



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:10 PM UTC

PDB ID : 7P1T / pdb_00007p1t
EMDB ID : EMD-13164
Title : Cryo-EM structure of encapsulin from Mycobacterium tuberculosis
Authors : Lewis, C.J.; Berger, C.; Ravelli, R.B.G.
Deposited on : 2021-07-02
Resolution : 2.29 Å(reported)
Based on initial model : 619G

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

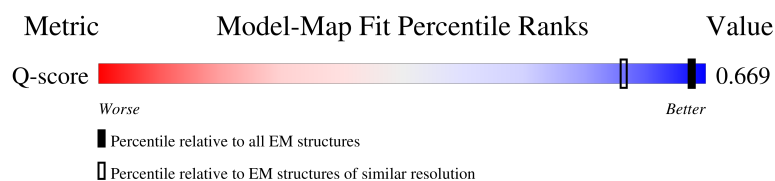
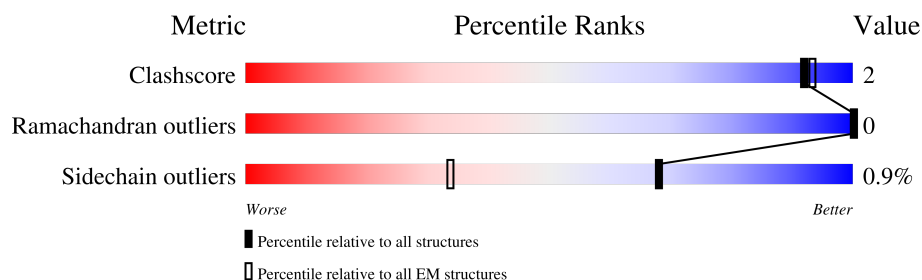
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

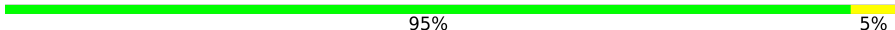
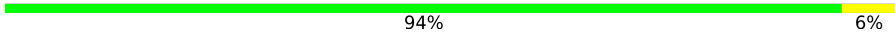
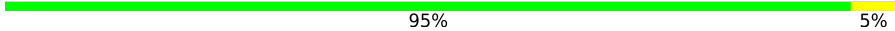
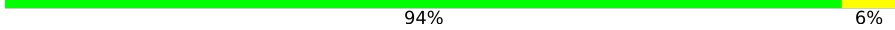
The reported resolution of this entry is 2.29 Å.

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.



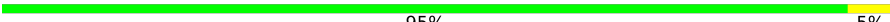
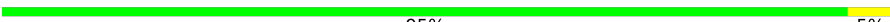
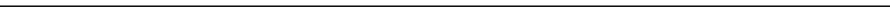
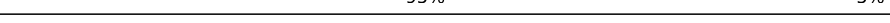
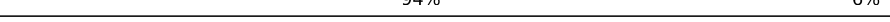
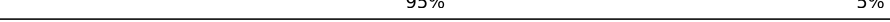
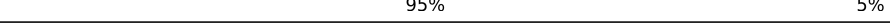
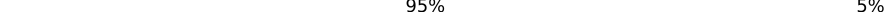
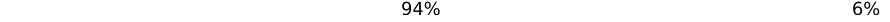
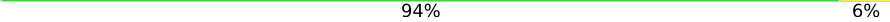
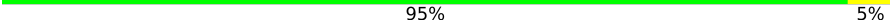
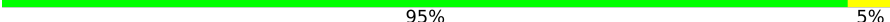
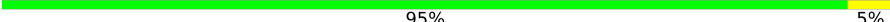
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3699 (1.79 - 2.79)

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

Mol	Chain	Length	Quality of chain
1	A	265	 95% 5%
1	AA	265	 94% 6%
1	AB	265	 95% 5%
1	B	265	 94% 6%

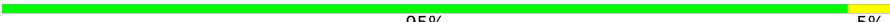
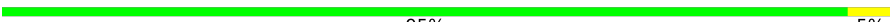
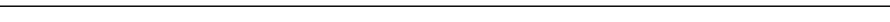
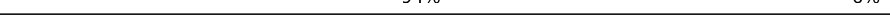
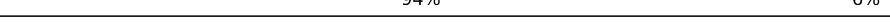
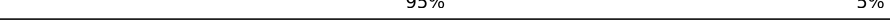
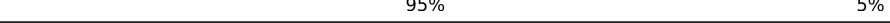
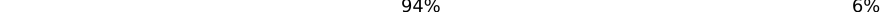
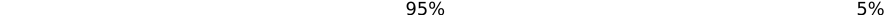
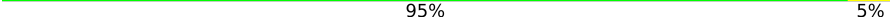
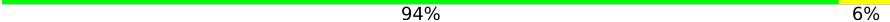
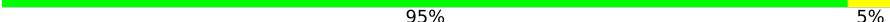
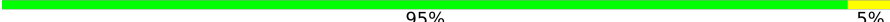
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Mol	Chain	Length	Quality of chain
1	BA	265	 95% 5%
1	BB	265	 95% 5%
1	C	265	 95% 5%
1	CA	265	 95% 5%
1	CB	265	 95% 5%
1	D	265	 94% 6%
1	DA	265	 95% 5%
1	DB	265	 94% 6%
1	E	265	 95% 5%
1	EA	265	 95% 5%
1	EB	265	 95% 5%
1	F	265	 95% 5%
1	FA	265	 95% 5%
1	FB	265	 95% 5%
1	G	265	 95% 5%
1	GA	265	 94% 6%
1	GB	265	 95% 5%
1	H	265	 95% 5%
1	HA	265	 95% 5%
1	HB	265	 94% 6%
1	I	265	 94% 6%
1	IA	265	 95% 5%
1	J	265	 95% 5%
1	JA	265	 95% 5%
1	K	265	 95% 5%

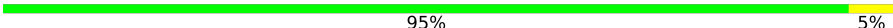
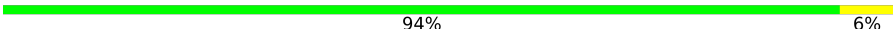
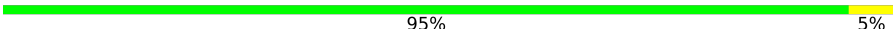
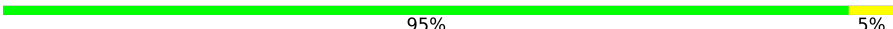
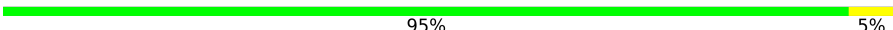
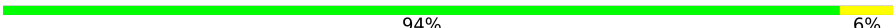
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Mol	Chain	Length	Quality of chain
1	KA	265	 95% 5%
1	L	265	 95% 5%
1	LA	265	 94% 6%
1	M	265	 95% 5%
1	MA	265	 95% 5%
1	N	265	 94% 6%
1	NA	265	 95% 5%
1	O	265	 95% 5%
1	OA	265	 95% 5%
1	P	265	 95% 5%
1	PA	265	 94% 6%
1	Q	265	 94% 6%
1	QA	265	 95% 5%
1	R	265	 95% 5%
1	RA	265	 94% 6%
1	S	265	 94% 6%
1	SA	265	 95% 5%
1	T	265	 95% 5%
1	TA	265	 94% 6%
1	U	265	 95% 5%
1	UA	265	 95% 5%
1	V	265	 94% 6%
1	VA	265	 95% 5%
1	W	265	 95% 5%
1	WA	265	 95% 5%

