



## Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 08:29 PM EDT

PDB ID : 6WL8 / pdb\_00006wl8  
EMDB ID : EMD-21817  
Title : Cryo-EM of Form 2 peptide filament  
Authors : Wang, F.; Gnewou, O.M.; Xu, C.; Su, Z.; Egelman, E.H.; Conticello, V.P.  
Deposited on : 2020-04-18  
Resolution : 4.10 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>.

---

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

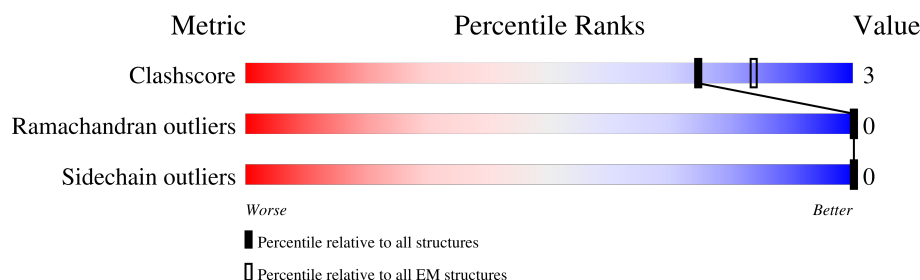
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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.



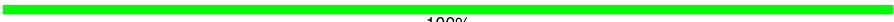




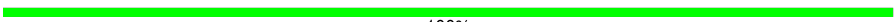

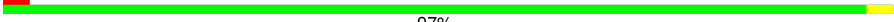



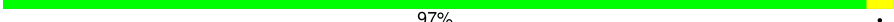



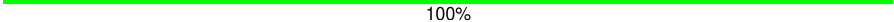

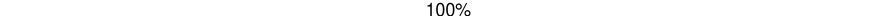

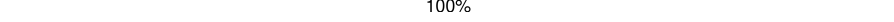

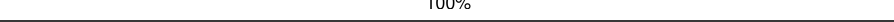

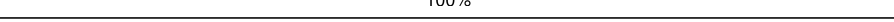

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0	29	100%
1	1	29	90%10%
1	2	29	97%.
1	3	29	100%
1	4	29	100%
1	5	29	97%.
1	6	29	100%
1	7	29	7%97%.

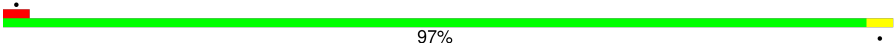

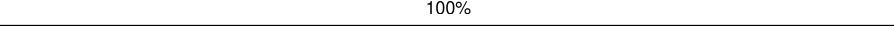
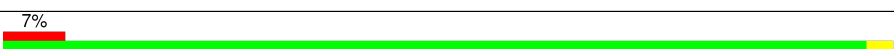

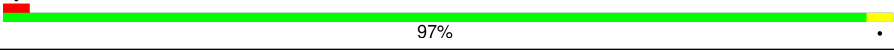

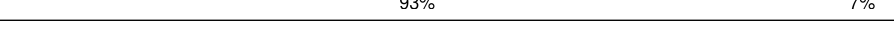


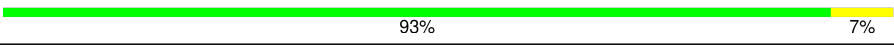
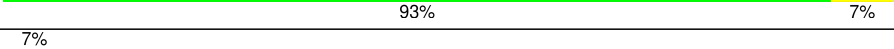
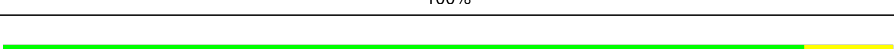
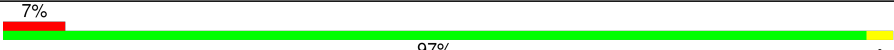

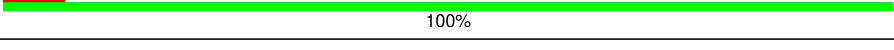
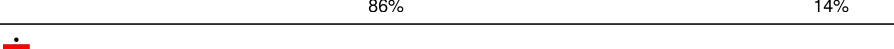



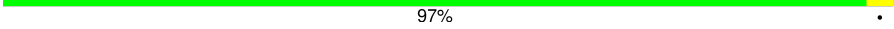



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	8	29	 100%
1	9	29	 97%
1	A	29	 79% 21%
1	AA	29	 100%
1	B	29	 83% 17%
1	BA	29	 100%
1	C	29	 79% 21%
1	CA	29	 97%
1	D	29	 83% 17%
1	DA	29	 100%
1	E	29	 86% 14%
1	EA	29	 97%
1	F	29	 83% 17%
1	FA	29	 100%
1	G	29	 86% 14%
1	GA	29	 100%
1	H	29	 86% 14%
1	HA	29	 100%
1	I	29	 86% 14%
1	IA	29	 100%
1	J	29	 90% 10%
1	JA	29	 100%
1	K	29	 86% 14%
1	KA	29	 100%
1	L	29	 90% 10%


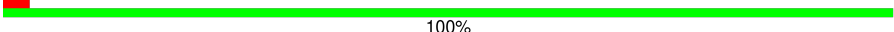

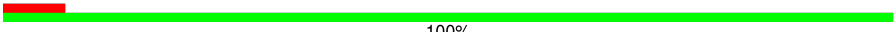








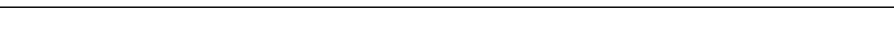

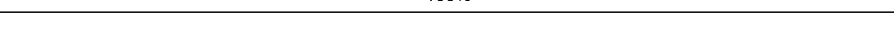
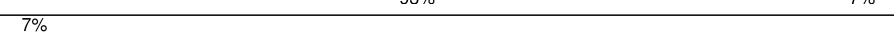
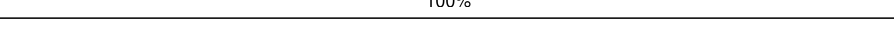

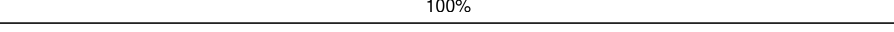

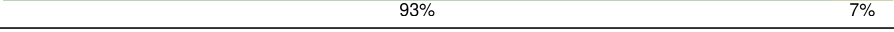

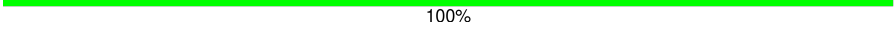

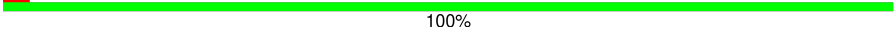
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	LA	29	
1	M	29	
1	MA	29	
1	N	29	
1	NA	29	
1	O	29	
1	OA	29	
1	P	29	
1	PA	29	
1	Q	29	
1	QA	29	
1	R	29	
1	RA	29	
1	S	29	
1	SA	29	
1	T	29	
1	TA	29	
1	U	29	
1	UA	29	
1	V	29	
1	VA	29	
1	W	29	
1	WA	29	
1	X	29	
1	XA	29	

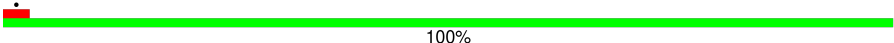

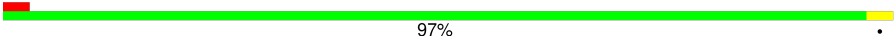

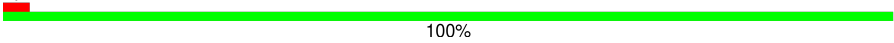

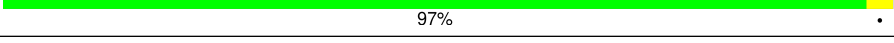

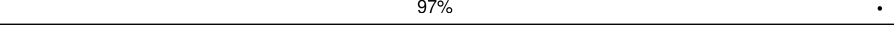
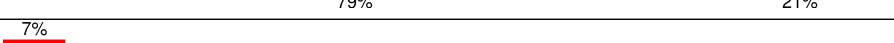
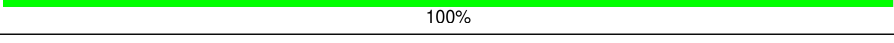
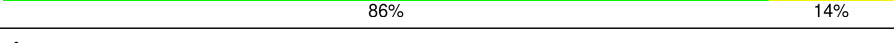
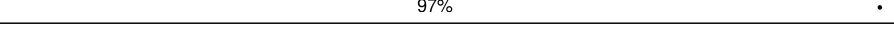





