

# wwPDB EM Validation Summary Report (i)

Jul 13, 2022 – 07:33 pm BST

PDB ID : 7PHM

EMDB ID : EMD-13420

Title : Cryo-EM structure of Mycobacterium tuberculosis encapsulin

Authors : Woodward, J.D.

 $Deposited \ on \quad : \quad 2021\text{-}08\text{-}17$ 

Resolution : 2.20 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev8

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

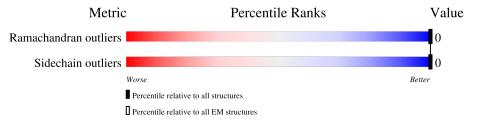
Validation Pipeline (wwPDB-VP) : 2.29

### 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 2.20 Å.

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



Metric	Whole archive $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	0	270	98%
1	1	270	98%
1	2	270	98%
1	3	270	98%
1	4	270	98%
1	5	270	98%
1	6	270	98%
1	7	270	98%
1	A	270	98%



Continued from previous page...

Mol	Chain	$oxed{ egin{array}{c} \mathbf{Length} \end{array} }$	Quality of chain
			•
1	В	270	98%
1	С	270	98%
1	D	270	98%
1	Е	270	98%
			•
1	F	270	98%
1	G	270	98%
1	Н	270	98%
1	I	270	98%
			·
1	J	270	98%
1	K	270	98%
1	L	270	98%
1	M	270	98%
			•
1	N	270	98%
1	О	270	98%
1	Р	270	98%
1	Q	270	98%
			•
1	R	270	98%
1	S	270	98%
1	Т	270	98%
1	U	270	98%
			·
1	V	270	98%
1	W	270	98%
1	X	270	98%
1	Y	270	98%
			•
1	Z	270	98%



 $Continued\ from\ previous\ page...$ 

Mol	Chain	$oxed{ egin{array}{c} \textit{Length} \end{array} }$	Quality of chain
1	a	270	98%
			•
1	b	270	98%
1	С	270	98%
1	d	270	98%
1	e	270	98%
1	f	270	98%
1	g	270	98%
1	h	270	98%
1	i	270	1000
			·
1	j	270	98%
1	k	270	98%
1	l	270	98%
1	m	270	98%
1	n	270	98%
1	О	270	98%
1		270	•
	p		•
1	q	270	98%
1	r	270	98%
1	S	270	98%
1	t	270	98%
1	u	270	98%
1	V	270	98%
1	W	270	98%
1	X	270	100
			·
1	У	270	98%



Continued from previous page...

Mol	Chain	Length	Quality of chain
1	${f z}$	270	98%



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 121560 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 29 kDa antigen CFP29.

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Mol	Chain	Residues		Ato	oms			AltConf	Trace
1       A       264       Total C N O S 2026 1273 353 399 1       0       0         1       B       264       Total C N O S 2026 1273 353 399 1       0       0         1       B       264       Total C N O S 2026 1273 353 399 1       0       0         1       C       264       Total C N O S 2026 1273 353 399 1       0       0         1       D       264       Total C N O S 2026 1273 353 399 1       0       0         1       E       264       Total C N O S 2026 1273 353 399 1       0       0         1       F       264       Total C N O S 2026 1273 353 399 1       0       0         1       F       264       Total C N O S 2026 1273 353 399 1       0       0         1       G       264       Total C N O S 2026 1273 353 399 1       0       0         1       H       264       Total C N O S 2026 1273 353 399 1       0       0         1       H       264       Total C N O S 2026 1273 353 399 1       0       0         1       J       264       Total C N O S 2026 1273 353 399 1       0       0         1       J       264       Total C N O S 2026 1273 353 399 1       0       0	1	7	264	Total	С	N	О	S	0	0
1       A       264       2026       1273       353       399       1       0       0         1       B       264       Total       C       N       O       S       0       0         1       C       264       Total       C       N       O       S       0       0         1       D       264       Total       C       N       O       S       0       0         1       E       264       Total       C       N       O       S       0       0         1       E       264       Total       C       N       O       S       0       0         1       F       264       Total       C       N       O       S       0       0         1       F       264       Total       C       N       O       S       0       0         1       F       264       Total       C       N       O       S       0       0         1       H       264       Total       C       N       O       S       0       0         1       H       264       Total<		L	204	2026	1273	353	399	1	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	۸	264	Total	С	N	О	S	0	0
1       B       264       2026       1273       353       399       1       0       0         1       C       264       Total       C       N       O       S       0       0         1       D       264       Total       C       N       O       S       0       0         1       E       264       Total       C       N       O       S       0       0         1       E       264       Total       C       N       O       S       0       0         1       F       264       Total       C       N       O       S       0       0         1       F       264       Total       C       N       O       S       0       0         1       G       264       Total       C       N       O       S       0       0         1       H       264       Total       C       N       O       S       0       0         1       J       264       Total       C       N       O       S       0       0         1       J       264       Total<	1	A	204	2026	1273	353	399	1	U	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Б	204	2026	1273	353	399	1	U	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	C	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1		204	2026	1273	353	399	1	U	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	D	264	Total	С	N	О	S	0	0
1       E       264       2026       1273       353       399       1       0       0         1       F       264       Total       C       N       O       S       0       0         1       G       264       Total       C       N       O       S       0       0         1       H       264       Total       C       N       O       S       0       0         1       I       264       Total       C       N       O       S       0       0         1       J       264       Total       C       N       O       S       0       0         1       J       264       Total       C       N       O       S       0       0         1       K       264       Total       C       N       O       S       0       0         1       K       264       Total       C       N       O       S       0       0         1       L       264       Total       C       N       O       S       0       0         1       M       264       Total<	1	D	204	2026	1273	353	399	1	U	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	E	264	Total	С	N	О	S	0	0
1       F       264       2026       1273       353       399       1       0       0         1       G       264       Total 2026       C       N       O       S       0       0         1       H       264       Total 2026       C       N       O       S       0       0         1       I       264       Total 2026       C       N       O       S       0       0         1       J       264       Total 2026       C       N       O       S       0       0         1       J       264       Total 2026       C       N       O       S       0       0         1       K       264       Total 2026       C       N       O       S       0       0         1       L       264       Total 2026       C       N       O       S       0       0         1       M       264       Total 2026       C       N       O       S       0       0         1       M       264       Total 2026       C       N       O       S       0       0 <td>1</td> <td>E</td> <td>204</td> <td>2026</td> <td>1273</td> <td>353</td> <td>399</td> <td>1</td> <td>0</td> <td>0</td>	1	E	204	2026	1273	353	399	1	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	E	264	Total	С	N	О	S	0	0
1       G       264       2026       1273       353       399       1       0       0         1       H       264       Total 2026       C       N       O       S       0       0         1       I       264       Total 2026       C       N       O       S       0       0         1       J       264       Total 2026       C       N       O       S       0       0         1       K       264       Total 2026       C       N       O       S       0       0         1       K       264       Total 2026       C       N       O       S       0       0         1       L       264       Total 2026       C       N       O       S       0       0         1       M       264       Total 2026       C       N       O       S       0       0         1       N       264       Total 2026       C       N       O       S       0       0         1       N       264       Total 2026       C       N       O       S       0       0 <td>1</td> <td>Г</td> <td>204</td> <td>2026</td> <td>1273</td> <td>353</td> <td>399</td> <td>1</td> <td>U</td> <td>0</td>	1	Г	204	2026	1273	353	399	1	U	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	C	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	G	204	2026	1273	353	399	1		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	П	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Π	204	2026	1273	353	399			
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Т	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	1	204	2026	1273	353	399		0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Ţ	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	J	204	2026	1273	353	399	1	0	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	T/	264	Total	С	N	О	S	0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	IX	204	2026		353	399		0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	Т	264	Total	С	N	О	S	0	0
1     M     264     2026     1273     353     399     1     0     0       1     N     264     Total     C     N     O     S     0     0       1     O     264     Total     C     N     O     S     0     0       1     O     264     Total     C     N     O     S       Total     C     N     O     S	1	L	204	2026	1273	353	399			0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	М	264	Total	С	N	О	S	0	0
1 N 264 2026 1273 353 399 1 0 0  1 O 264 Total C N O S 2026 1273 353 399 1 0 0  Total C N O S	1	1V1	204	2026	1273	353	399	1	U	U
1 O 264 Total C N O S 0 0 Total C N O S 0 0 Total C N O S 0 0	1	N	264	Total	С	N	О	S	0	0
1 0 264 2026 1273 353 399 1 0 0 Total C N O S	1	1.0	204	2026	1273		399		U	0
2026 1273 353 399 1 Total C N O S	1	0	264	Total	С	N	О	S	0	0
1 D Oct Total C N O S	1		204	2026	1273		399			U
1   P   '26/1	1	Р	264	Total	С	N	О		0	0
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	1	204	2026	1273	353	399	1	U	0