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Mol	Chain	Length	Quality of chain
1	X	265	 95%5%
1	XA	265	 94%6%
1	Y	265	 95%5%
1	YA	265	 95%5%
1	Z	265	 95%5%
1	ZA	265	 94%6%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 122040 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	B	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	C	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	D	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	E	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	F	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	G	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	H	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	I	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	J	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	K	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	L	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	M	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	N	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	O	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	P	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Q	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	S	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	T	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	U	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	V	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	W	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	X	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Y	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Z	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	BA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	CA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	DA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	EA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	FA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	GA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	HA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	IA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	JA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	KA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	LA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	NA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	OA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	PA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	QA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	RA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	SA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	TA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	UA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	VA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	WA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	XA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	YA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	ZA	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	BB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	CB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	DB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	EB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	FB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	GB	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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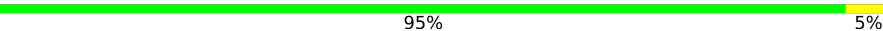
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		

3 Residue-property plots [i](#)

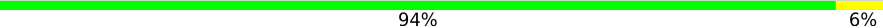
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 A: 

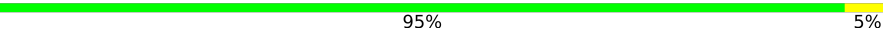


- Molecule 1: 29 kDa antigen, Cfp29

Chain B: 

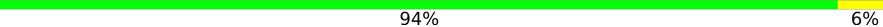


- Molecule 1: 29 kDa antigen, Cfp29

Chain C: 

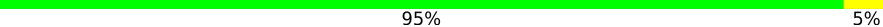


- Molecule 1: 29 kDa antigen, Cfp29

Chain D: 

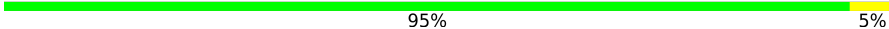


- Molecule 1: 29 kDa antigen, Cfp29

Chain E: 

