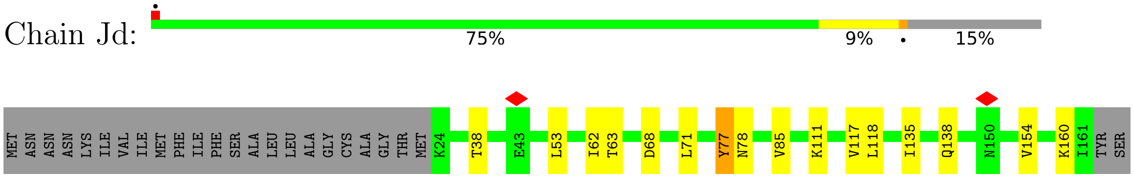


- Molecule 3: DotD

Chain Jd:



- Molecule 3: DotD

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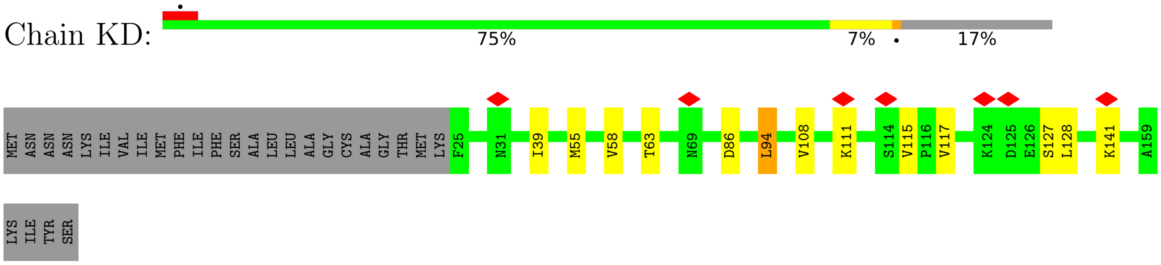
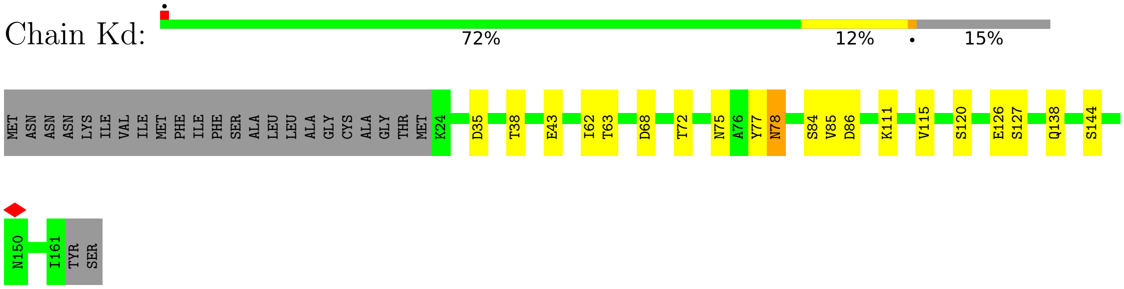


- Molecule 3: DotD

Chain Kd:



- Molecule 3: DotD

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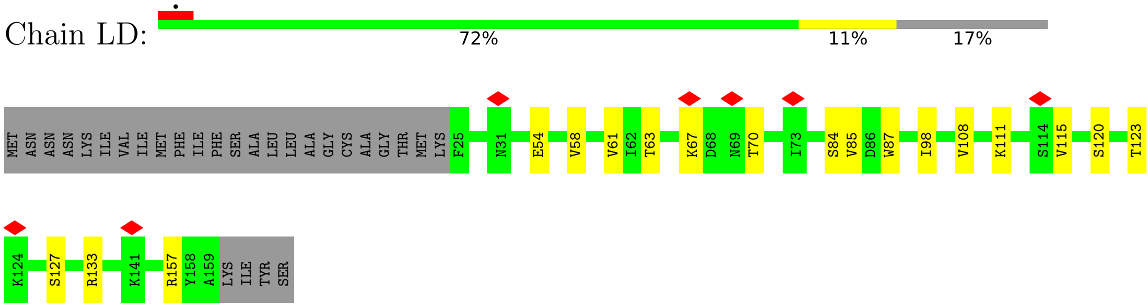
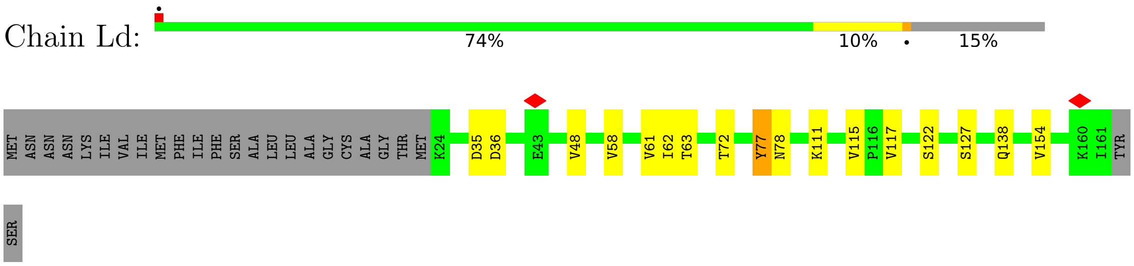


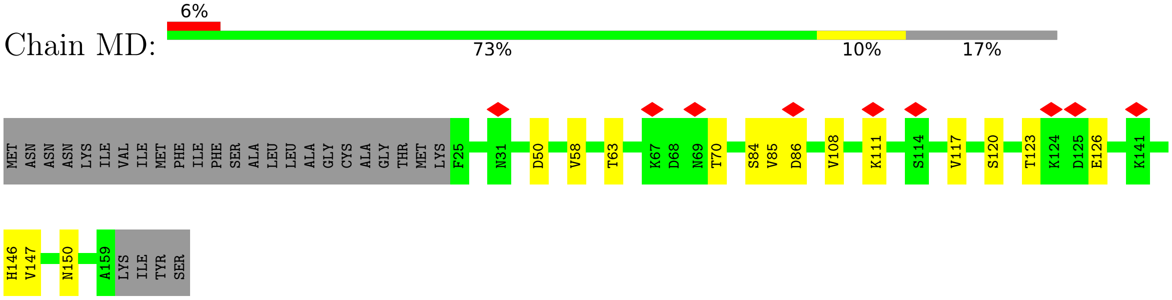
- Molecule 3: DotD

Chain Ld:



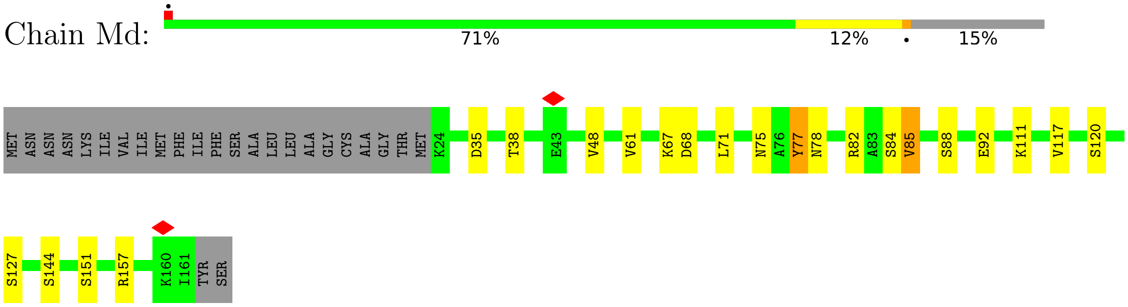
- Molecule 3: DotD

Chain MD:



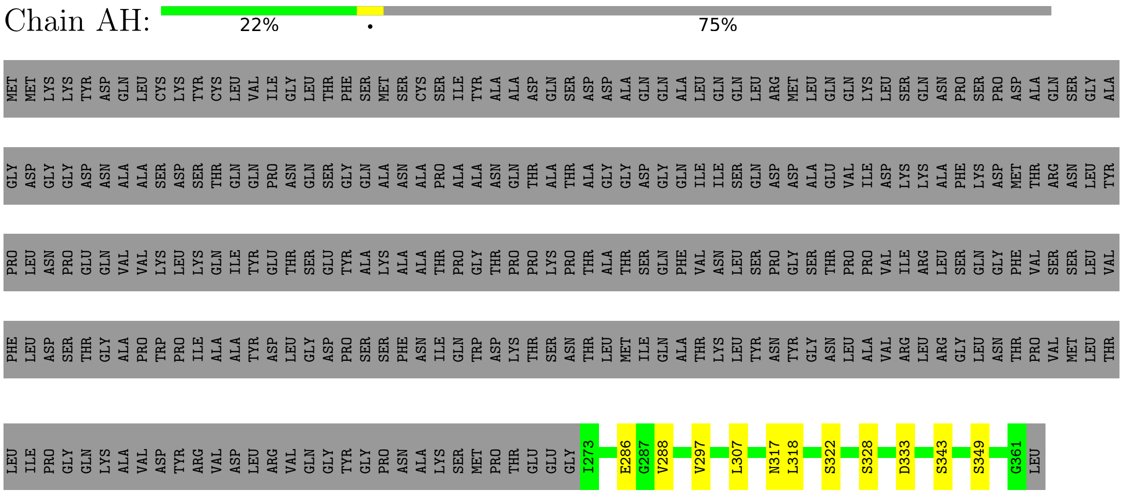
- Molecule 3: DotD

Chain Md:



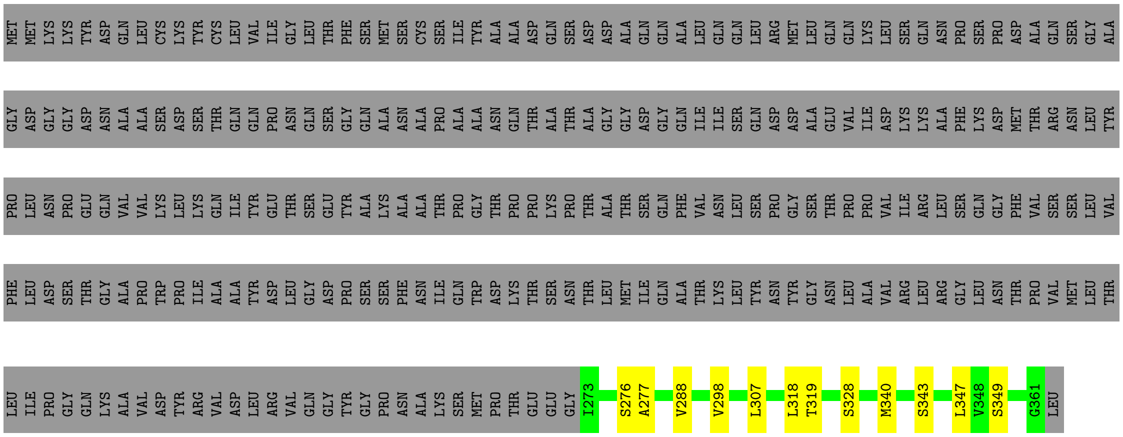
- Molecule 4: Type IV secretion protein IcmK

Chain AH:



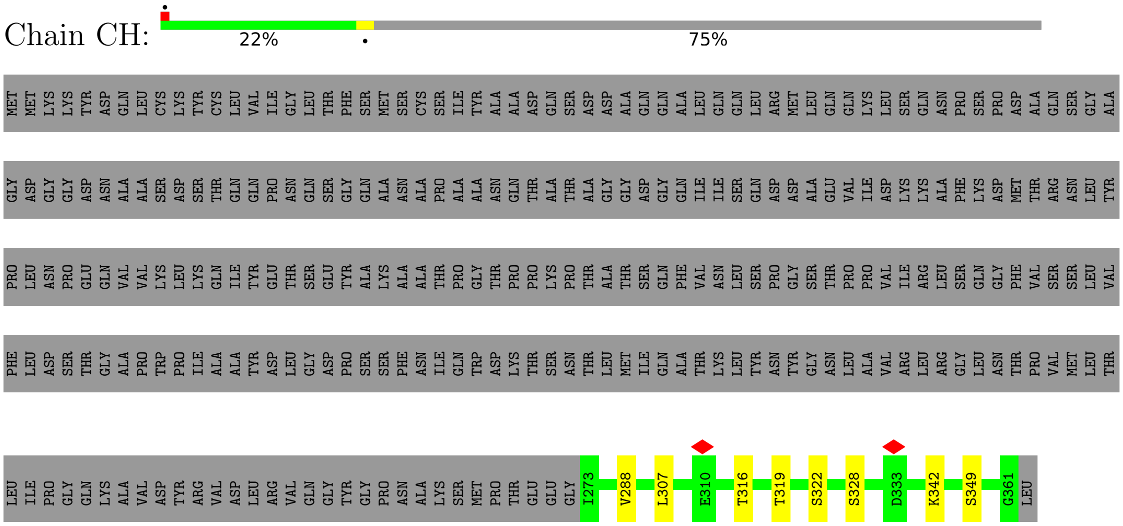
- Molecule 4: Type IV secretion protein IcmK

Chain BH:



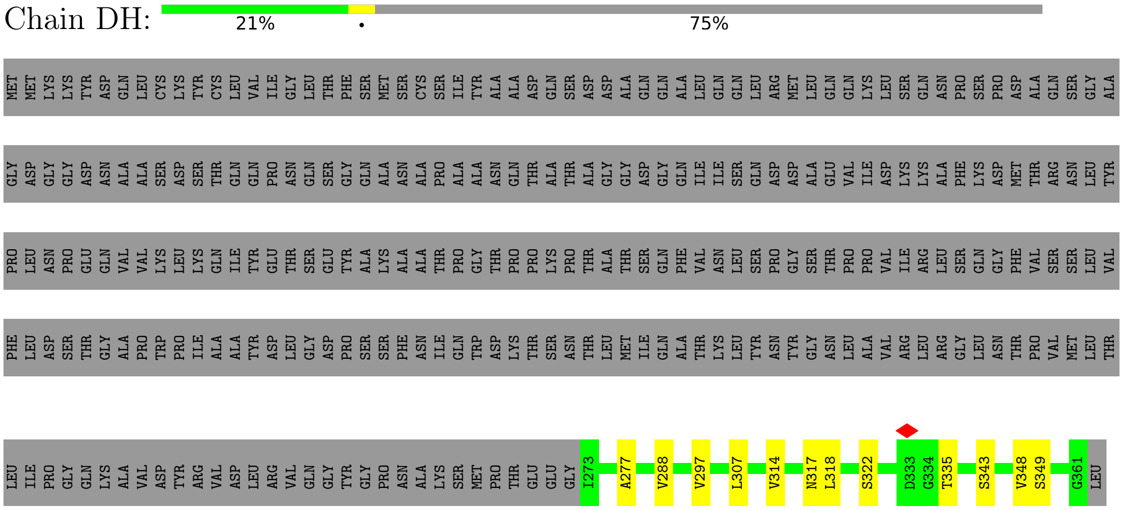
- Molecule 4: Type IV secretion protein IcmK

Chain CH:

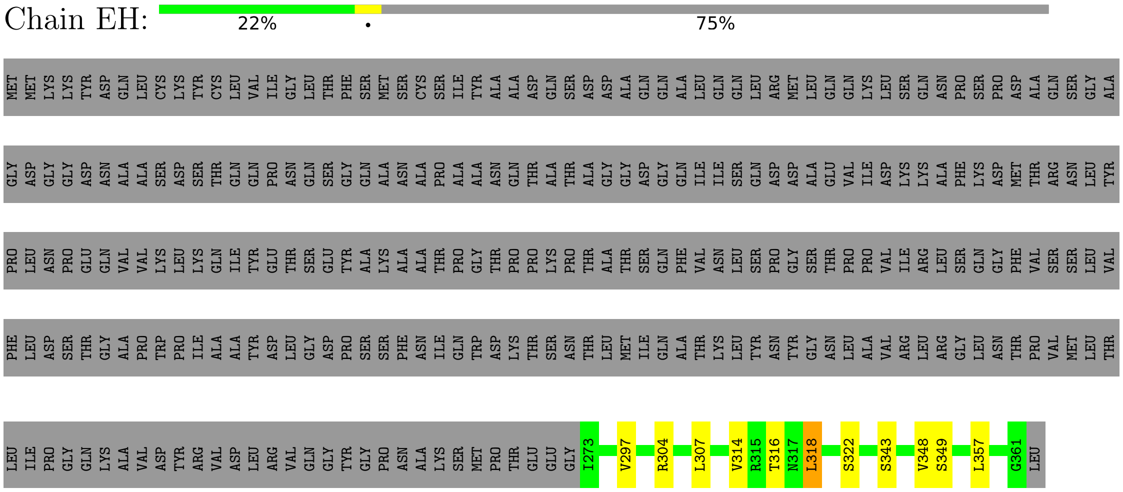


- Molecule 4: Type IV secretion protein IcmK

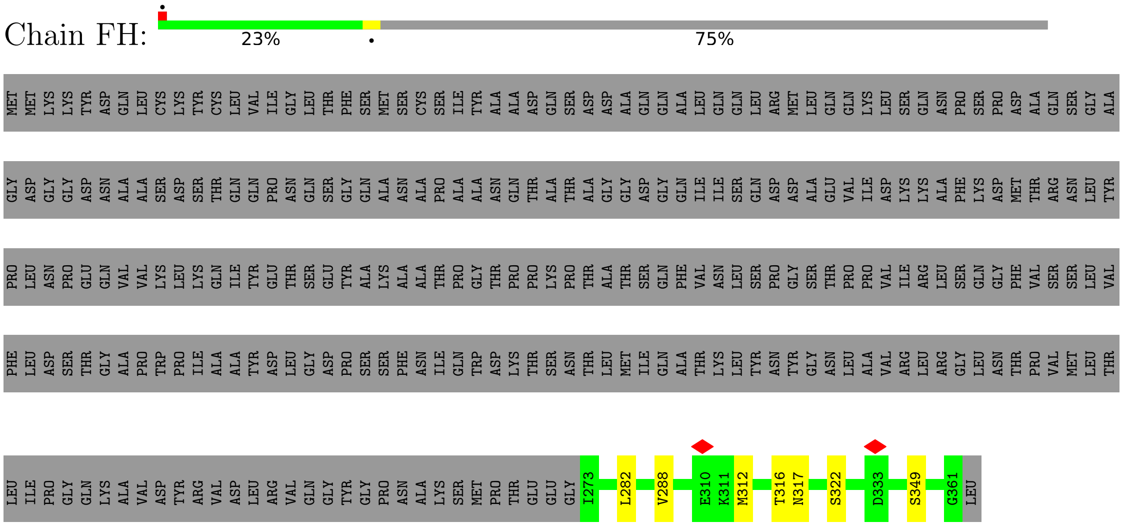
Chain DH:



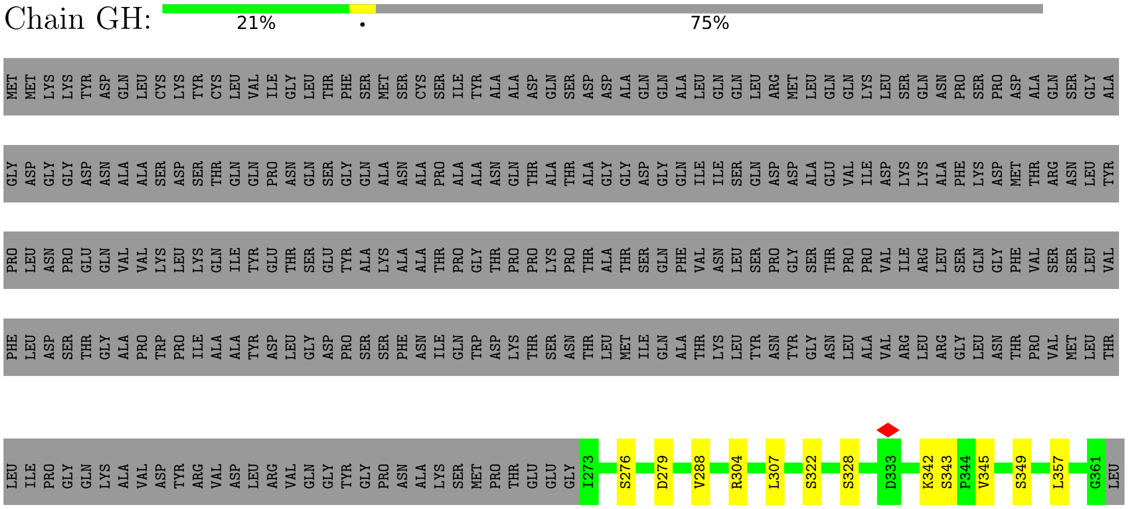
- Molecule 4: Type IV secretion protein IcmK



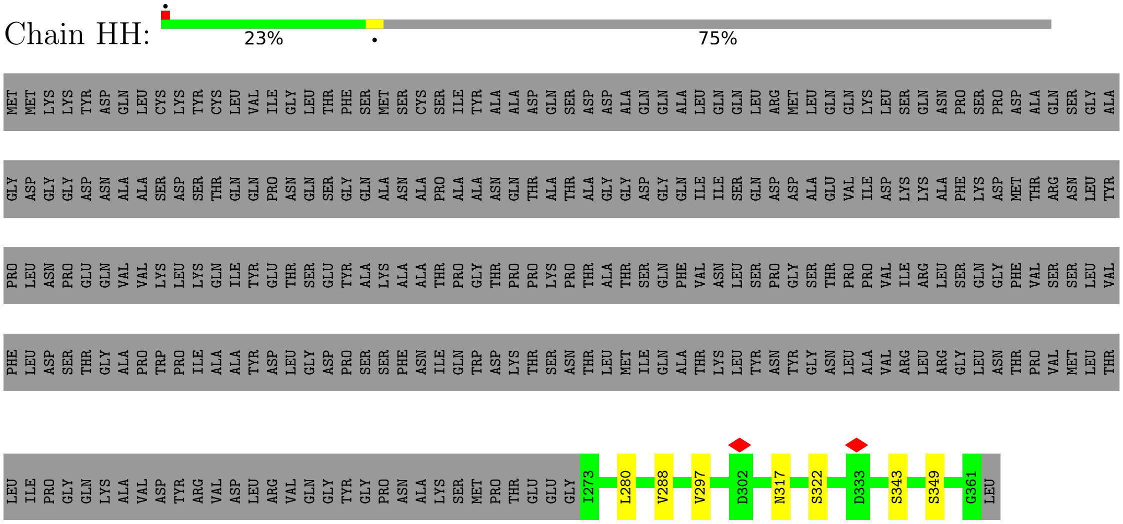
- Molecule 4: Type IV secretion protein IcmK



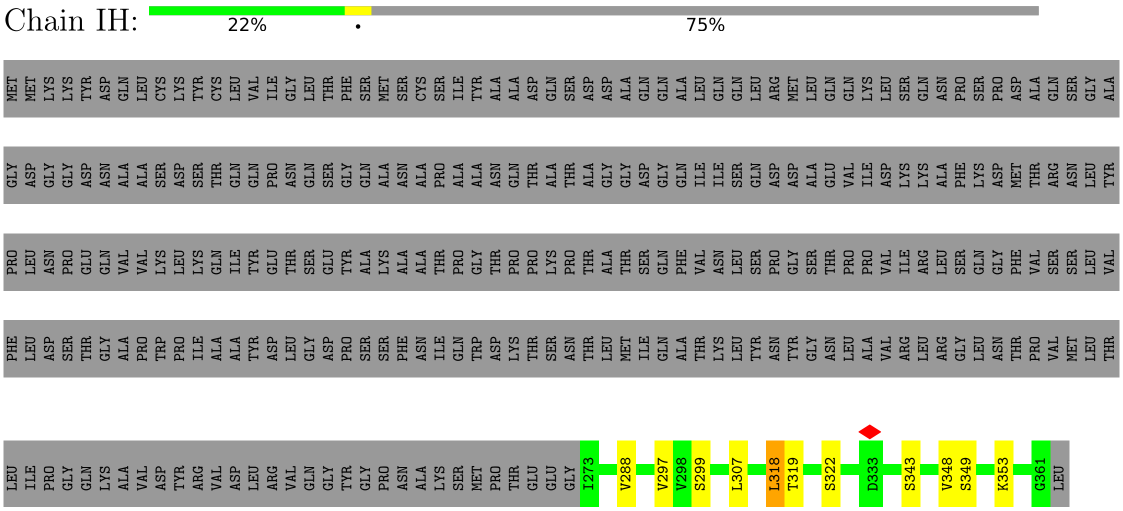
- Molecule 4: Type IV secretion protein IcmK



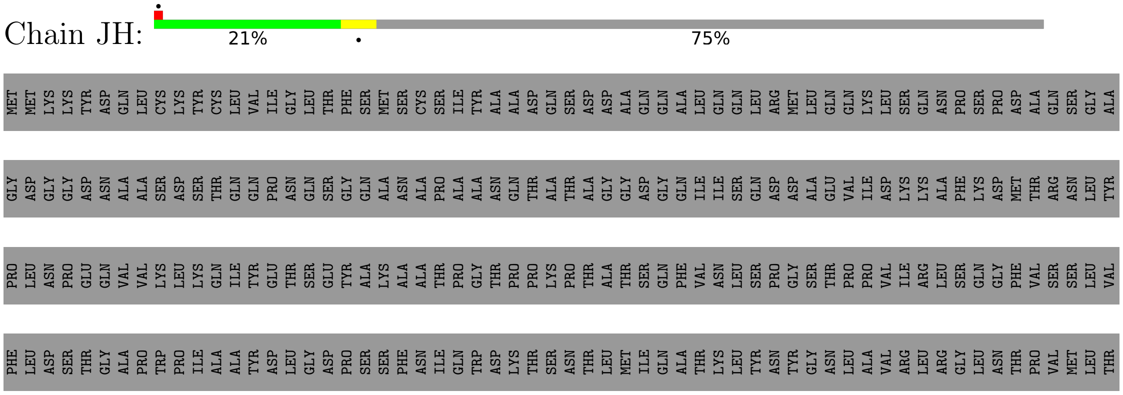
- Molecule 4: Type IV secretion protein IcmK

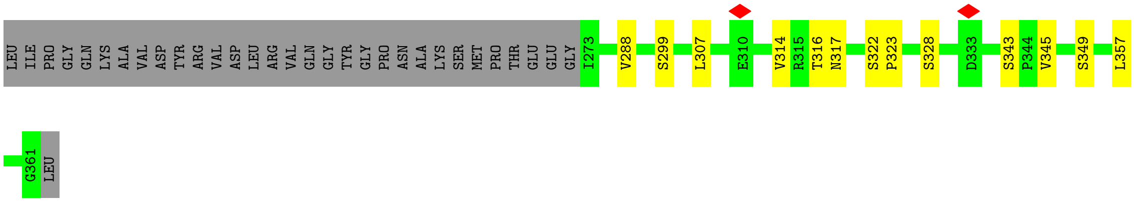


- Molecule 4: Type IV secretion protein IcmK

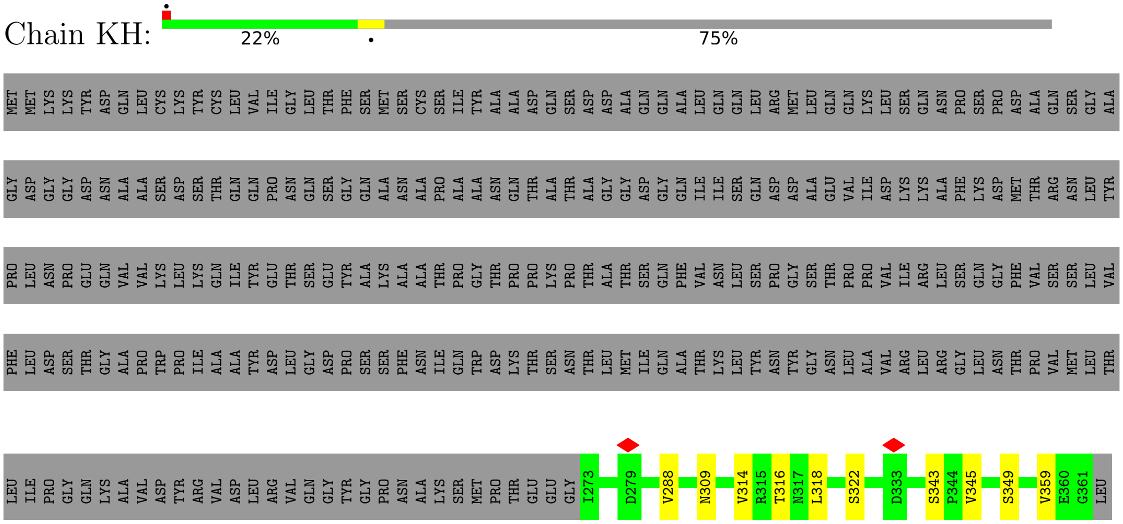


- Molecule 4: Type IV secretion protein IcmK

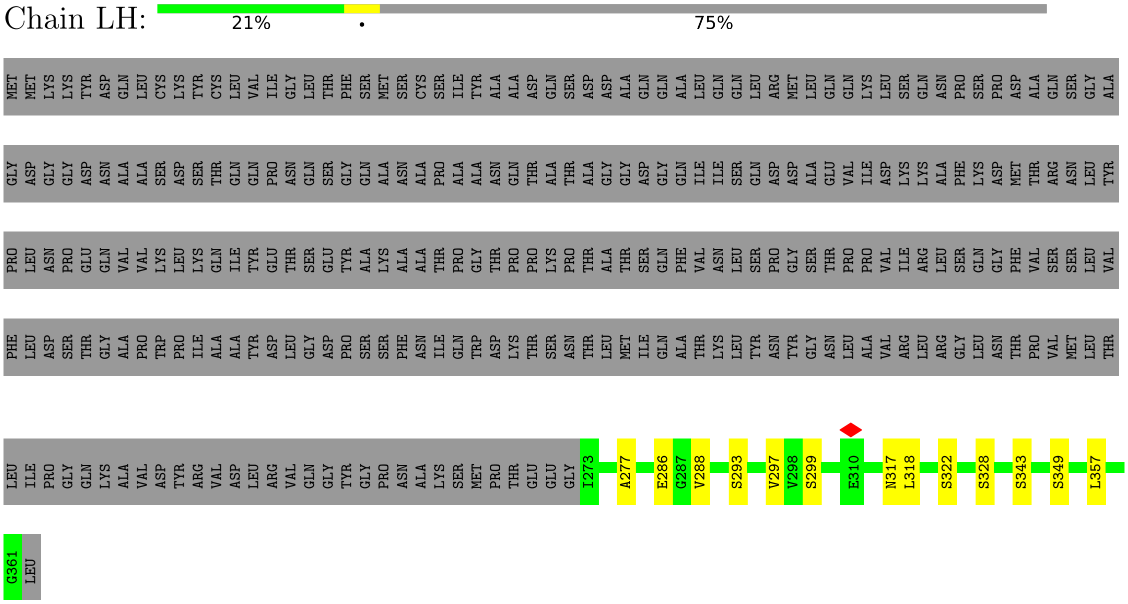




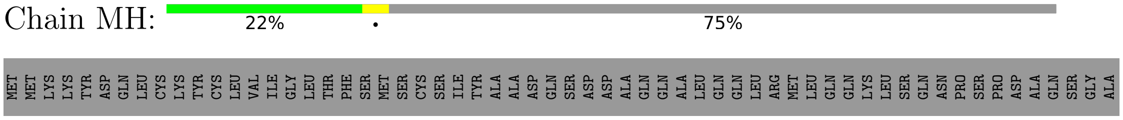
- Molecule 4: Type IV secretion protein IcmK

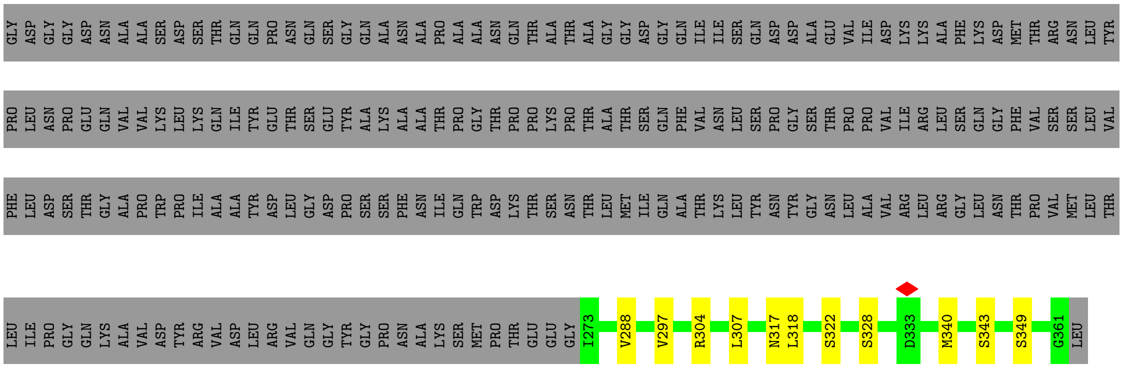


- Molecule 4: Type IV secretion protein IcmK



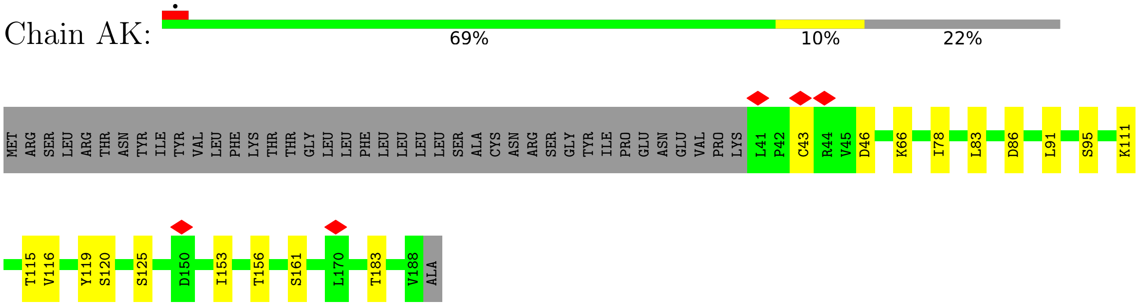
- Molecule 4: Type IV secretion protein IcmK





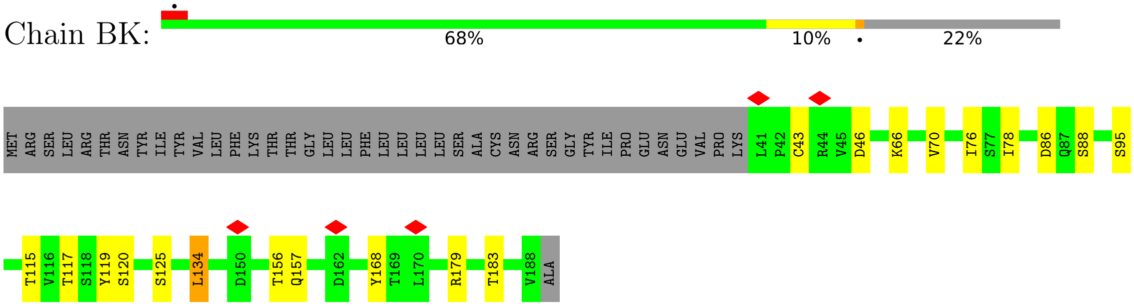
- Molecule 5: Inner membrane lipoprotein YiaD

Chain AK:



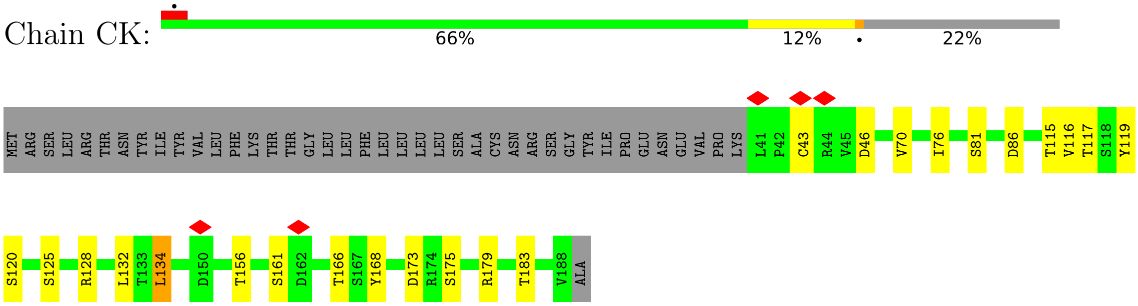
- Molecule 5: Inner membrane lipoprotein YiaD

Chain BK:



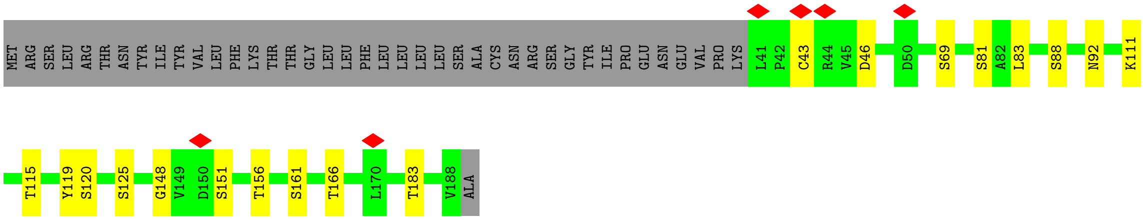
- Molecule 5: Inner membrane lipoprotein YiaD

Chain CK:



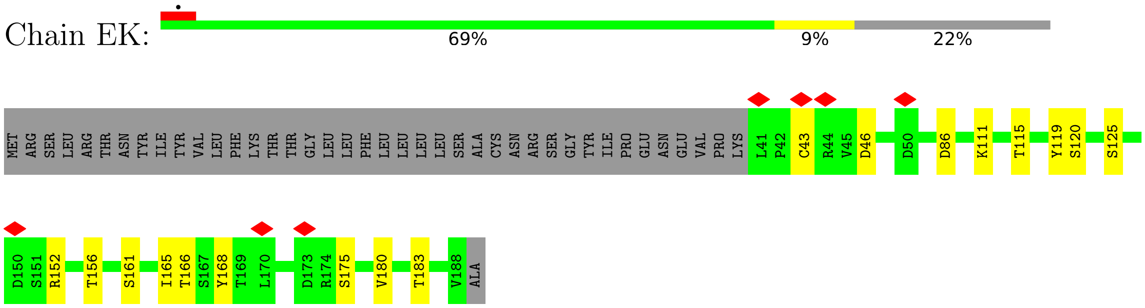
- Molecule 5: Inner membrane lipoprotein YiaD

Chain DK:



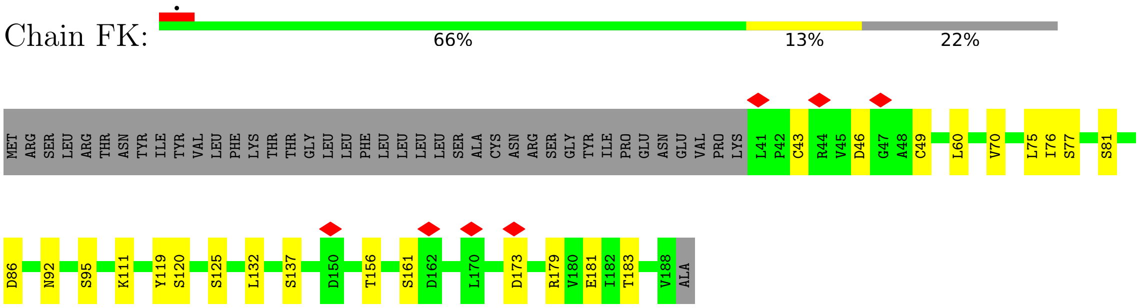
- Molecule 5: Inner membrane lipoprotein YiaD

Chain EK:



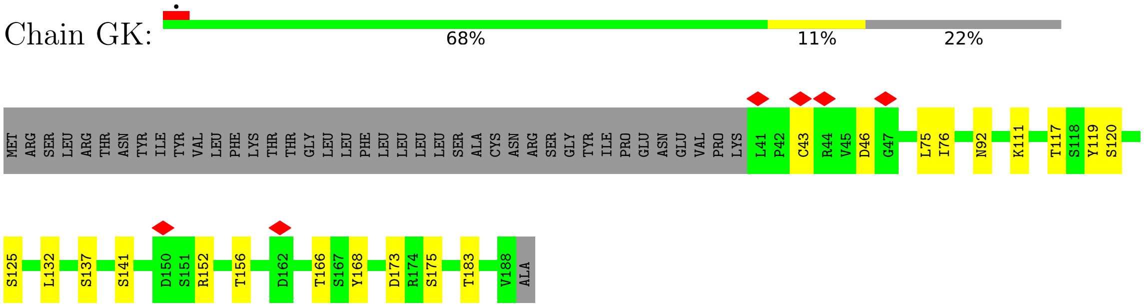
- Molecule 5: Inner membrane lipoprotein YiaD

Chain FK:



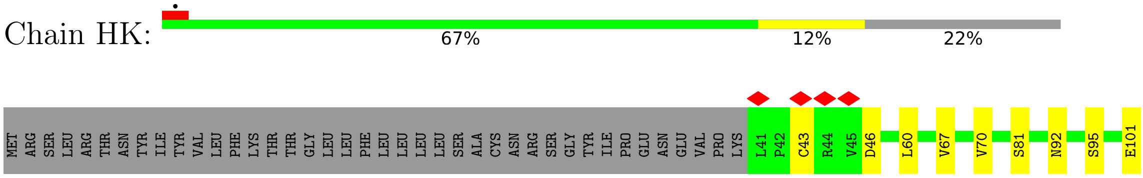
- Molecule 5: Inner membrane lipoprotein YiaD

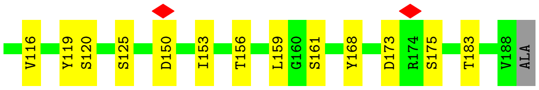
Chain GK:



- Molecule 5: Inner membrane lipoprotein YiaD

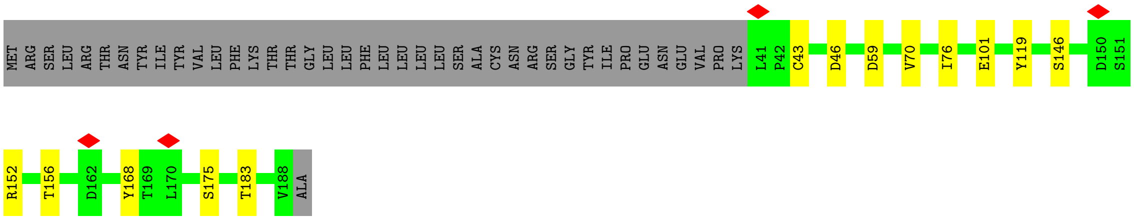
Chain HK:





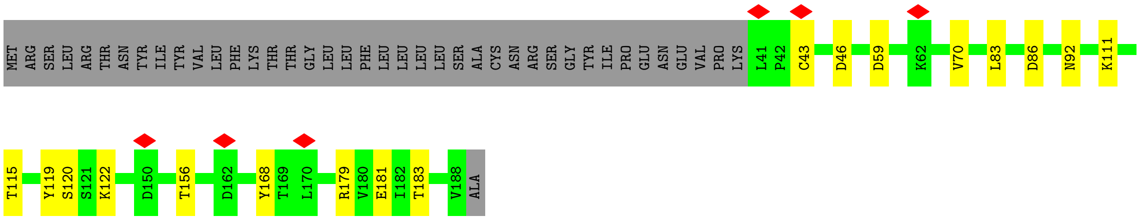
- Molecule 5: Inner membrane lipoprotein YiaD

Chain IK:



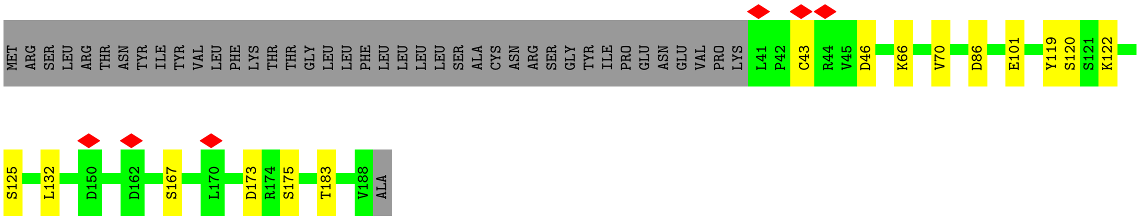
- Molecule 5: Inner membrane lipoprotein YiaD

Chain JK:



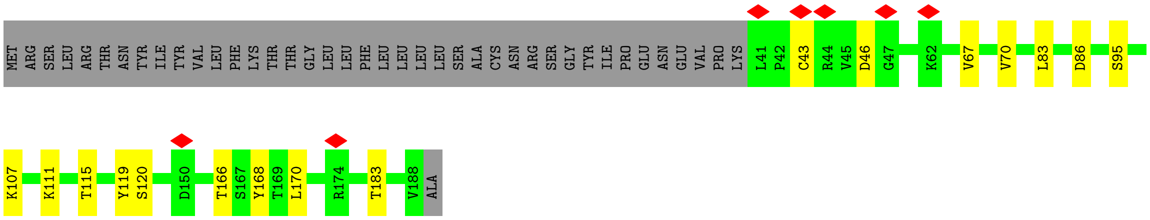
- Molecule 5: Inner membrane lipoprotein YiaD

Chain KK:

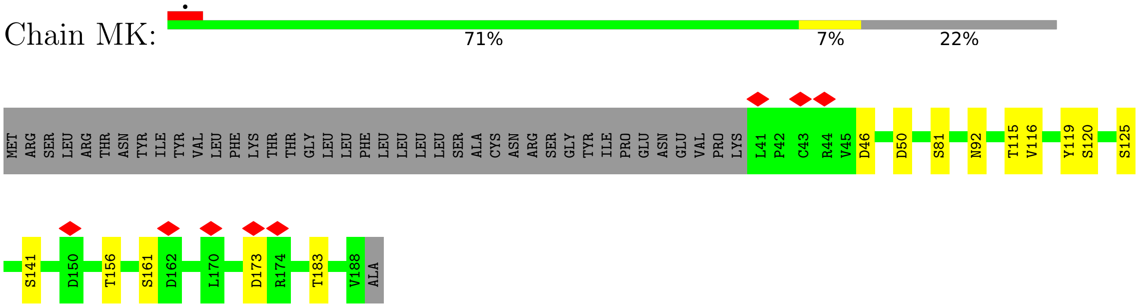


- Molecule 5: Inner membrane lipoprotein YiaD

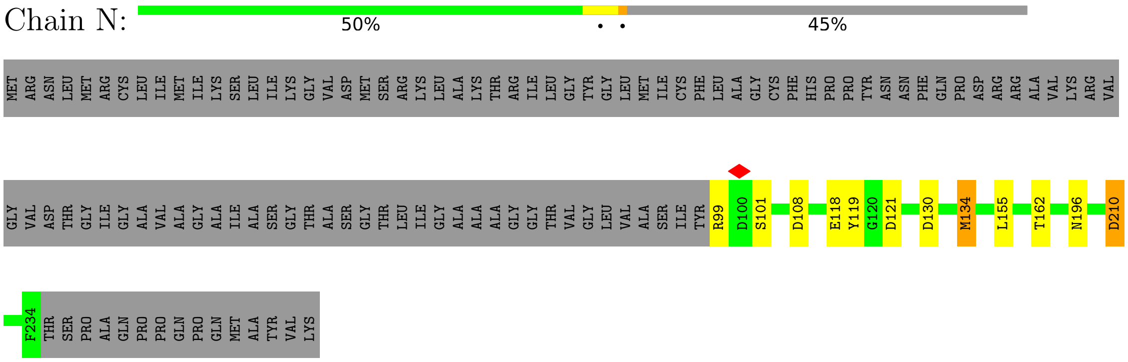
Chain LK:



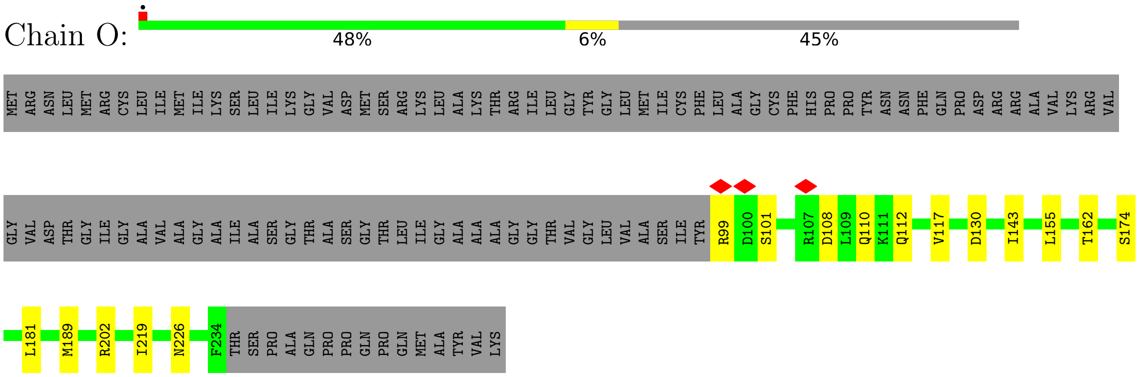
- Molecule 5: Inner membrane lipoprotein YiaD



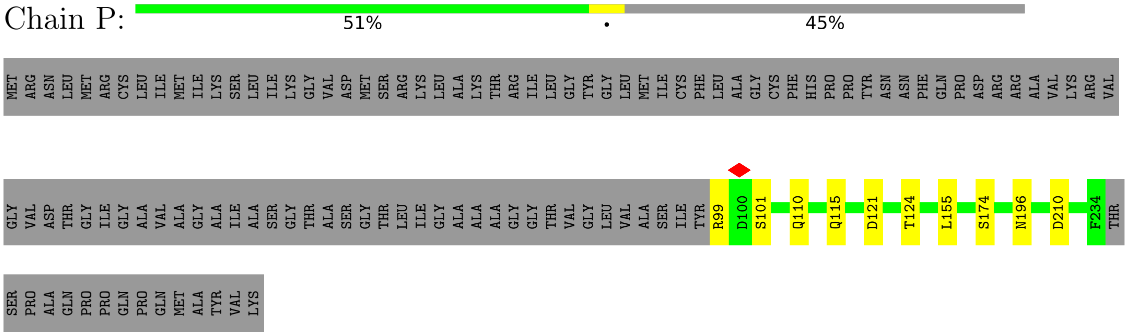
- Molecule 6: Outer membrane protein, OmpA family protein



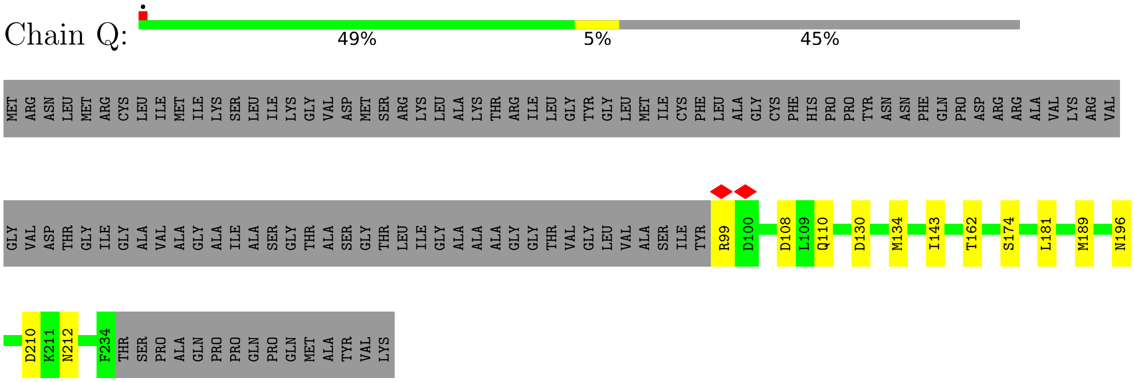
- Molecule 6: Outer membrane protein, OmpA family protein



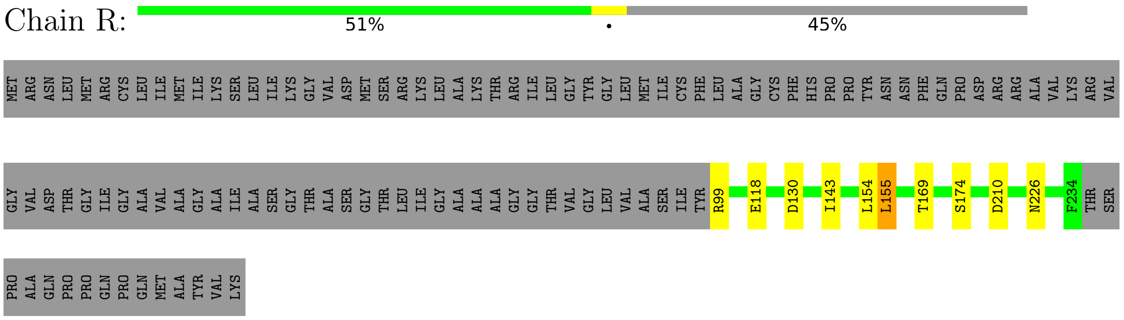
- Molecule 6: Outer membrane protein, OmpA family protein



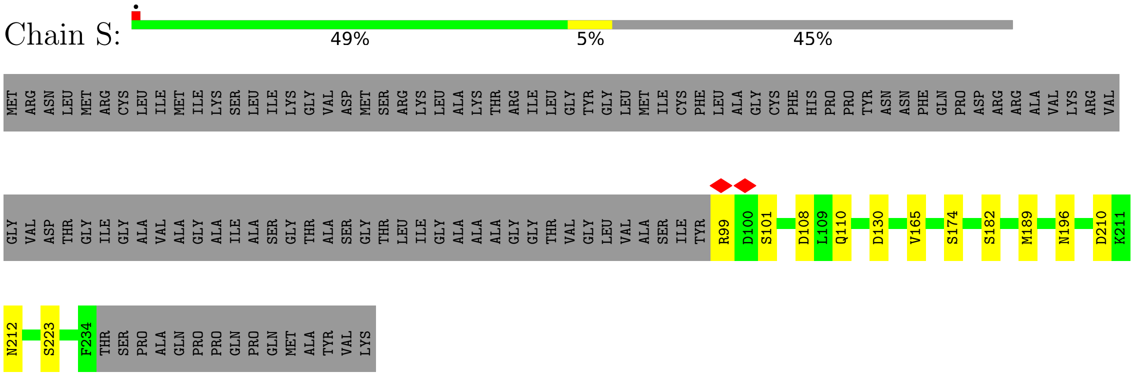
- Molecule 6: Outer membrane protein, OmpA family protein



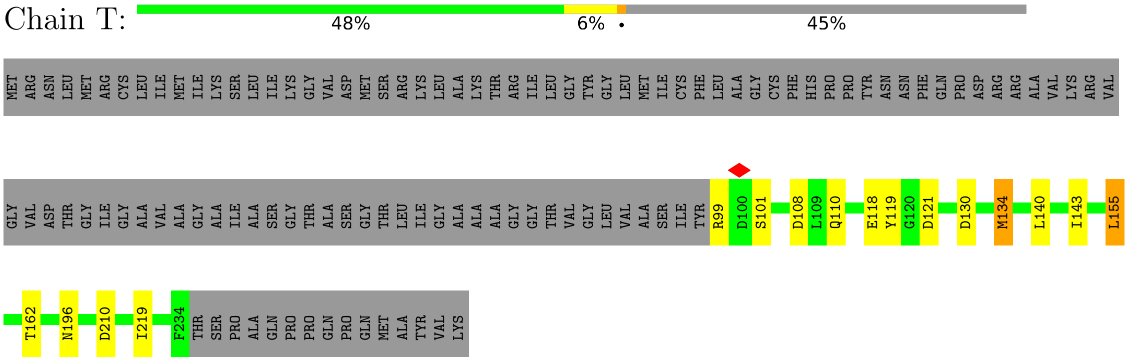
• Molecule 6: Outer membrane protein, OmpA family protein



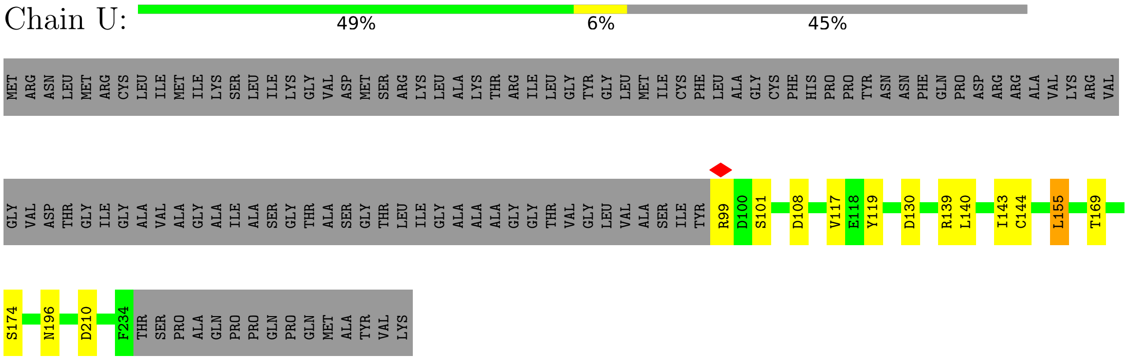
• Molecule 6: Outer membrane protein, OmpA family protein



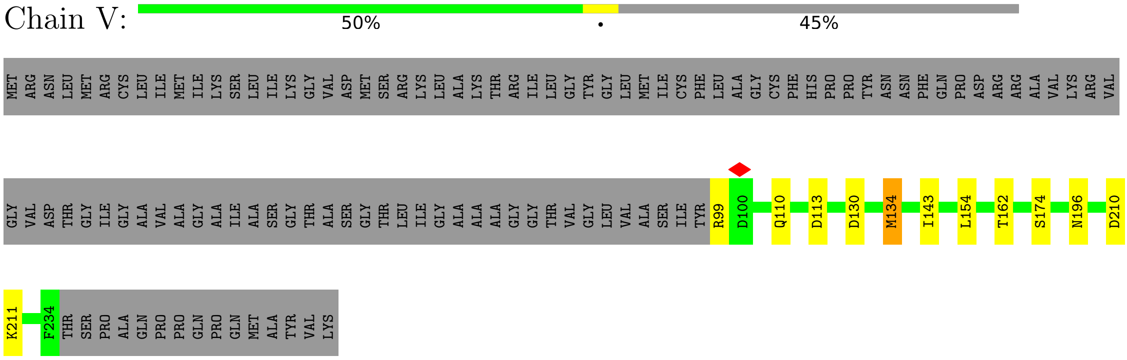
• Molecule 6: Outer membrane protein, OmpA family protein