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Residues	<u> </u>	Ato	oms			AltConf	Trace
-1	0	201	Total	С	N	О	S	0	0
1	Q	264	2026	1273	353	399	1	0	0
1	D	264	Total	С	N	О	S	0	0
1	R	264	2026	1273	353	399	1	0	0
1	a	004	Total	С	N	О	S	0	0
1	S	264	2026	1273	353	399	1	0	0
1	Т	264	Total	С	N	О	S	0	0
1	1	264	2026	1273	353	399	1	0	0
1	U	264	Total	С	N	О	S	0	0
1	U	204	2026	1273	353	399	1	0	U
1	V	264	Total	С	N	О	S	0	0
1	V	204	2026	1273	353	399	1	0	U
1	W	264	Total	С	N	О	S	0	0
1	VV	204	2026	1273	353	399	1	0	
1	X	264	Total	С	N	О	S	0	0
1	Λ	204	2026	1273	353	399	1	U	
1	Y	264	Total	С	N	О	S	0	0
1	1	204	2026	1273	353	399	1		
1		264	Total	С	N	О	S	0	0
1	a	204	2026	1273	353	399	1		U
1	b	264	Total	С	N	О	S	0	0
1	D	204	2026	1273	353	399	1		
1	c	264	Total	С	N	О	S	0	0
1		204	2026	1273	353	399	1		U
1	d	264	Total	С	N	Ο	S	0	0
1	u	204	2026	1273	353	399	1	U	U
1	e	264	Total	С	N	О	S	0	0
1	C	204	2026	1273	353	399	1	U	U
1	f	264	Total	$\mathbf{C}$	N	Ο	$\mathbf{S}$	0	0
1	1	204	2026	1273	353	399	1	0	U
1	g	264	Total	$\mathbf{C}$	N	O	S	0	0
	8	201	2026	1273	353	399	1	O O	O
1	h	264	Total	$\mathbf{C}$	N	O	S	0	0
	11	201	2026	1273	353	399	1	O O	O .
1	i	264	Total	С	N	О	$\mathbf{S}$	0	0
	1	201	2026	1273	353	399	1		
1	j	264	Total	С	N	О	$\mathbf{S}$	0	0
	J	201	2026	1273	353	399	1		0
1	k	264	Total	С	N	Ο	S	0	0
			2026	1273	353	399	1		
1	1	264	Total	C	N	0	S	0	0
	•		2026	1273	353	399	$\frac{1}{\gamma_{ontin}}$		



Continued from previous page...

Mol	Chain	$oxed{ \mathbf{Residues} }$	90	Ato	oms			AltConf	Trace
1,101	0 110111		Total	С	N	О	S		
1	m	264	2026	1273	353	399	1	0	0
1		264	Total	С	N	О	S	0	0
1	n	264	2026	1273	353	399	1	0	0
1	_	264	Total	С	N	О	S	0	0
1	О	264	2026	1273	353	399	1	0	0
1	n	264	Total	С	N	О	S	0	0
1	p	204	2026	1273	353	399	1	U	U
1	a	264	Total	С	N	О	S	0	0
1	q	204	2026	1273	353	399	1	U	U
1	r	264	Total	С	N	О	S	0	0
1	1	204	2026	1273	353	399	1	U	U
1	s	264	Total	$\mathbf{C}$	N	Ο	$\mathbf{S}$	0	0
1	ъ	204	2026	1273	353	399	1		0
1	t	264	Total	$\mathbf{C}$	N	O	S	0	0
	· ·	201	2026	1273	353	399	1		U
1	u	264	Total	$\mathbf{C}$	N	Ο	S	0	0
	u	201	2026	1273	353	399	1		
1	v	264	Total	С	N	Ο	$\mathbf{S}$	0	0
	·	201	2026	1273	353	399	1		Ů,
1	w	264	Total	С	N	О	S	0	0
	,,	201	2026	1273	353	399	1	Ü	
1	X	264	Total	С	N	О	S	0	0
		_01	2026	1273	353	399	1	Ű	Ü
1	у	264	Total	С	N	О	S	0	0
	J	_01	2026	1273	353	399	1	Ů	Ŭ.
1	$\mathbf{z}$	264	Total	С	N	O	S	0	0
	_		2026	1273	353	399	1	, and the second	
1	0	264	Total	C	N	0	S	0	0
			2026	1273	353	399	1	-	_
1	1	264	Total	C	N	0	S	0	0
			2026	1273	353	399	1		
1	2	264	Total	C	N	0	S	0	0
			2026	1273	353	399	1	Ů,	
1	3	264	Total	C	N	0	S	0	0
			2026	1273	353 N	399	1		
1	4	264	Total	C	N	0	S	0	0
			2026	1273	353 N	399	1		
1	5	264	Total	C	N	0	S	0	0
			2026 Total	$\frac{1273}{C}$	$\frac{353}{N}$	399	$\frac{1}{S}$	-	
1	6	264	Total	C 1272	N 252	O		0	0
			2026	1273	353	399	1		



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	264	Total 2026	C 1273	N 353	O 399	S 1	0	0

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	266	HIS	-	expression tag	UNP I6WZG6
Z	267	HIS	-	expression tag	UNP I6WZG6
Z	268	HIS	-	expression tag	UNP I6WZG6
Z	269	HIS	-	expression tag	UNP I6WZG6
Z	270	HIS	-	expression tag	UNP I6WZG6
A	266	HIS	-	expression tag	UNP I6WZG6
A	267	HIS	-	expression tag	UNP I6WZG6
A	268	HIS	-	expression tag	UNP I6WZG6
A	269	HIS	-	expression tag	UNP I6WZG6
A	270	HIS	-	expression tag	UNP I6WZG6
В	266	HIS	-	expression tag	UNP I6WZG6
В	267	HIS	-	expression tag	UNP I6WZG6
В	268	HIS	-	expression tag	UNP I6WZG6
В	269	HIS	-	expression tag	UNP I6WZG6
В	270	HIS	-	expression tag	UNP I6WZG6
С	266	HIS	-	expression tag	UNP I6WZG6
С	267	HIS	-	expression tag	UNP I6WZG6
С	268	HIS	-	expression tag	UNP I6WZG6
С	269	HIS	-	expression tag	UNP I6WZG6
С	270	HIS	_	expression tag	UNP I6WZG6
D	266	HIS	-	expression tag	UNP I6WZG6
D	267	HIS	-	expression tag	UNP I6WZG6
D	268	HIS	-	expression tag	UNP I6WZG6
D	269	HIS	-	expression tag	UNP I6WZG6
D	270	HIS	-	expression tag	UNP I6WZG6
Е	266	HIS	-	expression tag	UNP I6WZG6
Е	267	HIS	-	expression tag	UNP I6WZG6
Е	268	HIS	-	expression tag	UNP I6WZG6
Е	269	HIS	-	expression tag	UNP I6WZG6
Е	270	HIS	-	expression tag	UNP I6WZG6
F	266	HIS	-	expression tag	UNP I6WZG6
F	267	HIS	-	expression tag	UNP I6WZG6
F	268	HIS	-	expression tag	UNP I6WZG6
F	269	HIS	-	expression tag	UNP I6WZG6
F	270	HIS	-	expression tag	UNP I6WZG6
G	266	HIS	-	expression tag	UNP I6WZG6



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
G	267	HIS	-	expression tag	UNP I6WZG6
G	268	HIS	-	expression tag	UNP I6WZG6
G	269	HIS	-	expression tag	UNP I6WZG6
G	270	HIS	-	expression tag	UNP I6WZG6
Н	266	HIS	-	expression tag	UNP I6WZG6
Н	267	HIS	-	expression tag	UNP I6WZG6
Н	268	HIS	-	expression tag	UNP I6WZG6
Н	269	HIS	-	expression tag	UNP I6WZG6
Н	270	HIS	-	expression tag	UNP I6WZG6
I	266	HIS	-	expression tag	UNP I6WZG6
I	267	HIS	-	expression tag	UNP I6WZG6
I	268	HIS	-	expression tag	UNP I6WZG6
I	269	HIS	-	expression tag	UNP I6WZG6
I	270	HIS	-	expression tag	UNP I6WZG6
J	266	HIS	-	expression tag	UNP I6WZG6
J	267	HIS	-	expression tag	UNP I6WZG6
J	268	HIS	-	expression tag	UNP I6WZG6
J	269	HIS	-	expression tag	UNP I6WZG6
J	270	HIS	-	expression tag	UNP I6WZG6
K	266	HIS	-	expression tag	UNP I6WZG6
K	267	HIS	-	expression tag	UNP I6WZG6
K	268	HIS	-	expression tag	UNP I6WZG6
K	269	HIS	-	expression tag	UNP I6WZG6
K	270	HIS	-	expression tag	UNP I6WZG6
L	266	HIS	-	expression tag	UNP I6WZG6
L	267	HIS	-	expression tag	UNP I6WZG6
L	268	HIS	-	expression tag	UNP I6WZG6
L	269	HIS	-	expression tag	UNP I6WZG6
L	270	HIS	-	expression tag	UNP I6WZG6
M	266	HIS	-	expression tag	UNP I6WZG6
M	267	HIS	-	expression tag	UNP I6WZG6
M	268	HIS	-	expression tag	UNP I6WZG6
M	269	HIS	-	expression tag	UNP I6WZG6
M	270	HIS	-	expression tag	UNP I6WZG6
N	266	HIS	-	expression tag	UNP I6WZG6
N	267	HIS	-	expression tag	UNP I6WZG6
N	268	HIS		expression tag	UNP I6WZG6
N	269	HIS		expression tag	UNP I6WZG6
N	270	HIS		expression tag	UNP I6WZG6
О	266	HIS		expression tag	UNP I6WZG6
О	267	HIS	-	expression tag	UNP I6WZG6
О	268	HIS	_	expression tag	UNP I6WZG6



