



Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 12:05 pm BST

PDB ID : 6ZW5
EMDB ID : EMD-11481
Title : C15 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

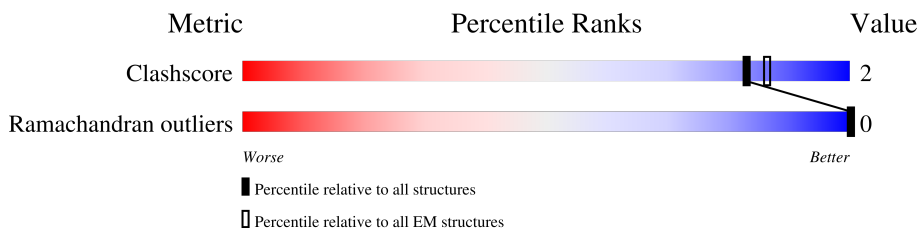
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

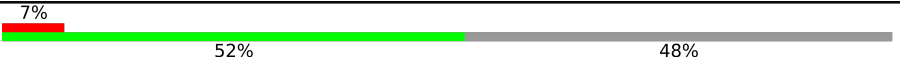





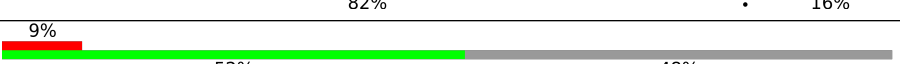
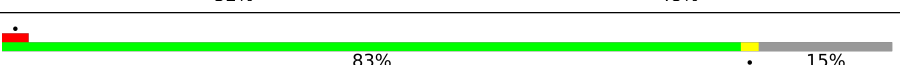

The reported resolution of this entry is 7.00 Å.

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 $\leq 5\%$. 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	
1	AA	258	
1	AB	258	
1	AC	258	
1	B	258	
1	BA	258	
1	BB	258	
1	BC	258	
1	C	258	

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Mol	Chain	Length	Quality of chain
1	CA	258	
1	CB	258	
1	CC	258	
1	D	258	
1	DA	258	
1	DB	258	
1	DC	258	
1	E	258	
1	EA	258	
1	EB	258	
1	EC	258	
1	F	258	
1	FA	258	
1	FB	258	
1	FC	258	
1	G	258	
1	GA	258	
1	GB	258	
1	GC	258	
1	H	258	
1	HA	258	
1	HB	258	
1	HC	258	
1	I	258	
1	IA	258	

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Mol	Chain	Length	Quality of chain
1	IB	258	
1	IC	258	
1	J	258	
1	JA	258	
1	JB	258	
1	JC	258	
1	K	258	
1	KA	258	
1	KB	258	
1	KC	258	
1	L	258	
1	LA	258	
1	LB	258	
1	LC	258	
1	M	258	
1	MA	258	
1	MB	258	
1	MC	258	
1	N	258	
1	NA	258	
1	NB	258	
1	O	258	
1	OA	258	
1	OB	258	
1	P	258	




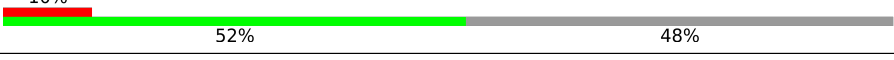
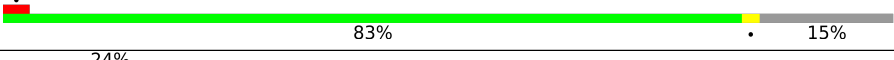
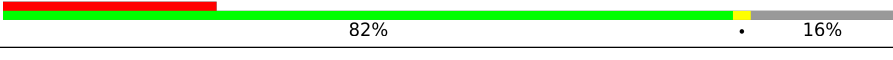
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Mol	Chain	Length	Quality of chain
1	PA	258	
1	PB	258	
1	Q	258	
1	QA	258	
1	QB	258	
1	R	258	
1	RA	258	
1	RB	258	
1	S	258	
1	SA	258	
1	SB	258	
1	T	258	
1	TA	258	
1	TB	258	
1	UA	258	
1	UB	258	
1	V	258	
1	VA	258	
1	VB	258	
1	W	258	
1	WA	258	
1	WB	258	
1	X	258	
1	XA	258	
1	XB	258	

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Mol	Chain	Length	Quality of chain
1	Y	258	
1	YA	258	
1	YB	258	
1	Z	258	
1	ZA	258	
1	ZB	258	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 86775 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	C	N	O	0	0
			661	395	133	133		
1	B	219	Total	C	N	O	0	0
			1086	648	219	219		
1	C	219	Total	C	N	O	0	0
			1086	648	219	219		
1	D	219	Total	C	N	O	0	0
			1086	648	219	219		
1	E	218	Total	C	N	O	0	0
			1081	645	218	218		
1	F	158	Total	C	N	O	0	0
			785	469	158	158		
1	G	133	Total	C	N	O	0	0
			661	395	133	133		
1	H	219	Total	C	N	O	0	0
			1086	648	219	219		
1	I	219	Total	C	N	O	0	0
			1086	648	219	219		
1	J	219	Total	C	N	O	0	0
			1086	648	219	219		
1	K	218	Total	C	N	O	0	0
			1081	645	218	218		
1	L	158	Total	C	N	O	0	0
			785	469	158	158		
1	M	133	Total	C	N	O	0	0
			661	395	133	133		
1	N	219	Total	C	N	O	0	0
			1086	648	219	219		
1	O	219	Total	C	N	O	0	0
			1086	648	219	219		
1	P	219	Total	C	N	O	0	0
			1086	648	219	219		
1	Q	218	Total	C	N	O	0	0
			1081	645	218	218		

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

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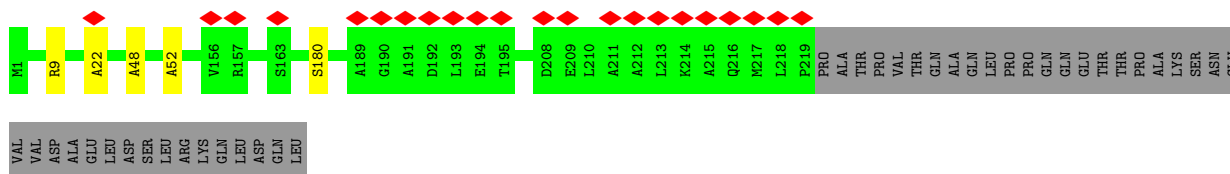
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Mol	Chain	Residues	Atoms				AltConf	Trace
1	IB	158	Total 785	C 469	N 158	O 158	0	0
1	JB	133	Total 661	C 395	N 133	O 133	0	0
1	KB	219	Total 1086	C 648	N 219	O 219	0	0
1	LB	219	Total 1086	C 648	N 219	O 219	0	0
1	MB	219	Total 1086	C 648	N 219	O 219	0	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
1	VB	133	Total 661	C 395	N 133	O 133	0	0
1	WB	219	Total 1086	C 648	N 219	O 219	0	0
1	XB	219	Total 1086	C 648	N 219	O 219	0	0
1	YB	219	Total 1086	C 648	N 219	O 219	0	0
1	ZB	218	Total 1081	C 645	N 218	O 218	0	0
1	AC	158	Total 785	C 469	N 158	O 158	0	0
1	BC	133	Total 661	C 395	N 133	O 133	0	0
1	CC	219	Total 1086	C 648	N 219	O 219	0	0

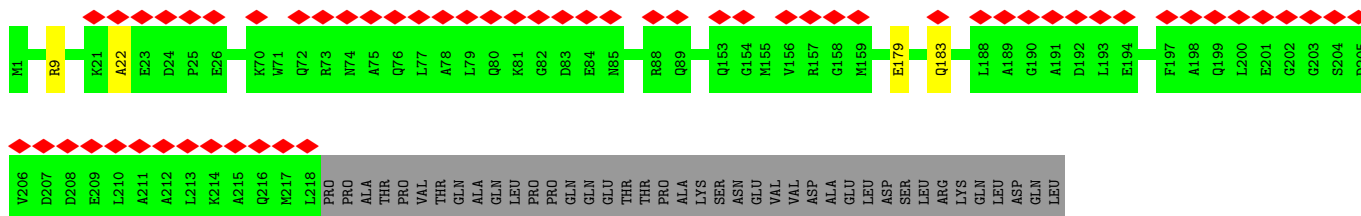
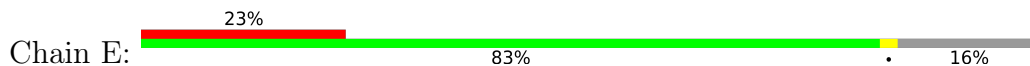
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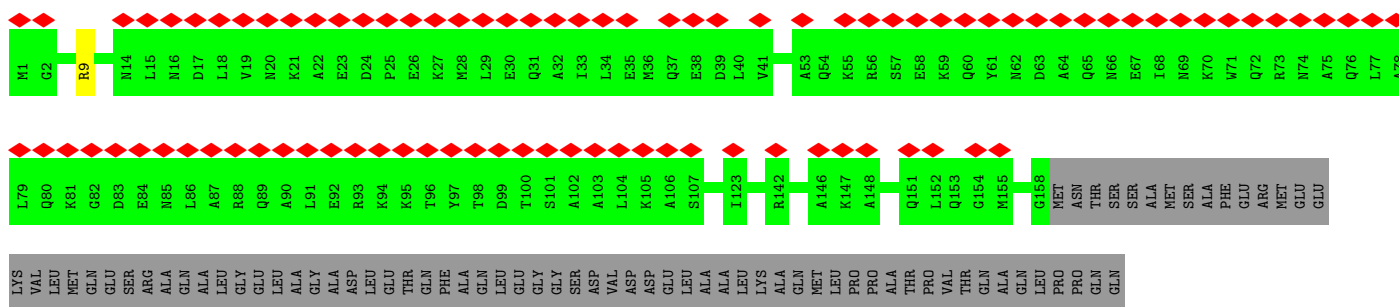
Mol	Chain	Residues	Atoms				AltConf	Trace
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			1086	648	219	219		
1	EC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	FC	218	Total	C	N	O	0	0
			1081	645	218	218		
1	GC	158	Total	C	N	O	0	0
			785	469	158	158		
1	HC	133	Total	C	N	O	0	0
			661	395	133	133		
1	IC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	JC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	KC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	LC	218	Total	C	N	O	0	0
			1081	645	218	218		
1	MC	158	Total	C	N	O	0	0
			785	469	158	158		



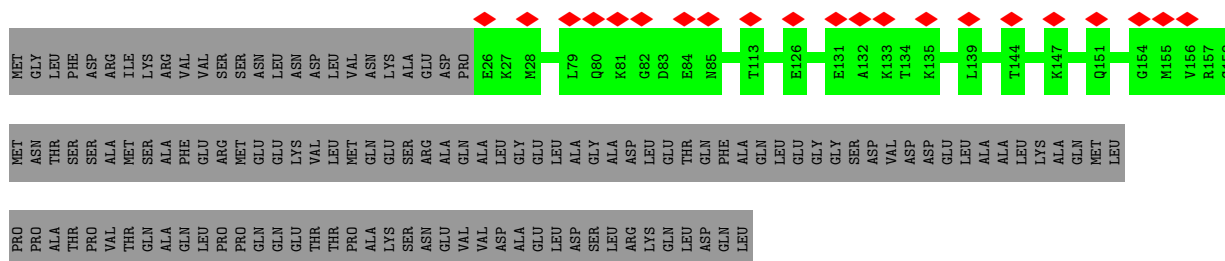
- Molecule 1: vipp1



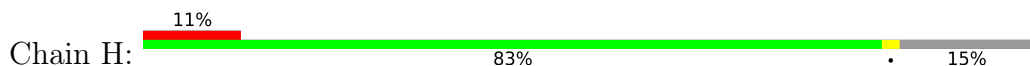
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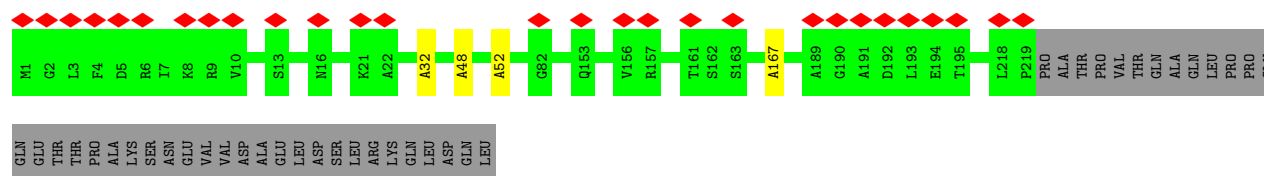


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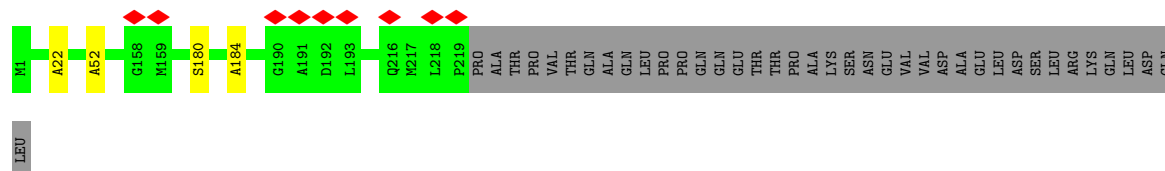
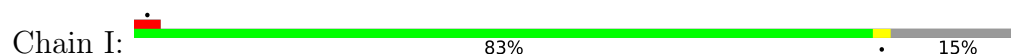


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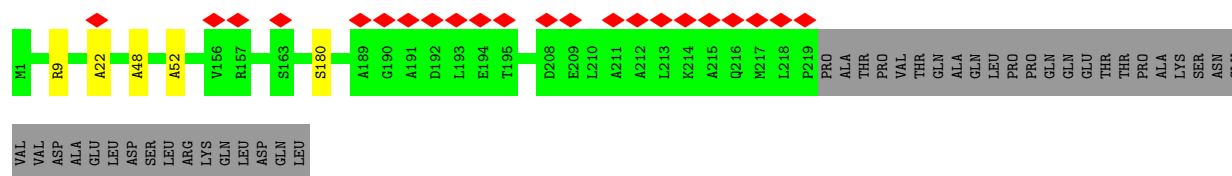
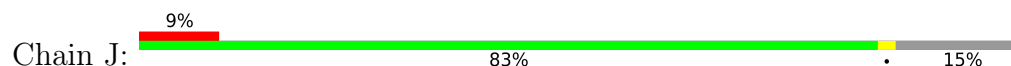




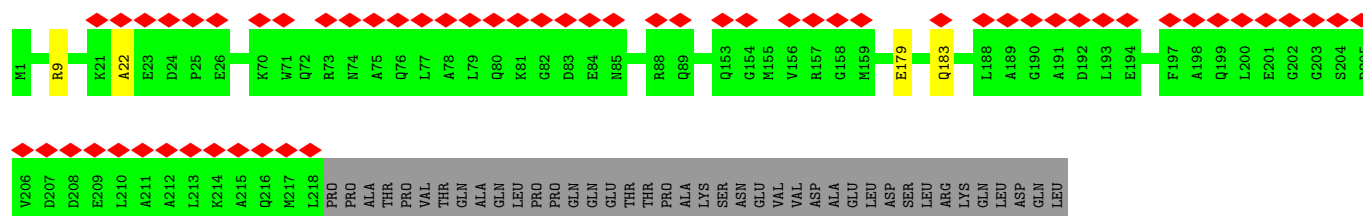
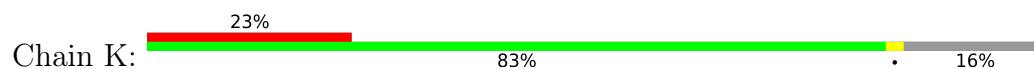
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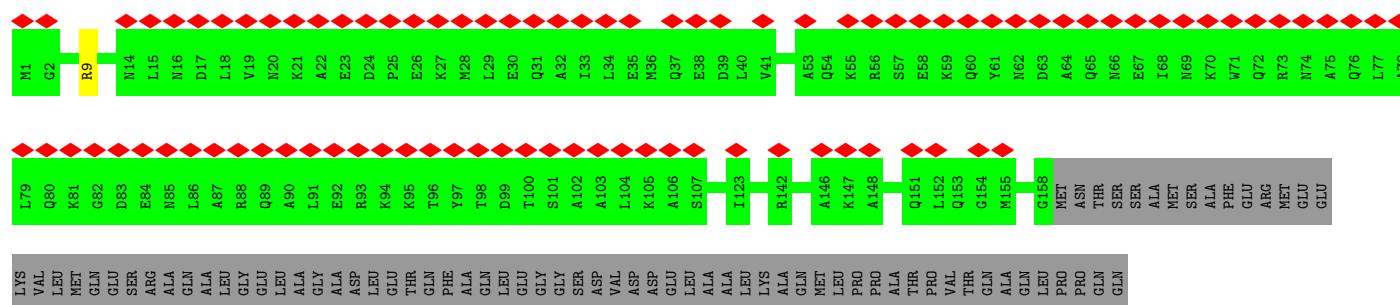
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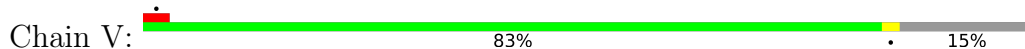


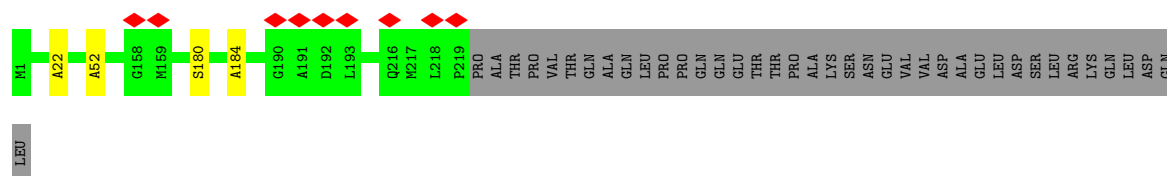
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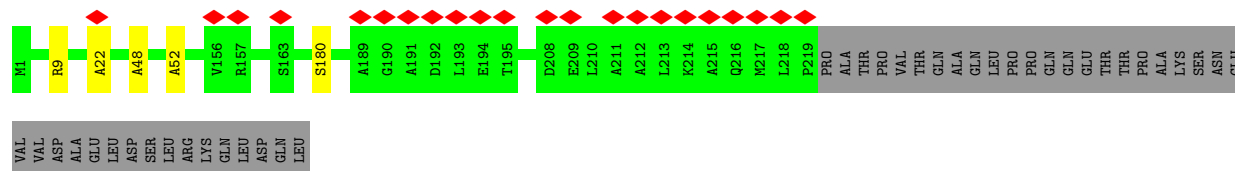
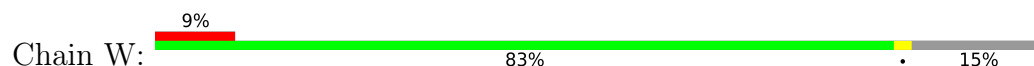
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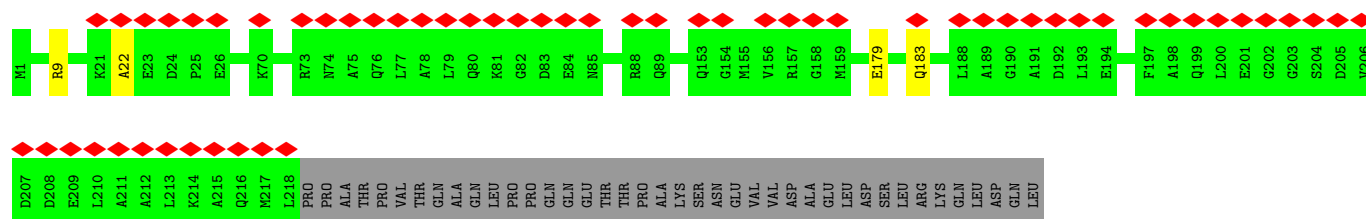
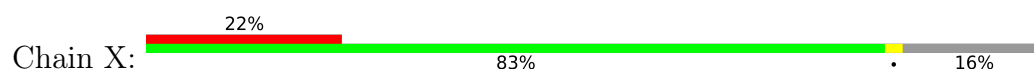




