



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:56 am GMT

PDB ID : 6ZW4  
EMDB ID : EMD-11478  
Title : C14 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 : 6.50 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](mailto: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>.

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

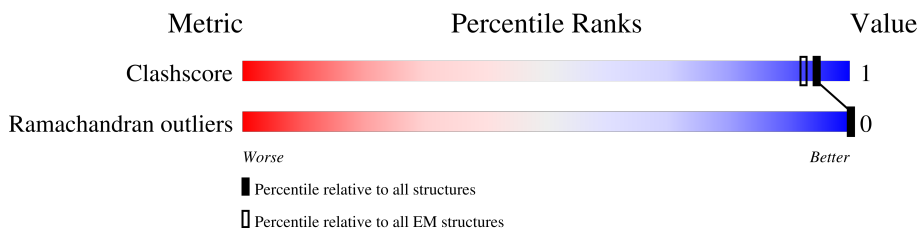
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 6.50 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  $\geq 3$ , 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	6% (red), 52% (green), 48% (grey)
1	AA	258	8% (red), 84% (green), 15% (grey)
1	AB	258	84% (green), 15% (grey)
1	AC	258	21% (red), 61% (green), 39% (grey)
1	B	258	9% (red), 84% (green), 15% (grey)
1	BA	258	83% (green), 15% (grey)
1	BB	258	13% (red), 84% (green), 16% (grey)
1	BC	258	6% (red), 52% (green), 48% (grey)
1	C	258	83% (green), 15% (grey)













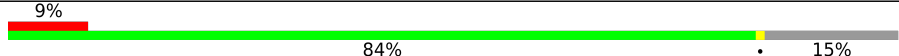
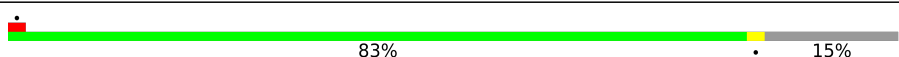
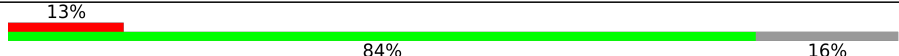

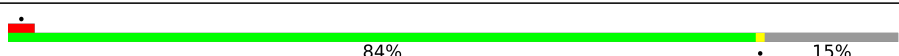
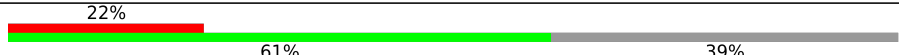
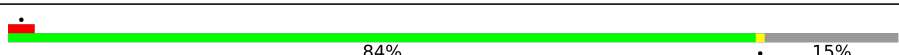
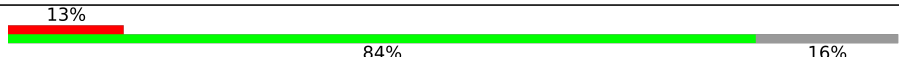
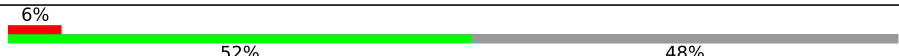



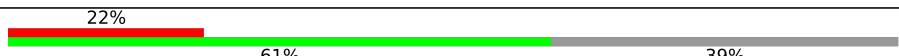
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Mol	Chain	Length	Quality of chain
1	CA	258	84% 15%
1	CB	258	21% 61% 39%
1	CC	258	84% 15%
1	D	258	84% 15%
1	DA	258	13% 84% 16%
1	DB	258	5% 52% 48%
1	DC	258	83% 15%
1	E	258	13% 84% 16%
1	EA	258	21% 61% 39%
1	EB	258	84% 15%
1	EC	258	84% 15%
1	F	258	21% 61% 39%
1	FA	258	6% 52% 48%
1	FB	258	83% 15%
1	FC	258	13% 84% 16%
1	G	258	6% 52% 48%
1	GA	258	84% 15%
1	GB	258	84% 15%
1	GC	258	22% 61% 39%
1	H	258	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	21% 61% 39%

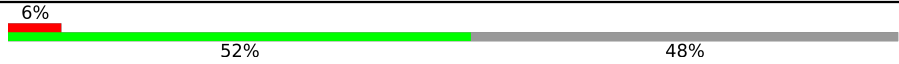
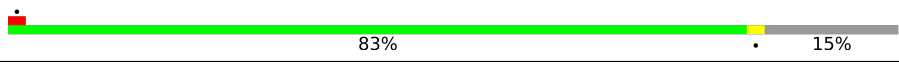
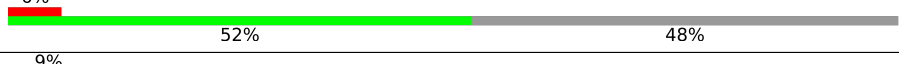


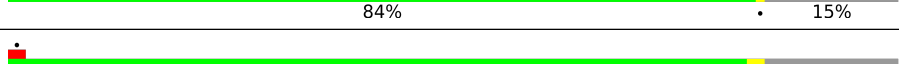
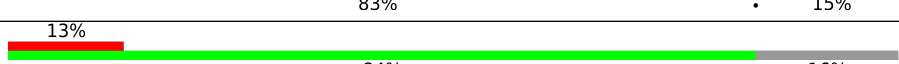
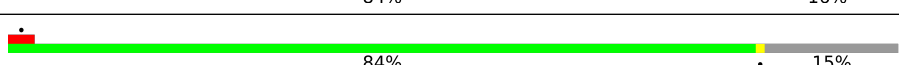
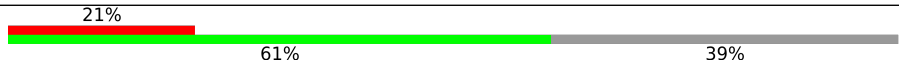


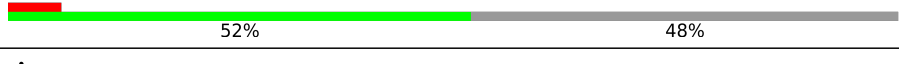
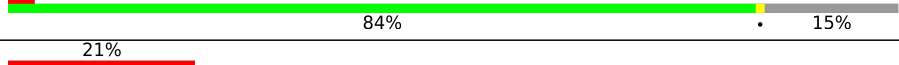

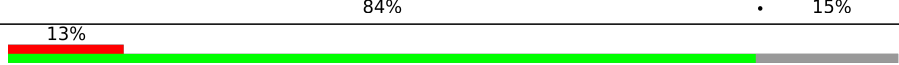
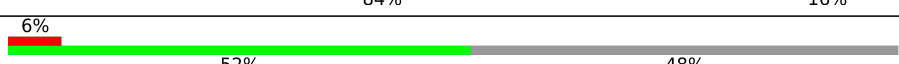




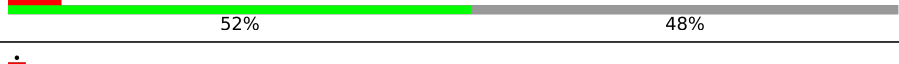

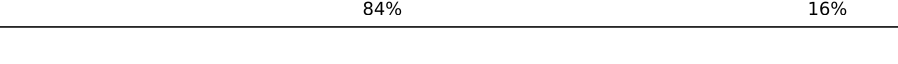


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Mol	Chain	Length	Quality of chain
1	J	258	 84% 13% 15%
1	JA	258	 84% 13% 16%
1	JB	258	 52% 6% 48%
1	K	258	 84% 13% 16%
1	KA	258	 61% 21% 39%
1	KB	258	 84% 8% 15%
1	L	258	 61% 21% 39%
1	LA	258	 52% 6% 48%
1	LB	258	 83% 5% 15%
1	M	258	 52% 9% 48%
1	MA	258	 84% 9% 15%
1	MB	258	 84% 5% 15%
1	N	258	 84% 9% 15%
1	NA	258	 83% 5% 15%
1	NB	258	 84% 13% 16%
1	O	258	 83% 5% 15%
1	OA	258	 84% 5% 15%
1	OB	258	 61% 22% 39%
1	P	258	 84% 5% 15%
1	PA	258	 84% 13% 16%
1	PB	258	 52% 6% 48%
1	Q	258	 84% 13% 16%
1	QA	258	 61% 21% 39%
1	QB	258	 84% 8% 15%
1	R	258	 61% 22% 39%

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

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 80990 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

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

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

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

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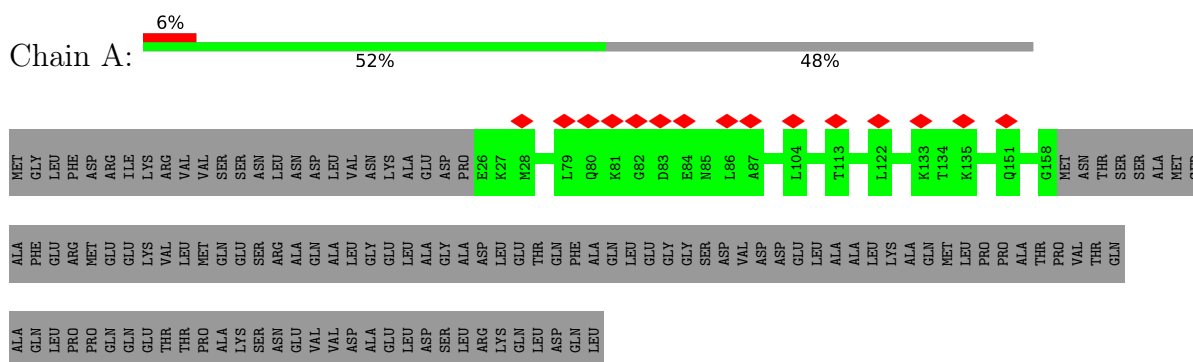
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>	<b>Trace</b>
1	DC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	EC	219	Total	C	N	O	0	0
			1086	648	219	219		
1	FC	218	Total	C	N	O	0	0
			1081	645	218	218		
1	GC	158	Total	C	N	O	0	0
			785	469	158	158		