- Molecule 6: Outer membrane protein, OmpA family protein

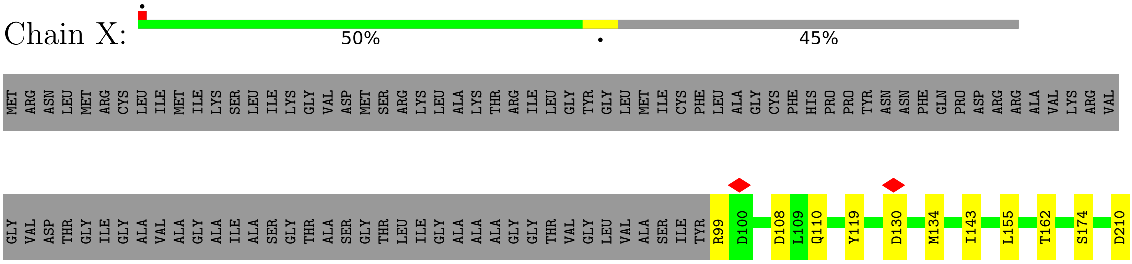


- Molecule 6: Outer membrane protein, OmpA family protein

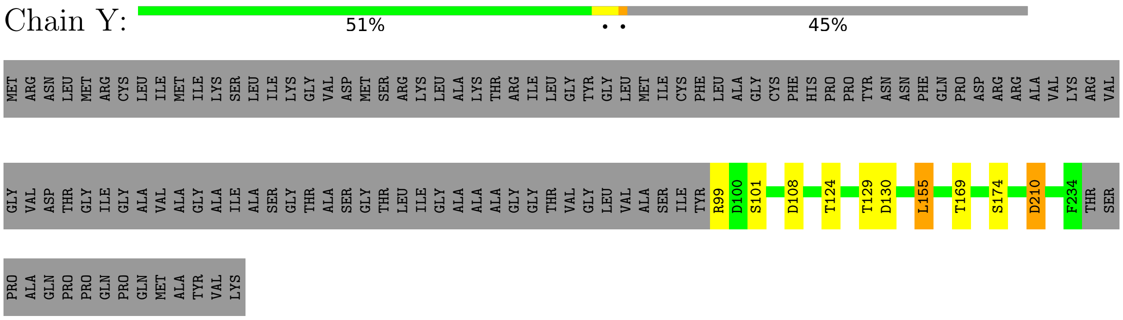


- Molecule 6: Outer membrane protein, OmpA family protein

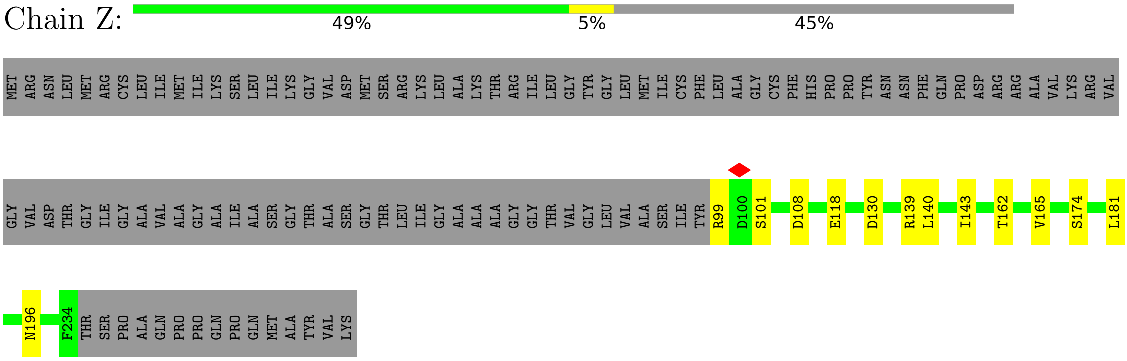
- Molecule 6: Outer membrane protein, OmpA family protein



- Molecule 6: Outer membrane protein, OmpA family protein



- Molecule 6: Outer membrane protein, OmpA family protein



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12200	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 ($e^-/\text{Å}^2$)	58.1	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	42.385	Depositor
Minimum map value	-19.636	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.109	Depositor
Recommended contour level	9.0	Depositor
Map size (Å)	836.39996, 836.39996, 836.39996	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.64, 1.64, 1.64	Depositor

5 Model quality ⓘ

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	$\#|Z| > 5$
2	AC	0.51	0/1629	0.67	0/2214
2	BC	0.51	0/1629	0.70	1/2214 (0.0%)
2	CC	0.52	0/1629	0.73	2/2214 (0.1%)
2	DC	0.49	0/1629	0.67	0/2214
2	EC	0.53	0/1629	0.74	2/2214 (0.1%)
2	FC	0.52	0/1629	0.71	2/2214 (0.1%)
2	GC	0.52	0/1629	0.78	3/2214 (0.1%)
2	HC	0.52	0/1629	0.79	3/2214 (0.1%)
2	IC	0.52	0/1629	0.74	2/2214 (0.1%)
2	JC	0.51	0/1629	0.74	2/2214 (0.1%)
2	KC	0.53	0/1629	0.75	1/2214 (0.0%)
2	LC	0.53	0/1629	0.71	1/2214 (0.0%)
2	MC	0.53	0/1629	0.73	3/2214 (0.1%)
3	AD	0.49	0/1060	0.76	3/1441 (0.2%)
3	Ad	0.50	0/1086	0.81	2/1474 (0.1%)
3	BD	0.50	0/1060	0.80	3/1441 (0.2%)
3	Bd	0.52	0/1086	0.78	1/1474 (0.1%)
3	CD	0.50	0/1060	0.80	1/1441 (0.1%)
3	Cd	0.53	1/1086 (0.1%)	0.82	2/1474 (0.1%)
3	DD	0.50	0/1060	0.78	2/1441 (0.1%)
3	Dd	0.53	0/1086	0.80	1/1474 (0.1%)
3	ED	0.52	0/1060	0.77	2/1441 (0.1%)
3	Ed	0.51	0/1086	0.77	1/1474 (0.1%)
3	FD	0.52	0/1060	0.75	1/1441 (0.1%)
3	Fd	0.55	0/1086	0.78	2/1474 (0.1%)
3	GD	0.50	0/1060	0.79	2/1441 (0.1%)
3	Gd	0.49	0/1086	0.78	2/1474 (0.1%)
3	HD	0.56	1/1060 (0.1%)	0.78	1/1441 (0.1%)
3	Hd	0.53	0/1086	0.82	2/1474 (0.1%)
3	ID	0.49	0/1060	0.76	0/1441
3	Id	0.52	0/1086	0.82	2/1474 (0.1%)
3	JD	0.49	0/1060	0.75	2/1441 (0.1%)
3	Jd	0.54	0/1086	0.82	2/1474 (0.1%)
3	KD	0.51	0/1060	0.77	3/1441 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	Kd	0.52	0/1086	0.77	1/1474 (0.1%)
3	LD	0.55	0/1060	0.80	1/1441 (0.1%)
3	Ld	0.51	0/1086	0.77	2/1474 (0.1%)
3	MD	0.51	0/1060	0.76	2/1441 (0.1%)
3	Md	0.53	0/1086	0.77	1/1474 (0.1%)
4	AH	0.61	0/695	0.79	0/947
4	BH	0.59	0/695	0.82	0/947
4	CH	0.59	0/695	0.78	0/947
4	DH	0.57	0/695	0.77	0/947
4	EH	0.61	0/695	0.79	1/947 (0.1%)
4	FH	0.59	0/695	0.76	0/947
4	GH	0.58	0/695	0.77	2/947 (0.2%)
4	HH	0.55	0/695	0.72	0/947
4	IH	0.57	0/695	0.76	1/947 (0.1%)
4	JH	0.64	0/695	0.79	1/947 (0.1%)
4	KH	0.59	0/695	0.81	1/947 (0.1%)
4	LH	0.62	0/695	0.80	1/947 (0.1%)
4	MH	0.59	0/695	0.78	0/947
5	AK	0.54	0/1171	0.70	0/1583
5	BK	0.52	0/1171	0.73	1/1583 (0.1%)
5	CK	0.52	0/1171	0.75	3/1583 (0.2%)
5	DK	0.53	0/1171	0.70	1/1583 (0.1%)
5	EK	0.53	0/1171	0.71	0/1583
5	FK	0.51	0/1171	0.73	1/1583 (0.1%)
5	GK	0.54	0/1171	0.74	1/1583 (0.1%)
5	HK	0.52	0/1171	0.70	0/1583
5	IK	0.53	0/1171	0.71	1/1583 (0.1%)
5	JK	0.53	0/1171	0.76	1/1583 (0.1%)
5	KK	0.53	0/1171	0.71	1/1583 (0.1%)
5	LK	0.53	0/1171	0.68	1/1583 (0.1%)
5	MK	0.50	0/1171	0.69	0/1583
6	N	0.52	0/1130	0.75	2/1522 (0.1%)
6	O	0.52	0/1130	0.71	0/1522
6	P	0.52	0/1130	0.74	0/1522
6	Q	0.49	0/1130	0.69	0/1522
6	R	0.50	0/1130	0.77	1/1522 (0.1%)
6	S	0.51	0/1130	0.71	0/1522
6	T	0.54	0/1130	0.74	1/1522 (0.1%)
6	U	0.49	0/1130	0.74	2/1522 (0.1%)
6	V	0.51	0/1130	0.77	1/1522 (0.1%)
6	W	0.52	0/1130	0.71	0/1522
6	X	0.53	0/1130	0.75	1/1522 (0.1%)
6	Y	0.54	0/1130	0.74	2/1522 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
6	Z	0.50	0/1130	0.69	0/1522
All	All	0.53	2/88023 (0.0%)	0.75	94/119353 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AX	0	2
1	AZ	0	2
1	BV	0	2
1	BX	0	2
1	BZ	0	2
1	CV	0	1
1	CX	0	2
1	CZ	0	1
1	DX	0	3
1	DZ	0	2
1	EX	0	3
1	EZ	0	1
1	FV	0	1
1	FX	0	3
1	FZ	0	1
1	GV	0	1
1	GX	0	2
1	GZ	0	1
1	HV	0	1
1	HX	0	2
1	HZ	0	1
1	IV	0	1
1	IX	0	2
1	IZ	0	1
1	JX	0	3
1	JZ	0	1
1	KV	0	1
1	KX	0	3
1	KZ	0	1
1	LX	0	3
1	LZ	0	2
1	MX	0	3
1	MZ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	NV	0	1
1	OV	0	2
1	PV	0	1
1	RV	0	1
2	BC	0	1
3	Bd	0	1
3	Ed	0	1
3	Fd	0	1
3	Id	0	1
3	Jd	0	1
3	Kd	0	1
3	Md	0	1
4	AH	0	1
4	BH	0	1
4	DH	0	2
4	EH	0	1
4	FH	0	1
4	GH	0	1
4	HH	0	1
4	IH	0	1
4	JH	0	1
4	KH	0	1
4	LH	0	1
5	DK	0	1
6	N	0	2
6	O	0	2
6	Q	0	2
6	T	0	1
6	V	0	2
6	W	0	1
6	X	0	1
6	Z	0	1
All	All	0	96

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Cd	58	VAL	CB-CG1	-5.97	1.40	1.52
3	HD	31	ASN	C-N	-5.41	1.21	1.34