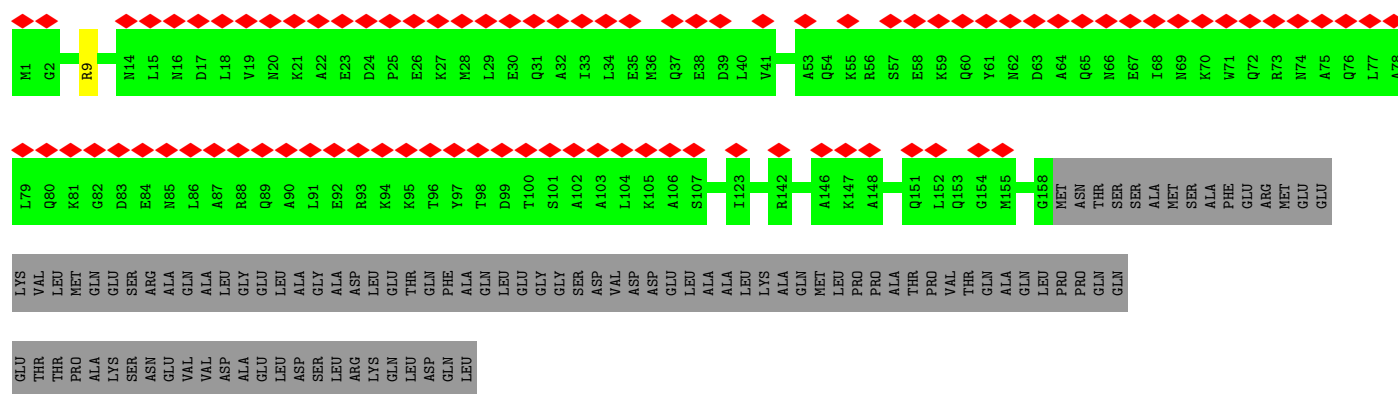
• Molecule 1: vipp1



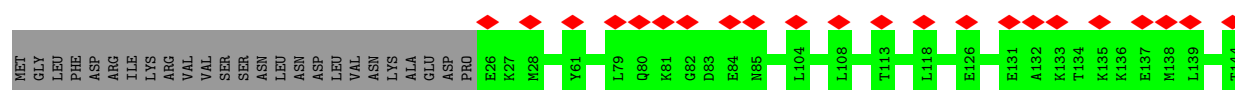
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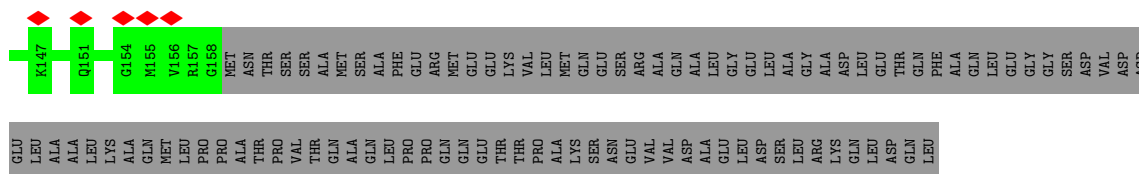


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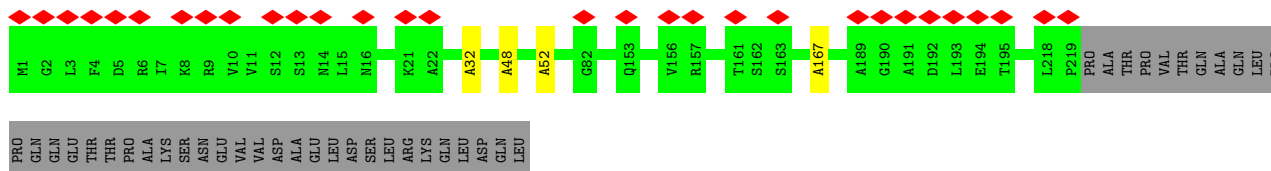
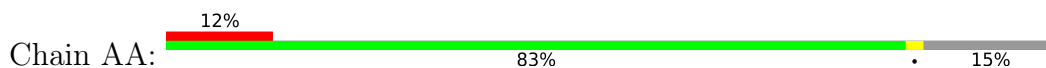


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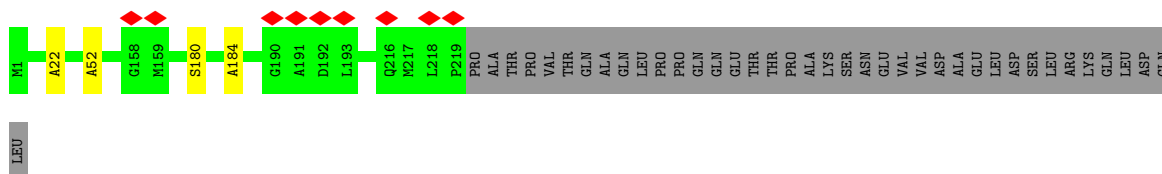
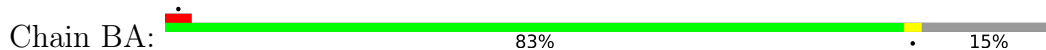




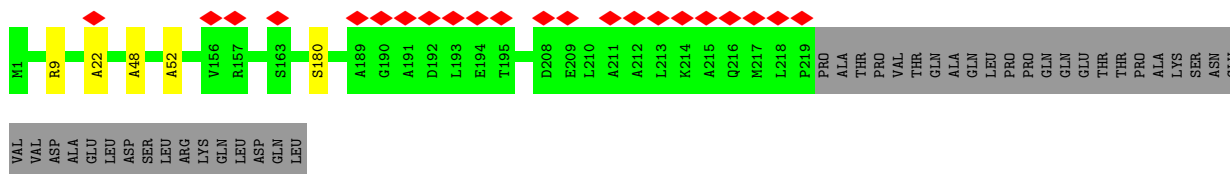
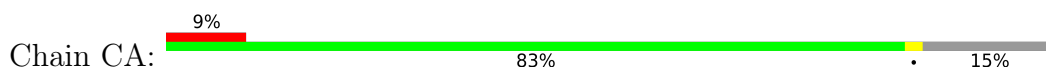
• Molecule 1: vipp1



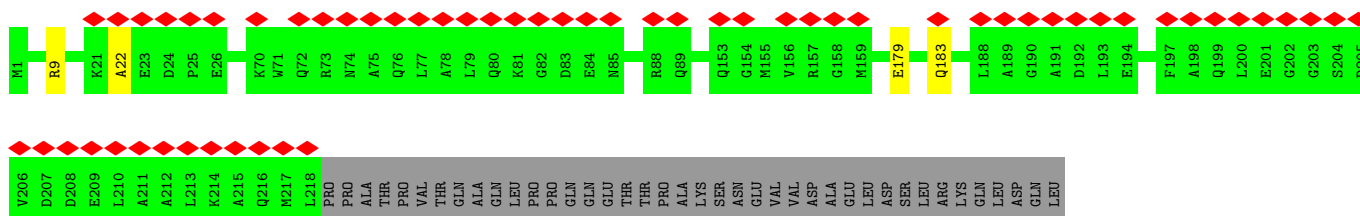
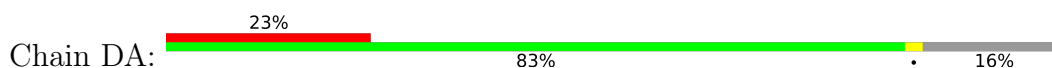
• Molecule 1: vipp1



• Molecule 1: vipp1

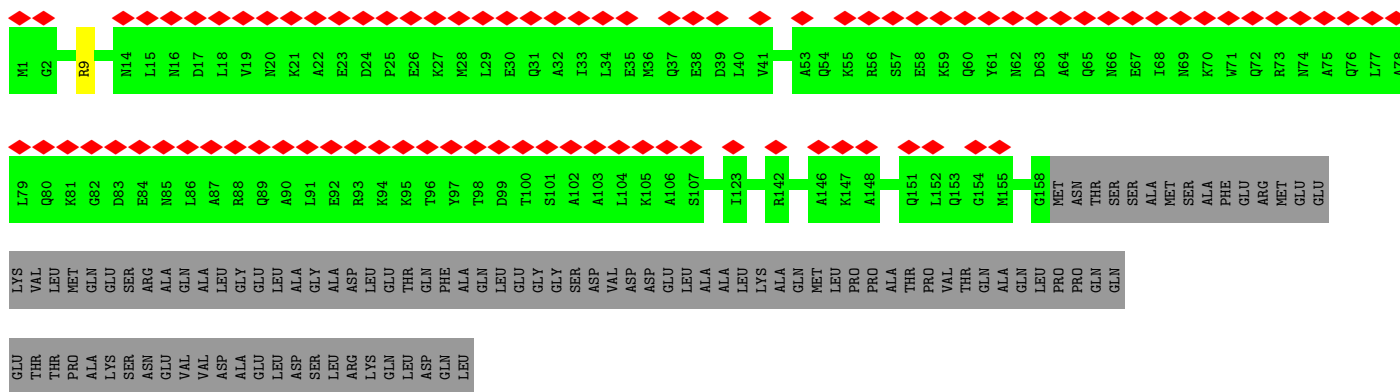


• Molecule 1: vipp1

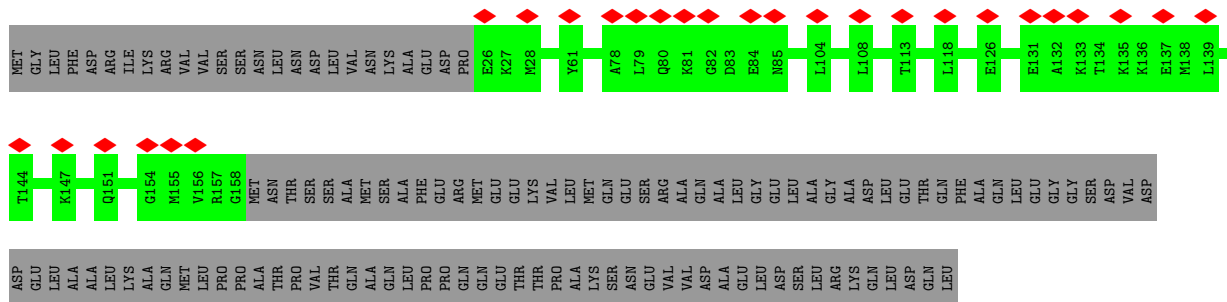


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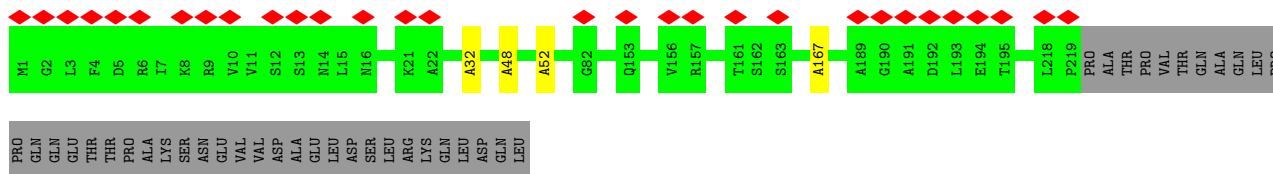
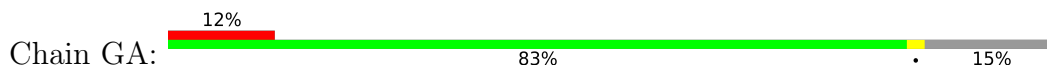




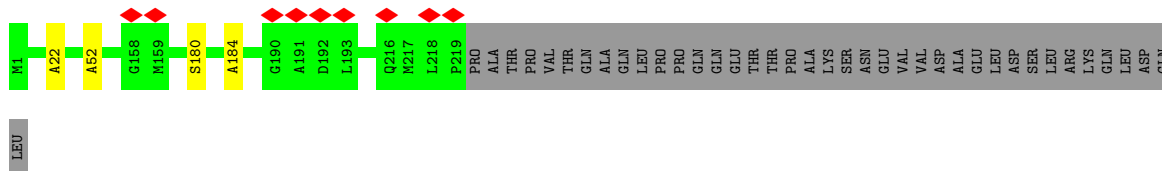
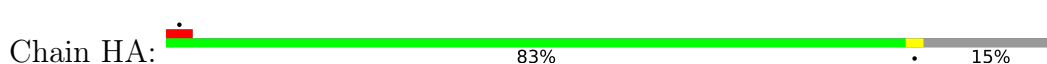
- Molecule 1: vippp1



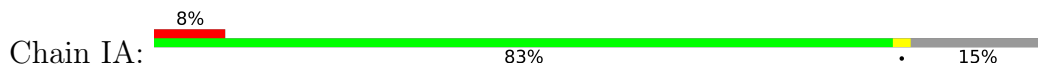
- Molecule 1: vippp1

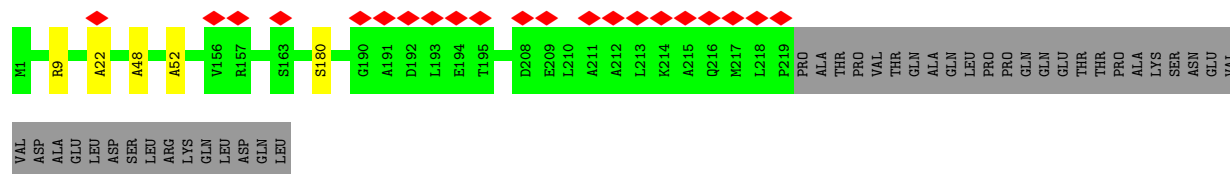


- Molecule 1: vippp1

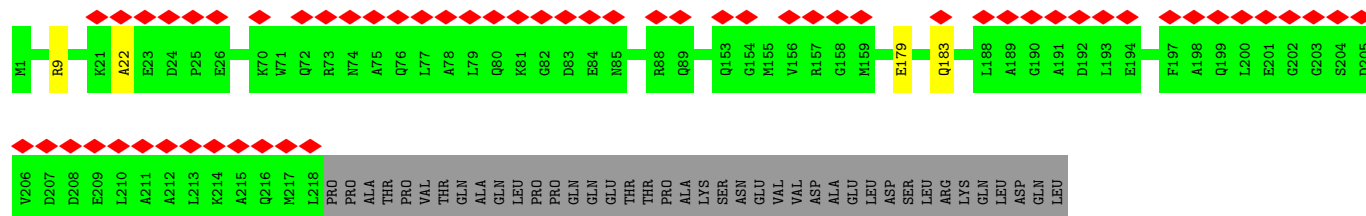
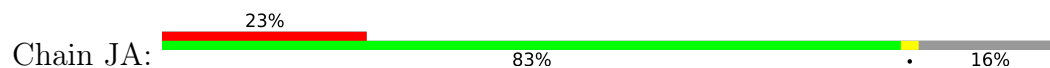