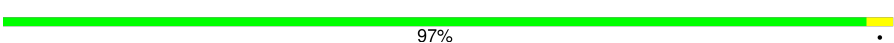




Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	Y	29	
1	YA	29	
1	Z	29	
1	ZA	29	
1	a	29	
1	aA	29	
1	b	29	
1	bA	29	
1	c	29	
1	cA	29	
1	d	29	
1	dA	29	
1	e	29	
1	eA	29	
1	f	29	
1	fA	29	
1	g	29	
1	gA	29	
1	h	29	
1	hA	29	
1	i	29	
1	iA	29	
1	j	29	
1	jA	29	
1	k	29	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	kA	29	
1	l	29	
1	lA	29	
1	m	29	
1	mA	29	
1	n	29	
1	nA	29	
1	o	29	
1	oA	29	
1	p	29	
1	pA	29	
1	q	29	
1	qA	29	
1	r	29	
1	rA	29	
1	s	29	
1	t	29	
1	u	29	
1	v	29	
1	w	29	
1	x	29	
1	y	29	
1	z	29	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 23850 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 Form 2 peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	29	Total	C	N	O	0	0
			225	145	37	43		
1	0	29	Total	C	N	O	0	0
			225	145	37	43		
1	B	29	Total	C	N	O	0	0
			225	145	37	43		
1	2	29	Total	C	N	O	0	0
			225	145	37	43		
1	C	29	Total	C	N	O	0	0
			225	145	37	43		
1	3	29	Total	C	N	O	0	0
			225	145	37	43		
1	D	29	Total	C	N	O	0	0
			225	145	37	43		
1	4	29	Total	C	N	O	0	0
			225	145	37	43		
1	E	29	Total	C	N	O	0	0
			225	145	37	43		
1	5	29	Total	C	N	O	0	0
			225	145	37	43		
1	F	29	Total	C	N	O	0	0
			225	145	37	43		
1	6	29	Total	C	N	O	0	0
			225	145	37	43		
1	G	29	Total	C	N	O	0	0
			225	145	37	43		
1	7	29	Total	C	N	O	0	0
			225	145	37	43		
1	H	29	Total	C	N	O	0	0
			225	145	37	43		
1	8	29	Total	C	N	O	0	0
			225	145	37	43		
1	I	29	Total	C	N	O	0	0
			225	145	37	43		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
1	9	29	Total	C	N	O	0	0
			225	145	37	43		
1	J	29	Total	C	N	O	0	0
			225	145	37	43		
1	AA	29	Total	C	N	O	0	0
			225	145	37	43		
1	K	29	Total	C	N	O	0	0
			225	145	37	43		
1	BA	29	Total	C	N	O	0	0
			225	145	37	43		
1	L	29	Total	C	N	O	0	0
			225	145	37	43		
1	CA	29	Total	C	N	O	0	0
			225	145	37	43		
1	M	29	Total	C	N	O	0	0
			225	145	37	43		
1	DA	29	Total	C	N	O	0	0
			225	145	37	43		
1	N	29	Total	C	N	O	0	0
			225	145	37	43		
1	EA	29	Total	C	N	O	0	0
			225	145	37	43		
1	O	29	Total	C	N	O	0	0
			225	145	37	43		
1	FA	29	Total	C	N	O	0	0
			225	145	37	43		
1	P	29	Total	C	N	O	0	0
			225	145	37	43		
1	GA	29	Total	C	N	O	0	0
			225	145	37	43		
1	Q	29	Total	C	N	O	0	0
			225	145	37	43		
1	HA	29	Total	C	N	O	0	0
			225	145	37	43		
1	R	29	Total	C	N	O	0	0
			225	145	37	43		
1	IA	29	Total	C	N	O	0	0
			225	145	37	43		
1	S	29	Total	C	N	O	0	0
			225	145	37	43		
1	JA	29	Total	C	N	O	0	0
			225	145	37	43		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
1	T	29	Total	C	N	O	0	0
			225	145	37	43		
1	KA	29	Total	C	N	O	0	0
			225	145	37	43		
1	U	29	Total	C	N	O	0	0
			225	145	37	43		
1	LA	29	Total	C	N	O	0	0
			225	145	37	43		
1	V	29	Total	C	N	O	0	0
			225	145	37	43		
1	MA	29	Total	C	N	O	0	0
			225	145	37	43		
1	W	29	Total	C	N	O	0	0
			225	145	37	43		
1	NA	29	Total	C	N	O	0	0
			225	145	37	43		
1	X	29	Total	C	N	O	0	0
			225	145	37	43		
1	OA	29	Total	C	N	O	0	0
			225	145	37	43		
1	Y	29	Total	C	N	O	0	0
			225	145	37	43		
1	PA	29	Total	C	N	O	0	0
			225	145	37	43		
1	Z	29	Total	C	N	O	0	0
			225	145	37	43		
1	QA	29	Total	C	N	O	0	0
			225	145	37	43		
1	a	29	Total	C	N	O	0	0
			225	145	37	43		
1	RA	29	Total	C	N	O	0	0
			225	145	37	43		
1	b	29	Total	C	N	O	0	0
			225	145	37	43		
1	SA	29	Total	C	N	O	0	0
			225	145	37	43		
1	c	29	Total	C	N	O	0	0
			225	145	37	43		
1	TA	29	Total	C	N	O	0	0
			225	145	37	43		
1	d	29	Total	C	N	O	0	0
			225	145	37	43		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
1	UA	29	Total 225	C 145	N 37	O 43	0	0
1	e	29	Total 225	C 145	N 37	O 43	0	0
1	VA	29	Total 225	C 145	N 37	O 43	0	0
1	f	29	Total 225	C 145	N 37	O 43	0	0
1	WA	29	Total 225	C 145	N 37	O 43	0	0
1	g	29	Total 225	C 145	N 37	O 43	0	0
1	XA	29	Total 225	C 145	N 37	O 43	0	0
1	h	29	Total 225	C 145	N 37	O 43	0	0
1	YA	29	Total 225	C 145	N 37	O 43	0	0
1	i	29	Total 225	C 145	N 37	O 43	0	0
1	ZA	29	Total 225	C 145	N 37	O 43	0	0
1	j	29	Total 225	C 145	N 37	O 43	0	0
1	aA	29	Total 225	C 145	N 37	O 43	0	0
1	k	29	Total 225	C 145	N 37	O 43	0	0
1	bA	29	Total 225	C 145	N 37	O 43	0	0
1	l	29	Total 225	C 145	N 37	O 43	0	0
1	cA	29	Total 225	C 145	N 37	O 43	0	0
1	m	29	Total 225	C 145	N 37	O 43	0	0
1	dA	29	Total 225	C 145	N 37	O 43	0	0
1	n	29	Total 225	C 145	N 37	O 43	0	0
1	eA	29	Total 225	C 145	N 37	O 43	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
1	o	29	Total	C	N	O	0	0
			225	145	37	43		
1	fA	29	Total	C	N	O	0	0
			225	145	37	43		
1	p	29	Total	C	N	O	0	0
			225	145	37	43		
1	gA	29	Total	C	N	O	0	0
			225	145	37	43		
1	q	29	Total	C	N	O	0	0
			225	145	37	43		
1	hA	29	Total	C	N	O	0	0
			225	145	37	43		
1	r	29	Total	C	N	O	0	0
			225	145	37	43		
1	iA	29	Total	C	N	O	0	0
			225	145	37	43		
1	s	29	Total	C	N	O	0	0
			225	145	37	43		
1	jA	29	Total	C	N	O	0	0
			225	145	37	43		
1	t	29	Total	C	N	O	0	0
			225	145	37	43		
1	kA	29	Total	C	N	O	0	0
			225	145	37	43		
1	u	29	Total	C	N	O	0	0
			225	145	37	43		
1	lA	29	Total	C	N	O	0	0
			225	145	37	43		
1	v	29	Total	C	N	O	0	0
			225	145	37	43		
1	mA	29	Total	C	N	O	0	0
			225	145	37	43		
1	w	29	Total	C	N	O	0	0
			225	145	37	43		
1	nA	29	Total	C	N	O	0	0
			225	145	37	43		
1	x	29	Total	C	N	O	0	0
			225	145	37	43		
1	oA	29	Total	C	N	O	0	0
			225	145	37	43		
1	y	29	Total	C	N	O	0	0
			225	145	37	43		

*Continued on next page...*


*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
1	pA	29	Total 225	C 145	N 37	O 43	0	0
1	z	29	Total 225	C 145	N 37	O 43	0	0
1	qA	29	Total 225	C 145	N 37	O 43	0	0
1	1	29	Total 225	C 145	N 37	O 43	0	0
1	rA	29	Total 225	C 145	N 37	O 43	0	0

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

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

- Molecule 1: Form 2 peptide

Chain A:  79% 21%




- Molecule 1: Form 2 peptide

Chain 0:  100%



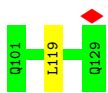
- Molecule 1: Form 2 peptide

Chain B:  83% 17%




- Molecule 1: Form 2 peptide

Chain 2:  97%



- Molecule 1: Form 2 peptide

Chain C:  79% 21%




- Molecule 1: Form 2 peptide

Chain 3:  100%



- Molecule 1: Form 2 peptide

Chain D:  83% 17%




- Molecule 1: Form 2 peptide

Chain 4:  100%



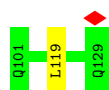
- Molecule 1: Form 2 peptide

Chain E:  86% 14%




- Molecule 1: Form 2 peptide

Chain 5:  97%



- Molecule 1: Form 2 peptide

Chain F:  83% 17%




- Molecule 1: Form 2 peptide

Chain 6:  100%



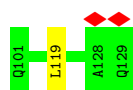
- Molecule 1: Form 2 peptide

Chain G:  86% 14%




- Molecule 1: Form 2 peptide

Chain 7:  7% 97% .



- Molecule 1: Form 2 peptide

Chain H:  86% 14%




- Molecule 1: Form 2 peptide

Chain 8:  100%

There are no outlier residues recorded for this chain.

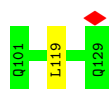
- Molecule 1: Form 2 peptide

Chain I:  86% 14%



- Molecule 1: Form 2 peptide

Chain 9:  7% 97% .



- Molecule 1: Form 2 peptide

Chain J:  90% 10%

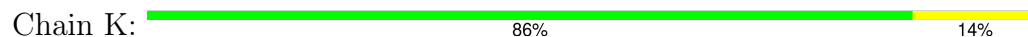


- Molecule 1: Form 2 peptide

Chain AA:  7% 100%



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide

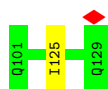


There are no outlier residues recorded for this chain.

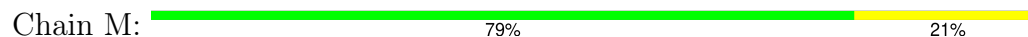
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



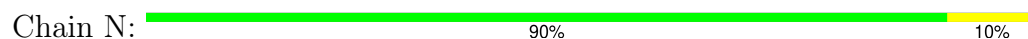
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



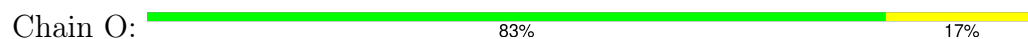




- Molecule 1: Form 2 peptide



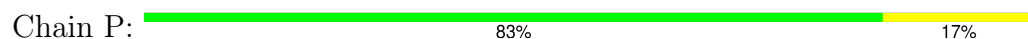
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



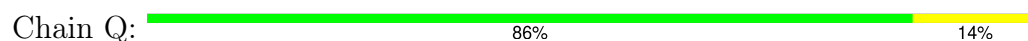
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide

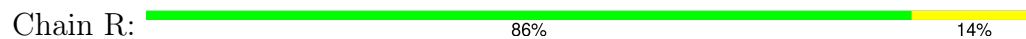


- Molecule 1: Form 2 peptide





- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



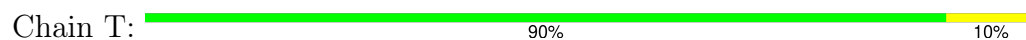
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide




- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



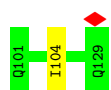
- Molecule 1: Form 2 peptide

Chain U:  83% 17%




- Molecule 1: Form 2 peptide

Chain LA:  97% .



- Molecule 1: Form 2 peptide

Chain V:  86% 14%




- Molecule 1: Form 2 peptide

Chain MA:  100%



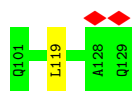
- Molecule 1: Form 2 peptide

Chain W:  79% 21%




- Molecule 1: Form 2 peptide

Chain NA:  7% 97% .



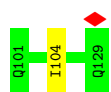
- Molecule 1: Form 2 peptide

Chain X:  79% 21%



- Molecule 1: Form 2 peptide

Chain OA:  97%



- Molecule 1: Form 2 peptide

Chain Y:  76% 24%




- Molecule 1: Form 2 peptide

Chain PA:  93% 7%



- Molecule 1: Form 2 peptide

Chain Z:  86% 14%



- Molecule 1: Form 2 peptide

Chain QA:  7% 97%



- Molecule 1: Form 2 peptide

Chain a:  90% 10%




- Molecule 1: Form 2 peptide

Chain RA:  93% 7%



- Molecule 1: Form 2 peptide

Chain b:  86% 14%




- Molecule 1: Form 2 peptide

Chain SA:  7% 100%



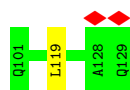
- Molecule 1: Form 2 peptide

Chain c:  79% 21%




- Molecule 1: Form 2 peptide

Chain TA:  7% 97%



- Molecule 1: Form 2 peptide

Chain d:  86% 14%




- Molecule 1: Form 2 peptide

Chain UA:  7% 100%



- Molecule 1: Form 2 peptide

Chain e:  79% 21%



- Molecule 1: Form 2 peptide

Chain VA:  100%



- Molecule 1: Form 2 peptide

Chain f:  93% 7%




- Molecule 1: Form 2 peptide

Chain WA:  100%



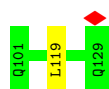
- Molecule 1: Form 2 peptide

Chain g:  83% 17%




- Molecule 1: Form 2 peptide

Chain XA:  97%



- Molecule 1: Form 2 peptide

Chain h:  79% 21%




- Molecule 1: Form 2 peptide

Chain YA:  100%



- Molecule 1: Form 2 peptide

Chain i:  83% 17%




- Molecule 1: Form 2 peptide

Chain ZA:  7% 100%



- Molecule 1: Form 2 peptide

Chain j:  83% 17%




- Molecule 1: Form 2 peptide

Chain aA:  100%



- Molecule 1: Form 2 peptide

Chain k:  90% 10%




- Molecule 1: Form 2 peptide

Chain bA:  97%



- Molecule 1: Form 2 peptide

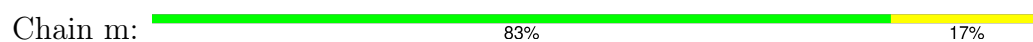
Chain l:  83% 17%



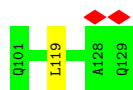
- Molecule 1: Form 2 peptide



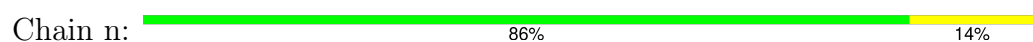
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



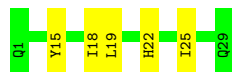
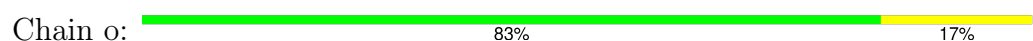
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



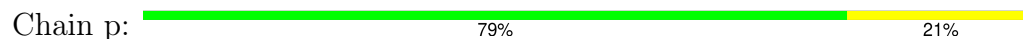
- Molecule 1: Form 2 peptide







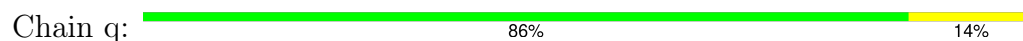
- Molecule 1: Form 2 peptide



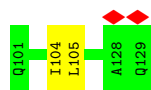
- Molecule 1: Form 2 peptide



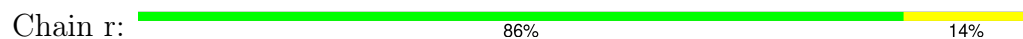
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



There are no outlier residues recorded for this chain.

