Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 05:43 am BST

PDB ID	:	6ZVT
EMDB ID	:	EMD-11470
Title	:	C13 symmetry: Bacterial Vipp1 and PspA are members of the ancient ESCRT-III membrane-remodeling superfamily.
Authors	:	Liu, J.W.; 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	:	7.00 Å(reported)

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

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

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

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

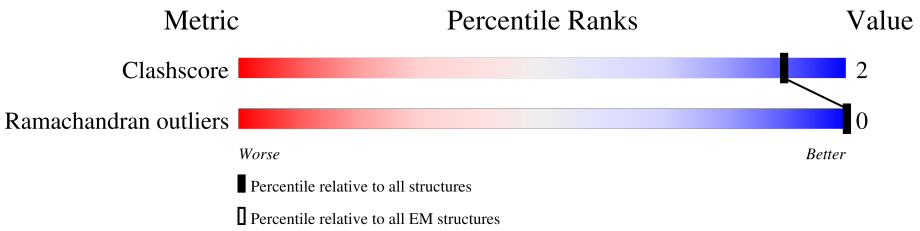
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 7.00 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	16% 52% 48%
1	AA	258	14% 84% 15%
1	AB	258	• 84% 15%
1	AC	258	18% 61% 39%
1	B	258	14% 84% 15%
1	BA	258	• 83% • 15%
1	BB	258	13% 84% 16%
1	C	258	• 83% • 15%
1	CA	258	• 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CB	258	18% 61% 39%
1	D	258	• 84% 15%
1	DA	258	12% 84% 16%
1	DB	258	16% 52% 48%
1	E	258	13% 84% 16%
1	EA	258	18% 61% 39%
1	EB	258	16% 84% 15%
1	F	258	18% 61% 39%
1	FA	258	16% 52% 48%
1	FB	258	• 83% • 15%
1	G	258	16% 52% 48%
1	GA	258	15% 84% 15%
1	GB	258	• 84% 15%
1	H	258	14% 84% 15%
1	HA	258	• 83% • 15%
1	HB	258	13% 84% 16%
1	I	258	• 83% • 15%
1	IA	258	• 84% 15%
1	IB	258	18% 61% 39%
1	J	258	5% 84% 15%
1	JA	258	13% 84% 16%
1	JB	258	15% 52% 48%
1	K	258	12% 84% 16%
1	KA	258	19% 61% 39%
1	KB	258	15% 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	L	258	18% 61% 39%
1	LA	258	16% 52% 48%
1	LB	258	83% 15%
1	M	258	15% 52% 48%
1	MA	258	15% 84% 15%
1	MB	258	5% 84% 15%
1	N	258	16% 84% 15%
1	NA	258	83% 15%
1	NB	258	12% 84% 16%
1	O	258	83% 15%
1	OA	258	84% 15%
1	OB	258	18% 61% 39%
1	P	258	5% 84% 15%
1	PA	258	12% 84% 16%
1	PB	258	15% 52% 48%
1	Q	258	13% 84% 16%
1	QA	258	18% 61% 39%
1	QB	258	16% 84% 15%
1	R	258	18% 61% 39%
1	RA	258	15% 52% 48%
1	RB	258	83% 15%
1	S	258	16% 52% 48%
1	SA	258	14% 84% 15%
1	SB	258	5% 84% 15%
1	T	258	15% 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	TA	258	83% · 15%
1	TB	258	13% 84% 16%
1	UA	258	84% 15%
1	UB	258	18% 61% 39%
1	V	258	83% · 15%
1	VA	258	12% 84% 16%
1	VB	258	16% 52% 48%
1	W	258	5% 84% 15%
1	WA	258	18% 61% 39%
1	WB	258	15% 84% 15%
1	X	258	12% 84% 16%
1	XA	258	15% 52% 48%
1	XB	258	83% · 15%
1	Y	258	18% 61% 39%
1	YA	258	16% 84% 15%
1	YB	258	84% 15%
1	Z	258	15% 52% 48%
1	ZA	258	83% · 15%
1	ZB	258	13% 84% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 75205 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
			Total	C	N	O		
1	A	133	661	395	133	133	0	0
1	B	219	1086	648	219	219	0	0
1	C	219	1086	648	219	219	0	0
1	D	219	1086	648	219	219	0	0
1	E	218	1081	645	218	218	0	0
1	F	158	785	469	158	158	0	0
1	G	133	661	395	133	133	0	0
1	H	219	1086	648	219	219	0	0
1	I	219	1086	648	219	219	0	0
1	J	219	1086	648	219	219	0	0
1	K	218	1081	645	218	218	0	0
1	L	158	785	469	158	158	0	0
1	M	133	661	395	133	133	0	0
1	N	219	1086	648	219	219	0	0
1	O	219	1086	648	219	219	0	0
1	P	219	1086	648	219	219	0	0
1	Q	218	1081	645	218	218	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

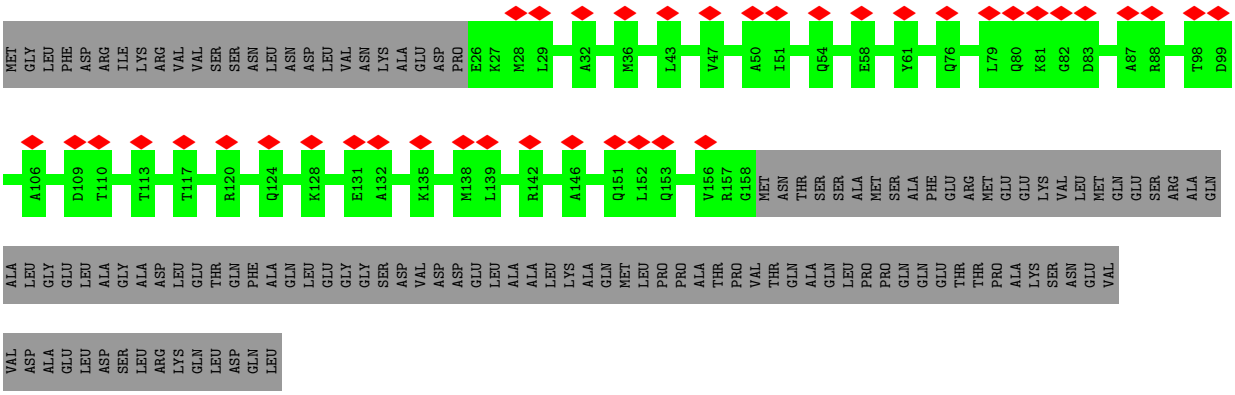
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	IB	158	785	469	158	158	0	0
1	JB	133	661	395	133	133	0	0
1	KB	219	1086	648	219	219	0	0
1	LB	219	1086	648	219	219	0	0
1	MB	219	1086	648	219	219	0	0
1	NB	218	1081	645	218	218	0	0
1	OB	158	785	469	158	158	0	0
1	PB	133	661	395	133	133	0	0
1	QB	219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

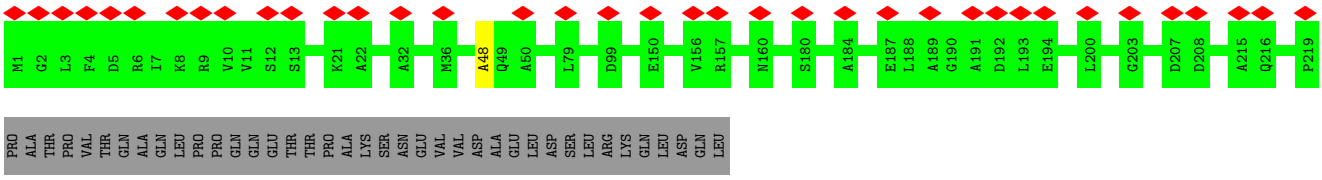
- Molecule 1: Vipp1

Chain A:



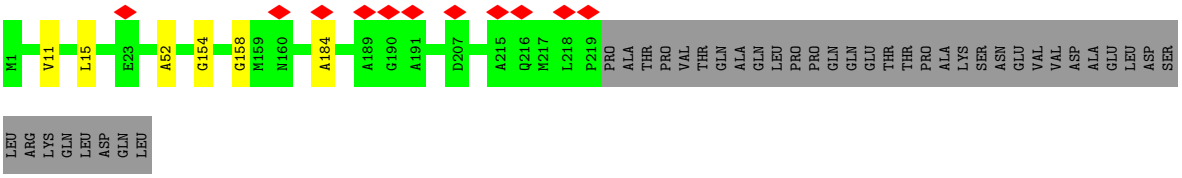
- Molecule 1: Vipp1

Chain B:



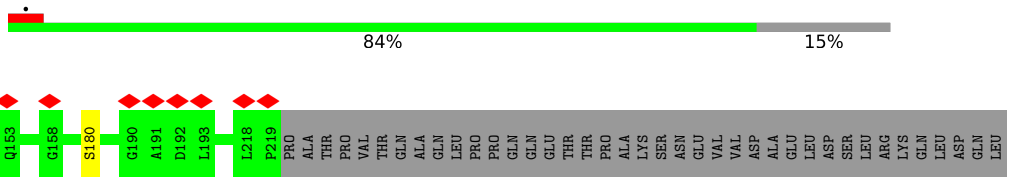
- Molecule 1: Vipp1

Chain C:



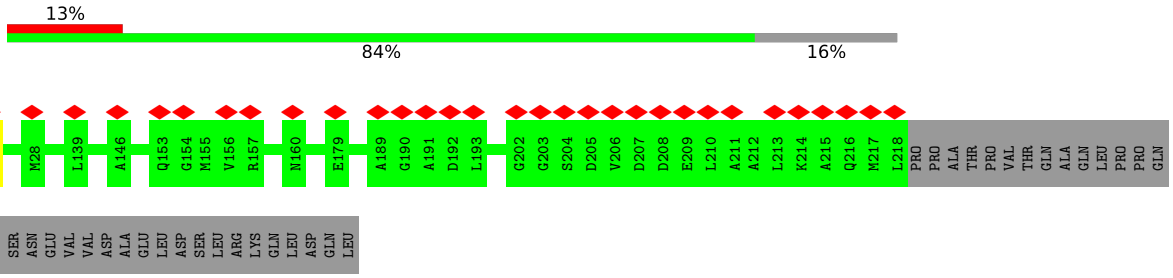
- Molecule 1: Vipp1

Chain D:



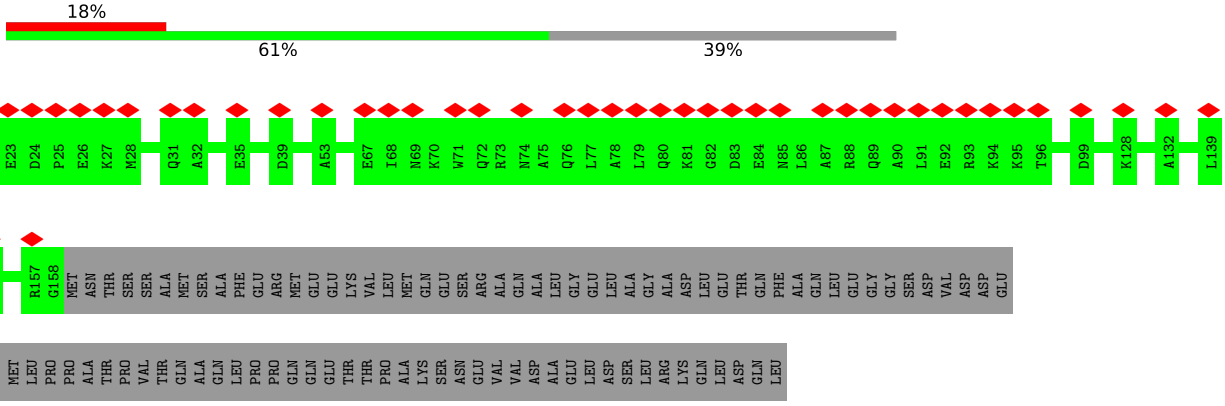
• Molecule 1: Vipp1

Chain E:



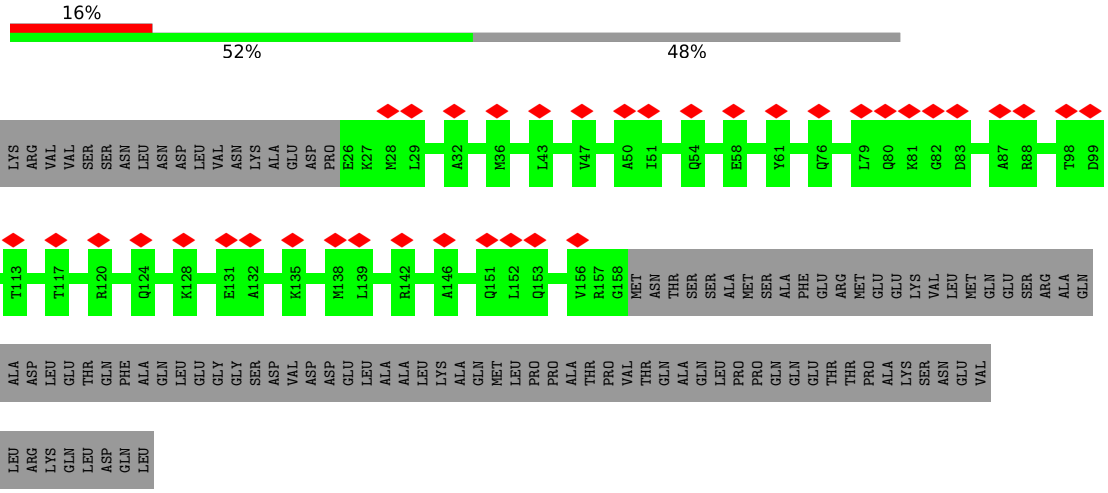
• Molecule 1: Vipp1

Chain F:



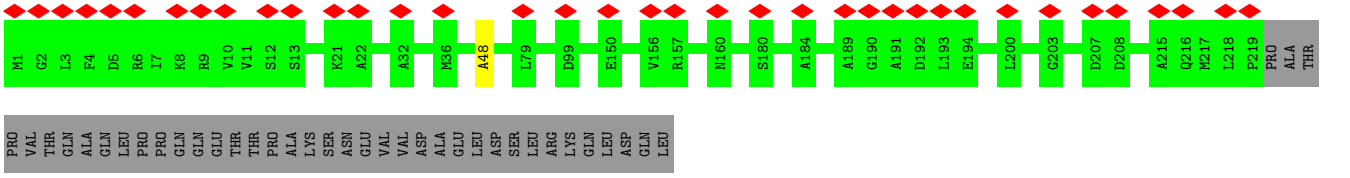
• Molecule 1: Vipp1

Chain G:



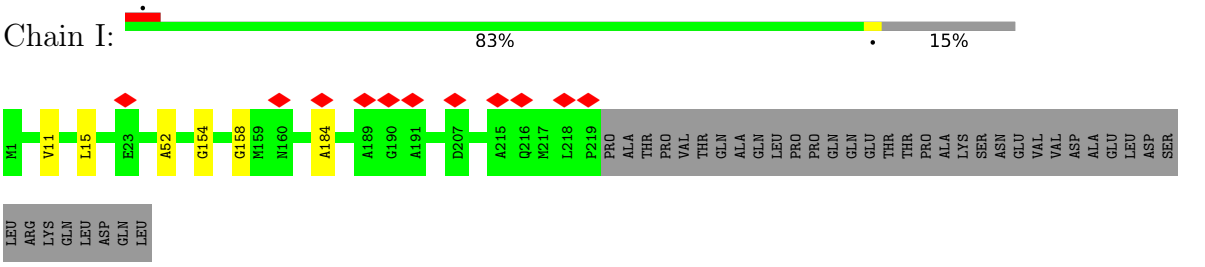
• Molecule 1: Vipp1

Chain H:



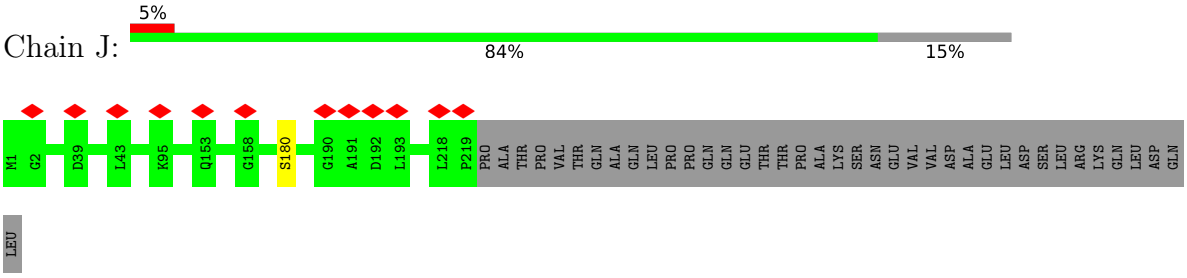
- Molecule 1: Vipp1

Chain I:



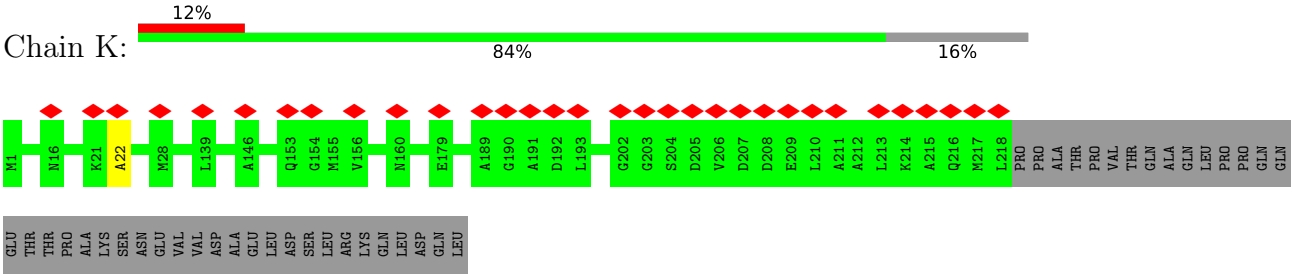
- Molecule 1: Vipp1

Chain J:



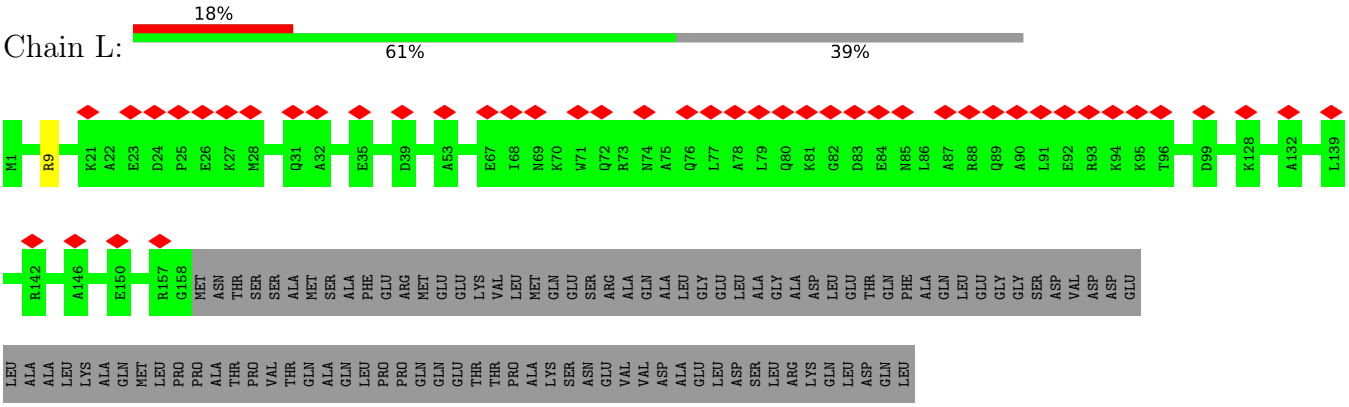
- Molecule 1: Vipp1

Chain K:



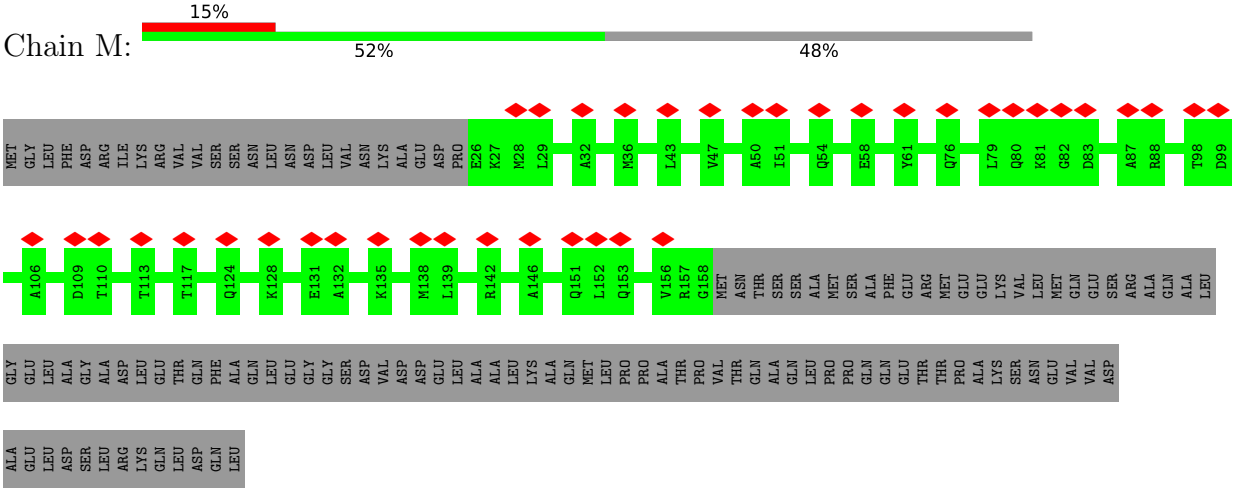
- Molecule 1: Vipp1

Chain L:



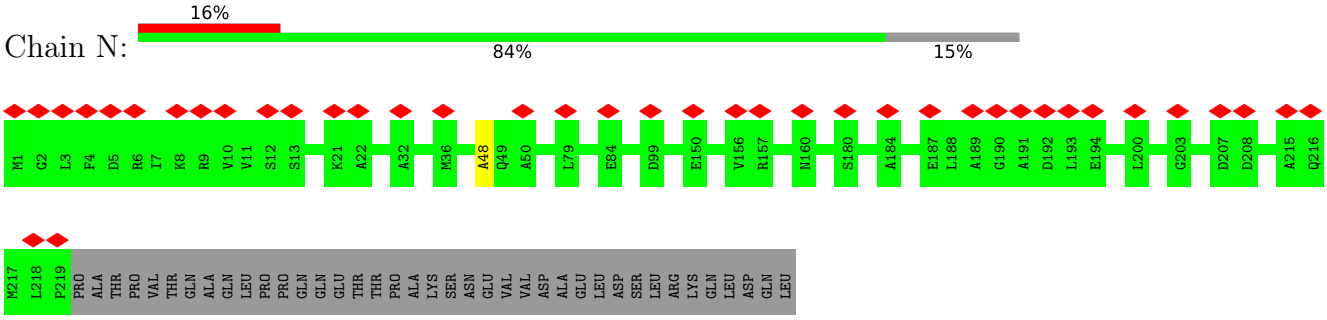
• Molecule 1: Vipp1

Chain M:



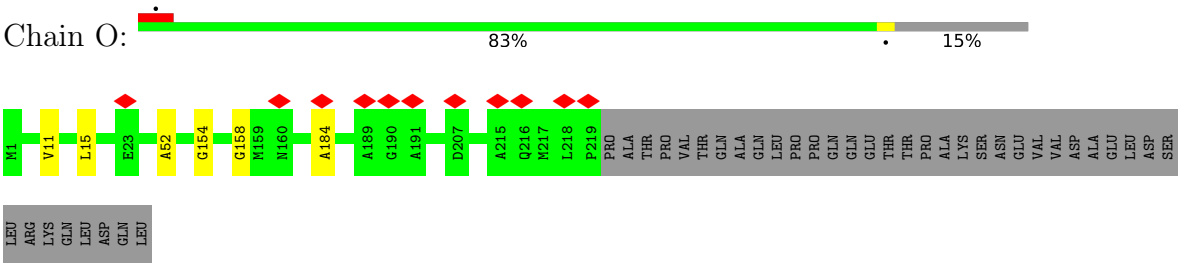
• Molecule 1: Vipp1

Chain N:



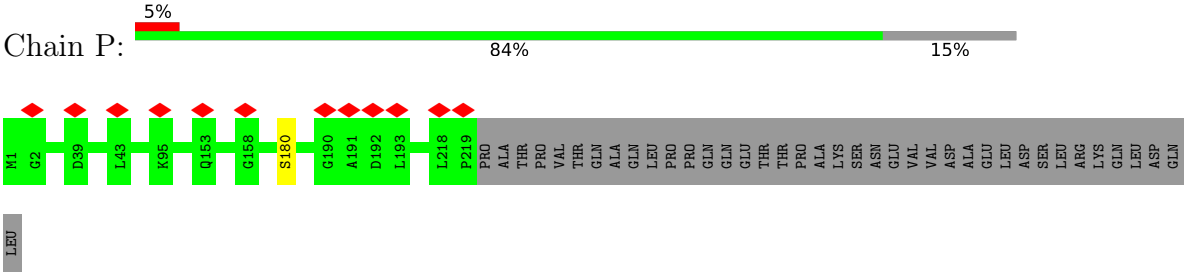
• Molecule 1: Vipp1

Chain O:



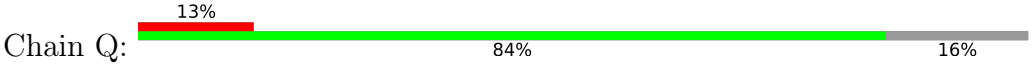
• Molecule 1: Vipp1

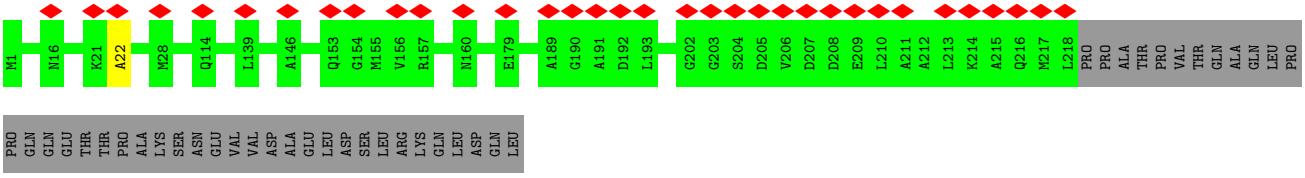
Chain P:



• Molecule 1: Vipp1

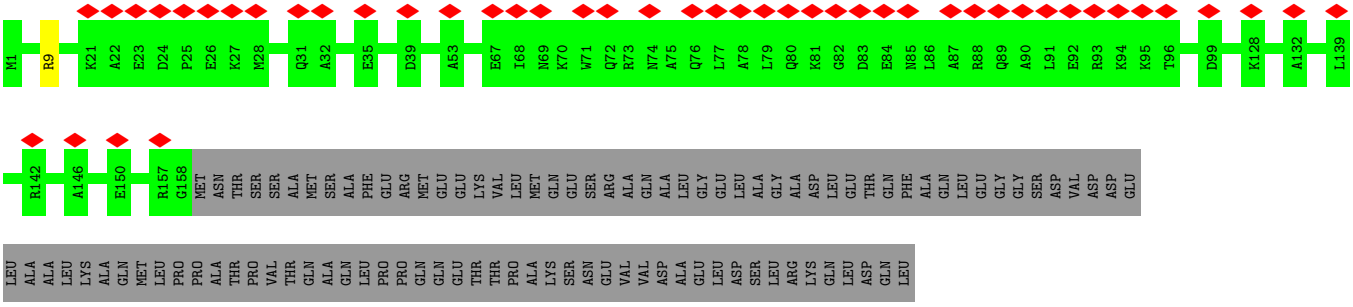
Chain Q:





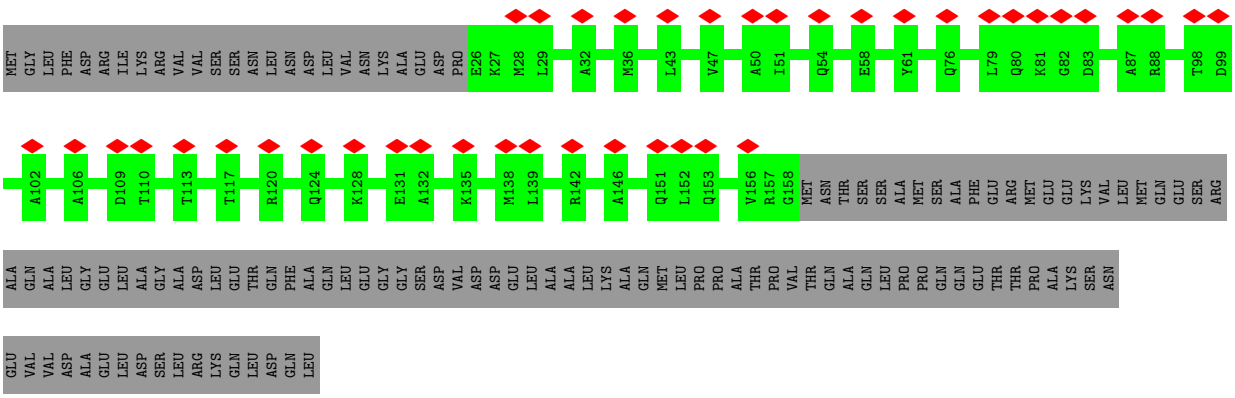
• Molecule 1: Vipp1

Chain R:



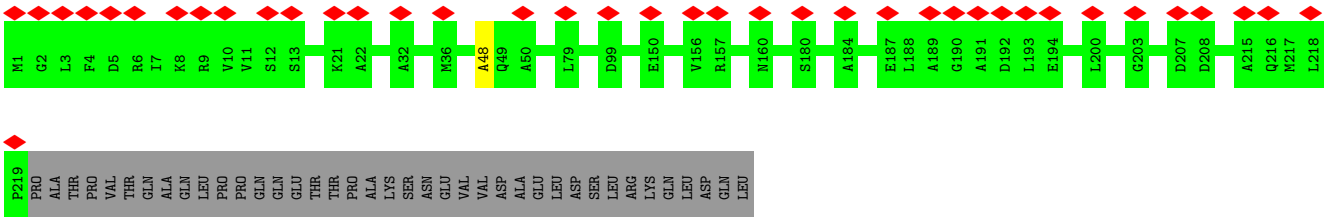
• Molecule 1: Vipp1

Chain S:



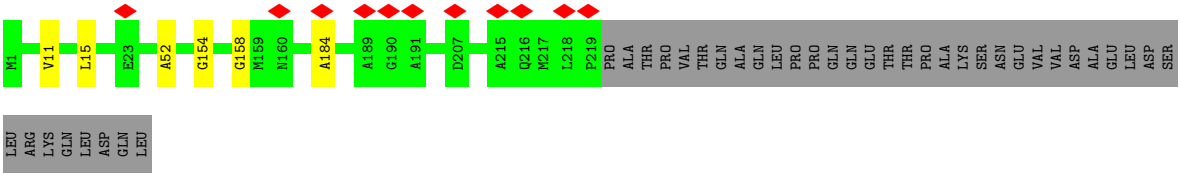
• Molecule 1: Vipp1

Chain T:



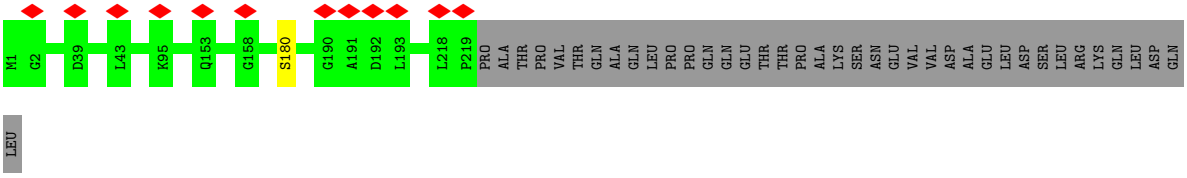
• Molecule 1: Vipp1

Chain V:



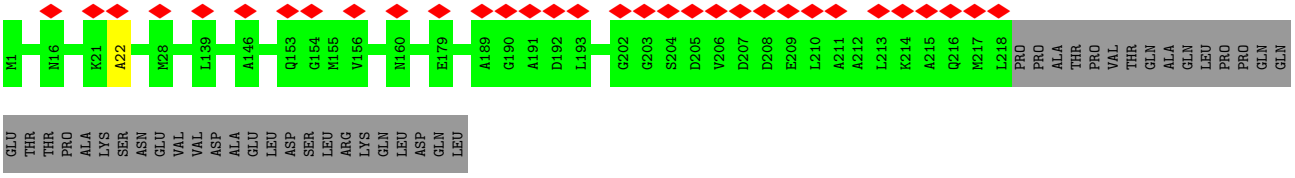
• Molecule 1: Vipp1

Chain W:



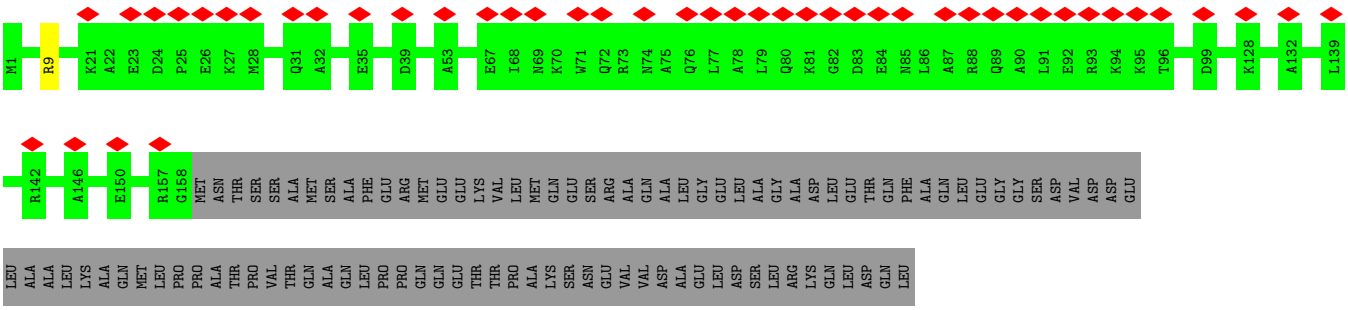
• Molecule 1: Vipp1

Chain X:



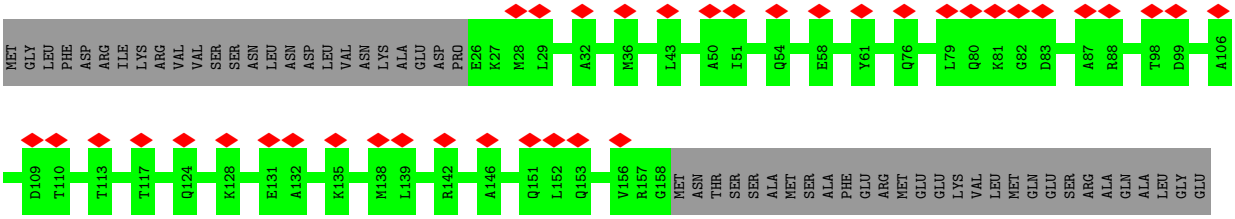
• Molecule 1: Vipp1

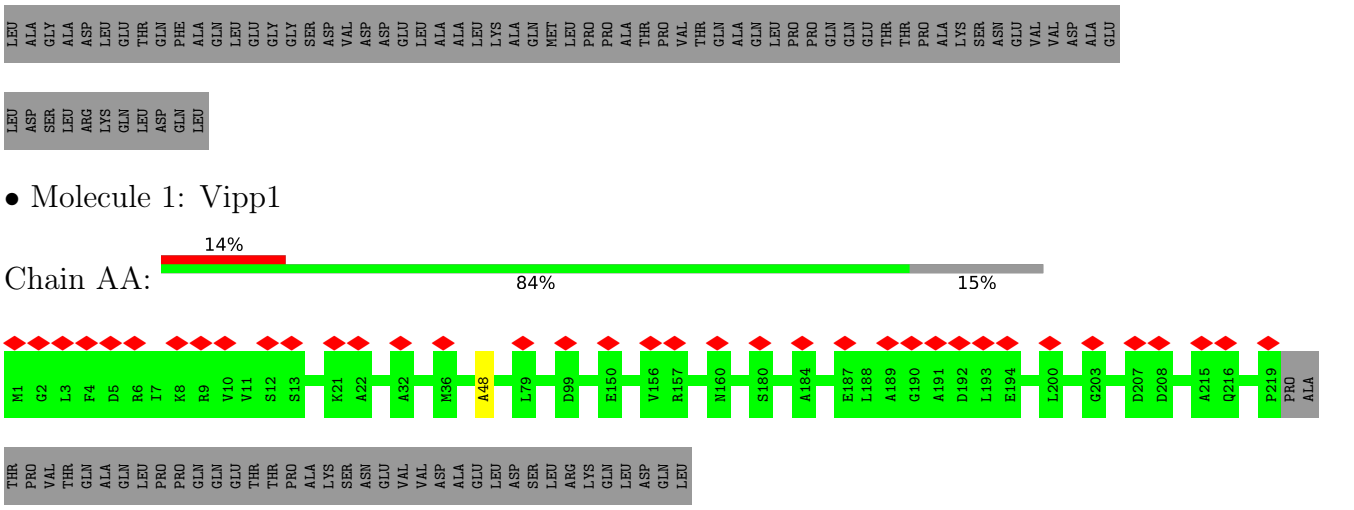
Chain Y:

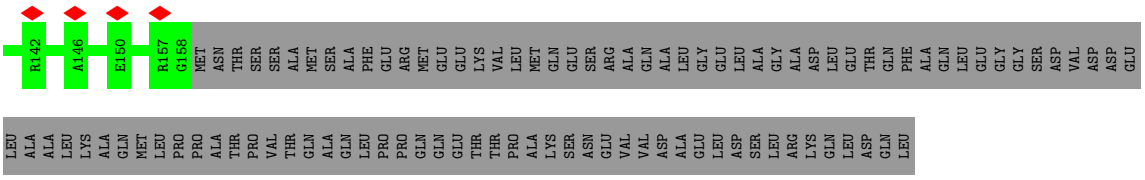


• Molecule 1: Vipp1

Chain Z:

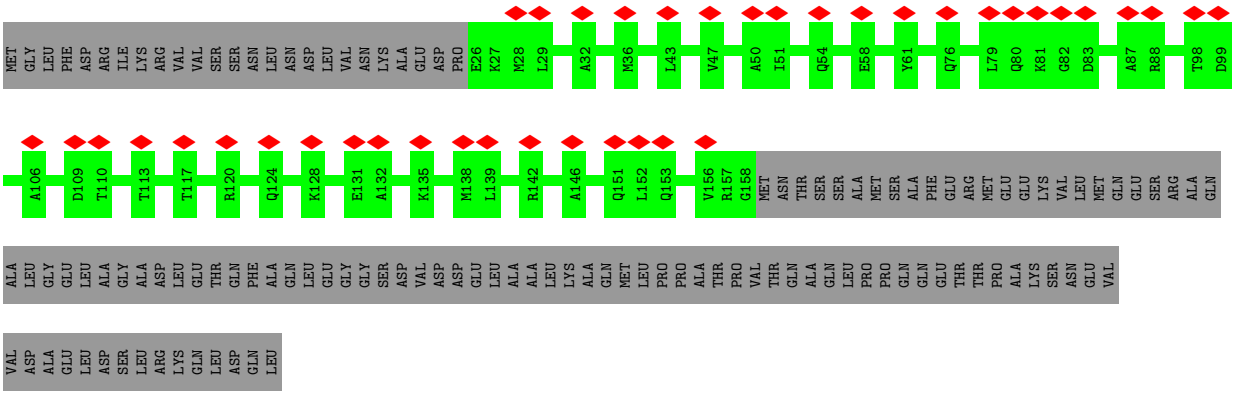



LEU ALA GLY ALA ASP LEU GLU THR GLN PHE ALA GLN LEU GLU GLY GLY SER ASP VAL ASP ASP GLU LEU ALA ALA LEU LYS ALA GLN MET LEU PRO PRO ALA THR PRO VAL THR GLN ALA GLN LEU PRO PRO GLN GLN GLU THR THR PRO ALA LYS SER ASN GLU VAL VAL ASP ALA GLU
LEU ASP SER LEU ARG LYS GLN LEU ASP GLN LEU
• Molecule 1: Vipp1
Chain AA:
14%
84%
15%
M1 G2 L3 F4 D5 R6 I7 K8 R9 V10 V11 S12 S13 K21 A22 A32 M36 A48 L79 D99 E150 V156 R157 N160 S180 A184 E187 L188 A189 G190 A191 D192 L193 E194 L200 G203 D207 D208 A215 Q216 P219 PRO ALA
THR PRO VAL THR GLN ALA GLN LEU PRO PRO GLN GLN GLU THR THR PRO ALA LYS SER ASN GLU VAL VAL ASP ALA GLU LEU ASP SER LEU ARG LYS GLN LEU ASP GLN LEU
• Molecule 1: Vipp1
Chain BA:
83%
15%
M1 V11 L15 E23 A52 G154 G158 M159 N160 A184 A189 G190 A191 D207 A215 Q216 M217 L218 P219 PRO ALA THR PRO VAL THR GLN ALA GLN LEU PRO PRO GLN GLN GLU THR THR PRO ALA LYS SER ASN GLU VAL VAL ASP ALA GLU LEU ASP SER
LEU ARG LYS GLN LEU ASP GLN LEU
• Molecule 1: Vipp1
Chain CA:
84%
15%
M1 D39 L43 K95 Q153 G158 S180 G190 A191 D192 L193 L218 P219 PRO ALA THR PRO VAL THR GLN ALA GLN LEU PRO PRO GLN GLN GLU THR THR PRO ALA LYS SER ASN GLU VAL VAL ASP ALA GLU LEU ASP SER LEU ARG LYS GLN LEU ASP GLN LEU
• Molecule 1: Vipp1
Chain DA:
12%
84%
16%
M1 N16 K21 A22 M28 L139 A146 Q153 G154 M155 V156 N160 E179 A189 G190 A191 D192 L193 G202 G203 S204 D205 V206 D207 D208 E209 L210 A211 A212 L213 K214 A215 Q216 M217 L218 PRO PRO ALA THR PRO VAL THR GLN ALA GLN LEU PRO PRO GLN GLN
GLU THR THR PRO ALA LYS SER ASN GLU VAL VAL ASP ALA GLU LEU ASP SER LEU ARG LYS GLN LEU ASP GLN LEU
• Molecule 1: Vipp1
Chain EA:
18%
61%
39%
M1 R9 K21 A22 E23 D24 P25 E26 K27 M28 Q31 A32 E35 D39 A53 E67 I68 N69 K70 W71 Q72 R73 N74 A75 Q76 L77 A78 L79 Q80 K81 G82 D83 E84 N85 L86 A87 R88 Q89 A90 L91 E92 R93 K94 K95 T96 D99 K128 A132 L139



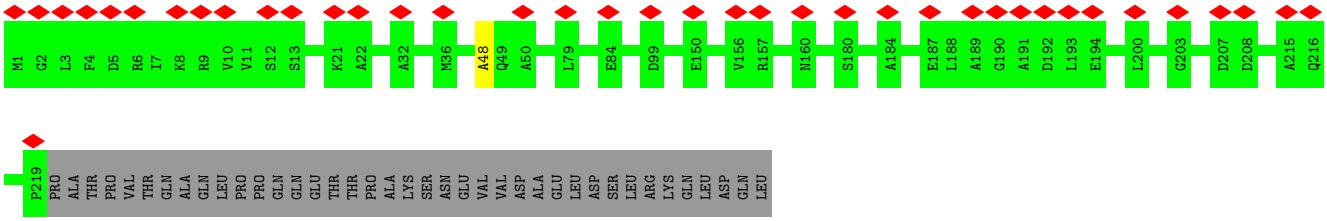
• Molecule 1: Vipp1

Chain FA:



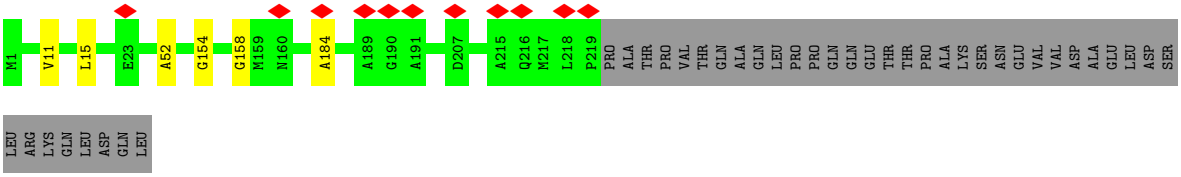
• Molecule 1: Vipp1

Chain GA:



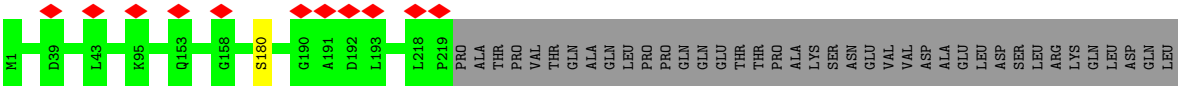
• Molecule 1: Vipp1

Chain HA:



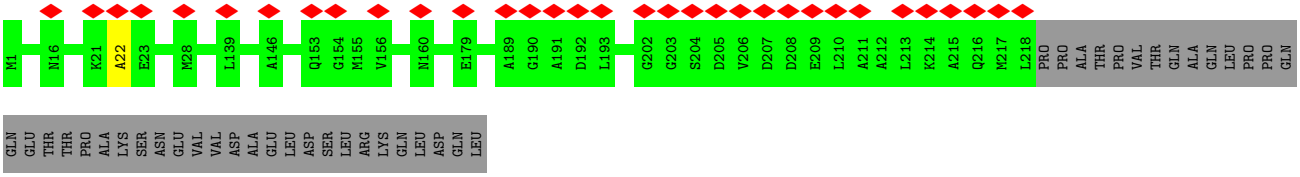
• Molecule 1: Vipp1

Chain IA:



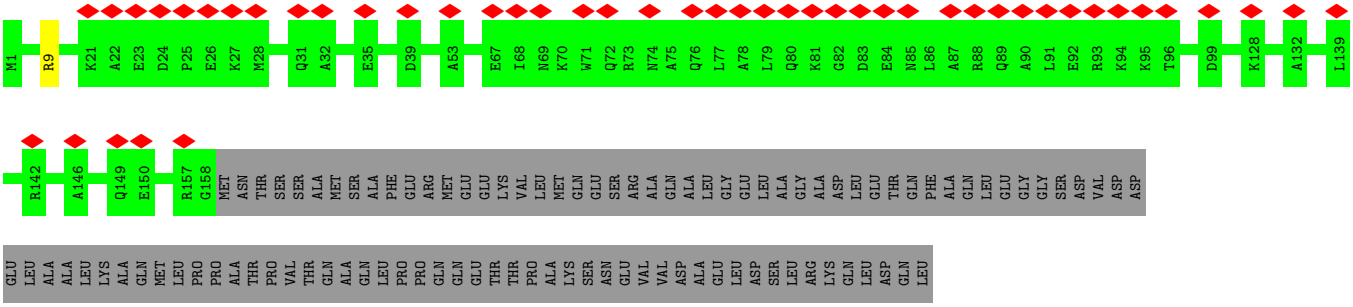
- Molecule 1: Vipp1

Chain JA:



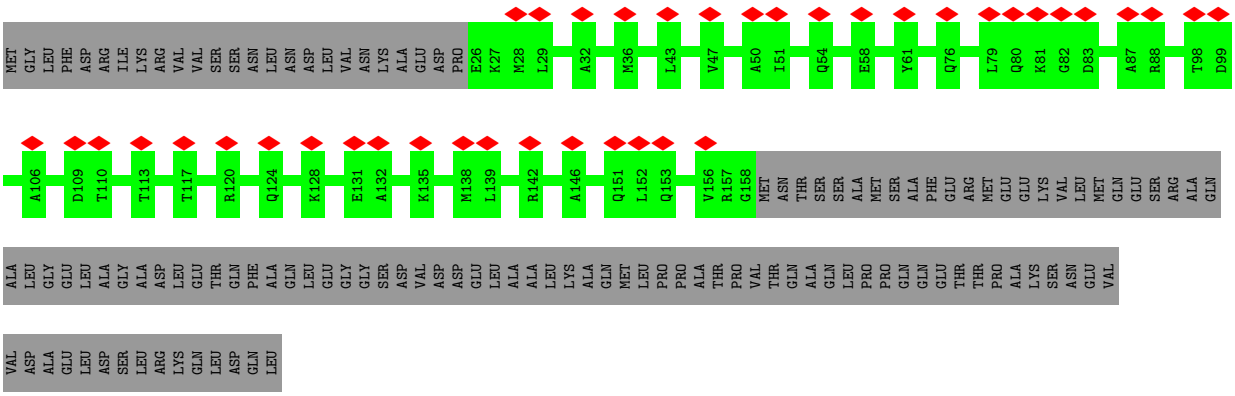
- Molecule 1: Vipp1

Chain KA:



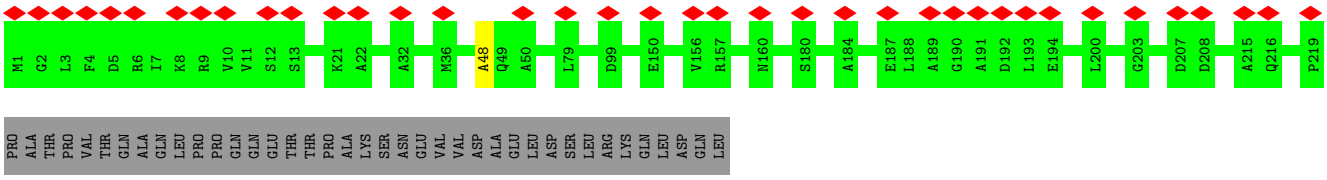
- Molecule 1: Vipp1

Chain LA:



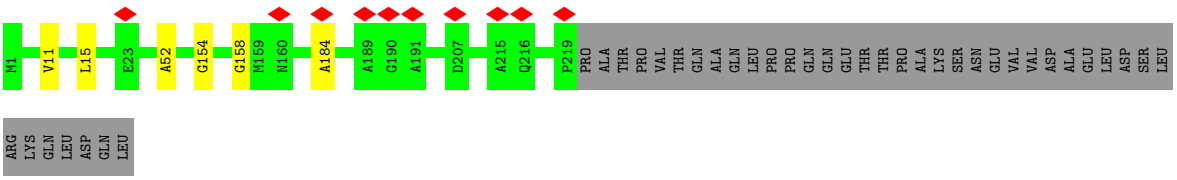
- Molecule 1: Vipp1

Chain MA:



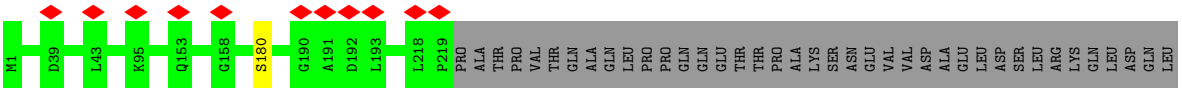
- Molecule 1: Vipp1

Chain NA:



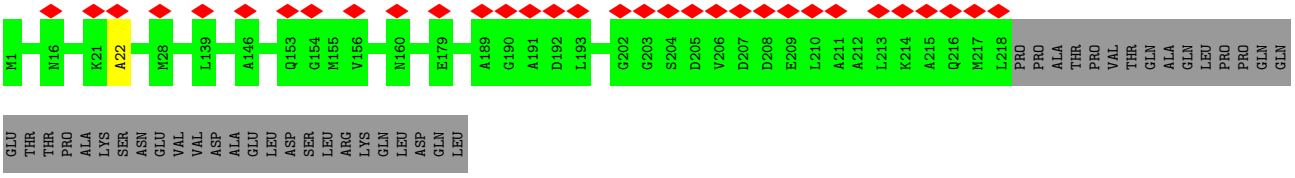
- Molecule 1: Vipp1

Chain OA:



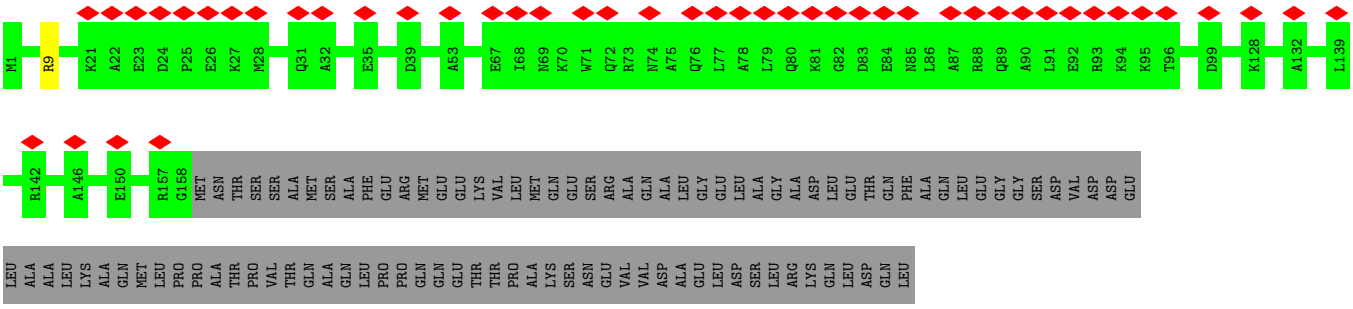
- Molecule 1: Vipp1

Chain PA:



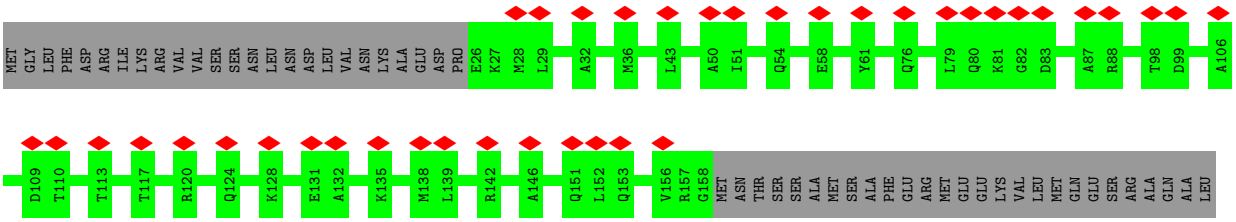
- Molecule 1: Vipp1

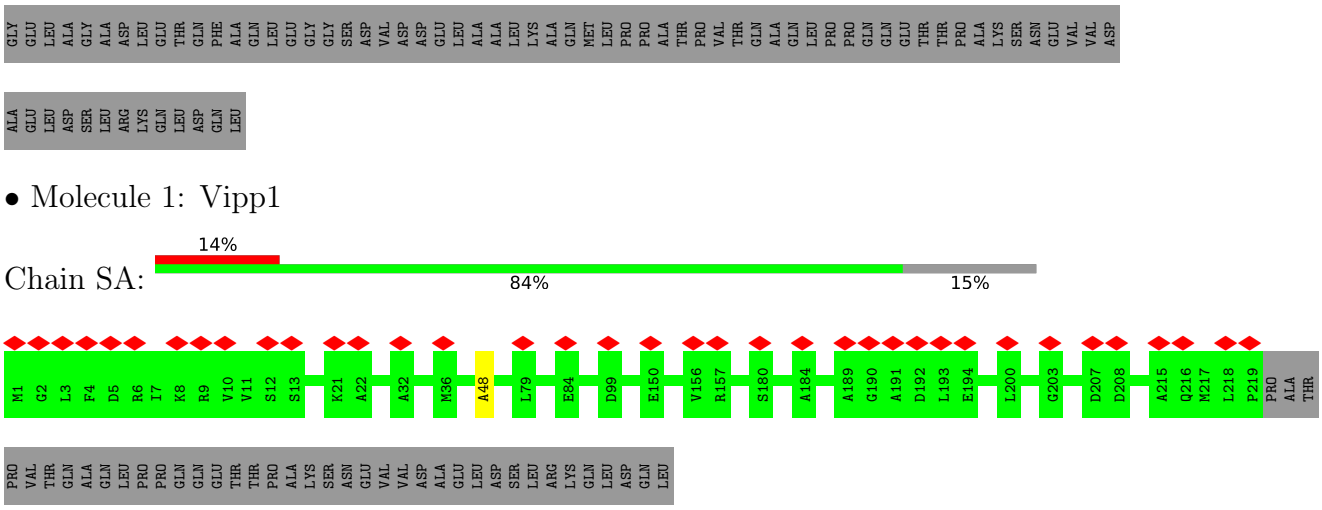
Chain QA:



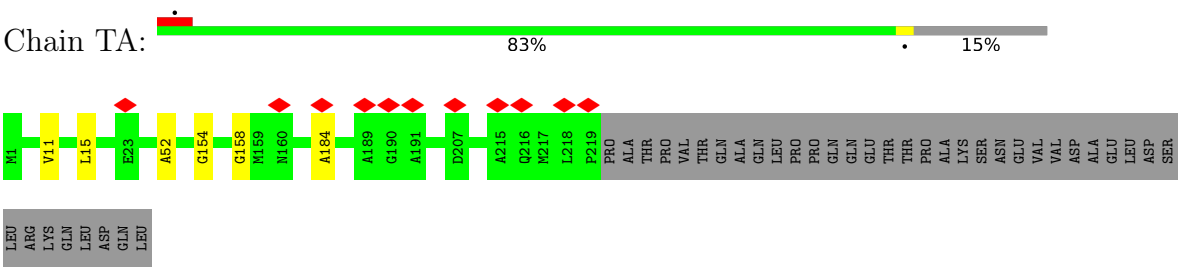
- Molecule 1: Vipp1

Chain RA:

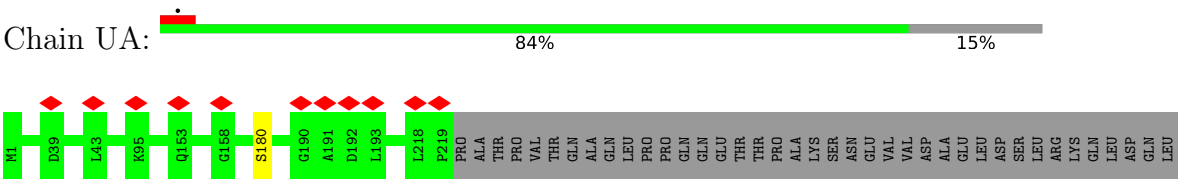




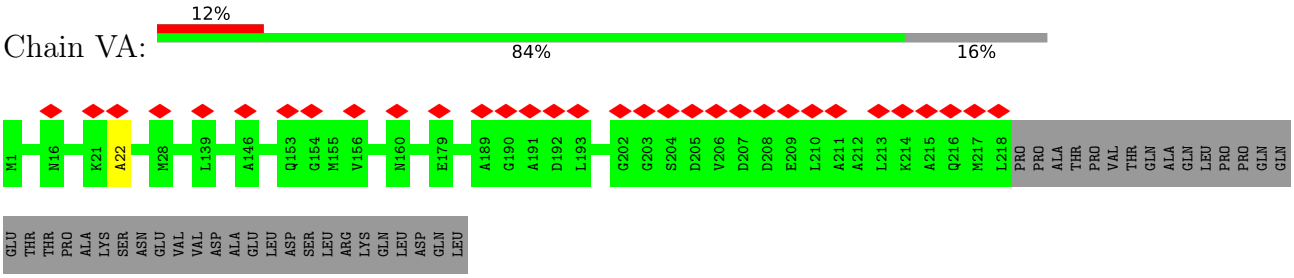
• Molecule 1: Vipp1



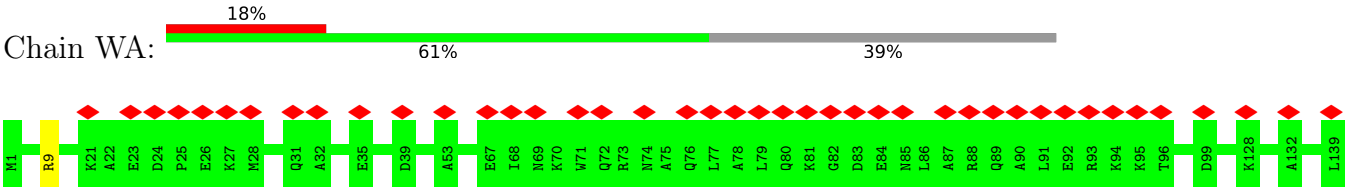
• Molecule 1: Vipp1

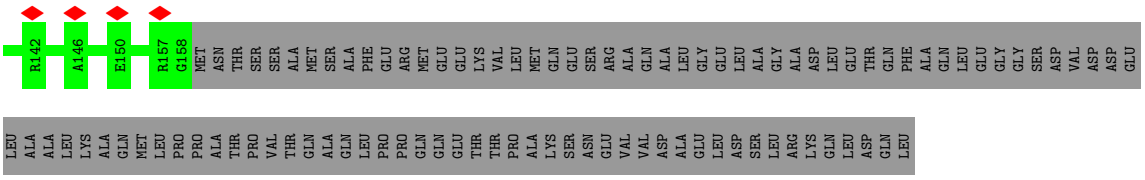


• Molecule 1: Vipp1



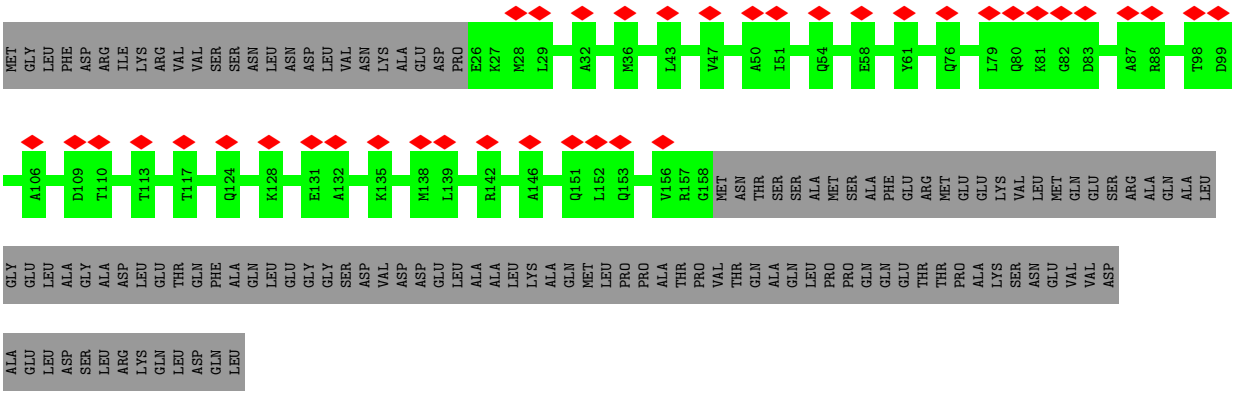
• Molecule 1: Vipp1





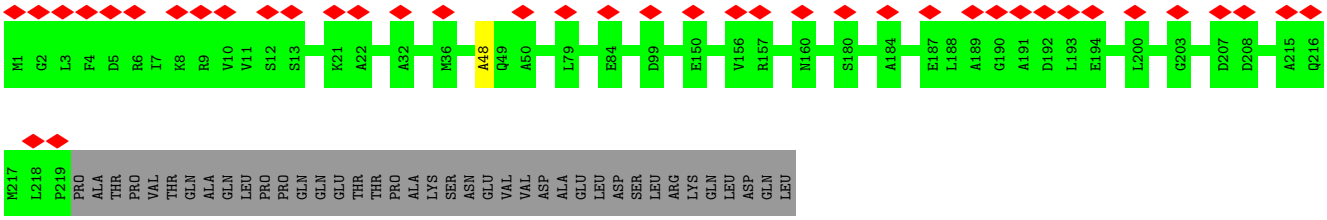
• Molecule 1: Vipp1

Chain XA:



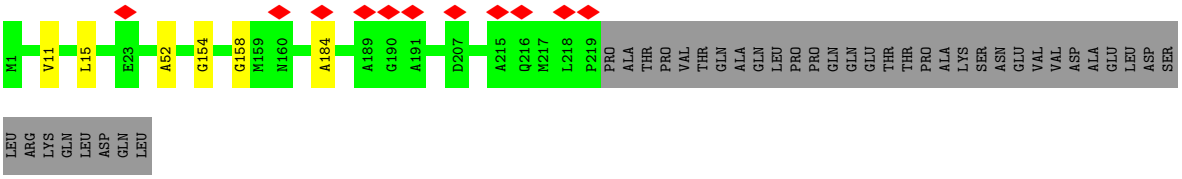
• Molecule 1: Vipp1

Chain YA:



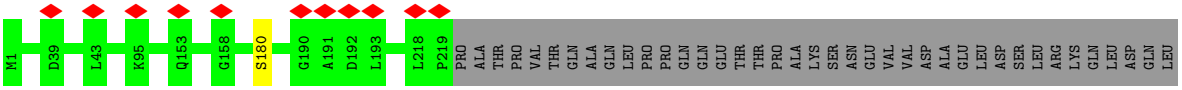
• Molecule 1: Vipp1

Chain ZA:



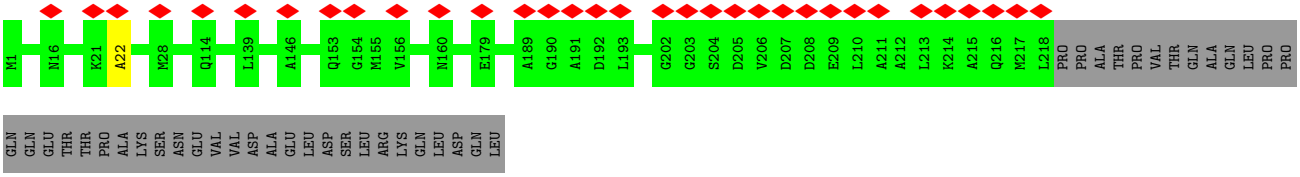
• Molecule 1: Vipp1

Chain AB:



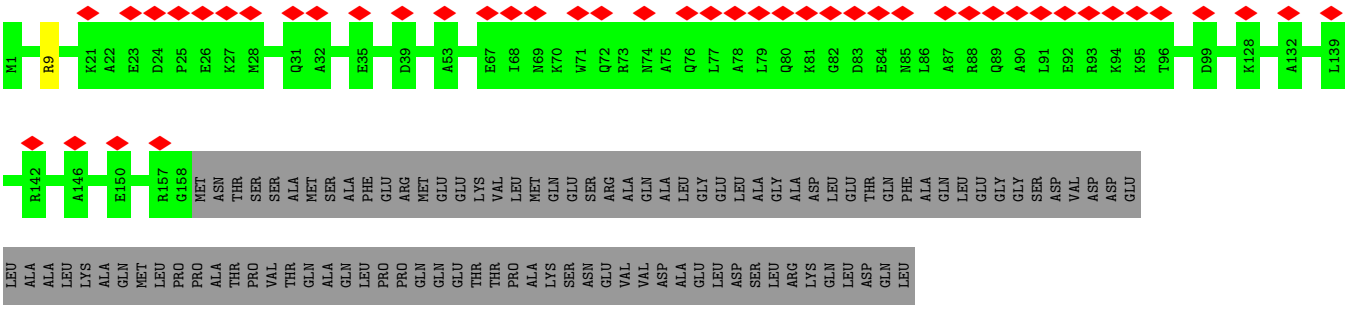
- Molecule 1: Vipp1

Chain BB:



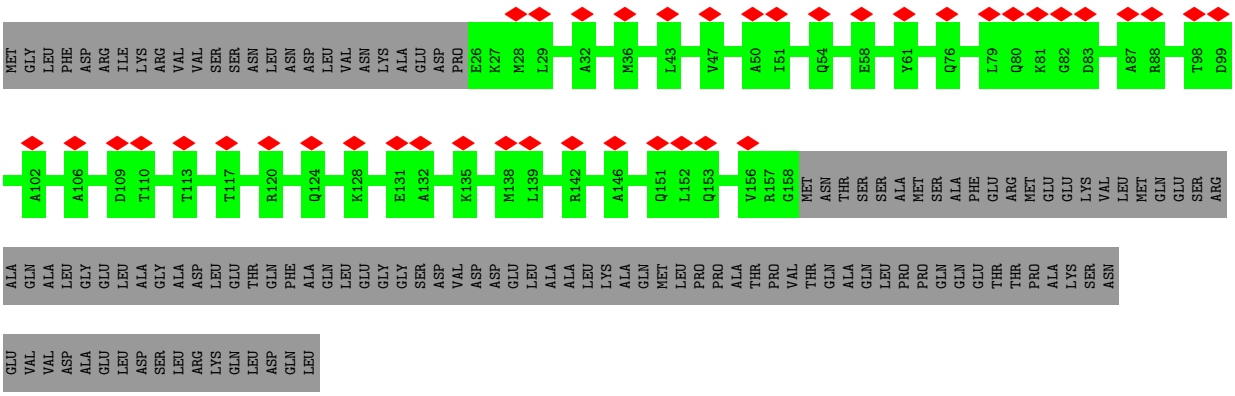
- Molecule 1: Vipp1

Chain CB:



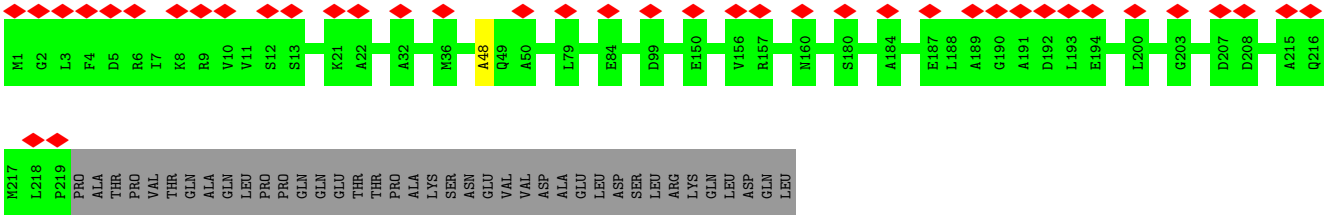
- Molecule 1: Vipp1

Chain DB:



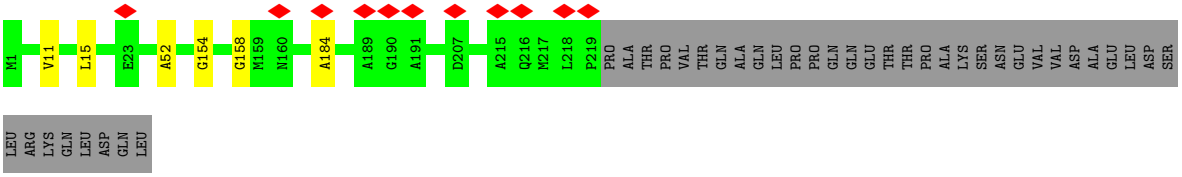
- Molecule 1: Vipp1

Chain EB:



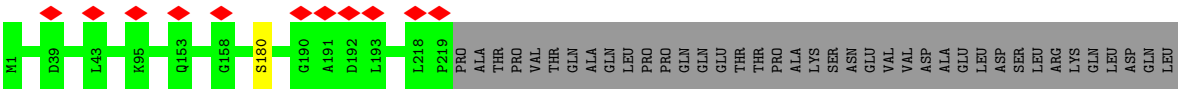
- Molecule 1: Vipp1

Chain FB:



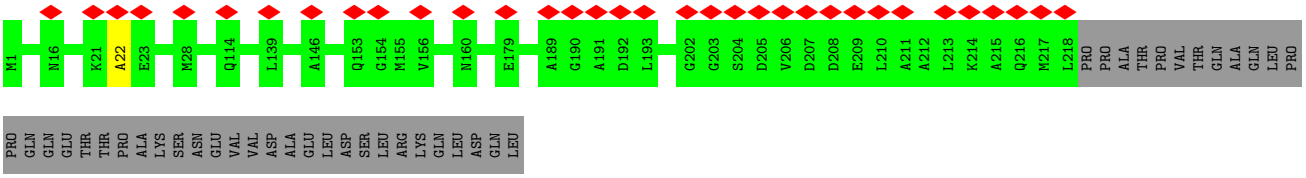
- Molecule 1: Vipp1

Chain GB:



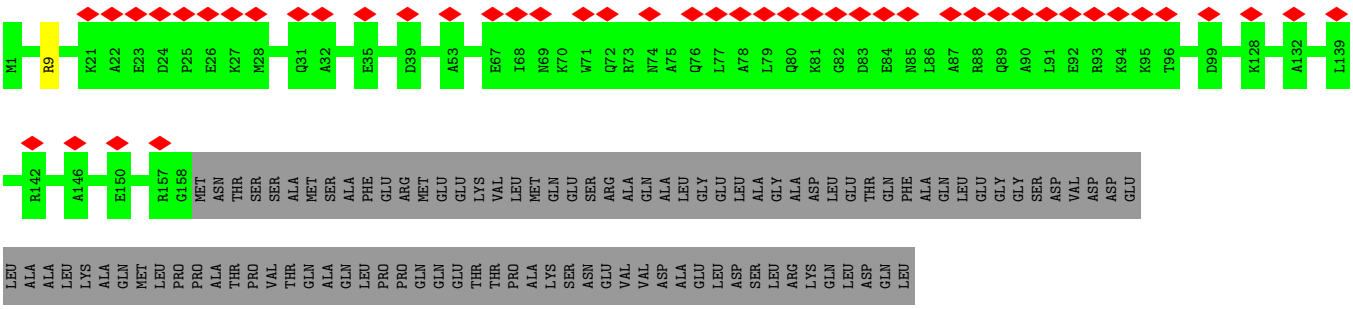
- Molecule 1: Vipp1

Chain HB:



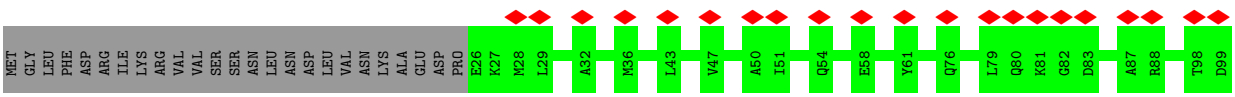
- Molecule 1: Vipp1

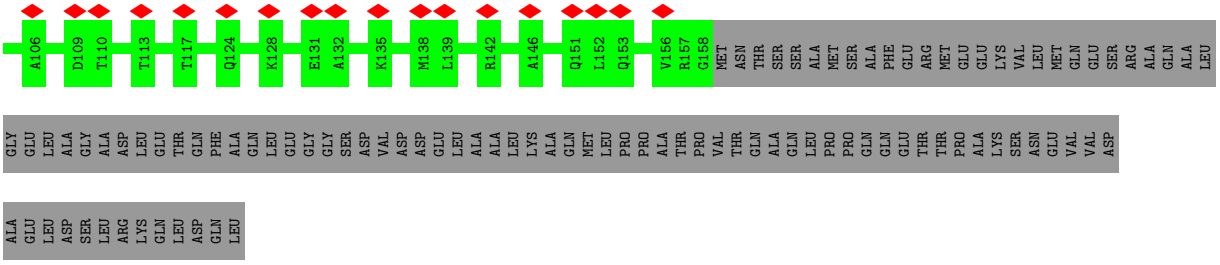
Chain IB:



- Molecule 1: Vipp1

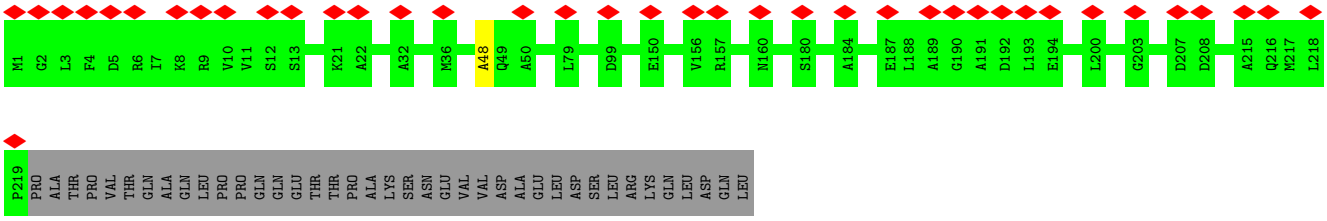
Chain JB:





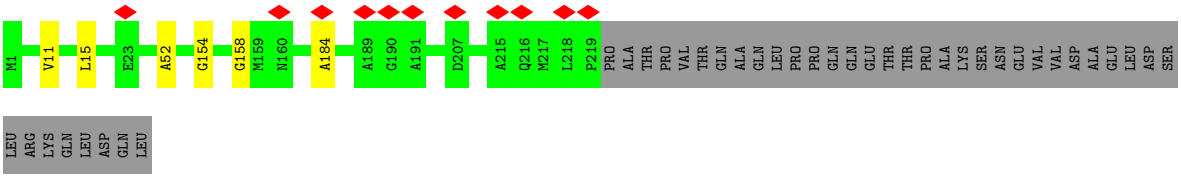
- Molecule 1: Vipp1

Chain KB:



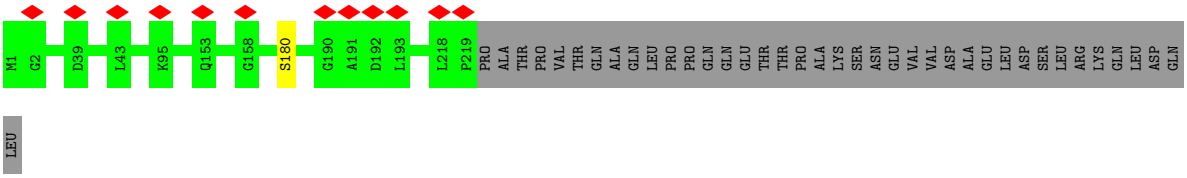
- Molecule 1: Vipp1

Chain LB:



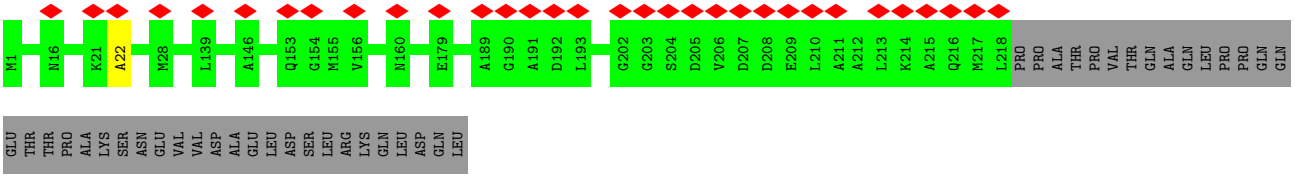
- Molecule 1: Vipp1

Chain MB:



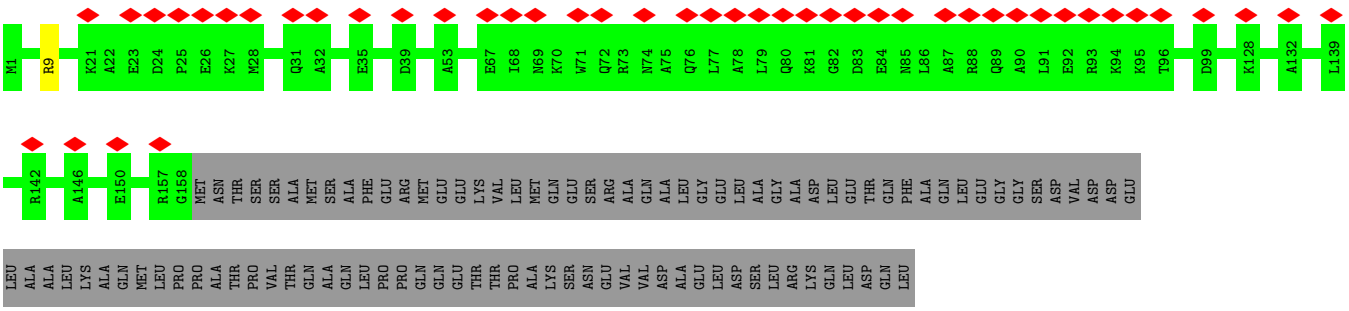
- Molecule 1: Vipp1

Chain NB:



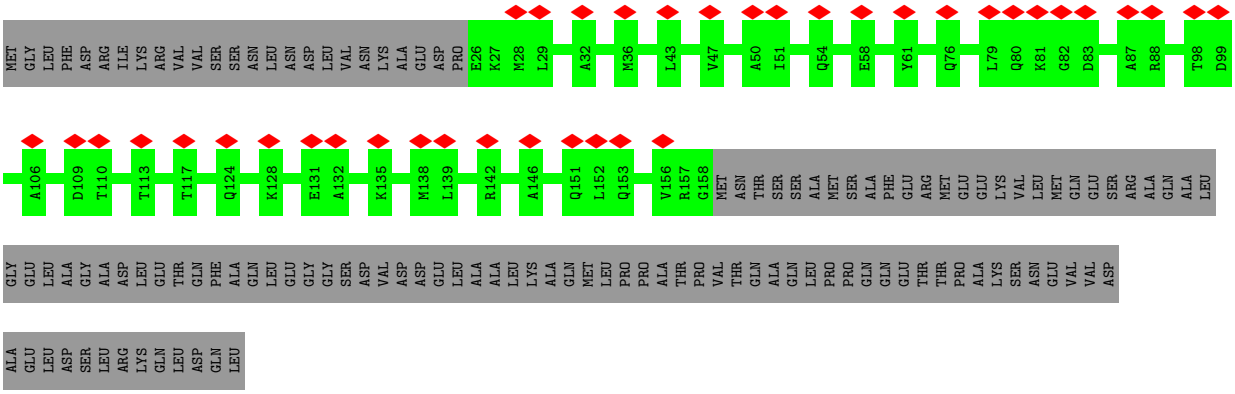
- Molecule 1: Vipp1

Chain OB:



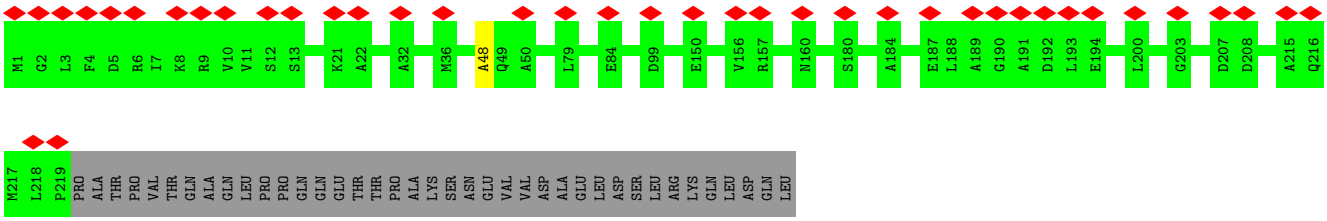
- Molecule 1: Vipp1

Chain PB:



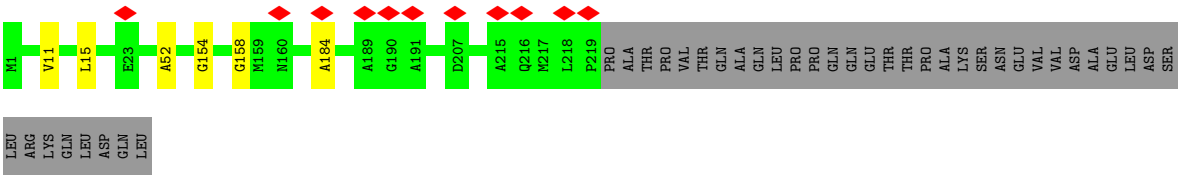
- Molecule 1: Vipp1

Chain QB:



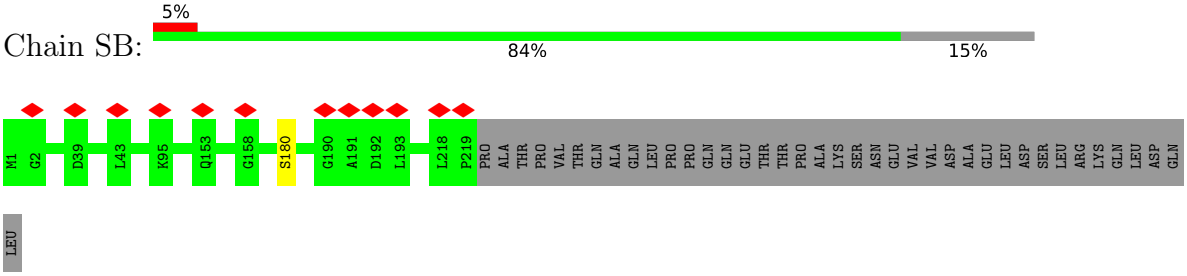
- Molecule 1: Vipp1

Chain RB:



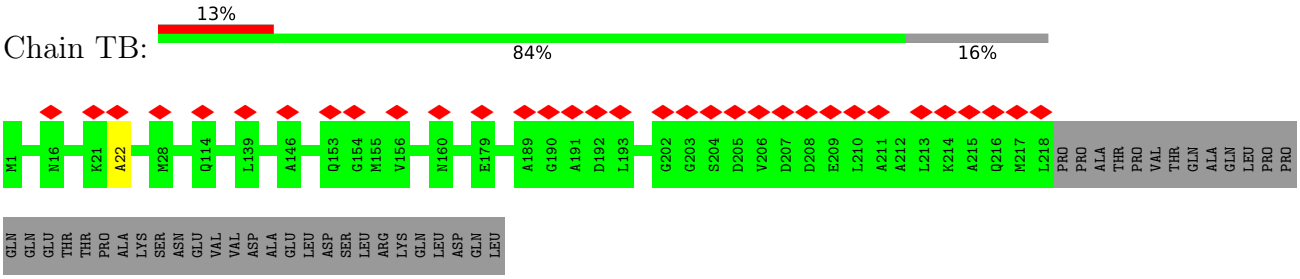
- Molecule 1: Vipp1

Chain SB:



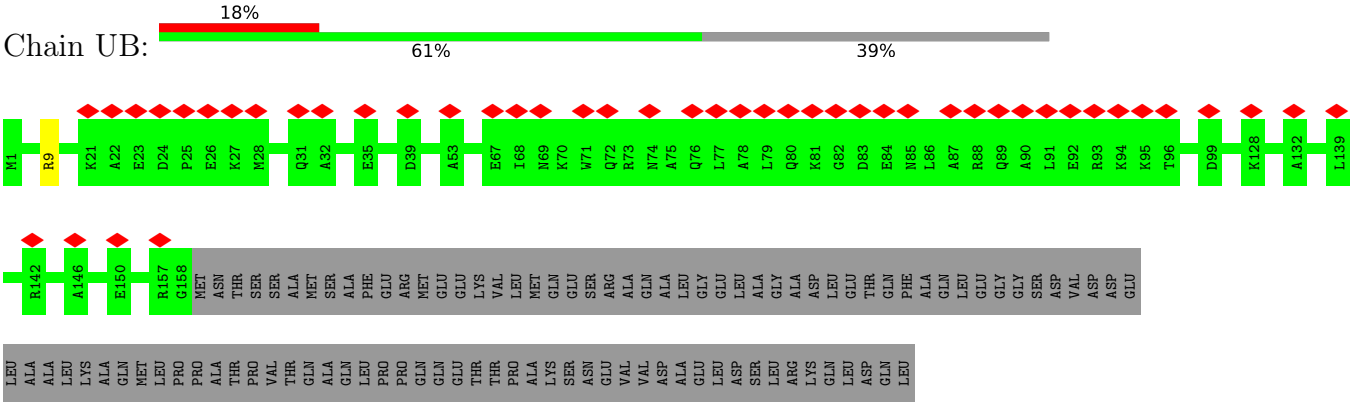
- Molecule 1: Vipp1

Chain TB:



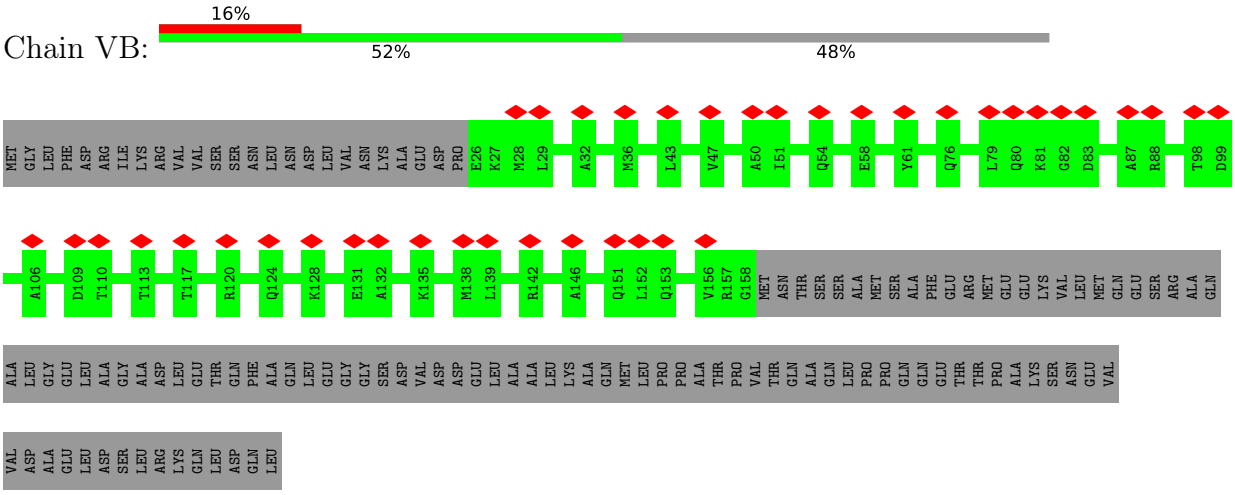
- Molecule 1: Vipp1

Chain UB:



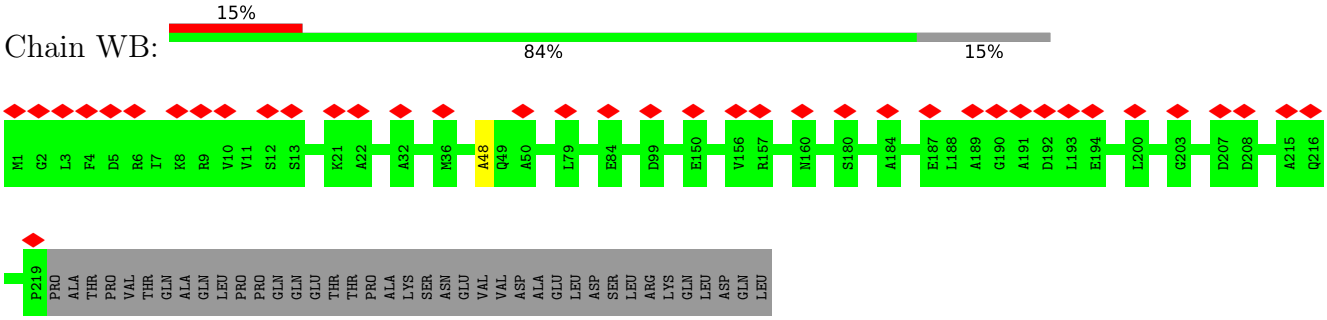
- Molecule 1: Vipp1

Chain VB:



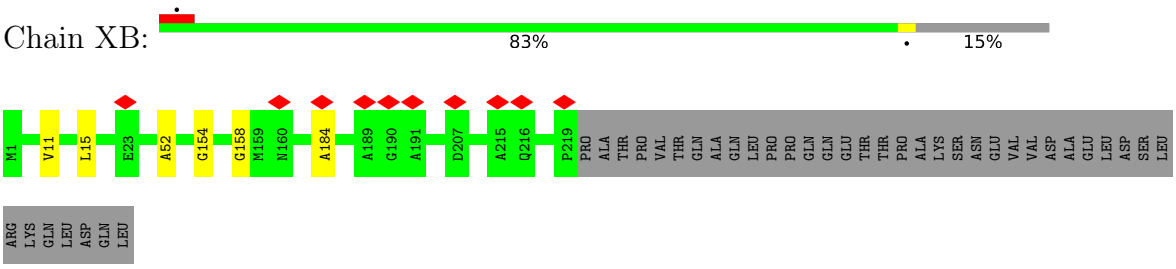
- Molecule 1: Vipp1

Chain WB:



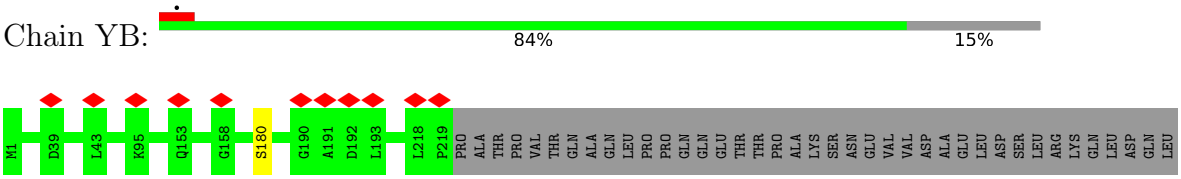
- Molecule 1: Vipp1

Chain XB:



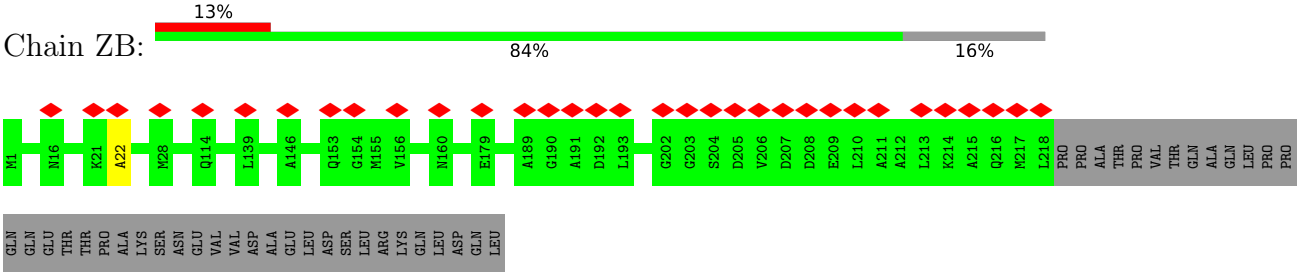
- Molecule 1: Vipp1

Chain YB:



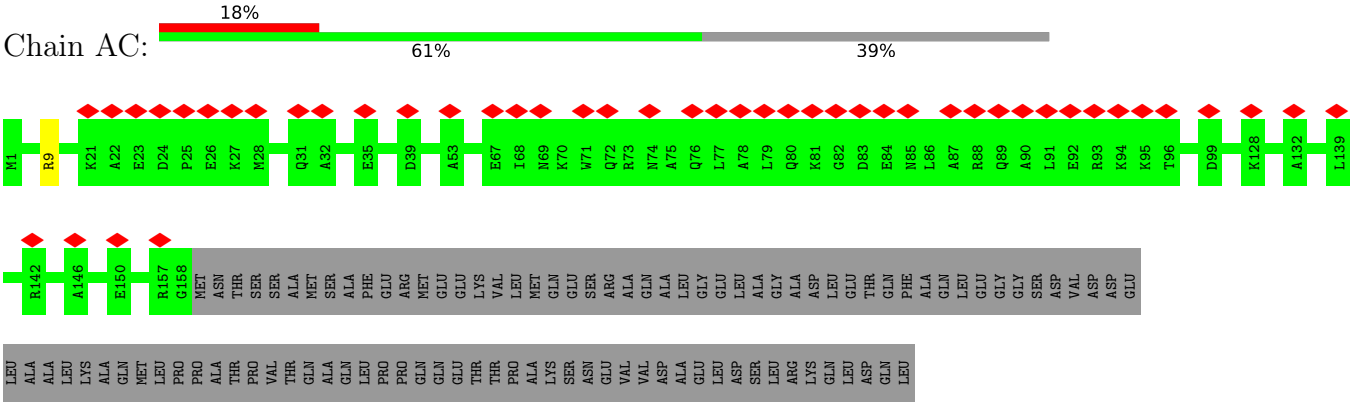
- Molecule 1: Vipp1

Chain ZB:



- Molecule 1: Vipp1

Chain AC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6920	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	0.055	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0187	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.19	0/660	0.37	0/920
1	AA	0.18	0/1085	0.35	0/1512
1	AB	0.19	0/1085	0.39	0/1512
1	AC	0.19	0/784	0.39	0/1093
1	B	0.18	0/1085	0.35	0/1512
1	BA	0.20	0/1085	0.39	0/1512
1	BB	0.20	0/1080	0.41	0/1505
1	C	0.20	0/1085	0.39	0/1512
1	CA	0.19	0/1085	0.39	0/1512
1	CB	0.20	0/784	0.39	0/1093
1	D	0.19	0/1085	0.39	0/1512
1	DA	0.20	0/1080	0.41	0/1505
1	DB	0.20	0/660	0.37	0/920
1	E	0.20	0/1080	0.41	0/1505
1	EA	0.20	0/784	0.39	0/1093
1	EB	0.18	0/1085	0.35	0/1512
1	F	0.20	0/784	0.39	0/1093
1	FA	0.19	0/660	0.37	0/920
1	FB	0.20	0/1085	0.39	0/1512
1	G	0.19	0/660	0.37	0/920
1	GA	0.18	0/1085	0.35	0/1512
1	GB	0.19	0/1085	0.39	0/1512
1	H	0.18	0/1085	0.35	0/1512
1	HA	0.20	0/1085	0.39	0/1512
1	HB	0.20	0/1080	0.41	0/1505
1	I	0.20	0/1085	0.39	0/1512
1	IA	0.19	0/1085	0.39	0/1512
1	IB	0.20	0/784	0.39	0/1093
1	J	0.19	0/1085	0.39	0/1512
1	JA	0.20	0/1080	0.41	0/1505
1	JB	0.20	0/660	0.37	0/920
1	K	0.20	0/1080	0.41	0/1505
1	KA	0.20	0/784	0.39	0/1093
1	KB	0.18	0/1085	0.35	0/1512

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	L	0.20	0/784	0.39	0/1093
1	LA	0.20	0/660	0.37	0/920
1	LB	0.20	0/1085	0.39	0/1512
1	M	0.19	0/660	0.37	0/920
1	MA	0.18	0/1085	0.35	0/1512
1	MB	0.19	0/1085	0.39	0/1512
1	N	0.18	0/1085	0.35	0/1512
1	NA	0.20	0/1085	0.39	0/1512
1	NB	0.20	0/1080	0.41	0/1505
1	O	0.20	0/1085	0.39	0/1512
1	OA	0.19	0/1085	0.39	0/1512
1	OB	0.20	0/784	0.39	0/1093
1	P	0.19	0/1085	0.39	0/1512
1	PA	0.20	0/1080	0.41	0/1505
1	PB	0.20	0/660	0.37	0/920
1	Q	0.20	0/1080	0.41	0/1505
1	QA	0.20	0/784	0.39	0/1093
1	QB	0.18	0/1085	0.35	0/1512
1	R	0.20	0/784	0.39	0/1093
1	RA	0.19	0/660	0.37	0/920
1	RB	0.20	0/1085	0.39	0/1512
1	S	0.20	0/660	0.37	0/920
1	SA	0.18	0/1085	0.35	0/1512
1	SB	0.19	0/1085	0.39	0/1512
1	T	0.18	0/1085	0.35	0/1512
1	TA	0.20	0/1085	0.39	0/1512
1	TB	0.20	0/1080	0.41	0/1505
1	UA	0.19	0/1085	0.39	0/1512
1	UB	0.20	0/784	0.39	0/1093
1	V	0.20	0/1085	0.39	0/1512
1	VA	0.20	0/1080	0.41	0/1505
1	VB	0.20	0/660	0.37	0/920
1	W	0.19	0/1085	0.39	0/1512
1	WA	0.19	0/784	0.39	0/1093
1	WB	0.18	0/1085	0.35	0/1512
1	X	0.20	0/1080	0.41	0/1505
1	XA	0.19	0/660	0.37	0/920
1	XB	0.20	0/1085	0.39	0/1512
1	Y	0.20	0/784	0.39	0/1093
1	YA	0.18	0/1085	0.35	0/1512
1	YB	0.19	0/1085	0.39	0/1512
1	Z	0.19	0/660	0.37	0/920
1	ZA	0.20	0/1085	0.39	0/1512

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	ZB	0.20	0/1080	0.41	0/1505
All	All	0.19	0/75127	0.38	0/104702

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	1	0
1	AB	1086	0	531	3	0
1	AC	785	0	376	2	0
1	B	1086	0	531	1	0
1	BA	1086	0	531	12	0
1	BB	1081	0	530	2	0
1	C	1086	0	531	12	0
1	CA	1086	0	531	3	0
1	CB	785	0	376	2	0
1	D	1086	0	531	3	0
1	DA	1081	0	530	2	0
1	DB	661	0	320	0	0
1	E	1081	0	530	2	0
1	EA	785	0	376	2	0
1	EB	1086	0	531	1	0
1	F	785	0	376	2	0
1	FA	661	0	320	0	0
1	FB	1086	0	531	13	0
1	G	661	0	320	0	0
1	GA	1086	0	531	1	0
1	GB	1086	0	531	3	0
1	H	1086	0	531	1	0
1	HA	1086	0	531	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HB	1081	0	530	2	0
1	I	1086	0	531	13	0
1	IA	1086	0	531	3	0
1	IB	785	0	376	2	0
1	J	1086	0	531	3	0
1	JA	1081	0	530	2	0
1	JB	661	0	320	0	0
1	K	1081	0	530	2	0
1	KA	785	0	376	2	0
1	KB	1086	0	531	1	0
1	L	785	0	376	2	0
1	LA	661	0	320	0	0
1	LB	1086	0	531	13	0
1	M	661	0	320	0	0
1	MA	1086	0	531	1	0
1	MB	1086	0	531	3	0
1	N	1086	0	531	1	0
1	NA	1086	0	531	12	0
1	NB	1081	0	530	2	0
1	O	1086	0	531	13	0
1	OA	1086	0	531	3	0
1	OB	785	0	376	2	0
1	P	1086	0	531	3	0
1	PA	1081	0	530	2	0
1	PB	661	0	320	0	0
1	Q	1081	0	530	2	0
1	QA	785	0	376	2	0
1	QB	1086	0	531	1	0
1	R	785	0	376	2	0
1	RA	661	0	320	0	0
1	RB	1086	0	531	13	0
1	S	661	0	320	0	0
1	SA	1086	0	531	1	0
1	SB	1086	0	531	3	0
1	T	1086	0	531	1	0
1	TA	1086	0	531	12	0
1	TB	1081	0	530	2	0
1	UA	1086	0	531	3	0
1	UB	785	0	376	2	0
1	V	1086	0	531	12	0
1	VA	1081	0	530	2	0
1	VB	661	0	320	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1086	0	531	3	0
1	WA	785	0	376	2	0
1	WB	1086	0	531	1	0
1	X	1081	0	530	2	0
1	XA	661	0	320	0	0
1	XB	1086	0	531	12	0
1	Y	785	0	376	2	0
1	YA	1086	0	531	1	0
1	YB	1086	0	531	3	0
1	Z	661	0	320	0	0
1	ZA	1086	0	531	13	0
1	ZB	1081	0	530	2	0
All	All	75205	0	36647	187	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 2.

All (187) 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:BA:154:GLY:O	1:BA:158:GLY:CA	2.11	0.98
1:XB:154:GLY:O	1:XB:158:GLY:CA	2.11	0.98
1:HA:154:GLY:O	1:HA:158:GLY:CA	2.11	0.98
1:C:154:GLY:O	1:C:158:GLY:CA	2.11	0.98
1:RB:154:GLY:O	1:RB:158:GLY:CA	2.12	0.98
1:ZA:154:GLY:O	1:ZA:158:GLY:CA	2.11	0.98
1:V:154:GLY:O	1:V:158:GLY:CA	2.11	0.98
1:FB:154:GLY:O	1:FB:158:GLY:CA	2.11	0.98
1:I:154:GLY:O	1:I:158:GLY:CA	2.11	0.97
1:NA:154:GLY:O	1:NA:158:GLY:CA	2.11	0.97
1:TA:154:GLY:O	1:TA:158:GLY:CA	2.11	0.97
1:O:154:GLY:O	1:O:158:GLY:CA	2.11	0.97
1:LB:154:GLY:O	1:LB:158:GLY:CA	2.11	0.97
1:V:154:GLY:O	1:V:158:GLY:HA3	1.66	0.96
1:RB:154:GLY:O	1:RB:158:GLY:HA3	1.66	0.96
1:I:154:GLY:O	1:I:158:GLY:HA3	1.66	0.96
1:C:154:GLY:O	1:C:158:GLY:HA3	1.66	0.96
1:O:154:GLY:O	1:O:158:GLY:HA3	1.66	0.96
1:XB:154:GLY:O	1:XB:158:GLY:HA3	1.66	0.95
1:HA:154:GLY:O	1:HA:158:GLY:HA3	1.66	0.95
1:FB:154:GLY:O	1:FB:158:GLY:HA3	1.66	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:154:GLY:O	1:FB:158:GLY:N	2.01	0.94
1:XB:154:GLY:O	1:XB:158:GLY:N	2.00	0.94
1:NA:154:GLY:O	1:NA:158:GLY:HA3	1.66	0.94
1:ZA:154:GLY:O	1:ZA:158:GLY:HA3	1.66	0.94
1:BA:154:GLY:O	1:BA:158:GLY:HA3	1.66	0.94
1:I:154:GLY:O	1:I:158:GLY:N	2.01	0.94
1:TA:154:GLY:O	1:TA:158:GLY:N	2.00	0.94
1:LB:154:GLY:O	1:LB:158:GLY:HA3	1.66	0.94
1:RB:154:GLY:O	1:RB:158:GLY:N	2.00	0.94
1:LB:154:GLY:O	1:LB:158:GLY:N	2.01	0.94
1:V:154:GLY:O	1:V:158:GLY:N	2.00	0.93
1:HA:154:GLY:O	1:HA:158:GLY:N	2.00	0.93
1:NA:154:GLY:O	1:NA:158:GLY:N	2.01	0.93
1:ZA:154:GLY:O	1:ZA:158:GLY:N	2.00	0.93
1:O:154:GLY:O	1:O:158:GLY:N	2.00	0.93
1:C:154:GLY:O	1:C:158:GLY:N	2.00	0.93
1:BA:154:GLY:O	1:BA:158:GLY:N	2.01	0.92
1:TA:154:GLY:O	1:TA:158:GLY:HA3	1.66	0.91
1:NA:52:ALA:CB	1:AB:180:SER:CB	2.51	0.89
1:D:180:SER:CB	1:RB:52:ALA:CB	2.51	0.89
1:HA:52:ALA:CB	1:UA:180:SER:CB	2.51	0.89
1:I:52:ALA:CB	1:W:180:SER:CB	2.51	0.89
1:C:52:ALA:CB	1:P:180:SER:CB	2.51	0.88
1:TA:52:ALA:CB	1:GB:180:SER:CB	2.51	0.88
1:BA:52:ALA:CB	1:OA:180:SER:CB	2.51	0.88
1:LB:52:ALA:CB	1:YB:180:SER:CB	2.51	0.88
1:ZA:52:ALA:CB	1:MB:180:SER:CB	2.51	0.88
1:O:52:ALA:CB	1:CA:180:SER:CB	2.51	0.88
1:J:180:SER:CB	1:XB:52:ALA:CB	2.51	0.88
1:V:52:ALA:CB	1:IA:180:SER:CB	2.51	0.88
1:FB:52:ALA:CB	1:SB:180:SER:CB	2.51	0.87
1:O:52:ALA:HB2	1:CA:180:SER:CB	2.13	0.77
1:J:180:SER:CB	1:XB:52:ALA:HB2	2.13	0.77
1:ZA:52:ALA:HB2	1:MB:180:SER:CB	2.14	0.77
1:FB:52:ALA:HB2	1:SB:180:SER:CB	2.13	0.77
1:D:180:SER:CB	1:RB:52:ALA:HB2	2.14	0.77
1:HA:52:ALA:HB2	1:UA:180:SER:CB	2.14	0.77
1:BA:52:ALA:HB2	1:OA:180:SER:CB	2.14	0.76
1:TA:52:ALA:HB2	1:GB:180:SER:CB	2.14	0.76
1:I:52:ALA:HB2	1:W:180:SER:CB	2.14	0.76
1:V:52:ALA:HB2	1:IA:180:SER:CB	2.14	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:ALA:HB2	1:P:180:SER:CB	2.14	0.76
1:NA:52:ALA:HB2	1:AB:180:SER:CB	2.14	0.75
1:LB:52:ALA:HB2	1:YB:180:SER:CB	2.15	0.75
1:LB:52:ALA:HB1	1:YB:180:SER:CB	2.23	0.68
1:TA:52:ALA:HB1	1:GB:180:SER:CB	2.25	0.67
1:D:180:SER:CB	1:RB:52:ALA:HB1	2.25	0.67
1:ZA:52:ALA:HB1	1:MB:180:SER:CB	2.25	0.66
1:NA:52:ALA:HB1	1:AB:180:SER:CB	2.25	0.66
1:FB:52:ALA:HB1	1:SB:180:SER:CB	2.25	0.66
1:C:52:ALA:HB1	1:P:180:SER:CB	2.24	0.65
1:V:52:ALA:HB1	1:IA:180:SER:CB	2.24	0.65
1:HA:52:ALA:HB1	1:UA:180:SER:CB	2.24	0.65
1:BA:52:ALA:HB1	1:OA:180:SER:CB	2.24	0.65
1:J:180:SER:CB	1:XB:52:ALA:HB1	2.26	0.65
1:I:52:ALA:HB1	1:W:180:SER:CB	2.25	0.64
1:O:52:ALA:HB1	1:CA:180:SER:CB	2.25	0.64
1:TB:22:ALA:HB2	1:UB:9:ARG:CB	2.29	0.63
1:BB:22:ALA:HB2	1:CB:9:ARG:CB	2.29	0.62
1:HB:22:ALA:HB2	1:IB:9:ARG:CB	2.29	0.62
1:NB:22:ALA:HB2	1:OB:9:ARG:CB	2.29	0.62
1:ZB:22:ALA:HB2	1:AC:9:ARG:CB	2.29	0.62
1:PA:22:ALA:HB2	1:QA:9:ARG:CB	2.29	0.62
1:VA:22:ALA:HB2	1:WA:9:ARG:CB	2.29	0.62
1:E:22:ALA:HB2	1:F:9:ARG:CB	2.29	0.62
1:JA:22:ALA:HB2	1:KA:9:ARG:CB	2.29	0.62
1:DA:22:ALA:HB2	1:EA:9:ARG:CB	2.29	0.61
1:X:22:ALA:HB2	1:Y:9:ARG:CB	2.29	0.61
1:K:22:ALA:HB2	1:L:9:ARG:CB	2.29	0.61
1:Q:22:ALA:HB2	1:R:9:ARG:CB	2.29	0.60
1:BA:154:GLY:HA2	1:BA:158:GLY:HA2	1.85	0.59
1:HA:154:GLY:HA2	1:HA:158:GLY:HA2	1.85	0.59
1:V:154:GLY:HA2	1:V:158:GLY:HA2	1.85	0.59
1:NA:154:GLY:HA2	1:NA:158:GLY:HA2	1.85	0.59
1:LB:154:GLY:HA2	1:LB:158:GLY:HA2	1.85	0.58
1:TA:154:GLY:HA2	1:TA:158:GLY:HA2	1.85	0.58
1:RB:154:GLY:HA2	1:RB:158:GLY:HA2	1.85	0.58
1:O:154:GLY:HA2	1:O:158:GLY:HA2	1.85	0.58
1:FB:154:GLY:HA2	1:FB:158:GLY:HA2	1.85	0.58
1:XB:154:GLY:HA2	1:XB:158:GLY:HA2	1.85	0.58
1:ZA:154:GLY:HA2	1:ZA:158:GLY:HA2	1.85	0.57
1:C:154:GLY:HA2	1:C:158:GLY:HA2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:GLY:HA2	1:I:158:GLY:HA2	1.85	0.57
1:PA:22:ALA:CB	1:QA:9:ARG:CB	2.85	0.55
1:HB:22:ALA:CB	1:IB:9:ARG:CB	2.85	0.55
1:NB:22:ALA:CB	1:OB:9:ARG:CB	2.85	0.55
1:TB:22:ALA:CB	1:UB:9:ARG:CB	2.85	0.55
1:JA:22:ALA:CB	1:KA:9:ARG:CB	2.85	0.54
1:VA:22:ALA:CB	1:WA:9:ARG:CB	2.85	0.54
1:ZB:22:ALA:CB	1:AC:9:ARG:CB	2.85	0.54
1:E:22:ALA:CB	1:F:9:ARG:CB	2.85	0.54
1:DA:22:ALA:CB	1:EA:9:ARG:CB	2.85	0.54
1:HA:11:VAL:O	1:HA:15:LEU:N	2.34	0.54
1:I:11:VAL:O	1:I:15:LEU:N	2.34	0.54
1:X:22:ALA:CB	1:Y:9:ARG:CB	2.85	0.54
1:BB:22:ALA:CB	1:CB:9:ARG:CB	2.85	0.54
1:Q:22:ALA:CB	1:R:9:ARG:CB	2.85	0.54
1:K:22:ALA:CB	1:L:9:ARG:CB	2.85	0.53
1:C:11:VAL:O	1:C:15:LEU:N	2.34	0.53
1:NA:11:VAL:O	1:NA:15:LEU:N	2.34	0.53
1:XB:11:VAL:O	1:XB:15:LEU:N	2.34	0.51
1:TA:11:VAL:O	1:TA:15:LEU:N	2.34	0.51
1:V:11:VAL:O	1:V:15:LEU:N	2.34	0.50
1:BA:11:VAL:O	1:BA:15:LEU:N	2.34	0.50
1:RB:11:VAL:O	1:RB:15:LEU:N	2.34	0.50
1:O:11:VAL:O	1:O:15:LEU:N	2.34	0.49
1:LB:11:VAL:O	1:LB:15:LEU:N	2.34	0.49
1:ZA:11:VAL:O	1:ZA:15:LEU:N	2.34	0.48
1:FB:11:VAL:O	1:FB:15:LEU:N	2.34	0.48
1:NA:154:GLY:HA2	1:NA:158:GLY:CA	2.45	0.47
1:TA:154:GLY:HA2	1:TA:158:GLY:CA	2.45	0.47
1:HA:154:GLY:HA2	1:HA:158:GLY:CA	2.45	0.47
1:ZA:154:GLY:HA2	1:ZA:158:GLY:CA	2.45	0.47
1:I:154:GLY:HA2	1:I:158:GLY:CA	2.45	0.46
1:C:154:GLY:HA2	1:C:158:GLY:CA	2.45	0.46
1:BA:154:GLY:HA2	1:BA:158:GLY:CA	2.45	0.46
1:FB:154:GLY:HA2	1:FB:158:GLY:CA	2.45	0.46
1:XB:154:GLY:HA2	1:XB:158:GLY:CA	2.45	0.46
1:I:154:GLY:CA	1:I:158:GLY:HA2	2.46	0.46
1:O:154:GLY:CA	1:O:158:GLY:HA2	2.46	0.46
1:LB:154:GLY:CA	1:LB:158:GLY:HA2	2.46	0.46
1:RB:154:GLY:CA	1:RB:158:GLY:HA2	2.46	0.46
1:V:154:GLY:HA2	1:V:158:GLY:CA	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RB:154:GLY:HA2	1:RB:158:GLY:CA	2.45	0.46
1:BA:154:GLY:CA	1:BA:158:GLY:HA2	2.46	0.46
1:ZA:154:GLY:CA	1:ZA:158:GLY:HA2	2.46	0.46
1:HA:154:GLY:CA	1:HA:158:GLY:HA2	2.46	0.45
1:TA:154:GLY:CA	1:TA:158:GLY:HA2	2.46	0.45
1:XB:154:GLY:CA	1:XB:158:GLY:HA2	2.46	0.45
1:C:154:GLY:CA	1:C:158:GLY:HA2	2.46	0.45
1:I:154:GLY:C	1:I:158:GLY:CA	2.84	0.45
1:V:154:GLY:CA	1:V:158:GLY:HA2	2.46	0.45
1:LB:154:GLY:HA2	1:LB:158:GLY:CA	2.45	0.45
1:O:154:GLY:HA2	1:O:158:GLY:CA	2.45	0.45
1:FB:154:GLY:CA	1:FB:158:GLY:HA2	2.46	0.45
1:O:154:GLY:C	1:O:158:GLY:CA	2.84	0.44
1:NA:154:GLY:CA	1:NA:158:GLY:HA2	2.46	0.44
1:FB:154:GLY:C	1:FB:158:GLY:CA	2.84	0.44
1:EB:48:ALA:HA	1:RB:184:ALA:HB1	1.99	0.44
1:GA:48:ALA:HA	1:TA:184:ALA:HB1	2.00	0.43
1:SA:48:ALA:HA	1:FB:184:ALA:HB1	2.00	0.43
1:AA:48:ALA:HA	1:NA:184:ALA:HB1	2.00	0.43
1:T:48:ALA:HA	1:HA:184:ALA:HB1	2.00	0.43
1:KB:48:ALA:HA	1:XB:184:ALA:HB1	1.99	0.43
1:V:154:GLY:C	1:V:158:GLY:CA	2.84	0.43
1:MA:48:ALA:HA	1:ZA:184:ALA:HB1	2.01	0.43
1:NA:154:GLY:C	1:NA:158:GLY:CA	2.84	0.42
1:YA:48:ALA:HA	1:LB:184:ALA:HB1	2.01	0.42
1:LB:154:GLY:C	1:LB:158:GLY:CA	2.84	0.42
1:B:48:ALA:HA	1:O:184:ALA:HB1	2.00	0.42
1:I:184:ALA:HB1	1:WB:48:ALA:HA	2.00	0.42
1:N:48:ALA:HA	1:BA:184:ALA:HB1	2.00	0.42
1:RB:154:GLY:C	1:RB:158:GLY:CA	2.84	0.41
1:C:184:ALA:HB1	1:QB:48:ALA:HA	2.01	0.41
1:FB:154:GLY:CA	1:FB:158:GLY:CA	2.99	0.41
1:RB:154:GLY:CA	1:RB:158:GLY:CA	2.99	0.41
1:C:154:GLY:CA	1:C:158:GLY:CA	2.99	0.41
1:I:154:GLY:CA	1:I:158:GLY:CA	2.99	0.41
1:ZA:154:GLY:C	1:ZA:158:GLY:CA	2.84	0.41
1:H:48:ALA:HA	1:V:184:ALA:HB1	2.02	0.40
1:O:154:GLY:CA	1:O:158:GLY:CA	2.99	0.40
1:XB:154:GLY:CA	1:XB:158:GLY:CA	2.99	0.40
1:TA:154:GLY:C	1:TA:158:GLY:CA	2.84	0.40
1:LB:154:GLY:CA	1:LB:158:GLY:CA	2.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:154:GLY:C	1:BA:158:GLY:CA	2.84	0.40
1:ZA:154:GLY:CA	1:ZA:158:GLY:CA	2.99	0.40

