wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 03:13 am GMT

PDB ID	:	6ZVS
EMDB ID	:	EMD-11469
Title	:	C12 symmetry: Bacterial Vipp1 and PspA are members of the ancient ESCRT-III membrane-remodeling superfamily.
Authors	:	Liu, J.; Tassinari, M.; Souza, D.P.; Naskar, S.; Noel, J.K.; Bohuszewicz, O.; Buck, M.; Williams, T.A.; Baum, B.; Low, H.H.
Deposited on	:	2020-07-27
Resolution	:	7.20 Å(reported)

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

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

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

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

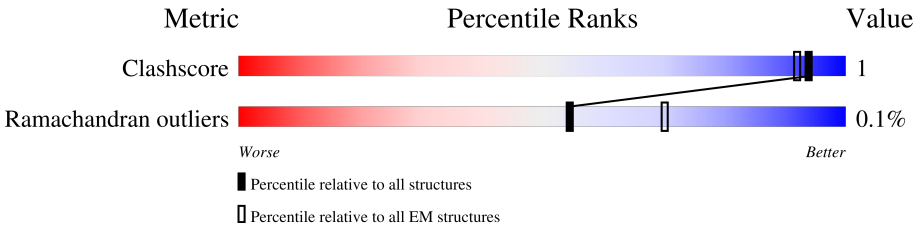
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	A	258	33% 52% 48%
1	AA	258	16% 84% 15%
1	AB	258	84% 15%
1	B	258	16% 84% 15%
1	BA	258	84% 15%
1	BB	258	5% 82% 16%
1	C	258	84% 15%
1	CA	258	84% 15%
1	CB	258	10% 61% 39%

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Mol	Chain	Length	Quality of chain
1	D	258	84% 15%
1	DA	258	82% 16%
1	DB	258	33% 52% 48%
1	E	258	82% 16%
1	EA	258	11% 61% 39%
1	EB	258	16% 84% 15%
1	F	258	11% 61% 39%
1	FA	258	34% 52% 48%
1	FB	258	84% 15%
1	G	258	34% 52% 48%
1	GA	258	16% 84% 15%
1	GB	258	84% 15%
1	H	258	16% 84% 15%
1	HA	258	84% 15%
1	HB	258	82% 16%
1	I	258	84% 15%
1	IA	258	84% 15%
1	IB	258	11% 61% 39%
1	J	258	84% 15%
1	JA	258	5% 82% 16%
1	JB	258	34% 52% 48%
1	K	258	82% 16%
1	KA	258	10% 61% 39%
1	KB	258	16% 84% 15%
1	L	258	10% 61% 39%

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Mol	Chain	Length	Quality of chain
1	LA	258	33% 52% 48%
1	LB	258	84% 15%
1	M	258	34% 52% 48%
1	MA	258	16% 84% 15%
1	MB	258	84% 15%
1	N	258	16% 84% 15%
1	NA	258	84% 15%
1	NB	258	82% 16%
1	O	258	84% 15%
1	OA	258	84% 15%
1	OB	258	11% 61% 39%
1	P	258	84% 15%
1	PA	258	82% 16%
1	PB	258	34% 52% 48%
1	Q	258	5% 82% 16%
1	QA	258	11% 61% 39%
1	QB	258	16% 84% 15%
1	R	258	10% 61% 39%
1	RA	258	34% 52% 48%
1	RB	258	84% 15%
1	S	258	33% 52% 48%
1	SA	258	16% 84% 15%
1	SB	258	84% 15%
1	T	258	16% 84% 15%
1	TA	258	84% 15%

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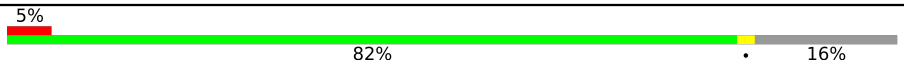
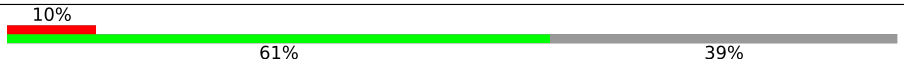
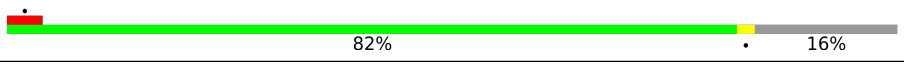
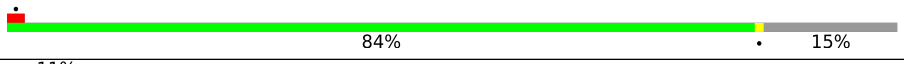
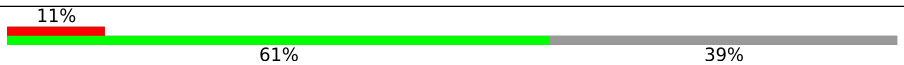
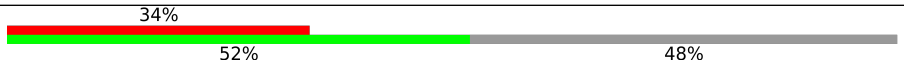
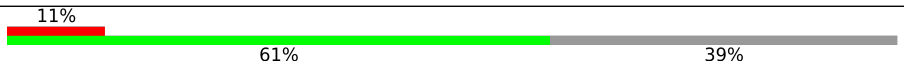
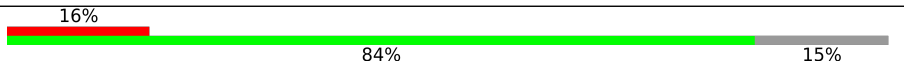
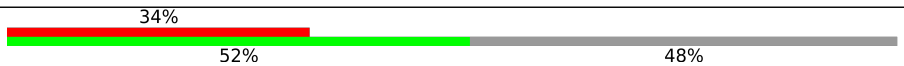
Mol	Chain	Length	Quality of chain
1	TB	258	
1	UA	258	
1	UB	258	
1	V	258	
1	VA	258	
1	W	258	
1	WA	258	
1	X	258	
1	XA	258	
1	Y	258	
1	YA	258	
1	Z	258	
1	ZA	258	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 69420 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 Vipp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	133	Total 661	C 395	N 133	O 133	0	0
1	B	219	Total 1086	C 648	N 219	O 219	0	0
1	C	219	Total 1086	C 648	N 219	O 219	0	0
1	D	219	Total 1086	C 648	N 219	O 219	0	0
1	E	218	Total 1081	C 645	N 218	O 218	0	0
1	F	158	Total 785	C 469	N 158	O 158	0	0
1	G	133	Total 661	C 395	N 133	O 133	0	0
1	H	219	Total 1086	C 648	N 219	O 219	0	0
1	I	219	Total 1086	C 648	N 219	O 219	0	0
1	J	219	Total 1086	C 648	N 219	O 219	0	0
1	K	218	Total 1081	C 645	N 218	O 218	0	0
1	L	158	Total 785	C 469	N 158	O 158	0	0
1	M	133	Total 661	C 395	N 133	O 133	0	0
1	N	219	Total 1086	C 648	N 219	O 219	0	0
1	O	219	Total 1086	C 648	N 219	O 219	0	0
1	P	219	Total 1086	C 648	N 219	O 219	0	0
1	Q	218	Total 1081	C 645	N 218	O 218	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	158	Total 785	C 469	N 158	O 158	0	0
1	S	133	Total 661	C 395	N 133	O 133	0	0
1	T	219	Total 1086	C 648	N 219	O 219	0	0
1	V	219	Total 1086	C 648	N 219	O 219	0	0
1	W	219	Total 1086	C 648	N 219	O 219	0	0
1	X	218	Total 1081	C 645	N 218	O 218	0	0
1	Y	158	Total 785	C 469	N 158	O 158	0	0
1	Z	133	Total 661	C 395	N 133	O 133	0	0
1	AA	219	Total 1086	C 648	N 219	O 219	0	0
1	BA	219	Total 1086	C 648	N 219	O 219	0	0
1	CA	219	Total 1086	C 648	N 219	O 219	0	0
1	DA	218	Total 1081	C 645	N 218	O 218	0	0
1	EA	158	Total 785	C 469	N 158	O 158	0	0
1	FA	133	Total 661	C 395	N 133	O 133	0	0
1	GA	219	Total 1086	C 648	N 219	O 219	0	0
1	HA	219	Total 1086	C 648	N 219	O 219	0	0
1	IA	219	Total 1086	C 648	N 219	O 219	0	0
1	JA	218	Total 1081	C 645	N 218	O 218	0	0
1	KA	158	Total 785	C 469	N 158	O 158	0	0
1	LA	133	Total 661	C 395	N 133	O 133	0	0
1	MA	219	Total 1086	C 648	N 219	O 219	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	NA	219	Total 1086	C 648	N 219	O 219	0	0
1	OA	219	Total 1086	C 648	N 219	O 219	0	0
1	PA	218	Total 1081	C 645	N 218	O 218	0	0
1	QA	158	Total 785	C 469	N 158	O 158	0	0
1	RA	133	Total 661	C 395	N 133	O 133	0	0
1	SA	219	Total 1086	C 648	N 219	O 219	0	0
1	TA	219	Total 1086	C 648	N 219	O 219	0	0
1	UA	219	Total 1086	C 648	N 219	O 219	0	0
1	VA	218	Total 1081	C 645	N 218	O 218	0	0
1	WA	158	Total 785	C 469	N 158	O 158	0	0
1	XA	133	Total 661	C 395	N 133	O 133	0	0
1	YA	219	Total 1086	C 648	N 219	O 219	0	0
1	ZA	219	Total 1086	C 648	N 219	O 219	0	0
1	AB	219	Total 1086	C 648	N 219	O 219	0	0
1	BB	218	Total 1081	C 645	N 218	O 218	0	0
1	CB	158	Total 785	C 469	N 158	O 158	0	0
1	DB	133	Total 661	C 395	N 133	O 133	0	0
1	EB	219	Total 1086	C 648	N 219	O 219	0	0
1	FB	219	Total 1086	C 648	N 219	O 219	0	0
1	GB	219	Total 1086	C 648	N 219	O 219	0	0
1	HB	218	Total 1081	C 645	N 218	O 218	0	0

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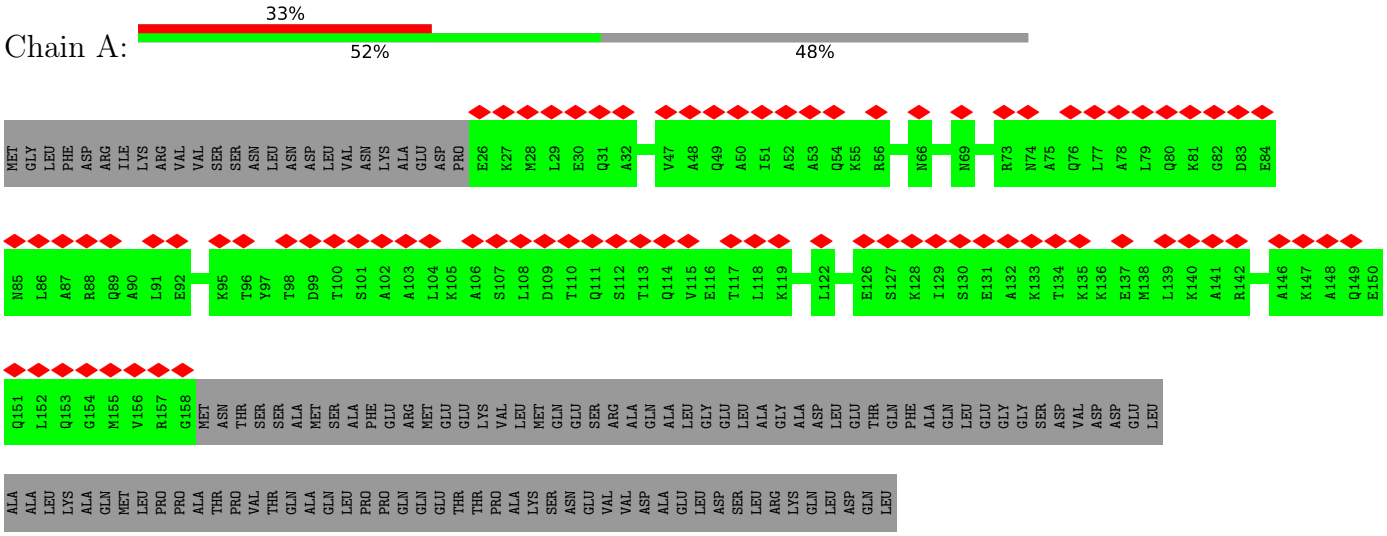
Mol	Chain	Residues	Atoms				AltConf	Trace
1	IB	158	Total 785	C 469	N 158	O 158	0	0
1	JB	133	Total 661	C 395	N 133	O 133	0	0
1	KB	219	Total 1086	C 648	N 219	O 219	0	0
1	LB	219	Total 1086	C 648	N 219	O 219	0	0
1	MB	219	Total 1086	C 648	N 219	O 219	0	0
1	NB	218	Total 1081	C 645	N 218	O 218	0	0
1	OB	158	Total 785	C 469	N 158	O 158	0	0
1	PB	133	Total 661	C 395	N 133	O 133	0	0
1	QB	219	Total 1086	C 648	N 219	O 219	0	0
1	RB	219	Total 1086	C 648	N 219	O 219	0	0
1	SB	219	Total 1086	C 648	N 219	O 219	0	0
1	TB	218	Total 1081	C 645	N 218	O 218	0	0
1	UB	158	Total 785	C 469	N 158	O 158	0	0

3 Residue-property plots (i)

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

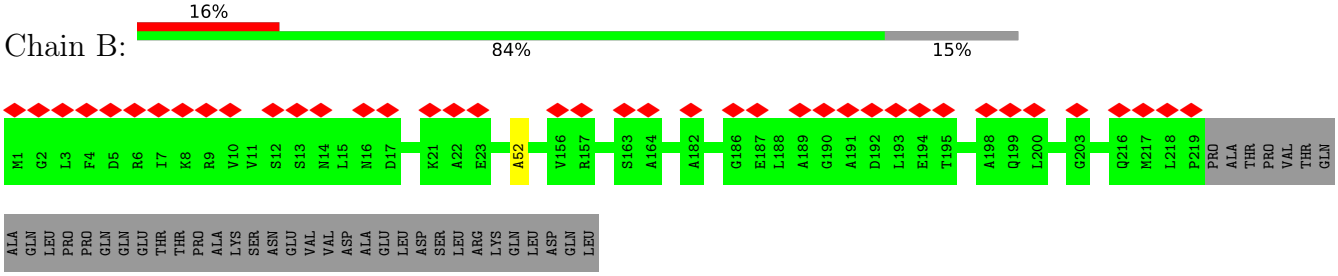
• Molecule 1: Vipp1

Chain A:



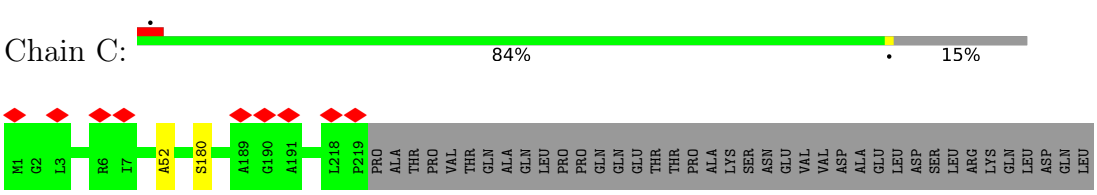
• Molecule 1: Vipp1

Chain B:



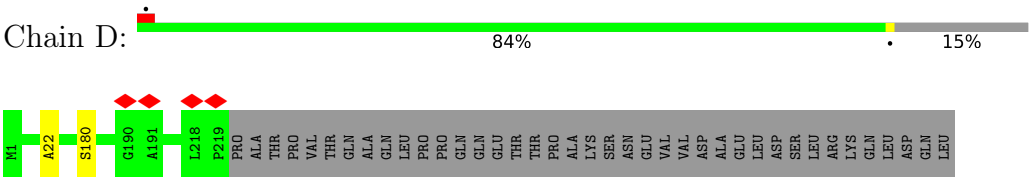
• Molecule 1: Vipp1

Chain C:



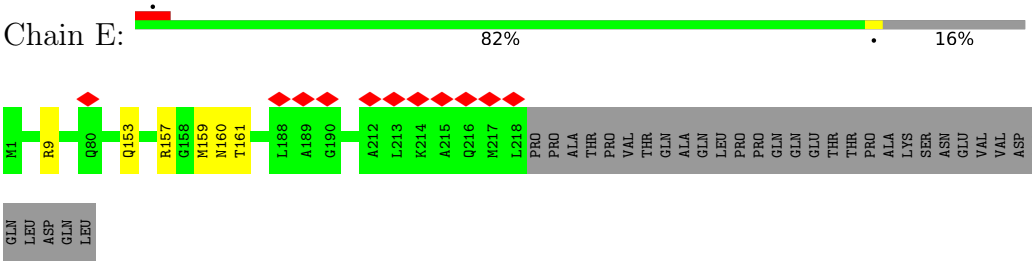
• Molecule 1: Vipp1

Chain D:



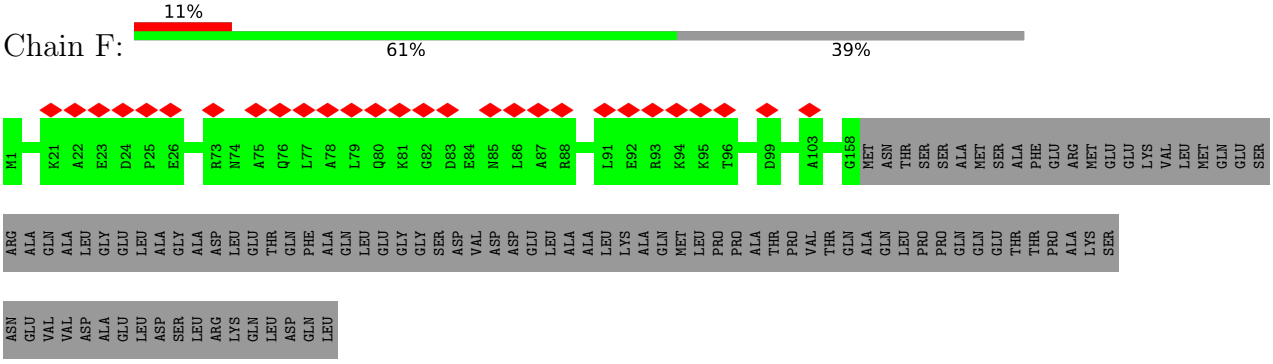
• Molecule 1: Vipp1

Chain E:



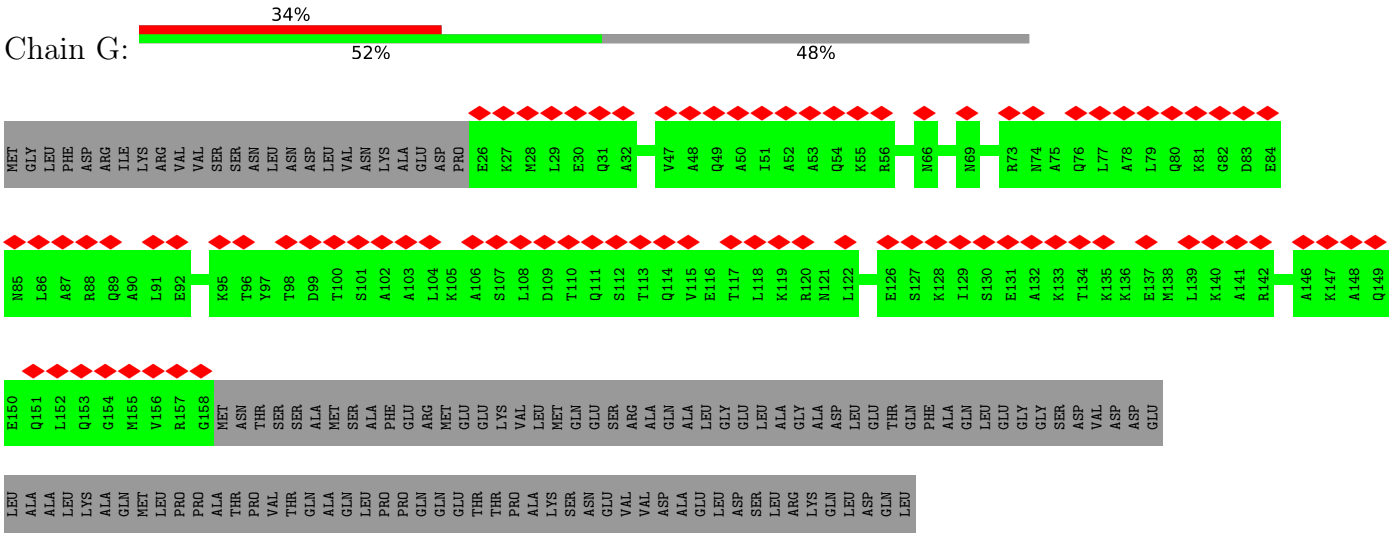
• Molecule 1: Vipp1

Chain F:



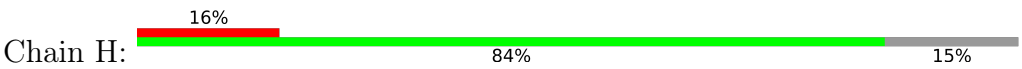
• Molecule 1: Vipp1

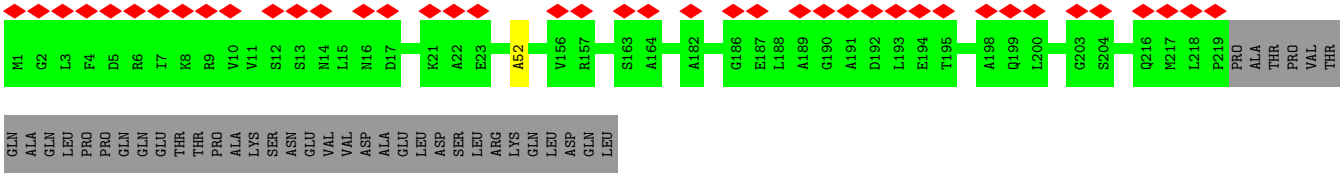
Chain G:



• Molecule 1: Vipp1

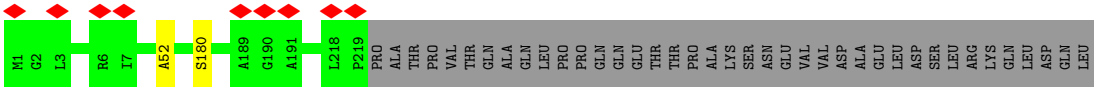
Chain H:





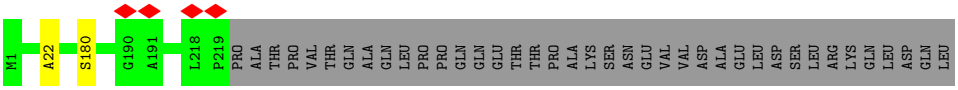
• Molecule 1: Vipp1

Chain I:



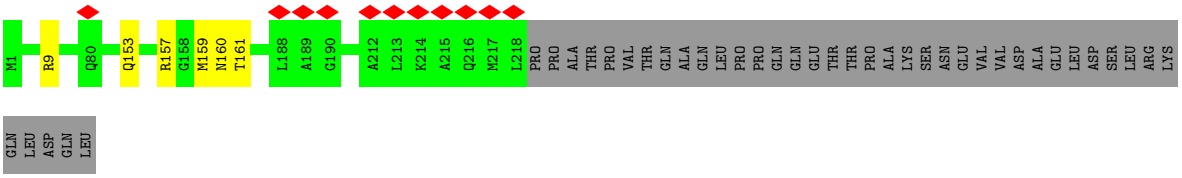
• Molecule 1: Vipp1

Chain J:



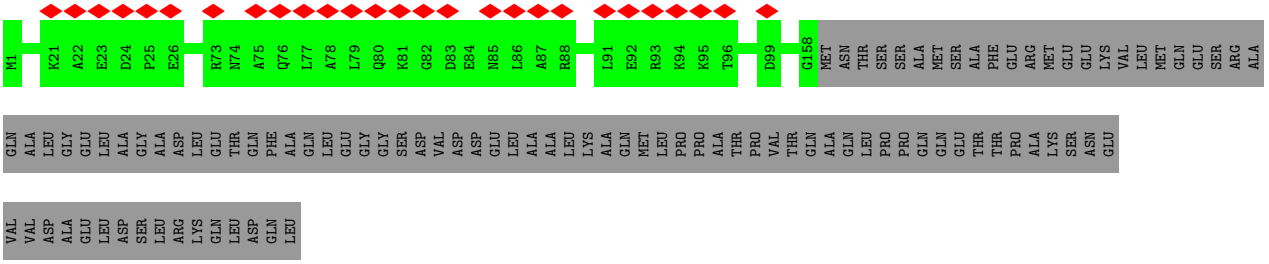
• Molecule 1: Vipp1

Chain K:



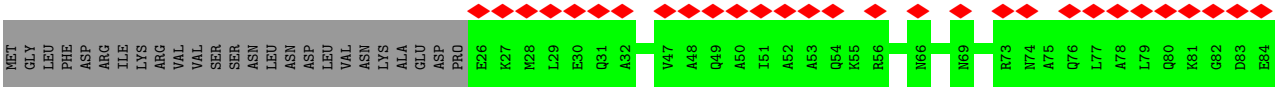
• Molecule 1: Vipp1

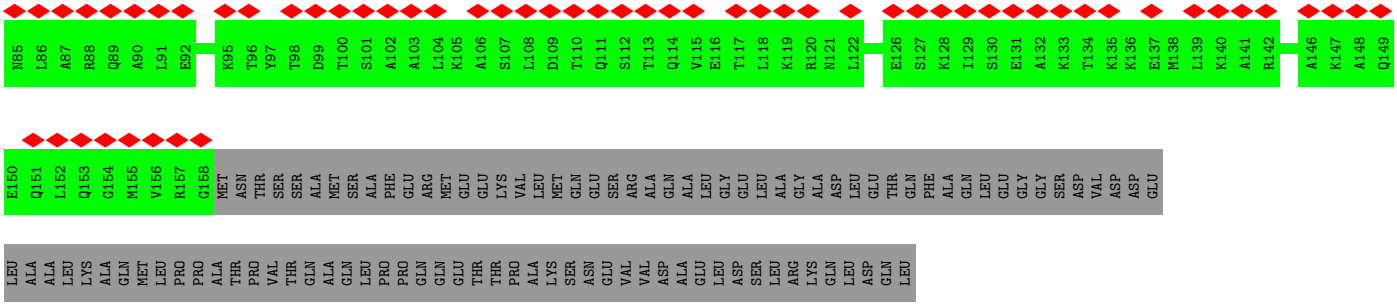
Chain L:



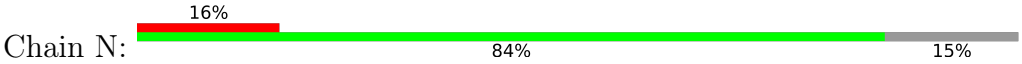
• Molecule 1: Vipp1

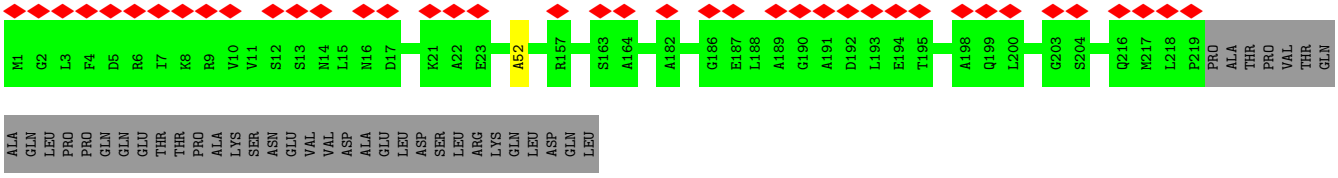
Chain M:



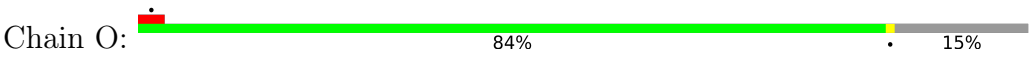


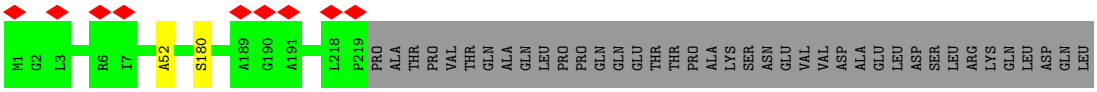
• Molecule 1: Vipp1



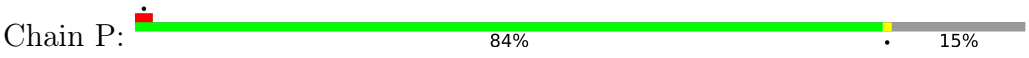


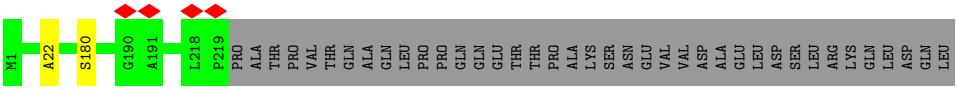
• Molecule 1: Vipp1



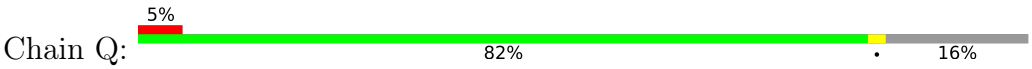


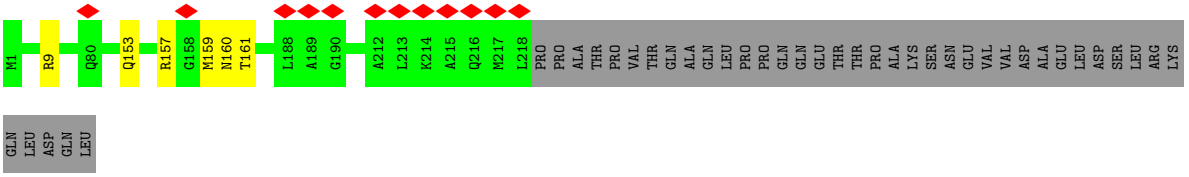
• Molecule 1: Vipp1



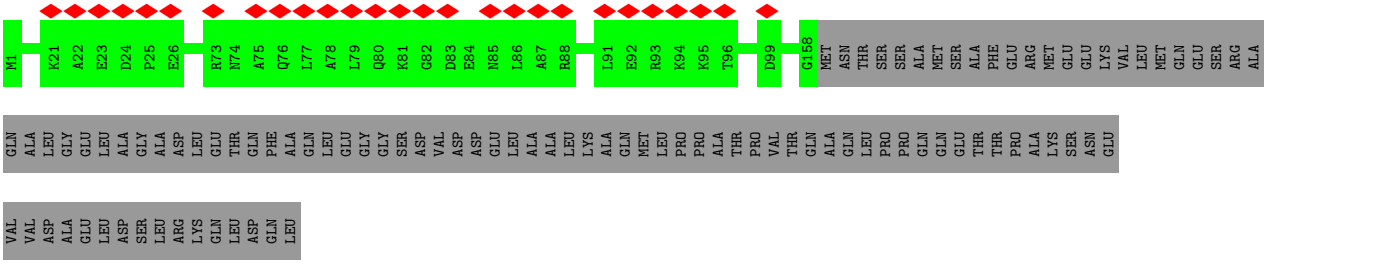


• Molecule 1: Vipp1





• Molecule 1: Vipp1



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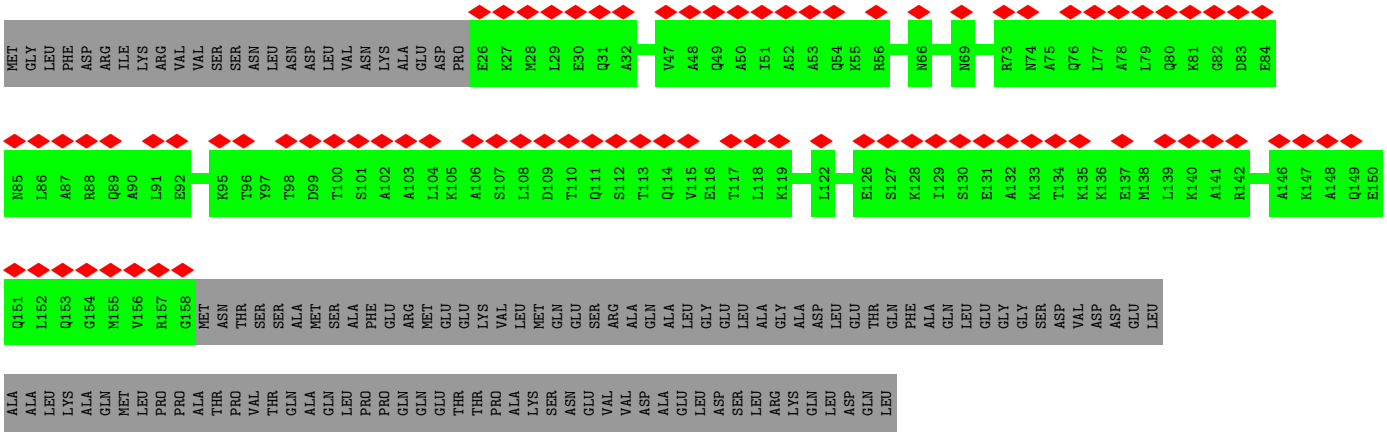