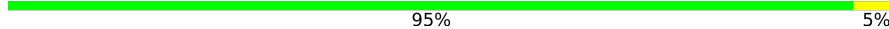


- Molecule 1: 29 kDa antigen, Cfp29

Chain F:  95% 5%

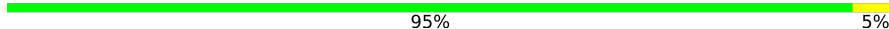


- Molecule 1: 29 kDa antigen, Cfp29

Chain G:  95% 5%



- Molecule 1: 29 kDa antigen, Cfp29

Chain H:  95% 5%

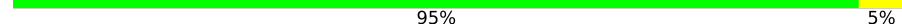


- Molecule 1: 29 kDa antigen, Cfp29

Chain I:  94% 6%

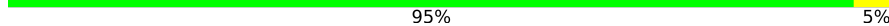


- Molecule 1: 29 kDa antigen, Cfp29

Chain J:  95% 5%

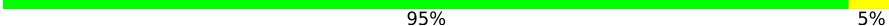


- Molecule 1: 29 kDa antigen, Cfp29

Chain K:  95% 5%

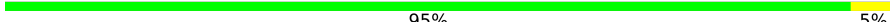


- Molecule 1: 29 kDa antigen, Cfp29

Chain L:  95% 5%



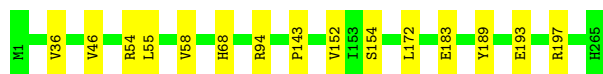
- Molecule 1: 29 kDa antigen, Cfp29

Chain M:  95% 5%

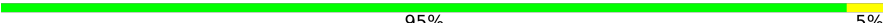


- Molecule 1: 29 kDa antigen, Cfp29

Chain N:  94% 6%



- Molecule 1: 29 kDa antigen, Cfp29

Chain O:  95% 5%

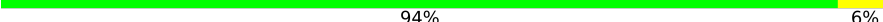


- Molecule 1: 29 kDa antigen, Cfp29

Chain P:  95% 5%

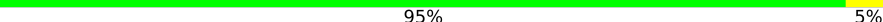


- Molecule 1: 29 kDa antigen, Cfp29

Chain Q:  94% 6%



- Molecule 1: 29 kDa antigen, Cfp29

Chain R:  95% 5%

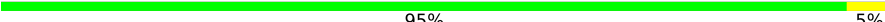


- Molecule 1: 29 kDa antigen, Cfp29

Chain S:  94% 6%

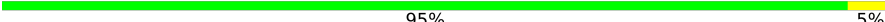


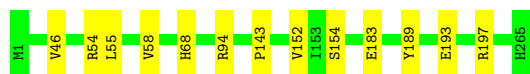
- Molecule 1: 29 kDa antigen, Cfp29

Chain T:  95% 5%



- Molecule 1: 29 kDa antigen, Cfp29

Chain U:  95% 5%

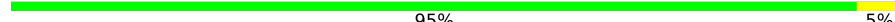


- Molecule 1: 29 kDa antigen, Cfp29

Chain V:  94% 6%

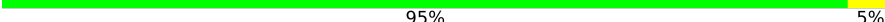


- Molecule 1: 29 kDa antigen, Cfp29

Chain W:  95% 5%

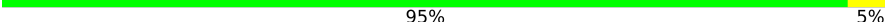


- Molecule 1: 29 kDa antigen, Cfp29

Chain X:  95% 5%

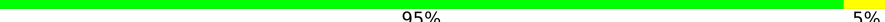


- Molecule 1: 29 kDa antigen, Cfp29

Chain Y:  95% 5%

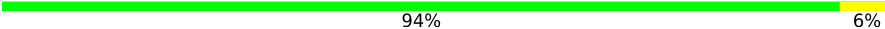


- Molecule 1: 29 kDa antigen, Cfp29

Chain Z:  95% 5%

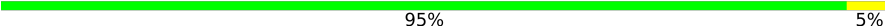


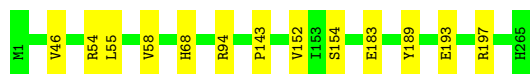
- Molecule 1: 29 kDa antigen, Cfp29

Chain AA:  94% 6%

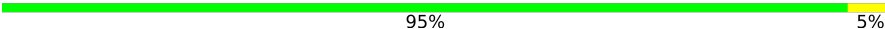


- Molecule 1: 29 kDa antigen, Cfp29

Chain BA:  95% 5%

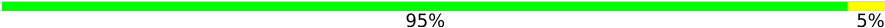


- Molecule 1: 29 kDa antigen, Cfp29

Chain CA:  95% 5%

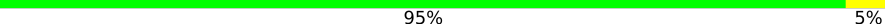


- Molecule 1: 29 kDa antigen, Cfp29

Chain DA:  95% 5%

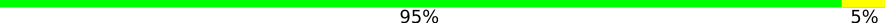


- Molecule 1: 29 kDa antigen, Cfp29

Chain EA:  95% 5%



- Molecule 1: 29 kDa antigen, Cfp29

Chain FA:  95% 5%

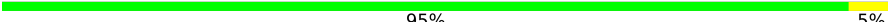


- Molecule 1: 29 kDa antigen, Cfp29

Chain GA:  94% 6%



- Molecule 1: 29 kDa antigen, Cfp29

Chain HA:  95% 5%

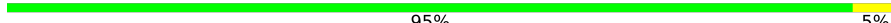


- Molecule 1: 29 kDa antigen, Cfp29

Chain IA:  95% 5%

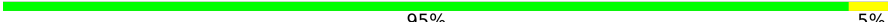


- Molecule 1: 29 kDa antigen, Cfp29

Chain JA:  95% 5%

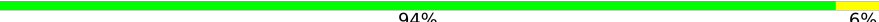


- Molecule 1: 29 kDa antigen, Cfp29

Chain KA:  95% 5%

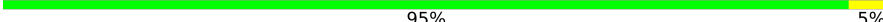


- Molecule 1: 29 kDa antigen, Cfp29

Chain LA:  94% 6%



- Molecule 1: 29 kDa antigen, Cfp29

Chain MA:  95% 5%

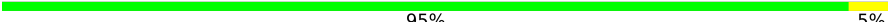


- Molecule 1: 29 kDa antigen, Cfp29

Chain NA:  95% 5%

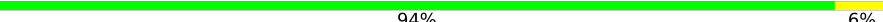


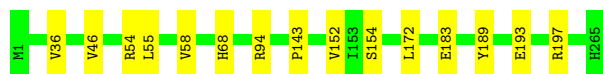
- Molecule 1: 29 kDa antigen, Cfp29

Chain OA:  95% 5%

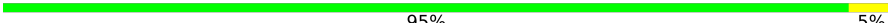


- Molecule 1: 29 kDa antigen, Cfp29

Chain PA:  94% 6%



- Molecule 1: 29 kDa antigen, Cfp29

Chain QA:  95% 5%



- Molecule 1: 29 kDa antigen, Cfp29

Chain RA:  94% 6%

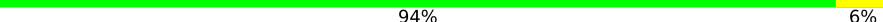


- Molecule 1: 29 kDa antigen, Cfp29

Chain SA:  95% 5%

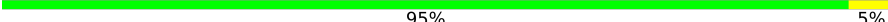


- Molecule 1: 29 kDa antigen, Cfp29

Chain TA:  94% 6%

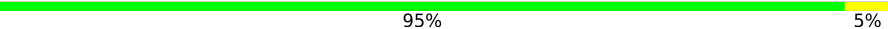


- Molecule 1: 29 kDa antigen, Cfp29

Chain UA:  95% 5%

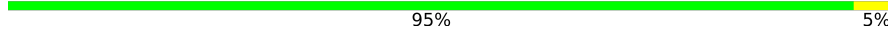


- Molecule 1: 29 kDa antigen, Cfp29

Chain VA:  95% 5%

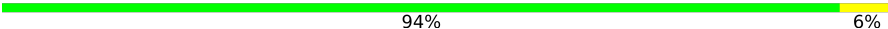


- Molecule 1: 29 kDa antigen, Cfp29

Chain WA:  95% 5%

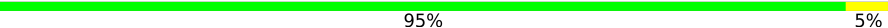


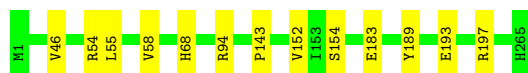
- Molecule 1: 29 kDa antigen, Cfp29

Chain XA:  94% 6%

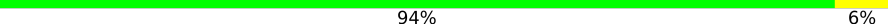


- Molecule 1: 29 kDa antigen, Cfp29

Chain YA:  95% 5%

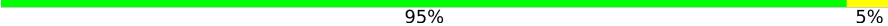


- Molecule 1: 29 kDa antigen, Cfp29

Chain ZA:  94% 6%



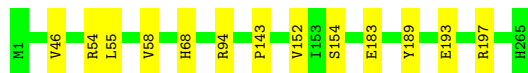
- Molecule 1: 29 kDa antigen, Cfp29

Chain AB:  95% 5%

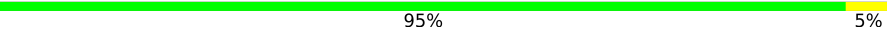


- Molecule 1: 29 kDa antigen, Cfp29

Chain BB:  95% 5%

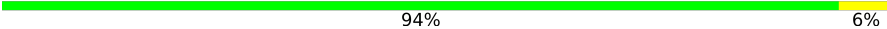


- Molecule 1: 29 kDa antigen, Cfp29

Chain CB:  95% 5%

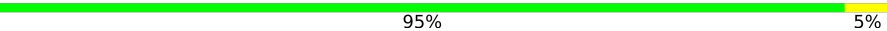


- Molecule 1: 29 kDa antigen, Cfp29

Chain DB:  94% 6%

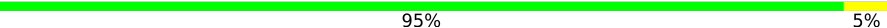


- Molecule 1: 29 kDa antigen, Cfp29

Chain EB:  95% 5%

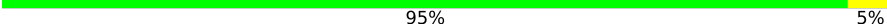


- Molecule 1: 29 kDa antigen, Cfp29

Chain FB:  95% 5%

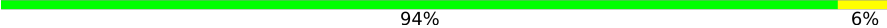


- Molecule 1: 29 kDa antigen, Cfp29

Chain GB:  95% 5%



- Molecule 1: 29 kDa antigen, Cfp29

Chain HB:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	57805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	163000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.839	Depositor
Minimum map value	0.000	Depositor
Average map value	0.438	Depositor
Map value standard deviation	1.797	Depositor
Recommended contour level	4.8	Depositor
Map size (Å)	320.25598, 320.25598, 320.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83399993, 0.83399993, 0.83399993	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/2074	0.71	0/2828
1	AA	0.44	0/2074	0.71	0/2828
1	AB	0.44	0/2074	0.71	0/2828
1	B	0.44	0/2074	0.71	0/2828
1	BA	0.44	0/2074	0.71	0/2828
1	BB	0.44	0/2074	0.71	0/2828
1	C	0.44	0/2074	0.71	0/2828
1	CA	0.44	0/2074	0.71	0/2828
1	CB	0.44	0/2074	0.71	0/2828
1	D	0.44	0/2074	0.71	0/2828
1	DA	0.45	0/2074	0.71	0/2828
1	DB	0.45	0/2074	0.71	0/2828
1	E	0.44	0/2074	0.71	0/2828
1	EA	0.44	0/2074	0.71	0/2828
1	EB	0.44	0/2074	0.71	0/2828
1	F	0.44	0/2074	0.71	0/2828
1	FA	0.44	0/2074	0.71	0/2828
1	FB	0.44	0/2074	0.71	0/2828
1	G	0.44	0/2074	0.71	0/2828
1	GA	0.44	0/2074	0.71	0/2828
1	GB	0.45	0/2074	0.71	0/2828
1	H	0.44	0/2074	0.71	0/2828
1	HA	0.44	0/2074	0.71	0/2828
1	HB	0.44	0/2074	0.71	0/2828
1	I	0.44	0/2074	0.71	0/2828
1	IA	0.44	0/2074	0.71	0/2828
1	J	0.45	0/2074	0.71	0/2828
1	JA	0.44	0/2074	0.71	0/2828
1	K	0.45	0/2074	0.71	0/2828
1	KA	0.44	0/2074	0.71	0/2828
1	L	0.45	0/2074	0.71	0/2828
1	LA	0.44	0/2074	0.71	0/2828
1	M	0.44	0/2074	0.71	0/2828
1	MA	0.44	0/2074	0.71	0/2828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	N	0.44	0/2074	0.71	0/2828
1	NA	0.44	0/2074	0.71	0/2828
1	O	0.44	0/2074	0.71	0/2828
1	OA	0.44	0/2074	0.71	0/2828
1	P	0.44	0/2074	0.71	0/2828
1	PA	0.44	0/2074	0.71	0/2828
1	Q	0.44	0/2074	0.71	0/2828
1	QA	0.44	0/2074	0.71	0/2828
1	R	0.44	0/2074	0.71	0/2828
1	RA	0.44	0/2074	0.71	0/2828
1	S	0.44	0/2074	0.71	0/2828
1	SA	0.44	0/2074	0.71	0/2828
1	T	0.44	0/2074	0.71	0/2828
1	TA	0.44	0/2074	0.71	0/2828
1	U	0.44	0/2074	0.71	0/2828
1	UA	0.44	0/2074	0.71	0/2828
1	V	0.44	0/2074	0.71	0/2828
1	VA	0.44	0/2074	0.71	0/2828
1	W	0.44	0/2074	0.71	0/2828
1	WA	0.44	0/2074	0.71	0/2828
1	X	0.44	0/2074	0.71	0/2828
1	XA	0.44	0/2074	0.71	0/2828
1	Y	0.45	0/2074	0.71	0/2828
1	YA	0.44	0/2074	0.71	0/2828
1	Z	0.44	0/2074	0.71	0/2828
1	ZA	0.45	0/2074	0.71	0/2828
All	All	0.44	0/124440	0.71	0/169680