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%)	129 (98%)	2 (2%)	0	100	100
1	AA	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	AB	217/258 (84%)	217 (100%)	0	0	100	100
1	AC	156/258 (60%)	156 (100%)	0	0	100	100
1	B	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	BA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	BB	216/258 (84%)	216 (100%)	0	0	100	100
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%)	216 (100%)	0	0	100	100
1	DB	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	E	216/258 (84%)	216 (100%)	0	0	100	100
1	EA	156/258 (60%)	156 (100%)	0	0	100	100
1	EB	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	F	156/258 (60%)	156 (100%)	0	0	100	100
1	FA	131/258 (51%)	129 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	G	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	GA	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	GB	217/258 (84%)	217 (100%)	0	0	100	100
1	H	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	HA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	HB	216/258 (84%)	216 (100%)	0	0	100	100
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%)	216 (100%)	0	0	100	100
1	JB	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	K	216/258 (84%)	216 (100%)	0	0	100	100
1	KA	156/258 (60%)	156 (100%)	0	0	100	100
1	KB	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	L	156/258 (60%)	156 (100%)	0	0	100	100
1	LA	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	LB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	M	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	MA	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	MB	217/258 (84%)	217 (100%)	0	0	100	100
1	N	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	NA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	NB	216/258 (84%)	216 (100%)	0	0	100	100
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
1	P	217/258 (84%)	217 (100%)	0	0	100	100
1	PA	216/258 (84%)	216 (100%)	0	0	100	100
1	PB	131/258 (51%)	129 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	216/258 (84%)	216 (100%)	0	0	100	100
1	QA	156/258 (60%)	156 (100%)	0	0	100	100
1	QB	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	R	156/258 (60%)	156 (100%)	0	0	100	100
1	RA	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	RB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	S	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	SA	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	SB	217/258 (84%)	217 (100%)	0	0	100	100
1	T	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	TA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	TB	216/258 (84%)	216 (100%)	0	0	100	100
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%)	216 (100%)	0	0	100	100
1	VB	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	W	217/258 (84%)	217 (100%)	0	0	100	100
1	WA	156/258 (60%)	156 (100%)	0	0	100	100
1	WB	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	X	216/258 (84%)	216 (100%)	0	0	100	100
1	XA	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	XB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	Y	156/258 (60%)	156 (100%)	0	0	100	100
1	YA	217/258 (84%)	210 (97%)	7 (3%)	0	100	100
1	YB	217/258 (84%)	217 (100%)	0	0	100	100
1	Z	131/258 (51%)	129 (98%)	2 (2%)	0	100	100
1	ZA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	ZB	216/258 (84%)	216 (100%)	0	0	100	100
All	All	15002/20124 (74%)	14872 (99%)	130 (1%)	0	100	100

There are no Ramachandran outliers to report.

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.

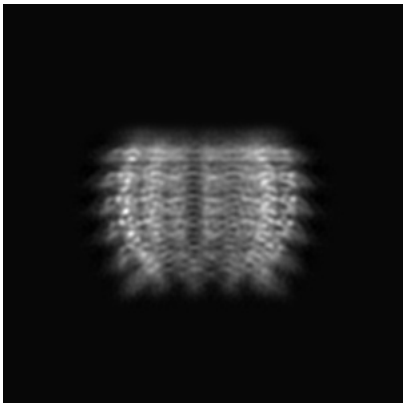
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11470. These allow visual inspection of the internal detail of the map and identification of artifacts.

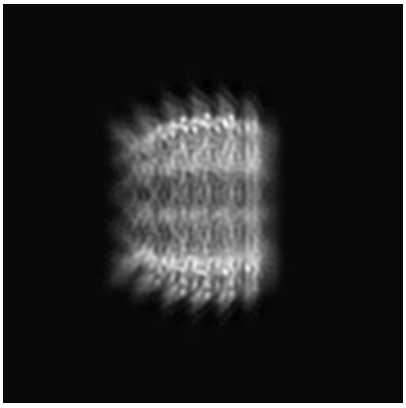
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



Y

Z

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

6.2 Central slices (i)

6.2.1 Primary map

X Index: 168

Y Index: 168

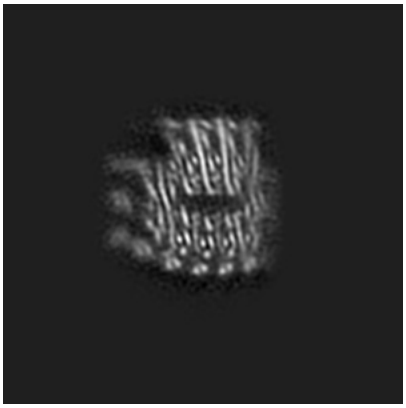
Z Index: 168

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: 232

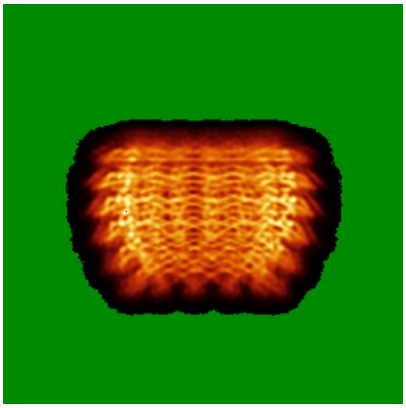

Y Index: 105

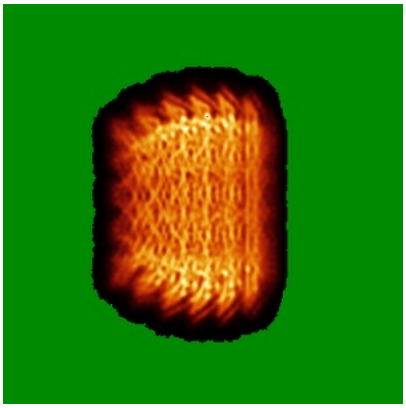
Z Index: 171

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

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

6.4.1 Primary map


X

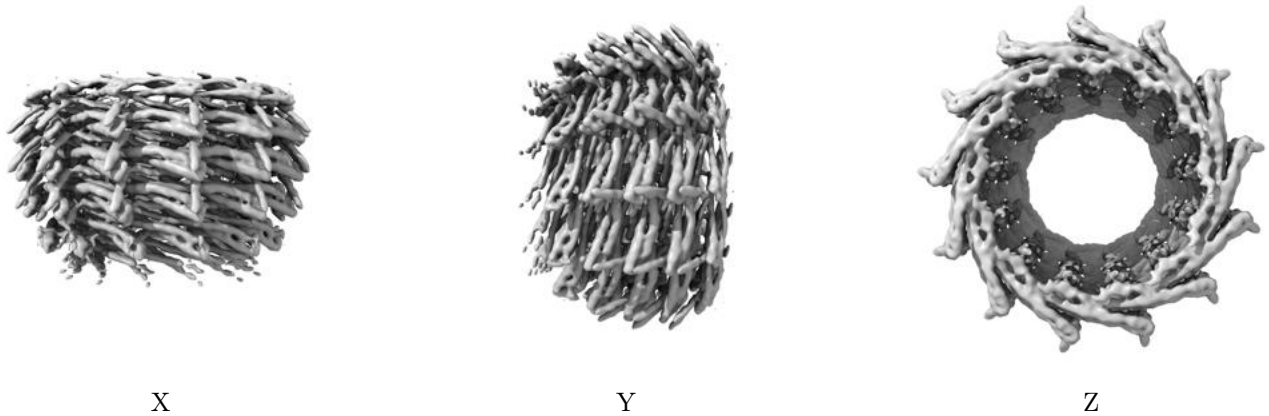

Y

Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

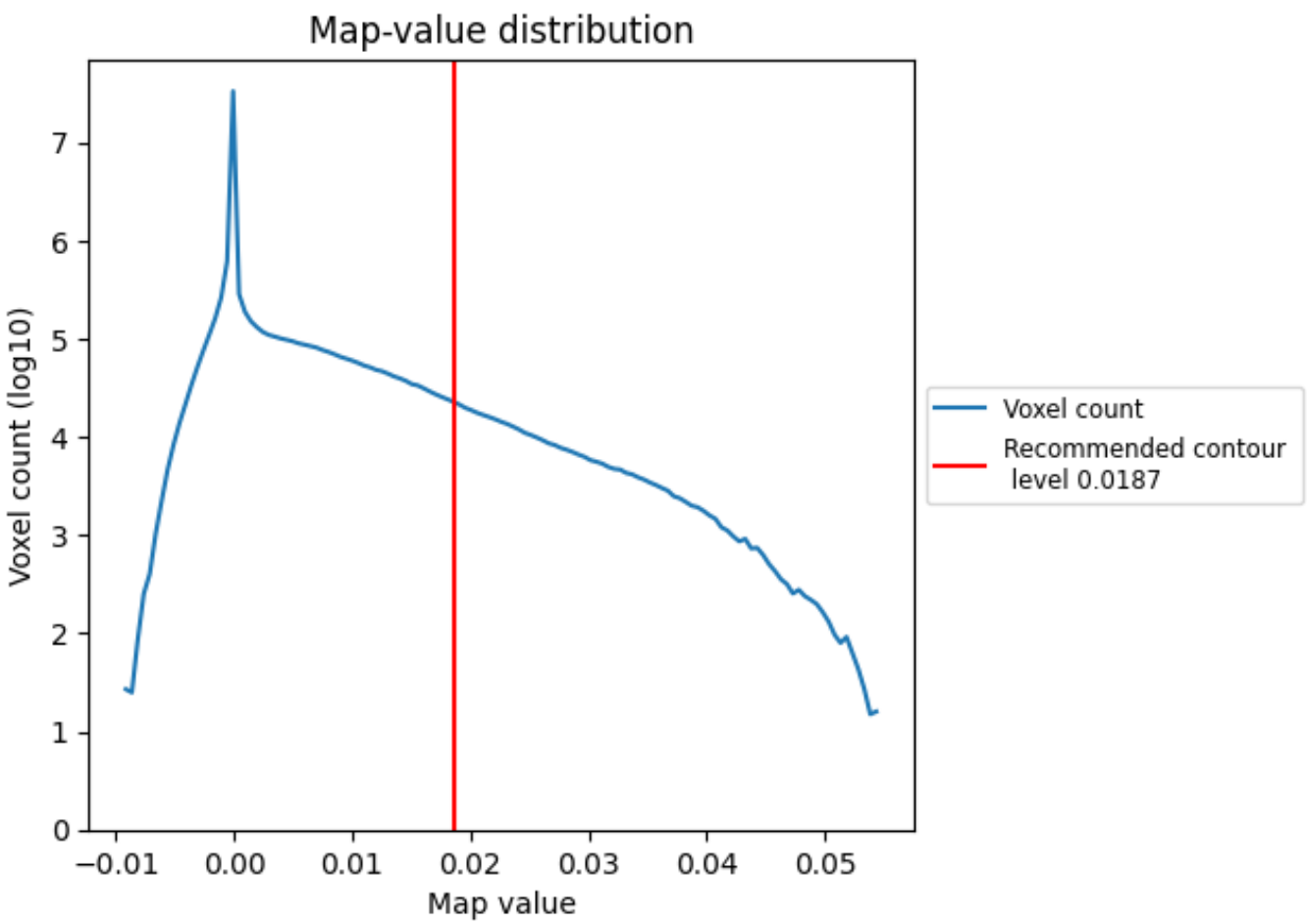
6.6 Mask visualisation (i)