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	JK	59	ASP	CB-CG-OD2	10.30	127.58	118.30
2	HC	117	LEU	CA-CB-CG	10.27	138.92	115.30
6	X	155	LEU	CA-CB-CG	9.98	138.26	115.30
6	V	113	ASP	CB-CG-OD1	9.90	127.21	118.30
2	GC	117	LEU	CA-CB-CG	9.13	136.30	115.30
2	GC	119	LEU	CA-CB-CG	8.36	134.54	115.30
2	KC	64	LEU	CA-CB-CG	8.35	134.50	115.30
6	R	155	LEU	CA-CB-CG	8.31	134.41	115.30
6	T	155	LEU	CA-CB-CG	7.86	133.38	115.30
3	HD	50	ASP	CB-CG-OD1	7.82	125.34	118.30
3	Jd	53	LEU	CB-CG-CD1	-7.56	98.14	111.00
3	Gd	71	LEU	CA-CB-CG	7.47	132.49	115.30
3	ED	50	ASP	CB-CG-OD1	7.42	124.98	118.30
2	IC	64	LEU	CA-CB-CG	7.39	132.29	115.30
3	AD	128	LEU	CA-CB-CG	7.35	132.21	115.30
2	MC	211	LEU	CA-CB-CG	7.23	131.94	115.30
2	IC	99	LEU	CA-CB-CG	7.17	131.79	115.30
2	JC	211	LEU	CA-CB-CG	7.05	131.53	115.30
3	MD	50	ASP	CB-CG-OD2	7.02	124.62	118.30
3	DD	50	ASP	CB-CG-OD2	6.84	124.46	118.30
2	BC	243	ASP	CB-CG-OD1	6.65	124.28	118.30
3	JD	94	LEU	CB-CG-CD2	6.58	122.19	111.00
6	U	108	ASP	CB-CG-OD2	6.52	124.17	118.30
5	LK	83	LEU	CA-CB-CG	6.51	130.27	115.30
3	GD	50	ASP	CB-CG-OD2	6.41	124.07	118.30
2	GC	243	ASP	CB-CG-OD1	6.39	124.05	118.30
5	CK	134	LEU	CA-CB-CG	6.30	129.79	115.30
5	IK	59	ASP	CB-CG-OD1	6.27	123.94	118.30
2	EC	72	LEU	CA-CB-CG	6.23	129.62	115.30
5	CK	132	LEU	CA-CB-CG	6.21	129.59	115.30
3	Fd	109	LEU	CA-CB-CG	6.21	129.58	115.30
4	KH	318	LEU	CA-CB-CG	6.20	129.56	115.30
3	ED	94	LEU	CA-CB-CG	6.17	129.48	115.30
3	AD	50	ASP	CB-CG-OD2	6.08	123.78	118.30
3	Hd	77	TYR	C-N-CA	6.03	136.78	121.70
3	Ld	77	TYR	C-N-CA	6.02	136.76	121.70
5	GK	132	LEU	CA-CB-CG	6.01	129.12	115.30
3	BD	94	LEU	CB-CG-CD2	6.01	121.21	111.00
2	CC	243	ASP	CB-CG-OD2	5.92	123.62	118.30
3	CD	59	GLU	CA-CB-CG	5.92	126.42	113.40
5	FK	132	LEU	CA-CB-CG	5.90	128.87	115.30
3	Ad	77	TYR	C-N-CA	5.88	136.41	121.70
5	BK	134	LEU	CA-CB-CG	5.86	128.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	KD	128	LEU	CA-CB-CG	5.84	128.74	115.30
3	Gd	77	TYR	C-N-CA	5.78	136.14	121.70
3	Ad	131	ILE	CG1-CB-CG2	-5.77	98.70	111.40
4	JH	357	LEU	CA-CB-CG	5.75	128.52	115.30
3	BD	98	ILE	CG1-CB-CG2	-5.71	98.84	111.40
2	MC	72	LEU	CA-CB-CG	5.71	128.43	115.30
3	Cd	58	VAL	CG1-CB-CG2	-5.69	101.79	110.90
3	Id	117	VAL	CG1-CB-CG2	-5.69	101.80	110.90
3	Hd	50	ASP	CB-CG-OD2	5.67	123.40	118.30
6	Y	155	LEU	CA-CB-CG	5.65	128.31	115.30
3	Dd	77	TYR	C-N-CA	5.64	135.79	121.70
5	DK	83	LEU	CA-CB-CG	5.62	128.22	115.30
3	BD	50	ASP	CB-CG-OD2	5.59	123.33	118.30
3	Cd	77	TYR	C-N-CA	5.58	135.66	121.70
2	HC	189	ASP	CB-CG-OD1	5.58	123.32	118.30
3	Id	77	TYR	C-N-CA	5.57	135.63	121.70
2	LC	243	ASP	CB-CG-OD1	5.52	123.27	118.30
6	N	121	ASP	CB-CG-OD1	5.49	123.24	118.30
3	Fd	53	LEU	CA-CB-CG	5.47	127.89	115.30
2	JC	90	LEU	CA-CB-CG	-5.46	102.73	115.30
3	Md	77	TYR	C-N-CA	5.43	135.27	121.70
3	LD	67	LYS	CA-CB-CG	5.42	125.33	113.40
3	Ed	71	LEU	CA-CB-CG	5.42	127.75	115.30
3	JD	125	ASP	CB-CG-OD2	5.36	123.13	118.30
2	FC	199	ILE	CG1-CB-CG2	-5.35	99.64	111.40
3	Bd	77	TYR	C-N-CA	5.34	135.05	121.70
3	Ld	58	VAL	CG1-CB-CG2	-5.34	102.36	110.90
3	DD	86	ASP	CB-CG-OD1	5.31	123.08	118.30
4	IH	318	LEU	CA-CB-CG	5.30	127.50	115.30
2	FC	64	LEU	CA-CB-CG	5.29	127.46	115.30
4	GH	357	LEU	CA-CB-CG	5.29	127.46	115.30
6	Y	210	ASP	CB-CG-OD1	5.27	123.05	118.30
3	AD	94	LEU	CB-CG-CD2	5.23	119.89	111.00
3	Kd	77	TYR	C-N-CA	5.23	134.77	121.70
6	N	210	ASP	CB-CG-OD1	5.20	122.98	118.30
4	GH	279	ASP	CB-CG-OD2	5.20	122.98	118.30
6	U	155	LEU	CA-CB-CG	5.19	127.23	115.30
2	CC	117	LEU	CA-CB-CG	5.19	127.23	115.30
3	MD	86	ASP	CB-CG-OD1	5.19	122.97	118.30
2	MC	243	ASP	CB-CG-OD1	5.18	122.96	118.30
5	KK	70	VAL	CG1-CB-CG2	-5.16	102.64	110.90
4	LH	357	LEU	CA-CB-CG	5.16	127.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	KD	86	ASP	CB-CG-OD1	5.16	122.94	118.30
3	GD	94	LEU	CB-CG-CD2	5.15	119.75	111.00
3	KD	94	LEU	CA-CB-CG	5.12	127.07	115.30
3	FD	50	ASP	CB-CG-OD2	5.10	122.89	118.30
2	EC	117	LEU	CA-CB-CG	5.07	126.97	115.30
5	CK	70	VAL	CG1-CB-CG2	-5.05	102.81	110.90
2	HC	90	LEU	CA-CB-CG	-5.03	103.72	115.30
3	Jd	77	TYR	C-N-CA	5.03	134.27	121.70
4	EH	318	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AH	322	SER	Peptide
1	AX	142	UNK	Peptide
1	AX	153	UNK	Peptide
1	AZ	20	UNK	Peptide
1	AZ	45	UNK	Peptide
2	BC	233	VAL	Peptide
4	BH	277	ALA	Peptide
1	BV	42	UNK	Peptide
1	BV	46	UNK	Peptide
1	BX	142	UNK	Peptide
1	BX	153	UNK	Peptide
1	BZ	20	UNK	Peptide
1	BZ	45	UNK	Peptide
3	Bd	27	LYS	Peptide
1	CV	77	UNK	Peptide
1	CX	142	UNK	Peptide
1	CX	153	UNK	Peptide
1	CZ	45	UNK	Peptide
4	DH	277	ALA	Peptide
4	DH	322	SER	Peptide
5	DK	148	GLY	Peptide
1	DX	142	UNK	Peptide
1	DX	153	UNK	Peptide
1	DX	219	UNK	Peptide
1	DZ	20	UNK	Peptide
1	DZ	45	UNK	Peptide
4	EH	322	SER	Peptide
1	EX	142	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	EX	153	UNK	Peptide
1	EX	43	UNK	Peptide
1	EZ	45	UNK	Peptide
3	Ed	78	ASN	Peptide
4	FH	322	SER	Peptide
1	FV	42	UNK	Peptide
1	FX	142	UNK	Peptide
1	FX	153	UNK	Peptide
1	FX	154	UNK	Peptide
1	FZ	45	UNK	Peptide
3	Fd	85	VAL	Peptide
4	GH	322	SER	Peptide
1	GV	77	UNK	Peptide
1	GX	142	UNK	Peptide
1	GX	153	UNK	Peptide
1	GZ	45	UNK	Peptide
4	HH	322	SER	Peptide
1	HV	77	UNK	Peptide
1	HX	142	UNK	Peptide
1	HX	153	UNK	Peptide
1	HZ	45	UNK	Peptide
4	IH	322	SER	Peptide
1	IV	77	UNK	Peptide
1	IX	142	UNK	Peptide
1	IX	153	UNK	Peptide
1	IZ	45	UNK	Peptide
3	Id	85	VAL	Peptide
4	JH	322	SER	Peptide
1	JX	142	UNK	Peptide
1	JX	153	UNK	Peptide
1	JX	43	UNK	Peptide
1	JZ	45	UNK	Peptide
3	Jd	85	VAL	Peptide
4	KH	322	SER	Peptide
1	KV	42	UNK	Peptide
1	KX	142	UNK	Peptide
1	KX	153	UNK	Peptide
1	KX	43	UNK	Peptide
1	KZ	45	UNK	Peptide
3	Kd	78	ASN	Peptide
4	LH	277	ALA	Peptide
1	LX	142	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	LX	153	UNK	Peptide
1	LX	154	UNK	Peptide
1	LZ	20	UNK	Peptide
1	LZ	45	UNK	Peptide
1	MX	142	UNK	Peptide
1	MX	153	UNK	Peptide
1	MX	43	UNK	Peptide
1	MZ	45	UNK	Peptide
3	Md	85	VAL	Peptide
6	N	134	MET	Peptide
6	N	196	ASN	Peptide
1	NV	42	UNK	Peptide
6	O	112	GLN	Peptide
6	O	155	LEU	Peptide
1	OV	41	UNK	Peptide
1	OV	42	UNK	Peptide
1	PV	77	UNK	Peptide
6	Q	134	MET	Peptide
6	Q	212	ASN	Peptide
1	RV	77	UNK	Peptide
6	T	134	MET	Peptide
6	V	134	MET	Peptide
6	V	196	ASN	Peptide
6	W	134	MET	Peptide
6	X	134	MET	Peptide
6	Z	196	ASN	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	AC	196/303 (65%)	190 (97%)	6 (3%)	0	100	100
2	BC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	CC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	DC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	EC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	FC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	GC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	HC	196/303 (65%)	190 (97%)	6 (3%)	0	100	100
2	IC	196/303 (65%)	191 (97%)	5 (3%)	0	100	100
2	JC	196/303 (65%)	187 (95%)	9 (5%)	0	100	100
2	KC	196/303 (65%)	189 (96%)	7 (4%)	0	100	100
2	LC	196/303 (65%)	188 (96%)	8 (4%)	0	100	100
2	MC	196/303 (65%)	191 (97%)	5 (3%)	0	100	100
3	AD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
3	Ad	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	BD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Bd	136/163 (83%)	125 (92%)	11 (8%)	0	100	100
3	CD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Cd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	DD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Dd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
3	ED	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Ed	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
3	FD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Fd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	GD	133/163 (82%)	125 (94%)	8 (6%)	0	100	100
3	Gd	136/163 (83%)	128 (94%)	8 (6%)	0	100	100
3	HD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Hd	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	ID	133/163 (82%)	129 (97%)	4 (3%)	0	100	100
3	Id	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	JD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Jd	136/163 (83%)	127 (93%)	9 (7%)	0	100	100
3	KD	133/163 (82%)	127 (96%)	6 (4%)	0	100	100
3	Kd	136/163 (83%)	130 (96%)	6 (4%)	0	100	100
3	LD	133/163 (82%)	126 (95%)	7 (5%)	0	100	100
3	Ld	136/163 (83%)	126 (93%)	10 (7%)	0	100	100
3	MD	133/163 (82%)	128 (96%)	5 (4%)	0	100	100
3	Md	136/163 (83%)	129 (95%)	7 (5%)	0	100	100
4	AH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	BH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	CH	87/361 (24%)	77 (88%)	10 (12%)	0	100	100
4	DH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	EH	87/361 (24%)	76 (87%)	11 (13%)	0	100	100
4	FH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	GH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	HH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	IH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	JH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
4	KH	87/361 (24%)	79 (91%)	8 (9%)	0	100	100
4	LH	87/361 (24%)	77 (88%)	10 (12%)	0	100	100
4	MH	87/361 (24%)	78 (90%)	9 (10%)	0	100	100
5	AK	146/189 (77%)	142 (97%)	4 (3%)	0	100	100
5	BK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	CK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	DK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	EK	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
5	FK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100
5	GK	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
5	HK	146/189 (77%)	138 (94%)	8 (6%)	0	100	100
5	IK	146/189 (77%)	140 (96%)	6 (4%)	0	100	100
5	JK	146/189 (77%)	141 (97%)	5 (3%)	0	100	100
5	KK	146/189 (77%)	137 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	LK	146/189 (77%)	139 (95%)	7 (5%)	0	100	100
5	MK	146/189 (77%)	136 (93%)	10 (7%)	0	100	100
6	N	134/249 (54%)	123 (92%)	11 (8%)	0	100	100
6	O	134/249 (54%)	124 (92%)	10 (8%)	0	100	100
6	P	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	Q	134/249 (54%)	127 (95%)	7 (5%)	0	100	100
6	R	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	S	134/249 (54%)	127 (95%)	7 (5%)	0	100	100
6	T	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	U	134/249 (54%)	128 (96%)	6 (4%)	0	100	100
6	V	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
6	W	134/249 (54%)	124 (92%)	10 (8%)	0	100	100
6	X	134/249 (54%)	125 (93%)	9 (7%)	0	100	100
6	Y	134/249 (54%)	125 (93%)	9 (7%)	0	100	100
6	Z	134/249 (54%)	126 (94%)	8 (6%)	0	100	100
All	All	10816/18564 (58%)	10205 (94%)	611 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	
2	AC	169/257 (66%)	157 (93%)	12 (7%)	14	45
2	BC	169/257 (66%)	153 (90%)	16 (10%)	8	34
2	CC	169/257 (66%)	154 (91%)	15 (9%)	9	37
2	DC	169/257 (66%)	149 (88%)	20 (12%)	5	26
2	EC	169/257 (66%)	152 (90%)	17 (10%)	7	31
2	FC	169/257 (66%)	155 (92%)	14 (8%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	GC	169/257 (66%)	153 (90%)	16 (10%)	8	34
2	HC	169/257 (66%)	156 (92%)	13 (8%)	13	43
2	IC	169/257 (66%)	152 (90%)	17 (10%)	7	31
2	JC	169/257 (66%)	156 (92%)	13 (8%)	13	43
2	KC	169/257 (66%)	154 (91%)	15 (9%)	9	37
2	LC	169/257 (66%)	154 (91%)	15 (9%)	9	37
2	MC	169/257 (66%)	157 (93%)	12 (7%)	14	45
3	AD	116/139 (84%)	101 (87%)	15 (13%)	4	22
3	Ad	119/139 (86%)	105 (88%)	14 (12%)	5	26
3	BD	116/139 (84%)	99 (85%)	17 (15%)	3	18
3	Bd	119/139 (86%)	106 (89%)	13 (11%)	6	29
3	CD	116/139 (84%)	93 (80%)	23 (20%)	1	8
3	Cd	119/139 (86%)	109 (92%)	10 (8%)	11	40
3	DD	116/139 (84%)	100 (86%)	16 (14%)	3	21
3	Dd	119/139 (86%)	104 (87%)	15 (13%)	4	23
3	ED	116/139 (84%)	98 (84%)	18 (16%)	2	17
3	Ed	119/139 (86%)	108 (91%)	11 (9%)	9	36
3	FD	116/139 (84%)	98 (84%)	18 (16%)	2	17
3	Fd	119/139 (86%)	106 (89%)	13 (11%)	6	29
3	GD	116/139 (84%)	101 (87%)	15 (13%)	4	22
3	Gd	119/139 (86%)	101 (85%)	18 (15%)	3	17
3	HD	116/139 (84%)	95 (82%)	21 (18%)	1	11
3	Hd	119/139 (86%)	102 (86%)	17 (14%)	3	19
3	ID	116/139 (84%)	102 (88%)	14 (12%)	5	24
3	Id	119/139 (86%)	110 (92%)	9 (8%)	13	43
3	JD	116/139 (84%)	100 (86%)	16 (14%)	3	21
3	Jd	119/139 (86%)	105 (88%)	14 (12%)	5	26
3	KD	116/139 (84%)	105 (90%)	11 (10%)	8	34
3	Kd	119/139 (86%)	100 (84%)	19 (16%)	2	15
3	LD	116/139 (84%)	99 (85%)	17 (15%)	3	18
3	Ld	119/139 (86%)	103 (87%)	16 (13%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	MD	116/139 (84%)	102 (88%)	14 (12%)	5	24
3	Md	119/139 (86%)	97 (82%)	22 (18%)	1	10
4	AH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	BH	75/300 (25%)	64 (85%)	11 (15%)	3	18
4	CH	75/300 (25%)	67 (89%)	8 (11%)	6	30
4	DH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	EH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	FH	75/300 (25%)	69 (92%)	6 (8%)	12	42
4	GH	75/300 (25%)	66 (88%)	9 (12%)	5	25
4	HH	75/300 (25%)	69 (92%)	6 (8%)	12	42
4	IH	75/300 (25%)	65 (87%)	10 (13%)	4	22
4	JH	75/300 (25%)	64 (85%)	11 (15%)	3	18
4	KH	75/300 (25%)	67 (89%)	8 (11%)	6	30
4	LH	75/300 (25%)	64 (85%)	11 (15%)	3	18
4	MH	75/300 (25%)	64 (85%)	11 (15%)	3	18
5	AK	126/163 (77%)	108 (86%)	18 (14%)	3	19
5	BK	126/163 (77%)	106 (84%)	20 (16%)	2	16
5	CK	126/163 (77%)	105 (83%)	21 (17%)	2	14
5	DK	126/163 (77%)	110 (87%)	16 (13%)	4	23
5	EK	126/163 (77%)	109 (86%)	17 (14%)	4	21
5	FK	126/163 (77%)	103 (82%)	23 (18%)	1	10
5	GK	126/163 (77%)	107 (85%)	19 (15%)	3	17
5	HK	126/163 (77%)	104 (82%)	22 (18%)	2	12
5	IK	126/163 (77%)	114 (90%)	12 (10%)	8	34
5	JK	126/163 (77%)	110 (87%)	16 (13%)	4	23
5	KK	126/163 (77%)	112 (89%)	14 (11%)	6	28
5	LK	126/163 (77%)	111 (88%)	15 (12%)	5	25
5	MK	126/163 (77%)	112 (89%)	14 (11%)	6	28
6	N	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	O	118/203 (58%)	104 (88%)	14 (12%)	5	25
6	P	118/203 (58%)	108 (92%)	10 (8%)	10	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Q	118/203 (58%)	107 (91%)	11 (9%)	9	35
6	R	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	S	118/203 (58%)	105 (89%)	13 (11%)	6	29
6	T	118/203 (58%)	102 (86%)	16 (14%)	3	21
6	U	118/203 (58%)	104 (88%)	14 (12%)	5	25
6	V	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	W	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	X	118/203 (58%)	109 (92%)	9 (8%)	13	43
6	Y	118/203 (58%)	108 (92%)	10 (8%)	10	40
6	Z	118/203 (58%)	106 (90%)	12 (10%)	7	31
All	All	9399/15613 (60%)	8301 (88%)	1098 (12%)	9	26

All (1098) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AC	61	GLU
2	AC	72	LEU
2	AC	102	GLU
2	AC	137	GLN
2	AC	141	ILE
2	AC	173	LYS
2	AC	177	CYS
2	AC	190	GLN
2	AC	229	THR
2	AC	246	VAL
2	AC	258	ASN
2	AC	259	SER
3	AD	47	SER
3	AD	58	VAL
3	AD	61	VAL
3	AD	63	THR
3	AD	70	THR
3	AD	86	ASP
3	AD	108	VAL
3	AD	111	LYS
3	AD	115	VAL
3	AD	117	VAL
3	AD	123	THR

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Mol	Chain	Res	Type
3	AD	126	GLU
3	AD	127	SER
3	AD	141	LYS
3	AD	157	ARG
4	AH	286	GLU
4	AH	288	VAL
4	AH	297	VAL
4	AH	307	LEU
4	AH	317	ASN
4	AH	318	LEU
4	AH	328	SER
4	AH	333	ASP
4	AH	343	SER
4	AH	349	SER
5	AK	43	CYS
5	AK	46	ASP
5	AK	66	LYS
5	AK	78	ILE
5	AK	83	LEU
5	AK	86	ASP
5	AK	91	LEU
5	AK	95	SER
5	AK	111	LYS
5	AK	115	THR
5	AK	116	VAL
5	AK	119	TYR
5	AK	120	SER
5	AK	125	SER
5	AK	153	ILE
5	AK	156	THR
5	AK	161	SER
5	AK	183	THR
3	Ad	38	THR
3	Ad	55	MET
3	Ad	63	THR
3	Ad	67	LYS
3	Ad	75	ASN
3	Ad	77	TYR
3	Ad	78	ASN
3	Ad	85	VAL
3	Ad	93	GLU
3	Ad	95	THR

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Mol	Chain	Res	Type
3	Ad	111	LYS
3	Ad	117	VAL
3	Ad	127	SER
3	Ad	130	GLU
2	BC	79	ILE
2	BC	126	ARG
2	BC	128	SER
2	BC	143	THR
2	BC	148	ARG
2	BC	174	GLU
2	BC	177	CYS
2	BC	180	THR
2	BC	189	ASP
2	BC	221	VAL
2	BC	228	HIS
2	BC	229	THR
2	BC	246	VAL
2	BC	256	ASN
2	BC	258	ASN
2	BC	259	SER
3	BD	52	MET
3	BD	58	VAL
3	BD	61	VAL
3	BD	63	THR
3	BD	85	VAL
3	BD	87	TRP
3	BD	88	SER
3	BD	93	GLU
3	BD	108	VAL
3	BD	111	LYS
3	BD	112	SER
3	BD	115	VAL
3	BD	117	VAL
3	BD	127	SER
3	BD	133	ARG
3	BD	144	SER
3	BD	151	SER
4	BH	276	SER
4	BH	288	VAL
4	BH	298	VAL
4	BH	307	LEU
4	BH	318	LEU

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Mol	Chain	Res	Type
4	BH	319	THR
4	BH	328	SER
4	BH	340	MET
4	BH	343	SER
4	BH	347	LEU
4	BH	349	SER
5	BK	43	CYS
5	BK	46	ASP
5	BK	66	LYS
5	BK	70	VAL
5	BK	76	ILE
5	BK	78	ILE
5	BK	86	ASP
5	BK	88	SER
5	BK	95	SER
5	BK	115	THR
5	BK	117	THR
5	BK	119	TYR
5	BK	120	SER
5	BK	125	SER
5	BK	134	LEU
5	BK	156	THR
5	BK	157	GLN
5	BK	168	TYR
5	BK	179	ARG
5	BK	183	THR
3	Bd	51	SER
3	Bd	61	VAL
3	Bd	62	ILE
3	Bd	63	THR
3	Bd	68	ASP
3	Bd	77	TYR
3	Bd	78	ASN
3	Bd	84	SER
3	Bd	85	VAL
3	Bd	115	VAL
3	Bd	117	VAL
3	Bd	127	SER
3	Bd	151	SER
2	CC	72	LEU
2	CC	91	ASP
2	CC	104	ASN

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Mol	Chain	Res	Type
2	CC	126	ARG
2	CC	173	LYS
2	CC	177	CYS
2	CC	180	THR
2	CC	189	ASP
2	CC	190	GLN
2	CC	221	VAL
2	CC	228	HIS
2	CC	229	THR
2	CC	234	THR
2	CC	239	GLU
2	CC	246	VAL
3	CD	31	ASN
3	CD	51	SER
3	CD	52	MET
3	CD	54	GLU
3	CD	59	GLU
3	CD	61	VAL
3	CD	70	THR
3	CD	84	SER
3	CD	85	VAL
3	CD	88	SER
3	CD	95	THR
3	CD	100	LYS
3	CD	108	VAL
3	CD	111	LYS
3	CD	117	VAL
3	CD	120	SER
3	CD	122	SER
3	CD	123	THR
3	CD	127	SER
3	CD	141	LYS
3	CD	147	VAL
3	CD	153	VAL
3	CD	157	ARG
4	CH	288	VAL
4	CH	307	LEU
4	CH	316	THR
4	CH	319	THR
4	CH	322	SER
4	CH	328	SER
4	CH	342	LYS

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Mol	Chain	Res	Type
4	CH	349	SER
5	CK	43	CYS
5	CK	46	ASP
5	CK	76	ILE
5	CK	81	SER
5	CK	86	ASP
5	CK	115	THR
5	CK	116	VAL
5	CK	117	THR
5	CK	119	TYR
5	CK	120	SER
5	CK	125	SER
5	CK	128	ARG
5	CK	134	LEU
5	CK	156	THR
5	CK	161	SER
5	CK	166	THR
5	CK	168	TYR
5	CK	173	ASP
5	CK	175	SER
5	CK	179	ARG
5	CK	183	THR
3	Cd	38	THR
3	Cd	43	GLU
3	Cd	61	VAL
3	Cd	63	THR
3	Cd	71	LEU
3	Cd	78	ASN
3	Cd	85	VAL
3	Cd	111	LYS
3	Cd	138	GLN
3	Cd	141	LYS
2	DC	62	THR
2	DC	72	LEU
2	DC	91	ASP
2	DC	98	SER
2	DC	104	ASN
2	DC	119	LEU
2	DC	126	ARG
2	DC	127	ILE
2	DC	128	SER
2	DC	140	PHE

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Mol	Chain	Res	Type
2	DC	143	THR
2	DC	157	LYS
2	DC	173	LYS
2	DC	177	CYS
2	DC	190	GLN
2	DC	231	LEU
2	DC	234	THR
2	DC	246	VAL
2	DC	256	ASN
2	DC	258	ASN
3	DD	31	ASN
3	DD	54	GLU
3	DD	63	THR
3	DD	70	THR
3	DD	85	VAL
3	DD	95	THR
3	DD	98	ILE
3	DD	108	VAL
3	DD	111	LYS
3	DD	120	SER
3	DD	122	SER
3	DD	133	ARG
3	DD	142	LYS
3	DD	144	SER
3	DD	151	SER
3	DD	157	ARG
4	DH	288	VAL
4	DH	297	VAL
4	DH	307	LEU
4	DH	314	VAL
4	DH	317	ASN
4	DH	318	LEU
4	DH	335	THR
4	DH	343	SER
4	DH	348	VAL
4	DH	349	SER
5	DK	43	CYS
5	DK	46	ASP
5	DK	69	SER
5	DK	81	SER
5	DK	88	SER
5	DK	92	ASN