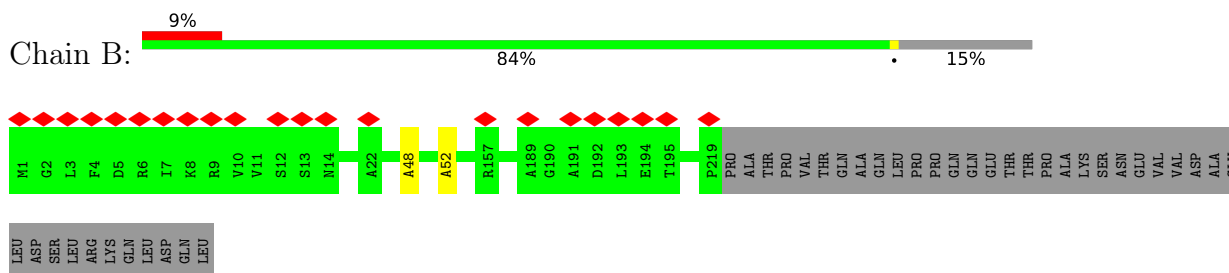
### 3 Residue-property plots [i](#)

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.

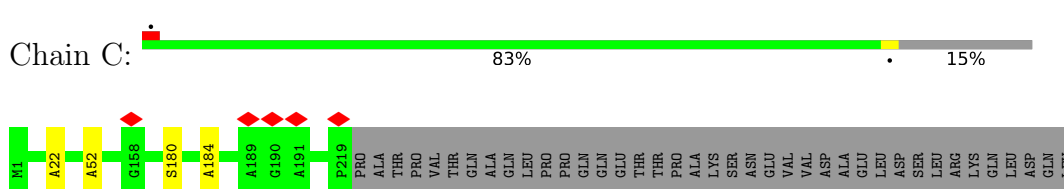
- Molecule 1: vipp1



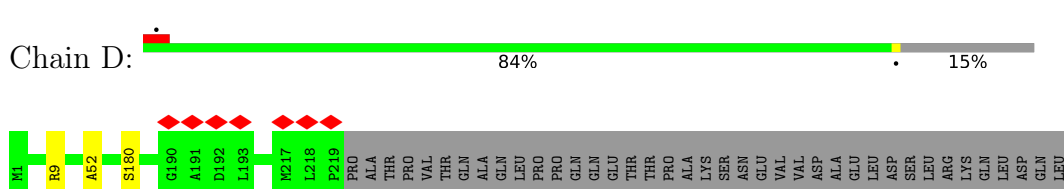
- Molecule 1: vipp1



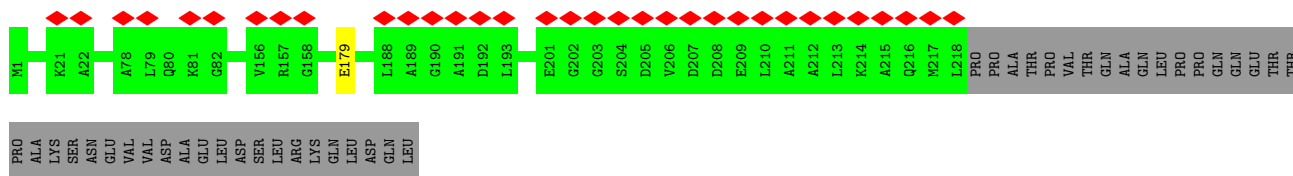
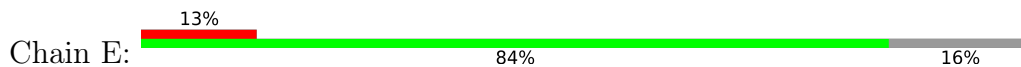
- Molecule 1: vipp1



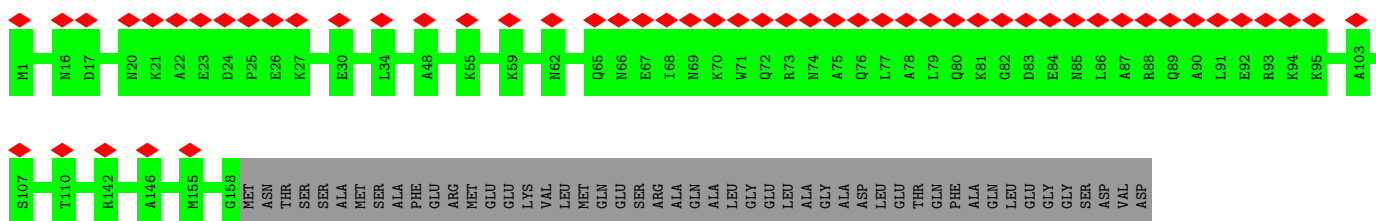
- Molecule 1: vipp1



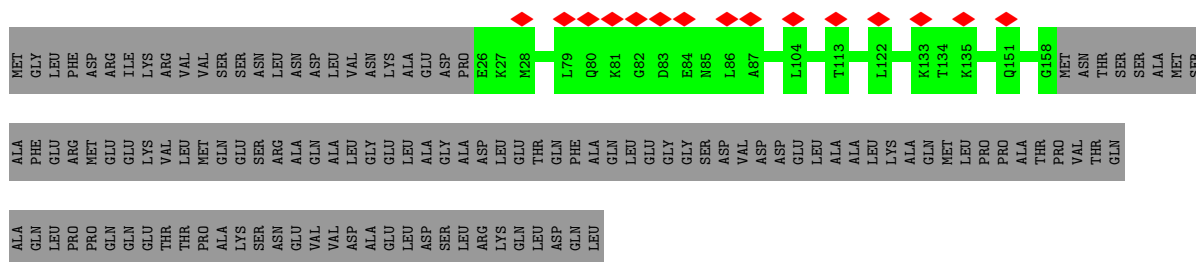
• Molecule 1: vipp1



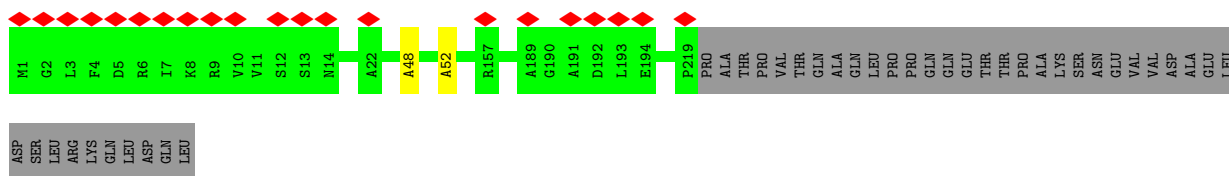
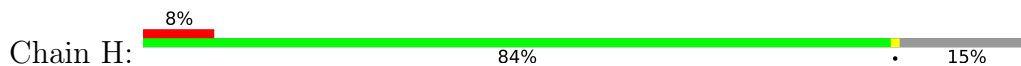
• Molecule 1: vipp1