- Molecule 1: vippp1

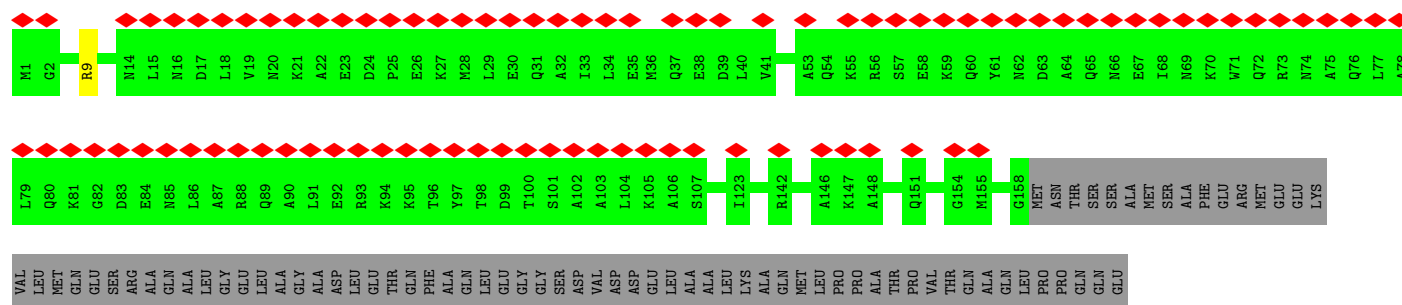




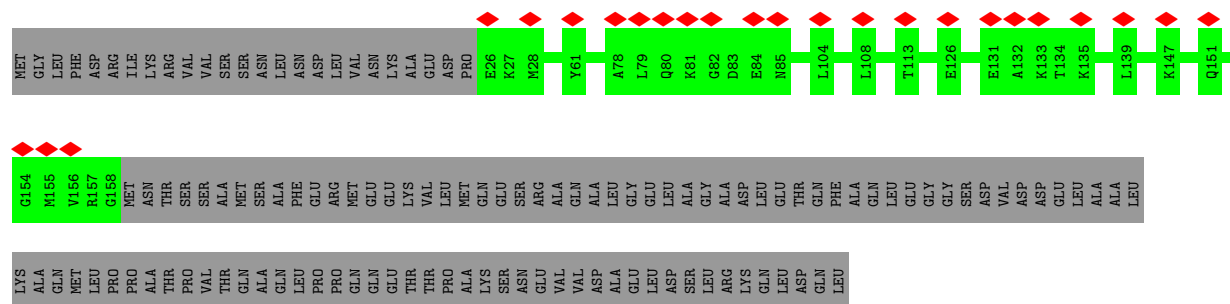
• Molecule 1: vipp1



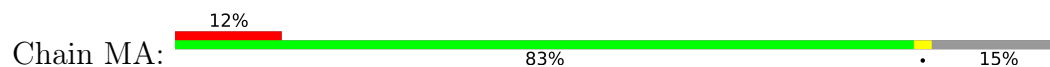
• Molecule 1: vipp1

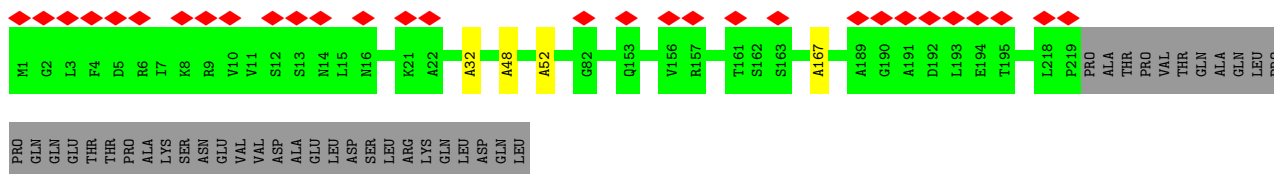


• Molecule 1: vipp1



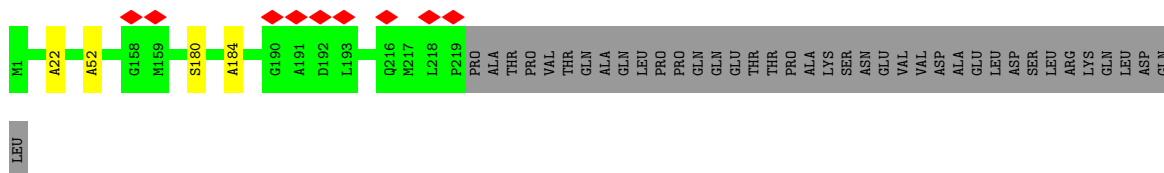
• Molecule 1: vipp1





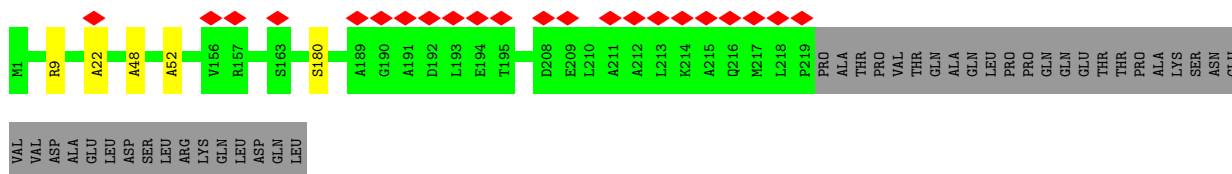
• Molecule 1: vipp1

Chain NA: 83% 15%



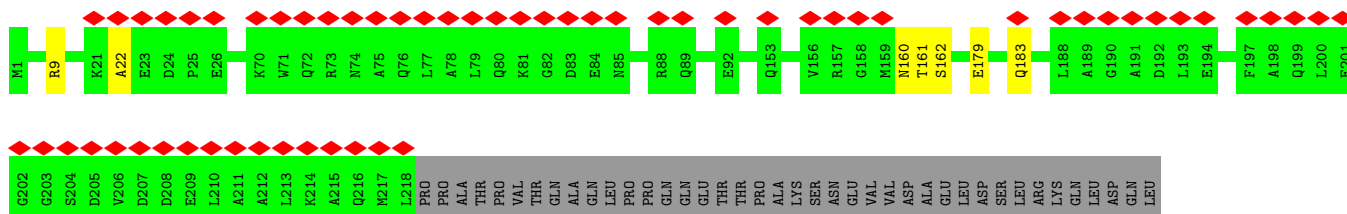
• Molecule 1: vipp1

Chain OA: 9% 83% 15%



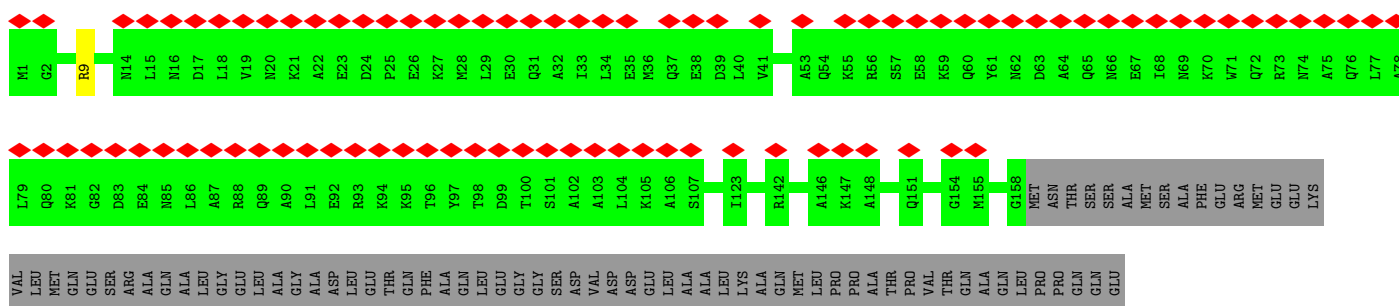
• Molecule 1: vipp1

Chain PA: 23% 82% 16%



• Molecule 1: vipp1

Chain QA: 35% 61% 39%



THR
THR
PRO
ALA
LYS
SER
ASN
GLU
VAL
VAL
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ALA
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ASP
SER
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ARG
LYS
GLN
LEU
ASP
GLN
LEU

• Molecule 1: vipp1

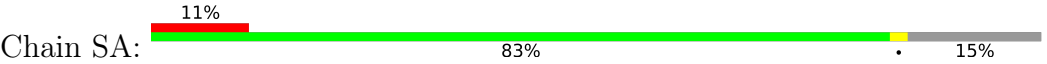


MET
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ASP
PRO
E26
L79
Q80
K91
G82
D83
E84
N85
L104
T113
E126
E131
A132
K133
T134
K135
L139
K147
Q151
G154
M155
V156
R157
G158
MET
ASN

THR
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ASP
ASP
GLU
LEU
ALA
ALA
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ALA
GLN
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GLU
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PRO
ALA
GLU
SER
LYS
GLN
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GLN
LEU

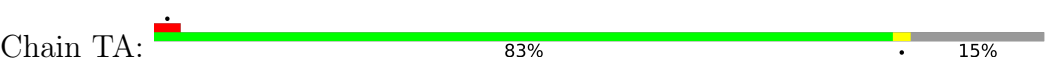
• Molecule 1: vipp1



M1
Q2
L3
F4
D5
R6
I7
K8
R9
V10
S13
M16
K21
A22
A32
A48
A52
G82
Q153
V156
R157
T161
S162
S163
A167
A189
G190
A191
D192
L193
E194
T195
L218
P219
PRO
ALA
THR
PRO
VAL
THR
GLN
ALA
GLN
LEU
PRO
GLN

GLN
GLU
THR
THR
PRO
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LYS
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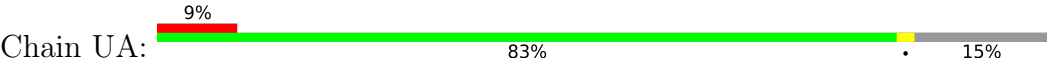
• Molecule 1: vipp1



M1
A22
A52
G158
M159
S180
A184
G190
A191
D192
L193
Q216
M217
L218
P219
PRO
ALA
THR
PRO
VAL
THR
GLN
GLN
GLN
LEU
PRO
PRO
GLN
GLU
THR
THR
PRO
ALA
LYS
SER
ASN
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GLN
GLN

LEU

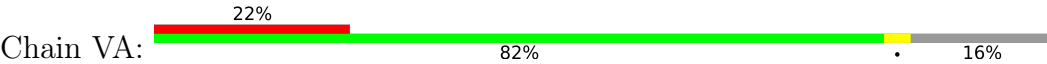
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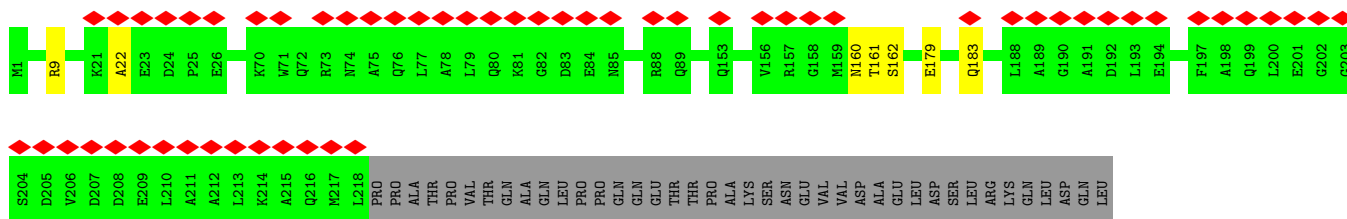


M1
R9
A22
A48
A52
V156
R157
S163
S180
A189
G190
A191
D192
L193
E194
T195
D208
E209
L210
A211
A212
L213
K214
A215
Q216
M217
L218
P219
PRO
ALA
THR
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THR
GLN
GLN
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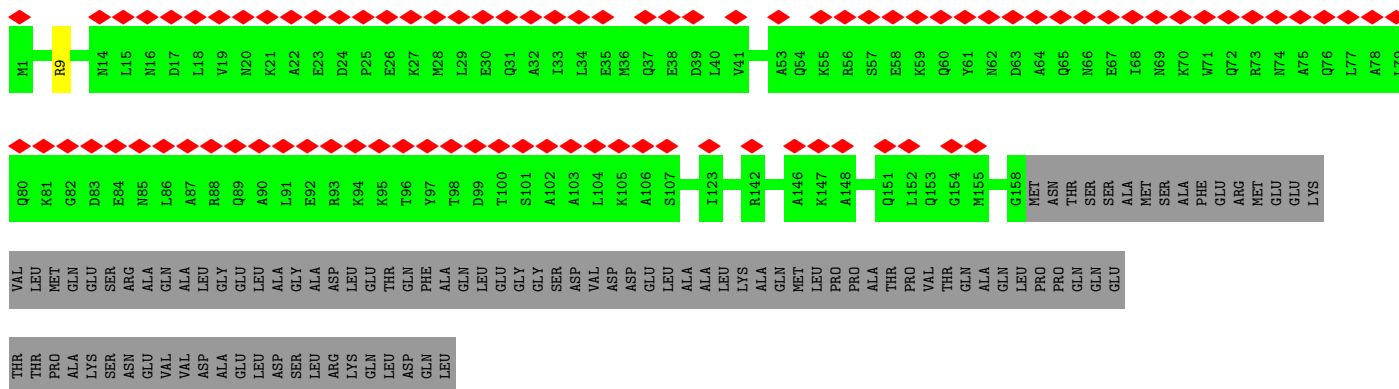
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VAL
ASP
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GLU
LEU
ASP
SER
LEU
LYS
ARG
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ASP
GLN
LEU

• Molecule 1: vipp1

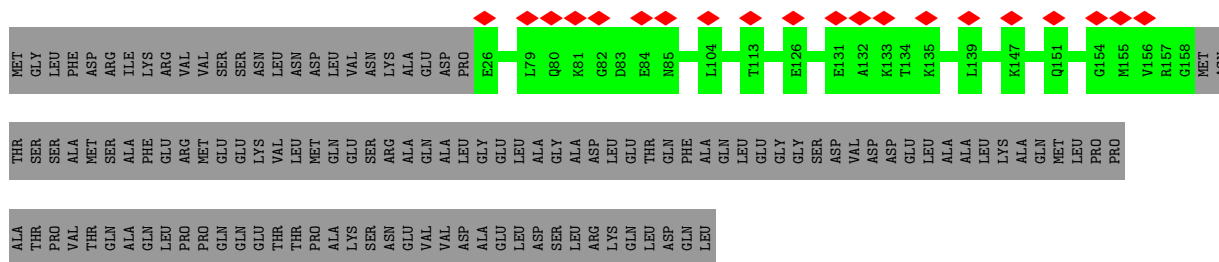




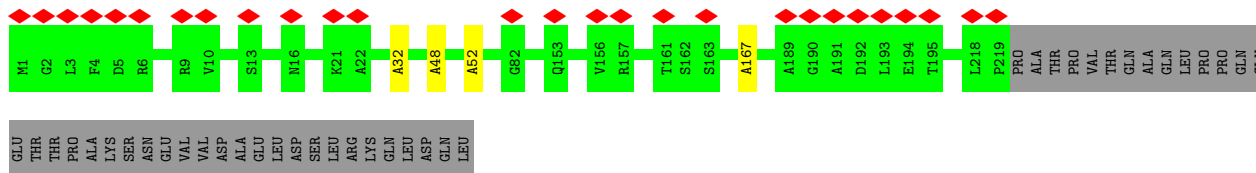
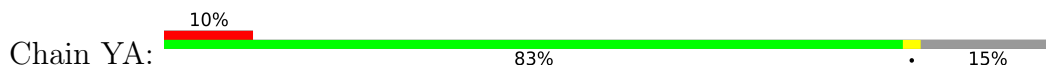
• Molecule 1: vipp1



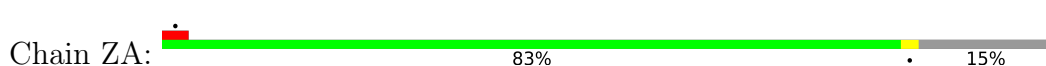
• Molecule 1: vipp1

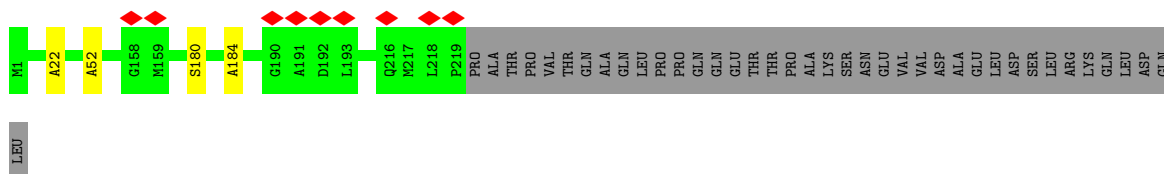


• Molecule 1: vipp1

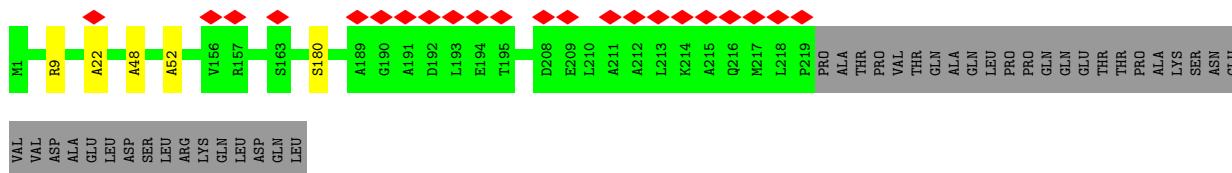
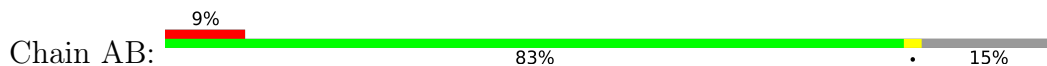


• Molecule 1: vipp1

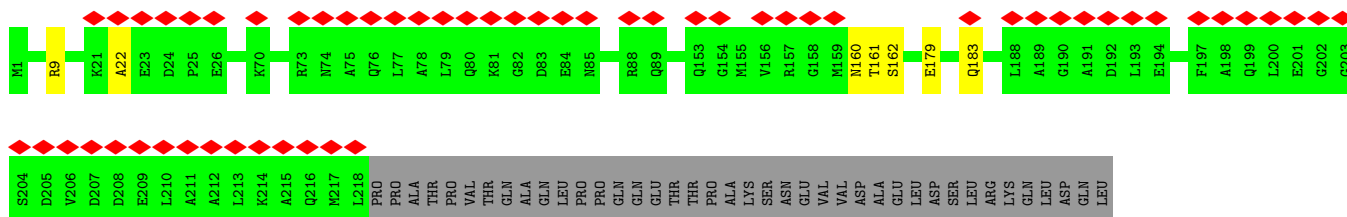
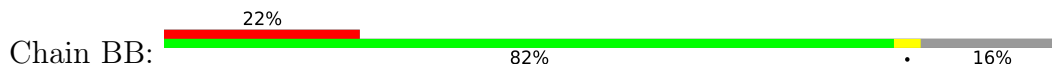




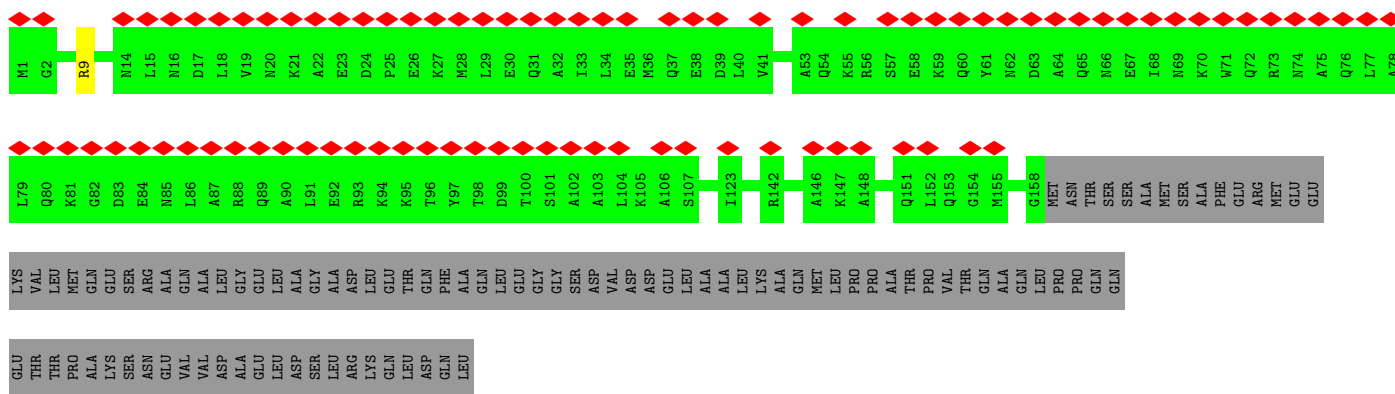
- Molecule 1: vipp1



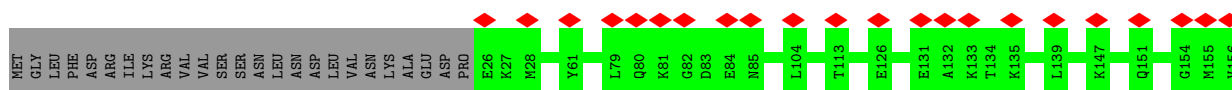
- Molecule 1: vipp1

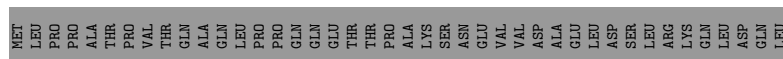
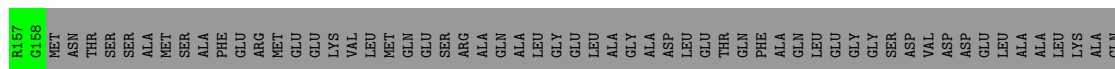


- Molecule 1: vipp1

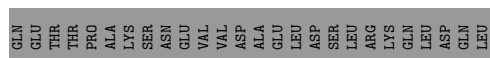
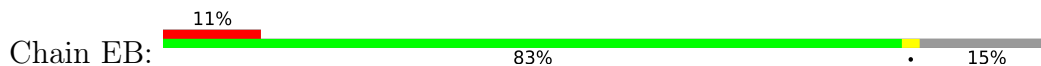