- Molecule 1: Form 2 peptide

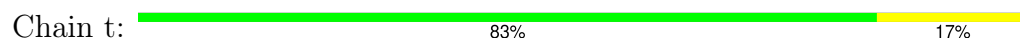




- Molecule 1: Form 2 peptide



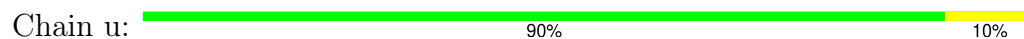
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



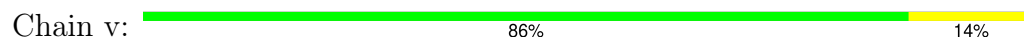
- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide



- Molecule 1: Form 2 peptide





- Molecule 1: Form 2 peptide

Chain w:  97%




- Molecule 1: Form 2 peptide

Chain nA:  97%



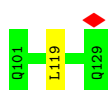
- Molecule 1: Form 2 peptide

Chain x:  90%




- Molecule 1: Form 2 peptide

Chain oA:  97%



- Molecule 1: Form 2 peptide

Chain y:  90%




- Molecule 1: Form 2 peptide

Chain pA:  7%



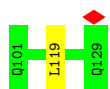
- Molecule 1: Form 2 peptide

Chain z:  90%




- Molecule 1: Form 2 peptide

Chain qA:  97%



- Molecule 1: Form 2 peptide

Chain 1:  90% 10%



- Molecule 1: Form 2 peptide

Chain rA:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=124.36°, rise=1.93 Å, axial sym=C1	Depositor
Number of segments used	408751	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0103	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0	0.17	0/226	0.34	0/301
1	1	0.21	0/226	0.37	0/301
1	2	0.18	0/226	0.34	0/301
1	3	0.18	0/226	0.35	0/301
1	4	0.17	0/226	0.34	0/301
1	5	0.18	0/226	0.37	0/301
1	6	0.17	0/226	0.35	0/301
1	7	0.18	0/226	0.33	0/301
1	8	0.17	0/226	0.34	0/301
1	9	0.17	0/226	0.35	0/301
1	A	0.27	0/226	0.40	0/301
1	AA	0.17	0/226	0.33	0/301
1	B	0.24	0/226	0.40	0/301
1	BA	0.18	0/226	0.36	0/301
1	C	0.26	0/226	0.39	0/301
1	CA	0.18	0/226	0.38	0/301
1	D	0.26	0/226	0.39	0/301
1	DA	0.17	0/226	0.31	0/301
1	E	0.27	0/226	0.40	0/301
1	EA	0.18	0/226	0.37	0/301
1	F	0.27	0/226	0.42	0/301
1	FA	0.18	0/226	0.37	0/301
1	G	0.26	0/226	0.41	0/301
1	GA	0.18	0/226	0.33	0/301
1	H	0.27	0/226	0.42	0/301
1	HA	0.18	0/226	0.37	0/301
1	I	0.24	0/226	0.41	0/301
1	IA	0.17	0/226	0.34	0/301
1	J	0.24	0/226	0.38	0/301
1	JA	0.18	0/226	0.37	0/301
1	K	0.26	0/226	0.39	0/301
1	KA	0.18	0/226	0.34	0/301
1	L	0.24	0/226	0.40	0/301
1	LA	0.17	0/226	0.35	0/301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	M	0.25	0/226	0.37	0/301
1	MA	0.18	0/226	0.34	0/301
1	N	0.26	0/226	0.42	0/301
1	NA	0.17	0/226	0.34	0/301
1	O	0.26	0/226	0.40	0/301
1	OA	0.18	0/226	0.39	0/301
1	P	0.27	0/226	0.40	0/301
1	PA	0.18	0/226	0.38	0/301
1	Q	0.25	0/226	0.39	0/301
1	QA	0.18	0/226	0.34	0/301
1	R	0.26	0/226	0.37	0/301
1	RA	0.18	0/226	0.38	0/301
1	S	0.24	0/226	0.42	0/301
1	SA	0.17	0/226	0.31	0/301
1	T	0.26	0/226	0.40	0/301
1	TA	0.18	0/226	0.34	0/301
1	U	0.27	0/226	0.41	0/301
1	UA	0.17	0/226	0.35	0/301
1	V	0.24	0/226	0.40	0/301
1	VA	0.18	0/226	0.34	0/301
1	W	0.27	0/226	0.44	0/301
1	WA	0.17	0/226	0.34	0/301
1	X	0.27	0/226	0.44	0/301
1	XA	0.18	0/226	0.32	0/301
1	Y	0.26	0/226	0.40	0/301
1	YA	0.16	0/226	0.32	0/301
1	Z	0.27	0/226	0.42	0/301
1	ZA	0.17	0/226	0.35	0/301
1	a	0.24	0/226	0.40	0/301
1	aA	0.18	0/226	0.34	0/301
1	b	0.25	0/226	0.39	0/301
1	bA	0.18	0/226	0.35	0/301
1	c	0.26	0/226	0.38	0/301
1	cA	0.17	0/226	0.35	0/301
1	d	0.24	0/226	0.38	0/301
1	dA	0.18	0/226	0.34	0/301
1	e	0.26	0/226	0.40	0/301
1	eA	0.17	0/226	0.34	0/301
1	f	0.24	0/226	0.39	0/301
1	fA	0.18	0/226	0.35	0/301
1	g	0.27	0/226	0.40	0/301
1	gA	0.18	0/226	0.36	0/301
1	h	0.26	0/226	0.42	0/301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	hA	0.19	0/226	0.37	0/301
1	i	0.26	0/226	0.41	0/301
1	iA	0.17	0/226	0.35	0/301
1	j	0.25	0/226	0.40	0/301
1	jA	0.17	0/226	0.33	0/301
1	k	0.23	0/226	0.39	0/301
1	kA	0.18	0/226	0.33	0/301
1	l	0.25	0/226	0.39	0/301
1	lA	0.17	0/226	0.36	0/301
1	m	0.24	0/226	0.39	0/301
1	mA	0.17	0/226	0.35	0/301
1	n	0.23	0/226	0.39	0/301
1	nA	0.18	0/226	0.34	0/301
1	o	0.27	0/226	0.39	0/301
1	oA	0.17	0/226	0.33	0/301
1	p	0.27	0/226	0.43	0/301
1	pA	0.17	0/226	0.31	0/301
1	q	0.26	0/226	0.37	0/301
1	qA	0.18	0/226	0.35	0/301
1	r	0.25	0/226	0.40	0/301
1	rA	0.17	0/226	0.32	0/301
1	s	0.23	0/226	0.36	0/301
1	t	0.24	0/226	0.40	0/301
1	u	0.24	0/226	0.41	0/301
1	v	0.25	0/226	0.38	0/301
1	w	0.23	0/226	0.36	0/301
1	x	0.24	0/226	0.36	0/301
1	y	0.22	0/226	0.39	0/301
1	z	0.24	0/226	0.38	0/301
All	All	0.22	0/23956	0.37	0/31906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	225	0	239	0	0
1	1	225	0	242	2	0
1	2	225	0	239	1	0
1	3	225	0	239	0	0
1	4	225	0	239	0	0
1	5	225	0	239	1	0
1	6	225	0	239	0	0
1	7	225	0	239	1	0
1	8	225	0	239	0	0
1	9	225	0	239	1	0
1	A	225	0	242	4	0
1	AA	225	0	239	0	0
1	B	225	0	242	4	0
1	BA	225	0	239	0	0
1	C	225	0	242	4	0
1	CA	225	0	239	1	0
1	D	225	0	242	3	0
1	DA	225	0	239	0	0
1	E	225	0	242	2	0
1	EA	225	0	239	1	0
1	F	225	0	242	4	0
1	FA	225	0	239	0	0
1	G	225	0	242	3	0
1	GA	225	0	239	0	0
1	H	225	0	242	3	0
1	HA	225	0	239	0	0
1	I	225	0	242	3	0
1	IA	225	0	239	0	0
1	J	225	0	242	2	0
1	JA	225	0	239	0	0
1	K	225	0	242	2	0
1	KA	225	0	239	0	0
1	L	225	0	242	2	0
1	LA	225	0	239	1	0
1	M	225	0	242	4	0
1	MA	225	0	239	0	0
1	N	225	0	242	2	0
1	NA	225	0	239	1	0
1	O	225	0	242	3	0
1	OA	225	0	239	1	0
1	P	225	0	242	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	PA	225	0	239	1	0
1	Q	225	0	242	3	0
1	QA	225	0	239	1	0
1	R	225	0	242	3	0
1	RA	225	0	239	2	0
1	S	225	0	242	1	0
1	SA	225	0	239	0	0
1	T	225	0	242	2	0
1	TA	225	0	239	1	0
1	U	225	0	242	3	0
1	UA	225	0	239	0	0
1	V	225	0	242	3	0
1	VA	225	0	239	0	0
1	W	225	0	242	5	0
1	WA	225	0	239	0	0
1	X	225	0	242	5	0
1	XA	225	0	239	1	0
1	Y	225	0	242	5	0
1	YA	225	0	239	0	0
1	Z	225	0	242	2	0
1	ZA	225	0	239	0	0
1	a	225	0	242	2	0
1	aA	225	0	239	0	0
1	b	225	0	242	2	0
1	bA	225	0	239	1	0
1	c	225	0	242	4	0
1	cA	225	0	239	0	0
1	d	225	0	242	3	0
1	dA	225	0	239	1	0
1	e	225	0	242	4	0
1	eA	225	0	239	0	0
1	f	225	0	242	1	0
1	fA	225	0	239	0	0
1	g	225	0	242	4	0
1	gA	225	0	239	0	0
1	h	225	0	242	4	0
1	hA	225	0	239	2	0
1	i	225	0	242	4	0
1	iA	225	0	239	0	0
1	j	225	0	242	3	0
1	jA	225	0	239	0	0
1	k	225	0	242	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	kA	225	0	239	0	0
1	l	225	0	242	3	0
1	lA	225	0	239	1	0
1	m	225	0	242	3	0
1	mA	225	0	239	0	0
1	n	225	0	242	3	0
1	nA	225	0	239	1	0
1	o	225	0	242	4	0
1	oA	225	0	239	1	0
1	p	225	0	242	4	0
1	pA	225	0	239	0	0
1	q	225	0	242	2	0
1	qA	225	0	239	1	0
1	r	225	0	242	2	0
1	rA	225	0	239	0	0
1	s	225	0	242	1	0
1	t	225	0	242	3	0
1	u	225	0	242	2	0
1	v	225	0	242	2	0
1	w	225	0	242	1	0
1	x	225	0	242	2	0
1	y	225	0	242	2	0
1	z	225	0	242	3	0
All	All	23850	0	25493	146	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 3.