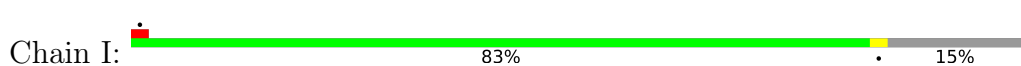
• Molecule 1: vipp1



• Molecule 1: vipp1



• Molecule 1: vipp1















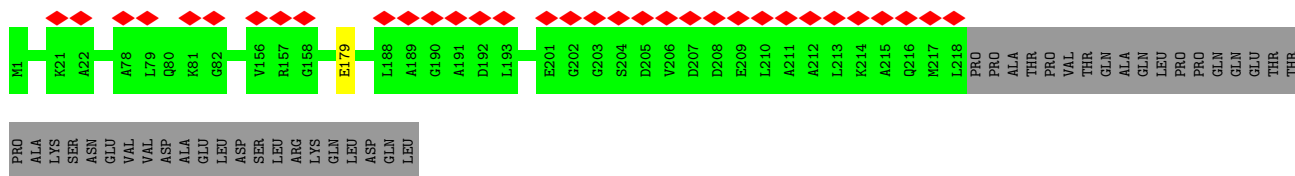




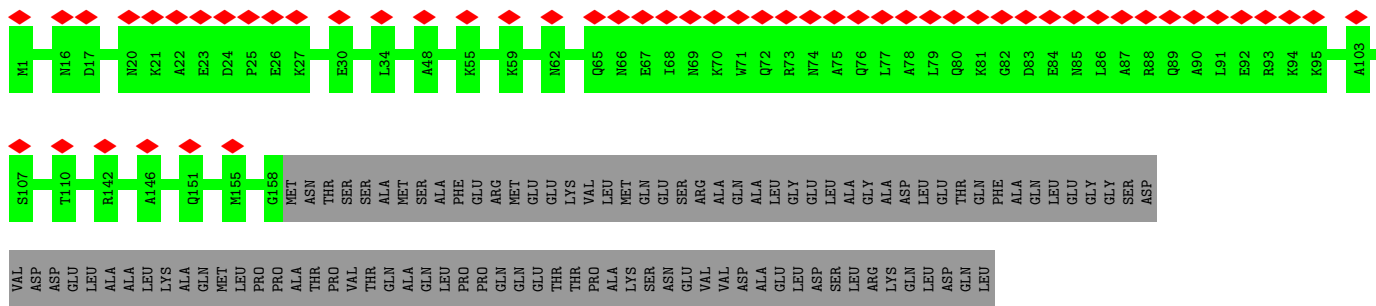




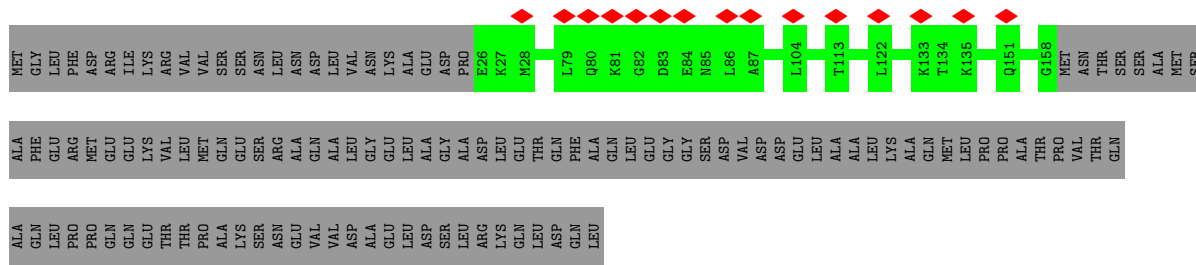




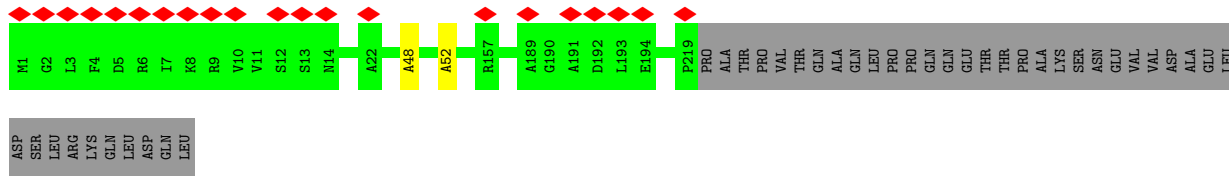
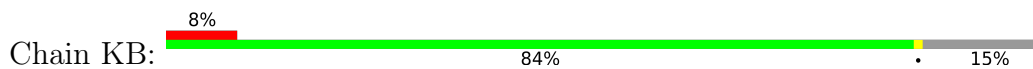
• Molecule 1: vipp1



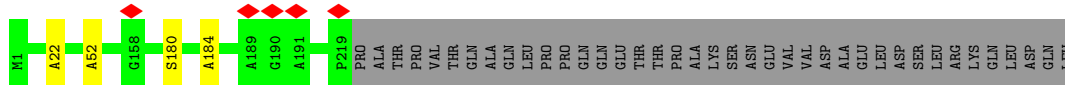
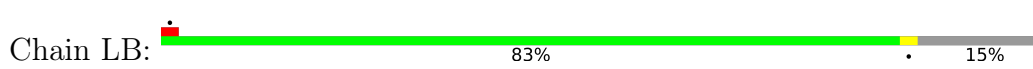
• Molecule 1: vipp1



• Molecule 1: vipp1



• Molecule 1: vipp1



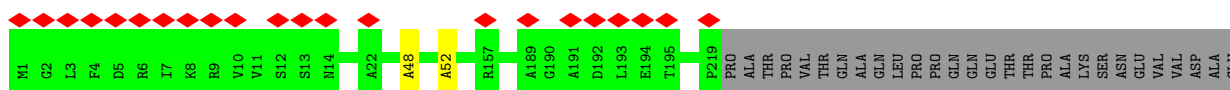
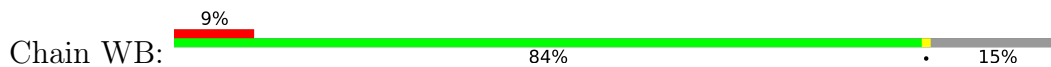






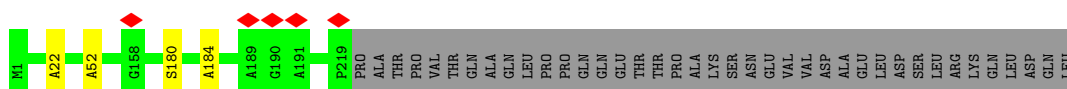
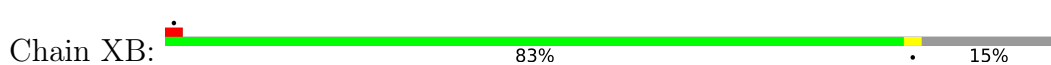
ALA  
GLN  
LEU  
ASP  
PRO  
PRO  
PRO  
GLN  
GLN  
GLU  
THR  
THR  
PRO  
PRO  
PRO  
ALA  
LYS  
LYS  
SER  
SER  
ASN  
GLU  
VAL  
VAL  
VAL  
ASP  
ASP  
ALA  
GLU  
LEU  
LEU  
ASP  
ASP  
GLN  
LEU

• Molecule 1: vipp1

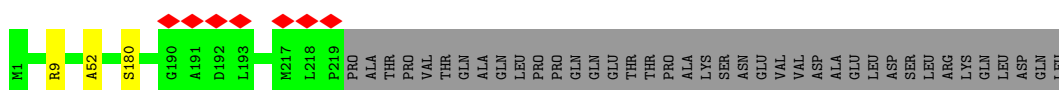
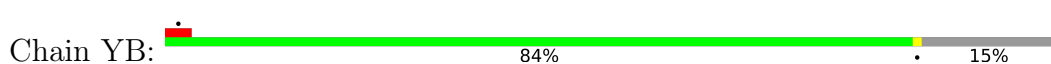


LEU  
ASP  
SER  
LEU  
ARG  
LYS  
GLN  
LEU  
ASP  
GLN  
LEU

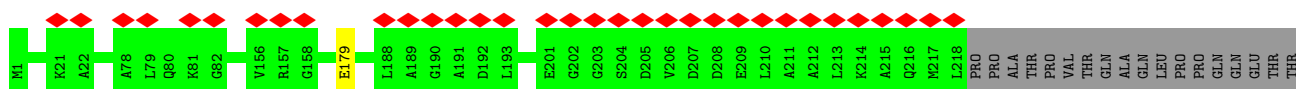
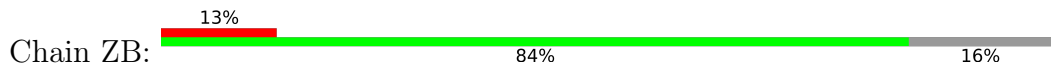
• Molecule 1: vipp1



• Molecule 1: vipp1

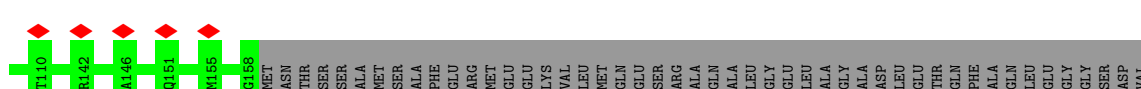
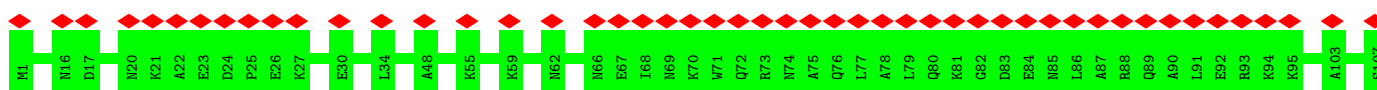


• Molecule 1: vipp1



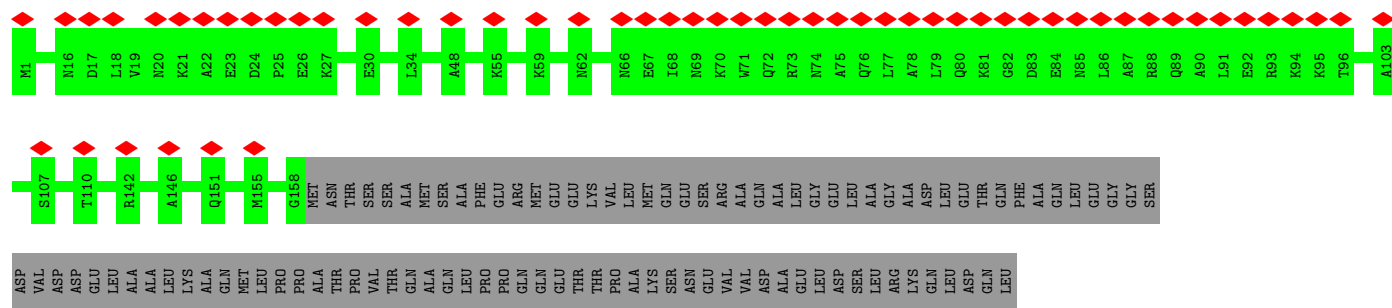
PRO  
ALA  
LYS  
SER  
ASN  
GLU  
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VAL  
VAL  
ALA  
ALA  
LEU  
LEU  
ASP  
SER  
SER  
ARG  
LYS  
GLN  
LEU  
ASP  
GLN