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled	Actual	Comment	Reference
О	269	HIS	-	expression tag	UNP I6WZG6
О	270	HIS	_	expression tag	UNP I6WZG6
Р	266	HIS	_	expression tag	UNP I6WZG6
Р	267	HIS	-	expression tag	UNP I6WZG6
Р	268	HIS	-	expression tag	UNP I6WZG6
Р	269	HIS	-	expression tag	UNP I6WZG6
Р	270	HIS	-	expression tag	UNP I6WZG6
Q	266	HIS	-	expression tag	UNP I6WZG6
Q	267	HIS	-	expression tag	UNP I6WZG6
Q	268	HIS	-	expression tag	UNP I6WZG6
Q	269	HIS	-	expression tag	UNP I6WZG6
Q	270	HIS	-	expression tag	UNP I6WZG6
R	266	HIS	-	expression tag	UNP I6WZG6
R	267	HIS	-	expression tag	UNP I6WZG6
R	268	HIS	-	expression tag	UNP I6WZG6
R	269	HIS	-	expression tag	UNP I6WZG6
R	270	HIS	-	expression tag	UNP I6WZG6
S	266	HIS	-	expression tag	UNP I6WZG6
S	267	HIS	-	expression tag	UNP I6WZG6
S	268	HIS	-	expression tag	UNP I6WZG6
S	269	HIS	-	expression tag	UNP I6WZG6
S	270	HIS	-	expression tag	UNP I6WZG6
Т	266	HIS	-	expression tag	UNP I6WZG6
Т	267	HIS	-	expression tag	UNP I6WZG6
Т	268	HIS	-	expression tag	UNP I6WZG6
Т	269	HIS	-	expression tag	UNP I6WZG6
Т	270	HIS	-	expression tag	UNP I6WZG6
U	266	HIS	-	expression tag	UNP I6WZG6
U	267	HIS	-	expression tag	UNP I6WZG6
U	268	HIS	-	expression tag	UNP I6WZG6
U	269	HIS	-	expression tag	UNP I6WZG6
U	270	HIS		expression tag	UNP I6WZG6
V	266	HIS	-	expression tag	UNP I6WZG6
V	267	HIS	-	expression tag	UNP I6WZG6
V	268	HIS	-	expression tag	UNP I6WZG6
V	269	HIS	-	expression tag	UNP I6WZG6
V	270	HIS	-	expression tag	UNP I6WZG6
W	266	HIS	-	expression tag	UNP I6WZG6
W	267	HIS	-	expression tag	UNP I6WZG6
W	268	HIS	-	expression tag	UNP I6WZG6
W	269	HIS	-	expression tag	UNP I6WZG6
W	270	HIS	-	expression tag	UNP I6WZG6



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
X	266	HIS	-	expression tag	UNP I6WZG6
X	267	HIS	-	expression tag	UNP I6WZG6
X	268	HIS	-	expression tag	UNP I6WZG6
X	269	HIS	-	expression tag	UNP I6WZG6
X	270	HIS	-	expression tag	UNP I6WZG6
Y	266	HIS	-	expression tag	UNP I6WZG6
Y	267	HIS	-	expression tag	UNP I6WZG6
Y	268	HIS	-	expression tag	UNP I6WZG6
Y	269	HIS	-	expression tag	UNP I6WZG6
Y	270	HIS	-	expression tag	UNP I6WZG6
a	266	HIS	-	expression tag	UNP I6WZG6
a	267	HIS	-	expression tag	UNP I6WZG6
a	268	HIS	-	expression tag	UNP I6WZG6
a	269	HIS	-	expression tag	UNP I6WZG6
a	270	HIS	-	expression tag	UNP I6WZG6
b	266	HIS	-	expression tag	UNP I6WZG6
b	267	HIS	-	expression tag	UNP I6WZG6
b	268	HIS	-	expression tag	UNP I6WZG6
b	269	HIS	-	expression tag	UNP I6WZG6
b	270	HIS	-	expression tag	UNP I6WZG6
С	266	HIS	-	expression tag	UNP I6WZG6
С	267	HIS	-	expression tag	UNP I6WZG6
С	268	HIS	-	expression tag	UNP I6WZG6
С	269	HIS	-	expression tag	UNP I6WZG6
c	270	HIS	-	expression tag	UNP I6WZG6
d	266	HIS	_	expression tag	UNP I6WZG6
d	267	HIS	-	expression tag	UNP I6WZG6
d	268	HIS	_	expression tag	UNP I6WZG6
d	269	HIS	-	expression tag	UNP I6WZG6
d	270	HIS	-	expression tag	UNP I6WZG6
е	266	HIS	-	expression tag	UNP I6WZG6
е	267	HIS	-	expression tag	UNP I6WZG6
е	268	HIS	-	expression tag	UNP I6WZG6
е	269	HIS	-	expression tag	UNP I6WZG6
е	270	HIS	-	expression tag	UNP I6WZG6
f	266	HIS	-	expression tag	UNP I6WZG6
f	267	HIS	-	expression tag	UNP I6WZG6
f	268	HIS	-	expression tag	UNP I6WZG6
f	269	HIS	-	expression tag	UNP I6WZG6
f	270	HIS	-	expression tag	UNP I6WZG6
g	266	HIS	-	expression tag	UNP I6WZG6
g	267	HIS	-	expression tag	UNP I6WZG6



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
g	268	HIS	-	expression tag	UNP I6WZG6
g	269	HIS	-	expression tag	UNP I6WZG6
g	270	HIS	-	expression tag	UNP I6WZG6
h	266	HIS	-	expression tag	UNP I6WZG6
h	267	HIS	-	expression tag	UNP I6WZG6
h	268	HIS	-	expression tag	UNP I6WZG6
h	269	HIS	-	expression tag	UNP I6WZG6
h	270	HIS	-	expression tag	UNP I6WZG6
i	266	HIS	-	expression tag	UNP I6WZG6
i	267	HIS	-	expression tag	UNP I6WZG6
i	268	HIS	-	expression tag	UNP I6WZG6
i	269	HIS	-	expression tag	UNP I6WZG6
i	270	HIS	-	expression tag	UNP I6WZG6
j	266	HIS	-	expression tag	UNP I6WZG6
j	267	HIS	-	expression tag	UNP I6WZG6
j	268	HIS	-	expression tag	UNP I6WZG6
j	269	HIS	-	expression tag	UNP I6WZG6
j	270	HIS	-	expression tag	UNP I6WZG6
k	266	HIS	-	expression tag	UNP I6WZG6
k	267	HIS	-	expression tag	UNP I6WZG6
k	268	HIS	-	expression tag	UNP I6WZG6
k	269	HIS	-	expression tag	UNP I6WZG6
k	270	HIS	-	expression tag	UNP I6WZG6
1	266	HIS	-	expression tag	UNP I6WZG6
1	267	HIS	-	expression tag	UNP I6WZG6
1	268	HIS	-	expression tag	UNP I6WZG6
1	269	HIS	-	expression tag	UNP I6WZG6
1	270	HIS	-	expression tag	UNP I6WZG6
m	266	HIS	-	expression tag	UNP I6WZG6
m	267	HIS	-	expression tag	UNP I6WZG6
m	268	HIS	-	expression tag	UNP I6WZG6
m	269	HIS	-	expression tag	UNP I6WZG6
m	270	HIS	-	expression tag	UNP I6WZG6
n	266	HIS	-	expression tag	UNP I6WZG6
n	267	HIS	-	expression tag	UNP I6WZG6
n	268	HIS	-	expression tag	UNP I6WZG6
n	269	HIS		expression tag	UNP I6WZG6
n	270	HIS		expression tag	UNP I6WZG6
О	266	HIS		expression tag	UNP I6WZG6
0	267	HIS	-	expression tag	UNP I6WZG6
О	268	HIS	-	expression tag	UNP I6WZG6
О	269	HIS	-	expression tag	UNP I6WZG6