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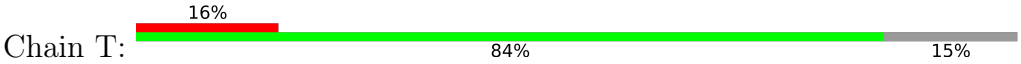

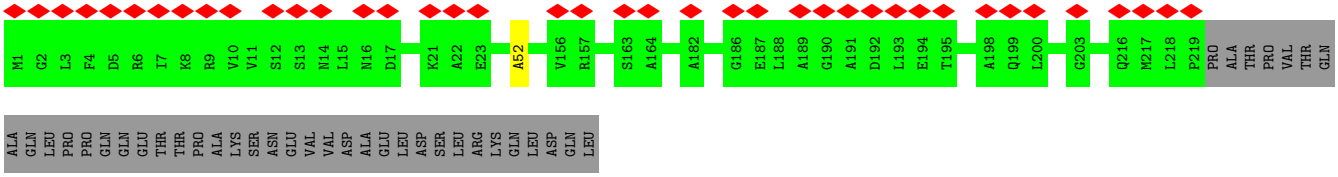

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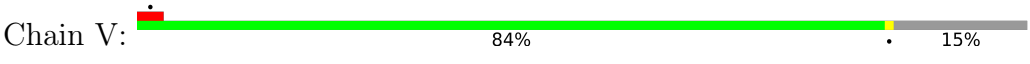

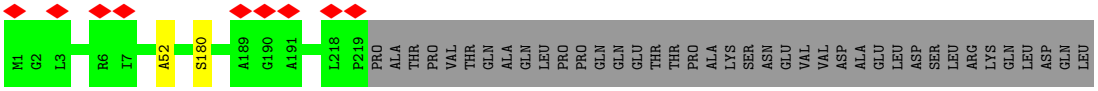

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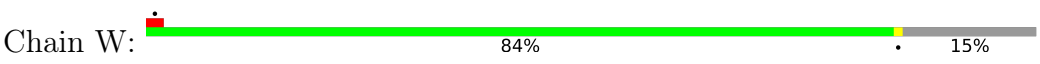
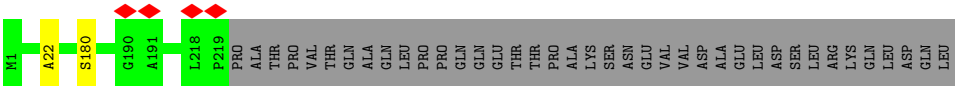
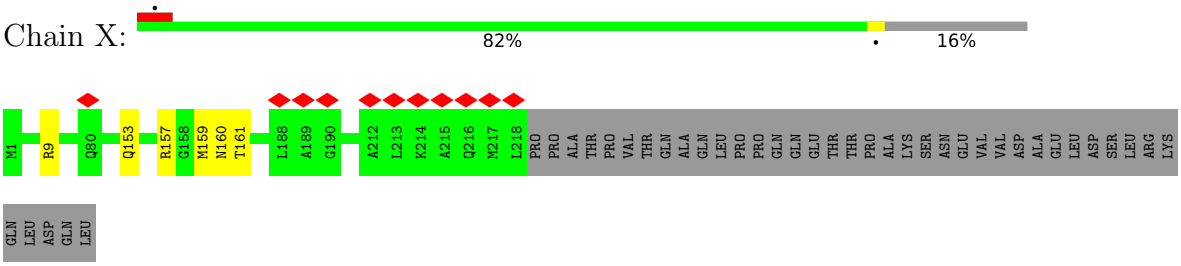




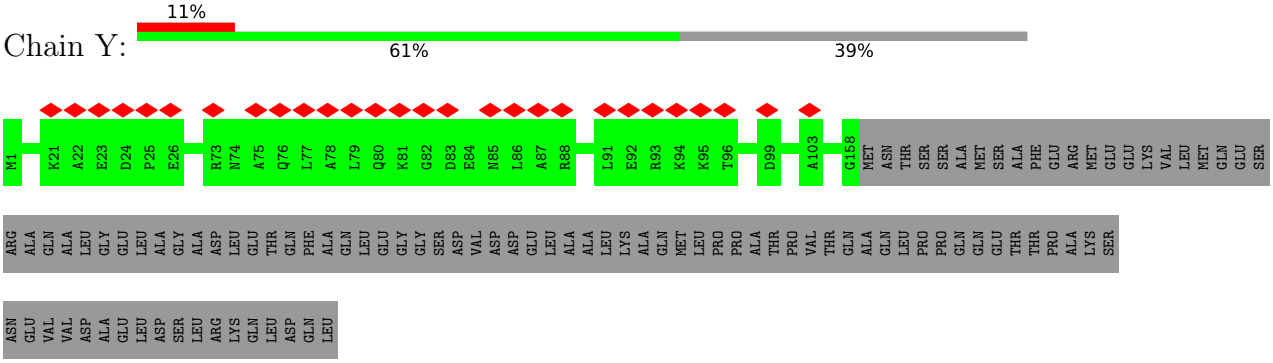
• Molecule 1: Vipp1

Chain X:



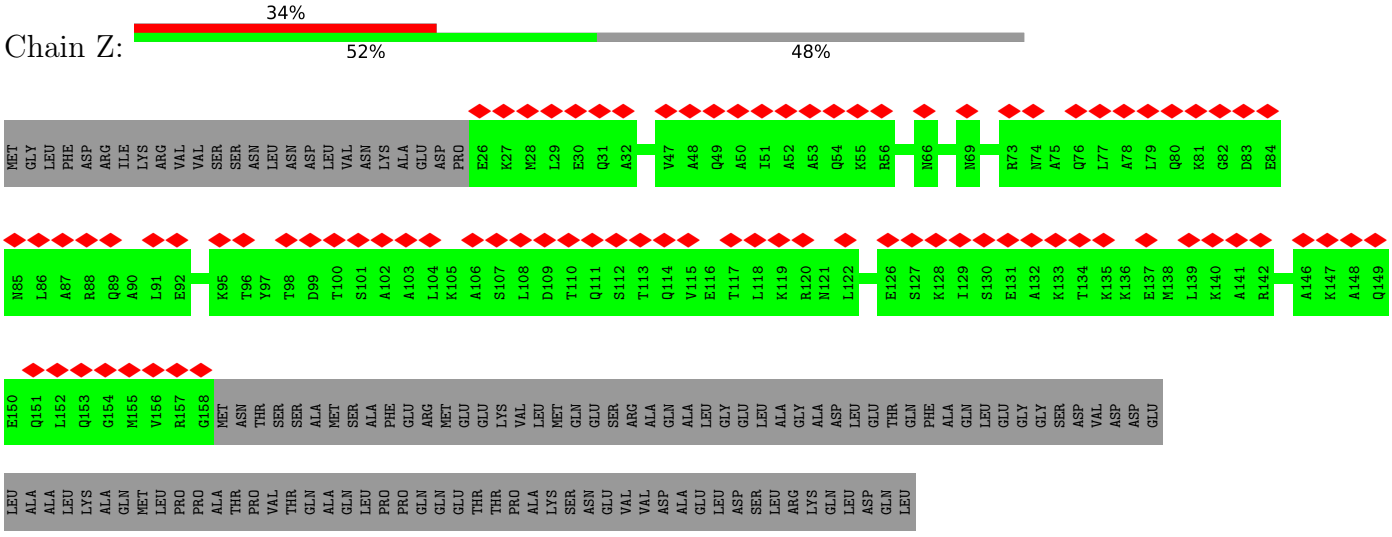
• Molecule 1: Vipp1

Chain Y:



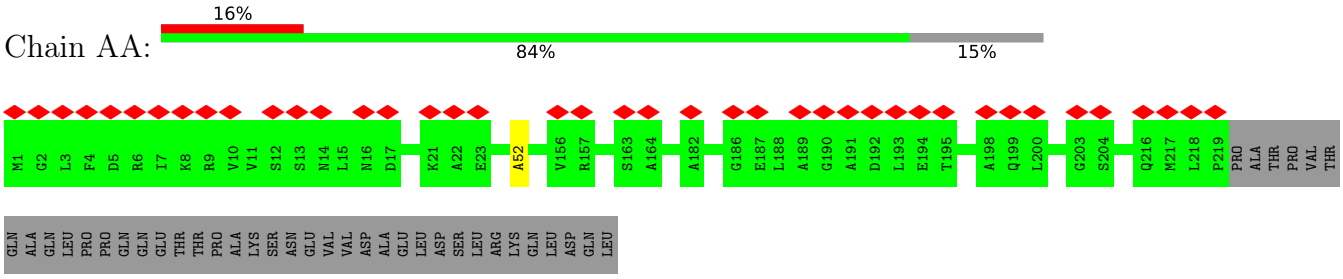
• Molecule 1: Vipp1

Chain Z:



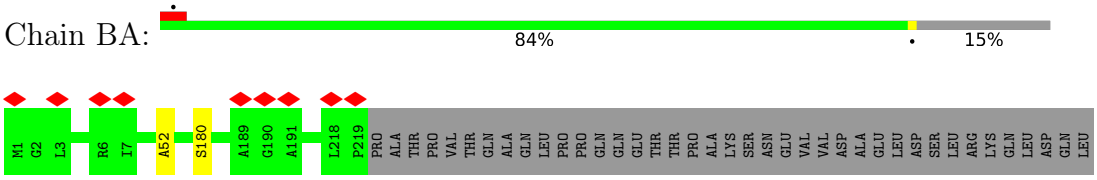
• Molecule 1: Vipp1

Chain AA:



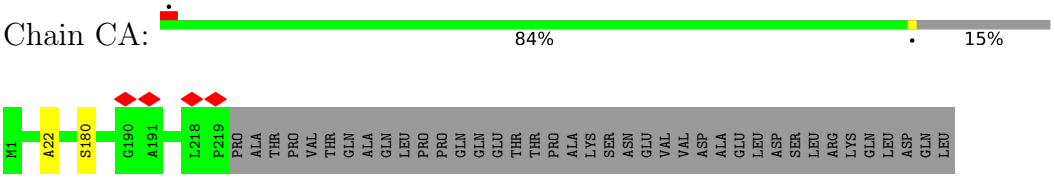
• Molecule 1: Vipp1

Chain BA:



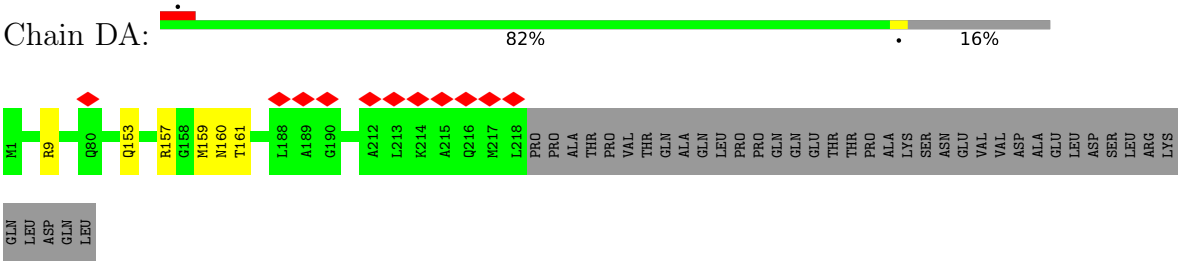
• Molecule 1: Vipp1

Chain CA:



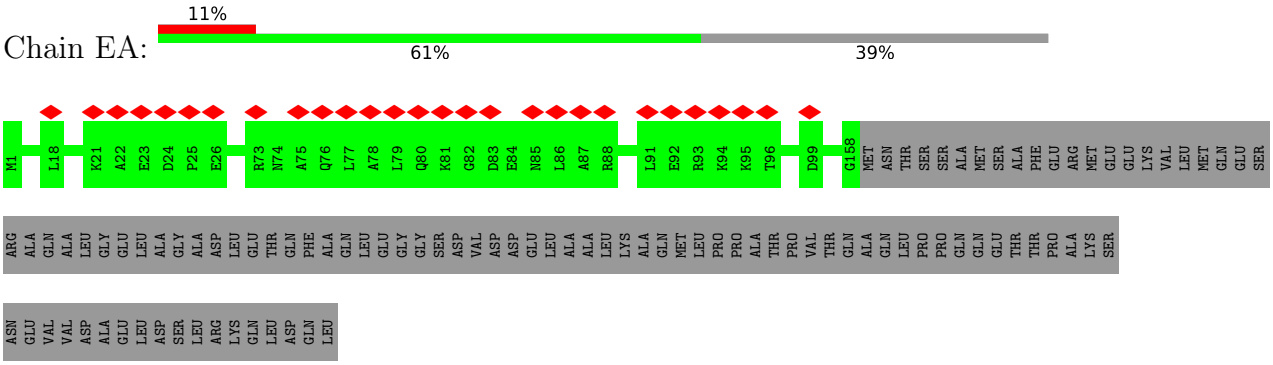
• Molecule 1: Vipp1

Chain DA:



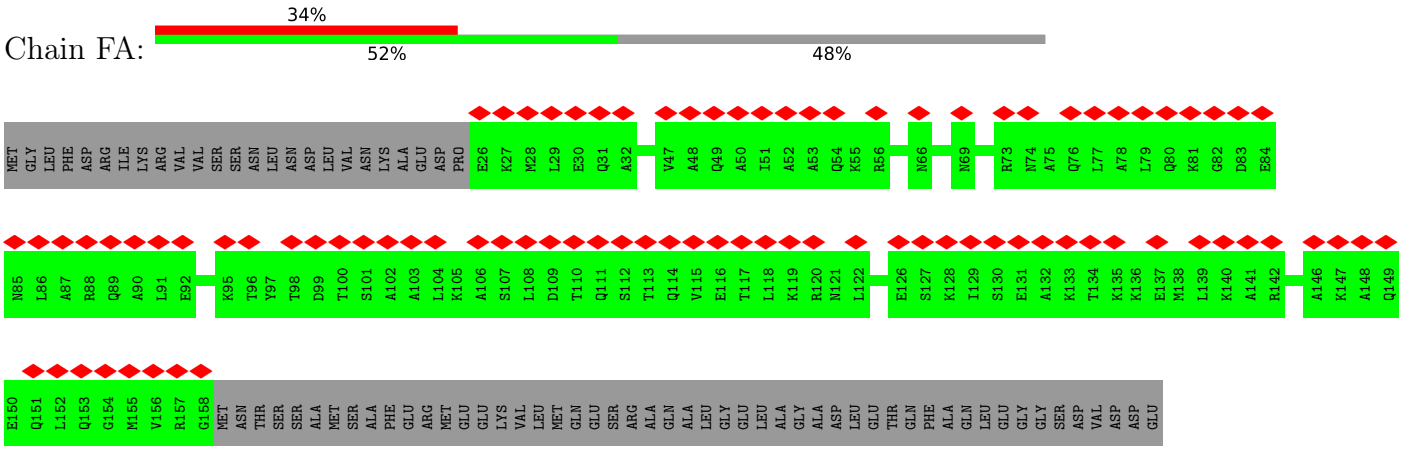
• Molecule 1: Vipp1

Chain EA:



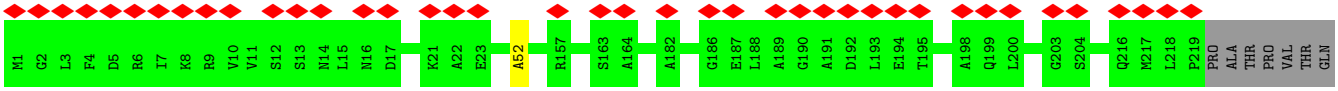
• Molecule 1: Vipp1

Chain FA:



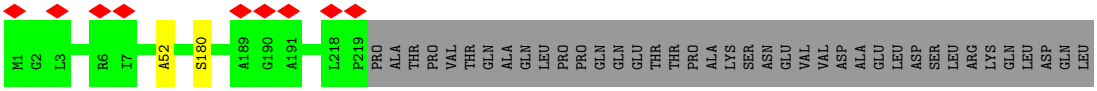
• Molecule 1: Vipp1

Chain GA:



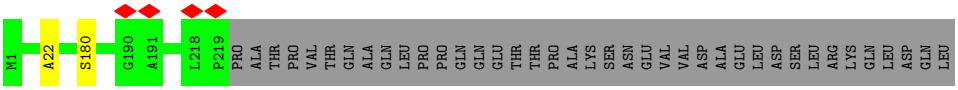
• Molecule 1: Vipp1

Chain HA:



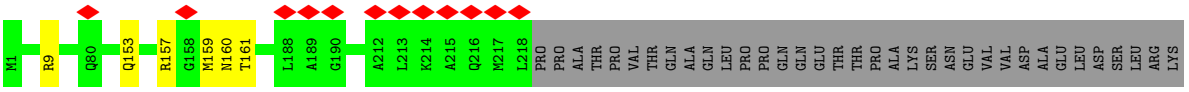
• Molecule 1: Vipp1

Chain IA:



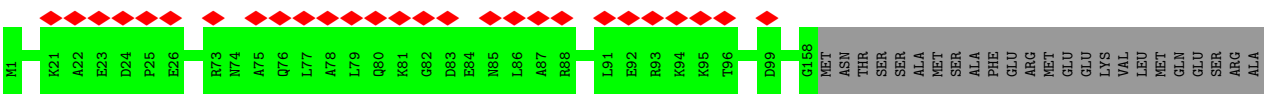
• Molecule 1: Vipp1

Chain JA:



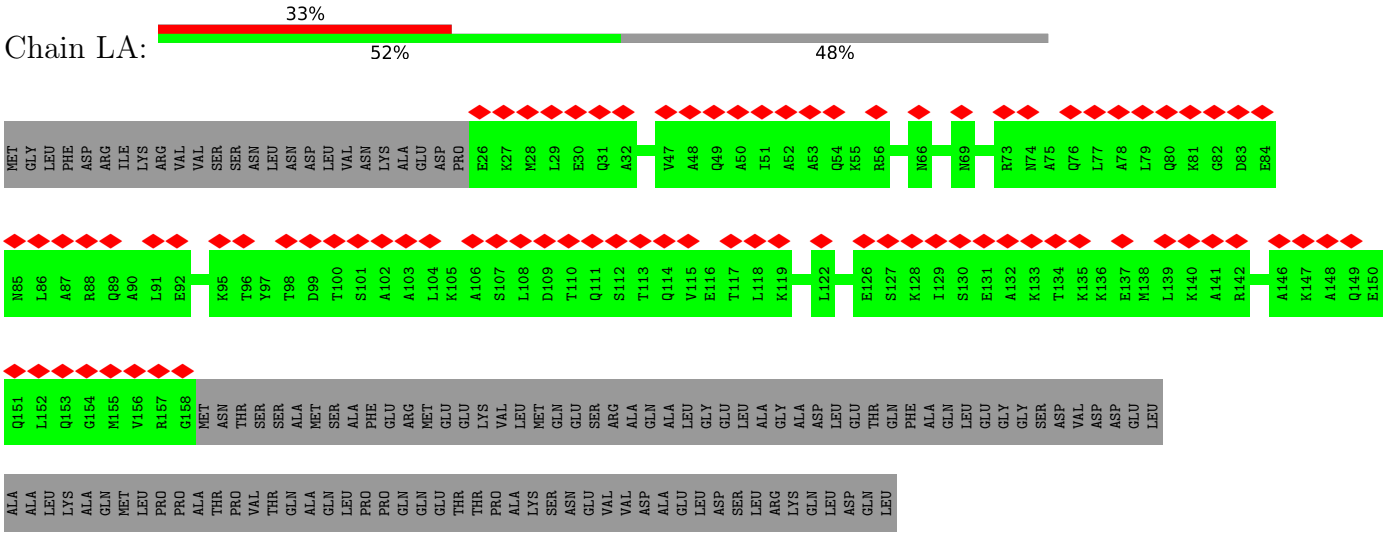
• Molecule 1: Vipp1

Chain KA:



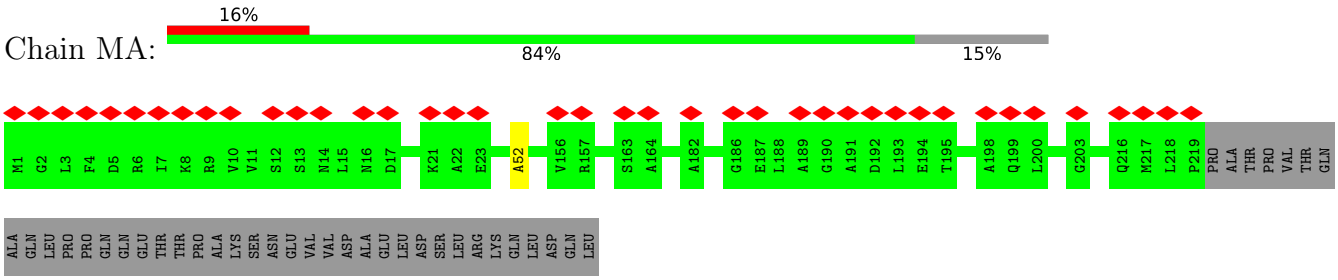
• Molecule 1: Vipp1

Chain LA:



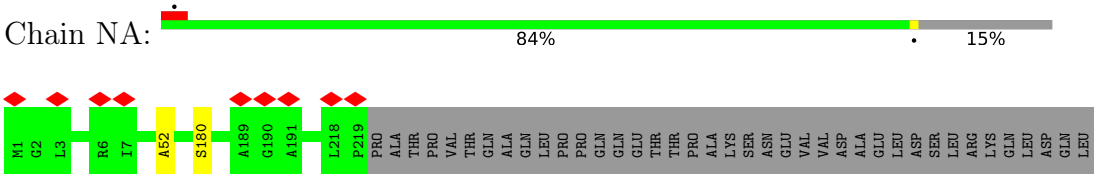
• Molecule 1: Vipp1

Chain MA:



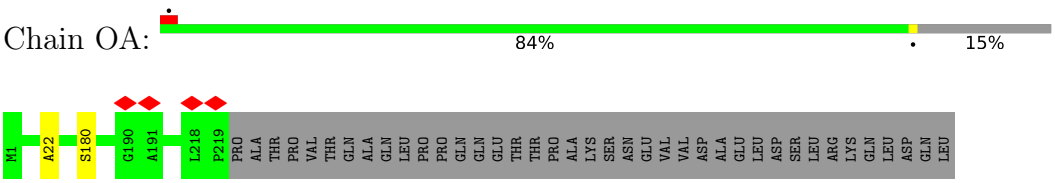
• Molecule 1: Vipp1

Chain NA:



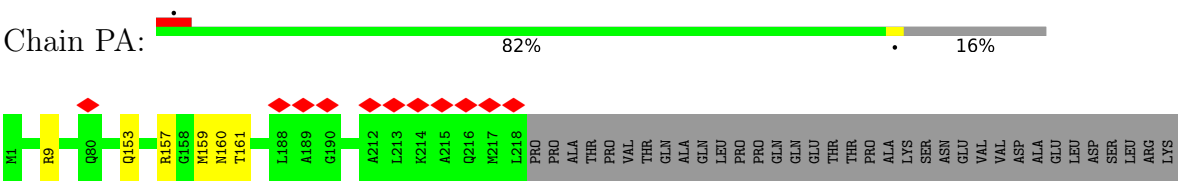
• Molecule 1: Vipp1

Chain OA:



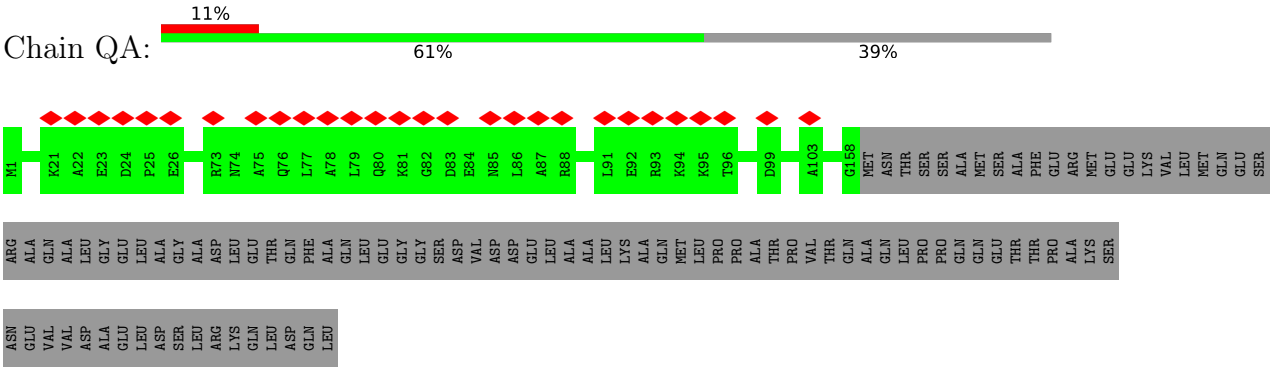
• Molecule 1: Vipp1

Chain PA:



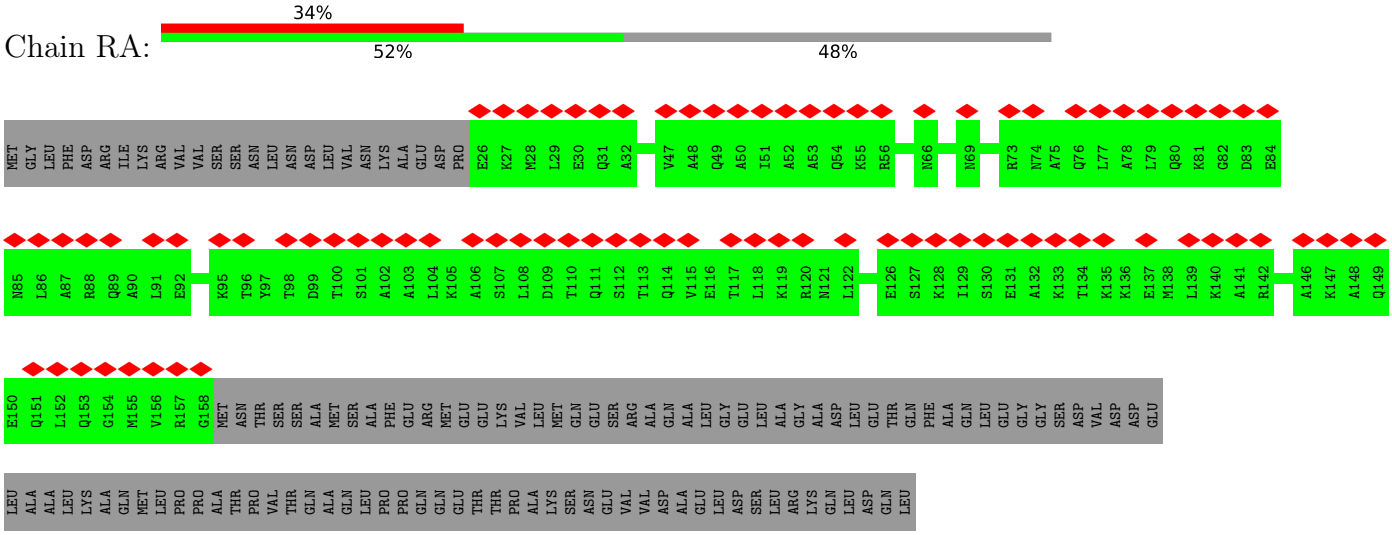
• Molecule 1: Vipp1

Chain QA:



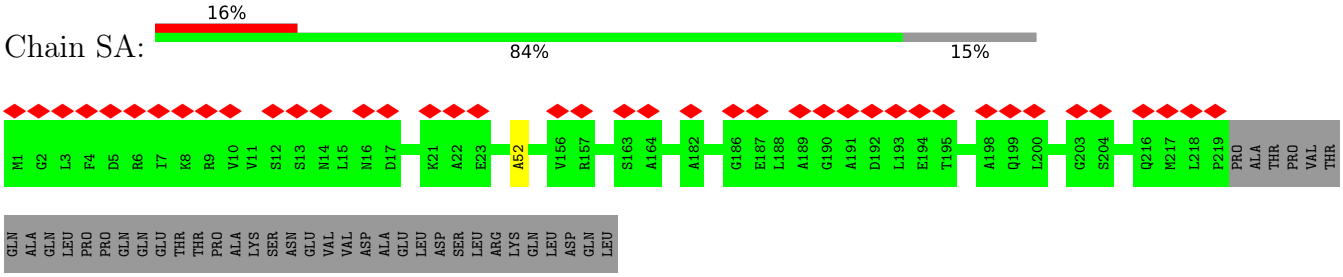
• Molecule 1: Vipp1

Chain RA:



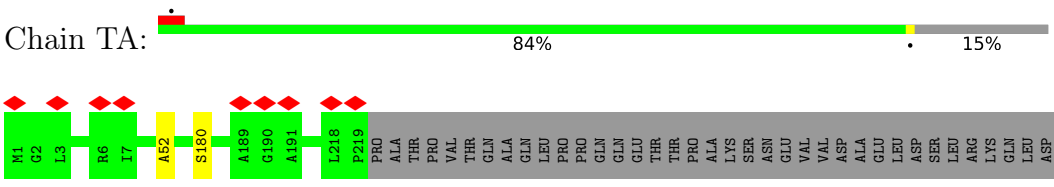
• Molecule 1: Vipp1

Chain SA:



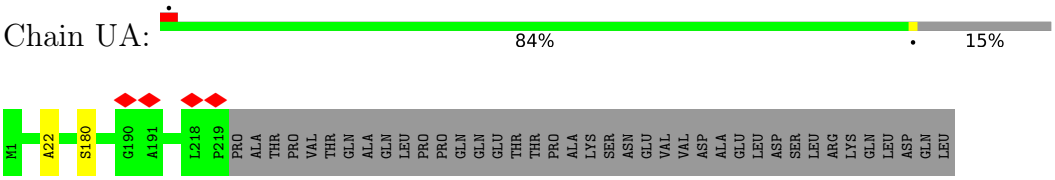
• Molecule 1: Vipp1

Chain TA:



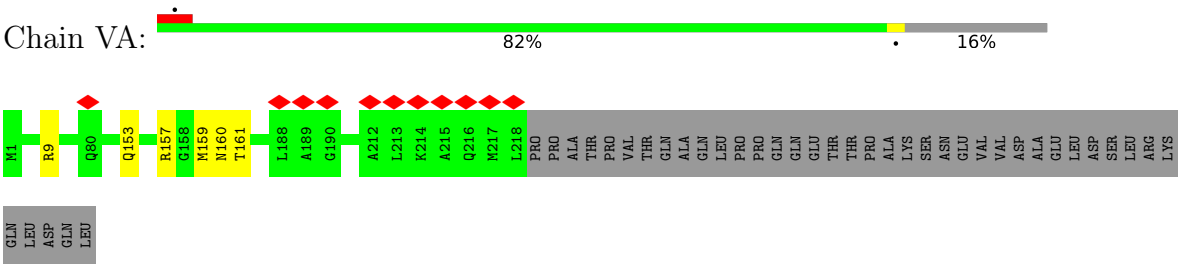
• Molecule 1: Vipp1

Chain UA:



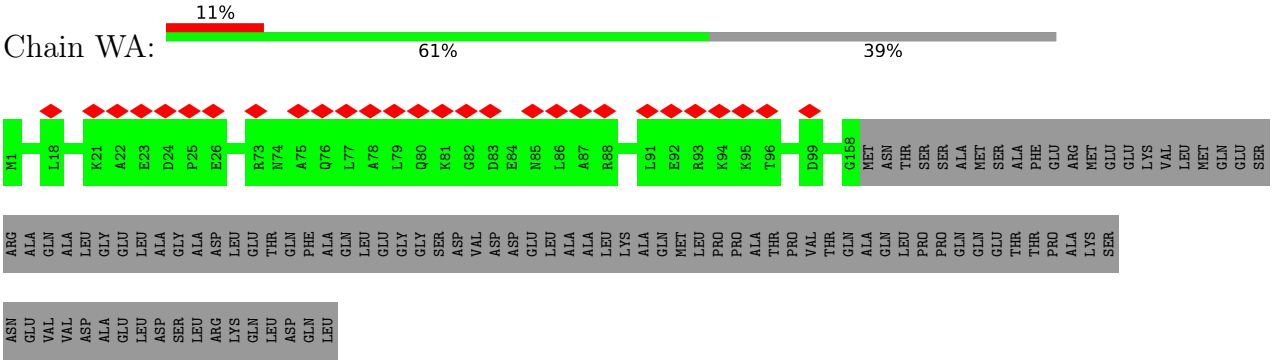
• Molecule 1: Vipp1

Chain VA:



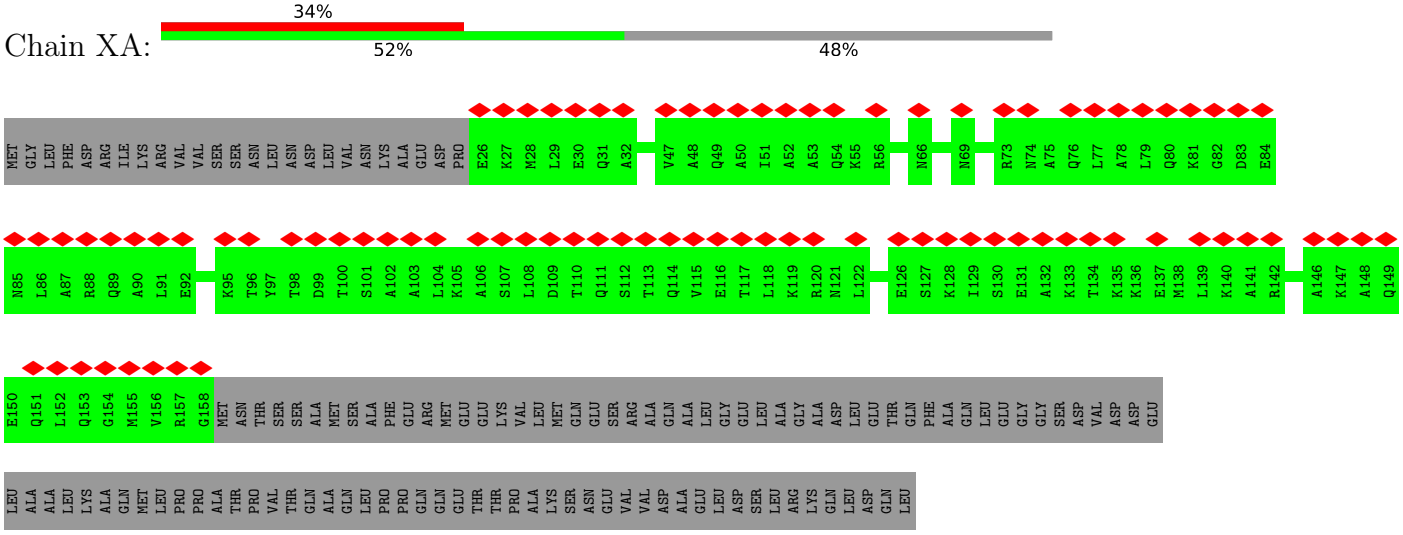
• Molecule 1: Vipp1

Chain WA:



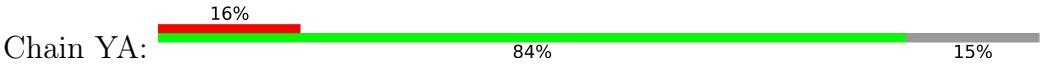
• Molecule 1: Vipp1

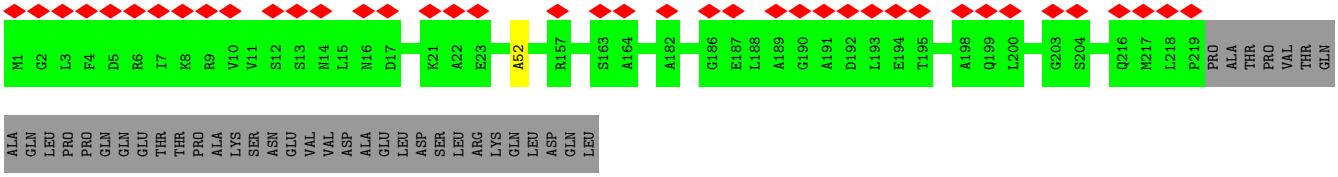
Chain XA:



• Molecule 1: Vipp1

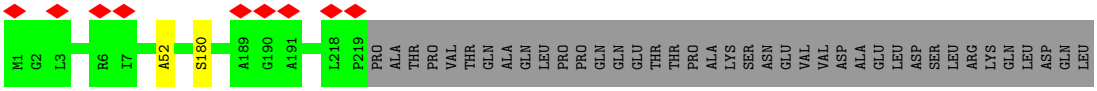
Chain YA:





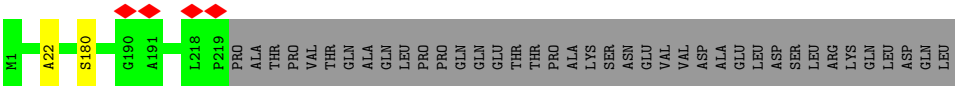
• Molecule 1: Vipp1

Chain ZA:



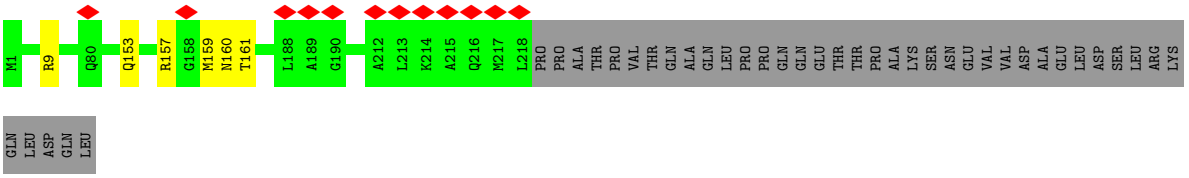
• Molecule 1: Vipp1

Chain AB:



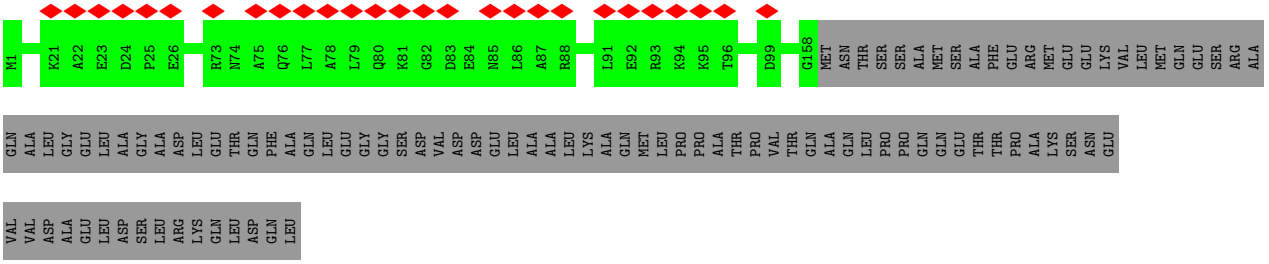
• Molecule 1: Vipp1

Chain BB:



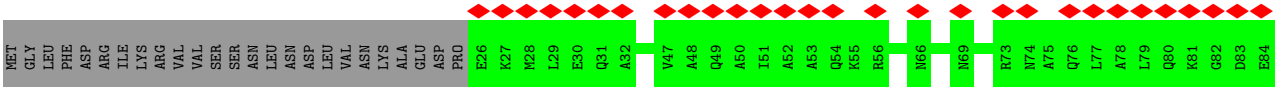
• Molecule 1: Vipp1

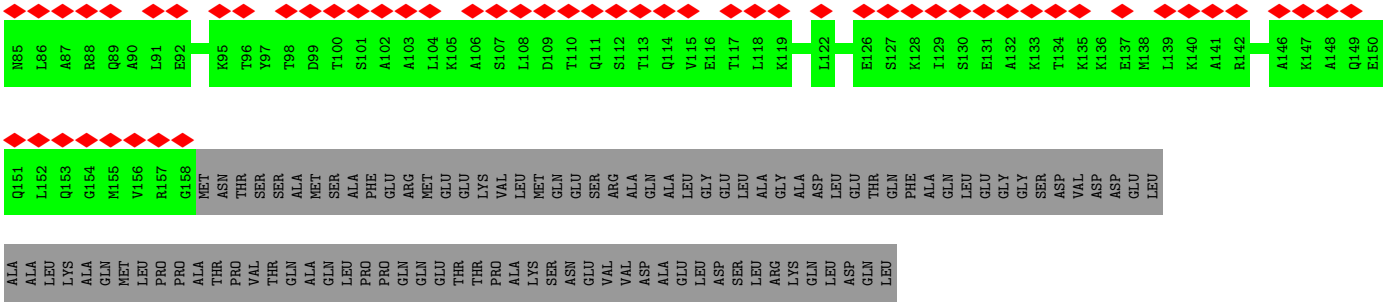
Chain CB:



• Molecule 1: Vipp1

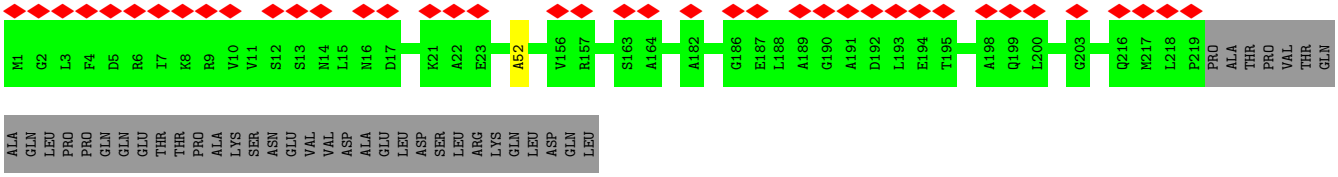
Chain DB:





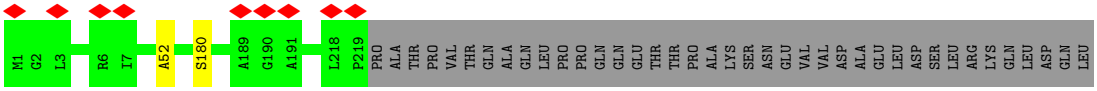
• Molecule 1: Vipp1

Chain EB:



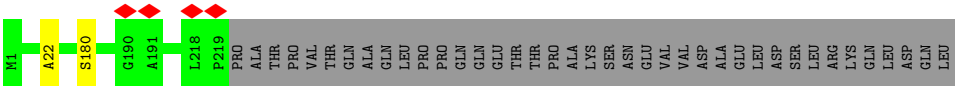
• Molecule 1: Vipp1

Chain FB:



• Molecule 1: Vipp1

Chain GB:

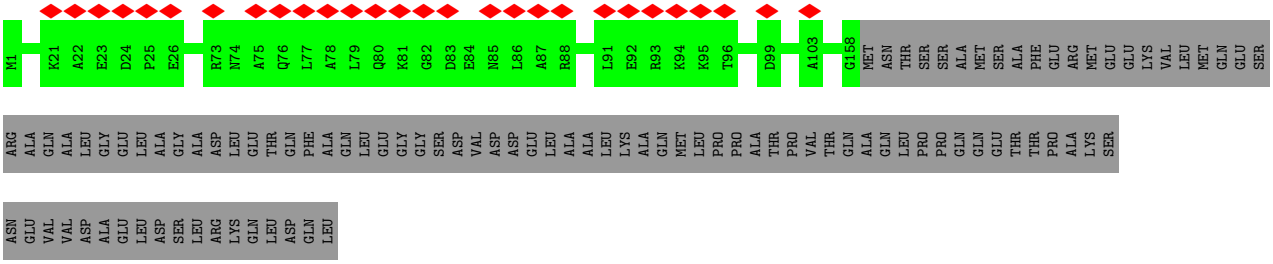


• Molecule 1: Vipp1

Chain HB:

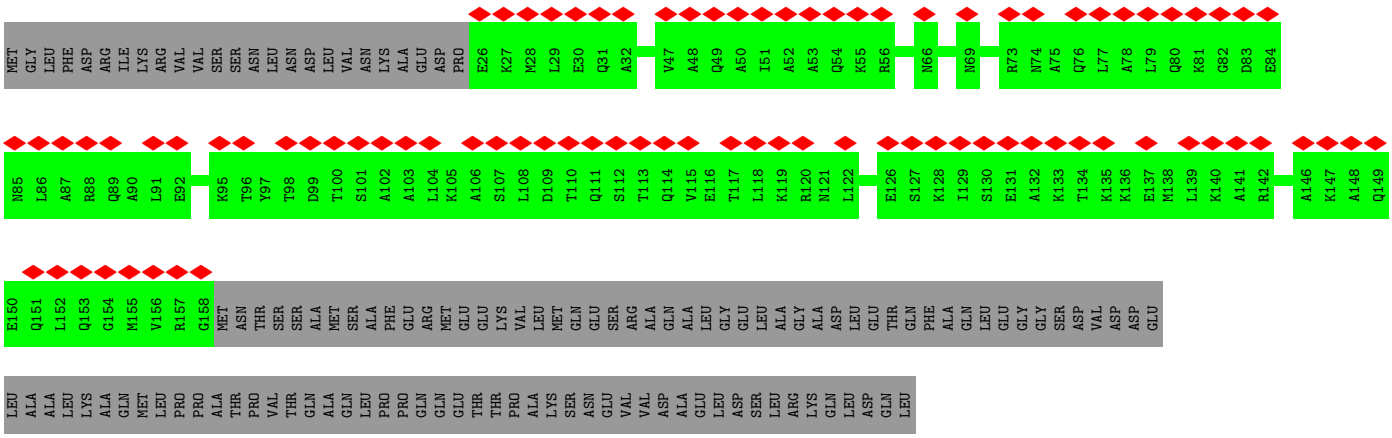
• Molecule 1: Vipp1

Chain IB:



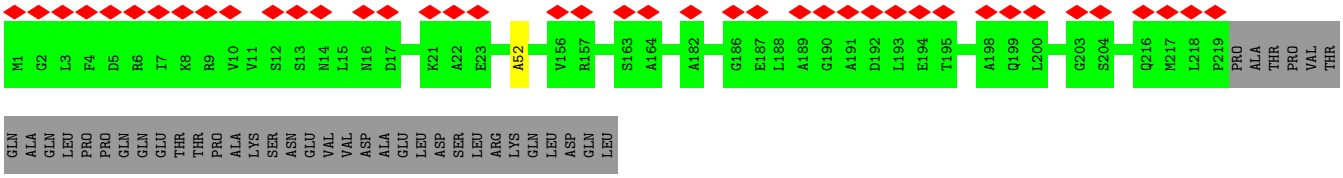
• Molecule 1: Vipp1

Chain JB:



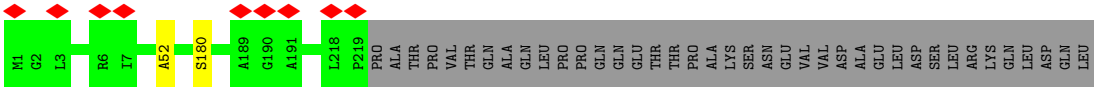
• Molecule 1: Vipp1

Chain KB:



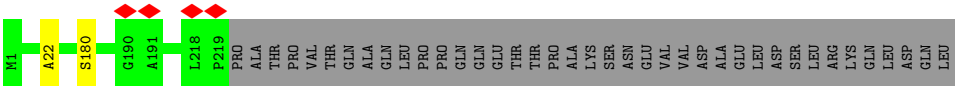
• Molecule 1: Vipp1

Chain LB:



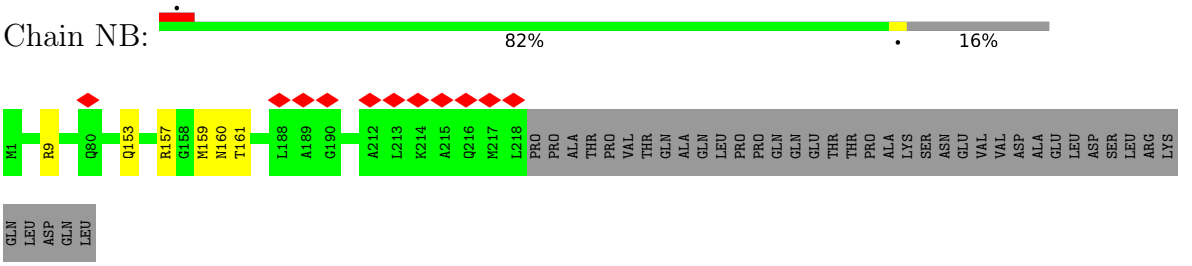
• Molecule 1: Vipp1

Chain MB:



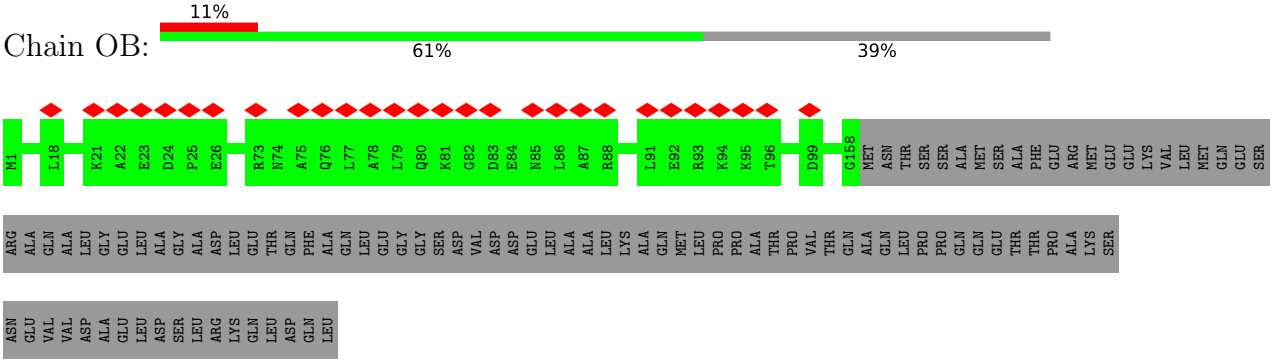
• Molecule 1: Vipp1

Chain NB:



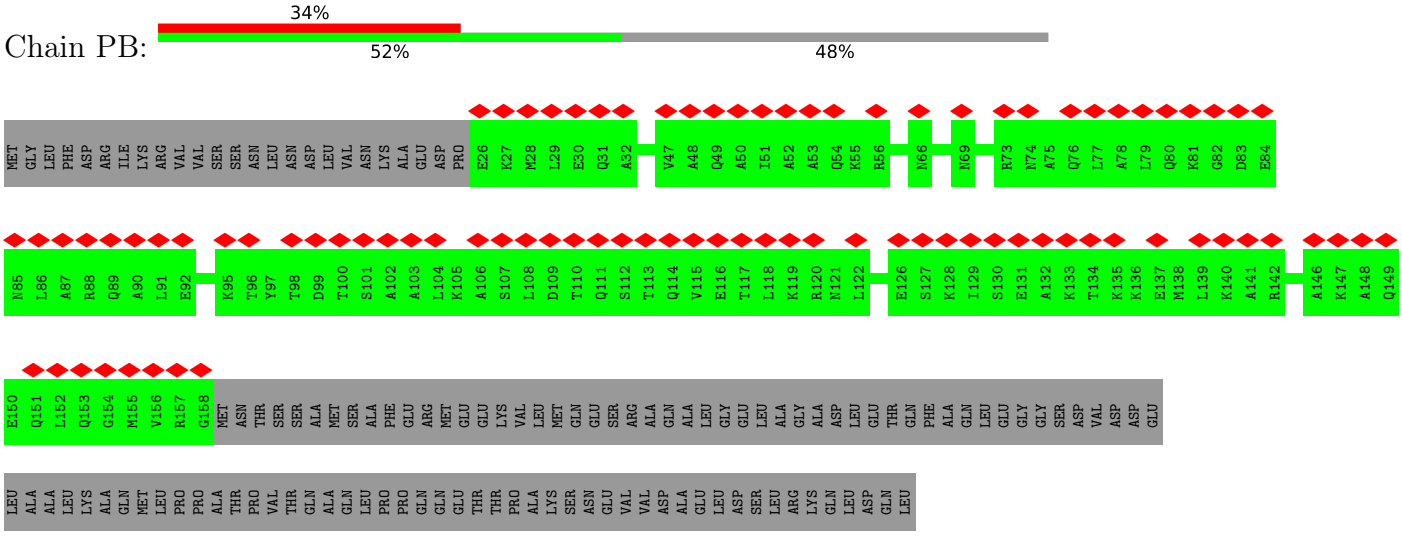
• Molecule 1: Vipp1

Chain OB:



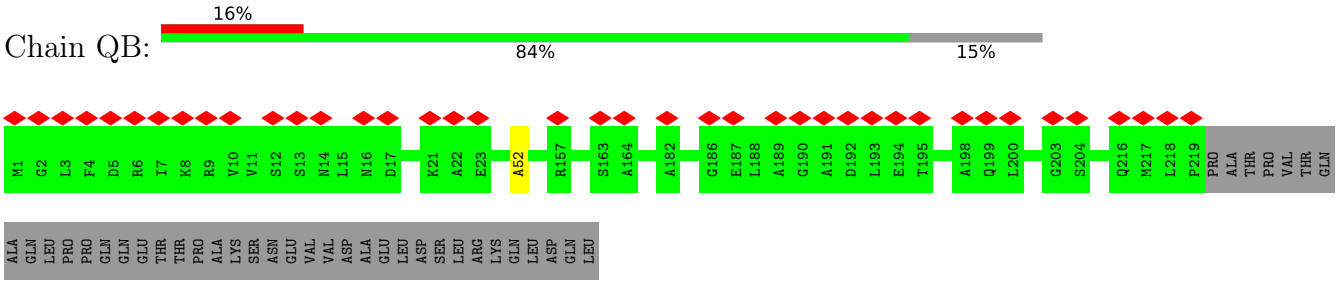
• Molecule 1: Vipp1

Chain PB:



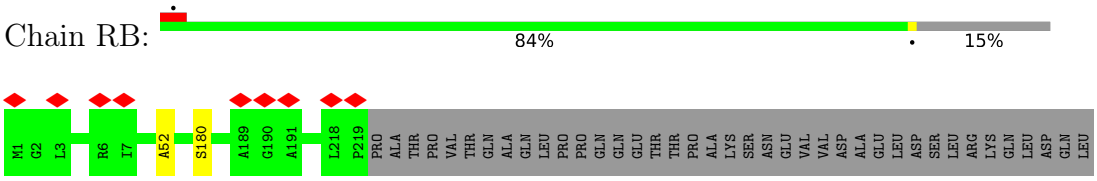
• Molecule 1: Vipp1

Chain QB:



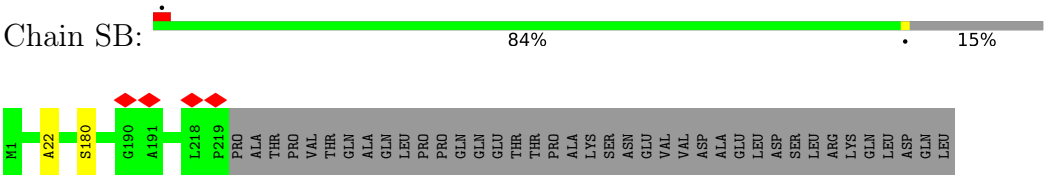
• Molecule 1: Vipp1

Chain RB:



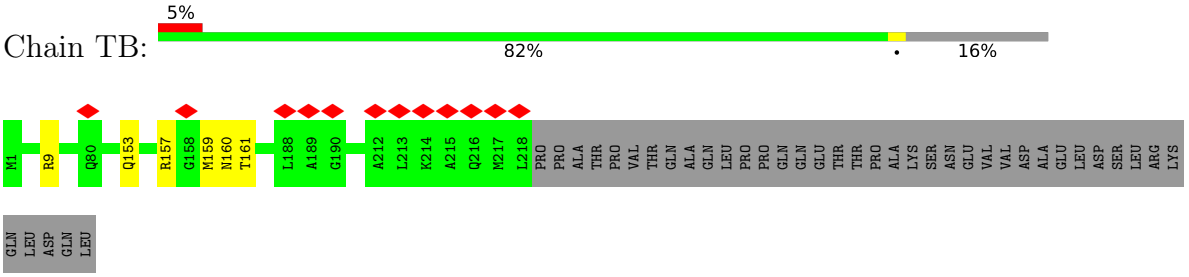
• Molecule 1: Vipp1

Chain SB:



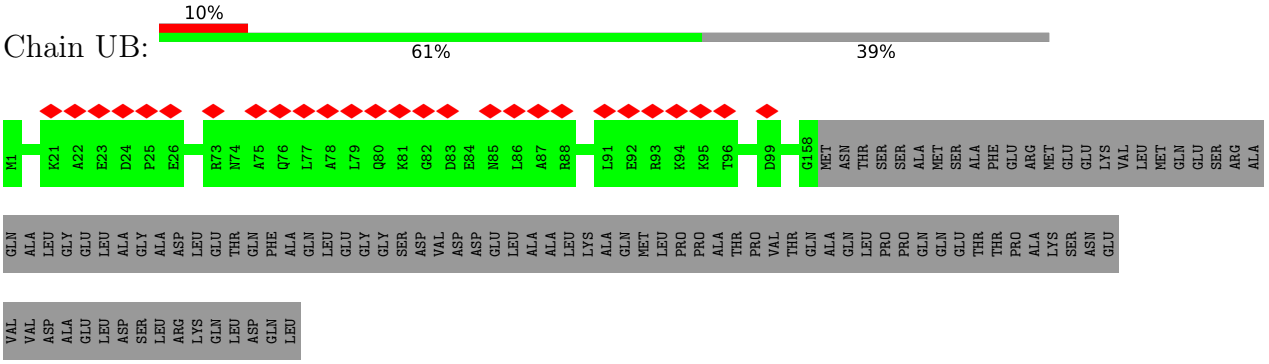
• Molecule 1: Vipp1

Chain TB:



• Molecule 1: Vipp1

Chain UB:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0178	Depositor
Map size (Å)	467.04, 467.04, 467.04	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.18	0/660	0.36	0/920
1	AA	0.19	0/1085	0.40	0/1512
1	AB	0.19	0/1085	0.40	0/1512
1	B	0.19	0/1085	0.40	0/1512
1	BA	0.19	0/1085	0.41	0/1512
1	BB	0.19	0/1080	0.42	0/1505
1	C	0.19	0/1085	0.41	0/1512
1	CA	0.19	0/1085	0.40	0/1512
1	CB	0.18	0/784	0.37	0/1093
1	D	0.19	0/1085	0.40	0/1512
1	DA	0.19	0/1080	0.42	0/1505
1	DB	0.18	0/660	0.36	0/920
1	E	0.19	0/1080	0.42	0/1505
1	EA	0.18	0/784	0.37	0/1093
1	EB	0.19	0/1085	0.40	0/1512
1	F	0.18	0/784	0.37	0/1093
1	FA	0.18	0/660	0.36	0/920
1	FB	0.19	0/1085	0.41	0/1512
1	G	0.18	0/660	0.36	0/920
1	GA	0.19	0/1085	0.40	0/1512
1	GB	0.19	0/1085	0.40	0/1512
1	H	0.19	0/1085	0.40	0/1512
1	HA	0.19	0/1085	0.41	0/1512
1	HB	0.19	0/1080	0.42	0/1505
1	I	0.19	0/1085	0.41	0/1512
1	IA	0.19	0/1085	0.40	0/1512
1	IB	0.18	0/784	0.37	0/1093
1	J	0.19	0/1085	0.40	0/1512
1	JA	0.19	0/1080	0.42	0/1505
1	JB	0.18	0/660	0.36	0/920
1	K	0.19	0/1080	0.42	0/1505
1	KA	0.18	0/784	0.37	0/1093
1	KB	0.19	0/1085	0.40	0/1512
1	L	0.18	0/784	0.37	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	LA	0.18	0/660	0.36	0/920
1	LB	0.19	0/1085	0.41	0/1512
1	M	0.18	0/660	0.36	0/920
1	MA	0.19	0/1085	0.40	0/1512
1	MB	0.19	0/1085	0.40	0/1512
1	N	0.19	0/1085	0.40	0/1512
1	NA	0.19	0/1085	0.41	0/1512
1	NB	0.19	0/1080	0.42	0/1505
1	O	0.19	0/1085	0.41	0/1512
1	OA	0.19	0/1085	0.40	0/1512
1	OB	0.18	0/784	0.37	0/1093
1	P	0.18	0/1085	0.40	0/1512
1	PA	0.19	0/1080	0.42	0/1505
1	PB	0.18	0/660	0.36	0/920
1	Q	0.19	0/1080	0.42	0/1505
1	QA	0.18	0/784	0.37	0/1093
1	QB	0.19	0/1085	0.40	0/1512
1	R	0.18	0/784	0.37	0/1093
1	RA	0.18	0/660	0.36	0/920
1	RB	0.19	0/1085	0.41	0/1512
1	S	0.18	0/660	0.36	0/920
1	SA	0.19	0/1085	0.40	0/1512
1	SB	0.19	0/1085	0.40	0/1512
1	T	0.19	0/1085	0.40	0/1512
1	TA	0.19	0/1085	0.41	0/1512
1	TB	0.19	0/1080	0.42	0/1505
1	UA	0.19	0/1085	0.40	0/1512
1	UB	0.18	0/784	0.37	0/1093
1	V	0.19	0/1085	0.41	0/1512
1	VA	0.19	0/1080	0.42	0/1505
1	W	0.19	0/1085	0.40	0/1512
1	WA	0.18	0/784	0.37	0/1093
1	X	0.19	0/1080	0.42	0/1505
1	XA	0.18	0/660	0.36	0/920
1	Y	0.18	0/784	0.37	0/1093
1	YA	0.19	0/1085	0.40	0/1512
1	Z	0.18	0/660	0.36	0/920
1	ZA	0.19	0/1085	0.41	0/1512
All	All	0.19	0/69348	0.40	0/96648