• Molecule 1: vipp1



ASP  
ASP  
GLU  
LEU  
ALA  
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ALA  
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MET  
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ALA  
ALA  
THR  
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PRO  
VAL  
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GLN  
GLN  
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GLU  
LEU  
ASP  
SER  
LEU  
LYS  
ARG  
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	17114	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	0.058	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0153	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	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	0.19	0/660	0.38	0/920
1	AA	0.36	0/1085	0.78	0/1512
1	AB	0.19	0/1085	0.40	0/1512
1	AC	0.18	0/784	0.38	0/1093
1	B	0.35	0/1085	0.78	0/1512
1	BA	0.19	0/1085	0.44	0/1512
1	BB	0.21	0/1080	0.42	0/1505
1	BC	0.19	0/660	0.38	0/920
1	C	0.19	0/1085	0.44	0/1512
1	CA	0.19	0/1085	0.40	0/1512
1	CB	0.18	0/784	0.38	0/1093
1	CC	0.36	0/1085	0.78	0/1512
1	D	0.19	0/1085	0.40	0/1512
1	DA	0.21	0/1080	0.42	0/1505
1	DB	0.19	0/660	0.38	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	0.38	0/1093
1	EB	0.36	0/1085	0.78	0/1512
1	EC	0.19	0/1085	0.40	0/1512
1	F	0.18	0/784	0.38	0/1093
1	FA	0.19	0/660	0.38	0/920
1	FB	0.19	0/1085	0.44	0/1512
1	FC	0.21	0/1080	0.42	0/1505
1	G	0.19	0/660	0.38	0/920
1	GA	0.36	0/1085	0.78	0/1512
1	GB	0.19	0/1085	0.40	0/1512
1	GC	0.18	0/784	0.38	0/1093
1	H	0.36	0/1085	0.78	0/1512
1	HA	0.19	0/1085	0.44	0/1512
1	HB	0.21	0/1080	0.42	0/1505
1	I	0.19	0/1085	0.44	0/1512
1	IA	0.19	0/1085	0.40	0/1512
1	IB	0.18	0/784	0.38	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	J	0.19	0/1085	0.40	0/1512
1	JA	0.21	0/1080	0.42	0/1505
1	JB	0.19	0/660	0.38	0/920
1	K	0.21	0/1080	0.42	0/1505
1	KA	0.18	0/784	0.38	0/1093
1	KB	0.35	0/1085	0.78	0/1512
1	L	0.18	0/784	0.38	0/1093
1	LA	0.19	0/660	0.38	0/920
1	LB	0.19	0/1085	0.44	0/1512
1	M	0.19	0/660	0.38	0/920
1	MA	0.36	0/1085	0.77	0/1512
1	MB	0.19	0/1085	0.40	0/1512
1	N	0.36	0/1085	0.78	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	0.40	0/1512
1	OB	0.18	0/784	0.38	0/1093
1	P	0.19	0/1085	0.40	0/1512
1	PA	0.21	0/1080	0.42	0/1505
1	PB	0.19	0/660	0.38	0/920
1	Q	0.21	0/1080	0.42	0/1505
1	QA	0.18	0/784	0.38	0/1093
1	QB	0.36	0/1085	0.78	0/1512
1	R	0.18	0/784	0.38	0/1093
1	RA	0.19	0/660	0.38	0/920
1	RB	0.19	0/1085	0.44	0/1512
1	S	0.19	0/660	0.38	0/920
1	SA	0.35	0/1085	0.78	0/1512
1	SB	0.19	0/1085	0.40	0/1512
1	T	0.36	0/1085	0.78	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	0.40	0/1512
1	UB	0.18	0/784	0.38	0/1093
1	V	0.19	0/1085	0.44	0/1512
1	VA	0.21	0/1080	0.42	0/1505
1	VB	0.19	0/660	0.38	0/920
1	W	0.19	0/1085	0.40	0/1512
1	WA	0.18	0/784	0.38	0/1093
1	WB	0.35	0/1085	0.78	0/1512
1	X	0.21	0/1080	0.42	0/1505
1	XA	0.19	0/660	0.38	0/920

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	XB	0.19	0/1085	0.44	0/1512
1	Y	0.18	0/784	0.38	0/1093
1	YA	0.36	0/1085	0.78	0/1512
1	YB	0.19	0/1085	0.40	0/1512
1	Z	0.19	0/660	0.38	0/920
1	ZA	0.19	0/1085	0.44	0/1512
1	ZB	0.21	0/1080	0.42	0/1505
All	All	0.23	0/80906	0.50	0/112756

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	2	0
1	AB	1086	0	531	7	0
1	AC	785	0	376	0	0
1	B	1086	0	531	2	0
1	BA	1086	0	531	7	0
1	BB	1081	0	530	2	0
1	BC	661	0	320	0	0
1	C	1086	0	531	7	0
1	CA	1086	0	531	7	0
1	CB	785	0	376	0	0
1	CC	1086	0	531	2	0
1	D	1086	0	531	7	0
1	DA	1081	0	530	2	0
1	DB	661	0	320	0	0
1	DC	1086	0	531	7	0
1	E	1081	0	530	2	0
1	EA	785	0	376	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EB	1086	0	531	2	0
1	EC	1086	0	531	7	0
1	F	785	0	376	0	0
1	FA	661	0	320	0	0
1	FB	1086	0	531	7	0
1	FC	1081	0	530	2	0
1	G	661	0	320	0	0
1	GA	1086	0	531	2	0
1	GB	1086	0	531	7	0
1	GC	785	0	376	0	0
1	H	1086	0	531	2	0
1	HA	1086	0	531	7	0
1	HB	1081	0	530	2	0
1	I	1086	0	531	7	0
1	IA	1086	0	531	7	0
1	IB	785	0	376	0	0
1	J	1086	0	531	7	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	0	0
1	KB	1086	0	531	2	0
1	L	785	0	376	0	0
1	LA	661	0	320	0	0
1	LB	1086	0	531	7	0
1	M	661	0	320	0	0
1	MA	1086	0	531	2	0
1	MB	1086	0	531	7	0
1	N	1086	0	531	2	0
1	NA	1086	0	531	7	0
1	NB	1081	0	530	2	0
1	O	1086	0	531	7	0
1	OA	1086	0	531	7	0
1	OB	785	0	376	0	0
1	P	1086	0	531	7	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	0	0
1	QB	1086	0	531	2	0
1	R	785	0	376	0	0
1	RA	661	0	320	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RB	1086	0	531	7	0
1	S	661	0	320	0	0
1	SA	1086	0	531	2	0
1	SB	1086	0	531	7	0
1	T	1086	0	531	2	0
1	TA	1086	0	531	7	0
1	TB	1081	0	530	2	0
1	UA	1086	0	531	7	0
1	UB	785	0	376	0	0
1	V	1086	0	531	7	0
1	VA	1081	0	530	2	0
1	VB	661	0	320	0	0
1	W	1086	0	531	7	0
1	WA	785	0	376	0	0
1	WB	1086	0	531	2	0
1	X	1081	0	530	2	0
1	XA	661	0	320	0	0
1	XB	1086	0	531	7	0
1	Y	785	0	376	0	0
1	YA	1086	0	531	2	0
1	YB	1086	0	531	7	0
1	Z	661	0	320	0	0
1	ZA	1086	0	531	7	0
1	ZB	1081	0	530	2	0
All	All	80990	0	39466	126	0