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2034	0	2013	9	0
1	AA	2034	0	2013	10	0
1	AB	2034	0	2013	9	0
1	B	2034	0	2013	10	0
1	BA	2034	0	2013	9	0
1	BB	2034	0	2013	9	0
1	C	2034	0	2013	9	0
1	CA	2034	0	2013	9	0
1	CB	2034	0	2013	9	0
1	D	2034	0	2013	10	0
1	DA	2034	0	2013	9	0
1	DB	2034	0	2013	11	0
1	E	2034	0	2013	8	0
1	EA	2034	0	2013	9	0
1	EB	2034	0	2013	8	0
1	F	2034	0	2013	8	0
1	FA	2034	0	2013	9	0
1	FB	2034	0	2013	9	0
1	G	2034	0	2013	10	0
1	GA	2034	0	2013	11	0
1	GB	2034	0	2013	8	0
1	H	2034	0	2013	9	0
1	HA	2034	0	2013	8	0
1	HB	2034	0	2013	10	0
1	I	2034	0	2013	11	0
1	IA	2034	0	2013	8	0
1	J	2034	0	2013	9	0
1	JA	2034	0	2013	9	0
1	K	2034	0	2013	8	0
1	KA	2034	0	2013	9	0
1	L	2034	0	2013	10	0
1	LA	2034	0	2013	10	0
1	M	2034	0	2013	8	0
1	MA	2034	0	2013	8	0
1	N	2034	0	2013	10	0
1	NA	2034	0	2013	8	0
1	O	2034	0	2013	9	0
1	OA	2034	0	2013	9	0
1	P	2034	0	2013	9	0
1	PA	2034	0	2013	10	0
1	Q	2034	0	2013	10	0
1	QA	2034	0	2013	9	0
1	R	2034	0	2013	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	RA	2034	0	2013	10	0
1	S	2034	0	2013	10	0
1	SA	2034	0	2013	9	0
1	T	2034	0	2013	8	0
1	TA	2034	0	2013	10	0
1	U	2034	0	2013	9	0
1	UA	2034	0	2013	9	0
1	V	2034	0	2013	11	0
1	VA	2034	0	2013	9	0
1	W	2034	0	2013	9	0
1	WA	2034	0	2013	8	0
1	X	2034	0	2013	9	0
1	XA	2034	0	2013	10	0
1	Y	2034	0	2013	9	0
1	YA	2034	0	2013	9	0
1	Z	2034	0	2013	9	0
1	ZA	2034	0	2013	10	0
All	All	122040	0	120780	371	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (371) 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:F:189:TYR:CE1	1:HA:197:ARG:HD3	2.48	0.49
1:K:189:TYR:CE1	1:MA:197:ARG:HD3	2.48	0.49
1:N:189:TYR:CE1	1:DA:197:ARG:HD3	2.48	0.49
1:EA:197:ARG:HD3	1:VA:189:TYR:CE1	2.48	0.49
1:IA:189:TYR:CE1	1:KA:197:ARG:HD3	2.48	0.49
1:SA:189:TYR:CE1	1:UA:197:ARG:HD3	2.48	0.49
1:H:189:TYR:CE1	1:YA:197:ARG:HD3	2.48	0.49
1:I:189:TYR:CE1	1:Y:197:ARG:HD3	2.48	0.49
1:J:197:ARG:HD3	1:BB:189:TYR:CE1	2.48	0.49
1:M:189:TYR:CE1	1:OA:197:ARG:HD3	2.48	0.49
1:O:197:ARG:HD3	1:RA:189:TYR:CE1	2.48	0.49
1:S:197:ARG:HD3	1:YA:189:TYR:CE1	2.48	0.49
1:FA:197:ARG:HD3	1:NA:189:TYR:CE1	2.48	0.49
1:JA:197:ARG:HD3	1:FB:189:TYR:CE1	2.48	0.49
1:A:189:TYR:CE1	1:X:197:ARG:HD3	2.48	0.49
1:D:197:ARG:HD3	1:OA:189:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:189:TYR:CE1	1:Q:197:ARG:HD3	2.48	0.49
1:CB:189:TYR:CE1	1:EB:197:ARG:HD3	2.48	0.49
1:C:189:TYR:CE1	1:TA:197:ARG:HD3	2.48	0.49
1:P:189:TYR:CE1	1:CA:197:ARG:HD3	2.48	0.49
1:R:189:TYR:CE1	1:DB:197:ARG:HD3	2.48	0.49
1:U:189:TYR:CE1	1:RA:197:ARG:HD3	2.48	0.49
1:Z:189:TYR:CE1	1:BB:197:ARG:HD3	2.48	0.49
1:B:189:TYR:CE1	1:QA:197:ARG:HD3	2.48	0.49
1:B:197:ARG:HD3	1:J:189:TYR:CE1	2.48	0.49
1:Q:189:TYR:CE1	1:AB:197:ARG:HD3	2.48	0.49
1:X:189:TYR:CE1	1:CB:197:ARG:HD3	2.48	0.49
1:CA:189:TYR:CE1	1:SA:197:ARG:HD3	2.48	0.49
1:GA:197:ARG:HD3	1:EB:189:TYR:CE1	2.48	0.49
1:HA:189:TYR:CE1	1:XA:197:ARG:HD3	2.48	0.49
1:LA:197:ARG:HD3	1:UA:189:TYR:CE1	2.48	0.49
1:G:189:TYR:CE1	1:FB:197:ARG:HD3	2.48	0.49
1:L:189:TYR:CE1	1:VA:197:ARG:HD3	2.48	0.49
1:MA:189:TYR:CE1	1:HB:197:ARG:HD3	2.48	0.49
1:K:197:ARG:HD3	1:BA:189:TYR:CE1	2.48	0.48
1:ZA:197:ARG:HD3	1:HB:189:TYR:CE1	2.48	0.48
1:F:197:ARG:HD3	1:W:189:TYR:CE1	2.48	0.48
1:P:197:ARG:HD3	1:LA:189:TYR:CE1	2.48	0.48
1:S:189:TYR:CE1	1:NA:197:ARG:HD3	2.48	0.48
1:A:197:ARG:HD3	1:GA:189:TYR:CE1	2.48	0.48
1:D:189:TYR:CE1	1:IA:197:ARG:HD3	2.48	0.48
1:H:197:ARG:HD3	1:FA:189:TYR:CE1	2.48	0.48
1:M:197:ARG:HD3	1:KA:189:TYR:CE1	2.48	0.48
1:I:197:ARG:HD3	1:DB:189:TYR:CE1	2.48	0.48
1:N:197:ARG:HD3	1:TA:189:TYR:CE1	2.48	0.48
1:Y:189:TYR:CE1	1:AA:197:ARG:HD3	2.48	0.48
1:EA:189:TYR:CE1	1:GB:197:ARG:HD3	2.48	0.48
1:PA:197:ARG:HD3	1:XA:189:TYR:CE1	2.48	0.48
1:U:197:ARG:HD3	1:AB:189:TYR:CE1	2.48	0.48
1:T:197:ARG:HD3	1:GB:189:TYR:CE1	2.48	0.48
1:V:197:ARG:HD3	1:DA:189:TYR:CE1	2.48	0.48
1:JA:189:TYR:CE1	1:WA:197:ARG:HD3	2.48	0.48
1:E:197:ARG:HD3	1:WA:189:TYR:CE1	2.48	0.48
1:R:197:ARG:HD3	1:AA:189:TYR:CE1	2.48	0.48
1:Z:197:ARG:HD3	1:QA:189:TYR:CE1	2.48	0.48
1:C:197:ARG:HD3	1:V:189:TYR:CE1	2.48	0.48
1:EB:143:PRO:HD3	1:EB:152:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:ARG:HD3	1:T:189:TYR:CE1	2.48	0.48
1:UA:143:PRO:HD3	1:UA:152:VAL:HG21	1.96	0.48
1:E:143:PRO:HD3	1:E:152:VAL:HG21	1.96	0.47
1:E:189:TYR:CE1	1:G:197:ARG:HD3	2.48	0.47
1:T:143:PRO:HD3	1:T:152:VAL:HG21	1.96	0.47
1:W:143:PRO:HD3	1:W:152:VAL:HG21	1.96	0.47
1:W:197:ARG:HD3	1:PA:189:TYR:CE1	2.48	0.47
1:B:143:PRO:HD3	1:B:152:VAL:HG21	1.96	0.47
1:I:143:PRO:HD3	1:I:152:VAL:HG21	1.96	0.47
1:BA:143:PRO:HD3	1:BA:152:VAL:HG21	1.96	0.47
1:JA:143:PRO:HD3	1:JA:152:VAL:HG21	1.96	0.47
1:RA:143:PRO:HD3	1:RA:152:VAL:HG21	1.96	0.47
1:N:143:PRO:HD3	1:N:152:VAL:HG21	1.96	0.47
1:Q:143:PRO:HD3	1:Q:152:VAL:HG21	1.96	0.47
1:U:143:PRO:HD3	1:U:152:VAL:HG21	1.96	0.47
1:BA:197:ARG:HD3	1:ZA:189:TYR:CE1	2.48	0.47
1:EA:143:PRO:HD3	1:EA:152:VAL:HG21	1.96	0.47
1:MA:143:PRO:HD3	1:MA:152:VAL:HG21	1.96	0.47
1:BB:143:PRO:HD3	1:BB:152:VAL:HG21	1.96	0.47
1:Z:143:PRO:HD3	1:Z:152:VAL:HG21	1.96	0.47