All (146) 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:l:22:HIS:HA	1:l:25:ILE:HD12	1.79	0.64
1:O:22:HIS:HA	1:O:25:ILE:HD12	1.80	0.64
1:o:22:HIS:HA	1:o:25:ILE:HD12	1.80	0.64
1:K:22:HIS:HA	1:K:25:ILE:HD12	1.81	0.63
1:t:22:HIS:HA	1:t:25:ILE:HD12	1.83	0.60
1:v:22:HIS:HA	1:v:25:ILE:HD12	1.84	0.60
1:e:22:HIS:HA	1:e:25:ILE:HD12	1.83	0.60
1:U:22:HIS:HA	1:U:25:ILE:HD12	1.84	0.60
1:m:22:HIS:HA	1:m:25:ILE:HD12	1.84	0.59
1:Q:15:TYR:HA	1:Q:18:ILE:HD12	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:u:15:TYR:HA	1:u:18:ILE:HD12	1.84	0.59
1:Y:22:HIS:HA	1:Y:25:ILE:HD12	1.84	0.59
1:s:15:TYR:HA	1:s:18:ILE:HD12	1.84	0.59
1:r:15:TYR:HA	1:r:18:ILE:HD12	1.85	0.59
1:t:15:TYR:HA	1:t:18:ILE:HD12	1.85	0.59
1:E:15:TYR:HA	1:E:18:ILE:HD12	1.85	0.59
1:L:15:TYR:HA	1:L:18:ILE:HD12	1.84	0.59
1:T:15:TYR:HA	1:T:18:ILE:HD12	1.84	0.59
1:n:15:TYR:HA	1:n:18:ILE:HD12	1.84	0.59
1:b:22:HIS:HA	1:b:25:ILE:HD12	1.83	0.59
1:h:22:HIS:HA	1:h:25:ILE:HD12	1.84	0.59
1:B:15:TYR:HA	1:B:18:ILE:HD12	1.85	0.58
1:I:15:TYR:HA	1:I:18:ILE:HD12	1.84	0.58
1:N:15:TYR:HA	1:N:18:ILE:HD12	1.86	0.58
1:C:15:TYR:HA	1:C:18:ILE:HD12	1.85	0.58
1:M:22:HIS:HA	1:M:25:ILE:HD12	1.85	0.58
1:F:15:TYR:HA	1:F:18:ILE:HD12	1.85	0.58
1:X:15:TYR:HA	1:X:18:ILE:HD12	1.84	0.58
1:p:15:TYR:HA	1:p:18:ILE:HD12	1.86	0.58
1:r:22:HIS:HA	1:r:25:ILE:HD12	1.86	0.58
1:A:22:HIS:HA	1:A:25:ILE:HD12	1.85	0.58
1:M:15:TYR:HA	1:M:18:ILE:HD12	1.85	0.58
1:W:15:TYR:HA	1:W:18:ILE:HD12	1.86	0.58
1:D:15:TYR:HA	1:D:18:ILE:HD12	1.85	0.58
1:z:15:TYR:HA	1:z:18:ILE:HD12	1.85	0.58
1:Y:15:TYR:HA	1:Y:18:ILE:HD12	1.84	0.58
1:a:15:TYR:HA	1:a:18:ILE:HD12	1.85	0.58
1:g:15:TYR:HA	1:g:18:ILE:HD12	1.86	0.57
1:S:15:TYR:HA	1:S:18:ILE:HD12	1.84	0.57
1:O:15:TYR:HA	1:O:18:ILE:HD12	1.85	0.57
1:f:15:TYR:HA	1:f:18:ILE:HD12	1.86	0.57
1:i:15:TYR:HA	1:i:18:ILE:HD12	1.86	0.57
1:v:15:TYR:HA	1:v:18:ILE:HD12	1.86	0.57
1:G:15:TYR:HA	1:G:18:ILE:HD12	1.85	0.57
1:K:15:TYR:HA	1:K:18:ILE:HD12	1.86	0.57
1:V:15:TYR:HA	1:V:18:ILE:HD12	1.85	0.57
1:q:15:TYR:HA	1:q:18:ILE:HD12	1.86	0.57
1:b:15:TYR:HA	1:b:18:ILE:HD12	1.86	0.57
1:o:15:TYR:HA	1:o:18:ILE:HD12	1.86	0.57
1:J:15:TYR:HA	1:J:18:ILE:HD12	1.85	0.57
1:A:15:TYR:HA	1:A:18:ILE:HD12	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:15:TYR:HA	1:m:18:ILE:HD12	1.86	0.56
1:e:15:TYR:HA	1:e:18:ILE:HD12	1.87	0.56
1:R:15:TYR:HA	1:R:18:ILE:HD12	1.87	0.56
1:x:15:TYR:HA	1:x:18:ILE:HD12	1.86	0.56
1:q:22:HIS:HA	1:q:25:ILE:HD12	1.88	0.56
1:U:15:TYR:HA	1:U:18:ILE:HD12	1.87	0.56
1:P:22:HIS:HA	1:P:25:ILE:HD12	1.89	0.55
1:c:15:TYR:HA	1:c:18:ILE:HD12	1.87	0.55
1:h:15:TYR:HA	1:h:18:ILE:HD12	1.87	0.55
1:E:22:HIS:HA	1:E:25:ILE:HD12	1.88	0.55
1:Z:15:TYR:HA	1:Z:18:ILE:HD12	1.87	0.55
1:g:22:HIS:HA	1:g:25:ILE:HD12	1.87	0.55
1:Z:22:HIS:HA	1:Z:25:ILE:HD12	1.89	0.55
1:d:15:TYR:HA	1:d:18:ILE:HD12	1.87	0.55
1:i:25:ILE:HD11	1:o:19:LEU:HG	1.87	0.55
1:P:15:TYR:HA	1:P:18:ILE:HD12	1.89	0.54
1:H:15:TYR:HA	1:H:18:ILE:HD12	1.89	0.53
1:C:22:HIS:HA	1:C:25:ILE:HD12	1.91	0.53
1:R:29:GLN:O	1:n:1:GLN:N	2.40	0.53
1:c:22:HIS:HA	1:c:25:ILE:HD12	1.91	0.52
1:j:22:HIS:HA	1:j:25:ILE:HD12	1.92	0.52
1:I:1:GLN:N	1:e:29:GLN:O	2.42	0.52
1:W:22:HIS:HA	1:W:25:ILE:HD12	1.93	0.51
1:i:22:HIS:HA	1:i:25:ILE:HD12	1.92	0.50
1:P:29:GLN:O	1:l:1:GLN:N	2.42	0.50
1:p:22:HIS:HA	1:p:25:ILE:HD12	1.93	0.50
1:a:1:GLN:N	1:w:29:GLN:O	2.41	0.50
1:O:1:GLN:N	1:k:29:GLN:O	2.42	0.49
1:c:1:GLN:N	1:y:29:GLN:O	2.43	0.49
1:I:29:GLN:O	1:N:1:GLN:N	2.43	0.48
1:F:22:HIS:HA	1:F:25:ILE:HD12	1.94	0.48
1:X:22:HIS:HA	1:X:25:ILE:HD12	1.95	0.48
1:k:15:TYR:HA	1:k:18:ILE:HD12	1.95	0.48
1:G:22:HIS:HA	1:G:25:ILE:HD12	1.96	0.47
1:l:15:TYR:HA	1:l:18:ILE:HD12	1.96	0.47
1:D:22:HIS:HA	1:D:25:ILE:HD12	1.96	0.46
1:A:19:LEU:HD12	1:F:25:ILE:HD11	1.96	0.46
1:B:1:GLN:N	1:U:29:GLN:O	2.45	0.46
1:1:15:TYR:HA	1:1:18:ILE:HD12	1.96	0.46
1:L:29:GLN:O	1:h:1:GLN:N	2.45	0.46
1:Q:25:ILE:HG12	1:W:23:ALA:HB2	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:23:ALA:HB2	1:d:25:ILE:HG12	1.97	0.46
1:d:29:GLN:O	1:z:1:GLN:N	2.44	0.45
1:M:1:GLN:N	1:i:29:GLN:O	2.43	0.45
1:W:25:ILE:HD11	1:c:19:LEU:HD12	1.99	0.44
1:A:29:GLN:O	1:V:1:GLN:N	2.41	0.44
1:R:19:LEU:HD12	1:X:25:ILE:HD11	2.00	0.43
1:y:15:TYR:HA	1:y:18:ILE:HD12	2.01	0.43
1:qA:119:LEU:HD23	1:qA:119:LEU:HA	1.88	0.43
1:NA:119:LEU:HD23	1:NA:119:LEU:HA	1.90	0.43
1:x:19:LEU:HD23	1:x:19:LEU:HA	1.87	0.43
1:Y:1:GLN:N	1:u:29:GLN:O	2.40	0.43
1:hA:105:LEU:HD12	1:nA:104:ILE:HD11	2.01	0.42
1:C:1:GLN:N	1:Y:29:GLN:O	2.43	0.42
1:RA:125:ILE:HD12	1:RA:125:ILE:HA	1.95	0.42
1:bA:105:LEU:HD12	1:hA:104:ILE:HD11	2.02	0.42
1:T:26:LEU:HD12	1:T:26:LEU:HA	1.92	0.42
1:t:12:LEU:HD12	1:z:18:ILE:HD11	2.00	0.42
1:lA:119:LEU:HD23	1:lA:119:LEU:HA	1.93	0.42
1:B:19:LEU:HD12	1:H:25:ILE:HD11	2.02	0.42
1:5:119:LEU:HD23	1:5:119:LEU:HA	1.94	0.42
1:H:22:HIS:HA	1:H:25:ILE:HD12	2.02	0.42
1:h:19:LEU:HD23	1:h:19:LEU:HA	1.91	0.42
1:D:23:ALA:HB2	1:J:25:ILE:HG12	2.02	0.42
1:n:19:LEU:HD23	1:n:19:LEU:HA	1.90	0.42
1:OA:104:ILE:H	1:OA:104:ILE:HG13	1.67	0.42
1:g:25:ILE:HD11	1:m:19:LEU:HD12	2.01	0.42
1:TA:119:LEU:HD23	1:TA:119:LEU:HA	1.92	0.42
1:j:15:TYR:HA	1:j:18:ILE:HD12	2.01	0.41
1:W:19:LEU:HD23	1:W:19:LEU:HA	1.89	0.41
1:RA:119:LEU:HD23	1:RA:119:LEU:HA	1.91	0.41
1:B:29:GLN:O	1:X:1:GLN:N	2.39	0.41
1:EA:119:LEU:HD23	1:EA:119:LEU:HA	1.93	0.41
1:o:19:LEU:HD12	1:o:19:LEU:HA	1.93	0.41
1:1:19:LEU:HD23	1:1:19:LEU:HA	1.86	0.41
1:PA:101:GLN:HB3	1:PA:104:ILE:HD12	2.03	0.41
1:2:119:LEU:HD23	1:2:119:LEU:HA	1.91	0.41
1:F:1:GLN:N	1:Q:29:GLN:O	2.44	0.41
1:G:25:ILE:HD11	1:M:19:LEU:HD12	2.02	0.41
1:7:119:LEU:HD23	1:7:119:LEU:HA	1.90	0.41
1:e:26:LEU:HD12	1:e:26:LEU:HA	1.88	0.41
1:oA:119:LEU:HD23	1:oA:119:LEU:HA	1.93	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:125:ILE:HD12	1:CA:125:ILE:HA	1.97	0.41
1:j:12:LEU:HD13	1:j:12:LEU:HA	1.95	0.40
1:Y:19:LEU:HD23	1:Y:19:LEU:HA	1.94	0.40
1:dA:119:LEU:HD23	1:dA:119:LEU:HA	1.91	0.40
1:V:19:LEU:HD23	1:V:19:LEU:HA	1.90	0.40
1:QA:119:LEU:HD23	1:QA:119:LEU:HA	1.92	0.40
1:p:26:LEU:HD12	1:p:26:LEU:HA	1.87	0.40
1:9:119:LEU:HD23	1:9:119:LEU:HA	1.89	0.40
1:LA:104:ILE:H	1:LA:104:ILE:HG13	1.68	0.40
1:XA:119:LEU:HD23	1:XA:119:LEU:HA	1.91	0.40
1:C:26:LEU:HD12	1:C:26:LEU:HA	1.91	0.40
1:g:12:LEU:HD13	1:g:12:LEU:HA	1.97	0.40
1:p:12:LEU:HD13	1:p:12:LEU:HA	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	27/29 (93%)	27 (100%)	0	0	100	100
1	1	27/29 (93%)	27 (100%)	0	0	100	100
1	2	27/29 (93%)	27 (100%)	0	0	100	100
1	3	27/29 (93%)	27 (100%)	0	0	100	100
1	4	27/29 (93%)	27 (100%)	0	0	100	100
1	5	27/29 (93%)	27 (100%)	0	0	100	100
1	6	27/29 (93%)	27 (100%)	0	0	100	100
1	7	27/29 (93%)	27 (100%)	0	0	100	100
1	8	27/29 (93%)	27 (100%)	0	0	100	100
1	9	27/29 (93%)	27 (100%)	0	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	27/29 (93%)	27 (100%)	0	0	100	100
1	AA	27/29 (93%)	27 (100%)	0	0	100	100
1	B	27/29 (93%)	27 (100%)	0	0	100	100
1	BA	27/29 (93%)	27 (100%)	0	0	100	100
1	C	27/29 (93%)	27 (100%)	0	0	100	100
1	CA	27/29 (93%)	27 (100%)	0	0	100	100
1	D	27/29 (93%)	27 (100%)	0	0	100	100
1	DA	27/29 (93%)	27 (100%)	0	0	100	100
1	E	27/29 (93%)	27 (100%)	0	0	100	100
1	EA	27/29 (93%)	27 (100%)	0	0	100	100
1	F	27/29 (93%)	27 (100%)	0	0	100	100
1	FA	27/29 (93%)	27 (100%)	0	0	100	100
1	G	27/29 (93%)	27 (100%)	0	0	100	100
1	GA	27/29 (93%)	27 (100%)	0	0	100	100
1	H	27/29 (93%)	27 (100%)	0	0	100	100
1	HA	27/29 (93%)	27 (100%)	0	0	100	100
1	I	27/29 (93%)	27 (100%)	0	0	100	100
1	IA	27/29 (93%)	27 (100%)	0	0	100	100
1	J	27/29 (93%)	27 (100%)	0	0	100	100
1	JA	27/29 (93%)	27 (100%)	0	0	100	100
1	K	27/29 (93%)	27 (100%)	0	0	100	100