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

All (126) 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:I:22:ALA:HB1	1:J:9:ARG:CB	2.12	0.80
1:O:22:ALA:HB1	1:P:9:ARG:CB	2.12	0.80
1:DC:22:ALA:HB1	1:EC:9:ARG:CB	2.12	0.80
1:LB:22:ALA:HB1	1:MB:9:ARG:CB	2.12	0.80
1:RB:22:ALA:HB1	1:SB:9:ARG:CB	2.12	0.80
1:C:22:ALA:HB1	1:D:9:ARG:CB	2.12	0.79
1:V:22:ALA:HB1	1:W:9:ARG:CB	2.12	0.79
1:XB:22:ALA:HB1	1:YB:9:ARG:CB	2.12	0.79
1:NA:22:ALA:HB1	1:OA:9:ARG:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:22:ALA:HB1	1:GB:9:ARG:CB	2.12	0.79
1:HA:22:ALA:HB1	1:IA:9:ARG:CB	2.12	0.79
1:BA:22:ALA:HB1	1:CA:9:ARG:CB	2.12	0.79
1:TA:22:ALA:HB1	1:UA:9:ARG:CB	2.12	0.79
1:ZA:22:ALA:HB1	1:AB:9:ARG:CB	2.12	0.78
1:SB:180:SER:CB	1:DC:52:ALA:CB	2.66	0.74
1:I:52:ALA:CB	1:EC:180:SER:CB	2.66	0.74
1:W:180:SER:CB	1:HA:52:ALA:CB	2.66	0.74
1:J:180:SER:CB	1:V:52:ALA:CB	2.66	0.74
1:C:52:ALA:CB	1:YB:180:SER:CB	2.66	0.73
1:D:180:SER:CB	1:O:52:ALA:CB	2.66	0.73
1:GB:180:SER:CB	1:RB:52:ALA:CB	2.66	0.73
1:OA:180:SER:CB	1:ZA:52:ALA:CB	2.66	0.73
1:AB:180:SER:CB	1:LB:52:ALA:CB	2.66	0.73
1:IA:180:SER:CB	1:TA:52:ALA:CB	2.66	0.73
1:P:180:SER:CB	1:BA:52:ALA:CB	2.66	0.73
1:UA:180:SER:CB	1:FB:52:ALA:CB	2.66	0.73
1:MB:180:SER:CB	1:XB:52:ALA:CB	2.66	0.72
1:CA:180:SER:CB	1:NA:52:ALA:CB	2.66	0.72
1:X:179:GLU:CB	1:IA:52:ALA:HB1	2.21	0.71
1:VA:179:GLU:CB	1:GB:52:ALA:HB1	2.21	0.71
1:HB:179:GLU:CB	1:SB:52:ALA:HB1	2.21	0.71
1:JA:179:GLU:CB	1:UA:52:ALA:HB1	2.21	0.71
1:K:179:GLU:CB	1:W:52:ALA:HB1	2.21	0.71
1:E:179:GLU:CB	1:P:52:ALA:HB1	2.21	0.71
1:D:52:ALA:HB1	1:ZB:179:GLU:CB	2.21	0.70
1:DA:179:GLU:CB	1:OA:52:ALA:HB1	2.20	0.70
1:J:52:ALA:HB1	1:FC:179:GLU:CB	2.21	0.70
1:NB:179:GLU:CB	1:YB:52:ALA:HB1	2.21	0.70
1:Q:179:GLU:CB	1:CA:52:ALA:HB1	2.21	0.70
1:BB:179:GLU:CB	1:MB:52:ALA:HB1	2.21	0.70
1:TB:179:GLU:CB	1:EC:52:ALA:HB1	2.21	0.70
1:PA:179:GLU:CB	1:AB:52:ALA:HB1	2.21	0.70
1:C:52:ALA:HB2	1:YB:180:SER:CB	2.25	0.67
1:D:180:SER:CB	1:O:52:ALA:HB2	2.25	0.67
1:I:52:ALA:HB2	1:EC:180:SER:CB	2.25	0.67
1:SB:180:SER:CB	1:DC:52:ALA:HB2	2.25	0.67
1:MB:180:SER:CB	1:XB:52:ALA:HB2	2.25	0.66
1:CA:180:SER:CB	1:NA:52:ALA:HB2	2.26	0.66
1:W:180:SER:CB	1:HA:52:ALA:HB2	2.25	0.66
1:GB:180:SER:CB	1:RB:52:ALA:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:SER:CB	1:V:52:ALA:HB2	2.25	0.66
1:P:180:SER:CB	1:BA:52:ALA:HB2	2.25	0.65
1:UA:180:SER:CB	1:FB:52:ALA:HB2	2.25	0.65
1:IA:180:SER:CB	1:TA:52:ALA:HB2	2.25	0.65
1:AB:180:SER:CB	1:LB:52:ALA:HB2	2.26	0.65
1:OA:180:SER:CB	1:ZA:52:ALA:HB2	2.25	0.64
1:TB:179:GLU:CB	1:EC:52:ALA:CB	2.77	0.63
1:HB:179:GLU:CB	1:SB:52:ALA:CB	2.77	0.63
1:J:52:ALA:CB	1:FC:179:GLU:CB	2.77	0.63
1:X:179:GLU:CB	1:IA:52:ALA:CB	2.77	0.63
1:Q:179:GLU:CB	1:CA:52:ALA:CB	2.77	0.62
1:VA:179:GLU:CB	1:GB:52:ALA:CB	2.77	0.62
1:D:52:ALA:CB	1:ZB:179:GLU:CB	2.76	0.62
1:DA:179:GLU:CB	1:OA:52:ALA:CB	2.77	0.62
1:NB:179:GLU:CB	1:YB:52:ALA:CB	2.77	0.62
1:PA:179:GLU:CB	1:AB:52:ALA:CB	2.77	0.62
1:E:179:GLU:CB	1:P:52:ALA:CB	2.76	0.62
1:K:179:GLU:CB	1:W:52:ALA:CB	2.76	0.62
1:JA:179:GLU:CB	1:UA:52:ALA:CB	2.77	0.62
1:BB:179:GLU:CB	1:MB:52:ALA:CB	2.77	0.61
1:DC:22:ALA:CB	1:EC:9:ARG:CB	2.79	0.61
1:C:22:ALA:CB	1:D:9:ARG:CB	2.79	0.61
1:O:22:ALA:CB	1:P:9:ARG:CB	2.79	0.61
1:LB:22:ALA:CB	1:MB:9:ARG:CB	2.79	0.61
1:RB:22:ALA:CB	1:SB:9:ARG:CB	2.79	0.61
1:NA:22:ALA:CB	1:OA:9:ARG:CB	2.79	0.60
1:I:22:ALA:CB	1:J:9:ARG:CB	2.79	0.60
1:XB:22:ALA:CB	1:YB:9:ARG:CB	2.79	0.60
1:BA:22:ALA:CB	1:CA:9:ARG:CB	2.79	0.60
1:V:22:ALA:CB	1:W:9:ARG:CB	2.79	0.60
1:ZA:22:ALA:CB	1:AB:9:ARG:CB	2.79	0.60
1:FB:22:ALA:CB	1:GB:9:ARG:CB	2.79	0.60
1:TA:22:ALA:CB	1:UA:9:ARG:CB	2.79	0.59
1:HA:22:ALA:CB	1:IA:9:ARG:CB	2.79	0.59
1:AB:180:SER:CB	1:LB:52:ALA:HB1	2.32	0.59
1:CA:180:SER:CB	1:NA:52:ALA:HB1	2.33	0.58
1:W:180:SER:CB	1:HA:52:ALA:HB1	2.33	0.58
1:UA:180:SER:CB	1:FB:52:ALA:HB1	2.33	0.58
1:C:52:ALA:HB1	1:YB:180:SER:CB	2.33	0.58
1:SB:180:SER:CB	1:DC:52:ALA:HB1	2.33	0.58
1:IA:180:SER:CB	1:TA:52:ALA:HB1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:180:SER:CB	1:BA:52:ALA:HB1	2.33	0.58
1:MB:180:SER:CB	1:XB:52:ALA:HB1	2.33	0.58
1:I:52:ALA:HB1	1:EC:180:SER:CB	2.33	0.58
1:GB:180:SER:CB	1:RB:52:ALA:HB1	2.33	0.58
1:OA:180:SER:CB	1:ZA:52:ALA:HB1	2.33	0.57
1:J:180:SER:CB	1:V:52:ALA:HB1	2.34	0.56
1:D:180:SER:CB	1:O:52:ALA:HB1	2.33	0.56
1:RB:180:SER:CB	1:CC:52:ALA:HB1	2.42	0.49
1:B:52:ALA:HB1	1:XB:180:SER:CB	2.44	0.48
1:C:180:SER:CB	1:N:52:ALA:HB1	2.44	0.47
1:LB:180:SER:CB	1:WB:52:ALA:HB1	2.44	0.47
1:I:180:SER:CB	1:T:52:ALA:HB1	2.45	0.47
1:O:180:SER:CB	1:AA:52:ALA:HB1	2.45	0.47
1:HA:180:SER:CB	1:SA:52:ALA:HB1	2.45	0.47
1:FB:180:SER:CB	1:QB:52:ALA:HB1	2.44	0.47
1:V:180:SER:CB	1:GA:52:ALA:HB1	2.45	0.47
1:NA:180:SER:CB	1:YA:52:ALA:HB1	2.44	0.47
1:H:52:ALA:HB1	1:DC:180:SER:CB	2.44	0.46
1:BA:180:SER:CB	1:MA:52:ALA:HB1	2.45	0.46
1:ZA:180:SER:CB	1:KB:52:ALA:HB1	2.45	0.46
1:I:184:ALA:CB	1:T:48:ALA:HB1	2.46	0.46
1:TA:180:SER:CB	1:EB:52:ALA:HB1	2.45	0.46
1:BA:184:ALA:CB	1:MA:48:ALA:HB1	2.46	0.46
1:TA:184:ALA:CB	1:EB:48:ALA:HB1	2.47	0.45
1:HA:184:ALA:CB	1:SA:48:ALA:HB1	2.47	0.45
1:NA:184:ALA:CB	1:YA:48:ALA:HB1	2.47	0.45
1:O:184:ALA:CB	1:AA:48:ALA:HB1	2.47	0.44
1:FB:184:ALA:CB	1:QB:48:ALA:HB1	2.48	0.44
1:V:184:ALA:CB	1:GA:48:ALA:HB1	2.47	0.44
1:LB:184:ALA:CB	1:WB:48:ALA:HB1	2.48	0.44
1:B:48:ALA:HB1	1:XB:184:ALA:CB	2.48	0.43
1:C:184:ALA:CB	1:N:48:ALA:HB1	2.47	0.43
1:ZA:184:ALA:CB	1:KB:48:ALA:HB1	2.48	0.43
1:H:48:ALA:HB1	1:DC:184:ALA:CB	2.48	0.43
1:RB:184:ALA:CB	1:CC:48:ALA:HB1	2.50	0.42

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
1	AA	217/258 (84%)	213 (98%)	4 (2%)	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%)	213 (98%)	4 (2%)	0	100	100
1	BA	217/258 (84%)	217 (100%)	0	0	100	100
1	BB	216/258 (84%)	216 (100%)	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%)	213 (98%)	4 (2%)	0	100	100
1	D	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	DA	216/258 (84%)	216 (100%)	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%)	216 (100%)	0	0	100	100
1	EA	156/258 (60%)	156 (100%)	0	0	100	100
1	EB	217/258 (84%)	213 (98%)	4 (2%)	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%)	216 (100%)	0	0	100	100
1	G	131/258 (51%)	131 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GA	217/258 (84%)	213 (98%)	4 (2%)	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%)	213 (98%)	4 (2%)	0	100	100
1	HA	217/258 (84%)	217 (100%)	0	0	100	100
1	HB	216/258 (84%)	216 (100%)	0	0	100	100
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	J	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	JA	216/258 (84%)	216 (100%)	0	0	100	100
1	JB	131/258 (51%)	131 (100%)	0	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%)	213 (98%)	4 (2%)	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	M	131/258 (51%)	131 (100%)	0	0	100	100
1	MA	217/258 (84%)	213 (98%)	4 (2%)	0	100	100
1	MB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	N	217/258 (84%)	213 (98%)	4 (2%)	0	100	100
1	NA	217/258 (84%)	217 (100%)	0	0	100	100
1	NB	216/258 (84%)	216 (100%)	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%)	216 (100%)	0	0	100	100
1	PB	131/258 (51%)	131 (100%)	0	0	100	100
1	Q	216/258 (84%)	216 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	QA	156/258 (60%)	156 (100%)	0	0	100	100
1	QB	217/258 (84%)	213 (98%)	4 (2%)	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%)	213 (98%)	4 (2%)	0	100	100
1	SB	217/258 (84%)	216 (100%)	1 (0%)	0	100	100
1	T	217/258 (84%)	213 (98%)	4 (2%)	0	100	100
1	TA	217/258 (84%)	217 (100%)	0	0	100	100
1	TB	216/258 (84%)	216 (100%)	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%)	216 (100%)	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%)	213 (98%)	4 (2%)	0	100	100
1	X	216/258 (84%)	216 (100%)	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%)	213 (98%)	4 (2%)	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%)	216 (100%)	0	0	100	100
All	All	16156/21672 (74%)	16086 (100%)	70 (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.