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

7 Map analysis (i)

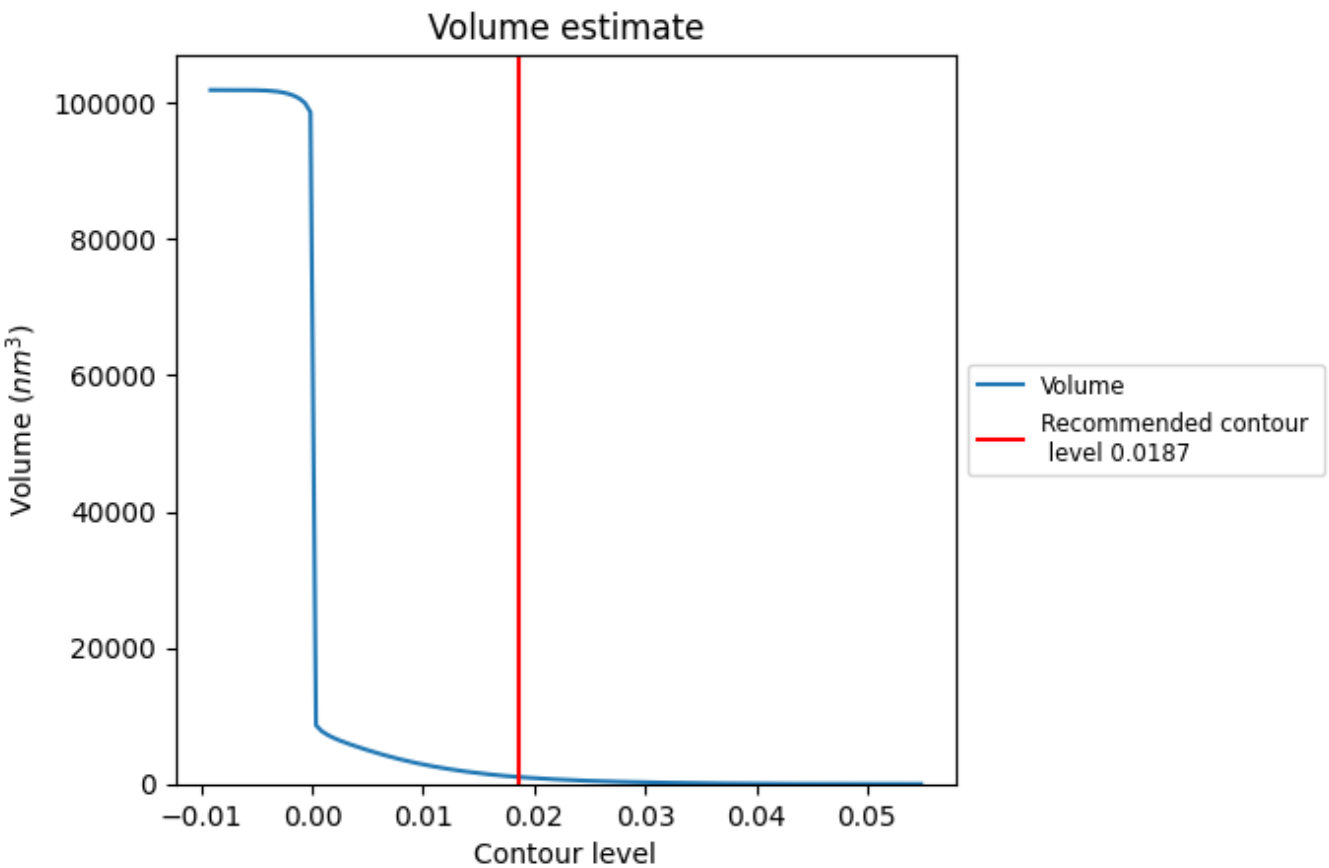
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

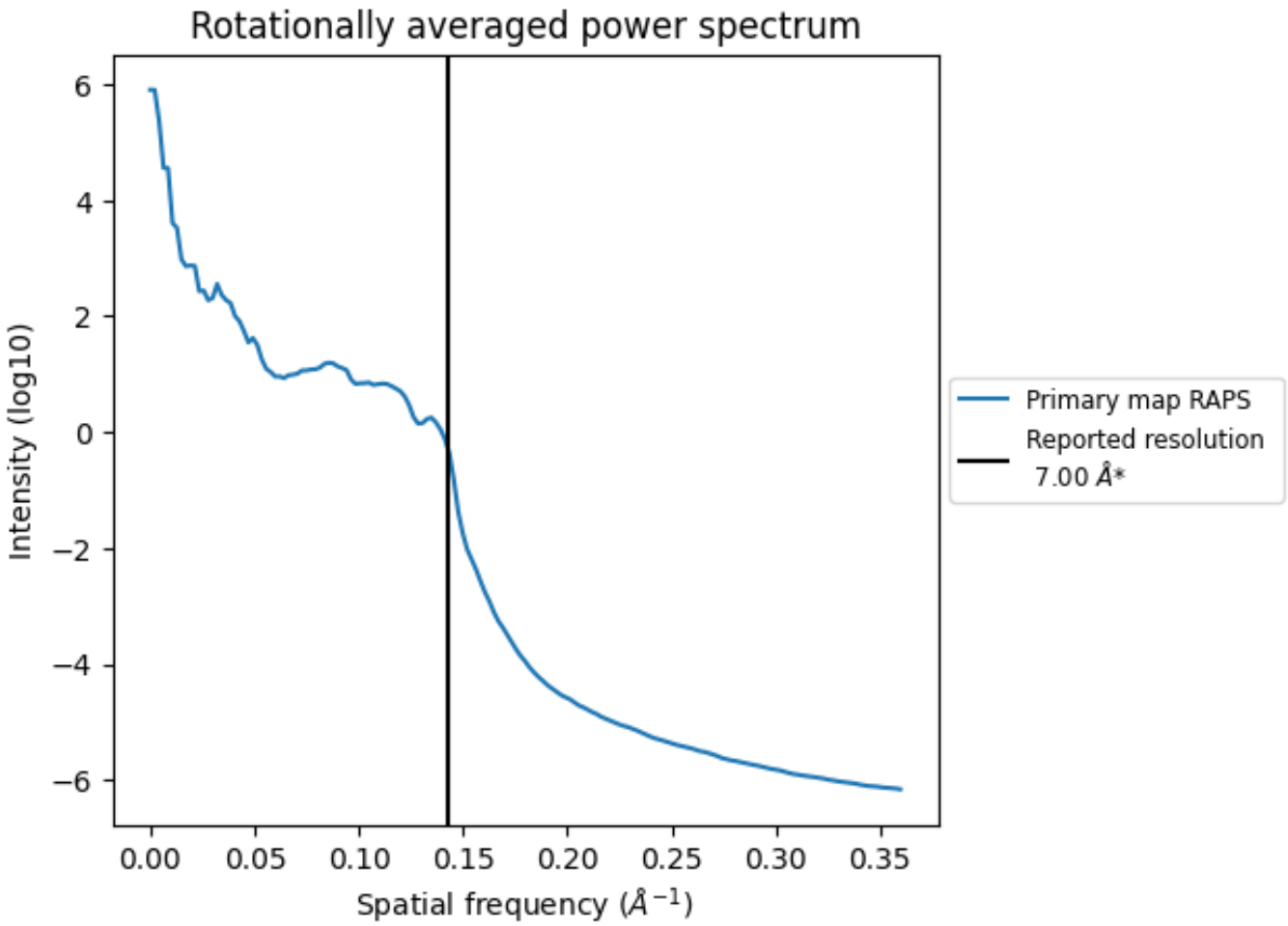
7.2 Volume estimate (i)



The volume at the recommended contour level is 1006 nm^3; this corresponds to an approximate mass of 909 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 0.143 Å^{-1}

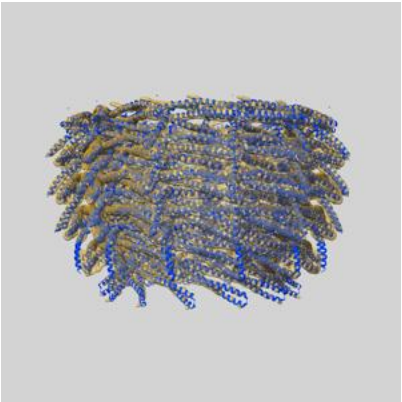
8 Fourier-Shell correlation (i)

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

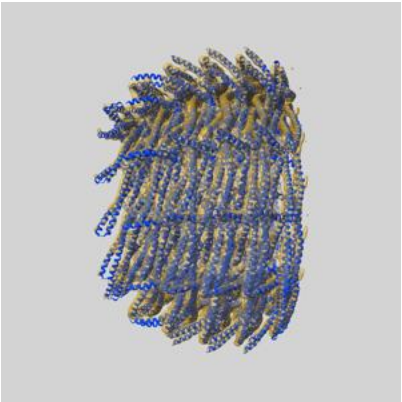
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11470 and PDB model 6ZVT. Per-residue inclusion information can be found in section 3 on page 10.

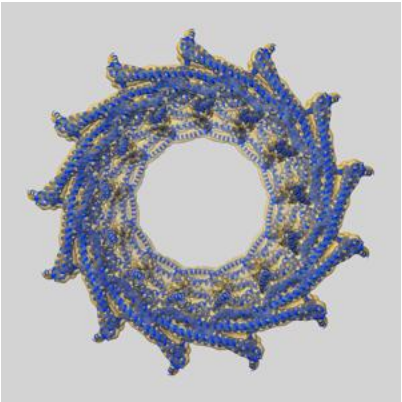
9.1 Map-model overlay (i)



X



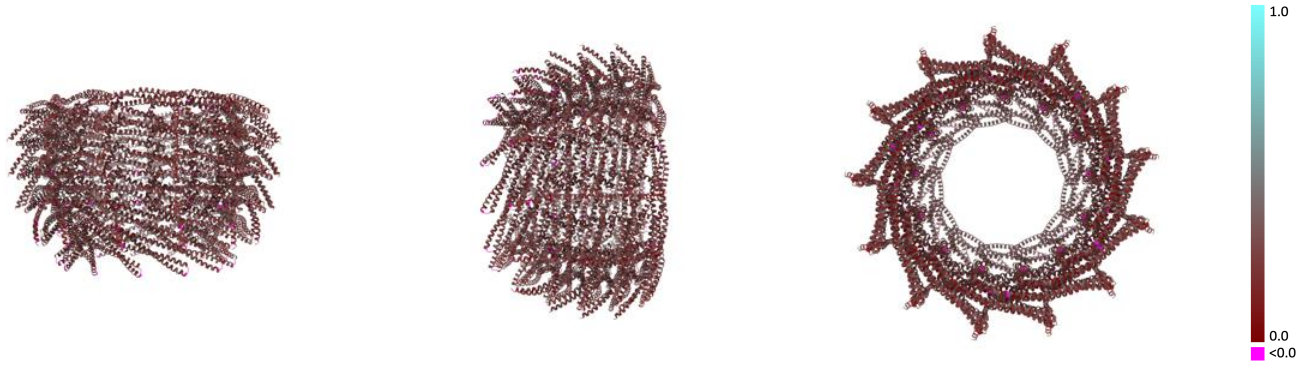
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

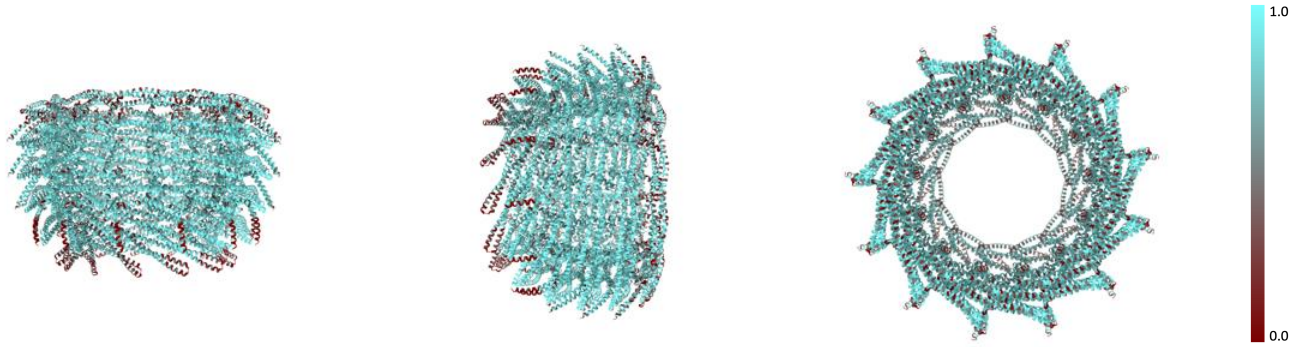
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

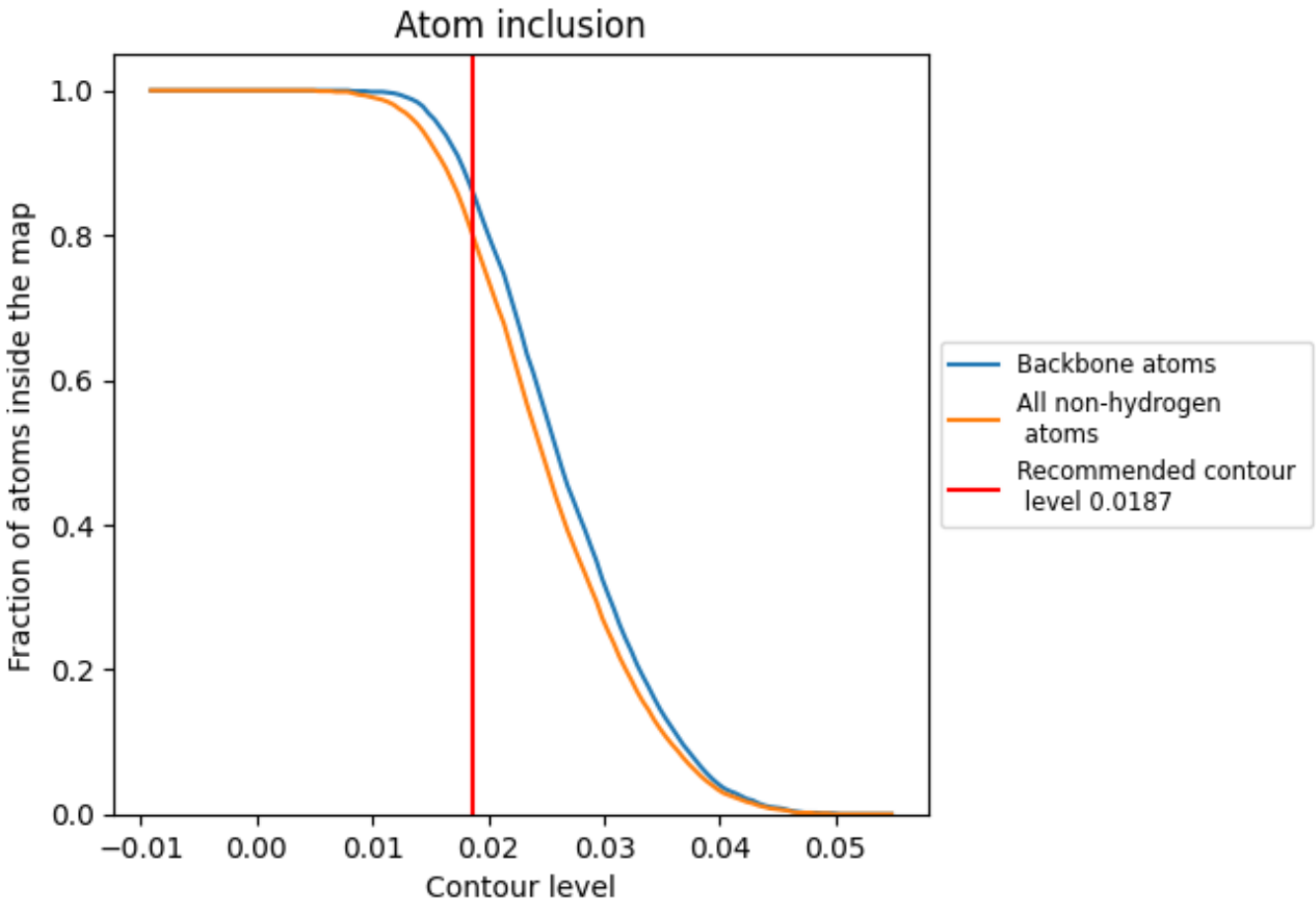
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0187).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.2580
A	0.6960	0.2520
AA	0.7820	0.2520
AB	0.8840	0.2690
AC	0.6660	0.2560
B	0.7840	0.2520
BA	0.8840	0.2620
BB	0.7960	0.2550
C	0.8880	0.2640
CA	0.8830	0.2660
CB	0.6710	0.2560
D	0.8870	0.2690
DA	0.7970	0.2560
DB	0.6900	0.2530
E	0.8010	0.2560
EA	0.6700	0.2560
EB	0.7800	0.2550
F	0.6690	0.2560
FA	0.6930	0.2550
FB	0.8830	0.2630
G	0.6960	0.2540
GA	0.7790	0.2530
GB	0.8830	0.2680
H	0.7840	0.2520
HA	0.8850	0.2630
HB	0.7960	0.2550
I	0.8840	0.2630
IA	0.8850	0.2670
IB	0.6700	0.2560
J	0.8840	0.2650
JA	0.7960	0.2580
JB	0.6940	0.2520
K	0.7960	0.2550
KA	0.6690	0.2540
KB	0.7810	0.2500

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
L	0.6730	0.2540
LA	0.6930	0.2550
LB	0.8850	0.2630
M	0.6940	0.2530
MA	0.7840	0.2540
MB	0.8820	0.2660
N	0.7820	0.2500
NA	0.8840	0.2650
NB	0.7960	0.2540
O	0.8860	0.2620
OA	0.8840	0.2700
OB	0.6730	0.2560
P	0.8800	0.2680
PA	0.8010	0.2570
PB	0.6960	0.2520
Q	0.7970	0.2570
QA	0.6710	0.2560
QB	0.7800	0.2520
R	0.6730	0.2550
RA	0.6960	0.2510
RB	0.8840	0.2640
S	0.6930	0.2540
SA	0.7860	0.2540
SB	0.8830	0.2670
T	0.7810	0.2520
TA	0.8850	0.2650
TB	0.7960	0.2550
UA	0.8850	0.2690
UB	0.6690	0.2550
V	0.8820	0.2640
VA	0.8010	0.2570
VB	0.6910	0.2530
W	0.8820	0.2660
WA	0.6730	0.2550
WB	0.7800	0.2520
X	0.7990	0.2570
XA	0.6940	0.2540
XB	0.8850	0.2620
Y	0.6750	0.2550
YA	0.7790	0.2540
YB	0.8830	0.2660
Z	0.6970	0.2530

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ZA	0.8830	0.2660
ZB	0.8000	0.2550