1:CA:143:PRO:HD3	1:CA:152:VAL:HG21	1.96	0.47
1:HA:143:PRO:HD3	1:HA:152:VAL:HG21	1.96	0.47
1:PA:143:PRO:HD3	1:PA:152:VAL:HG21	1.96	0.47
1:K:143:PRO:HD3	1:K:152:VAL:HG21	1.96	0.47
1:X:143:PRO:HD3	1:X:152:VAL:HG21	1.96	0.47
1:GA:143:PRO:HD3	1:GA:152:VAL:HG21	1.96	0.47
1:ZA:143:PRO:HD3	1:ZA:152:VAL:HG21	1.96	0.47
1:J:143:PRO:HD3	1:J:152:VAL:HG21	1.96	0.47
1:LA:143:PRO:HD3	1:LA:152:VAL:HG21	1.96	0.47
1:TA:143:PRO:HD3	1:TA:152:VAL:HG21	1.96	0.47
1:DB:143:PRO:HD3	1:DB:152:VAL:HG21	1.96	0.47
1:F:143:PRO:HD3	1:F:152:VAL:HG21	1.96	0.47
1:O:143:PRO:HD3	1:O:152:VAL:HG21	1.97	0.47
1:SA:143:PRO:HD3	1:SA:152:VAL:HG21	1.96	0.47
1:CB:143:PRO:HD3	1:CB:152:VAL:HG21	1.96	0.47
1:XA:143:PRO:HD3	1:XA:152:VAL:HG21	1.96	0.47
1:HB:143:PRO:HD3	1:HB:152:VAL:HG21	1.96	0.47
1:R:143:PRO:HD3	1:R:152:VAL:HG21	1.96	0.47
1:Y:143:PRO:HD3	1:Y:152:VAL:HG21	1.96	0.47
1:C:143:PRO:HD3	1:C:152:VAL:HG21	1.96	0.47
1:DA:143:PRO:HD3	1:DA:152:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:143:PRO:HD3	1:M:152:VAL:HG21	1.96	0.46
1:V:143:PRO:HD3	1:V:152:VAL:HG21	1.96	0.46
1:AA:143:PRO:HD3	1:AA:152:VAL:HG21	1.96	0.46
1:H:143:PRO:HD3	1:H:152:VAL:HG21	1.96	0.46
1:WA:143:PRO:HD3	1:WA:152:VAL:HG21	1.96	0.46
1:GB:143:PRO:HD3	1:GB:152:VAL:HG21	1.96	0.46
1:QA:143:PRO:HD3	1:QA:152:VAL:HG21	1.96	0.46
1:P:143:PRO:HD3	1:P:152:VAL:HG21	1.96	0.46
1:D:143:PRO:HD3	1:D:152:VAL:HG21	1.96	0.46
1:S:143:PRO:HD3	1:S:152:VAL:HG21	1.96	0.46
1:OA:143:PRO:HD3	1:OA:152:VAL:HG21	1.96	0.46
1:YA:143:PRO:HD3	1:YA:152:VAL:HG21	1.96	0.46
1:AB:143:PRO:HD3	1:AB:152:VAL:HG21	1.96	0.46
1:A:143:PRO:HD3	1:A:152:VAL:HG21	1.96	0.46
1:G:143:PRO:HD3	1:G:152:VAL:HG21	1.96	0.46
1:FA:143:PRO:HD3	1:FA:152:VAL:HG21	1.96	0.46
1:VA:143:PRO:HD3	1:VA:152:VAL:HG21	1.96	0.46
1:L:143:PRO:HD3	1:L:152:VAL:HG21	1.96	0.46
1:IA:143:PRO:HD3	1:IA:152:VAL:HG21	1.97	0.46
1:KA:143:PRO:HD3	1:KA:152:VAL:HG21	1.96	0.46
1:NA:143:PRO:HD3	1:NA:152:VAL:HG21	1.96	0.46
1:FB:143:PRO:HD3	1:FB:152:VAL:HG21	1.96	0.46
1:N:55:LEU:HD22	1:N:68:HIS:HB3	2.01	0.43
1:U:55:LEU:HD22	1:U:68:HIS:HB3	2.01	0.43
1:Z:55:LEU:HD22	1:Z:68:HIS:HB3	2.01	0.43
1:AA:55:LEU:HD22	1:AA:68:HIS:HB3	2.01	0.43
1:I:55:LEU:HD22	1:I:68:HIS:HB3	2.01	0.43
1:V:55:LEU:HD22	1:V:68:HIS:HB3	2.01	0.43
1:UA:55:LEU:HD22	1:UA:68:HIS:HB3	2.01	0.43
1:XA:55:LEU:HD22	1:XA:68:HIS:HB3	2.01	0.43
1:HB:55:LEU:HD22	1:HB:68:HIS:HB3	2.01	0.43
1:C:55:LEU:HD22	1:C:68:HIS:HB3	2.01	0.43
1:H:55:LEU:HD22	1:H:68:HIS:HB3	2.01	0.43
1:M:55:LEU:HD22	1:M:68:HIS:HB3	2.01	0.43
1:R:55:LEU:HD22	1:R:68:HIS:HB3	2.01	0.43
1:EB:55:LEU:HD22	1:EB:68:HIS:HB3	2.01	0.43
1:E:55:LEU:HD22	1:E:68:HIS:HB3	2.01	0.43
1:T:55:LEU:HD22	1:T:68:HIS:HB3	2.01	0.43
1:B:55:LEU:HD22	1:B:68:HIS:HB3	2.01	0.43
1:DA:55:LEU:HD22	1:DA:68:HIS:HB3	2.01	0.43
1:Q:55:LEU:HD22	1:Q:68:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:55:LEU:HD22	1:W:68:HIS:HB3	2.01	0.42
1:Y:55:LEU:HD22	1:Y:68:HIS:HB3	2.01	0.42
1:BA:55:LEU:HD22	1:BA:68:HIS:HB3	2.01	0.42
1:GA:55:LEU:HD22	1:GA:68:HIS:HB3	2.01	0.42
1:LA:55:LEU:HD22	1:LA:68:HIS:HB3	2.01	0.42
1:C:154:SER:OG	1:V:183:GLU:HG2	2.20	0.42
1:F:55:LEU:HD22	1:F:68:HIS:HB3	2.01	0.42
1:K:55:LEU:HD22	1:K:68:HIS:HB3	2.01	0.42
1:GA:154:SER:OG	1:EB:183:GLU:HG2	2.20	0.42
1:LA:154:SER:OG	1:UA:183:GLU:HG2	2.20	0.42
1:MA:183:GLU:HG2	1:HB:154:SER:OG	2.20	0.42
1:D:46:VAL:HA	1:TA:94:ARG:O	2.20	0.42
1:E:46:VAL:HA	1:IA:94:ARG:O	2.20	0.42
1:I:46:VAL:HA	1:YA:94:ARG:O	2.20	0.42
1:T:154:SER:OG	1:GB:183:GLU:HG2	2.20	0.42
1:FA:46:VAL:HA	1:GB:94:ARG:O	2.20	0.42
1:HA:55:LEU:HD22	1:HA:68:HIS:HB3	2.01	0.42
1:HA:183:GLU:HG2	1:XA:154:SER:OG	2.20	0.42
1:KA:46:VAL:HA	1:WA:94:ARG:O	2.20	0.42
1:MA:55:LEU:HD22	1:MA:68:HIS:HB3	2.01	0.42
1:OA:55:LEU:HD22	1:OA:68:HIS:HB3	2.01	0.42
1:WA:55:LEU:HD22	1:WA:68:HIS:HB3	2.01	0.42
1:YA:55:LEU:HD22	1:YA:68:HIS:HB3	2.01	0.42
1:GB:55:LEU:HD22	1:GB:68:HIS:HB3	2.01	0.42
1:E:154:SER:OG	1:WA:183:GLU:HG2	2.20	0.42
1:F:94:ARG:O	1:X:46:VAL:HA	2.20	0.42
1:H:94:ARG:O	1:GA:46:VAL:HA	2.20	0.42
1:M:94:ARG:O	1:LA:46:VAL:HA	2.20	0.42
1:N:46:VAL:HA	1:OA:94:ARG:O	2.20	0.42
1:N:94:ARG:O	1:UA:46:VAL:HA	2.20	0.42
1:O:154:SER:OG	1:RA:183:GLU:HG2	2.20	0.42
1:R:154:SER:OG	1:AA:183:GLU:HG2	2.20	0.42
1:U:183:GLU:HG2	1:RA:154:SER:OG	2.20	0.42
1:Y:46:VAL:HA	1:CB:94:ARG:O	2.20	0.42
1:Z:183:GLU:HG2	1:BB:154:SER:OG	2.20	0.42
1:DA:46:VAL:HA	1:SA:94:ARG:O	2.20	0.42
1:DB:55:LEU:HD22	1:DB:68:HIS:HB3	2.01	0.42
1:A:94:ARG:O	1:HA:46:VAL:HA	2.20	0.42
1:B:183:GLU:HG2	1:QA:154:SER:OG	2.20	0.42
1:D:154:SER:OG	1:OA:183:GLU:HG2	2.20	0.42
1:I:94:ARG:O	1:EB:46:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:SER:OG	1:BB:183:GLU:HG2	2.20	0.42
1:P:94:ARG:O	1:MA:46:VAL:HA	2.20	0.42
1:S:46:VAL:HA	1:DB:94:ARG:O	2.20	0.42
1:S:154:SER:OG	1:YA:183:GLU:HG2	2.20	0.42
1:T:46:VAL:HA	1:NA:94:ARG:O	2.20	0.42
1:KA:55:LEU:HD22	1:KA:68:HIS:HB3	2.01	0.42
1:A:46:VAL:HA	1:G:94:ARG:O	2.20	0.42
1:G:183:GLU:HG2	1:FB:154:SER:OG	2.20	0.42
1:K:94:ARG:O	1:CA:46:VAL:HA	2.20	0.42
1:L:183:GLU:HG2	1:VA:154:SER:OG	2.20	0.42
1:N:183:GLU:HG2	1:DA:154:SER:OG	2.20	0.42