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Mol	Chain	Res	Type
5	DK	111	LYS
5	DK	115	THR
5	DK	119	TYR
5	DK	120	SER
5	DK	125	SER
5	DK	151	SER
5	DK	156	THR
5	DK	161	SER
5	DK	166	THR
5	DK	183	THR
3	Dd	38	THR
3	Dd	53	LEU
3	Dd	54	GLU
3	Dd	61	VAL
3	Dd	62	ILE
3	Dd	63	THR
3	Dd	68	ASP
3	Dd	75	ASN
3	Dd	78	ASN
3	Dd	93	GLU
3	Dd	111	LYS
3	Dd	117	VAL
3	Dd	118	LEU
3	Dd	144	SER
3	Dd	151	SER
2	EC	61	GLU
2	EC	72	LEU
2	EC	81	GLU
2	EC	97	ASN
2	EC	102	GLU
2	EC	105	ILE
2	EC	126	ARG
2	EC	139	HIS
2	EC	173	LYS
2	EC	177	CYS
2	EC	189	ASP
2	EC	199	ILE
2	EC	228	HIS
2	EC	229	THR
2	EC	238	SER
2	EC	244	ASP
2	EC	246	VAL

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Mol	Chain	Res	Type
3	ED	39	ILE
3	ED	58	VAL
3	ED	61	VAL
3	ED	63	THR
3	ED	87	TRP
3	ED	88	SER
3	ED	94	LEU
3	ED	95	THR
3	ED	98	ILE
3	ED	108	VAL
3	ED	111	LYS
3	ED	120	SER
3	ED	122	SER
3	ED	123	THR
3	ED	124	LYS
3	ED	126	GLU
3	ED	127	SER
3	ED	151	SER
4	EH	297	VAL
4	EH	304	ARG
4	EH	307	LEU
4	EH	314	VAL
4	EH	316	THR
4	EH	318	LEU
4	EH	343	SER
4	EH	348	VAL
4	EH	349	SER
4	EH	357	LEU
5	EK	43	CYS
5	EK	46	ASP
5	EK	86	ASP
5	EK	111	LYS
5	EK	115	THR
5	EK	119	TYR
5	EK	120	SER
5	EK	125	SER
5	EK	152	ARG
5	EK	156	THR
5	EK	161	SER
5	EK	165	ILE
5	EK	166	THR
5	EK	168	TYR

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Mol	Chain	Res	Type
5	EK	175	SER
5	EK	180	VAL
5	EK	183	THR
3	Ed	38	THR
3	Ed	62	ILE
3	Ed	72	THR
3	Ed	75	ASN
3	Ed	77	TYR
3	Ed	86	ASP
3	Ed	111	LYS
3	Ed	115	VAL
3	Ed	138	GLN
3	Ed	141	LYS
3	Ed	153	VAL
2	FC	72	LEU
2	FC	81	GLU
2	FC	119	LEU
2	FC	126	ARG
2	FC	134	VAL
2	FC	143	THR
2	FC	157	LYS
2	FC	173	LYS
2	FC	180	THR
2	FC	190	GLN
2	FC	228	HIS
2	FC	233	VAL
2	FC	246	VAL
2	FC	258	ASN
3	FD	31	ASN
3	FD	52	MET
3	FD	54	GLU
3	FD	63	THR
3	FD	69	ASN
3	FD	70	THR
3	FD	84	SER
3	FD	95	THR
3	FD	98	ILE
3	FD	100	LYS
3	FD	108	VAL
3	FD	111	LYS
3	FD	122	SER
3	FD	123	THR

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Mol	Chain	Res	Type
3	FD	127	SER
3	FD	142	LYS
3	FD	144	SER
3	FD	154	VAL
4	FH	282	LEU
4	FH	288	VAL
4	FH	312	MET
4	FH	316	THR
4	FH	317	ASN
4	FH	349	SER
5	FK	43	CYS
5	FK	46	ASP
5	FK	49	CYS
5	FK	60	LEU
5	FK	70	VAL
5	FK	75	LEU
5	FK	76	ILE
5	FK	77	SER
5	FK	81	SER
5	FK	86	ASP
5	FK	92	ASN
5	FK	95	SER
5	FK	111	LYS
5	FK	119	TYR
5	FK	120	SER
5	FK	125	SER
5	FK	137	SER
5	FK	156	THR
5	FK	161	SER
5	FK	173	ASP
5	FK	179	ARG
5	FK	181	GLU
5	FK	183	THR
3	Fd	38	THR
3	Fd	48	VAL
3	Fd	54	GLU
3	Fd	63	THR
3	Fd	67	LYS
3	Fd	71	LEU
3	Fd	72	THR
3	Fd	77	TYR
3	Fd	80	GLN

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Mol	Chain	Res	Type
3	Fd	111	LYS
3	Fd	115	VAL
3	Fd	117	VAL
3	Fd	127	SER
2	GC	97	ASN
2	GC	109	VAL
2	GC	134	VAL
2	GC	136	LYS
2	GC	173	LYS
2	GC	178	ILE
2	GC	180	THR
2	GC	189	ASP
2	GC	190	GLN
2	GC	213	ARG
2	GC	221	VAL
2	GC	228	HIS
2	GC	233	VAL
2	GC	234	THR
2	GC	246	VAL
2	GC	256	ASN
3	GD	31	ASN
3	GD	52	MET
3	GD	53	LEU
3	GD	61	VAL
3	GD	63	THR
3	GD	70	THR
3	GD	97	ARG
3	GD	108	VAL
3	GD	111	LYS
3	GD	117	VAL
3	GD	120	SER
3	GD	123	THR
3	GD	127	SER
3	GD	142	LYS
3	GD	157	ARG
4	GH	276	SER
4	GH	288	VAL
4	GH	304	ARG
4	GH	307	LEU
4	GH	328	SER
4	GH	342	LYS
4	GH	343	SER

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Mol	Chain	Res	Type
4	GH	345	VAL
4	GH	349	SER
5	GK	43	CYS
5	GK	46	ASP
5	GK	75	LEU
5	GK	76	ILE
5	GK	92	ASN
5	GK	111	LYS
5	GK	117	THR
5	GK	119	TYR
5	GK	120	SER
5	GK	125	SER
5	GK	137	SER
5	GK	141	SER
5	GK	152	ARG
5	GK	156	THR
5	GK	166	THR
5	GK	168	TYR
5	GK	173	ASP
5	GK	175	SER
5	GK	183	THR
3	Gd	36	ASP
3	Gd	61	VAL
3	Gd	62	ILE
3	Gd	68	ASP
3	Gd	71	LEU
3	Gd	75	ASN
3	Gd	77	TYR
3	Gd	78	ASN
3	Gd	82	ARG
3	Gd	85	VAL
3	Gd	93	GLU
3	Gd	108	VAL
3	Gd	111	LYS
3	Gd	117	VAL
3	Gd	122	SER
3	Gd	127	SER
3	Gd	141	LYS
3	Gd	156	LEU
2	HC	81	GLU
2	HC	99	LEU
2	HC	116	THR

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Mol	Chain	Res	Type
2	HC	126	ARG
2	HC	173	LYS
2	HC	177	CYS
2	HC	180	THR
2	HC	228	HIS
2	HC	229	THR
2	HC	233	VAL
2	HC	234	THR
2	HC	246	VAL
2	HC	266	VAL
3	HD	31	ASN
3	HD	47	SER
3	HD	58	VAL
3	HD	61	VAL
3	HD	63	THR
3	HD	70	THR
3	HD	84	SER
3	HD	85	VAL
3	HD	100	LYS
3	HD	108	VAL
3	HD	111	LYS
3	HD	115	VAL
3	HD	117	VAL
3	HD	119	ILE
3	HD	123	THR
3	HD	124	LYS
3	HD	126	GLU
3	HD	127	SER
3	HD	141	LYS
3	HD	146	HIS
3	HD	151	SER
4	HH	280	LEU
4	HH	288	VAL
4	HH	297	VAL
4	HH	317	ASN
4	HH	343	SER
4	HH	349	SER
5	HK	43	CYS
5	HK	46	ASP
5	HK	60	LEU
5	HK	67	VAL
5	HK	70	VAL

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Mol	Chain	Res	Type
5	HK	81	SER
5	HK	92	ASN
5	HK	95	SER
5	HK	101	GLU
5	HK	116	VAL
5	HK	119	TYR
5	HK	120	SER
5	HK	125	SER
5	HK	150	ASP
5	HK	153	ILE
5	HK	156	THR
5	HK	159	LEU
5	HK	161	SER
5	HK	168	TYR
5	HK	173	ASP
5	HK	175	SER
5	HK	183	THR
3	Hd	29	PRO
3	Hd	35	ASP
3	Hd	38	THR
3	Hd	55	MET
3	Hd	57	LYS
3	Hd	60	LYS
3	Hd	77	TYR
3	Hd	85	VAL
3	Hd	93	GLU
3	Hd	111	LYS
3	Hd	122	SER
3	Hd	123	THR
3	Hd	126	GLU
3	Hd	138	GLN
3	Hd	152	GLN
3	Hd	153	VAL
3	Hd	161	ILE
2	IC	61	GLU
2	IC	72	LEU
2	IC	91	ASP
2	IC	99	LEU
2	IC	100	VAL
2	IC	119	LEU
2	IC	126	ARG
2	IC	140	PHE

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Mol	Chain	Res	Type
2	IC	173	LYS
2	IC	177	CYS
2	IC	189	ASP
2	IC	226	VAL
2	IC	229	THR
2	IC	246	VAL
2	IC	256	ASN
2	IC	258	ASN
2	IC	266	VAL
3	ID	39	ILE
3	ID	61	VAL
3	ID	63	THR
3	ID	70	THR
3	ID	87	TRP
3	ID	108	VAL
3	ID	111	LYS
3	ID	115	VAL
3	ID	123	THR
3	ID	126	GLU
3	ID	133	ARG
3	ID	141	LYS
3	ID	144	SER
3	ID	151	SER
4	IH	288	VAL
4	IH	297	VAL
4	IH	299	SER
4	IH	307	LEU
4	IH	318	LEU
4	IH	319	THR
4	IH	343	SER
4	IH	348	VAL
4	IH	349	SER
4	IH	353	LYS
5	IK	43	CYS
5	IK	46	ASP
5	IK	70	VAL
5	IK	76	ILE
5	IK	101	GLU
5	IK	119	TYR
5	IK	146	SER
5	IK	152	ARG
5	IK	156	THR

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Mol	Chain	Res	Type
5	IK	168	TYR
5	IK	175	SER
5	IK	183	THR
3	Id	38	THR
3	Id	43	GLU
3	Id	63	THR
3	Id	75	ASN
3	Id	78	ASN
3	Id	82	ARG
3	Id	108	VAL
3	Id	111	LYS
3	Id	127	SER
2	JC	61	GLU
2	JC	143	THR
2	JC	149	GLN
2	JC	173	LYS
2	JC	177	CYS
2	JC	180	THR
2	JC	181	GLU
2	JC	189	ASP
2	JC	211	LEU
2	JC	228	HIS
2	JC	229	THR
2	JC	246	VAL
2	JC	258	ASN
3	JD	54	GLU
3	JD	63	THR
3	JD	70	THR
3	JD	85	VAL
3	JD	87	TRP
3	JD	108	VAL
3	JD	111	LYS
3	JD	117	VAL
3	JD	123	THR
3	JD	126	GLU
3	JD	127	SER
3	JD	144	SER
3	JD	147	VAL
3	JD	150	ASN
3	JD	153	VAL
3	JD	157	ARG
4	JH	288	VAL

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Mol	Chain	Res	Type
4	JH	299	SER
4	JH	307	LEU
4	JH	314	VAL
4	JH	316	THR
4	JH	317	ASN
4	JH	323	PRO
4	JH	328	SER
4	JH	343	SER
4	JH	345	VAL
4	JH	349	SER
5	JK	43	CYS
5	JK	46	ASP
5	JK	70	VAL
5	JK	83	LEU
5	JK	86	ASP
5	JK	92	ASN
5	JK	111	LYS
5	JK	115	THR
5	JK	119	TYR
5	JK	120	SER
5	JK	122	LYS
5	JK	156	THR
5	JK	168	TYR
5	JK	179	ARG
5	JK	181	GLU
5	JK	183	THR
3	Jd	38	THR
3	Jd	62	ILE
3	Jd	63	THR
3	Jd	68	ASP
3	Jd	71	LEU
3	Jd	77	TYR
3	Jd	78	ASN
3	Jd	111	LYS
3	Jd	117	VAL
3	Jd	118	LEU
3	Jd	135	ILE
3	Jd	138	GLN
3	Jd	154	VAL
3	Jd	160	LYS
2	KC	61	GLU
2	KC	85	LYS

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Mol	Chain	Res	Type
2	KC	130	ARG
2	KC	139	HIS
2	KC	157	LYS
2	KC	177	CYS
2	KC	180	THR
2	KC	190	GLN
2	KC	228	HIS
2	KC	239	GLU
2	KC	243	ASP
2	KC	246	VAL
2	KC	256	ASN
2	KC	258	ASN
2	KC	266	VAL
3	KD	39	ILE
3	KD	55	MET
3	KD	58	VAL
3	KD	63	THR
3	KD	94	LEU
3	KD	108	VAL
3	KD	111	LYS
3	KD	115	VAL
3	KD	117	VAL
3	KD	127	SER
3	KD	141	LYS
4	KH	288	VAL
4	KH	309	ASN
4	KH	314	VAL
4	KH	316	THR
4	KH	343	SER
4	KH	345	VAL
4	KH	349	SER
4	KH	359	VAL
5	KK	43	CYS
5	KK	46	ASP
5	KK	66	LYS
5	KK	86	ASP
5	KK	101	GLU
5	KK	119	TYR
5	KK	120	SER
5	KK	122	LYS
5	KK	125	SER
5	KK	132	LEU

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Mol	Chain	Res	Type
5	KK	167	SER
5	KK	173	ASP
5	KK	175	SER
5	KK	183	THR
3	Kd	35	ASP
3	Kd	38	THR
3	Kd	43	GLU
3	Kd	62	ILE
3	Kd	63	THR
3	Kd	68	ASP
3	Kd	72	THR
3	Kd	75	ASN
3	Kd	78	ASN
3	Kd	84	SER
3	Kd	85	VAL
3	Kd	86	ASP
3	Kd	111	LYS
3	Kd	115	VAL
3	Kd	120	SER
3	Kd	126	GLU
3	Kd	127	SER
3	Kd	138	GLN
3	Kd	144	SER
2	LC	81	GLU
2	LC	104	ASN
2	LC	116	THR
2	LC	134	VAL
2	LC	153	MET
2	LC	173	LYS
2	LC	177	CYS
2	LC	180	THR
2	LC	189	ASP
2	LC	221	VAL
2	LC	228	HIS
2	LC	229	THR
2	LC	244	ASP
2	LC	246	VAL
2	LC	256	ASN
3	LD	54	GLU
3	LD	58	VAL
3	LD	61	VAL
3	LD	63	THR

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Mol	Chain	Res	Type
3	LD	70	THR
3	LD	84	SER
3	LD	85	VAL
3	LD	87	TRP
3	LD	98	ILE
3	LD	108	VAL
3	LD	111	LYS
3	LD	115	VAL
3	LD	120	SER
3	LD	123	THR
3	LD	127	SER
3	LD	133	ARG
3	LD	157	ARG
4	LH	286	GLU
4	LH	288	VAL
4	LH	293	SER
4	LH	297	VAL
4	LH	299	SER
4	LH	317	ASN
4	LH	318	LEU
4	LH	322	SER
4	LH	328	SER
4	LH	343	SER
4	LH	349	SER
5	LK	43	CYS
5	LK	46	ASP
5	LK	67	VAL
5	LK	70	VAL
5	LK	86	ASP
5	LK	95	SER
5	LK	107	LYS
5	LK	111	LYS
5	LK	115	THR
5	LK	119	TYR
5	LK	120	SER
5	LK	166	THR
5	LK	168	TYR
5	LK	170	LEU
5	LK	183	THR
3	Ld	35	ASP
3	Ld	36	ASP
3	Ld	48	VAL

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Mol	Chain	Res	Type
3	Ld	61	VAL
3	Ld	62	ILE
3	Ld	63	THR
3	Ld	72	THR
3	Ld	77	TYR
3	Ld	78	ASN
3	Ld	111	LYS
3	Ld	115	VAL
3	Ld	117	VAL
3	Ld	122	SER
3	Ld	127	SER
3	Ld	138	GLN
3	Ld	154	VAL
2	MC	91	ASP
2	MC	126	ARG
2	MC	134	VAL
2	MC	143	THR
2	MC	177	CYS
2	MC	211	LEU
2	MC	228	HIS
2	MC	229	THR
2	MC	246	VAL
2	MC	255	LEU
2	MC	258	ASN
2	MC	268	LYS
3	MD	58	VAL
3	MD	63	THR
3	MD	70	THR
3	MD	84	SER
3	MD	85	VAL
3	MD	108	VAL
3	MD	111	LYS
3	MD	117	VAL
3	MD	120	SER
3	MD	123	THR
3	MD	126	GLU
3	MD	146	HIS
3	MD	147	VAL
3	MD	150	ASN
4	MH	288	VAL
4	MH	297	VAL
4	MH	304	ARG

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Mol	Chain	Res	Type
4	MH	307	LEU
4	MH	317	ASN
4	MH	318	LEU
4	MH	322	SER
4	MH	328	SER
4	MH	340	MET
4	MH	343	SER
4	MH	349	SER
5	MK	46	ASP
5	MK	50	ASP
5	MK	81	SER
5	MK	92	ASN
5	MK	115	THR
5	MK	116	VAL
5	MK	119	TYR
5	MK	120	SER
5	MK	125	SER
5	MK	141	SER
5	MK	156	THR
5	MK	161	SER
5	MK	173	ASP
5	MK	183	THR
3	Md	35	ASP
3	Md	38	THR
3	Md	48	VAL
3	Md	61	VAL
3	Md	67	LYS
3	Md	68	ASP
3	Md	71	LEU
3	Md	75	ASN
3	Md	77	TYR
3	Md	78	ASN
3	Md	82	ARG
3	Md	84	SER
3	Md	85	VAL
3	Md	88	SER
3	Md	92	GLU
3	Md	111	LYS
3	Md	117	VAL
3	Md	120	SER
3	Md	127	SER
3	Md	144	SER

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Mol	Chain	Res	Type
3	Md	151	SER
3	Md	157	ARG
6	N	99	ARG
6	N	101	SER
6	N	108	ASP
6	N	118	GLU
6	N	119	TYR
6	N	130	ASP
6	N	134	MET
6	N	155	LEU
6	N	162	THR
6	N	210	ASP
6	O	99	ARG
6	O	101	SER
6	O	108	ASP
6	O	110	GLN
6	O	117	VAL
6	O	130	ASP
6	O	143	ILE
6	O	162	THR
6	O	174	SER
6	O	181	LEU
6	O	189	MET
6	O	202	ARG
6	O	219	ILE
6	O	226	ASN
6	P	99	ARG
6	P	101	SER
6	P	110	GLN
6	P	115	GLN
6	P	121	ASP
6	P	124	THR
6	P	155	LEU
6	P	174	SER
6	P	196	ASN
6	P	210	ASP
6	Q	99	ARG
6	Q	108	ASP
6	Q	110	GLN
6	Q	130	ASP
6	Q	143	ILE
6	Q	162	THR