 $Continued\ from\ previous\ page...$ 

Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
О	270	HIS	-	expression tag	UNP I6WZG6
р	266	HIS	-	expression tag	UNP I6WZG6
р	267	HIS	-	expression tag	UNP I6WZG6
р	268	HIS	-	expression tag	UNP I6WZG6
р	269	HIS	-	expression tag	UNP I6WZG6
p	270	HIS	-	expression tag	UNP I6WZG6
q	266	HIS	-	expression tag	UNP I6WZG6
q	267	HIS	-	expression tag	UNP I6WZG6
q	268	HIS	-	expression tag	UNP I6WZG6
q	269	HIS	-	expression tag	UNP I6WZG6
q	270	HIS	-	expression tag	UNP I6WZG6
r	266	HIS	-	expression tag	UNP I6WZG6
r	267	HIS	-	expression tag	UNP I6WZG6
r	268	HIS	-	expression tag	UNP I6WZG6
r	269	HIS	-	expression tag	UNP I6WZG6
r	270	HIS	-	expression tag	UNP I6WZG6
S	266	HIS	-	expression tag	UNP I6WZG6
S	267	HIS	-	expression tag	UNP I6WZG6
S	268	HIS	-	expression tag	UNP I6WZG6
S	269	HIS	-	expression tag	UNP I6WZG6
S	270	HIS	-	expression tag	UNP I6WZG6
t	266	HIS	-	expression tag	UNP I6WZG6
t	267	HIS	_	expression tag	UNP I6WZG6
t	268	HIS	-	expression tag	UNP I6WZG6
t	269	HIS	-	expression tag	UNP I6WZG6
t	270	HIS	-	expression tag	UNP I6WZG6
u	266	HIS	-	expression tag	UNP I6WZG6
u	267	HIS	-	expression tag	UNP I6WZG6
u	268	HIS	-	expression tag	UNP I6WZG6
u	269	HIS	-	expression tag	UNP I6WZG6
u	270	HIS	-	expression tag	UNP I6WZG6
V	266	HIS	-	expression tag	UNP I6WZG6
V	267	HIS	-	expression tag	UNP I6WZG6
V	268	HIS	-	expression tag	UNP I6WZG6
V	269	HIS	-	expression tag	UNP I6WZG6
V	270	HIS	-	expression tag	UNP I6WZG6
W	266	HIS	-	expression tag	UNP I6WZG6
W	267	HIS	-	expression tag	UNP I6WZG6
W	268	HIS	-	expression tag	UNP I6WZG6
W	269	HIS	-	expression tag	UNP I6WZG6
W	270	HIS	-	expression tag	UNP I6WZG6
X	266	HIS	-	expression tag	UNP I6WZG6
	l	·	<u> </u>		l on mort mage