- Molecule 1: vipp1

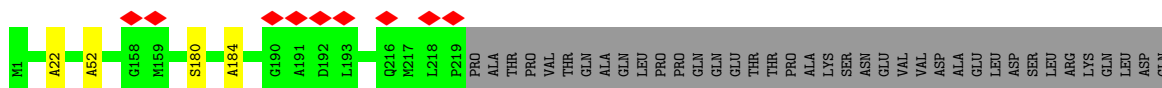
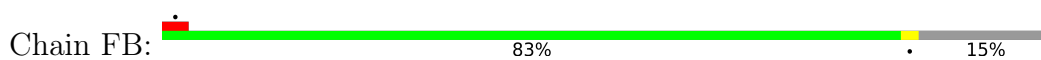




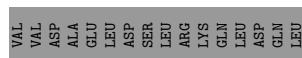
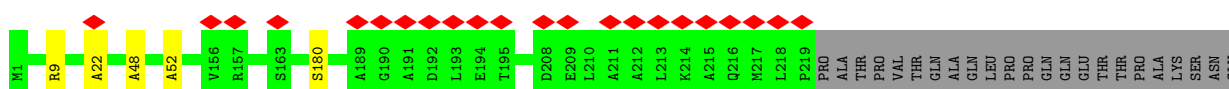
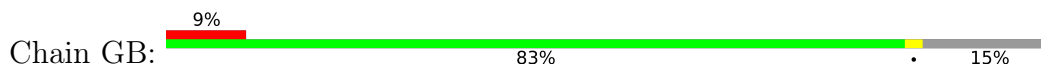
• Molecule 1: vipp1



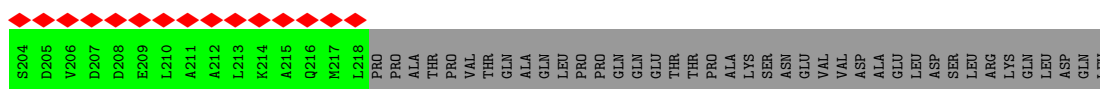
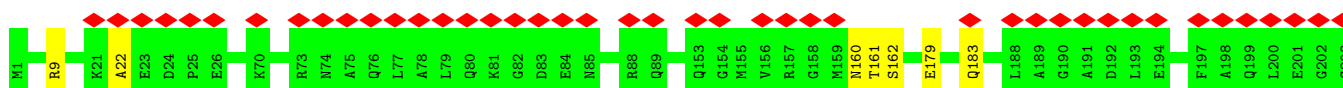
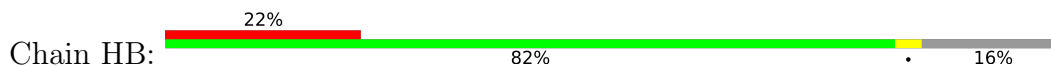
• Molecule 1: vipp1



• Molecule 1: vipp1

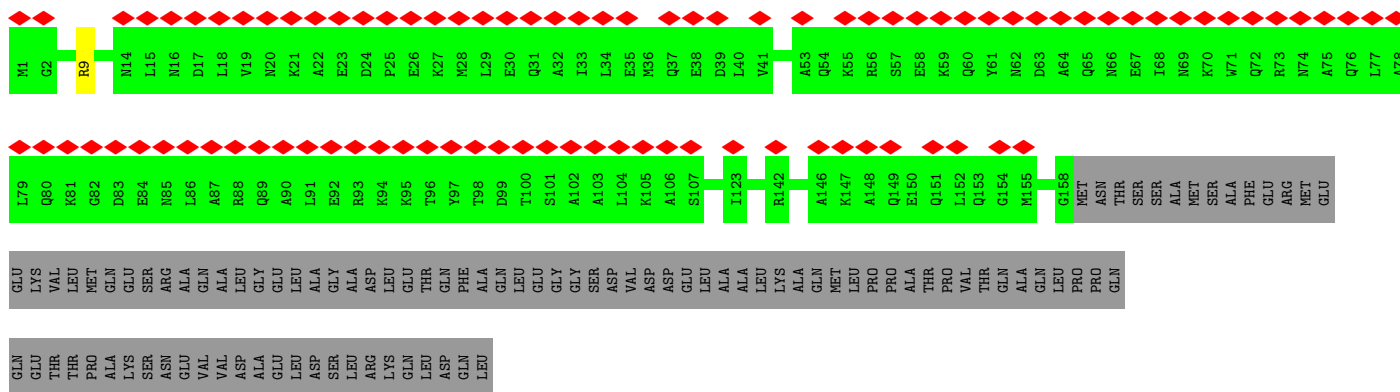


• Molecule 1: vipp1

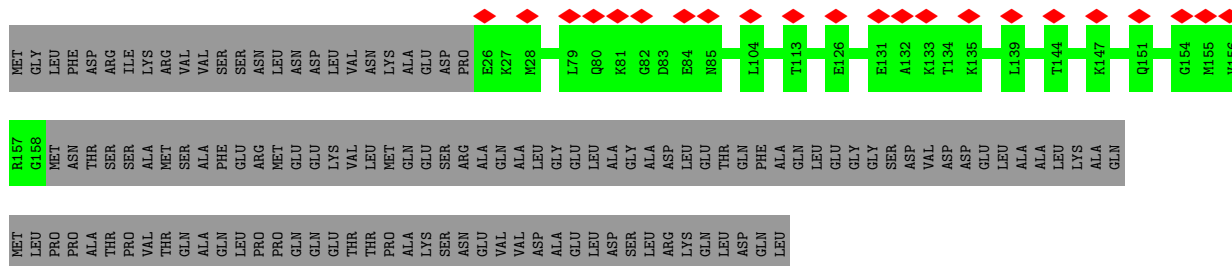


• Molecule 1: vipp1

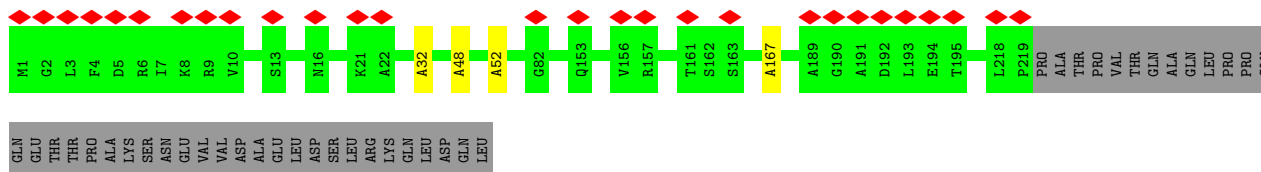
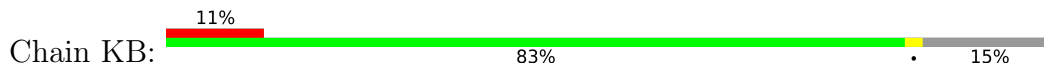




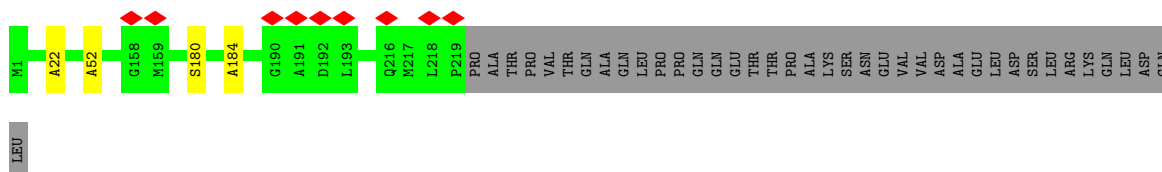
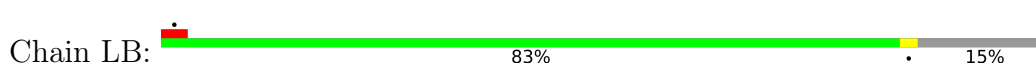
- Molecule 1: vippp1



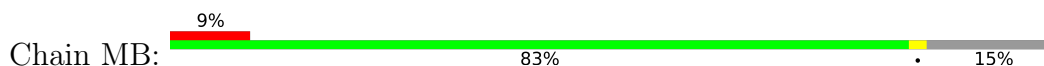
- Molecule 1: vippp1

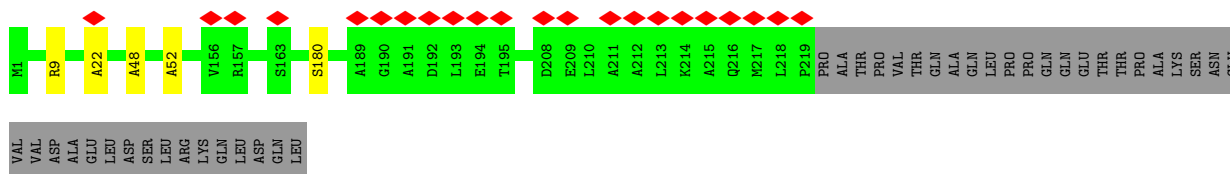


- Molecule 1: vippp1

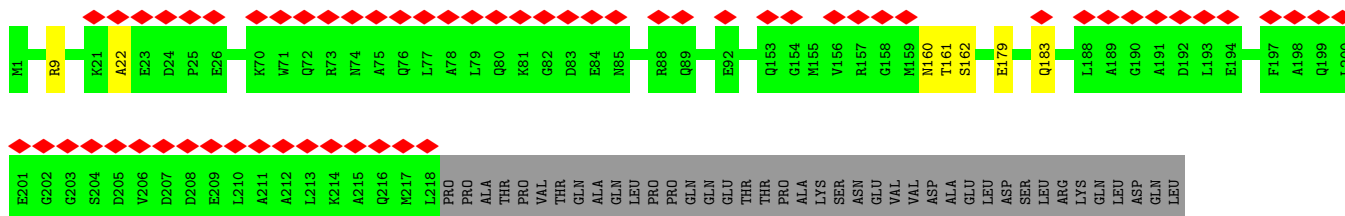
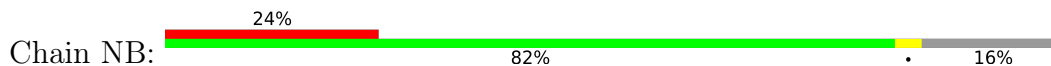


- Molecule 1: vippp1

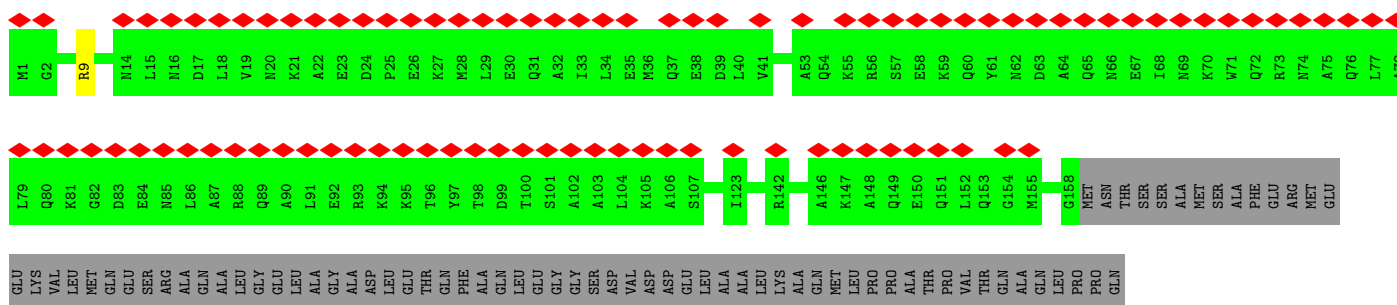




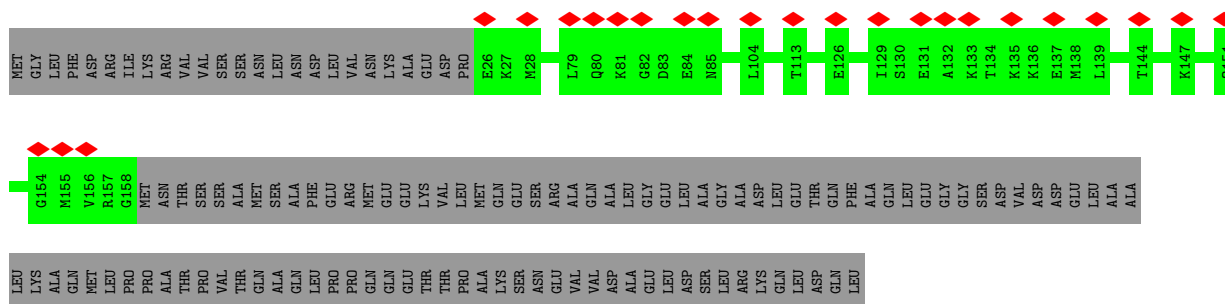
- Molecule 1: vipp1



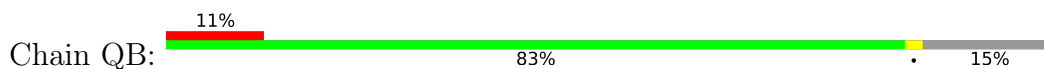
- Molecule 1: vipp1

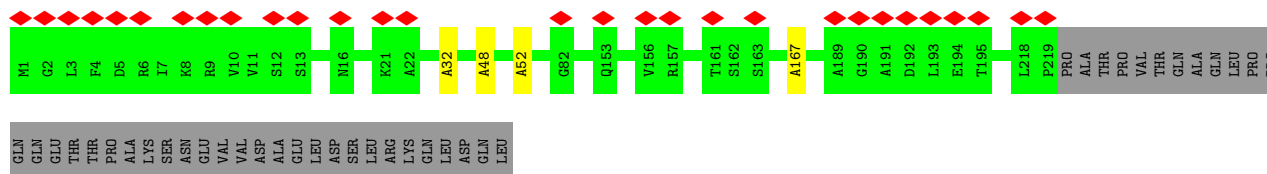


- Molecule 1: vipp1



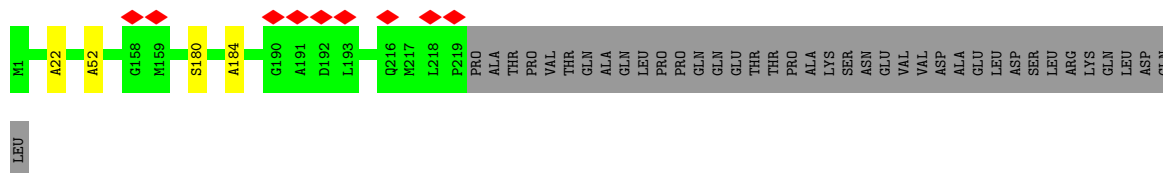
- Molecule 1: vipp1





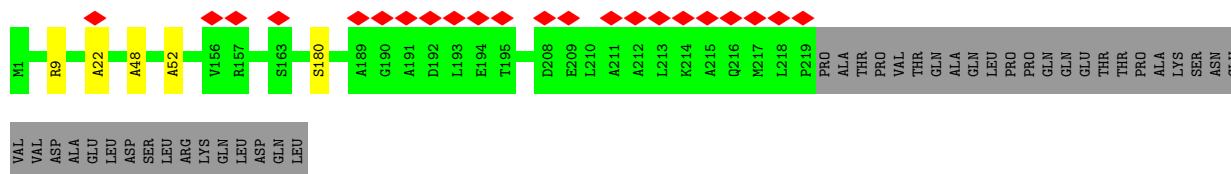
• Molecule 1: vipp1

Chain RB: 83% 15%



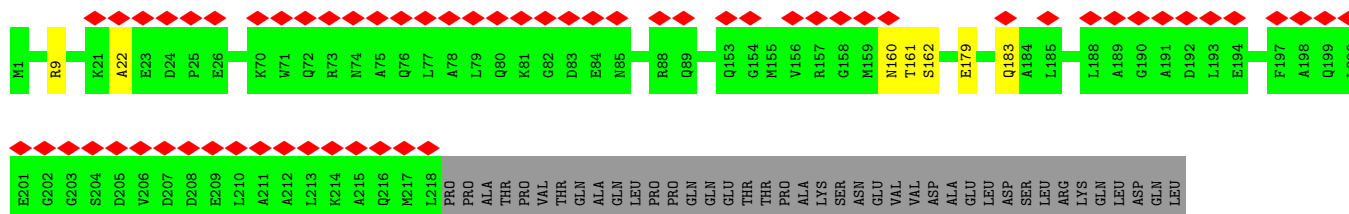
• Molecule 1: vipp1

Chain SB: 9% 83% 15%



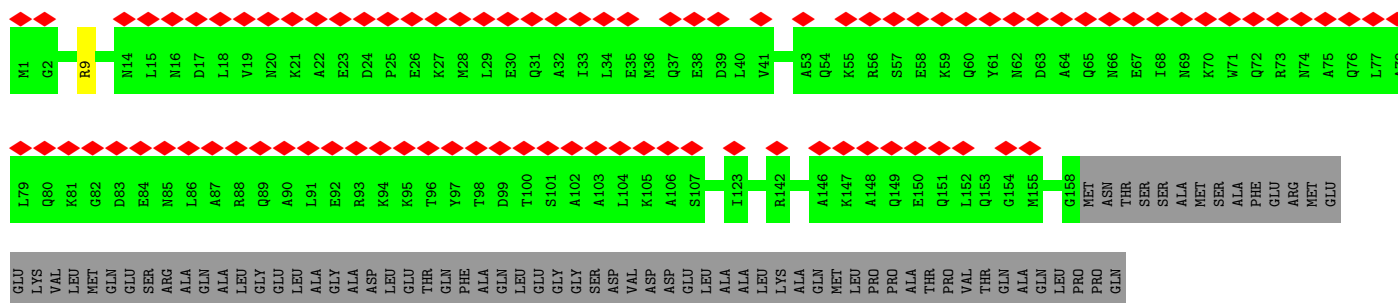
• Molecule 1: vipp1

Chain TB: 24% 82% 16%



• Molecule 1: vipp1

Chain UB: 36% 61% 39%



GLN
GLU
THR
THR
PRO
ALA
LYS
SER
ASN
GLU
VAL
VAL
SER
ASP
ALA
GLU
LEU
ASP
SER
LEU
ARG
LYS
GLN
LEU
ASP
GLN
LEU

• Molecule 1: vipp1

Chain VB: 9% 52% 48%

MET
GLY
PHE
ASP
ASN
ILE
LYS
ARG
VAL
VAL
SER
SER
ASN
ALA
GLU
LEU
ASP
PRO
E26
K27
M28
L79
Q80
K81
G82
D83
E84
N85
L104
L108
T113
E126
I129
S130
E131
A132
K133
T134
K135
L139
K147
Q151
G154

M155
V156
R157
G158
MET
THR
SER
SER
ALA
MET
PHE
ALA
GLN
LEU
PRO
ARG
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GLN
GLU
LYS
VAL
LEU
MET
GLN
LYS
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LEU
THR
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SER
ASP
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LEU
LYS

ALA
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GLN
THR
THR
PRO
PRO
LYS
SER
ASN
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VAL
VAL
ASP
ALA
GLY
LEU
LEU
ASP
SER
LEU
ARG
LYS
GLN
ASP
GLN
LEU