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	661	0	320	0	0
1	AA	1086	0	531	3	0
1	AB	1086	0	531	4	0
1	B	1086	0	531	3	0
1	BA	1086	0	531	6	0
1	BB	1081	0	530	4	0
1	C	1086	0	531	6	0
1	CA	1086	0	531	4	0
1	CB	785	0	376	0	0
1	D	1086	0	531	4	0
1	DA	1081	0	530	5	0
1	DB	661	0	320	0	0
1	E	1081	0	530	5	0
1	EA	785	0	376	0	0
1	EB	1086	0	531	3	0
1	F	785	0	376	0	0
1	FA	661	0	320	0	0
1	FB	1086	0	531	6	0
1	G	661	0	320	0	0
1	GA	1086	0	531	3	0
1	GB	1086	0	531	4	0
1	H	1086	0	531	4	0
1	HA	1086	0	531	6	0
1	HB	1081	0	530	4	0
1	I	1086	0	531	6	0
1	IA	1086	0	531	4	0
1	IB	785	0	376	0	0
1	J	1086	0	531	4	0
1	JA	1081	0	530	4	0
1	JB	661	0	320	0	0
1	K	1081	0	530	5	0
1	KA	785	0	376	0	0
1	KB	1086	0	531	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	785	0	376	0	0
1	LA	661	0	320	0	0
1	LB	1086	0	531	6	0
1	M	661	0	320	0	0
1	MA	1086	0	531	3	0
1	MB	1086	0	531	4	0
1	N	1086	0	531	3	0
1	NA	1086	0	531	6	0
1	NB	1081	0	530	5	0
1	O	1086	0	531	6	0
1	OA	1086	0	531	4	0
1	OB	785	0	376	0	0
1	P	1086	0	531	4	0
1	PA	1081	0	530	4	0
1	PB	661	0	320	0	0
1	Q	1081	0	530	5	0
1	QA	785	0	376	0	0
1	QB	1086	0	531	3	0
1	R	785	0	376	0	0
1	RA	661	0	320	0	0
1	RB	1086	0	531	6	0
1	S	661	0	320	0	0
1	SA	1086	0	531	3	0
1	SB	1086	0	531	4	0
1	T	1086	0	531	3	0
1	TA	1086	0	531	6	0
1	TB	1081	0	530	5	0
1	UA	1086	0	531	4	0
1	UB	785	0	376	0	0
1	V	1086	0	531	7	0
1	VA	1081	0	530	4	0
1	W	1086	0	531	4	0
1	WA	785	0	376	0	0
1	X	1081	0	530	5	0
1	XA	661	0	320	0	0
1	Y	785	0	376	0	0
1	YA	1086	0	531	3	0
1	Z	661	0	320	0	0
1	ZA	1086	0	531	6	0
All	All	69420	0	33828	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 128 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:52:ALA:HB1	1:BA:180:SER:CB	1.30	1.61
1:AA:52:ALA:HB1	1:NA:180:SER:CB	1.30	1.61
1:T:52:ALA:HB1	1:HA:180:SER:CB	1.30	1.61
1:GA:52:ALA:HB1	1:TA:180:SER:CB	1.30	1.61
1:MA:52:ALA:HB1	1:ZA:180:SER:CB	1.30	1.61

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/258 (51%)	131 (100%)	0	0	100	100
1	AA	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	AB	217/258 (84%)	217 (100%)	0	0	100	100
1	B	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	BA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	BB	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	C	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	CA	217/258 (84%)	217 (100%)	0	0	100	100
1	CB	156/258 (60%)	156 (100%)	0	0	100	100
1	D	217/258 (84%)	217 (100%)	0	0	100	100
1	DA	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	DB	131/258 (51%)	131 (100%)	0	0	100	100
1	E	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	EA	156/258 (60%)	156 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EB	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	F	156/258 (60%)	156 (100%)	0	0	100	100
1	FA	131/258 (51%)	131 (100%)	0	0	100	100
1	FB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	G	131/258 (51%)	131 (100%)	0	0	100	100
1	GA	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	GB	217/258 (84%)	217 (100%)	0	0	100	100
1	H	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	HA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	HB	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	I	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	IA	217/258 (84%)	217 (100%)	0	0	100	100
1	IB	156/258 (60%)	156 (100%)	0	0	100	100
1	J	217/258 (84%)	217 (100%)	0	0	100	100
1	JA	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	JB	131/258 (51%)	131 (100%)	0	0	100	100
1	K	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	KA	156/258 (60%)	156 (100%)	0	0	100	100
1	KB	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	L	156/258 (60%)	156 (100%)	0	0	100	100
1	LA	131/258 (51%)	131 (100%)	0	0	100	100
1	LB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	M	131/258 (51%)	131 (100%)	0	0	100	100
1	MA	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	MB	217/258 (84%)	217 (100%)	0	0	100	100
1	N	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	NA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	NB	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	O	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	OA	217/258 (84%)	217 (100%)	0	0	100	100
1	OB	156/258 (60%)	156 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	217/258 (84%)	217 (100%)	0	0	100	100
1	PA	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	PB	131/258 (51%)	131 (100%)	0	0	100	100
1	Q	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	QA	156/258 (60%)	156 (100%)	0	0	100	100
1	QB	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	R	156/258 (60%)	156 (100%)	0	0	100	100
1	RA	131/258 (51%)	131 (100%)	0	0	100	100
1	RB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	S	131/258 (51%)	131 (100%)	0	0	100	100
1	SA	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	SB	217/258 (84%)	217 (100%)	0	0	100	100
1	T	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	TA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	TB	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	UA	217/258 (84%)	217 (100%)	0	0	100	100
1	UB	156/258 (60%)	156 (100%)	0	0	100	100
1	V	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	VA	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	W	217/258 (84%)	217 (100%)	0	0	100	100
1	WA	156/258 (60%)	156 (100%)	0	0	100	100
1	X	216/258 (84%)	215 (100%)	0	1 (0%)	29	69
1	XA	131/258 (51%)	131 (100%)	0	0	100	100
1	Y	156/258 (60%)	156 (100%)	0	0	100	100
1	YA	217/258 (84%)	215 (99%)	2 (1%)	0	100	100
1	Z	131/258 (51%)	131 (100%)	0	0	100	100
1	ZA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
All	All	13848/18576 (74%)	13800 (100%)	36 (0%)	12 (0%)	54	86

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	160	ASN

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Mol	Chain	Res	Type
1	K	160	ASN
1	Q	160	ASN
1	X	160	ASN
1	DA	160	ASN

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

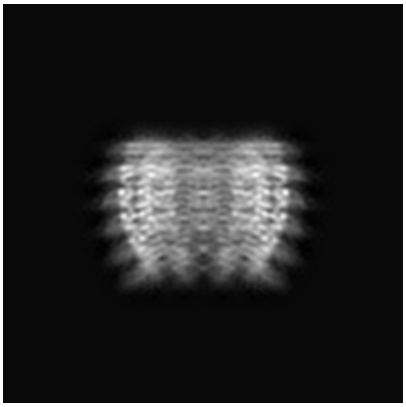
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11469. These allow visual inspection of the internal detail of the map and identification of artifacts.

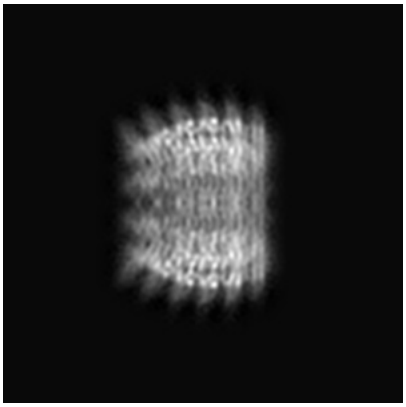
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 168

Y Index: 168

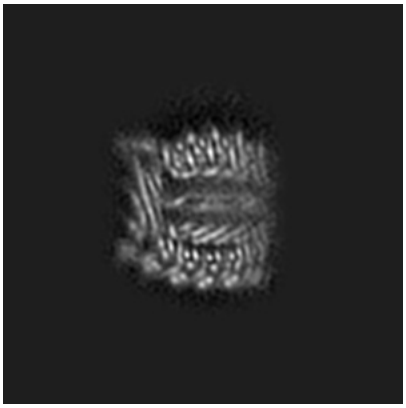
Z Index: 168

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 215



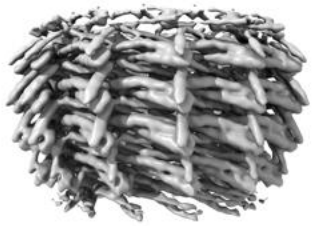
Y Index: 121

Z Index: 157

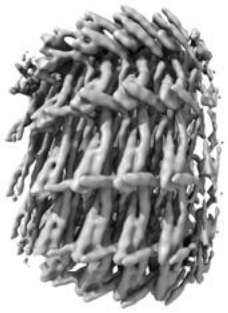
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0178. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

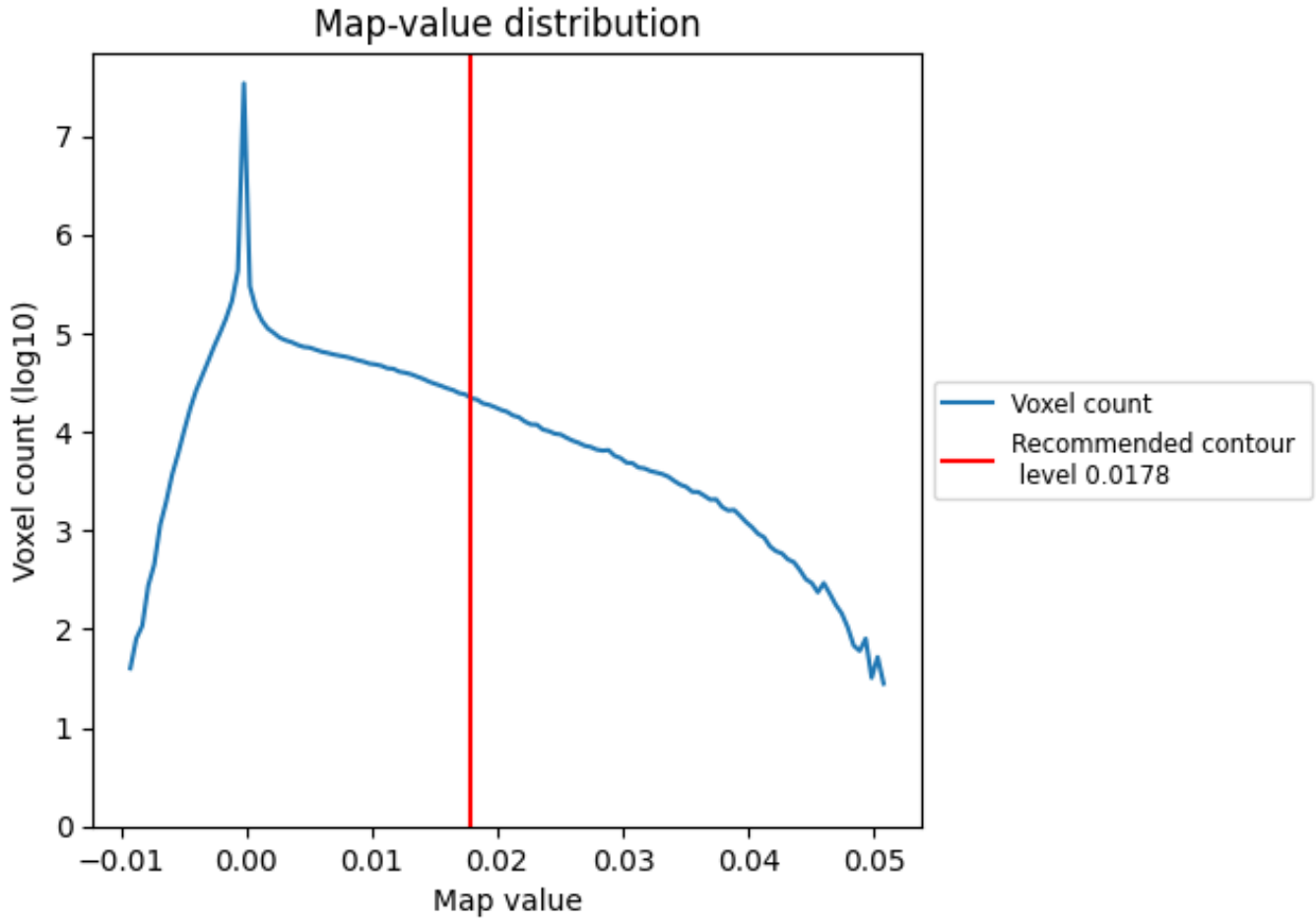
6.5 Mask visualisation (i)

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

7 Map analysis

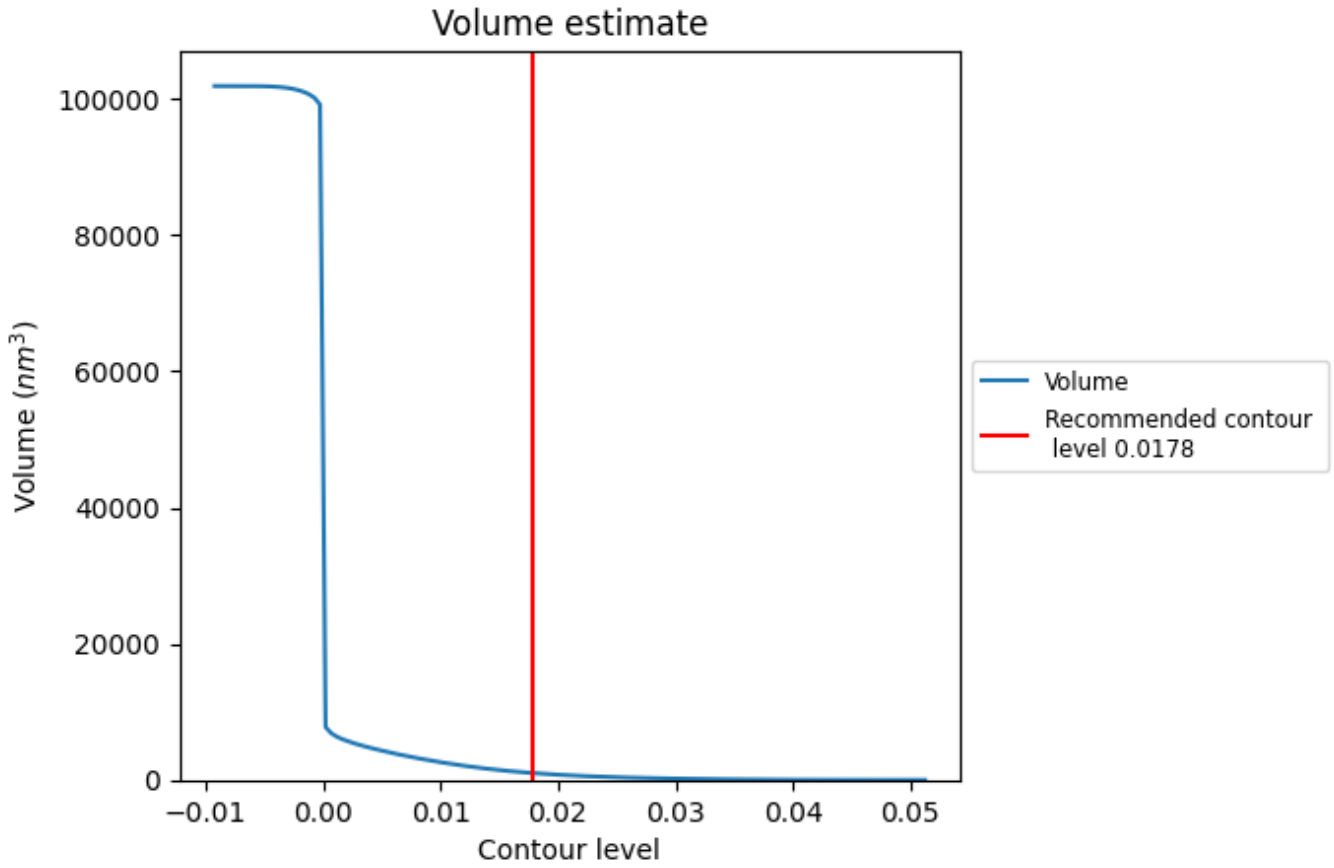
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