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Mol	Chain	Res	Type
6	Q	174	SER
6	Q	181	LEU
6	Q	189	MET
6	Q	196	ASN
6	Q	210	ASP
6	R	99	ARG
6	R	118	GLU
6	R	130	ASP
6	R	143	ILE
6	R	154	LEU
6	R	155	LEU
6	R	169	THR
6	R	174	SER
6	R	210	ASP
6	R	226	ASN
6	S	99	ARG
6	S	101	SER
6	S	108	ASP
6	S	110	GLN
6	S	130	ASP
6	S	165	VAL
6	S	174	SER
6	S	182	SER
6	S	189	MET
6	S	196	ASN
6	S	210	ASP
6	S	212	ASN
6	S	223	SER
6	T	99	ARG
6	T	101	SER
6	T	108	ASP
6	T	110	GLN
6	T	118	GLU
6	T	119	TYR
6	T	121	ASP
6	T	130	ASP
6	T	134	MET
6	T	140	LEU
6	T	143	ILE
6	T	155	LEU
6	T	162	THR
6	T	196	ASN

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Mol	Chain	Res	Type
6	T	210	ASP
6	T	219	ILE
6	U	99	ARG
6	U	101	SER
6	U	117	VAL
6	U	119	TYR
6	U	130	ASP
6	U	139	ARG
6	U	140	LEU
6	U	143	ILE
6	U	144	CYS
6	U	155	LEU
6	U	169	THR
6	U	174	SER
6	U	196	ASN
6	U	210	ASP
6	V	99	ARG
6	V	110	GLN
6	V	130	ASP
6	V	134	MET
6	V	143	ILE
6	V	154	LEU
6	V	162	THR
6	V	174	SER
6	V	210	ASP
6	V	211	LYS
6	W	99	ARG
6	W	101	SER
6	W	110	GLN
6	W	121	ASP
6	W	143	ILE
6	W	154	LEU
6	W	162	THR
6	W	174	SER
6	W	210	ASP
6	W	212	ASN
6	X	99	ARG
6	X	108	ASP
6	X	110	GLN
6	X	119	TYR
6	X	130	ASP
6	X	143	ILE

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Mol	Chain	Res	Type
6	X	162	THR
6	X	174	SER
6	X	210	ASP
6	Y	99	ARG
6	Y	101	SER
6	Y	108	ASP
6	Y	124	THR
6	Y	129	THR
6	Y	130	ASP
6	Y	155	LEU
6	Y	169	THR
6	Y	174	SER
6	Y	210	ASP
6	Z	99	ARG
6	Z	101	SER
6	Z	108	ASP
6	Z	118	GLU
6	Z	130	ASP
6	Z	139	ARG
6	Z	140	LEU
6	Z	143	ILE
6	Z	162	THR
6	Z	165	VAL
6	Z	174	SER
6	Z	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
2	AC	103	HIS
3	AD	152	GLN
5	AK	147	GLN
3	Ad	152	GLN
2	BC	82	GLN
2	BC	103	HIS
3	BD	138	GLN
3	BD	152	GLN
3	Bd	78	ASN
3	Bd	152	GLN
2	CC	103	HIS
2	CC	228	HIS
3	CD	152	GLN

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Mol	Chain	Res	Type
5	CK	147	GLN
3	Cd	78	ASN
3	Cd	152	GLN
2	DC	103	HIS
3	DD	152	GLN
3	Dd	152	GLN
2	EC	103	HIS
3	ED	138	GLN
3	ED	152	GLN
4	EH	341	GLN
5	EK	100	ASN
5	EK	147	GLN
3	Ed	31	ASN
3	Ed	32	ASN
2	FC	256	ASN
2	FC	258	ASN
3	FD	32	ASN
3	FD	138	GLN
3	FD	152	GLN
3	Fd	32	ASN
2	GC	103	HIS
3	GD	138	GLN
3	GD	152	GLN
4	GH	351	HIS
3	Gd	78	ASN
3	HD	138	GLN
3	HD	152	GLN
5	HK	61	ASN
2	IC	103	HIS
3	ID	138	GLN
3	ID	152	GLN
3	Id	80	GLN
3	Id	103	HIS
3	Id	152	GLN
2	JC	103	HIS
2	JC	241	HIS
3	JD	138	GLN
3	JD	152	GLN
4	JH	351	HIS
5	JK	87	GLN
3	Jd	31	ASN
3	Jd	32	ASN

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Mol	Chain	Res	Type
3	Jd	78	ASN
2	KC	103	HIS
3	KD	152	GLN
3	Kd	32	ASN
3	Kd	152	GLN
2	LC	103	HIS
3	LD	138	GLN
3	LD	152	GLN
5	LK	87	GLN
3	Ld	32	ASN
3	Ld	152	GLN
2	MC	103	HIS
3	MD	138	GLN
3	Md	32	ASN
3	Md	78	ASN
6	N	112	GLN
6	N	150	ASN
6	N	156	ASN
6	N	177	HIS
6	N	212	ASN
6	N	232	GLN
6	O	141	ASN
6	O	212	ASN
6	O	232	GLN
6	P	112	GLN
6	P	141	ASN
6	P	149	ASN
6	P	212	ASN
6	P	232	GLN
6	Q	112	GLN
6	Q	150	ASN
6	Q	232	GLN
6	R	112	GLN
6	R	149	ASN
6	R	156	ASN
6	R	177	HIS
6	R	212	ASN
6	R	232	GLN
6	S	112	GLN
6	S	141	ASN
6	S	150	ASN
6	S	156	ASN

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Mol	Chain	Res	Type
6	S	185	GLN
6	S	212	ASN
6	S	232	GLN
6	T	112	GLN
6	T	141	ASN
6	T	149	ASN
6	T	150	ASN
6	T	212	ASN
6	T	232	GLN
6	U	112	GLN
6	U	141	ASN
6	U	150	ASN
6	U	185	GLN
6	U	212	ASN
6	U	232	GLN
6	V	112	GLN
6	V	141	ASN
6	V	150	ASN
6	V	212	ASN
6	V	232	GLN
6	W	112	GLN
6	W	141	ASN
6	W	177	HIS
6	W	232	GLN
6	X	112	GLN
6	X	150	ASN
6	X	212	ASN
6	X	232	GLN
6	Y	112	GLN
6	Y	141	ASN
6	Y	150	ASN
6	Y	212	ASN
6	Y	232	GLN
6	Z	112	GLN
6	Z	141	ASN
6	Z	149	ASN
6	Z	212	ASN
6	Z	232	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

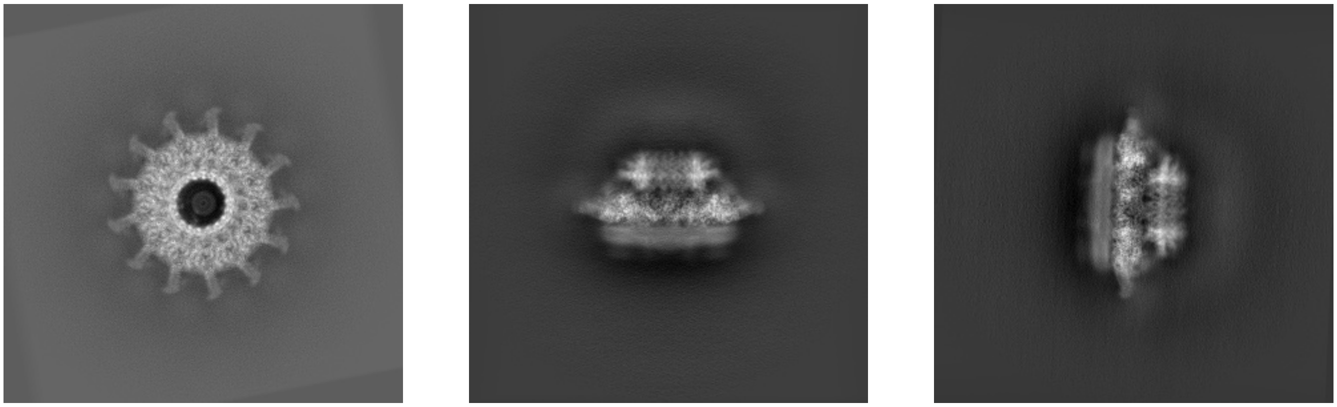
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-22070. 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

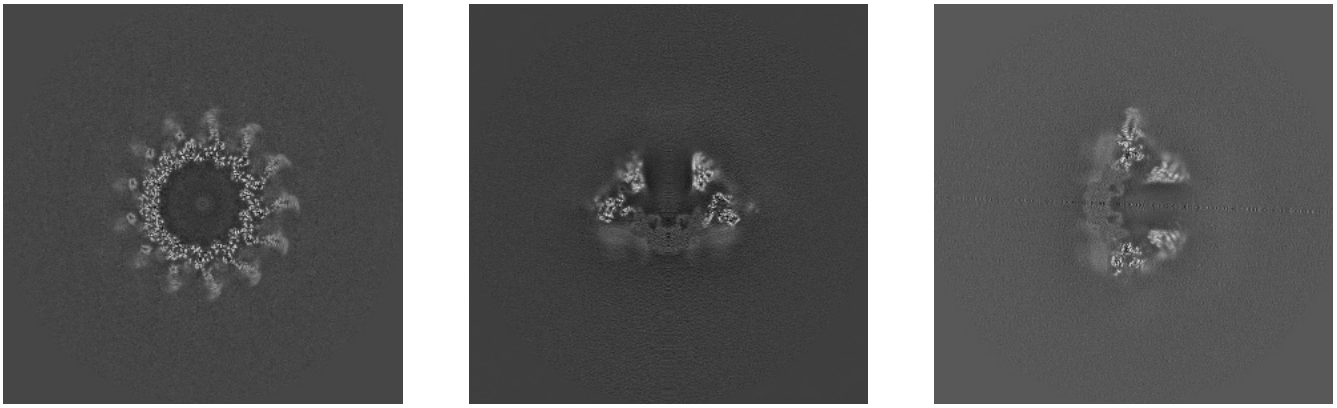


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

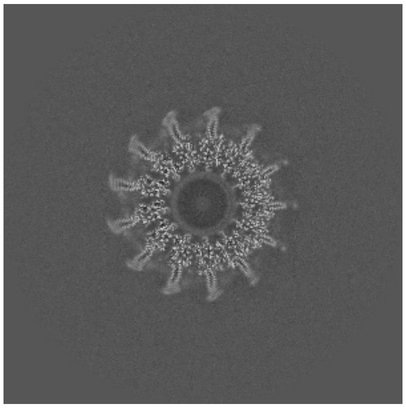


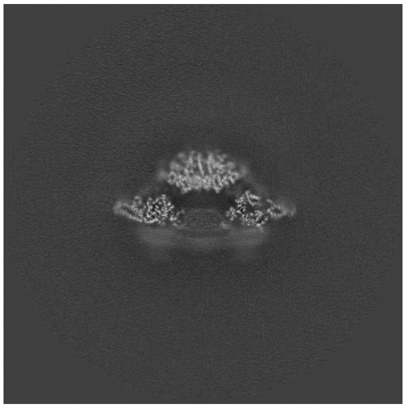
X Index: 255 Y Index: 255 Z Index: 255

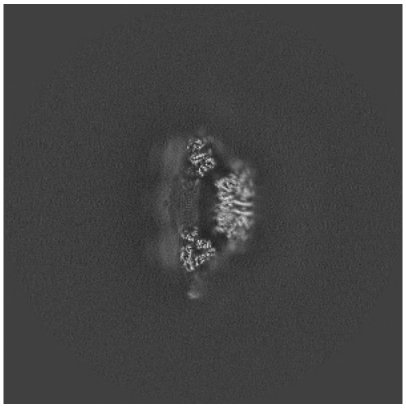
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map


X Index: 245

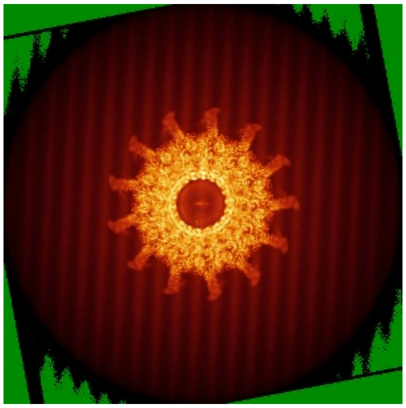

Y Index: 218

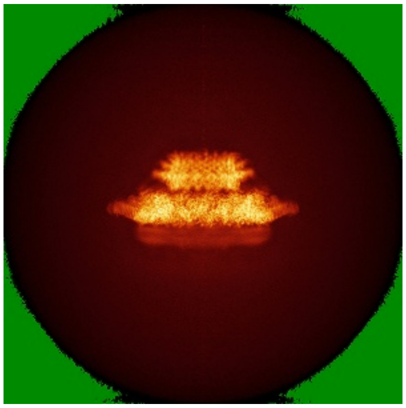

Z Index: 288

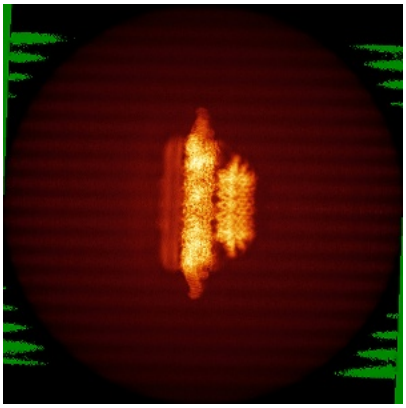
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map


X

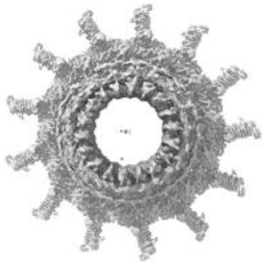

Y


Z

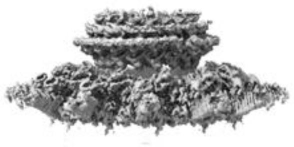
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

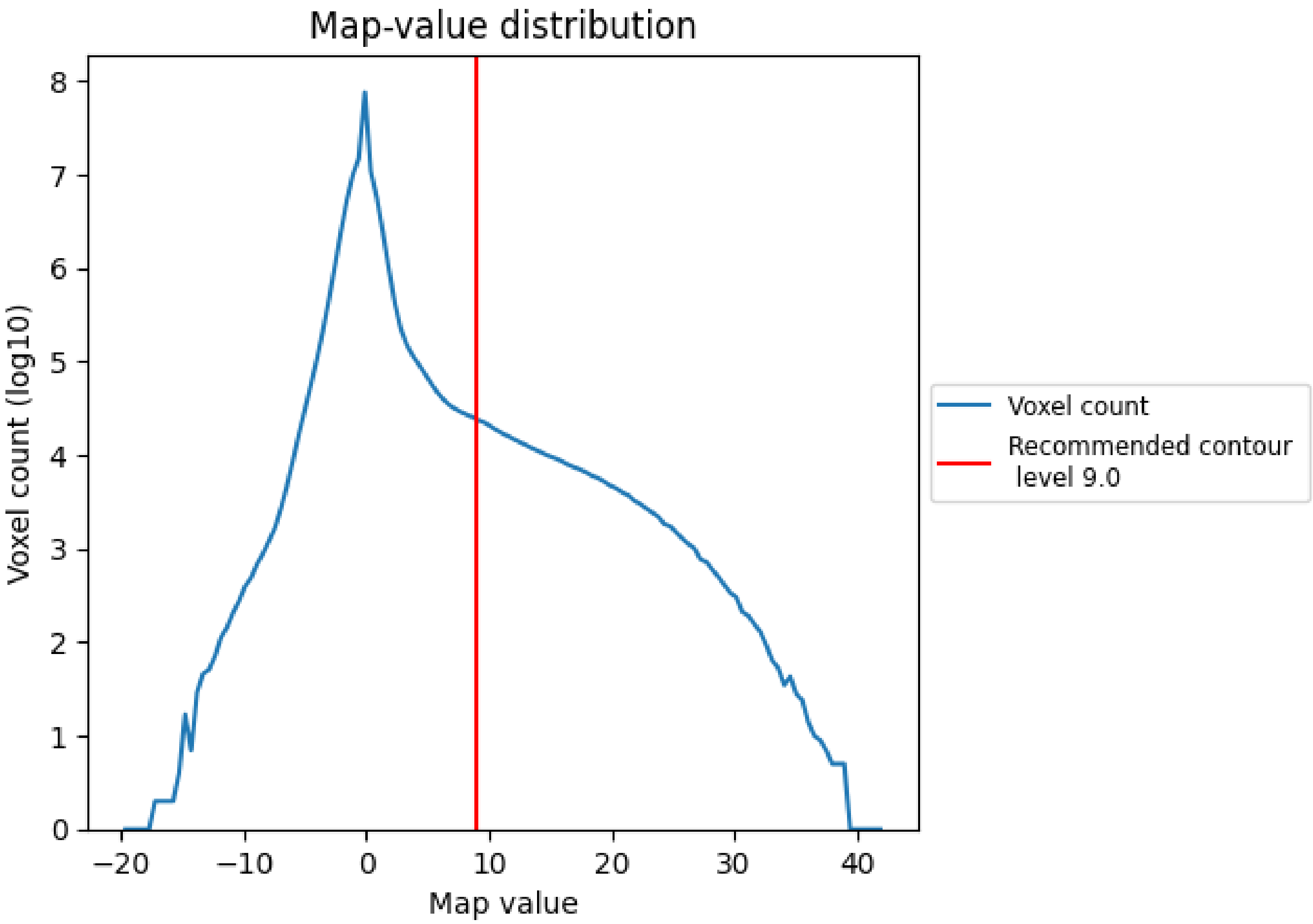
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

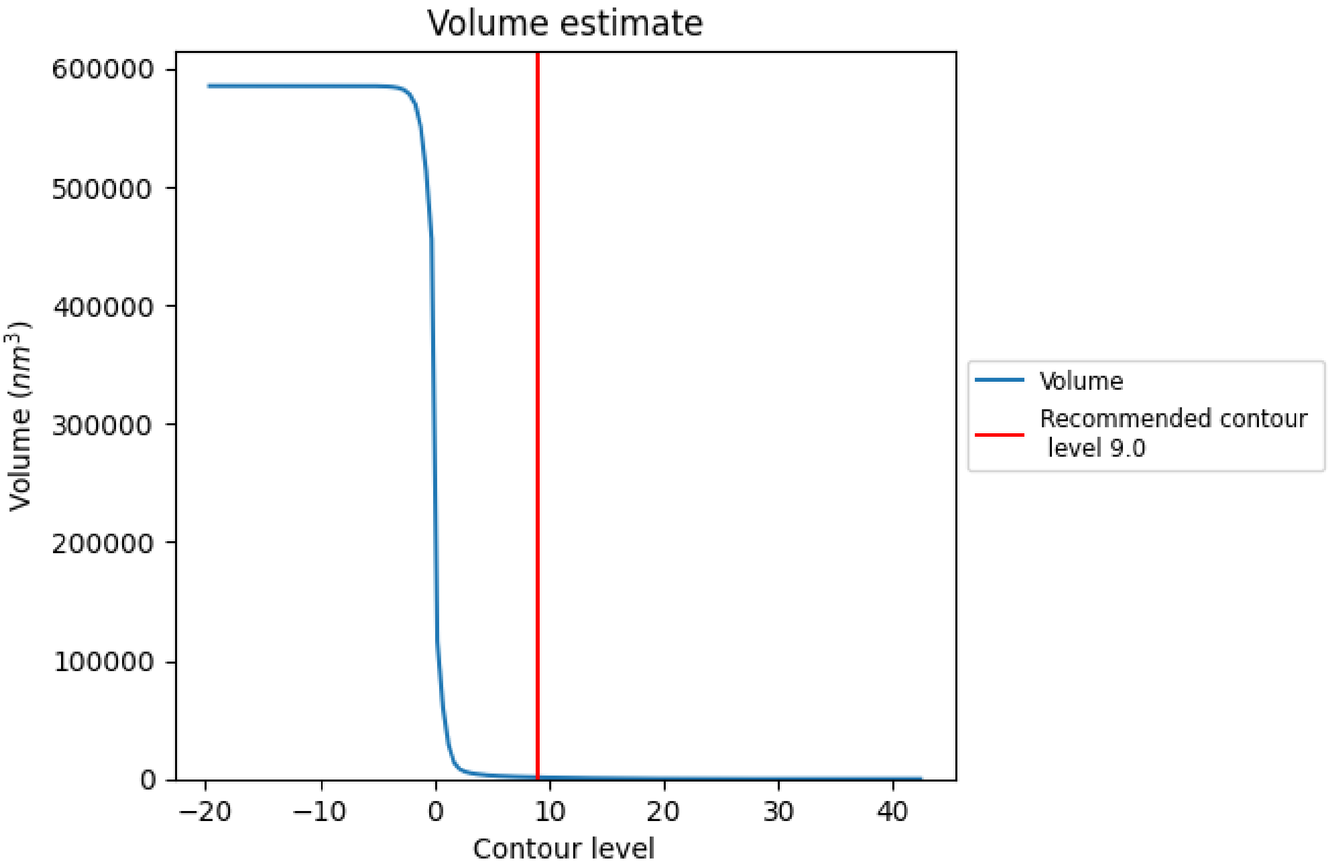
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