1	KA	27/29 (93%)	27 (100%)	0	0	100	100
1	L	27/29 (93%)	27 (100%)	0	0	100	100
1	LA	27/29 (93%)	27 (100%)	0	0	100	100
1	M	27/29 (93%)	27 (100%)	0	0	100	100
1	MA	27/29 (93%)	27 (100%)	0	0	100	100
1	N	27/29 (93%)	27 (100%)	0	0	100	100
1	NA	27/29 (93%)	27 (100%)	0	0	100	100
1	O	27/29 (93%)	27 (100%)	0	0	100	100
1	OA	27/29 (93%)	27 (100%)	0	0	100	100
1	P	27/29 (93%)	27 (100%)	0	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	PA	27/29 (93%)	27 (100%)	0	0	100	100
1	Q	27/29 (93%)	27 (100%)	0	0	100	100
1	QA	27/29 (93%)	27 (100%)	0	0	100	100
1	R	27/29 (93%)	27 (100%)	0	0	100	100
1	RA	27/29 (93%)	27 (100%)	0	0	100	100
1	S	27/29 (93%)	27 (100%)	0	0	100	100
1	SA	27/29 (93%)	27 (100%)	0	0	100	100
1	T	27/29 (93%)	27 (100%)	0	0	100	100
1	TA	27/29 (93%)	27 (100%)	0	0	100	100
1	U	27/29 (93%)	27 (100%)	0	0	100	100
1	UA	27/29 (93%)	27 (100%)	0	0	100	100
1	V	27/29 (93%)	27 (100%)	0	0	100	100
1	VA	27/29 (93%)	27 (100%)	0	0	100	100
1	W	27/29 (93%)	27 (100%)	0	0	100	100
1	WA	27/29 (93%)	27 (100%)	0	0	100	100
1	X	27/29 (93%)	27 (100%)	0	0	100	100
1	XA	27/29 (93%)	27 (100%)	0	0	100	100
1	Y	27/29 (93%)	27 (100%)	0	0	100	100
1	YA	27/29 (93%)	27 (100%)	0	0	100	100
1	Z	27/29 (93%)	27 (100%)	0	0	100	100
1	ZA	27/29 (93%)	27 (100%)	0	0	100	100
1	a	27/29 (93%)	27 (100%)	0	0	100	100
1	aA	27/29 (93%)	27 (100%)	0	0	100	100
1	b	27/29 (93%)	27 (100%)	0	0	100	100
1	bA	27/29 (93%)	27 (100%)	0	0	100	100
1	c	27/29 (93%)	27 (100%)	0	0	100	100
1	cA	27/29 (93%)	27 (100%)	0	0	100	100
1	d	27/29 (93%)	27 (100%)	0	0	100	100
1	dA	27/29 (93%)	27 (100%)	0	0	100	100
1	e	27/29 (93%)	27 (100%)	0	0	100	100
1	eA	27/29 (93%)	27 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	f	27/29 (93%)	27 (100%)	0	0	100	100
1	fA	27/29 (93%)	27 (100%)	0	0	100	100
1	g	27/29 (93%)	27 (100%)	0	0	100	100
1	gA	27/29 (93%)	27 (100%)	0	0	100	100
1	h	27/29 (93%)	27 (100%)	0	0	100	100
1	hA	27/29 (93%)	27 (100%)	0	0	100	100
1	i	27/29 (93%)	27 (100%)	0	0	100	100
1	iA	27/29 (93%)	27 (100%)	0	0	100	100
1	j	27/29 (93%)	27 (100%)	0	0	100	100
1	jA	27/29 (93%)	27 (100%)	0	0	100	100
1	k	27/29 (93%)	27 (100%)	0	0	100	100
1	kA	27/29 (93%)	27 (100%)	0	0	100	100
1	l	27/29 (93%)	27 (100%)	0	0	100	100
1	lA	27/29 (93%)	27 (100%)	0	0	100	100
1	m	27/29 (93%)	27 (100%)	0	0	100	100
1	mA	27/29 (93%)	27 (100%)	0	0	100	100
1	n	27/29 (93%)	27 (100%)	0	0	100	100
1	nA	27/29 (93%)	27 (100%)	0	0	100	100
1	o	27/29 (93%)	27 (100%)	0	0	100	100
1	oA	27/29 (93%)	27 (100%)	0	0	100	100
1	p	27/29 (93%)	27 (100%)	0	0	100	100
1	pA	27/29 (93%)	27 (100%)	0	0	100	100
1	q	27/29 (93%)	27 (100%)	0	0	100	100
1	qA	27/29 (93%)	27 (100%)	0	0	100	100
1	r	27/29 (93%)	27 (100%)	0	0	100	100
1	rA	27/29 (93%)	27 (100%)	0	0	100	100
1	s	27/29 (93%)	27 (100%)	0	0	100	100
1	t	27/29 (93%)	27 (100%)	0	0	100	100
1	u	27/29 (93%)	27 (100%)	0	0	100	100
1	v	27/29 (93%)	27 (100%)	0	0	100	100
1	w	27/29 (93%)	27 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	27/29 (93%)	27 (100%)	0	0	100	100
1	y	27/29 (93%)	27 (100%)	0	0	100	100
1	z	27/29 (93%)	27 (100%)	0	0	100	100
All	All	2862/3074 (93%)	2862 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	21/21 (100%)	21 (100%)	0	100	100
1	1	21/21 (100%)	21 (100%)	0	100	100
1	2	21/21 (100%)	21 (100%)	0	100	100
1	3	21/21 (100%)	21 (100%)	0	100	100
1	4	21/21 (100%)	21 (100%)	0	100	100
1	5	21/21 (100%)	21 (100%)	0	100	100
1	6	21/21 (100%)	21 (100%)	0	100	100
1	7	21/21 (100%)	21 (100%)	0	100	100
1	8	21/21 (100%)	21 (100%)	0	100	100
1	9	21/21 (100%)	21 (100%)	0	100	100
1	A	21/21 (100%)	21 (100%)	0	100	100
1	AA	21/21 (100%)	21 (100%)	0	100	100
1	B	21/21 (100%)	21 (100%)	0	100	100
1	BA	21/21 (100%)	21 (100%)	0	100	100
1	C	21/21 (100%)	21 (100%)	0	100	100
1	CA	21/21 (100%)	21 (100%)	0	100	100
1	D	21/21 (100%)	21 (100%)	0	100	100
1	DA	21/21 (100%)	21 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	21/21 (100%)	21 (100%)	0	100	100
1	EA	21/21 (100%)	21 (100%)	0	100	100
1	F	21/21 (100%)	21 (100%)	0	100	100
1	FA	21/21 (100%)	21 (100%)	0	100	100
1	G	21/21 (100%)	21 (100%)	0	100	100
1	GA	21/21 (100%)	21 (100%)	0	100	100
1	H	21/21 (100%)	21 (100%)	0	100	100
1	HA	21/21 (100%)	21 (100%)	0	100	100
1	I	21/21 (100%)	21 (100%)	0	100	100
1	IA	21/21 (100%)	21 (100%)	0	100	100
1	J	21/21 (100%)	21 (100%)	0	100	100
1	JA	21/21 (100%)	21 (100%)	0	100	100
1	K	21/21 (100%)	21 (100%)	0	100	100
1	KA	21/21 (100%)	21 (100%)	0	100	100
1	L	21/21 (100%)	21 (100%)	0	100	100
1	LA	21/21 (100%)	21 (100%)	0	100	100
1	M	21/21 (100%)	21 (100%)	0	100	100
1	MA	21/21 (100%)	21 (100%)	0	100	100
1	N	21/21 (100%)	21 (100%)	0	100	100
1	NA	21/21 (100%)	21 (100%)	0	100	100
1	O	21/21 (100%)	21 (100%)	0	100	100
1	OA	21/21 (100%)	21 (100%)	0	100	100
1	P	21/21 (100%)	21 (100%)	0	100	100
1	PA	21/21 (100%)	21 (100%)	0	100	100
1	Q	21/21 (100%)	21 (100%)	0	100	100
1	QA	21/21 (100%)	21 (100%)	0	100	100
1	R	21/21 (100%)	21 (100%)	0	100	100
1	RA	21/21 (100%)	21 (100%)	0	100	100
1	S	21/21 (100%)	21 (100%)	0	100	100
1	SA	21/21 (100%)	21 (100%)	0	100	100
1	T	21/21 (100%)	21 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TA	21/21 (100%)	21 (100%)	0	100	100
1	U	21/21 (100%)	21 (100%)	0	100	100
1	UA	21/21 (100%)	21 (100%)	0	100	100
1	V	21/21 (100%)	21 (100%)	0	100	100
1	VA	21/21 (100%)	21 (100%)	0	100	100
1	W	21/21 (100%)	21 (100%)	0	100	100
1	WA	21/21 (100%)	21 (100%)	0	100	100
1	X	21/21 (100%)	21 (100%)	0	100	100
1	XA	21/21 (100%)	21 (100%)	0	100	100
1	Y	21/21 (100%)	21 (100%)	0	100	100
1	YA	21/21 (100%)	21 (100%)	0	100	100
1	Z	21/21 (100%)	21 (100%)	0	100	100
1	ZA	21/21 (100%)	21 (100%)	0	100	100
1	a	21/21 (100%)	21 (100%)	0	100	100
1	aA	21/21 (100%)	21 (100%)	0	100	100
1	b	21/21 (100%)	21 (100%)	0	100	100
1	bA	21/21 (100%)	21 (100%)	0	100	100
1	c	21/21 (100%)	21 (100%)	0	100	100
1	cA	21/21 (100%)	21 (100%)	0	100	100
1	d	21/21 (100%)	21 (100%)	0	100	100
1	dA	21/21 (100%)	21 (100%)	0	100	100
1	e	21/21 (100%)	21 (100%)	0	100	100
1	eA	21/21 (100%)	21 (100%)	0	100	100
1	f	21/21 (100%)	21 (100%)	0	100	100
1	fA	21/21 (100%)	21 (100%)	0	100	100
1	g	21/21 (100%)	21 (100%)	0	100	100
1	gA	21/21 (100%)	21 (100%)	0	100	100
1	h	21/21 (100%)	21 (100%)	0	100	100
1	hA	21/21 (100%)	21 (100%)	0	100	100
1	i	21/21 (100%)	21 (100%)	0	100	100
1	iA	21/21 (100%)	21 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	21/21 (100%)	21 (100%)	0	100	100
1	jA	21/21 (100%)	21 (100%)	0	100	100
1	k	21/21 (100%)	21 (100%)	0	100	100
1	kA	21/21 (100%)	21 (100%)	0	100	100
1	l	21/21 (100%)	21 (100%)	0	100	100
1	lA	21/21 (100%)	21 (100%)	0	100	100
1	m	21/21 (100%)	21 (100%)	0	100	100
1	mA	21/21 (100%)	21 (100%)	0	100	100
1	n	21/21 (100%)	21 (100%)	0	100	100
1	nA	21/21 (100%)	21 (100%)	0	100	100
1	o	21/21 (100%)	21 (100%)	0	100	100
1	oA	21/21 (100%)	21 (100%)	0	100	100
1	p	21/21 (100%)	21 (100%)	0	100	100
1	pA	21/21 (100%)	21 (100%)	0	100	100
1	q	21/21 (100%)	21 (100%)	0	100	100
1	qA	21/21 (100%)	21 (100%)	0	100	100
1	r	21/21 (100%)	21 (100%)	0	100	100
1	rA	21/21 (100%)	21 (100%)	0	100	100
1	s	21/21 (100%)	21 (100%)	0	100	100
1	t	21/21 (100%)	21 (100%)	0	100	100
1	u	21/21 (100%)	21 (100%)	0	100	100
1	v	21/21 (100%)	21 (100%)	0	100	100
1	w	21/21 (100%)	21 (100%)	0	100	100
1	x	21/21 (100%)	21 (100%)	0	100	100
1	y	21/21 (100%)	21 (100%)	0	100	100
1	z	21/21 (100%)	21 (100%)	0	100	100
All	All	2226/2226 (100%)	2226 (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. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	CA	122	HIS
1	EA	122	HIS
1	JA	122	HIS
1	MA	122	HIS
1	j	22	HIS
1	eA	122	HIS
1	t	1	GLN
1	u	22	HIS
1	y	22	HIS