 $Continued\ from\ previous\ page...$ 

X   268   HIS   -	Chain	Residue	Modelled  Modelled	Actual	Comment	Reference
X   269	X	267	HIS	-	expression tag	UNP I6WZG6
X	X	268	HIS	-	expression tag	UNP I6WZG6
y         266         HIS         -         expression tag         UNP 16WZG6           y         267         HIS         -         expression tag         UNP 16WZG6           y         268         HIS         -         expression tag         UNP 16WZG6           y         269         HIS         -         expression tag         UNP 16WZG6           z         266         HIS         -         expression tag         UNP 16WZG6           z         267         HIS         -         expression tag         UNP 16WZG6           z         268         HIS         -         expression tag         UNP 16WZG6           z         269         HIS         -         expression tag         UNP 16WZG6           z         269         HIS         -         expression tag         UNP 16WZG6           z         270         HIS         -         expression tag         UNP 16WZG6           0         266         HIS         -         expression tag         UNP 16WZG6           0         268         HIS         -         expression tag         UNP 16WZG6           0         267         HIS         -         expression tag         UNP	X	269	HIS	-	expression tag	UNP I6WZG6
y         267         HIS         -         expression tag         UNP I6WZG6           y         268         HIS         -         expression tag         UNP I6WZG6           y         269         HIS         -         expression tag         UNP I6WZG6           y         270         HIS         -         expression tag         UNP I6WZG6           z         266         HIS         -         expression tag         UNP I6WZG6           z         267         HIS         -         expression tag         UNP I6WZG6           z         269         HIS         -         expression tag         UNP I6WZG6           z         269         HIS         -         expression tag         UNP I6WZG6           z         270         HIS         -         expression tag         UNP I6WZG6           0         266         HIS         -         expression tag         UNP I6WZG6           0         267         HIS         -         expression tag         UNP I6WZG6           0         269         HIS         -         expression tag         UNP I6WZG6           0         270         HIS         -         expression tag         UNP	X	270	HIS	-	expression tag	UNP I6WZG6
y         268         HIS         -         expression tag         UNP 16WZG6           y         269         HIS         -         expression tag         UNP 16WZG6           y         270         HIS         -         expression tag         UNP 16WZG6           z         266         HIS         -         expression tag         UNP 16WZG6           z         267         HIS         -         expression tag         UNP 16WZG6           z         268         HIS         -         expression tag         UNP 16WZG6           z         269         HIS         -         expression tag         UNP 16WZG6           z         270         HIS         -         expression tag         UNP 16WZG6           0         266         HIS         -         expression tag         UNP 16WZG6           0         268         HIS         -         expression tag         UNP 16WZG6           0         269         HIS         -         expression tag         UNP 16WZG6           1         266         HIS         -         expression tag         UNP 16WZG6           1         267         HIS         -         expression tag         UNP	У	266	HIS	-	expression tag	UNP I6WZG6
y         269         HIS         -         expression tag         UNP 16WZG6           y         270         HIS         -         expression tag         UNP 16WZG6           z         266         HIS         -         expression tag         UNP 16WZG6           z         268         HIS         -         expression tag         UNP 16WZG6           z         268         HIS         -         expression tag         UNP 16WZG6           z         269         HIS         -         expression tag         UNP 16WZG6           z         270         HIS         -         expression tag         UNP 16WZG6           0         266         HIS         -         expression tag         UNP 16WZG6           0         267         HIS         -         expression tag         UNP 16WZG6           0         269         HIS         -         expression tag         UNP 16WZG6           0         269         HIS         -         expression tag         UNP 16WZG6           1         266         HIS         -         expression tag         UNP 16WZG6           1         267         HIS         -         expression tag         UNP	у	267	HIS	-	expression tag	UNP I6WZG6
y         270         HIS         -         expression tag         UNP 16WZG6           z         266         HIS         -         expression tag         UNP 16WZG6           z         267         HIS         -         expression tag         UNP 16WZG6           z         268         HIS         -         expression tag         UNP 16WZG6           z         269         HIS         -         expression tag         UNP 16WZG6           0         266         HIS         -         expression tag         UNP 16WZG6           0         266         HIS         -         expression tag         UNP 16WZG6           0         267         HIS         -         expression tag         UNP 16WZG6           0         268         HIS         -         expression tag         UNP 16WZG6           0         269         HIS         -         expression tag         UNP 16WZG6           1         266         HIS         -         expression tag         UNP 16WZG6           1         267         HIS         -         expression tag         UNP 16WZG6           1         269         HIS         -         expression tag         UNP	у	268	HIS	-	expression tag	UNP I6WZG6
Z   266	У	269	HIS	-	expression tag	UNP I6WZG6
z         267         HIS         -         expression tag         UNP I6WZG6           z         268         HIS         -         expression tag         UNP I6WZG6           z         269         HIS         -         expression tag         UNP I6WZG6           z         270         HIS         -         expression tag         UNP I6WZG6           0         266         HIS         -         expression tag         UNP I6WZG6           0         267         HIS         -         expression tag         UNP I6WZG6           0         268         HIS         -         expression tag         UNP I6WZG6           0         269         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP	У	270	HIS	-	expression tag	UNP I6WZG6
z         268         HIS         -         expression tag         UNP I6WZG6           z         269         HIS         -         expression tag         UNP I6WZG6           z         270         HIS         -         expression tag         UNP I6WZG6           0         266         HIS         -         expression tag         UNP I6WZG6           0         267         HIS         -         expression tag         UNP I6WZG6           0         269         HIS         -         expression tag         UNP I6WZG6           0         269         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP	Z	266	HIS	-	expression tag	UNP I6WZG6
z         269         HIS         -         expression tag         UNP I6WZG6           z         270         HIS         -         expression tag         UNP I6WZG6           0         266         HIS         -         expression tag         UNP I6WZG6           0         267         HIS         -         expression tag         UNP I6WZG6           0         268         HIS         -         expression tag         UNP I6WZG6           0         269         HIS         -         expression tag         UNP I6WZG6           0         270         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP	Z	267	HIS	-	expression tag	UNP I6WZG6
z         270         HIS         - expression tag         UNP I6WZG6           0         266         HIS         - expression tag         UNP I6WZG6           0         267         HIS         - expression tag         UNP I6WZG6           0         268         HIS         - expression tag         UNP I6WZG6           0         269         HIS         - expression tag         UNP I6WZG6           0         270         HIS         - expression tag         UNP I6WZG6           1         266         HIS         - expression tag         UNP I6WZG6           1         266         HIS         - expression tag         UNP I6WZG6           1         268         HIS         - expression tag         UNP I6WZG6           1         269         HIS         - expression tag         UNP I6WZG6           2         266         HIS         - expression tag         UNP I6WZG6           2         267         HIS         - expression tag         UNP I6WZG6           2         268         HIS         - expression tag         UNP I6WZG6           2         269         HIS         - expression tag         UNP I6WZG6           3         266	Z	268	HIS	-	expression tag	UNP I6WZG6
0         266         HIS         -         expression tag         UNP 16WZG6           0         267         HIS         -         expression tag         UNP 16WZG6           0         268         HIS         -         expression tag         UNP 16WZG6           0         269         HIS         -         expression tag         UNP 16WZG6           0         270         HIS         -         expression tag         UNP 16WZG6           1         266         HIS         -         expression tag         UNP 16WZG6           1         267         HIS         -         expression tag         UNP 16WZG6           1         268         HIS         -         expression tag         UNP 16WZG6           1         269         HIS         -         expression tag         UNP 16WZG6           1         270         HIS         -         expression tag         UNP 16WZG6           2         266         HIS         -         expression tag         UNP 16WZG6           2         267         HIS         -         expression tag         UNP 16WZG6           2         269         HIS         -         expression tag         UNP	Z	269	HIS	-	expression tag	UNP I6WZG6
0         267         HIS         -         expression tag         UNP 16WZG6           0         268         HIS         -         expression tag         UNP 16WZG6           0         269         HIS         -         expression tag         UNP 16WZG6           0         270         HIS         -         expression tag         UNP 16WZG6           1         266         HIS         -         expression tag         UNP 16WZG6           1         267         HIS         -         expression tag         UNP 16WZG6           1         268         HIS         -         expression tag         UNP 16WZG6           1         269         HIS         -         expression tag         UNP 16WZG6           2         266         HIS         -         expression tag         UNP 16WZG6           2         267         HIS         -         expression tag         UNP 16WZG6           2         268         HIS         -         expression tag         UNP 16WZG6           2         269         HIS         -         expression tag         UNP 16WZG6           3         266         HIS         -         expression tag         UNP	Z	270	HIS	-	expression tag	UNP I6WZG6
0         268         HIS         -         expression tag         UNP I6WZG6           0         269         HIS         -         expression tag         UNP I6WZG6           0         270         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP	0	266	HIS	-	expression tag	UNP I6WZG6
0         269         HIS         -         expression tag         UNP I6WZG6           0         270         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP	0	267	HIS	-	expression tag	UNP I6WZG6
0         270         HIS         -         expression tag         UNP I6WZG6           1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           1         270         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP	0	268	HIS	-	expression tag	UNP I6WZG6
1         266         HIS         -         expression tag         UNP I6WZG6           1         267         HIS         -         expression tag         UNP I6WZG6           1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           1         270         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP	0	269	HIS	_	expression tag	UNP I6WZG6
1         267         HIS         -         expression tag         UNP I6WZG6           1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           1         270         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP	0	270	HIS	-	expression tag	UNP I6WZG6
1         268         HIS         -         expression tag         UNP I6WZG6           1         269         HIS         -         expression tag         UNP I6WZG6           1         270         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP	1	266	HIS	-	expression tag	UNP I6WZG6
1         269         HIS         -         expression tag         UNP I6WZG6           1         270         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP	1	267	HIS	-	expression tag	UNP I6WZG6
1         270         HIS         -         expression tag         UNP I6WZG6           2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP	1	268	HIS	-	expression tag	UNP I6WZG6
2         266         HIS         -         expression tag         UNP I6WZG6           2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP	1	269	HIS	-	expression tag	UNP I6WZG6
2         267         HIS         -         expression tag         UNP I6WZG6           2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP	1	270	HIS	-	expression tag	UNP I6WZG6
2         268         HIS         -         expression tag         UNP I6WZG6           2         269         HIS         -         expression tag         UNP I6WZG6           2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP	2	266	HIS	-	expression tag	UNP I6WZG6
2         269         HIS         -         expression tag         UNP I6WZG6           2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP	2	267	HIS	-	expression tag	UNP I6WZG6
2         270         HIS         -         expression tag         UNP I6WZG6           3         266         HIS         -         expression tag         UNP I6WZG6           3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           3         270         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	2	268	HIS	-	expression tag	UNP I6WZG6
3 266 HIS - expression tag UNP I6WZG6 3 267 HIS - expression tag UNP I6WZG6 3 268 HIS - expression tag UNP I6WZG6 3 269 HIS - expression tag UNP I6WZG6 3 270 HIS - expression tag UNP I6WZG6 4 266 HIS - expression tag UNP I6WZG6 4 267 HIS - expression tag UNP I6WZG6 4 268 HIS - expression tag UNP I6WZG6 4 269 HIS - expression tag UNP I6WZG6 4 270 HIS - expression tag UNP I6WZG6 5 266 HIS - expression tag UNP I6WZG6 5 267 HIS - expression tag UNP I6WZG6 5 267 HIS - expression tag UNP I6WZG6 6 Expression tag UNP I6WZG6 7 Expression tag UNP I6WZG6 8 Expression tag UNP I6WZG6 9 Expression tag UNP I6WZG6 9 Expression tag UNP I6WZG6 9 Expression tag UNP I6WZG6	2	269	HIS	-	expression tag	UNP I6WZG6
3         267         HIS         -         expression tag         UNP I6WZG6           3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           3         270         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	2	270	HIS	-	expression tag	UNP I6WZG6
3         268         HIS         -         expression tag         UNP I6WZG6           3         269         HIS         -         expression tag         UNP I6WZG6           3         270         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	3	266	HIS	-	expression tag	UNP I6WZG6
3         269         HIS         -         expression tag         UNP I6WZG6           3         270         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	3	267	HIS	-	expression tag	UNP I6WZG6
3         270         HIS         -         expression tag         UNP I6WZG6           4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	3	268	HIS	-	expression tag	UNP I6WZG6
4         266         HIS         -         expression tag         UNP I6WZG6           4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	3	269	HIS	-	expression tag	UNP I6WZG6
4         267         HIS         -         expression tag         UNP I6WZG6           4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	3	270	HIS	-	expression tag	UNP I6WZG6
4         268         HIS         -         expression tag         UNP I6WZG6           4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	4	266	HIS	-	expression tag	UNP I6WZG6
4         269         HIS         -         expression tag         UNP I6WZG6           4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	4	267	HIS	-	expression tag	UNP I6WZG6
4         270         HIS         -         expression tag         UNP I6WZG6           5         266         HIS         -         expression tag         UNP I6WZG6           5         267         HIS         -         expression tag         UNP I6WZG6	4	268	HIS	-	expression tag	UNP I6WZG6
5 266 HIS - expression tag UNP I6WZG6 5 267 HIS - expression tag UNP I6WZG6	4	269	HIS	-	expression tag	UNP I6WZG6
5 267 HIS - expression tag UNP I6WZG6	4	270	HIS	-	expression tag	UNP I6WZG6
	5	266	HIS	-	expression tag	UNP I6WZG6
5 268 HIS - expression tag UNP I6WZG6	5	267	HIS	-	expression tag	UNP I6WZG6
	5	268	HIS	-	expression tag	UNP I6WZG6



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
5	269	HIS	-	expression tag	UNP I6WZG6
5	270	HIS	-	expression tag	UNP I6WZG6
6	266	HIS	-	expression tag	UNP I6WZG6
6	267	HIS	-	expression tag	UNP I6WZG6
6	268	HIS	-	expression tag	UNP I6WZG6
6	269	HIS	_	expression tag	UNP I6WZG6
6	270	HIS	-	expression tag	UNP I6WZG6
7	266	HIS	-	expression tag	UNP I6WZG6
7	267	HIS	-	expression tag	UNP I6WZG6
7	268	HIS	-	expression tag	UNP I6WZG6
7	269	HIS	-	expression tag	UNP I6WZG6
7	270	HIS	-	expression tag	UNP I6WZG6

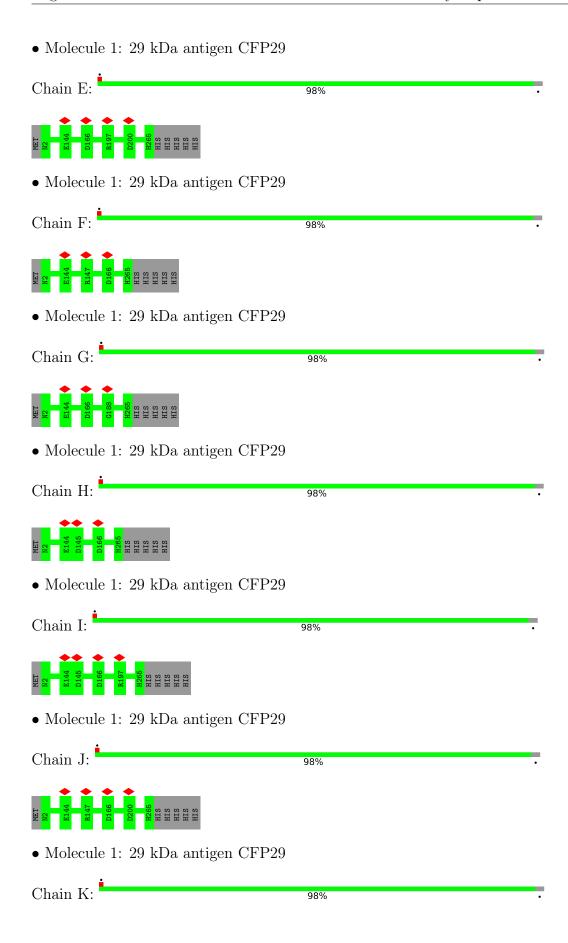


### 3 Residue-property plots (i)

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: 29 kDa antigen CFP29 Chain Z: • Molecule 1: 29 kDa antigen CFP29 Chain A: • Molecule 1: 29 kDa antigen CFP29 Chain B: 98% • Molecule 1: 29 kDa antigen CFP29 Chain C: 98% • Molecule 1: 29 kDa antigen CFP29 Chain D: 98%