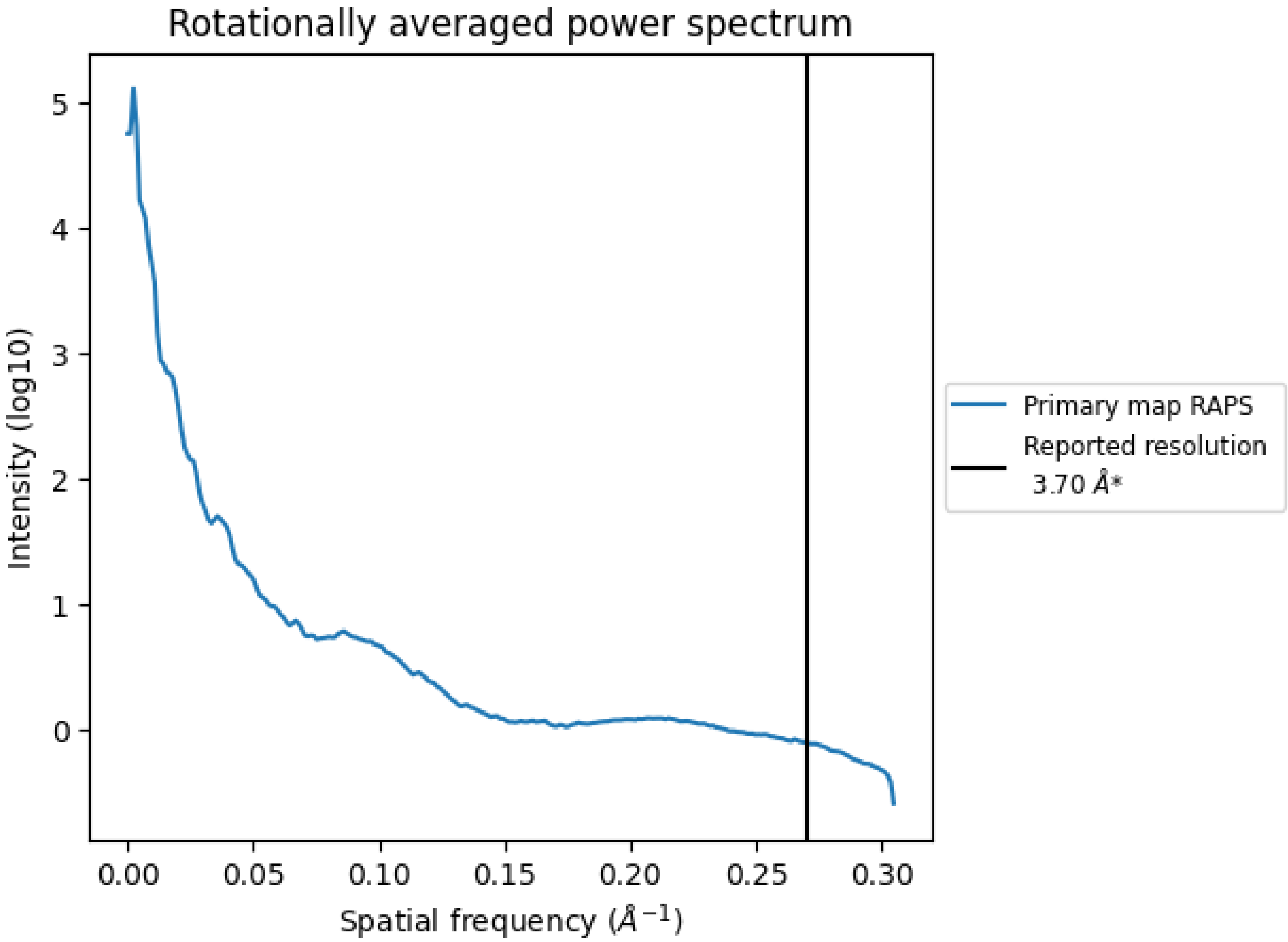
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1402 nm^3; this corresponds to an approximate mass of 1266 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

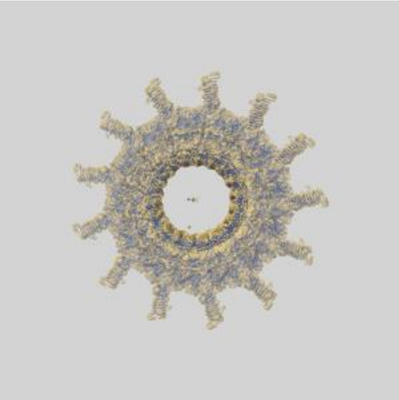
8 Fourier-Shell correlation ⓘ

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

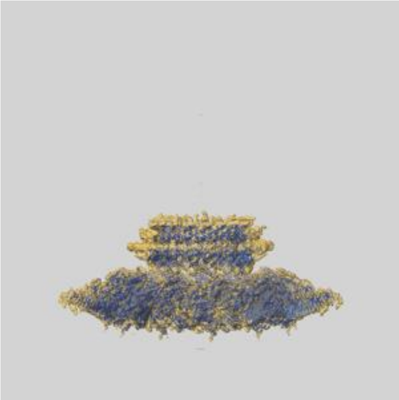
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-22070 and PDB model 6X65. Per-residue inclusion information can be found in section 3 on page 17.

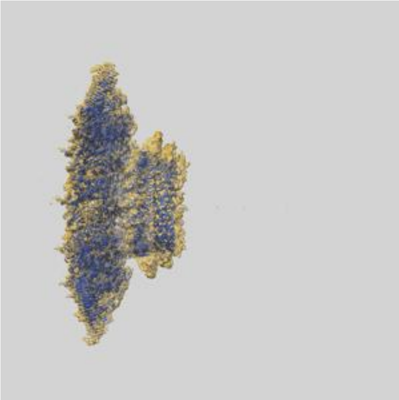
9.1 Map-model overlay ⓘ



X



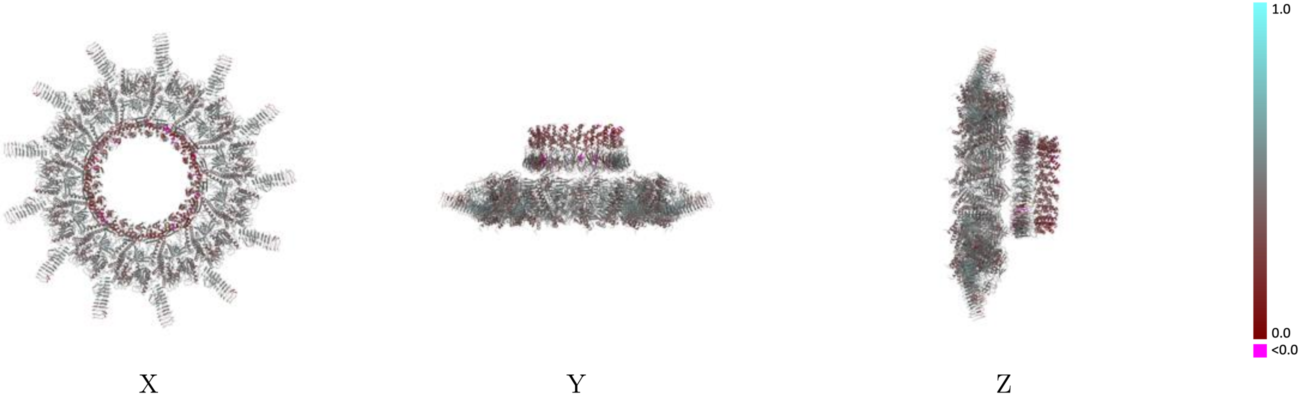
Y



Z

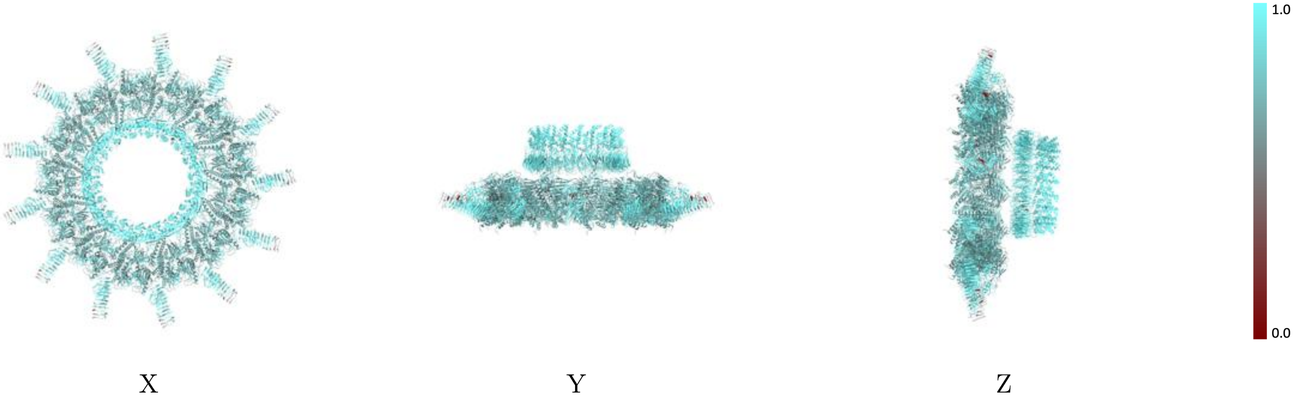
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



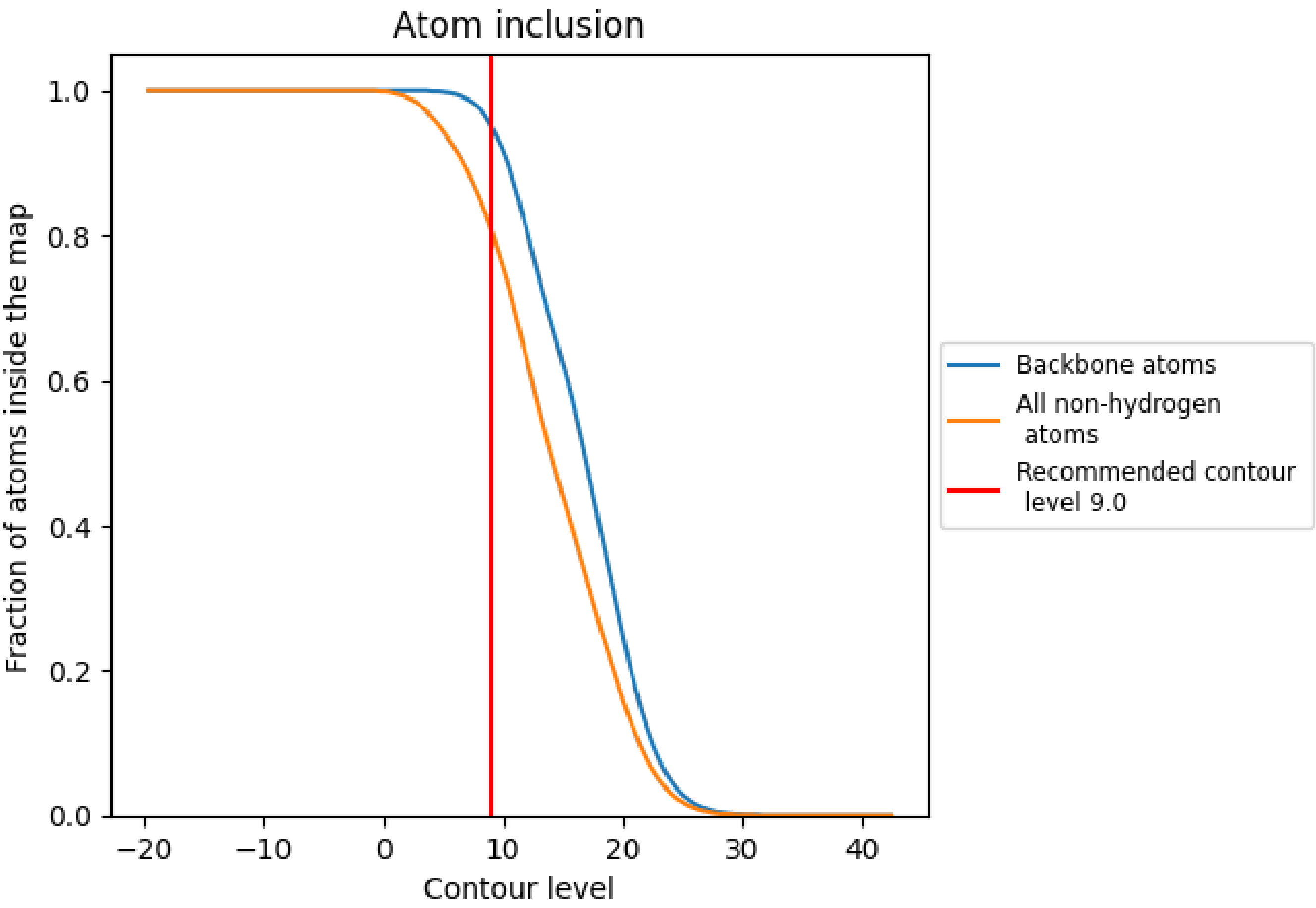
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (9.0).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 81% 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 (9.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4470
AC	0.7620	0.4530
AD	0.7180	0.4220
AH	0.8070	0.5070
AK	0.7700	0.4580
AV	0.9760	0.3580
AW	0.9810	0.3400
AX	0.8610	0.4630
AY	0.8460	0.4500
AZ	0.8860	0.5180
Ad	0.7510	0.4540
BC	0.7660	0.4570
BD	0.7250	0.4290
BH	0.8150	0.5090
BK	0.7620	0.4450
BV	0.9610	0.2800
BW	0.9630	0.3040
BX	0.8580	0.4760
BY	0.8420	0.4470
BZ	0.8970	0.5160
Bd	0.7500	0.4560
CC	0.7700	0.4530
CD	0.7230	0.4170
CH	0.7950	0.5060
CK	0.7660	0.4510
CV	0.9810	0.3860
CW	0.9750	0.3280
CX	0.8590	0.4620
CY	0.8580	0.4410
CZ	0.8910	0.5130
Cd	0.7430	0.4470
DC	0.7690	0.4560
DD	0.7290	0.4350
DH	0.8070	0.5020
DK	0.7620	0.4540

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Chain	Atom inclusion	Q-score
DV	0.9820	0.3910
DW	0.9380	0.3030
DX	0.8540	0.4700
DY	0.8500	0.4410
DZ	0.9030	0.5150
Dd	0.7640	0.4570
EC	0.7670	0.4590
ED	0.7260	0.4310
EH	0.7970	0.4990
EK	0.7700	0.4520
EV	0.9390	0.2740
EW	0.9690	0.3310
EX	0.8590	0.4730
EY	0.8500	0.4540
EZ	0.9090	0.5190
Ed	0.7430	0.4570
FC	0.7760	0.4610
FD	0.7150	0.4230
FH	0.7980	0.5080
FK	0.7700	0.4530
FV	0.9360	0.2930
FW	0.8750	0.2360
FX	0.8500	0.4730
FY	0.8350	0.4580
FZ	0.9060	0.5080
Fd	0.7460	0.4580
GC	0.7720	0.4620
GD	0.7200	0.4230
GH	0.7980	0.5090
GK	0.7740	0.4550
GV	0.9960	0.4300
GW	0.9560	0.2900
GX	0.8500	0.4690
GY	0.8460	0.4480
GZ	0.8860	0.5140
Gd	0.7550	0.4670
HC	0.7700	0.4600
HD	0.7350	0.4330
HH	0.8040	0.5030
HK	0.7660	0.4490
HV	0.9960	0.4550
HW	0.9440	0.3390

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Chain	Atom inclusion	Q-score
HX	0.8570	0.4730
HY	0.8540	0.4360
HZ	0.8890	0.5010
Hd	0.7470	0.4510
IC	0.7680	0.4600
ID	0.7170	0.4300
IH	0.7950	0.4980
IK	0.7720	0.4530
IV	0.9860	0.4410
IW	0.9940	0.3720
IX	0.8580	0.4700
IY	0.8540	0.4480
IZ	0.8860	0.5150
Id	0.7450	0.4550
JC	0.7660	0.4510
JD	0.7270	0.4290
JH	0.8010	0.5050
JK	0.7570	0.4510
JV	0.9460	0.2930
JW	0.9750	0.3670
JX	0.8490	0.4680
JY	0.8390	0.4440
JZ	0.8910	0.5080
Jd	0.7560	0.4580
KC	0.7680	0.4570
KD	0.7250	0.4320
KH	0.7980	0.5070
KK	0.7640	0.4470
KV	0.9690	0.3160
KW	0.9500	0.3300
KX	0.8580	0.4710
KY	0.8310	0.4380
KZ	0.9030	0.5180
Kd	0.7460	0.4560
LC	0.7750	0.4550
LD	0.7210	0.4250
LH	0.8060	0.5050
LK	0.7590	0.4500
LV	0.9940	0.3760
LW	0.9690	0.3240
LX	0.8610	0.4700
LY	0.8460	0.4470

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Chain	Atom inclusion	Q-score
LZ	0.8890	0.5160
Ld	0.7420	0.4470
MC	0.7610	0.4620
MD	0.7200	0.4260
MH	0.8150	0.5050
MK	0.7590	0.4450
MV	0.9960	0.4090
MW	0.9690	0.3240
MX	0.8550	0.4660
MY	0.8690	0.4590
MZ	0.8970	0.5130
Md	0.7490	0.4500
N	0.7830	0.4560
NV	0.9890	0.3740
NW	0.9500	0.2530
O	0.7820	0.4500
OV	0.9360	0.3130
OW	0.8870	0.2990
P	0.7900	0.4660
PV	0.9930	0.4050
PW	0.9560	0.3400
Q	0.7850	0.4570
QV	0.9970	0.4140
QW	0.9940	0.3590
R	0.7810	0.4480
RV	0.9960	0.4260
RW	0.9880	0.3870
S	0.7710	0.4430
T	0.7790	0.4540
U	0.7700	0.4440
V	0.7710	0.4440
W	0.7870	0.4550
X	0.7810	0.4560
Y	0.7880	0.4600
Z	0.7740	0.4420