• Molecule 1: vipp1

Chain WB: 11% 83% 15%

M1
Q2
L3
F4
D5
R6
I7
K8
R9
V10
S13
M14
L15
N16
K21
A22
A32
A48
A52
G82
Q153
V156
R157
T161
S162
S163
A167
A189
G190
A191
D192
L193
E194
T195
L218
P219
PRO
ALA
THR
PRO
VAL
GLN
GLN
LEU
PRO
PRO

GLN
GLN
THR
THR
PRO
PRO
ALA
LYS
SER
ASN
GLU
VAL
VAL
ASP
GLN
GLN
GLU
LEU
LEU
ASP
SER
LEU
ARG
LYS
GLN
LEU
ASP
GLN
LEU

• Molecule 1: vipp1

Chain XB: 83% 15%

M1
A22
A52
G158
M159
S180
A184
G190
A191
D192
Q216
M217
L218
P219
PRO
ALA
THR
PRO
VAL
THR
GLN
ALA
GLN
LEU
PRO
PRO
GLN
GLN
THR
THR
PRO
ALA
LYS
SER
ASN
GLU
VAL
VAL
ASP
GLU
GLU
LEU
SER
SER
LEU
ARG
LYS
GLN
LEU
ASP
GLN
LEU

• Molecule 1: vipp1

Chain YB: 9% 83% 15%

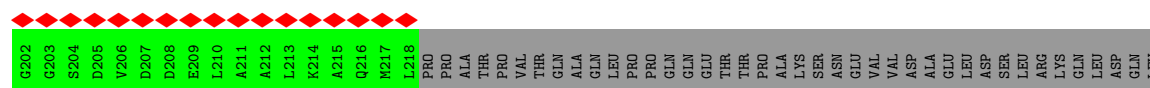
M1
R9
A22
A48
A52
V156
R157
S163
S180
A189
G190
A191
D192
L193
E194
T195
D208
E209
L210
A211
A212
L213
K214
A215
Q216
M217
L218
P219
PRO
ALA
THR
PRO
VAL
THR
GLN
GLN
GLN
LEU
PRO
PRO
GLN
GLN
THR
THR
PRO
ALA
GLU
ASN
GLU

VAL
VAL
ASP
ALA
GLU
LEU
ASP
SER
ARG
LYS
GLN
GLN
ASP
GLN
LEU

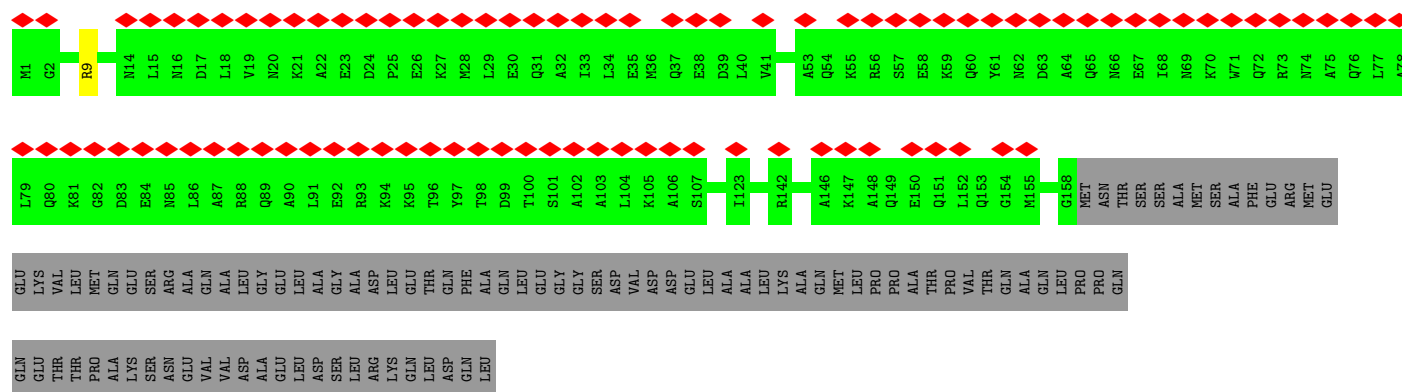
• Molecule 1: vipp1

Chain ZB: 24% 82% 16%

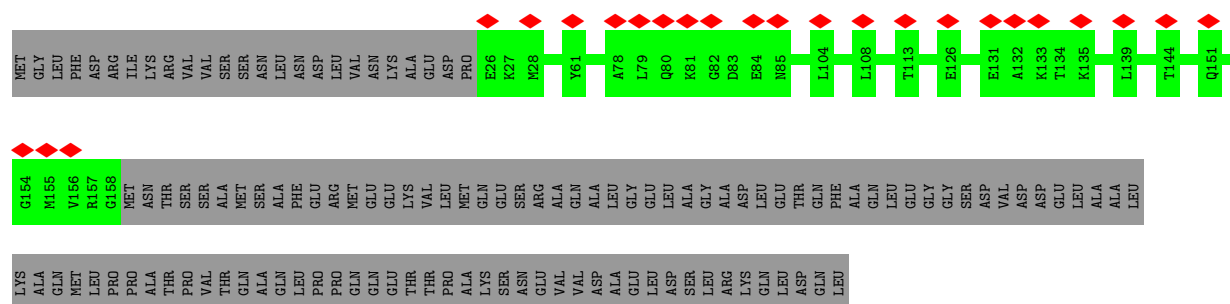
M1
R9
K21
A22
E23
D24
P25
E26
K70
W71
Q72
R73
N74
A75
Q76
L77
A78
L79
Q80
K81
G82
D83
E84
N85
R88
Q89
E92
Q153
G154
M155
V156
R157
G158
M159
M160
T161
E179
Q183
L188
A189
G190
A191
D192
L193
E194
F197
A198
Q199
L200
E201



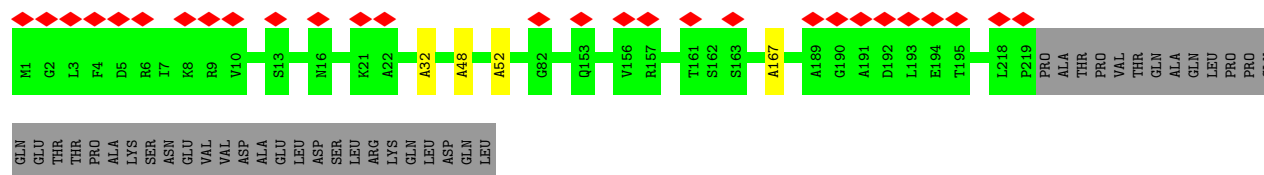
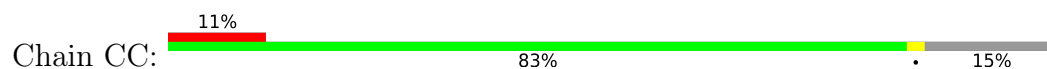
• Molecule 1: vipp1



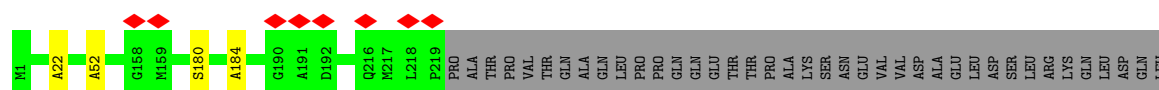
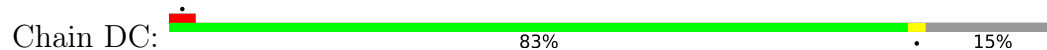
• Molecule 1: vipp1



• Molecule 1: vipp1



• Molecule 1: vipp1



GLU
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LEU
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SER
LEU
ARG
LYS
GLN
LEU
ASP
GLN
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18217	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 ($e^-/\text{\AA}^2$)	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	0.046	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0182	Depositor
Map size (\AA)	467.04, 467.04, 467.04	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.18	0/660	0.37	0/920
1	AA	0.18	0/1085	0.39	0/1512
1	AB	0.19	0/1085	0.39	0/1512
1	AC	0.18	0/784	0.37	0/1093
1	B	0.18	0/1085	0.39	0/1512
1	BA	0.19	0/1085	0.44	0/1512
1	BB	0.21	0/1080	0.42	0/1505
1	BC	0.18	0/660	0.37	0/920
1	C	0.19	0/1085	0.44	0/1512
1	CA	0.19	0/1085	0.39	0/1512
1	CB	0.18	0/784	0.37	0/1093
1	CC	0.18	0/1085	0.39	0/1512
1	D	0.19	0/1085	0.39	0/1512
1	DA	0.21	0/1080	0.42	0/1505
1	DB	0.18	0/660	0.37	0/920
1	DC	0.19	0/1085	0.44	0/1512
1	E	0.21	0/1080	0.42	0/1505
1	EA	0.18	0/784	0.37	0/1093
1	EB	0.18	0/1085	0.39	0/1512
1	EC	0.19	0/1085	0.39	0/1512
1	F	0.18	0/784	0.37	0/1093
1	FA	0.18	0/660	0.37	0/920
1	FB	0.19	0/1085	0.44	0/1512
1	FC	0.21	0/1080	0.42	0/1505
1	G	0.18	0/660	0.37	0/920
1	GA	0.19	0/1085	0.39	0/1512
1	GB	0.19	0/1085	0.39	0/1512
1	GC	0.18	0/784	0.37	0/1093
1	H	0.19	0/1085	0.39	0/1512
1	HA	0.19	0/1085	0.44	0/1512
1	HB	0.21	0/1080	0.42	0/1505
1	HC	0.18	0/660	0.37	0/920
1	I	0.19	0/1085	0.44	0/1512
1	IA	0.19	0/1085	0.39	0/1512

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	IB	0.18	0/784	0.37	0/1093
1	IC	0.18	0/1085	0.39	0/1512
1	J	0.19	0/1085	0.39	0/1512
1	JA	0.21	0/1080	0.42	0/1505
1	JB	0.18	0/660	0.37	0/920
1	JC	0.19	0/1085	0.44	0/1512
1	K	0.21	0/1080	0.42	0/1505
1	KA	0.18	0/784	0.37	0/1093
1	KB	0.18	0/1085	0.39	0/1512
1	KC	0.19	0/1085	0.39	0/1512
1	L	0.18	0/784	0.37	0/1093
1	LA	0.18	0/660	0.37	0/920
1	LB	0.19	0/1085	0.44	0/1512
1	LC	0.20	0/1080	0.42	0/1505
1	M	0.18	0/660	0.37	0/920
1	MA	0.18	0/1085	0.39	0/1512
1	MB	0.19	0/1085	0.39	0/1512
1	MC	0.18	0/784	0.37	0/1093
1	N	0.18	0/1085	0.39	0/1512
1	NA	0.19	0/1085	0.44	0/1512
1	NB	0.21	0/1080	0.42	0/1505
1	O	0.19	0/1085	0.44	0/1512
1	OA	0.19	0/1085	0.39	0/1512
1	OB	0.18	0/784	0.37	0/1093
1	P	0.19	0/1085	0.39	0/1512
1	PA	0.21	0/1080	0.42	0/1505
1	PB	0.18	0/660	0.37	0/920
1	Q	0.21	0/1080	0.42	0/1505
1	QA	0.18	0/784	0.37	0/1093
1	QB	0.19	0/1085	0.39	0/1512
1	R	0.18	0/784	0.37	0/1093
1	RA	0.18	0/660	0.37	0/920
1	RB	0.19	0/1085	0.44	0/1512
1	S	0.18	0/660	0.37	0/920
1	SA	0.18	0/1085	0.39	0/1512
1	SB	0.19	0/1085	0.39	0/1512
1	T	0.19	0/1085	0.39	0/1512
1	TA	0.19	0/1085	0.44	0/1512
1	TB	0.21	0/1080	0.42	0/1505
1	UA	0.19	0/1085	0.39	0/1512
1	UB	0.18	0/784	0.37	0/1093
1	V	0.19	0/1085	0.44	0/1512
1	VA	0.20	0/1080	0.42	0/1505

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	VB	0.18	0/660	0.37	0/920
1	W	0.19	0/1085	0.39	0/1512
1	WA	0.18	0/784	0.37	0/1093
1	WB	0.18	0/1085	0.39	0/1512
1	X	0.21	0/1080	0.42	0/1505
1	XA	0.18	0/660	0.37	0/920
1	XB	0.19	0/1085	0.44	0/1512
1	Y	0.18	0/784	0.37	0/1093
1	YA	0.18	0/1085	0.39	0/1512
1	YB	0.19	0/1085	0.39	0/1512
1	Z	0.18	0/660	0.37	0/920
1	ZA	0.19	0/1085	0.44	0/1512
1	ZB	0.21	0/1080	0.42	0/1505
All	All	0.19	0/86685	0.40	0/120810