1:W:154:SER:OG	1:PA:183:GLU:HG2	2.20	0.42
1:X:55:LEU:HD22	1:X:68:HIS:HB3	2.01	0.42
1:SA:55:LEU:HD22	1:SA:68:HIS:HB3	2.01	0.42
1:TA:55:LEU:HD22	1:TA:68:HIS:HB3	2.01	0.42
1:A:154:SER:OG	1:GA:183:GLU:HG2	2.20	0.42
1:A:183:GLU:HG2	1:X:154:SER:OG	2.20	0.42
1:C:94:ARG:O	1:W:46:VAL:HA	2.20	0.42
1:I:183:GLU:HG2	1:Y:154:SER:OG	2.20	0.42
1:P:154:SER:OG	1:LA:183:GLU:HG2	2.20	0.42
1:P:183:GLU:HG2	1:CA:154:SER:OG	2.20	0.42
1:Q:183:GLU:HG2	1:AB:154:SER:OG	2.20	0.42
1:R:94:ARG:O	1:BA:46:VAL:HA	2.20	0.42
1:S:55:LEU:HD22	1:S:68:HIS:HB3	2.01	0.42
1:V:154:SER:OG	1:DA:183:GLU:HG2	2.20	0.42
1:Y:183:GLU:HG2	1:AA:154:SER:OG	2.20	0.42
1:BA:154:SER:OG	1:ZA:183:GLU:HG2	2.20	0.42
1:CA:55:LEU:HD22	1:CA:68:HIS:HB3	2.01	0.42
1:EA:55:LEU:HD22	1:EA:68:HIS:HB3	2.01	0.42
1:FA:55:LEU:HD22	1:FA:68:HIS:HB3	2.01	0.42
1:IA:46:VAL:HA	1:XA:94:ARG:O	2.20	0.42
1:PA:154:SER:OG	1:XA:183:GLU:HG2	2.20	0.42
1:SA:183:GLU:HG2	1:UA:154:SER:OG	2.20	0.42
1:ZA:154:SER:OG	1:HB:183:GLU:HG2	2.20	0.42
1:CB:55:LEU:HD22	1:CB:68:HIS:HB3	2.01	0.42
1:C:46:VAL:HA	1:QA:94:ARG:O	2.20	0.42
1:F:183:GLU:HG2	1:HA:154:SER:OG	2.20	0.42
1:G:46:VAL:HA	1:HA:94:ARG:O	2.20	0.42
1:O:183:GLU:HG2	1:Q:154:SER:OG	2.20	0.42
1:R:46:VAL:HA	1:AB:94:ARG:O	2.20	0.42
1:JA:55:LEU:HD22	1:JA:68:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NA:46:VAL:HA	1:HB:94:ARG:O	2.20	0.42
1:CB:183:GLU:HG2	1:EB:154:SER:OG	2.20	0.42
1:D:55:LEU:HD22	1:D:68:HIS:HB3	2.01	0.42
1:H:154:SER:OG	1:FA:183:GLU:HG2	2.20	0.42
1:K:183:GLU:HG2	1:MA:154:SER:OG	2.20	0.42
1:L:46:VAL:HA	1:MA:94:ARG:O	2.20	0.42
1:L:94:ARG:O	1:P:46:VAL:HA	2.20	0.42
1:O:55:LEU:HD22	1:O:68:HIS:HB3	2.01	0.42
1:CA:183:GLU:HG2	1:SA:154:SER:OG	2.20	0.42
1:OA:46:VAL:HA	1:UA:94:ARG:O	2.20	0.42
1:ZA:55:LEU:HD22	1:ZA:68:HIS:HB3	2.01	0.42
1:B:154:SER:OG	1:J:183:GLU:HG2	2.20	0.42
1:J:55:LEU:HD22	1:J:68:HIS:HB3	2.01	0.42
1:M:154:SER:OG	1:KA:183:GLU:HG2	2.20	0.42
1:X:183:GLU:HG2	1:CB:154:SER:OG	2.20	0.42
1:EA:94:ARG:O	1:WA:46:VAL:HA	2.20	0.42
1:PA:55:LEU:HD22	1:PA:68:HIS:HB3	2.01	0.42
1:YA:46:VAL:HA	1:EB:94:ARG:O	2.20	0.42
1:F:154:SER:OG	1:W:183:GLU:HG2	2.20	0.41
1:M:46:VAL:HA	1:VA:94:ARG:O	2.20	0.41
1:V:94:ARG:O	1:Z:46:VAL:HA	2.20	0.41
1:PA:94:ARG:O	1:TA:46:VAL:HA	2.20	0.41
1:VA:55:LEU:HD22	1:VA:68:HIS:HB3	2.01	0.41
1:ZA:94:ARG:O	1:DB:46:VAL:HA	2.20	0.41
1:FB:55:LEU:HD22	1:FB:68:HIS:HB3	2.01	0.41
1:H:46:VAL:HA	1:FB:94:ARG:O	2.20	0.41
1:I:154:SER:OG	1:DB:183:GLU:HG2	2.20	0.41
1:K:154:SER:OG	1:BA:183:GLU:HG2	2.20	0.41
1:P:55:LEU:HD22	1:P:68:HIS:HB3	2.01	0.41
1:U:46:VAL:HA	1:AA:94:ARG:O	2.20	0.41
1:W:94:ARG:O	1:QA:46:VAL:HA	2.20	0.41
1:FA:154:SER:OG	1:NA:183:GLU:HG2	2.20	0.41
1:IA:183:GLU:HG2	1:KA:154:SER:OG	2.20	0.41
1:JA:94:ARG:O	1:GB:46:VAL:HA	2.20	0.41
1:NA:55:LEU:HD22	1:NA:68:HIS:HB3	2.01	0.41
1:BB:55:LEU:HD22	1:BB:68:HIS:HB3	2.01	0.41
1:A:55:LEU:HD22	1:A:68:HIS:HB3	2.01	0.41
1:G:55:LEU:HD22	1:G:68:HIS:HB3	2.01	0.41
1:J:46:VAL:HA	1:Y:94:ARG:O	2.20	0.41
1:N:154:SER:OG	1:TA:183:GLU:HG2	2.20	0.41
1:AA:46:VAL:HA	1:BB:94:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:55:LEU:HD22	1:QA:68:HIS:HB3	2.01	0.41
1:RA:55:LEU:HD22	1:RA:68:HIS:HB3	2.01	0.41
1:AB:55:LEU:HD22	1:AB:68:HIS:HB3	2.01	0.41
1:B:94:ARG:O	1:F:46:VAL:HA	2.20	0.41
1:K:46:VAL:HA	1:Q:94:ARG:O	2.20	0.41
1:L:55:LEU:HD22	1:L:68:HIS:HB3	2.01	0.41
1:BA:94:ARG:O	1:AB:46:VAL:HA	2.20	0.41
1:L:154:SER:OG	1:T:183:GLU:HG2	2.20	0.41
1:O:46:VAL:HA	1:DA:94:ARG:O	2.20	0.41
1:Q:46:VAL:HA	1:CA:94:ARG:O	2.20	0.41
1:R:183:GLU:HG2	1:DB:154:SER:OG	2.20	0.41
1:U:154:SER:OG	1:AB:183:GLU:HG2	2.20	0.41
1:V:46:VAL:HA	1:RA:94:ARG:O	2.20	0.41
1:Z:94:ARG:O	1:RA:46:VAL:HA	2.20	0.41
1:IA:55:LEU:HD22	1:IA:68:HIS:HB3	2.01	0.41
1:C:183:GLU:HG2	1:TA:154:SER:OG	2.20	0.41
1:E:183:GLU:HG2	1:G:154:SER:OG	2.20	0.41
1:B:46:VAL:HA	1:X:94:ARG:O	2.20	0.41
1:E:94:ARG:O	1:XA:46:VAL:HA	2.20	0.41
1:H:183:GLU:HG2	1:YA:154:SER:OG	2.20	0.41
1:J:94:ARG:O	1:CB:46:VAL:HA	2.20	0.41
1:M:183:GLU:HG2	1:OA:154:SER:OG	2.20	0.41
1:O:94:ARG:O	1:SA:46:VAL:HA	2.20	0.41
1:T:94:ARG:O	1:HB:46:VAL:HA	2.20	0.41
1:U:94:ARG:O	1:BB:46:VAL:HA	2.20	0.41
1:Z:154:SER:OG	1:QA:183:GLU:HG2	2.20	0.41
1:EA:154:SER:OG	1:VA:183:GLU:HG2	2.20	0.41
1:JA:154:SER:OG	1:FB:183:GLU:HG2	2.20	0.41
1:LA:94:ARG:O	1:VA:46:VAL:HA	2.20	0.41
1:D:94:ARG:O	1:PA:46:VAL:HA	2.20	0.41
1:S:94:ARG:O	1:ZA:46:VAL:HA	2.20	0.41
1:EA:46:VAL:HA	1:KA:94:ARG:O	2.20	0.41
1:FA:94:ARG:O	1:JA:46:VAL:HA	2.20	0.41
1:GA:94:ARG:O	1:FB:46:VAL:HA	2.20	0.41
1:HB:28:LYS:HB2	1:HB:28:LYS:HE2	1.96	0.41
1:D:183:GLU:HG2	1:IA:154:SER:OG	2.20	0.41
1:S:60:ALA:HA	1:S:61:PRO:HD3	1.99	0.41
1:S:183:GLU:HG2	1:NA:154:SER:OG	2.20	0.41
1:EA:183:GLU:HG2	1:GB:154:SER:OG	2.20	0.41
1:JA:183:GLU:HG2	1:WA:154:SER:OG	2.20	0.41
1:DB:28:LYS:HB2	1:DB:28:LYS:HE2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LYS:HB2	1:G:28:LYS:HE2	1.96	0.41
1:N:193:GLU:O	1:N:197:ARG:HG3	2.21	0.41
1:RA:193:GLU:O	1:RA:197:ARG:HG3	2.21	0.41
1:SA:193:GLU:O	1:SA:197:ARG:HG3	2.21	0.41
1:DB:36:VAL:HG11	1:DB:172:LEU:HD11	2.04	0.41
1:J:193:GLU:O	1:J:197:ARG:HG3	2.22	0.40