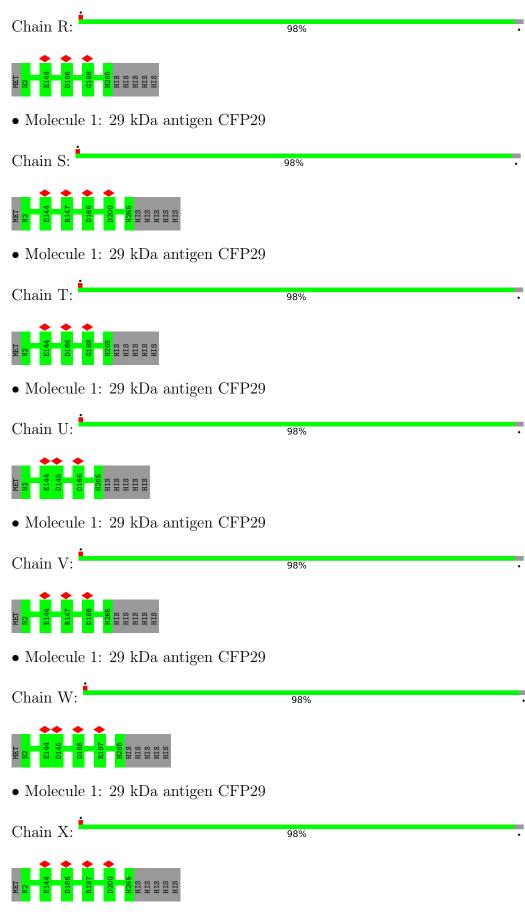








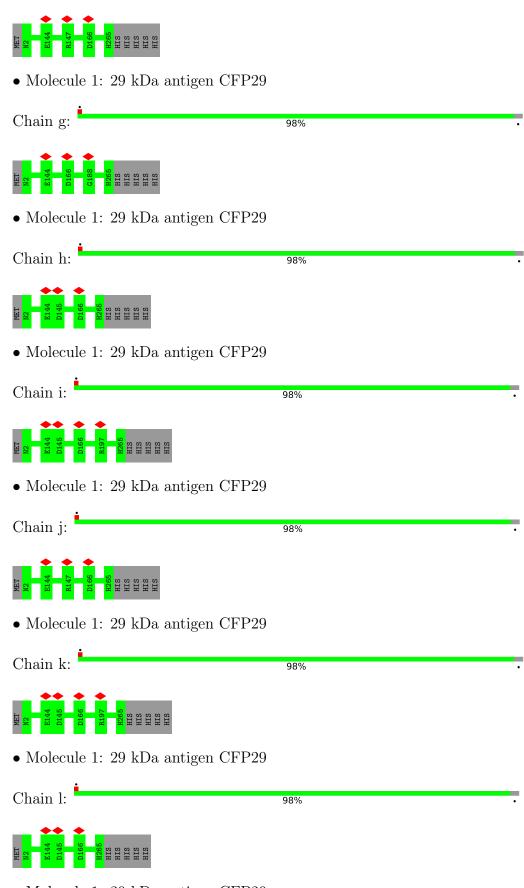






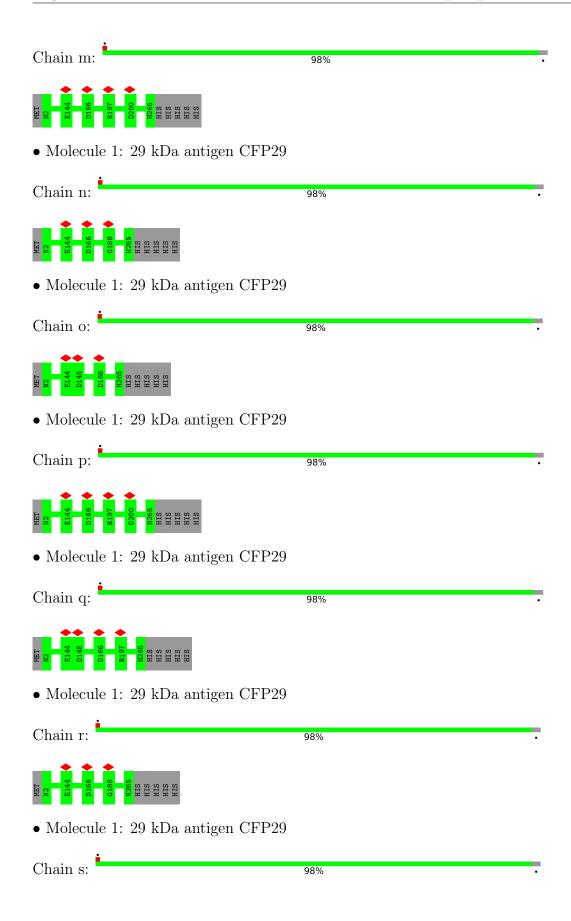






• Molecule 1: 29 kDa antigen CFP29

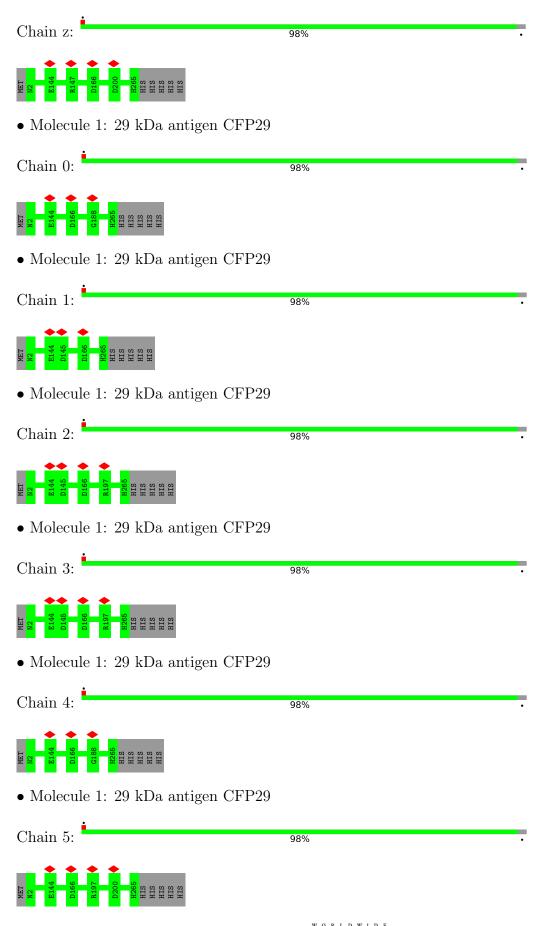














• Molecule 1: 29 kDa antigen CFP29

Chain 6: 98% .



• Molecule 1: 29 kDa antigen CFP29

Chain 7: 98% .





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1000000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	457.91998, 457.91998, 457.91998	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	langles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	0	0.45	0/2066	0.57	0/2818
1	1	0.45	0/2066	0.57	0/2818
1	2	0.45	0/2066	0.57	0/2818
1	3	0.45	0/2066	0.57	0/2818
1	4	0.45	0/2066	0.57	0/2818
1	5	0.45	0/2066	0.57	0/2818
1	6	0.44	0/2066	0.57	0/2818
1	7	0.45	0/2066	0.57	0/2818
1	A	0.45	0/2066	0.57	0/2818
1	В	0.45	0/2066	0.57	0/2818
1	С	0.45	0/2066	0.57	0/2818
1	D	0.45	0/2066	0.57	0/2818
1	Е	0.45	0/2066	0.57	0/2818
1	F	0.45	0/2066	0.57	0/2818
1	G	0.45	0/2066	0.57	0/2818
1	Н	0.45	0/2066	0.57	0/2818
1	I	0.45	0/2066	0.57	0/2818
1	J	0.45	0/2066	0.57	0/2818
1	K	0.44	0/2066	0.57	0/2818
1	L	0.45	0/2066	0.57	0/2818
1	M	0.45	0/2066	0.57	0/2818
1	N	0.45	0/2066	0.57	0/2818
1	О	0.45	0/2066	0.57	0/2818
1	Р	0.45	0/2066	0.57	0/2818
1	Q	0.45	0/2066	0.57	0/2818
1	R	0.45	0/2066	0.57	0/2818
1	S	0.44	0/2066	0.57	0/2818
1	Т	0.45	0/2066	0.57	0/2818
1	U	0.45	0/2066	0.57	0/2818
1	V	0.45	0/2066	0.57	0/2818
1	W	0.45	0/2066	0.57	0/2818
1	X	0.45	0/2066	0.57	0/2818
1	Y	0.44	0/2066	0.57	0/2818
1	Z	0.45	0/2066	0.57	0/2818