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

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	13	0
1	AB	1086	0	531	9	0
1	AC	785	0	376	2	0
1	B	1086	0	531	13	0
1	BA	1086	0	531	9	0
1	BB	1081	0	530	9	0
1	BC	661	0	320	0	0
1	C	1086	0	531	9	0
1	CA	1086	0	531	9	0
1	CB	785	0	376	2	0
1	CC	1086	0	531	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1086	0	531	9	0
1	DA	1081	0	530	7	0
1	DB	661	0	320	0	0
1	DC	1086	0	531	9	0
1	E	1081	0	530	7	0
1	EA	785	0	376	2	0
1	EB	1086	0	531	13	0
1	EC	1086	0	531	9	0
1	F	785	0	376	2	0
1	FA	661	0	320	0	0
1	FB	1086	0	531	9	0
1	FC	1081	0	530	8	0
1	G	661	0	320	0	0
1	GA	1086	0	531	13	0
1	GB	1086	0	531	9	0
1	GC	785	0	376	2	0
1	H	1086	0	531	13	0
1	HA	1086	0	531	9	0
1	HB	1081	0	530	9	0
1	HC	661	0	320	0	0
1	I	1086	0	531	9	0
1	IA	1086	0	531	9	0
1	IB	785	0	376	2	0
1	IC	1086	0	531	13	0
1	J	1086	0	531	9	0
1	JA	1081	0	530	7	0
1	JB	661	0	320	0	0
1	JC	1086	0	531	9	0
1	K	1081	0	530	7	0
1	KA	785	0	376	2	0
1	KB	1086	0	531	13	0
1	KC	1086	0	531	9	0
1	L	785	0	376	2	0
1	LA	661	0	320	0	0
1	LB	1086	0	531	9	0
1	LC	1081	0	530	7	0
1	M	661	0	320	0	0
1	MA	1086	0	531	13	0
1	MB	1086	0	531	9	0
1	MC	785	0	376	2	0
1	N	1086	0	531	12	0
1	NA	1086	0	531	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	NB	1081	0	530	9	0
1	O	1086	0	531	9	0
1	OA	1086	0	531	9	0
1	OB	785	0	376	2	0
1	P	1086	0	531	9	0
1	PA	1081	0	530	9	0
1	PB	661	0	320	0	0
1	Q	1081	0	530	7	0
1	QA	785	0	376	2	0
1	QB	1086	0	531	13	0
1	R	785	0	376	2	0
1	RA	661	0	320	0	0
1	RB	1086	0	531	9	0
1	S	661	0	320	0	0
1	SA	1086	0	531	13	0
1	SB	1086	0	531	9	0
1	T	1086	0	531	12	0
1	TA	1086	0	531	9	0
1	TB	1081	0	530	9	0
1	UA	1086	0	531	9	0
1	UB	785	0	376	2	0
1	V	1086	0	531	9	0
1	VA	1081	0	530	9	0
1	VB	661	0	320	0	0
1	W	1086	0	531	9	0
1	WA	785	0	376	2	0
1	WB	1086	0	531	13	0
1	X	1081	0	530	7	0
1	XA	661	0	320	0	0
1	XB	1086	0	531	9	0
1	Y	785	0	376	2	0
1	YA	1086	0	531	13	0
1	YB	1086	0	531	9	0
1	Z	661	0	320	0	0
1	ZA	1086	0	531	9	0
1	ZB	1081	0	530	8	0
All	All	86775	0	42285	313	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 (313) 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:ZA:184:ALA:HB1	1:KB:48:ALA:HB1	1.21	1.18
1:TA:184:ALA:HB1	1:EB:48:ALA:HB1	1.21	1.18
1:NA:184:ALA:HB1	1:YA:48:ALA:HB1	1.23	1.17
1:HA:184:ALA:HB1	1:SA:48:ALA:HB1	1.22	1.16
1:LB:184:ALA:HB1	1:WB:48:ALA:HB1	1.22	1.15
1:FB:184:ALA:HB1	1:QB:48:ALA:HB1	1.22	1.15
1:RB:184:ALA:HB1	1:CC:48:ALA:HB1	1.20	1.14
1:BA:184:ALA:HB1	1:MA:48:ALA:HB1	1.21	1.12
1:XB:184:ALA:HB1	1:IC:48:ALA:HB1	1.19	1.12
1:V:184:ALA:HB1	1:GA:48:ALA:HB1	1.22	1.12
1:O:184:ALA:HB1	1:AA:48:ALA:HB1	1.22	1.10
1:B:48:ALA:HB1	1:DC:184:ALA:HB1	1.24	1.09
1:I:184:ALA:HB1	1:T:48:ALA:HB1	1.22	1.09
1:H:48:ALA:HB1	1:JC:184:ALA:HB1	1.22	1.08
1:C:184:ALA:HB1	1:N:48:ALA:HB1	1.20	1.08
1:B:52:ALA:HB1	1:DC:180:SER:CB	1.87	1.04
1:LB:180:SER:CB	1:WB:52:ALA:HB1	1.87	1.04
1:V:180:SER:CB	1:GA:52:ALA:HB1	1.88	1.03
1:O:180:SER:CB	1:AA:52:ALA:HB1	1.89	1.03
1:H:52:ALA:HB1	1:JC:180:SER:CB	1.88	1.02
1:RB:180:SER:CB	1:CC:52:ALA:HB1	1.90	1.02
1:NA:180:SER:CB	1:YA:52:ALA:HB1	1.88	1.02
1:TA:180:SER:CB	1:EB:52:ALA:HB1	1.88	1.02
1:I:180:SER:CB	1:T:52:ALA:HB1	1.90	1.02
1:C:180:SER:CB	1:N:52:ALA:HB1	1.89	1.02
1:BA:180:SER:CB	1:MA:52:ALA:HB1	1.89	1.02
1:HA:180:SER:CB	1:SA:52:ALA:HB1	1.89	1.01
1:FB:180:SER:CB	1:QB:52:ALA:HB1	1.89	1.01
1:XB:184:ALA:CB	1:IC:48:ALA:HB1	1.91	1.01
1:ZA:180:SER:CB	1:KB:52:ALA:HB1	1.89	1.00
1:ZA:184:ALA:CB	1:KB:48:ALA:HB1	1.91	1.00
1:XB:180:SER:CB	1:IC:52:ALA:HB1	1.92	1.00
1:BA:184:ALA:CB	1:MA:48:ALA:HB1	1.92	1.00
1:LB:184:ALA:CB	1:WB:48:ALA:HB1	1.92	1.00
1:C:184:ALA:CB	1:N:48:ALA:HB1	1.90	1.00
1:RB:184:ALA:CB	1:CC:48:ALA:HB1	1.91	1.00
1:H:48:ALA:HB1	1:JC:184:ALA:CB	1.92	0.99
1:NA:184:ALA:CB	1:YA:48:ALA:HB1	1.93	0.99
1:TA:184:ALA:CB	1:EB:48:ALA:HB1	1.91	0.99
1:V:184:ALA:CB	1:GA:48:ALA:HB1	1.92	0.99
1:FB:184:ALA:CB	1:QB:48:ALA:HB1	1.92	0.98
1:O:184:ALA:CB	1:AA:48:ALA:HB1	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:184:ALA:CB	1:SA:48:ALA:HB1	1.92	0.98
1:I:184:ALA:CB	1:T:48:ALA:HB1	1.94	0.97
1:B:48:ALA:HB1	1:DC:184:ALA:CB	1.93	0.96
1:C:184:ALA:HB1	1:N:48:ALA:CB	1.98	0.94
1:RB:184:ALA:HB1	1:CC:48:ALA:CB	1.99	0.93
1:XB:184:ALA:HB1	1:IC:48:ALA:CB	1.98	0.92
1:TA:184:ALA:HB1	1:EB:48:ALA:CB	1.99	0.92
1:V:184:ALA:HB1	1:GA:48:ALA:CB	2.00	0.92
1:HA:184:ALA:HB1	1:SA:48:ALA:CB	2.00	0.92
1:FB:184:ALA:HB1	1:QB:48:ALA:CB	2.00	0.92
1:BA:184:ALA:HB1	1:MA:48:ALA:CB	1.99	0.91
1:ZA:184:ALA:HB1	1:KB:48:ALA:CB	1.99	0.91
1:LB:184:ALA:HB1	1:WB:48:ALA:CB	2.00	0.91
1:O:184:ALA:HB1	1:AA:48:ALA:CB	2.00	0.91
1:B:48:ALA:CB	1:DC:184:ALA:HB1	2.01	0.91
1:H:48:ALA:CB	1:JC:184:ALA:HB1	2.00	0.91
1:I:184:ALA:HB1	1:T:48:ALA:CB	2.01	0.90
1:NA:184:ALA:HB1	1:YA:48:ALA:CB	2.01	0.90
1:I:52:ALA:CB	1:KC:180:SER:CB	2.65	0.74
1:NB:179:GLU:CB	1:YB:52:ALA:CB	2.65	0.74
1:ZB:179:GLU:CB	1:KC:52:ALA:HB1	2.17	0.74
1:C:52:ALA:CB	1:EC:180:SER:CB	2.65	0.74
1:JA:179:GLU:CB	1:UA:52:ALA:CB	2.66	0.74
1:TB:179:GLU:CB	1:EC:52:ALA:CB	2.66	0.74
1:Q:179:GLU:CB	1:CA:52:ALA:CB	2.66	0.74
1:OA:180:SER:CB	1:ZA:52:ALA:CB	2.65	0.74
1:MB:180:SER:CB	1:XB:52:ALA:CB	2.65	0.74
1:K:179:GLU:CB	1:W:52:ALA:CB	2.66	0.74
1:PA:179:GLU:CB	1:AB:52:ALA:CB	2.66	0.74
1:D:180:SER:CB	1:O:52:ALA:CB	2.66	0.74
1:DA:179:GLU:CB	1:OA:52:ALA:CB	2.66	0.74
1:UA:180:SER:CB	1:FB:52:ALA:CB	2.66	0.74
1:W:180:SER:CB	1:HA:52:ALA:CB	2.65	0.73
1:X:179:GLU:CB	1:IA:52:ALA:CB	2.66	0.73
1:HB:179:GLU:CB	1:SB:52:ALA:CB	2.66	0.73
1:ZB:179:GLU:CB	1:KC:52:ALA:CB	2.66	0.73
1:D:52:ALA:CB	1:FC:179:GLU:CB	2.66	0.73
1:CA:180:SER:CB	1:NA:52:ALA:CB	2.66	0.73
1:K:179:GLU:CB	1:W:52:ALA:HB1	2.18	0.73
1:DA:179:GLU:CB	1:OA:52:ALA:HB1	2.18	0.73
1:TB:179:GLU:CB	1:EC:52:ALA:HB1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZB:183:GLN:CB	1:KC:48:ALA:HB1	2.18	0.73
1:E:179:GLU:CB	1:P:52:ALA:HB1	2.19	0.73
1:P:180:SER:CB	1:BA:52:ALA:CB	2.66	0.73
1:BB:179:GLU:CB	1:MB:52:ALA:CB	2.66	0.73
1:J:52:ALA:CB	1:LC:179:GLU:CB	2.66	0.73
1:IA:180:SER:CB	1:TA:52:ALA:CB	2.66	0.73
1:BB:179:GLU:CB	1:MB:52:ALA:HB1	2.19	0.73
1:E:179:GLU:CB	1:P:52:ALA:CB	2.66	0.73
1:PA:179:GLU:CB	1:AB:52:ALA:HB1	2.19	0.73
1:VA:179:GLU:CB	1:GB:52:ALA:CB	2.66	0.73
1:GB:180:SER:CB	1:RB:52:ALA:CB	2.66	0.73
1:J:180:SER:CB	1:V:52:ALA:CB	2.66	0.73
1:AB:180:SER:CB	1:LB:52:ALA:CB	2.66	0.73
1:TB:183:GLN:CB	1:EC:48:ALA:HB1	2.19	0.73
1:VA:179:GLU:CB	1:GB:52:ALA:HB1	2.19	0.73
1:YB:180:SER:CB	1:JC:52:ALA:CB	2.67	0.73
1:E:183:GLN:CB	1:P:48:ALA:HB1	2.19	0.73
1:Q:179:GLU:CB	1:CA:52:ALA:HB1	2.18	0.73
1:SB:180:SER:CB	1:DC:52:ALA:CB	2.66	0.73
1:HB:179:GLU:CB	1:SB:52:ALA:HB1	2.18	0.72
1:J:52:ALA:HB1	1:LC:179:GLU:CB	2.19	0.72
1:JA:179:GLU:CB	1:UA:52:ALA:HB1	2.19	0.72
1:VA:183:GLN:CB	1:GB:48:ALA:HB1	2.20	0.72
1:X:179:GLU:CB	1:IA:52:ALA:HB1	2.19	0.72
1:HB:183:GLN:CB	1:SB:48:ALA:HB1	2.20	0.72
1:X:183:GLN:CB	1:IA:48:ALA:HB1	2.21	0.71
1:JA:183:GLN:CB	1:UA:48:ALA:HB1	2.21	0.71
1:D:52:ALA:HB1	1:FC:179:GLU:CB	2.19	0.71
1:K:183:GLN:CB	1:W:48:ALA:HB1	2.21	0.71
1:NB:179:GLU:CB	1:YB:52:ALA:HB1	2.19	0.71
1:BB:183:GLN:CB	1:MB:48:ALA:HB1	2.20	0.71
1:DA:183:GLN:CB	1:OA:48:ALA:HB1	2.20	0.71
1:NB:183:GLN:CB	1:YB:48:ALA:HB1	2.21	0.70
1:J:48:ALA:HB1	1:LC:183:GLN:CB	2.20	0.70
1:Q:183:GLN:CB	1:CA:48:ALA:HB1	2.21	0.70
1:D:48:ALA:HB1	1:FC:183:GLN:CB	2.22	0.70
1:PA:183:GLN:CB	1:AB:48:ALA:HB1	2.21	0.69
1:J:180:SER:CB	1:V:52:ALA:HB1	2.23	0.69
1:C:52:ALA:HB1	1:EC:180:SER:CB	2.23	0.69
1:P:180:SER:CB	1:BA:52:ALA:HB1	2.23	0.68
1:OA:180:SER:CB	1:ZA:52:ALA:HB1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:180:SER:CB	1:FB:52:ALA:HB1	2.24	0.68
1:I:52:ALA:HB1	1:KC:180:SER:CB	2.24	0.68
1:CA:180:SER:CB	1:NA:52:ALA:HB1	2.24	0.68
1:MB:180:SER:CB	1:XB:52:ALA:HB1	2.24	0.68
1:SB:180:SER:CB	1:DC:52:ALA:HB1	2.24	0.68
1:W:180:SER:CB	1:HA:52:ALA:HB1	2.24	0.68
1:IA:180:SER:CB	1:TA:52:ALA:HB1	2.23	0.68
1:YB:180:SER:CB	1:JC:52:ALA:HB1	2.23	0.67
1:AB:180:SER:CB	1:LB:52:ALA:HB1	2.24	0.67
1:GB:180:SER:CB	1:RB:52:ALA:HB1	2.23	0.67
1:D:180:SER:CB	1:O:52:ALA:HB1	2.24	0.67
1:TA:180:SER:CB	1:EB:52:ALA:CB	2.72	0.66
1:V:180:SER:CB	1:GA:52:ALA:CB	2.71	0.66
1:O:180:SER:CB	1:AA:52:ALA:CB	2.72	0.66
1:ZA:180:SER:CB	1:KB:52:ALA:CB	2.72	0.64
1:H:52:ALA:CB	1:JC:180:SER:CB	2.71	0.64
1:RB:180:SER:CB	1:CC:52:ALA:CB	2.73	0.64
1:BA:180:SER:CB	1:MA:52:ALA:CB	2.72	0.63
1:FB:180:SER:CB	1:QB:52:ALA:CB	2.73	0.62
1:LB:180:SER:CB	1:WB:52:ALA:CB	2.71	0.62
1:HA:180:SER:CB	1:SA:52:ALA:CB	2.72	0.62
1:B:52:ALA:CB	1:DC:180:SER:CB	2.71	0.60
1:NA:180:SER:CB	1:YA:52:ALA:CB	2.72	0.60
1:C:180:SER:CB	1:N:52:ALA:CB	2.72	0.58
1:MB:180:SER:CB	1:XB:52:ALA:HB2	2.34	0.58
1:I:52:ALA:HB2	1:KC:180:SER:CB	2.34	0.58
1:YA:167:ALA:HB2	1:EB:32:ALA:HB2	1.86	0.58
1:QB:167:ALA:HB2	1:WB:32:ALA:HB2	1.85	0.58
1:D:180:SER:CB	1:O:52:ALA:HB2	2.34	0.57
1:I:180:SER:CB	1:T:52:ALA:CB	2.74	0.57
1:C:52:ALA:HB2	1:EC:180:SER:CB	2.34	0.57
1:XB:180:SER:CB	1:IC:52:ALA:CB	2.75	0.57
1:UA:180:SER:CB	1:FB:52:ALA:HB2	2.34	0.57
1:EB:167:ALA:HB2	1:KB:32:ALA:HB2	1.86	0.57
1:AB:180:SER:CB	1:LB:52:ALA:HB2	2.34	0.57
1:W:180:SER:CB	1:HA:52:ALA:HB2	2.34	0.57
1:WB:167:ALA:HB2	1:CC:32:ALA:HB2	1.87	0.57
1:CC:167:ALA:HB2	1:IC:32:ALA:HB2	1.86	0.57
1:B:167:ALA:HB2	1:H:32:ALA:HB2	1.86	0.57
1:OA:180:SER:CB	1:ZA:52:ALA:HB2	2.35	0.57
1:SB:180:SER:CB	1:DC:52:ALA:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:180:SER:CB	1:TA:52:ALA:HB2	2.35	0.56
1:ZB:183:GLN:CB	1:KC:48:ALA:CB	2.83	0.56
1:SA:167:ALA:HB2	1:YA:32:ALA:HB2	1.86	0.56
1:GB:180:SER:CB	1:RB:52:ALA:HB2	2.35	0.56
1:H:167:ALA:HB2	1:N:32:ALA:HB2	1.86	0.56
1:KB:167:ALA:HB2	1:QB:32:ALA:HB2	1.87	0.56
1:AA:167:ALA:HB2	1:GA:32:ALA:HB2	1.86	0.56
1:CA:180:SER:CB	1:NA:52:ALA:HB2	2.35	0.56
1:B:32:ALA:HB2	1:IC:167:ALA:HB2	1.87	0.56
1:T:167:ALA:HB2	1:AA:32:ALA:HB2	1.86	0.56
1:MA:167:ALA:HB2	1:SA:32:ALA:HB2	1.86	0.56
1:TB:183:GLN:CB	1:EC:48:ALA:CB	2.84	0.56
1:GA:167:ALA:HB2	1:MA:32:ALA:HB2	1.87	0.56
1:E:183:GLN:CB	1:P:48:ALA:CB	2.84	0.55
1:BB:183:GLN:CB	1:MB:48:ALA:CB	2.84	0.55
1:N:167:ALA:HB2	1:T:32:ALA:HB2	1.88	0.55
1:P:180:SER:CB	1:BA:52:ALA:HB2	2.35	0.55
1:VA:183:GLN:CB	1:GB:48:ALA:CB	2.84	0.55
1:NB:183:GLN:CB	1:YB:48:ALA:CB	2.85	0.55
1:X:183:GLN:CB	1:IA:48:ALA:CB	2.85	0.55
1:JA:183:GLN:CB	1:UA:48:ALA:CB	2.85	0.55
1:J:48:ALA:CB	1:LC:183:GLN:CB	2.85	0.55
1:WB:167:ALA:CB	1:CC:32:ALA:HB2	2.37	0.54
1:DA:183:GLN:CB	1:OA:48:ALA:CB	2.84	0.54
1:EB:167:ALA:CB	1:KB:32:ALA:HB2	2.38	0.54
1:PA:183:GLN:CB	1:AB:48:ALA:CB	2.85	0.54
1:YB:180:SER:CB	1:JC:52:ALA:HB2	2.36	0.54
1:B:167:ALA:CB	1:H:32:ALA:HB2	2.37	0.54
1:AA:167:ALA:CB	1:GA:32:ALA:HB2	2.38	0.54
1:GA:167:ALA:CB	1:MA:32:ALA:HB2	2.38	0.54
1:HB:183:GLN:CB	1:SB:48:ALA:CB	2.85	0.54
1:YA:167:ALA:CB	1:EB:32:ALA:HB2	2.38	0.54
1:K:183:GLN:CB	1:W:48:ALA:CB	2.86	0.54
1:D:48:ALA:CB	1:FC:183:GLN:CB	2.86	0.53
1:CC:167:ALA:CB	1:IC:32:ALA:HB2	2.38	0.53
1:J:180:SER:CB	1:V:52:ALA:HB2	2.36	0.53
1:Q:183:GLN:CB	1:CA:48:ALA:CB	2.85	0.53
1:MA:167:ALA:CB	1:SA:32:ALA:HB2	2.38	0.53
1:SA:167:ALA:CB	1:YA:32:ALA:HB2	2.38	0.53
1:QB:167:ALA:CB	1:WB:32:ALA:HB2	2.38	0.53
1:KB:167:ALA:CB	1:QB:32:ALA:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:ALA:CB	1:N:32:ALA:HB2	2.38	0.53
1:N:167:ALA:CB	1:T:32:ALA:HB2	2.38	0.52
1:B:32:ALA:HB2	1:IC:167:ALA:CB	2.39	0.52
1:T:167:ALA:CB	1:AA:32:ALA:HB2	2.39	0.52
1:LC:22:ALA:CB	1:MC:9:ARG:CB	2.90	0.50
1:Q:22:ALA:CB	1:R:9:ARG:CB	2.90	0.50
1:TB:22:ALA:CB	1:UB:9:ARG:CB	2.90	0.50
1:E:22:ALA:CB	1:F:9:ARG:CB	2.90	0.49
1:ZB:22:ALA:CB	1:AC:9:ARG:CB	2.90	0.49
1:X:22:ALA:CB	1:Y:9:ARG:CB	2.90	0.49
1:FC:22:ALA:CB	1:GC:9:ARG:CB	2.90	0.49
1:K:22:ALA:CB	1:L:9:ARG:CB	2.90	0.49
1:PA:22:ALA:CB	1:QA:9:ARG:CB	2.90	0.49
1:NB:22:ALA:CB	1:OB:9:ARG:CB	2.90	0.49
1:AA:167:ALA:CB	1:GA:32:ALA:CB	2.91	0.49
1:VA:22:ALA:CB	1:WA:9:ARG:CB	2.90	0.49
1:GA:167:ALA:CB	1:MA:32:ALA:CB	2.91	0.49
1:JA:22:ALA:CB	1:KA:9:ARG:CB	2.90	0.49
1:HB:22:ALA:CB	1:IB:9:ARG:CB	2.90	0.49
1:WB:167:ALA:CB	1:CC:32:ALA:CB	2.91	0.49
1:SA:167:ALA:CB	1:YA:32:ALA:CB	2.91	0.48
1:YA:167:ALA:CB	1:EB:32:ALA:CB	2.91	0.48
1:BB:22:ALA:CB	1:CB:9:ARG:CB	2.90	0.48
1:CC:167:ALA:CB	1:IC:32:ALA:CB	2.91	0.48
1:DA:22:ALA:CB	1:EA:9:ARG:CB	2.90	0.48
1:EB:167:ALA:CB	1:KB:32:ALA:CB	2.91	0.48
1:N:167:ALA:CB	1:T:32:ALA:CB	2.91	0.48
1:B:32:ALA:CB	1:IC:167:ALA:CB	2.91	0.48
1:B:167:ALA:CB	1:H:32:ALA:CB	2.91	0.48
1:T:167:ALA:CB	1:AA:32:ALA:CB	2.91	0.48
1:H:167:ALA:CB	1:N:32:ALA:CB	2.91	0.48
1:KB:167:ALA:CB	1:QB:32:ALA:CB	2.91	0.48
1:MA:167:ALA:CB	1:SA:32:ALA:CB	2.91	0.48
1:QB:167:ALA:CB	1:WB:32:ALA:CB	2.91	0.48
1:Q:22:ALA:HB1	1:R:9:ARG:CB	2.46	0.46
1:E:22:ALA:HB1	1:F:9:ARG:CB	2.46	0.46
1:K:22:ALA:HB1	1:L:9:ARG:CB	2.46	0.46
1:ZB:22:ALA:HB1	1:AC:9:ARG:CB	2.46	0.46
1:X:22:ALA:HB1	1:Y:9:ARG:CB	2.46	0.46
1:LC:22:ALA:HB1	1:MC:9:ARG:CB	2.46	0.46
1:TB:22:ALA:HB1	1:UB:9:ARG:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:22:ALA:HB1	1:EA:9:ARG:CB	2.46	0.46
1:FC:22:ALA:HB1	1:GC:9:ARG:CB	2.46	0.46
1:JA:22:ALA:HB1	1:KA:9:ARG:CB	2.46	0.45
1:NB:22:ALA:HB1	1:OB:9:ARG:CB	2.46	0.45
1:PA:22:ALA:HB1	1:QA:9:ARG:CB	2.46	0.45
1:VA:22:ALA:HB1	1:WA:9:ARG:CB	2.46	0.45
1:HB:22:ALA:HB1	1:IB:9:ARG:CB	2.46	0.45
1:BB:22:ALA:HB1	1:CB:9:ARG:CB	2.46	0.45
1:T:167:ALA:HB2	1:AA:32:ALA:CB	2.49	0.43
1:CA:22:ALA:HB2	1:DA:9:ARG:CB	2.49	0.43
1:EC:22:ALA:HB2	1:FC:9:ARG:CB	2.49	0.43
1:W:22:ALA:HB2	1:X:9:ARG:CB	2.49	0.43
1:SA:167:ALA:HB2	1:YA:32:ALA:CB	2.49	0.43
1:MB:22:ALA:HB2	1:NB:9:ARG:CB	2.49	0.43
1:J:22:ALA:HB2	1:K:9:ARG:CB	2.49	0.42
1:BA:22:ALA:HB1	1:CA:9:ARG:CB	2.50	0.42
1:GA:167:ALA:HB2	1:MA:32:ALA:CB	2.50	0.42
1:IA:22:ALA:HB2	1:JA:9:ARG:CB	2.49	0.42
1:NA:22:ALA:HB1	1:OA:9:ARG:CB	2.49	0.42
1:GB:22:ALA:HB2	1:HB:9:ARG:CB	2.49	0.42
1:SB:22:ALA:HB2	1:TB:9:ARG:CB	2.49	0.42
1:D:22:ALA:HB2	1:E:9:ARG:CB	2.49	0.42
1:P:22:ALA:HB2	1:Q:9:ARG:CB	2.49	0.42
1:FB:22:ALA:HB1	1:GB:9:ARG:CB	2.50	0.42
1:EB:167:ALA:HB2	1:KB:32:ALA:CB	2.50	0.42
1:B:167:ALA:HB2	1:H:32:ALA:CB	2.49	0.42
1:OA:22:ALA:HB2	1:PA:9:ARG:CB	2.49	0.42
1:ZA:22:ALA:HB1	1:AB:9:ARG:CB	2.49	0.42
1:YB:22:ALA:HB2	1:ZB:9:ARG:CB	2.49	0.42
1:TA:22:ALA:HB1	1:UA:9:ARG:CB	2.49	0.42
1:AB:22:ALA:HB2	1:BB:9:ARG:CB	2.49	0.42
1:KB:167:ALA:HB2	1:QB:32:ALA:CB	2.49	0.42
1:RB:22:ALA:HB1	1:SB:9:ARG:CB	2.49	0.42
1:C:22:ALA:HB1	1:D:9:ARG:CB	2.50	0.42
1:YA:167:ALA:HB2	1:EB:32:ALA:CB	2.49	0.42
1:KC:22:ALA:HB2	1:LC:9:ARG:CB	2.49	0.42
1:JC:22:ALA:HB1	1:KC:9:ARG:CB	2.49	0.42
1:HA:22:ALA:HB1	1:IA:9:ARG:CB	2.49	0.41
1:O:22:ALA:HB1	1:P:9:ARG:CB	2.50	0.41
1:V:22:ALA:HB1	1:W:9:ARG:CB	2.49	0.41
1:LB:22:ALA:HB1	1:MB:9:ARG:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MA:167:ALA:HB2	1:SA:32:ALA:CB	2.49	0.41
1:UA:22:ALA:HB2	1:VA:9:ARG:CB	2.49	0.41
1:XB:22:ALA:HB1	1:YB:9:ARG:CB	2.50	0.41
1:H:167:ALA:HB2	1:N:32:ALA:CB	2.49	0.41
1:I:22:ALA:HB1	1:J:9:ARG:CB	2.49	0.41
1:B:32:ALA:CB	1:IC:167:ALA:HB2	2.49	0.41
1:CC:167:ALA:HB2	1:IC:32:ALA:CB	2.49	0.41
1:BB:160:ASN:O	1:BB:161:THR:C	2.58	0.41
1:WB:167:ALA:HB2	1:CC:32:ALA:CB	2.50	0.41
1:HB:160:ASN:O	1:HB:161:THR:C	2.58	0.41
1:TB:160:ASN:O	1:TB:161:THR:C	2.58	0.41
1:ZB:160:ASN:O	1:ZB:161:THR:C	2.58	0.41
1:AA:167:ALA:HB2	1:GA:32:ALA:CB	2.49	0.41
1:PA:160:ASN:O	1:PA:161:THR:C	2.58	0.41
1:DC:22:ALA:HB1	1:EC:9:ARG:CB	2.50	0.41
1:VA:160:ASN:O	1:VA:161:THR:C	2.58	0.41
1:FC:160:ASN:O	1:FC:161:THR:C	2.58	0.41
1:BB:161:THR:O	1:BB:162:SER:C	2.60	0.40
1:NB:160:ASN:O	1:NB:161:THR:C	2.58	0.40
1:VA:161:THR:O	1:VA:162:SER:C	2.60	0.40
1:HB:161:THR:O	1:HB:162:SER:C	2.60	0.40
1:NB:161:THR:O	1:NB:162:SER:C	2.60	0.40
1:QB:167:ALA:HB2	1:WB:32:ALA:CB	2.49	0.40
1:PA:161:THR:O	1:PA:162:SER:C	2.60	0.40
1:TB:161:THR:O	1:TB:162:SER:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/258 (51%)	131 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	AB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	AC	156/258 (60%)	156 (100%)	0	0	100	100
1	B	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	BA	217/258 (84%)	217 (100%)	0	0	100	100
1	BB	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	BC	131/258 (51%)	131 (100%)	0	0	100	100
1	C	217/258 (84%)	217 (100%)	0	0	100	100
1	CA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	CB	156/258 (60%)	156 (100%)	0	0	100	100
1	CC	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	D	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	DA	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	DB	131/258 (51%)	131 (100%)	0	0	100	100
1	DC	217/258 (84%)	217 (100%)	0	0	100	100
1	E	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	EA	156/258 (60%)	156 (100%)	0	0	100	100
1	EB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	EC	217/258 (84%)	216 (100%)	1 (0%)	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%)	217 (100%)	0	0	100	100
1	FC	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	G	131/258 (51%)	131 (100%)	0	0	100	100
1	GA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	GB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	GC	156/258 (60%)	156 (100%)	0	0	100	100
1	H	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	HA	217/258 (84%)	217 (100%)	0	0	100	100
1	HB	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	HC	131/258 (51%)	131 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	217/258 (84%)	217 (100%)	0	0	100	100
1	IA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	IB	156/258 (60%)	156 (100%)	0	0	100	100
1	IC	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	J	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	JA	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	JB	131/258 (51%)	131 (100%)	0	0	100	100
1	JC	217/258 (84%)	217 (100%)	0	0	100	100
1	K	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	KA	156/258 (60%)	156 (100%)	0	0	100	100
1	KB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	KC	217/258 (84%)	216 (100%)	1 (0%)	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%)	217 (100%)	0	0	100	100
1	LC	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	M	131/258 (51%)	131 (100%)	0	0	100	100
1	MA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	MB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	MC	156/258 (60%)	156 (100%)	0	0	100	100
1	N	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	NA	217/258 (84%)	217 (100%)	0	0	100	100
1	NB	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	O	217/258 (84%)	217 (100%)	0	0	100	100
1	OA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	OB	156/258 (60%)	156 (100%)	0	0	100	100
1	P	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	PA	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	PB	131/258 (51%)	131 (100%)	0	0	100	100
1	Q	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	QA	156/258 (60%)	156 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QB	217/258 (84%)	216 (100%)	1 (0%)	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%)	217 (100%)	0	0	100	100
1	S	131/258 (51%)	131 (100%)	0	0	100	100
1	SA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	SB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	T	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	TA	217/258 (84%)	217 (100%)	0	0	100	100
1	TB	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	UA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	UB	156/258 (60%)	156 (100%)	0	0	100	100
1	V	217/258 (84%)	217 (100%)	0	0	100	100
1	VA	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	VB	131/258 (51%)	131 (100%)	0	0	100	100
1	W	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	WA	156/258 (60%)	156 (100%)	0	0	100	100
1	WB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	X	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
1	XA	131/258 (51%)	131 (100%)	0	0	100	100
1	XB	217/258 (84%)	217 (100%)	0	0	100	100
1	Y	156/258 (60%)	156 (100%)	0	0	100	100
1	YA	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	YB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	Z	131/258 (51%)	131 (100%)	0	0	100	100
1	ZA	217/258 (84%)	217 (100%)	0	0	100	100
1	ZB	216/258 (84%)	215 (100%)	1 (0%)	0	100	100
All	All	17310/23220 (74%)	17265 (100%)	45 (0%)	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.