1:L:28:LYS:HB2	1:L:28:LYS:HE2	1.96	0.40
1:O:193:GLU:O	1:O:197:ARG:HG3	2.22	0.40
1:V:28:LYS:HB2	1:V:28:LYS:HE2	1.96	0.40
1:LA:36:VAL:HG11	1:LA:172:LEU:HD11	2.04	0.40
1:TA:36:VAL:HG11	1:TA:172:LEU:HD11	2.04	0.40
1:CB:193:GLU:O	1:CB:197:ARG:HG3	2.22	0.40
1:B:36:VAL:HG11	1:B:172:LEU:HD11	2.04	0.40
1:C:193:GLU:O	1:C:197:ARG:HG3	2.22	0.40
1:D:60:ALA:HA	1:D:61:PRO:HD3	1.99	0.40
1:I:193:GLU:O	1:I:197:ARG:HG3	2.22	0.40
1:R:193:GLU:O	1:R:197:ARG:HG3	2.22	0.40
1:U:193:GLU:O	1:U:197:ARG:HG3	2.21	0.40
1:W:193:GLU:O	1:W:197:ARG:HG3	2.22	0.40
1:Z:193:GLU:O	1:Z:197:ARG:HG3	2.21	0.40
1:GA:36:VAL:HG11	1:GA:172:LEU:HD11	2.04	0.40
1:VA:36:VAL:HG11	1:VA:172:LEU:HD11	2.04	0.40
1:XA:28:LYS:HB2	1:XA:28:LYS:HE2	1.96	0.40
1:XA:36:VAL:HG11	1:XA:172:LEU:HD11	2.04	0.40
1:BB:193:GLU:O	1:BB:197:ARG:HG3	2.22	0.40
1:FB:36:VAL:HG11	1:FB:172:LEU:HD11	2.04	0.40
1:HB:36:VAL:HG11	1:HB:172:LEU:HD11	2.04	0.40
1:B:60:ALA:HA	1:B:61:PRO:HD3	1.99	0.40
1:Q:36:VAL:HG11	1:Q:172:LEU:HD11	2.04	0.40
1:Q:60:ALA:HA	1:Q:61:PRO:HD3	1.99	0.40
1:V:36:VAL:HG11	1:V:172:LEU:HD11	2.04	0.40
1:X:60:ALA:HA	1:X:61:PRO:HD3	1.99	0.40
1:AA:36:VAL:HG11	1:AA:172:LEU:HD11	2.04	0.40
1:AA:193:GLU:O	1:AA:197:ARG:HG3	2.22	0.40
1:BA:193:GLU:O	1:BA:197:ARG:HG3	2.22	0.40
1:FA:193:GLU:O	1:FA:197:ARG:HG3	2.22	0.40
1:GA:193:GLU:O	1:GA:197:ARG:HG3	2.22	0.40
1:KA:193:GLU:O	1:KA:197:ARG:HG3	2.22	0.40
1:QA:193:GLU:O	1:QA:197:ARG:HG3	2.22	0.40
1:YA:193:GLU:O	1:YA:197:ARG:HG3	2.21	0.40
1:D:193:GLU:O	1:D:197:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:GLU:O	1:G:197:ARG:HG3	2.22	0.40
1:I:84:LEU:HD23	1:I:84:LEU:HA	1.93	0.40
1:L:193:GLU:O	1:L:197:ARG:HG3	2.22	0.40
1:V:193:GLU:O	1:V:197:ARG:HG3	2.22	0.40
1:EA:193:GLU:O	1:EA:197:ARG:HG3	2.22	0.40
1:GA:34:ARG:HH11	1:GA:34:ARG:HD3	1.77	0.40
1:JA:193:GLU:O	1:JA:197:ARG:HG3	2.22	0.40
1:LA:193:GLU:O	1:LA:197:ARG:HG3	2.22	0.40
1:OA:193:GLU:O	1:OA:197:ARG:HG3	2.22	0.40
1:RA:60:ALA:HA	1:RA:61:PRO:HD3	1.99	0.40
1:TA:193:GLU:O	1:TA:197:ARG:HG3	2.22	0.40
1:AB:193:GLU:O	1:AB:197:ARG:HG3	2.22	0.40
1:A:36:VAL:HG11	1:A:172:LEU:HD11	2.04	0.40
1:H:36:VAL:HG11	1:H:172:LEU:HD11	2.04	0.40
1:I:36:VAL:HG11	1:I:172:LEU:HD11	2.04	0.40
1:N:36:VAL:HG11	1:N:172:LEU:HD11	2.04	0.40
1:P:36:VAL:HG11	1:P:172:LEU:HD11	2.04	0.40
1:S:193:GLU:O	1:S:197:ARG:HG3	2.22	0.40
1:Y:36:VAL:HG11	1:Y:172:LEU:HD11	2.04	0.40
1:CA:60:ALA:HA	1:CA:61:PRO:HD3	1.99	0.40
1:DA:36:VAL:HG11	1:DA:172:LEU:HD11	2.04	0.40
1:PA:36:VAL:HG11	1:PA:172:LEU:HD11	2.04	0.40
1:PA:193:GLU:O	1:PA:197:ARG:HG3	2.22	0.40
1:UA:193:GLU:O	1:UA:197:ARG:HG3	2.22	0.40
1:ZA:36:VAL:HG11	1:ZA:172:LEU:HD11	2.04	0.40
1:ZA:193:GLU:O	1:ZA:197:ARG:HG3	2.21	0.40
1:DB:193:GLU:O	1:DB:197:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	B	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	BA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	BB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	C	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	CA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	CB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	D	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	DA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	DB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	E	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	EA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	EB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	F	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	FA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	FB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	G	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	GA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	GB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	H	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	HA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	HB	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	I	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	IA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	J	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	JA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	K	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	KA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	L	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	LA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	MA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	N	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	NA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	O	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	OA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	P	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	PA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Q	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	QA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	R	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	RA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	S	