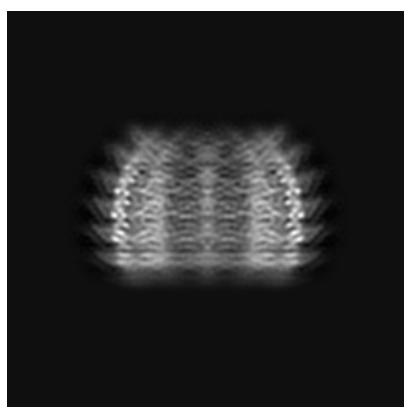
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11478. These allow visual inspection of the internal detail of the map and identification of artifacts.

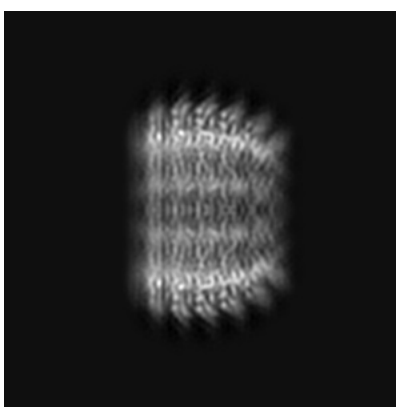
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



X



Y

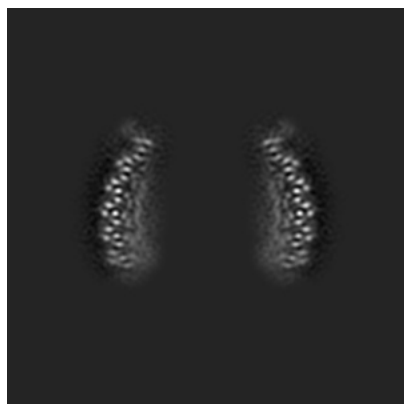


Z

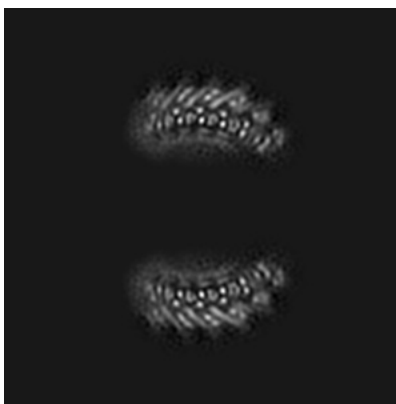
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 168



Y Index: 168



Z Index: 168

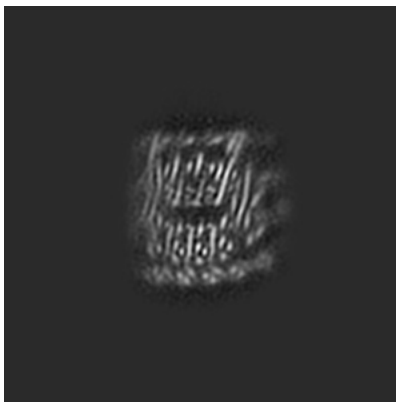
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 232



Y Index: 237

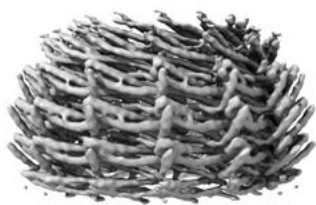


Z Index: 164

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0153. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

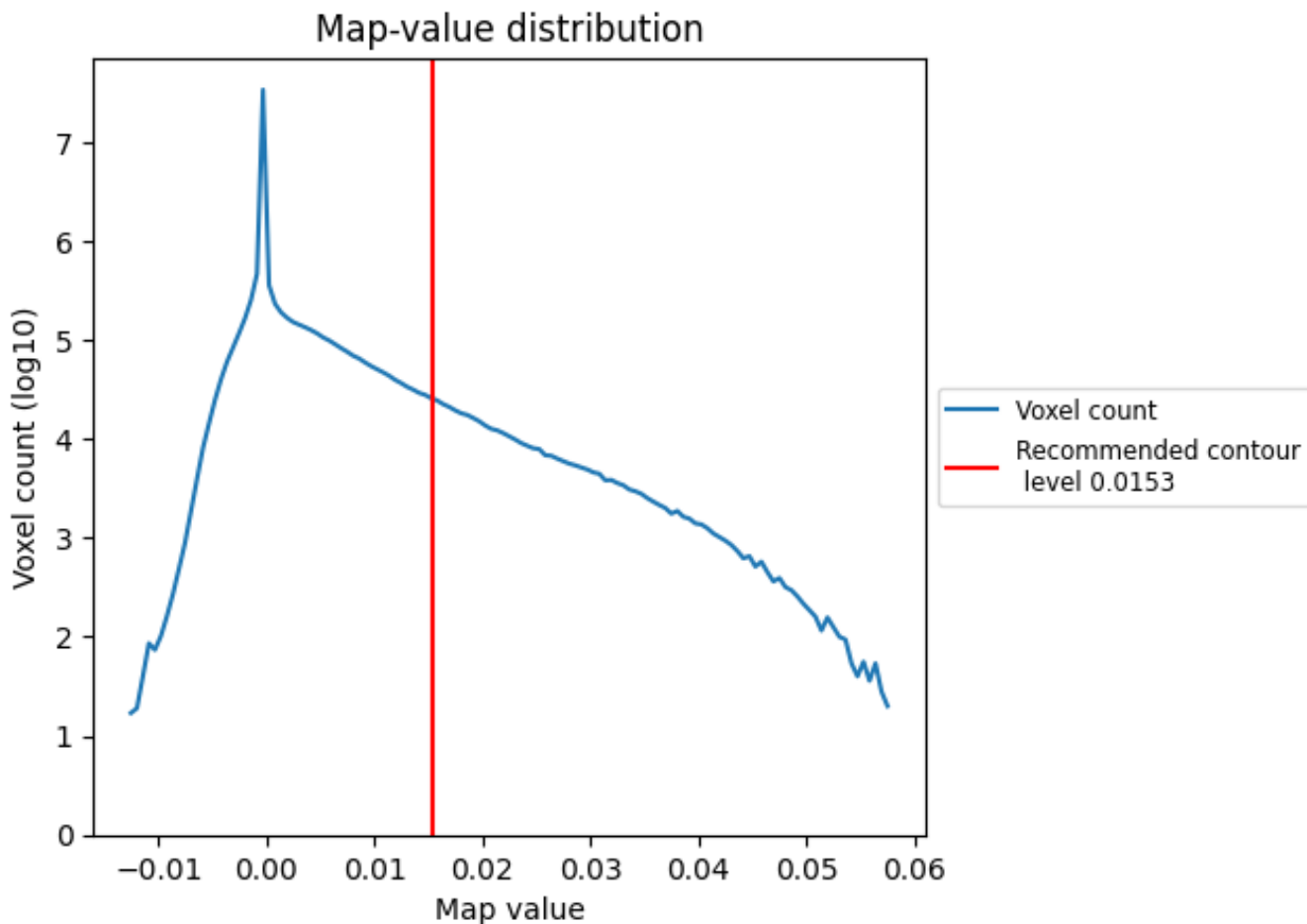
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