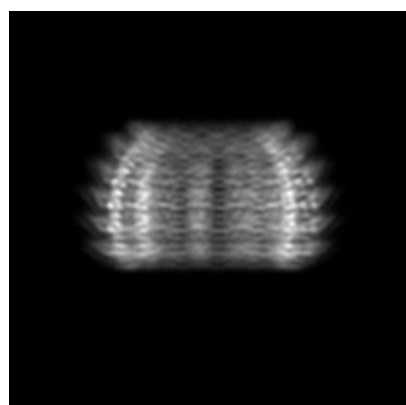
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11481. These allow visual inspection of the internal detail of the map and identification of artifacts.

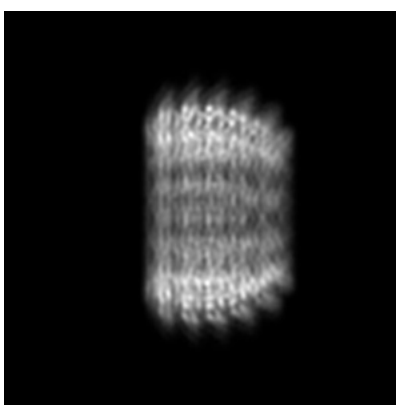
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

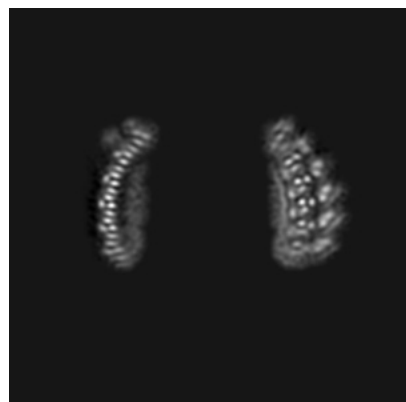


Z

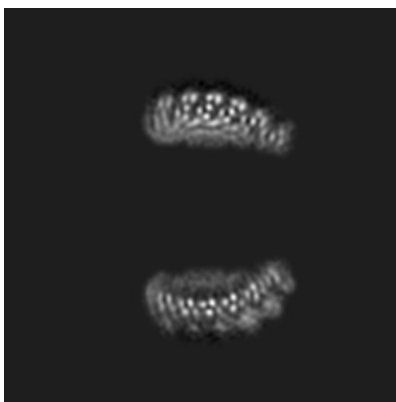
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 168



Y Index: 168



Z Index: 168

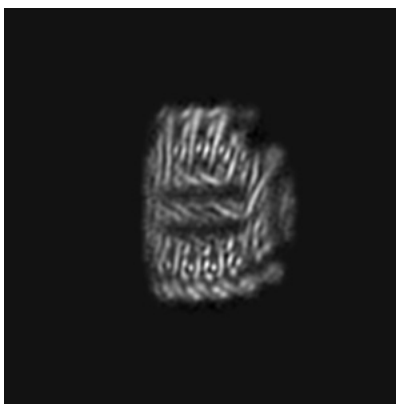
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 108



Y Index: 235

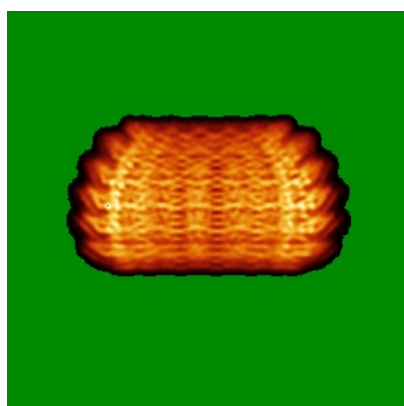


Z Index: 172

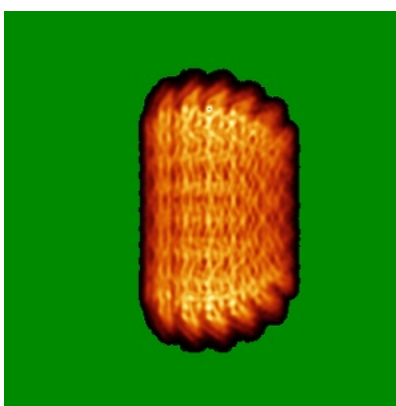
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

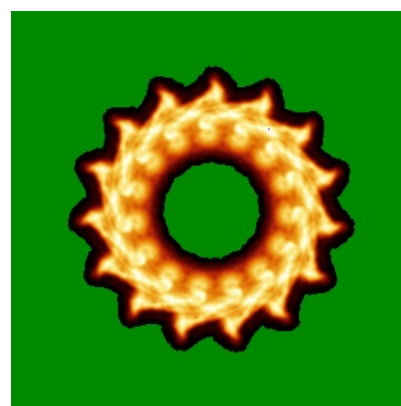
6.4.1 Primary map



X



Y

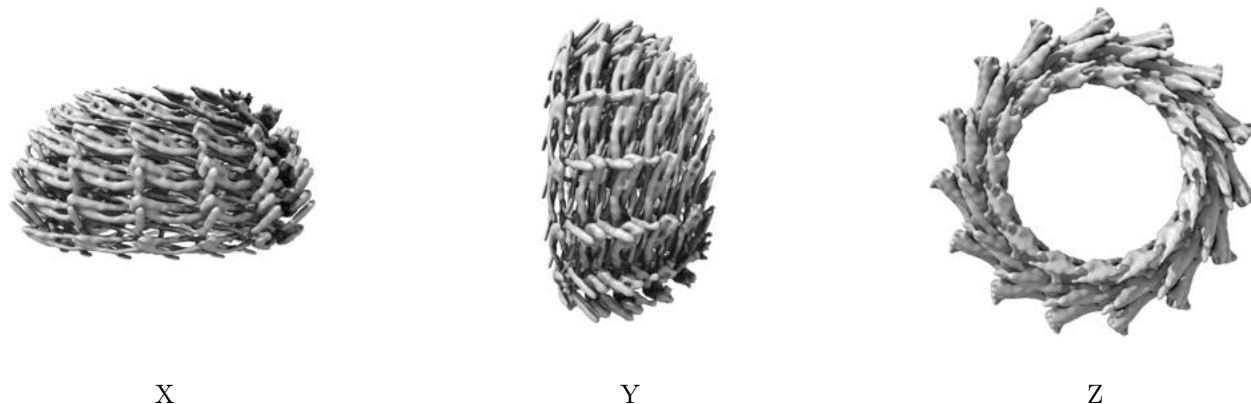


Z

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 0.0182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

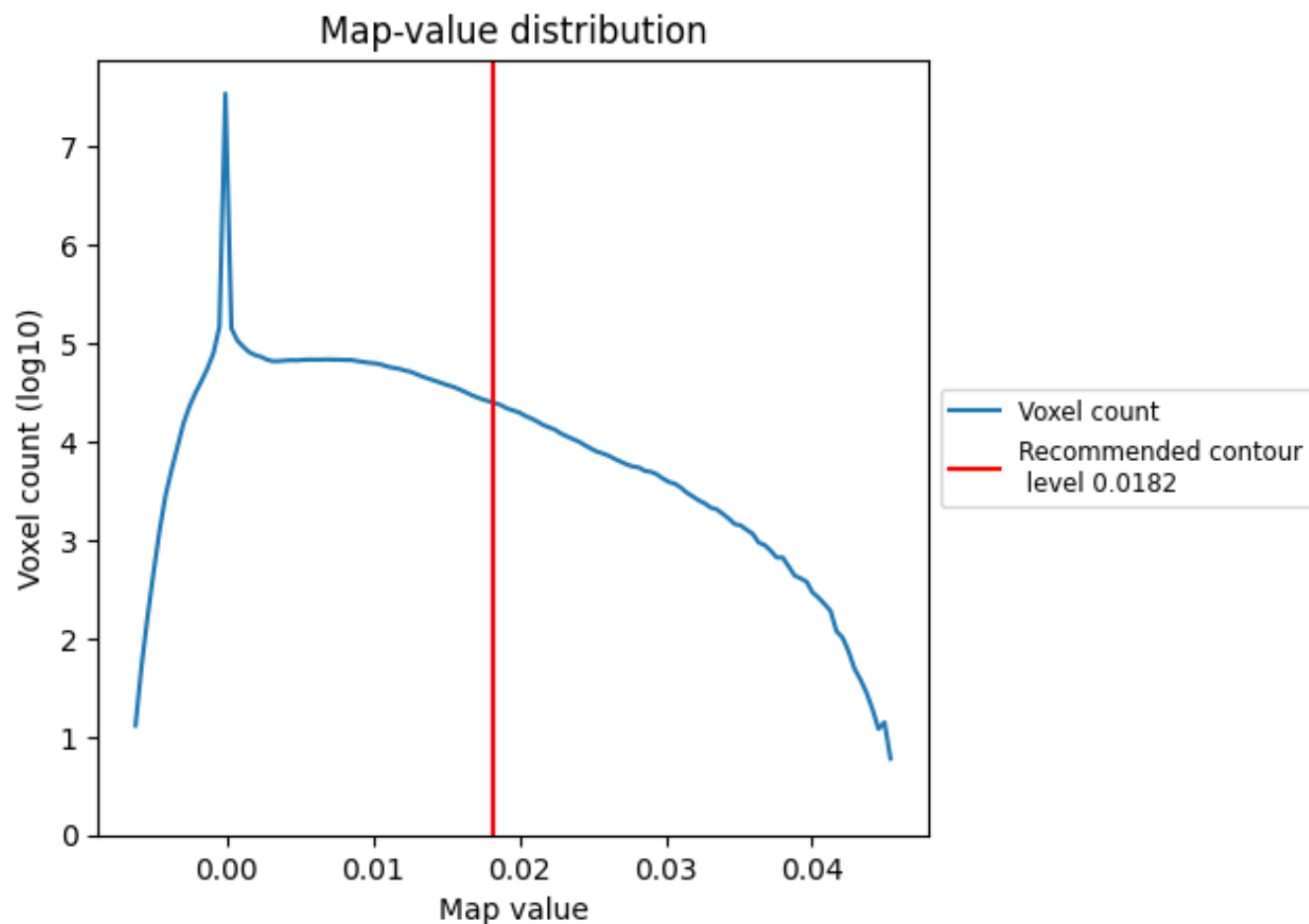
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

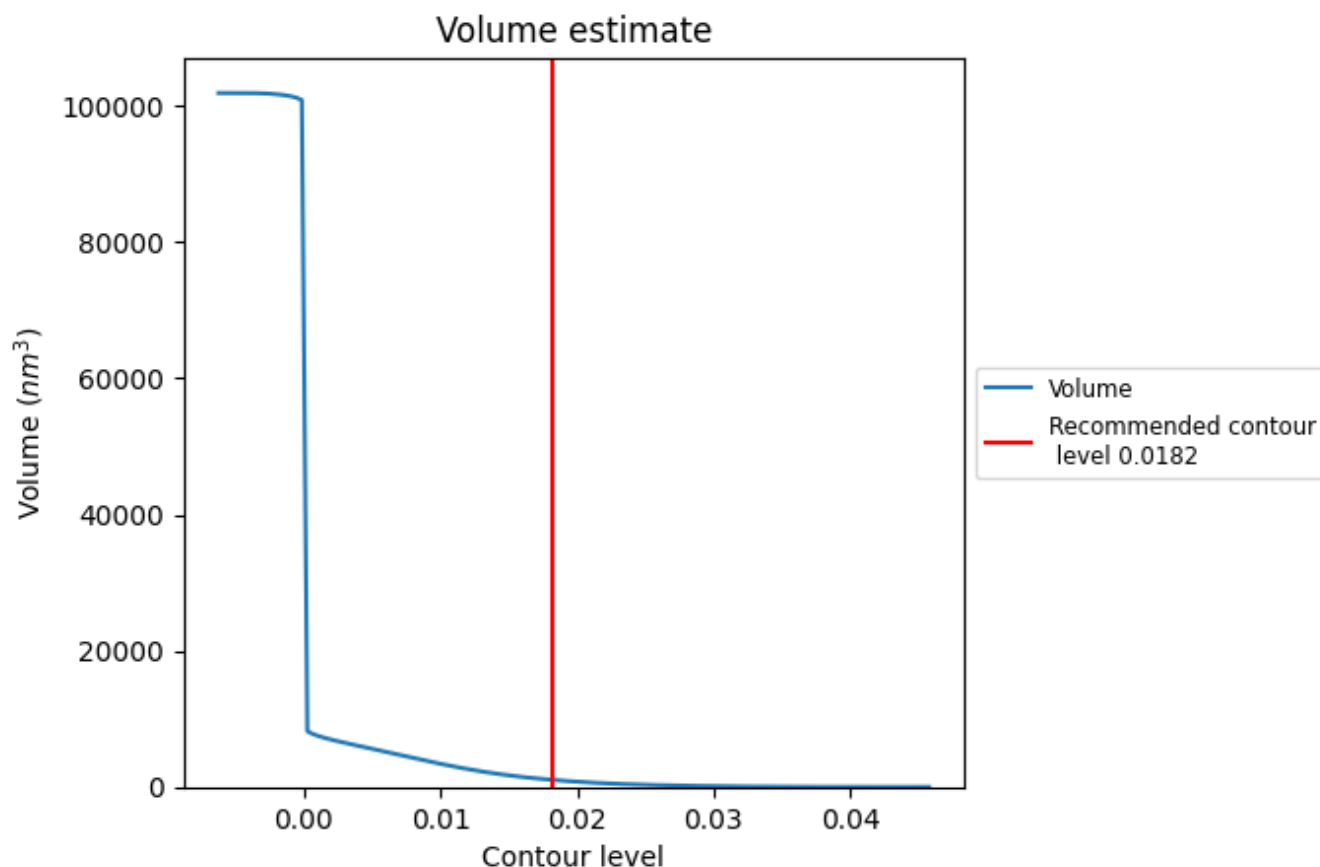
This section contains the results of statistical analysis of the map.