### 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 oligosaccharides 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.

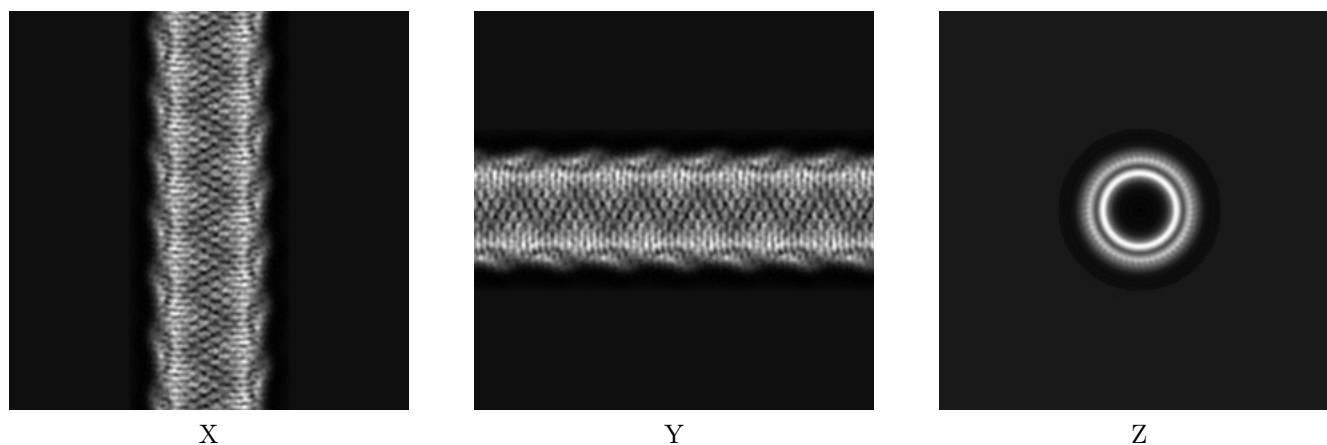
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21817. 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](#)

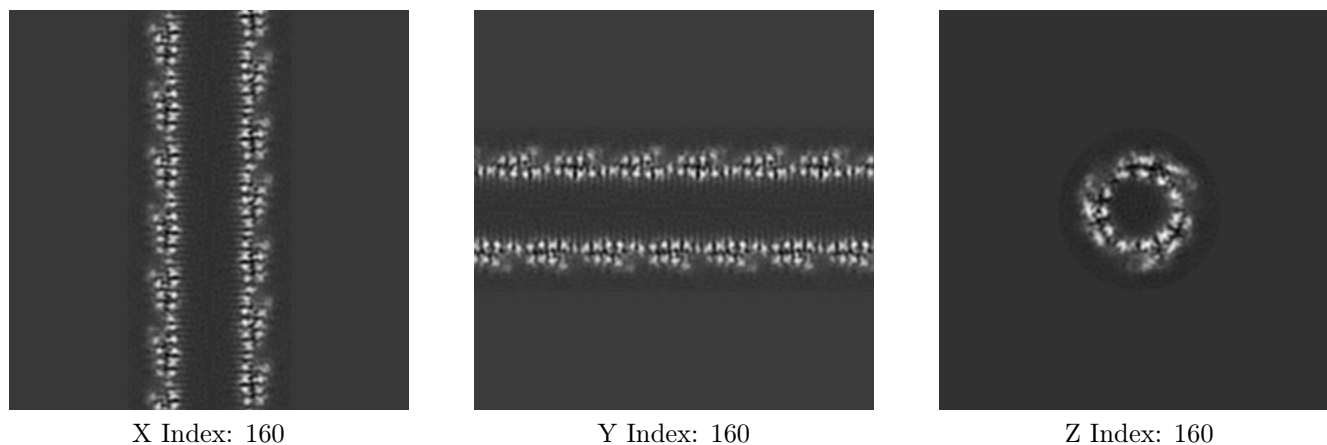
#### 6.1.1 Primary map



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

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

#### 6.2.1 Primary map

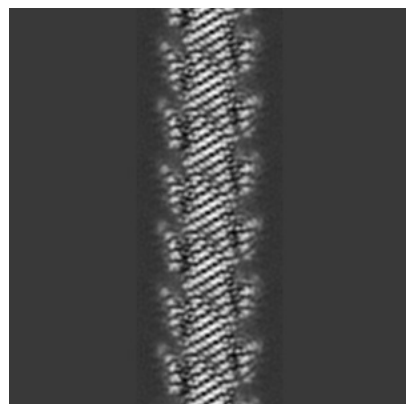




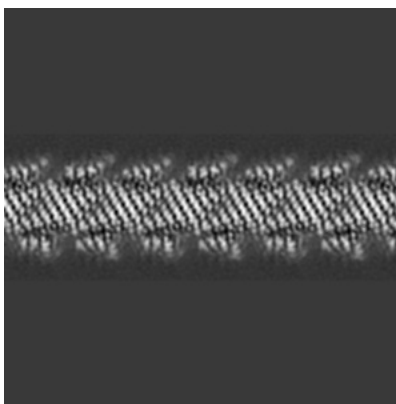
The images above show central slices of the map in three orthogonal directions.

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

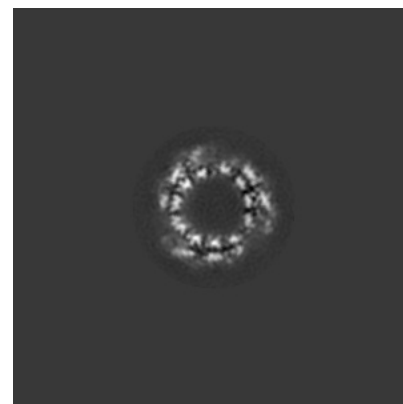
### 6.3.1 Primary map



X Index: 132



Y Index: 132

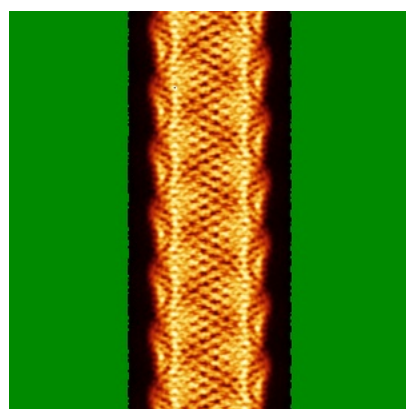


Z Index: 91

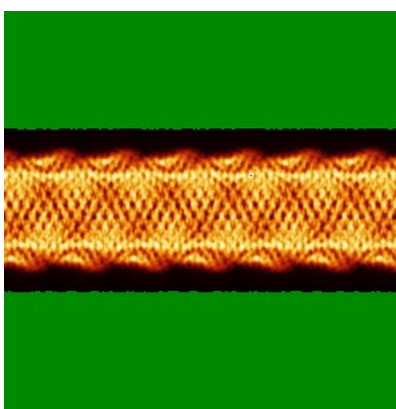
The images above show the largest variance slices of the map in three orthogonal directions.