N (f = 1	Cl :	Bond	lengths	Bond	langles
Mol	Chain	RMSZ	# Z  > 5	RMSZ	$\mid \# \mid Z \mid > 5 \mid$
1	a	0.45	0/2066	0.57	0/2818
1	b	0.45	0/2066	0.57	0/2818
1	С	0.45	0/2066	0.57	0/2818
1	d	0.45	0/2066	0.57	0/2818
1	е	0.45	0/2066	0.57	0/2818
1	f	0.45	0/2066	0.57	0/2818
1	g	0.45	0/2066	0.57	0/2818
1	h	0.45	0/2066	0.57	0/2818
1	i	0.45	0/2066	0.57	0/2818
1	j	0.45	0/2066	0.57	0/2818
1	k	0.45	0/2066	0.57	0/2818
1	1	0.45	0/2066	0.57	0/2818
1	m	0.45	0/2066	0.57	0/2818
1	n	0.44	0/2066	0.57	0/2818
1	О	0.45	0/2066	0.57	0/2818
1	р	0.45	0/2066	0.57	0/2818
1	q	0.44	0/2066	0.57	0/2818
1	r	0.45	0/2066	0.57	0/2818
1	s	0.45	0/2066	0.57	0/2818
1	t	0.45	0/2066	0.57	0/2818
1	u	0.44	0/2066	0.57	0/2818
1	V	0.45	0/2066	0.57	0/2818
1	W	0.44	0/2066	0.57	0/2818
1	X	0.45	0/2066	0.57	0/2818
1	у	0.45	0/2066	0.57	0/2818
1	Z	0.45	0/2066	0.57	0/2818
All	All	0.45	0/123960	0.57	0/169080

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)

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



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	0	262/270~(97%)	258 (98%)	4 (2%)	0	100	100
1	1	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	2	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	3	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	4	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	5	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	6	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	7	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	A	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	В	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	С	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	D	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	Е	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	F	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	G	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	Н	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	I	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	J	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	K	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	L	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	M	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	N	$262/270 \; (97\%)$	258 (98%)	4 (2%)	0	100	100
1	О	$262/270 \; (97\%)$	258 (98%)	4 (2%)	0	100	100
1	Р	$262/270 \ (97\%)$	258 (98%)	4 (2%)	0	100	100
1	Q	$262/270 \; (97\%)$	258 (98%)	4 (2%)	0	100	100



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	R	262/270~(97%)	258 (98%)	4 (2%)	0	100	100
1	S	$262/270\ (97\%)$	258 (98%)	4 (2%)	0	100	100
1	T	262/270~(97%)	258 (98%)	4 (2%)	0	100	100
1	U	262/270~(97%)	258 (98%)	4 (2%)	0	100	100
1	V	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	W	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	X	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	Y	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	Z	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	a	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	b	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	c	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	d	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	е	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	f	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	g	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	h	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	i	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	j	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	k	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	1	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	m	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	n	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	О	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	p	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	q	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	r	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	S	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	t	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	u	262/270 (97%)	258 (98%)	4 (2%)	0	100	100
1	V	262/270 (97%)	258 (98%)	4 (2%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	W	262/270~(97%)	258 (98%)	4 (2%)	0	100	100
1	X	$262/270 \ (97\%)$	258 (98%)	4 (2%)	0	100	100
1	У	262/270~(97%)	258 (98%)	4 (2%)	0	100	100
1	Z	$262/270 \ (97\%)$	258 (98%)	4 (2%)	0	100	100
All	All	15720/16200 (97%)	15480 (98%)	240 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	$217/223\ (97\%)$	217 (100%)	0	100 100
1	1	$217/223\ (97\%)$	217 (100%)	0	100 100
1	2	$217/223\ (97\%)$	217 (100%)	0	100 100
1	3	$217/223\ (97\%)$	217 (100%)	0	100 100
1	4	$217/223\ (97\%)$	217 (100%)	0	100 100
1	5	$217/223\ (97\%)$	217 (100%)	0	100 100
1	6	$217/223\ (97\%)$	217 (100%)	0	100 100
1	7	$217/223\ (97\%)$	217 (100%)	0	100 100
1	A	$217/223\ (97\%)$	217 (100%)	0	100 100
1	В	$217/223\ (97\%)$	217 (100%)	0	100 100
1	$\mathbf{C}$	$217/223\ (97\%)$	217 (100%)	0	100 100
1	D	$217/223\ (97\%)$	217 (100%)	0	100 100
1	E	$217/223\ (97\%)$	217 (100%)	0	100 100
1	F	$217/223\ (97\%)$	217 (100%)	0	100 100
1	G	217/223 (97%)	217 (100%)	0	100 100
1	Н	$217/223\ (97\%)$	217 (100%)	0	100 100
1	I	$217/223\ (97\%)$	217 (100%)	0	100 100



 $Continued\ from\ previous\ page...$ 

Mol	Chain	Analysed	Rotameric	Outliers	Percei	ntiles
1	J	$217/223\ (97\%)$	217 (100%)	0	100	100
1	K	$217/223\ (97\%)$	217 (100%)	0	100	100
1	L	$217/223\ (97\%)$	217 (100%)	0	100	100
1	M	$217/223\ (97\%)$	217 (100%)	0	100	100
1	N	$217/223\ (97\%)$	217 (100%)	0	100	100
1	О	$217/223\ (97\%)$	217 (100%)	0	100	100
1	Р	$217/223\ (97\%)$	217 (100%)	0	100	100
1	Q	$217/223\ (97\%)$	217 (100%)	0	100	100
1	R	$217/223\ (97\%)$	217 (100%)	0	100	100
1	S	217/223 (97%)	217 (100%)	0	100	100
1	Т	217/223 (97%)	217 (100%)	0	100	100
1	U	217/223 (97%)	217 (100%)	0	100	100
1	V	217/223 (97%)	217 (100%)	0	100	100
1	W	217/223 (97%)	217 (100%)	0	100	100
1	X	217/223 (97%)	217 (100%)	0	100	100
1	Y	217/223 (97%)	217 (100%)	0	100	100
1	Z	217/223 (97%)	217 (100%)	0	100	100
1	a	217/223 (97%)	217 (100%)	0	100	100
1	b	217/223 (97%)	217 (100%)	0	100	100
1	С	217/223 (97%)	217 (100%)	0	100	100
1	d	$217/223 \ (97\%)$	217 (100%)	0	100	100
1	е	217/223 (97%)	217 (100%)	0	100	100
1	f	$217/223 \ (97\%)$	217 (100%)	0	100	100
1	g	$217/223 \ (97\%)$	217 (100%)	0	100	100
1	h	$217/223\ (97\%)$	217 (100%)	0	100	100
1	i	$217/223 \ (97\%)$	217 (100%)	0	100	100
1	j	$217/223 \ (97\%)$	217 (100%)	0	100	100
1	k	217/223 (97%)	217 (100%)	0	100	100
1	1	$217/223\ (97\%)$	217 (100%)	0	100	100
1	m	217/223 (97%)	217 (100%)	0	100	100
1	n	$217/223 \ (97\%)$	217 (100%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Rotameric Outliers		Percentiles	
1	О	$217/223\ (97\%)$	217 (100%)	0	100 100	
1	p	217/223~(97%)	217 (100%)	0	100 100	
1	q	$217/223\ (97\%)$	217 (100%)	0	100 100	
1	r	217/223~(97%)	217 (100%)	0	100 100	
1	S	$217/223 \ (97\%)$	217 (100%)	0	100 100	
1	t	$217/223 \ (97\%)$	217 (100%)	0	100 100	
1	u	217/223~(97%)	217 (100%)	0	100 100	
1	V	$217/223\ (97\%)$	217 (100%)	0	100 100	
1	W	$217/223\ (97\%)$	217 (100%)	0	100 100	
1	X	$217/223\ (97\%)$	217 (100%)	0	100 100	
1	У	$217/223 \ (97\%)$	217 (100%)	0	100 100	
1	Z	217/223~(97%)	217 (100%)	0	100 100	
All	All	13020/13380 (97%)	13020 (100%)	0	100 100	

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	c	137	ASN
1	3	137	ASN
1	j	137	ASN
1	2	137	ASN
1	7	137	ASN