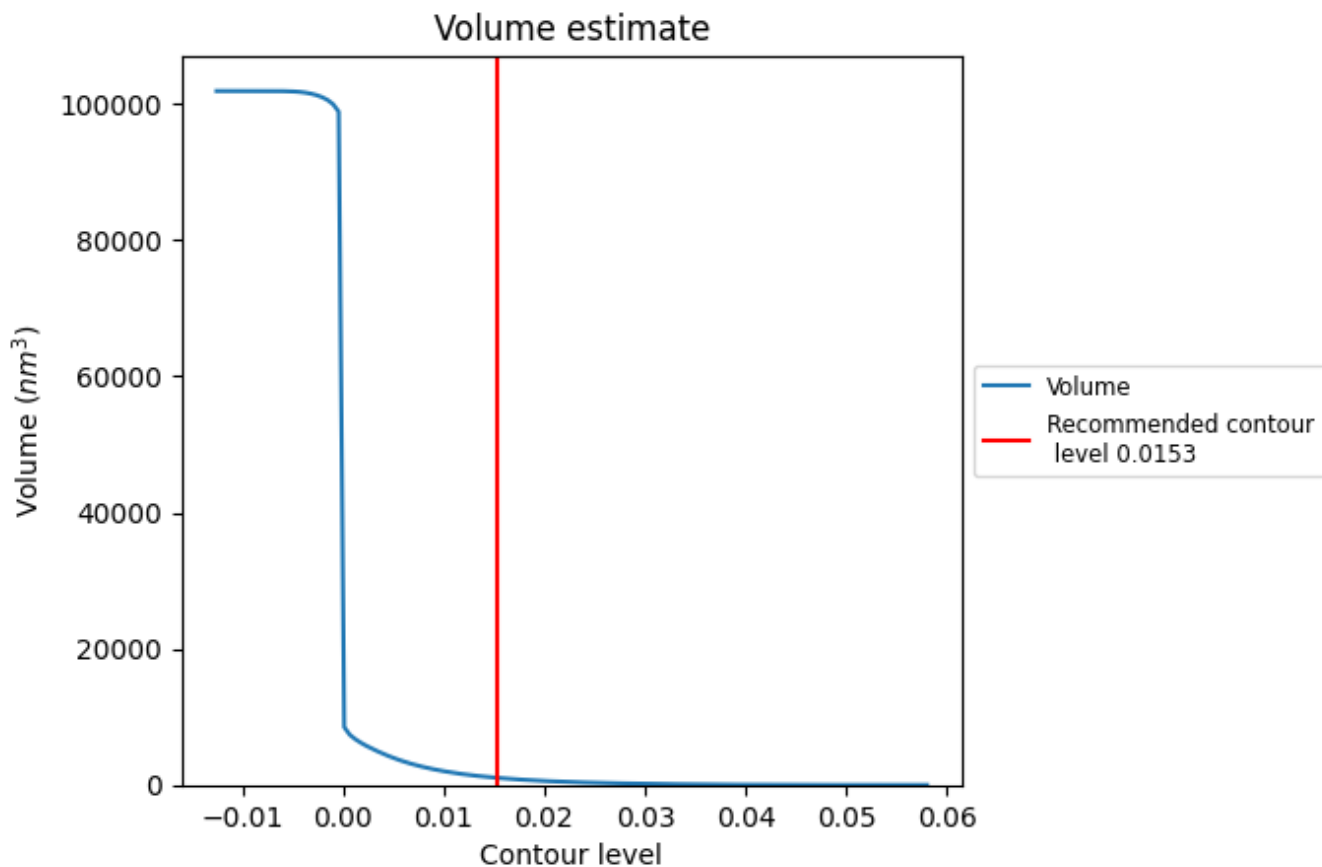
This section contains the results of statistical analysis of the map.

### 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.

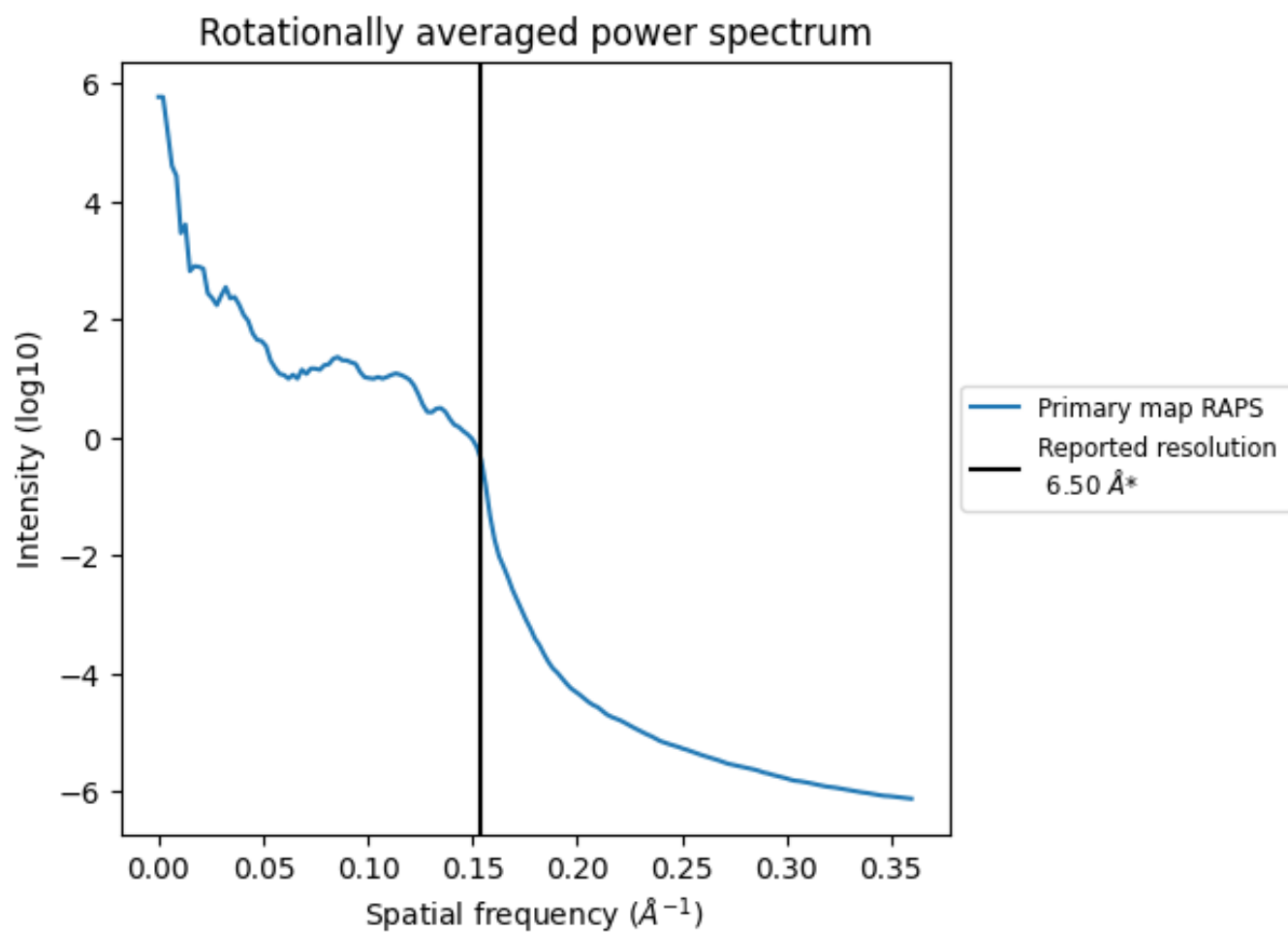
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1051 nm<sup>3</sup>; this corresponds to an approximate mass of 949 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 0.154 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

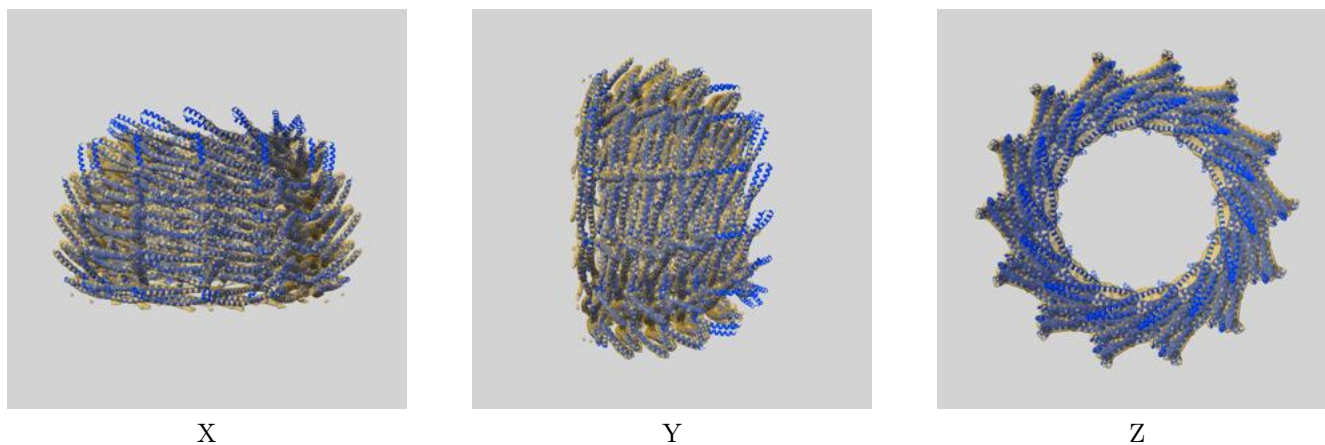
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

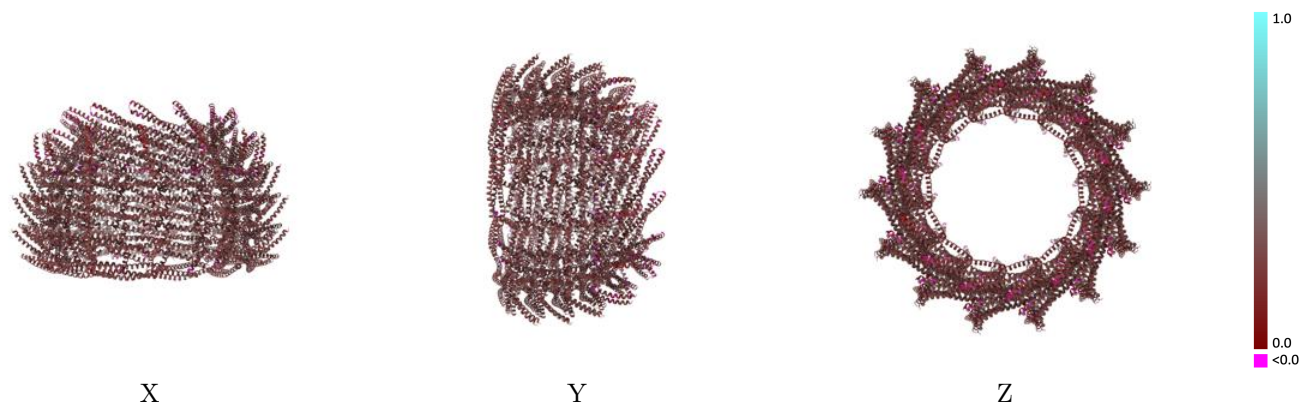
This section contains information regarding the fit between EMDB map EMD-11478 and PDB model 6ZW4. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