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

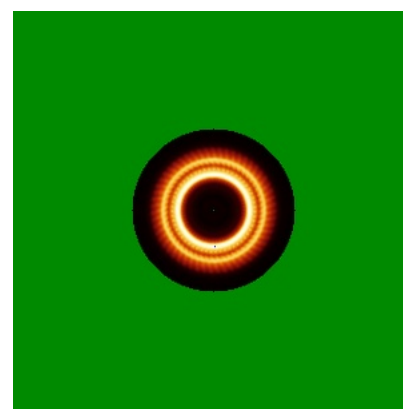
### 6.4.1 Primary map



X



Y

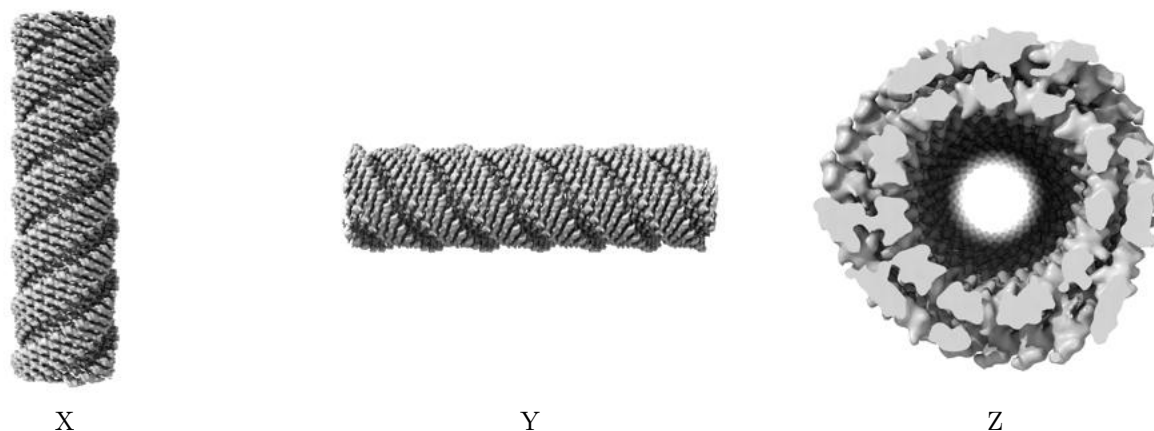


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

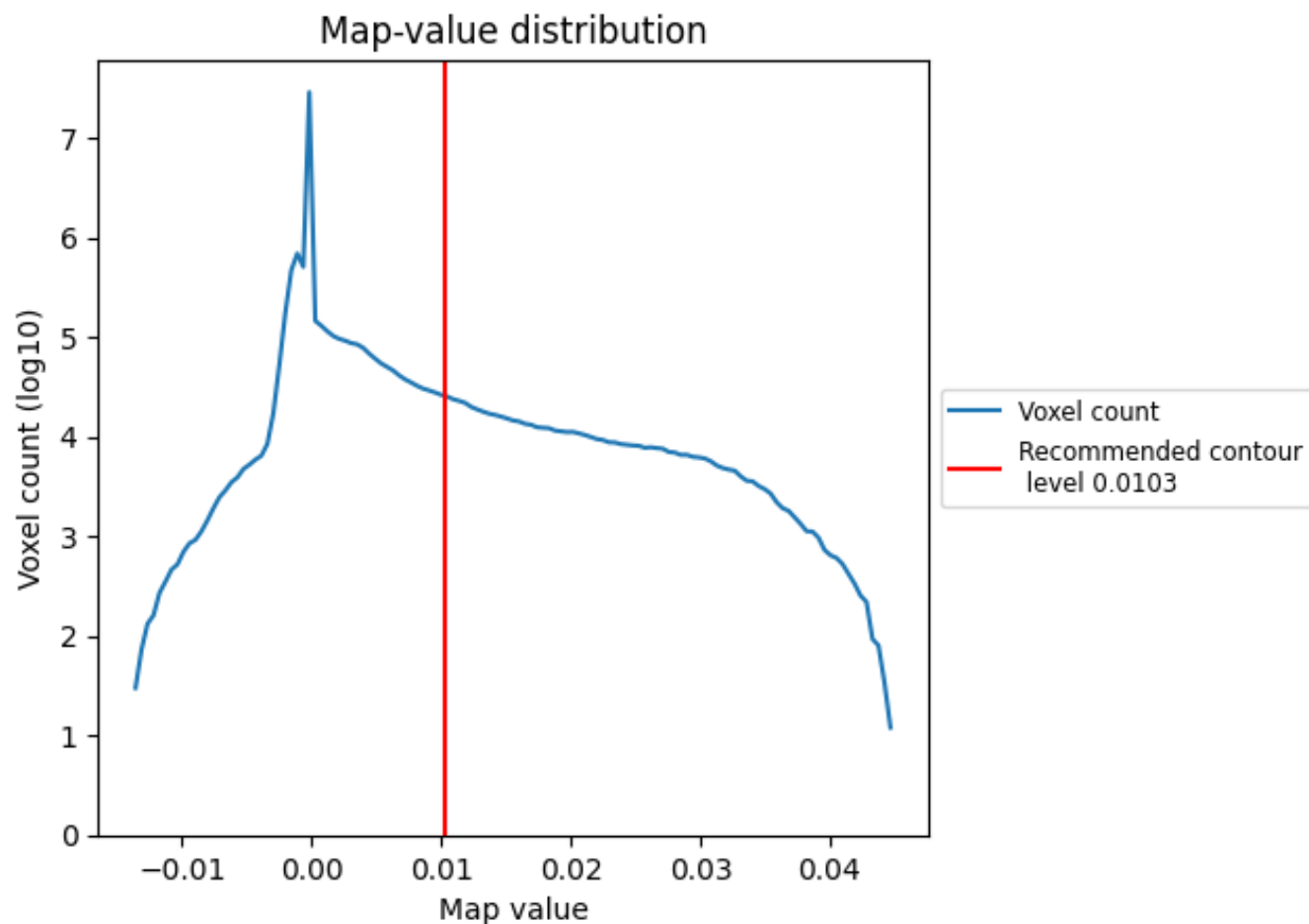
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

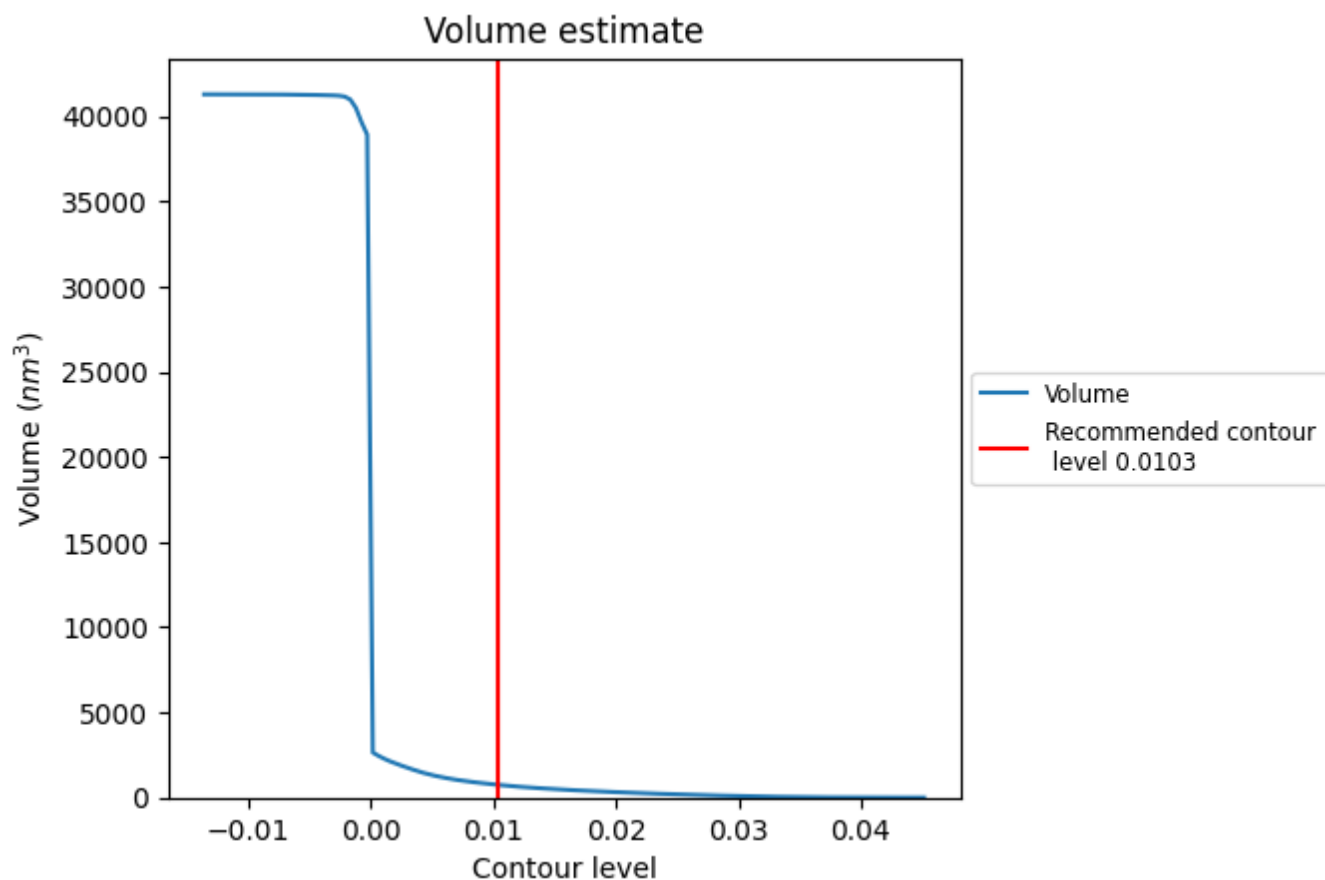
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

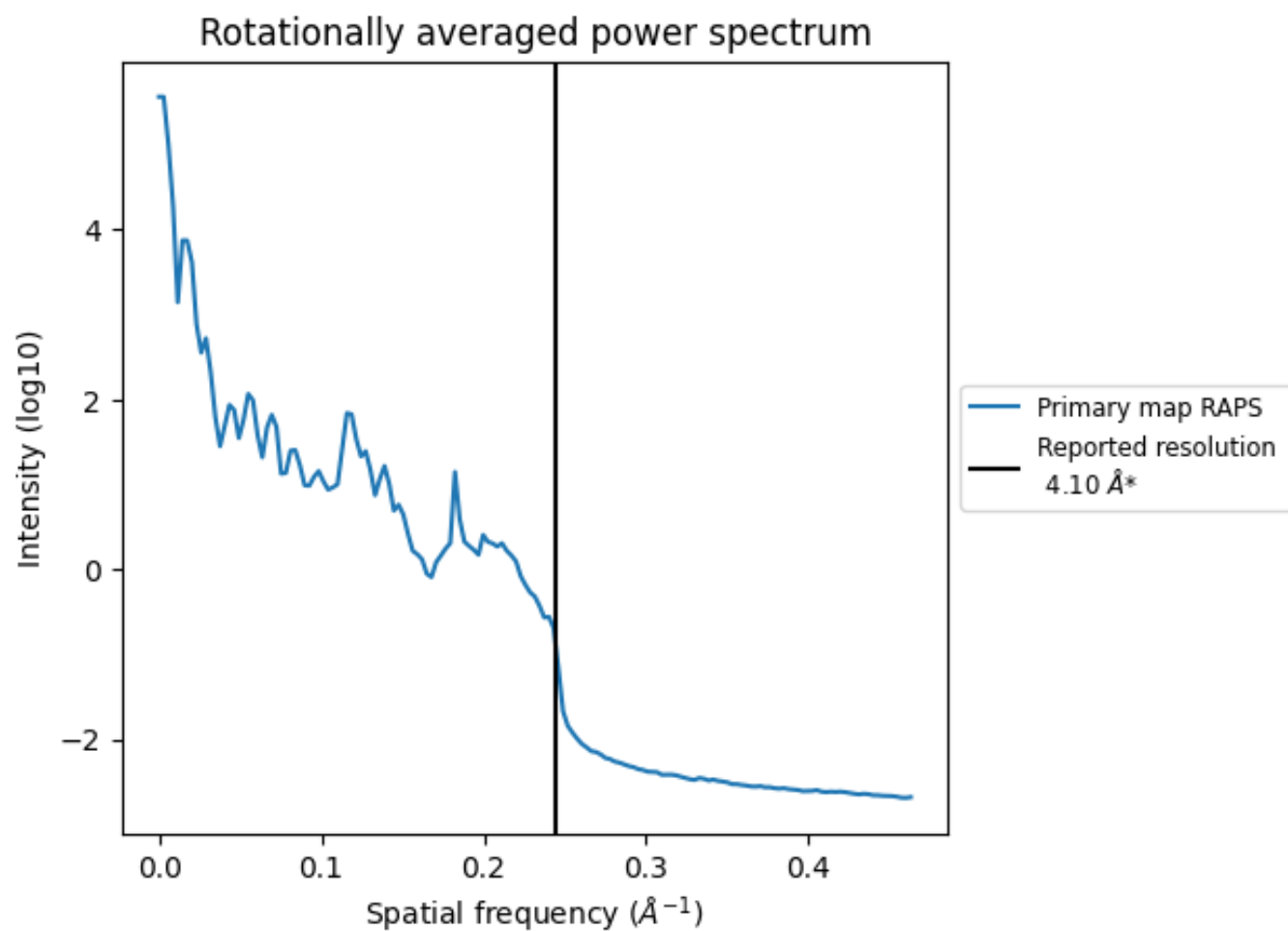
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 754  $\text{nm}^3$ ; this corresponds to an approximate mass of 681 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