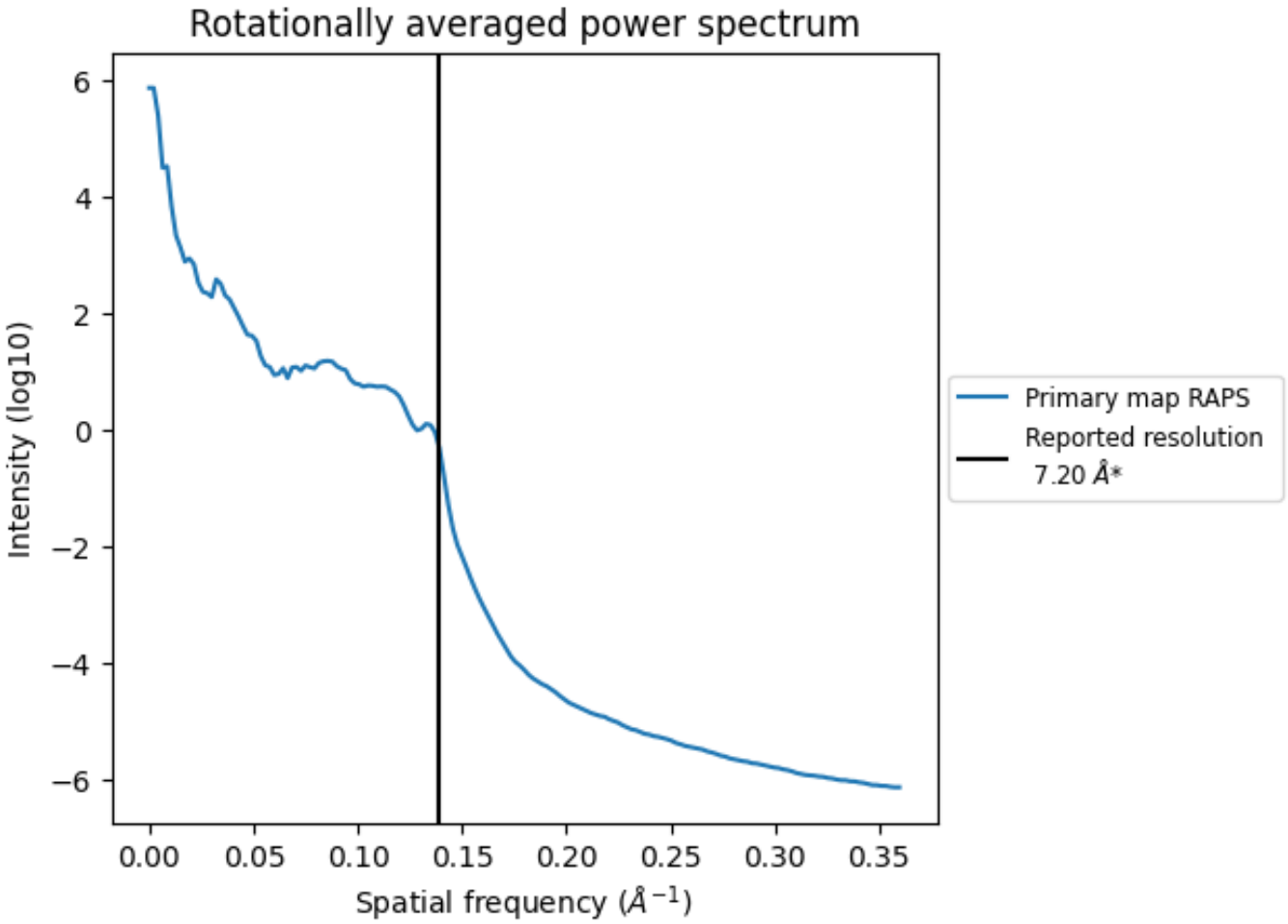
7.2 Volume estimate (i)



The volume at the recommended contour level is 1022 nm^3; this corresponds to an approximate mass of 923 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.139 Å^{-1}

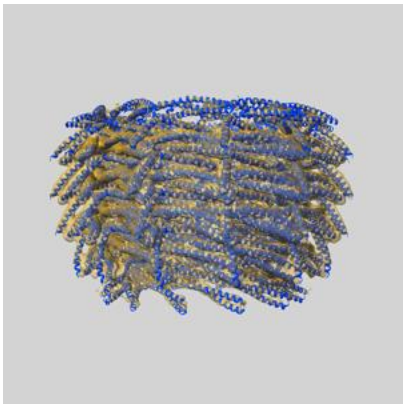
8 Fourier-Shell correlation (i)

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

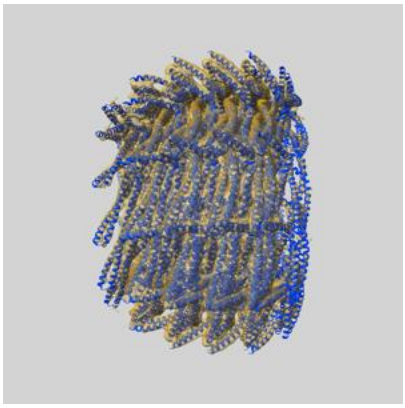
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11469 and PDB model 6ZVS. Per-residue inclusion information can be found in section 3 on page 10.

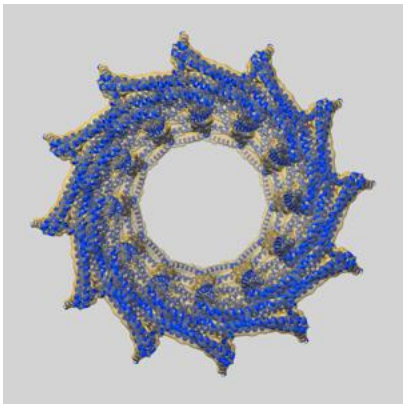
9.1 Map-model overlay



X



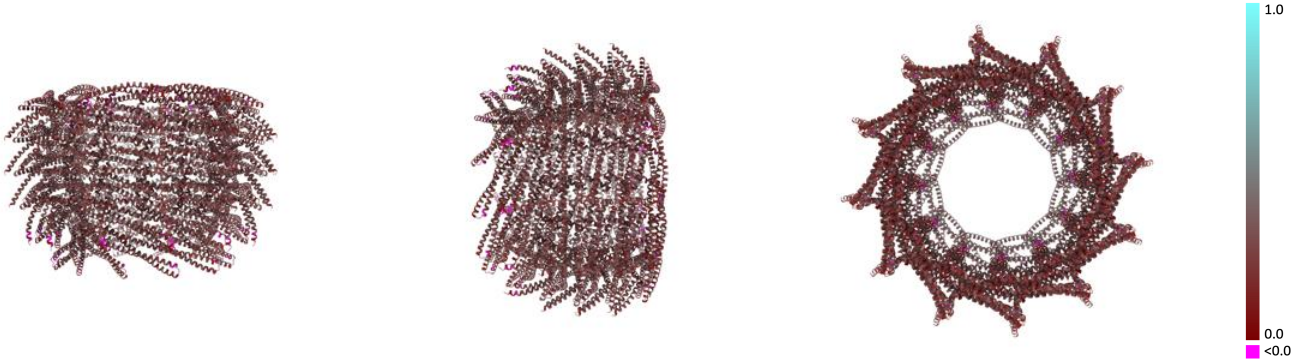
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0178 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.

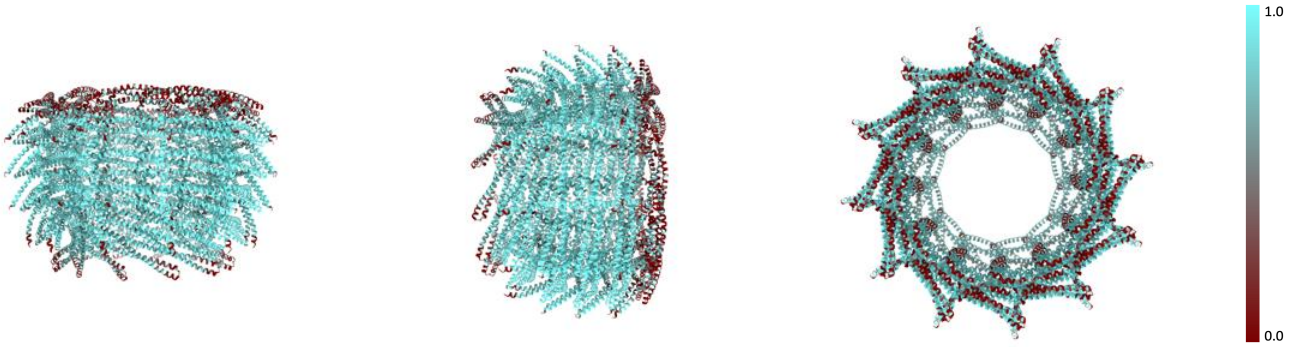
9.2 Q-score mapped to coordinate model



X Y Z

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

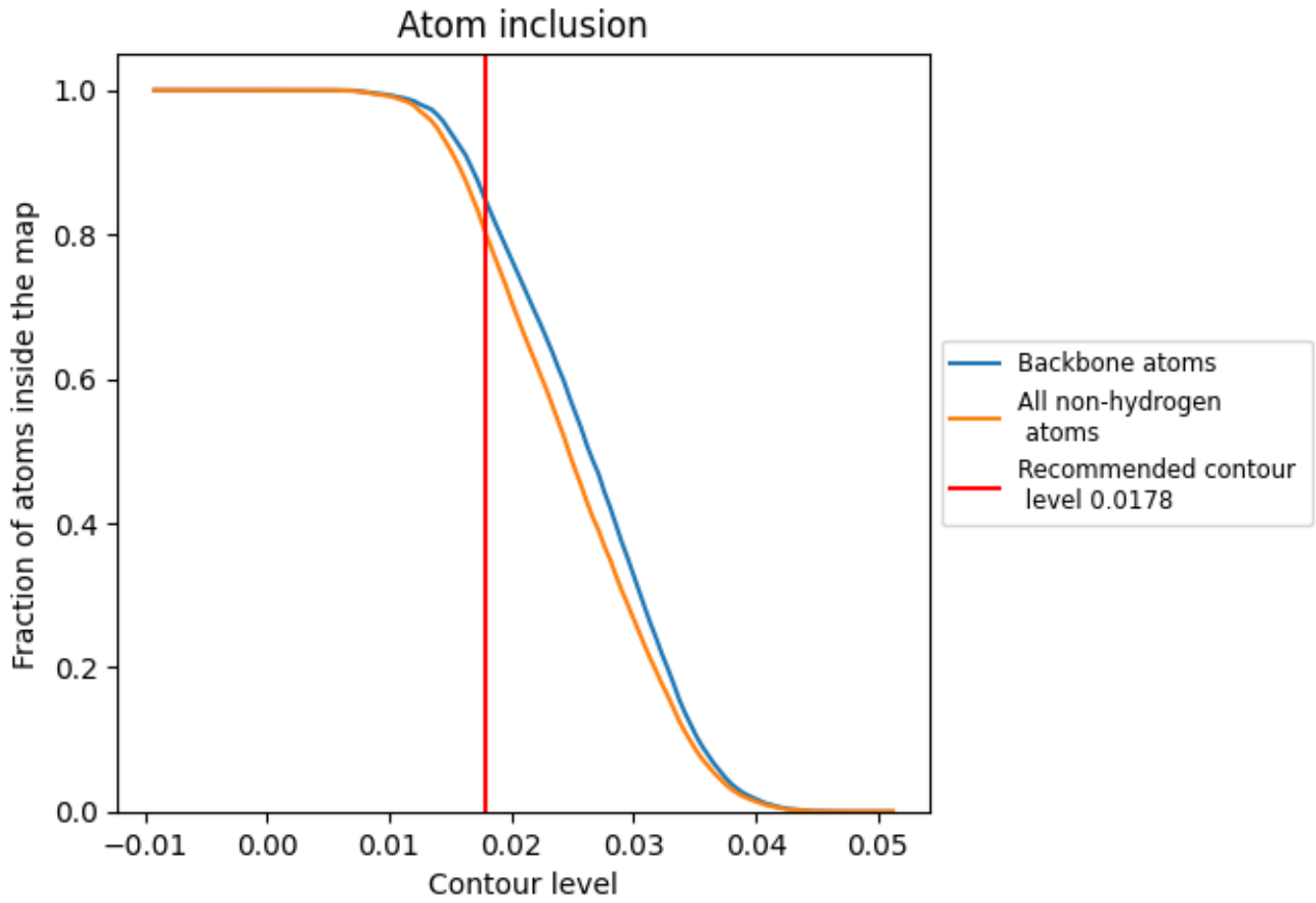
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0178).

9.4 Atom inclusion (i)



At the recommended contour level, 85% 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 (0.0178) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8057	0.2610
A	0.3268	0.2420
AA	0.7762	0.2490
AB	0.9558	0.2760
B	0.7781	0.2510
BA	0.9236	0.2680
BB	0.8992	0.2600
C	0.9227	0.2710
CA	0.9549	0.2740
CB	0.7478	0.2600
D	0.9576	0.2760
DA	0.9019	0.2580
DB	0.3268	0.2390
E	0.9029	0.2580
EA	0.7465	0.2580
EB	0.7781	0.2500
F	0.7465	0.2580
FA	0.3207	0.2410
FB	0.9227	0.2710
G	0.3222	0.2390
GA	0.7790	0.2520
GB	0.9576	0.2770
H	0.7762	0.2500
HA	0.9236	0.2730
HB	0.9029	0.2580
I	0.9245	0.2690
IA	0.9558	0.2770
IB	0.7465	0.2590
J	0.9558	0.2730
JA	0.8992	0.2610
JB	0.3238	0.2400
K	0.9019	0.2570
KA	0.7478	0.2600
KB	0.7762	0.2510
L	0.7452	0.2560

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Chain	Atom inclusion	Q-score
LA	0.3268	0.2400
LB	0.9245	0.2710
M	0.3238	0.2420
MA	0.7781	0.2510
MB	0.9558	0.2750
N	0.7790	0.2490
NA	0.9227	0.2710
NB	0.9019	0.2590
O	0.9236	0.2680
OA	0.9576	0.2780
OB	0.7452	0.2570
P	0.9558	0.2730
PA	0.9029	0.2600
PB	0.3222	0.2420
Q	0.8992	0.2590
QA	0.7465	0.2610
QB	0.7781	0.2520
R	0.7478	0.2580
RA	0.3238	0.2390
RB	0.9236	0.2710
S	0.3268	0.2410
SA	0.7762	0.2510
SB	0.9558	0.2740
T	0.7781	0.2490
TA	0.9245	0.2740
TB	0.8992	0.2580
UA	0.9558	0.2780
UB	0.7478	0.2580
V	0.9227	0.2690
VA	0.9019	0.2610
W	0.9576	0.2740
WA	0.7452	0.2600
X	0.9029	0.2580
XA	0.3222	0.2400
Y	0.7465	0.2600
YA	0.7790	0.2530
Z	0.3238	0.2390
ZA	0.9236	0.2720