#### 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.



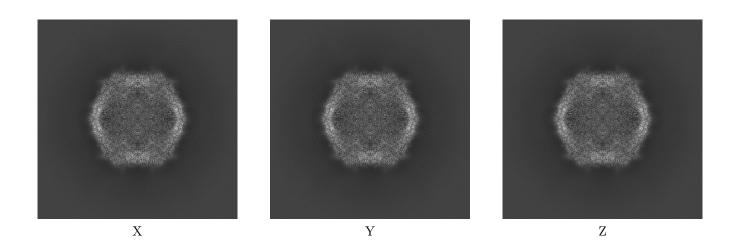
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13420. 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)

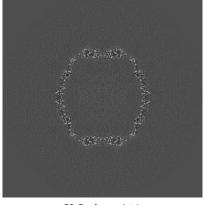
#### 6.1.1 Primary map



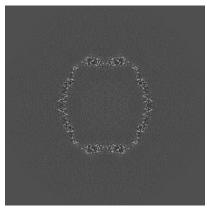
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

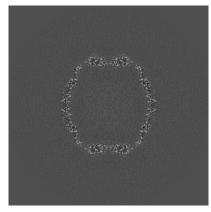
#### 6.2.1 Primary map







Y Index: 216



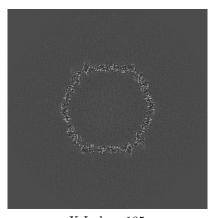
Z Index: 216

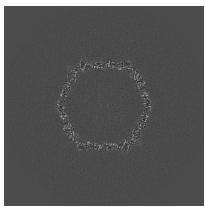


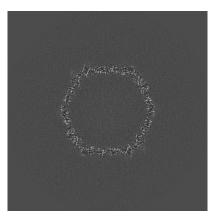
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map







X Index: 195

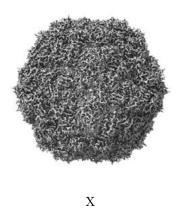
Y Index: 195

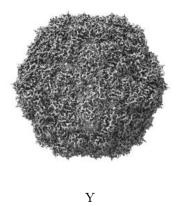
Z Index: 195

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







 $\mathbf{Z}$ 

The images above show the 3D surface view of the map at the recommended contour level 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation (i)

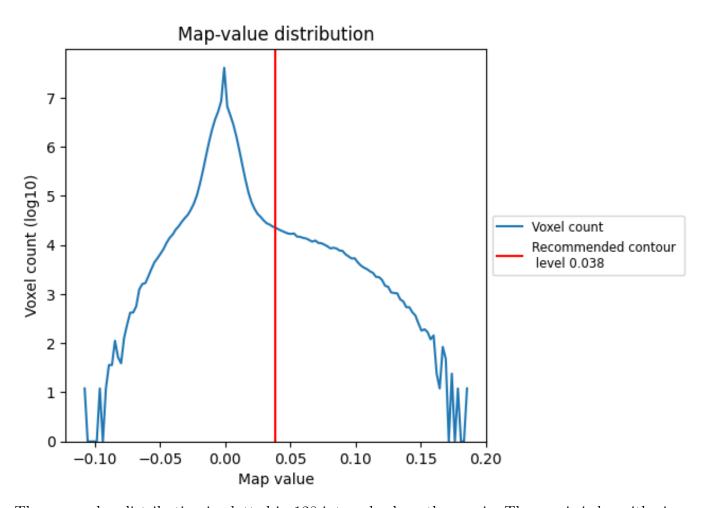
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

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

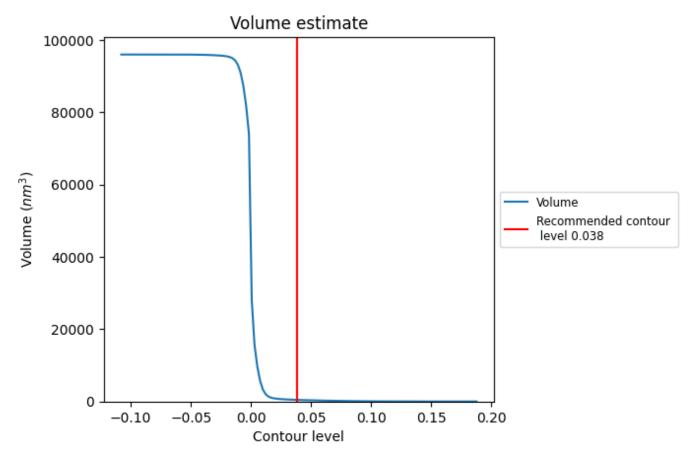
### 7.1 Map-value distribution (i)



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)

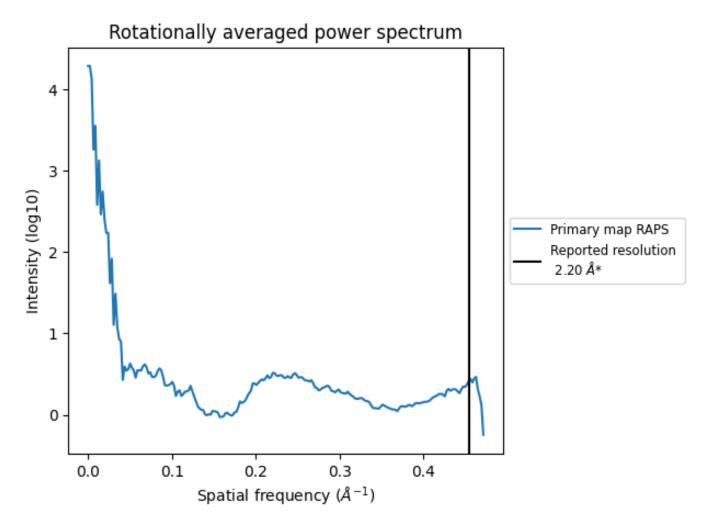


The volume at the recommended contour level is  $447~\mathrm{nm^3}$ ; this corresponds to an approximate mass of  $404~\mathrm{kDa}$ .

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)



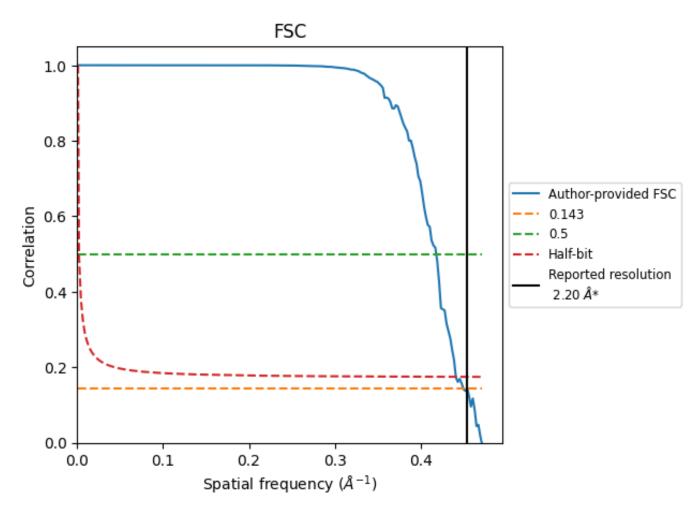
\*Reported resolution corresponds to spatial frequency of 0.455  $\rm \AA^{-1}$ 



## 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.455  $\rm \AA^{-1}$ 



## 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.22	2.39	2.27
Unmasked-calculated*	-	-	-

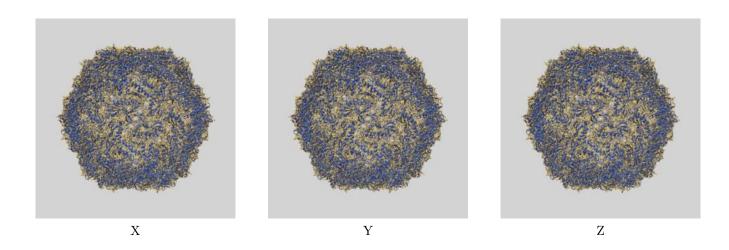
<sup>\*</sup>Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13420 and PDB model 7PHM. Per-residue inclusion information can be found in section 3 on page 17.

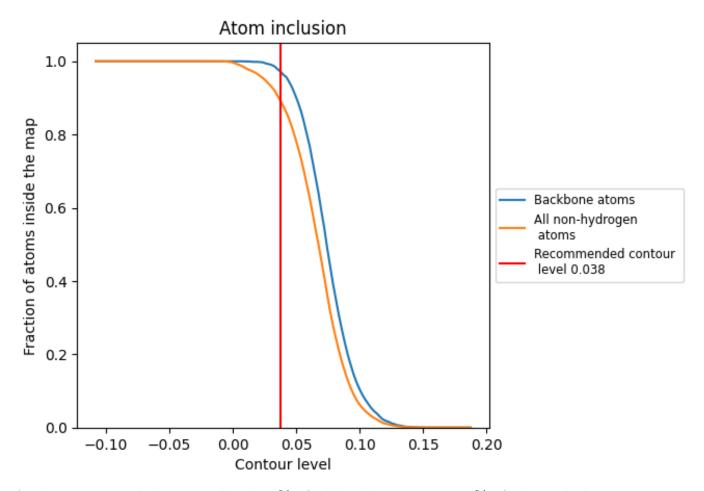
### 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.038 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 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