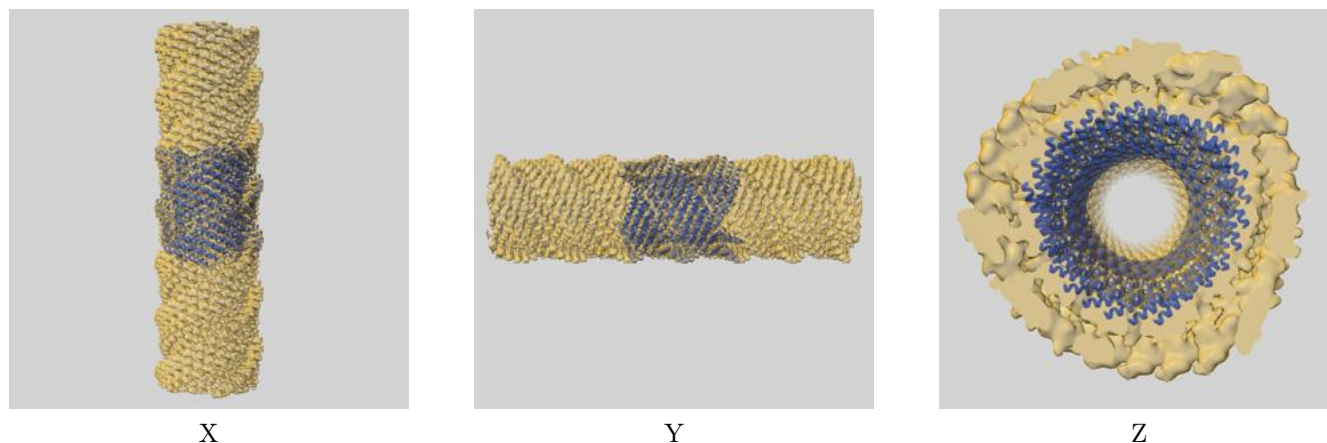
## 8 Fourier-Shell correlation

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

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

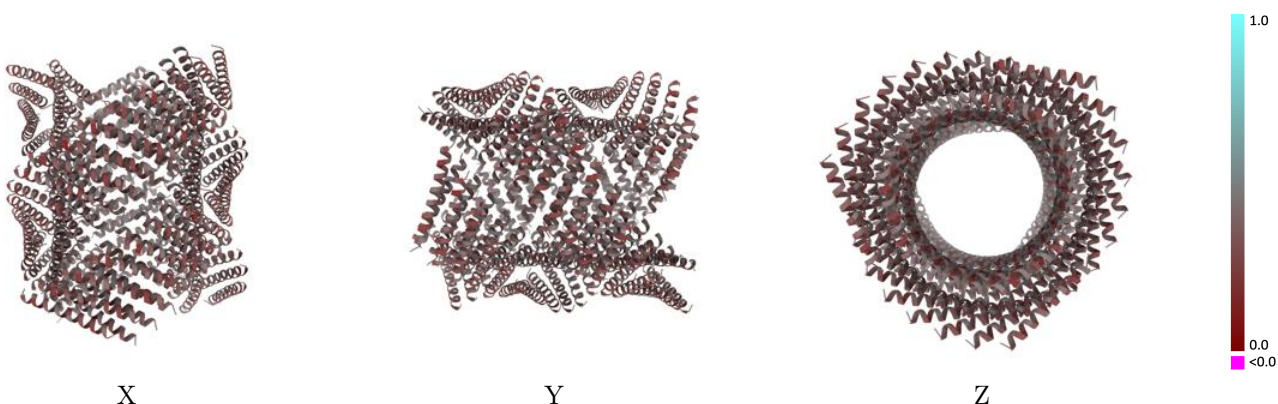
This section contains information regarding the fit between EMDB map EMD-21817 and PDB model 6WL8. Per-residue inclusion information can be found in section 3 on page 13.

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



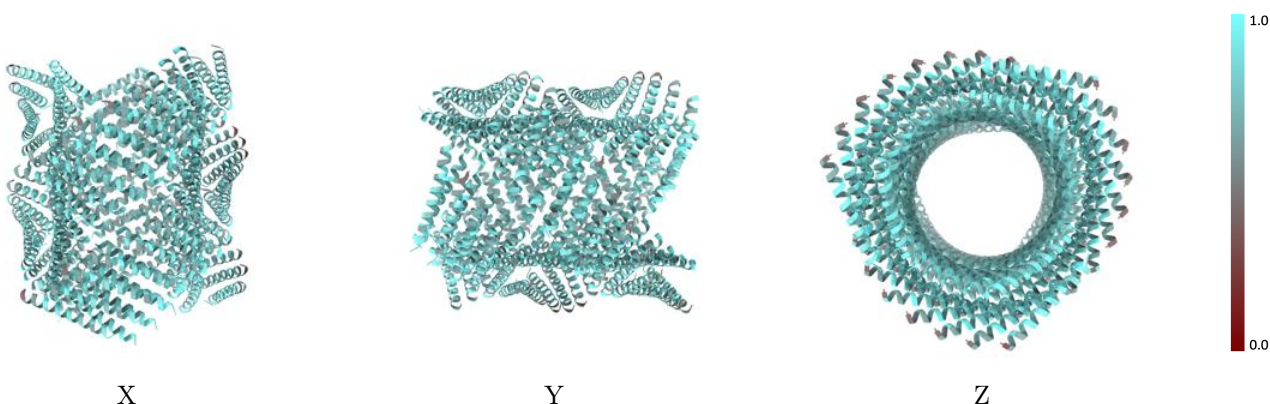
The images above show the 3D surface view of the map at the recommended contour level 0.0103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

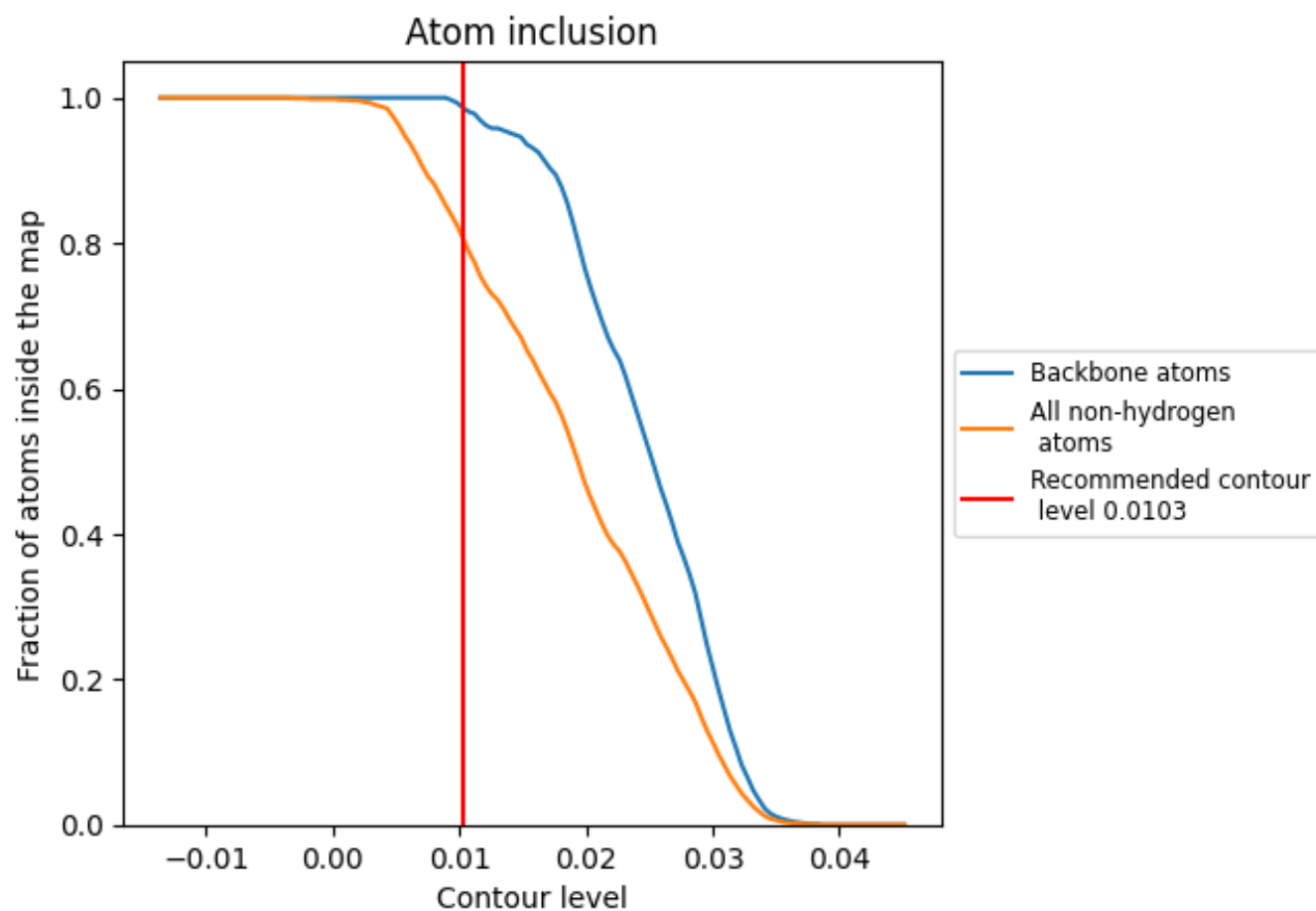
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0103).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.3640
0	 0.7810	 0.3450
1	 0.8350	 0.3830
2	 0.7770	 0.3480
3	 0.7680	 0.3470
4	 0.7720	 0.3440
5	 0.7680	 0.3450
6	 0.7860	 0.3540
7	 0.7680	 0.3500
8	 0.7810	 0.3460
9	 0.7770	 0.3460
A	 0.8350	 0.3780
AA	 0.7770	 0.3500
B	 0.8390	 0.3800
BA	 0.7900	 0.3520
C	 0.8440	 0.3850
CA	 0.7900	 0.3490
D	 0.8440	 0.3790
DA	 0.7590	 0.3470
E	 0.8390	 0.3810
EA	 0.7720	 0.3400
F	 0.8350	 0.3810
FA	 0.7720	 0.3450
G	 0.8260	 0.3830
GA	 0.7770	 0.3520
H	 0.8350	 0.3750
HA	 0.7720	 0.3410
I	 0.8390	 0.3760
IA	 0.7770	 0.3520
J	 0.8300	 0.3810
JA	 0.7630	 0.3510
K	 0.8350	 0.3850
KA	 0.7680	 0.3470
L	 0.8390	 0.3750
LA	 0.7770	 0.3510































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
M	 0.8260	 0.3790
MA	 0.7770	 0.3470
N	 0.8300	 0.3810
NA	 0.7680	 0.3490
O	 0.8440	 0.3810
OA	 0.7860	 0.3510
P	 0.8350	 0.3780
PA	 0.7770	 0.3460
Q	 0.8390	 0.3840
QA	 0.7630	 0.3530
R	 0.8300	 0.3780
RA	 0.7860	 0.3500
S	 0.8350	 0.3790
SA	 0.7770	 0.3480
T	 0.8300	 0.3820
TA	 0.7720	 0.3490
U	 0.8260	 0.3750
UA	 0.7770	 0.3490
V	 0.8300	 0.3800
VA	 0.7770	 0.3470
W	 0.8300	 0.3820
WA	 0.7720	 0.3520
X	 0.8350	 0.3740
XA	 0.7770	 0.3530
Y	 0.8350	 0.3850
YA	 0.7770	 0.3530
Z	 0.8260	 0.3760
ZA	 0.7770	 0.3520
a	 0.8350	 0.3830
aA	 0.7810	 0.3510
b	 0.8300	 0.3770
bA	 0.7770	 0.3460
c	 0.8300	 0.3760
cA	 0.7720	 0.3510
d	 0.8350	 0.3820
dA	 0.7810	 0.3460
e	 0.8260	 0.3790
eA	 0.7770	 0.3460
f	 0.8350	 0.3770
fA	 0.7680	 0.3530
g	 0.8350	 0.3770
gA	 0.7860	 0.3530

*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
h	 0.8350	 0.3770
hA	 0.7680	 0.3460
i	 0.8350	 0.3780
iA	 0.7810	 0.3480
j	 0.8260	 0.3770
jA	 0.7860	 0.3430
k	 0.8390	 0.3750
kA	 0.7720	 0.3430
l	 0.8390	 0.3800
lA	 0.7810	 0.3490
m	 0.8210	 0.3770
mA	 0.7770	 0.3480
n	 0.8390	 0.3780
nA	 0.7900	 0.3460
o	 0.8260	 0.3760
oA	 0.7770	 0.3430
p	 0.8390	 0.3820
pA	 0.7720	 0.3520
q	 0.8440	 0.3840
qA	 0.7720	 0.3450
r	 0.8300	 0.3800
rA	 0.7860	 0.3500
s	 0.8390	 0.3780
t	 0.8390	 0.3800
u	 0.8480	 0.3780
v	 0.8530	 0.3840
w	 0.8210	 0.3810
x	 0.8390	 0.3810
y	 0.8350	 0.3770
z	 0.8480	 0.3770