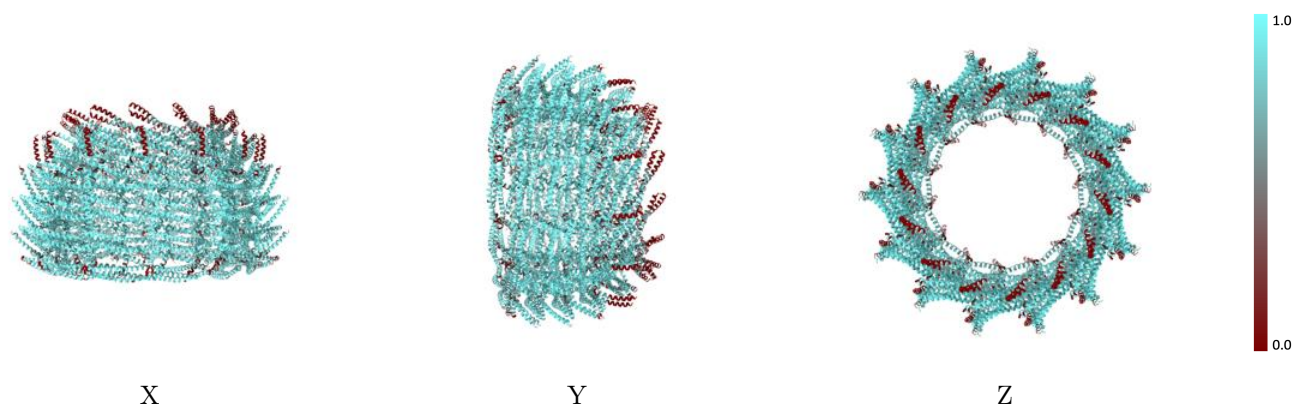
The images above show the 3D surface view of the map at the recommended contour level 0.0153 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



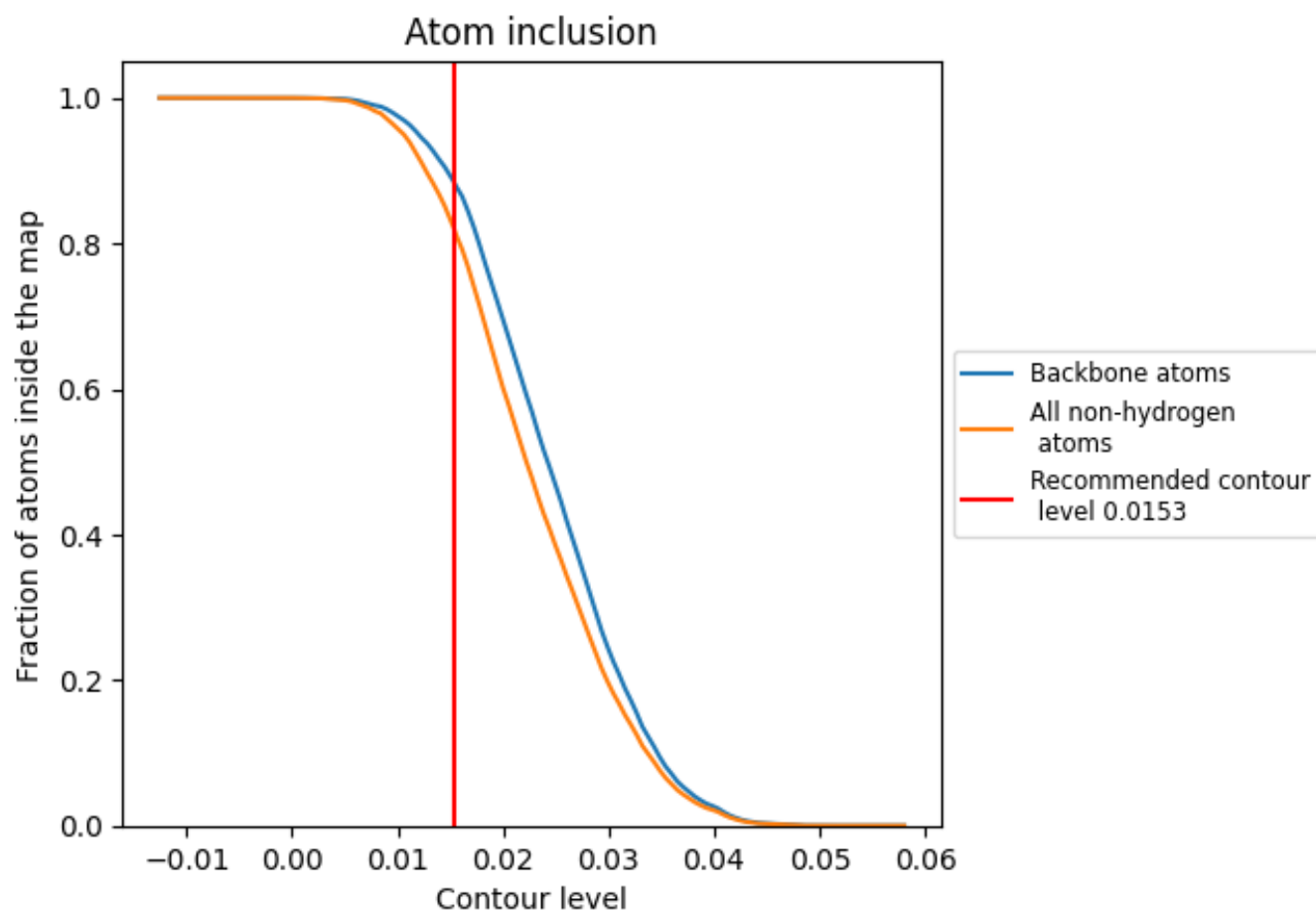
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0153).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.0153) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8224	 0.2600
A	 0.7897	 0.2640
AA	 0.8471	 0.2640
AB	 0.9162	 0.2680
AC	 0.6000	 0.2390
B	 0.8471	 0.2660
BA	 0.9282	 0.2680
BB	 0.7826	 0.2500
BC	 0.7882	 0.2670
C	 0.9282	 0.2670
CA	 0.9134	 0.2670
CB	 0.6013	 0.2400
CC	 0.8444	 0.2660
D	 0.9134	 0.2660
DA	 0.7789	 0.2520
DB	 0.7852	 0.2660
DC	 0.9273	 0.2680
E	 0.7808	 0.2480
EA	 0.6000	 0.2380
EB	 0.8499	 0.2670
EC	 0.9116	 0.2660
F	 0.6000	 0.2370
FA	 0.7852	 0.2650
FB	 0.9282	 0.2670
FC	 0.7817	 0.2500
G	 0.7897	 0.2640
GA	 0.8481	 0.2640
GB	 0.9162	 0.2670
GC	 0.5975	 0.2380
H	 0.8517	 0.2660
HA	 0.9291	 0.2660
HB	 0.7845	 0.2540
I	 0.9291	 0.2690
IA	 0.9153	 0.2660
IB	 0.6000	 0.2420



















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Chain	Atom inclusion	Q-score
J	 0.9134	 0.2690
JA	 0.7789	 0.2490
JB	 0.7867	 0.2660
K	 0.7817	 0.2530
KA	 0.6000	 0.2390
KB	 0.8517	 0.2660
L	 0.6025	 0.2400
LA	 0.7882	 0.2670
LB	 0.9291	 0.2670
M	 0.7882	 0.2620
MA	 0.8444	 0.2680
MB	 0.9144	 0.2670
N	 0.8490	 0.2650
NA	 0.9273	 0.2690
NB	 0.7798	 0.2510
O	 0.9282	 0.2660
OA	 0.9116	 0.2670
OB	 0.5949	 0.2390
P	 0.9153	 0.2650
PA	 0.7798	 0.2500
PB	 0.7867	 0.2620
Q	 0.7826	 0.2490
QA	 0.6000	 0.2390
QB	 0.8490	 0.2650
R	 0.5975	 0.2380
RA	 0.7897	 0.2670
RB	 0.9300	 0.2650
S	 0.7852	 0.2640
SA	 0.8471	 0.2660
SB	 0.9144	 0.2640
T	 0.8508	 0.2650
TA	 0.9282	 0.2680
TB	 0.7808	 0.2490
UA	 0.9134	 0.2680
UB	 0.5962	 0.2390
V	 0.9300	 0.2670
VA	 0.7817	 0.2520
VB	 0.7867	 0.2630
W	 0.9162	 0.2650
WA	 0.6000	 0.2410
WB	 0.8471	 0.2650
X	 0.7789	 0.2500

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Chain	Atom inclusion	Q-score
XA	 0.7897	 0.2650
XB	 0.9291	 0.2650
Y	 0.5949	 0.2380
YA	 0.8508	 0.2660
YB	 0.9162	 0.2650
Z	 0.7882	 0.2640
ZA	 0.9300	 0.2670
ZB	 0.7789	 0.2490