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.

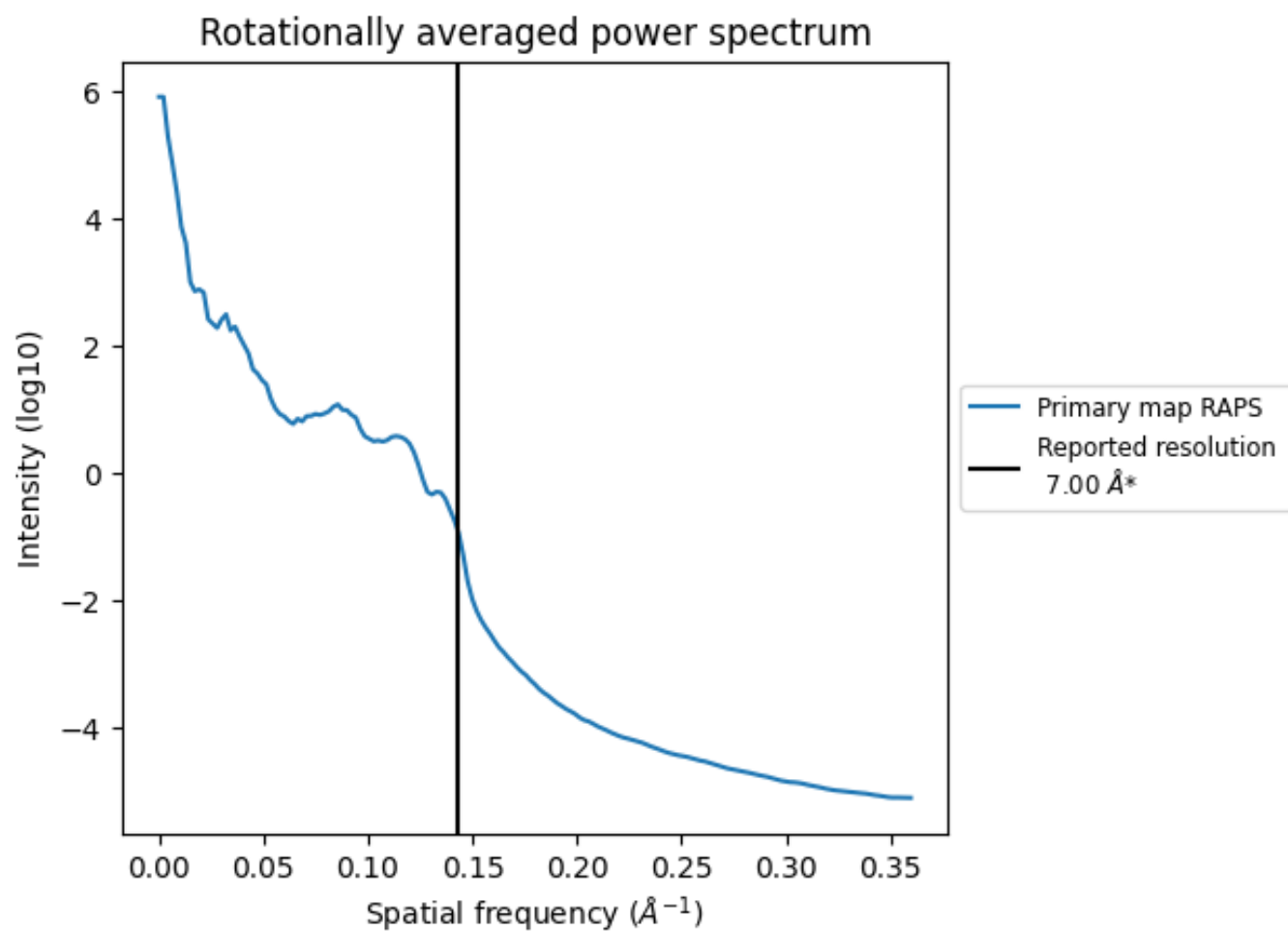
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1040 nm^3 ; this corresponds to an approximate mass of 939 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

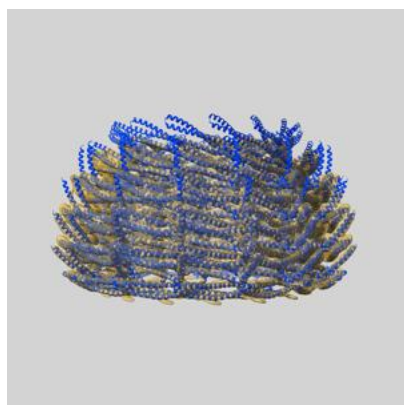
8 Fourier-Shell correlation ⓘ

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

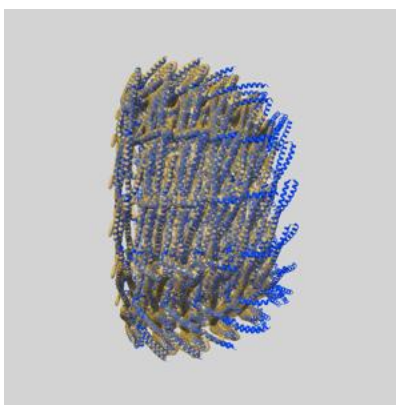
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11481 and PDB model 6ZW5. Per-residue inclusion information can be found in section 3 on page 12.

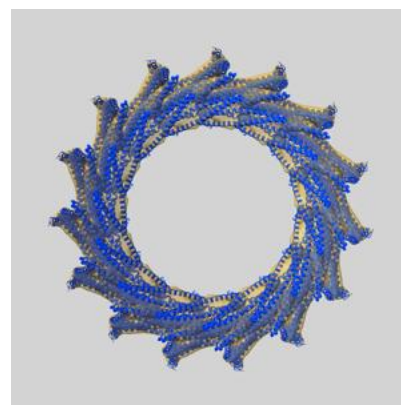
9.1 Map-model overlay [i](#)



X



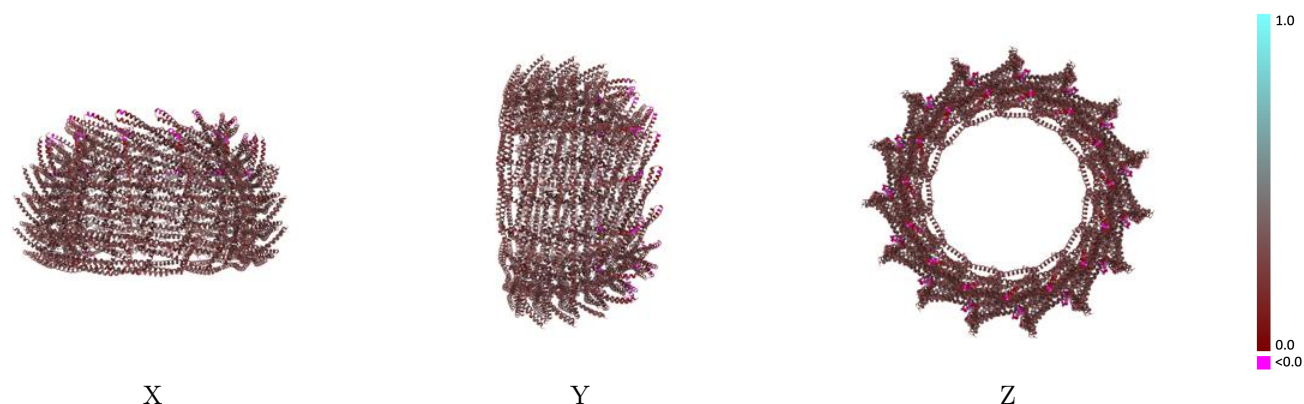
Y



Z

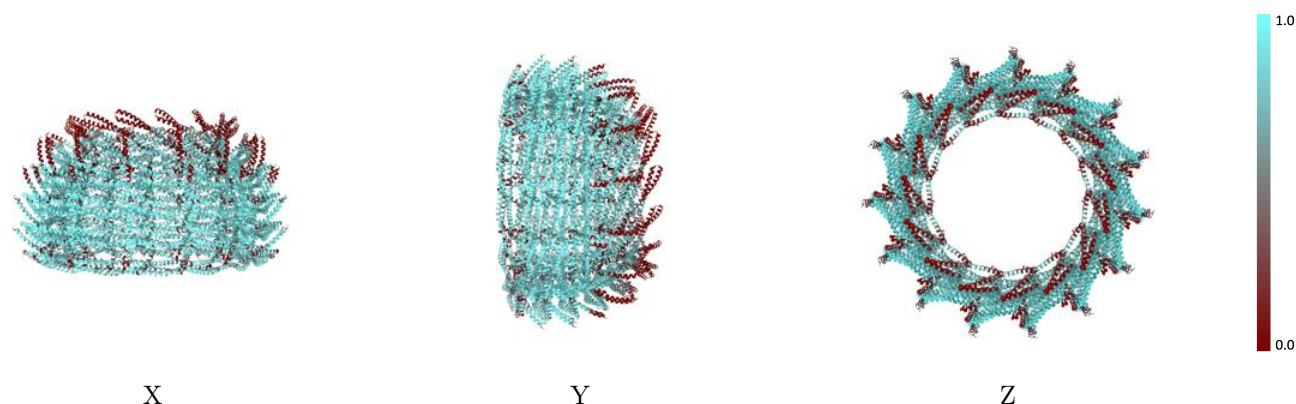
The images above show the 3D surface view of the map at the recommended contour level 0.0182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



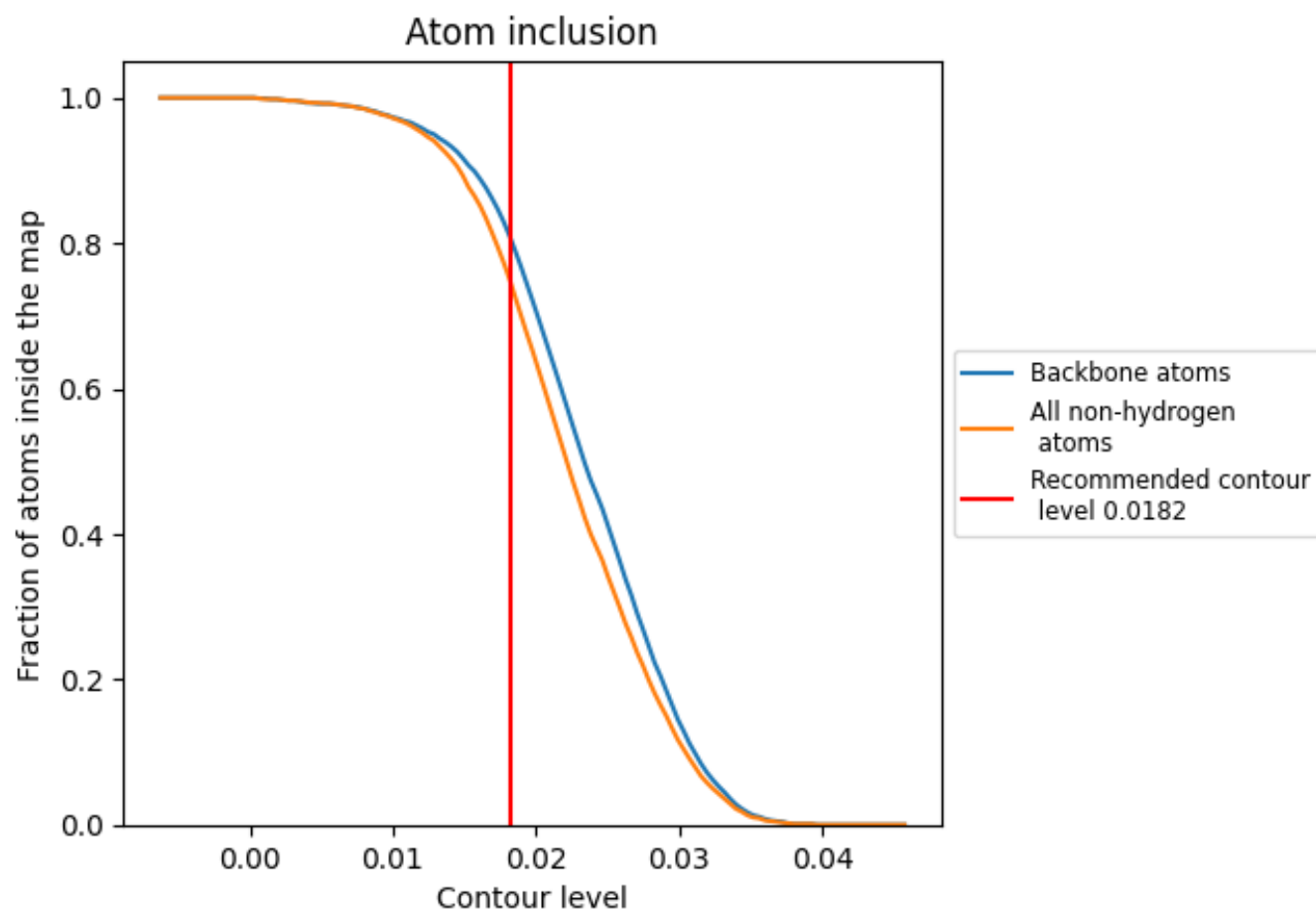
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0182).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.0182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.2580
A	 0.7730	 0.2660
AA	 0.8060	 0.2610
AB	 0.8590	 0.2680
AC	 0.3730	 0.2370
B	 0.8240	 0.2610
BA	 0.9160	 0.2720
BB	 0.6770	 0.2410
BC	 0.7440	 0.2690
C	 0.9210	 0.2730
CA	 0.8540	 0.2690
CB	 0.3950	 0.2390
CC	 0.8200	 0.2590
D	 0.8560	 0.2700
DA	 0.6650	 0.2410
DB	 0.7550	 0.2680
DC	 0.9160	 0.2730
E	 0.6660	 0.2420
EA	 0.3950	 0.2350
EB	 0.8200	 0.2620
EC	 0.8510	 0.2690
F	 0.3910	 0.2350
FA	 0.7170	 0.2690
FB	 0.9200	 0.2740
FC	 0.6540	 0.2410
G	 0.7620	 0.2660
GA	 0.8080	 0.2590
GB	 0.8530	 0.2700
GC	 0.3860	 0.2350
H	 0.8190	 0.2590
HA	 0.9180	 0.2710
HB	 0.6690	 0.2440
HC	 0.7650	 0.2670
I	 0.9210	 0.2730
IA	 0.8580	 0.2690































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Chain	Atom inclusion	Q-score
IB	 0.3780	 0.2380
IC	 0.8250	 0.2590
J	 0.8590	 0.2700
JA	 0.6700	 0.2400
JB	 0.7500	 0.2700
JC	 0.9180	 0.2720
K	 0.6680	 0.2420
KA	 0.3910	 0.2360
KB	 0.8160	 0.2600
KC	 0.8470	 0.2690
L	 0.3960	 0.2360
LA	 0.7440	 0.2700
LB	 0.9170	 0.2740
LC	 0.6580	 0.2400
M	 0.7370	 0.2660
MA	 0.8110	 0.2620
MB	 0.8470	 0.2690
MC	 0.3860	 0.2360
N	 0.8080	 0.2580
NA	 0.9170	 0.2740
NB	 0.6530	 0.2430
O	 0.9180	 0.2710
OA	 0.8540	 0.2690
OB	 0.3720	 0.2380
P	 0.8540	 0.2670
PA	 0.6680	 0.2410
PB	 0.7440	 0.2680
Q	 0.6670	 0.2390
QA	 0.3960	 0.2360
QB	 0.8080	 0.2600
R	 0.3920	 0.2330
RA	 0.7580	 0.2700
RB	 0.9150	 0.2720
S	 0.7310	 0.2690
SA	 0.8220	 0.2610
SB	 0.8460	 0.2680
T	 0.8040	 0.2600
TA	 0.9210	 0.2720
TB	 0.6540	 0.2410
UA	 0.8520	 0.2690
UB	 0.3640	 0.2380
V	 0.9150	 0.2730

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Chain	Atom inclusion	Q-score
VA	 0.6720	 0.2430
VB	 0.7440	 0.2650
W	 0.8470	 0.2690
WA	 0.3990	 0.2390
WB	 0.8140	 0.2570
X	 0.6640	 0.2410
XA	 0.7640	 0.2680
XB	 0.9180	 0.2710
Y	 0.3980	 0.2350
YA	 0.8230	 0.2610
YB	 0.8510	 0.2670
Z	 0.7290	 0.2660
ZA	 0.9240	 0.2720
ZB	 0.6540	 0.2410