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	SA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	T	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	TA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	U	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	UA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	V	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	VA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	W	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	WA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	X	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	XA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Y	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	YA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Z	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	ZA	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
All	All	15780/15900 (99%)	15540 (98%)	240 (2%)	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	A	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	AA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	AB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	B	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	BA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	BB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	C	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	CA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	CB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	D	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	DA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	DB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	E	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	EA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	EB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	F	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	FA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	FB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	G	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	GA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	GB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	H	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	HA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	HB	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	I	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	IA	218/218 (100%)	216 (99%)	2 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	JA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	K	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	KA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	L	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	LA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	M	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	MA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	N	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	NA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	O	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	OA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	P	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	PA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	Q	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	QA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	R	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	RA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	S	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	SA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	T	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	TA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	U	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	UA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	V	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	VA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	W	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	WA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	X	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	XA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	Y	218/218 (100%)	216 (99%)	2 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	YA	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	Z	218/218 (100%)	216 (99%)	2 (1%)	70	84
1	ZA	218/218 (100%)	216 (99%)	2 (1%)	70	84
All	All	13080/13080 (100%)	12960 (99%)	120 (1%)	68	84

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	58	VAL
1	B	54	ARG
1	B	58	VAL
1	C	54	ARG
1	C	58	VAL
1	D	54	ARG
1	D	58	VAL
1	E	54	ARG
1	E	58	VAL
1	F	54	ARG
1	F	58	VAL
1	G	54	ARG
1	G	58	VAL
1	H	54	ARG
1	H	58	VAL
1	I	54	ARG
1	I	58	VAL
1	J	54	ARG
1	J	58	VAL
1	K	54	ARG
1	K	58	VAL
1	L	54	ARG
1	L	58	VAL
1	M	54	ARG
1	M	58	VAL
1	N	54	ARG
1	N	58	VAL
1	O	54	ARG
1	O	58	VAL
1	P	54	ARG
1	P	58	VAL
1	Q	54	ARG

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Mol	Chain	Res	Type
1	Q	58	VAL
1	R	54	ARG
1	R	58	VAL
1	S	54	ARG
1	S	58	VAL
1	T	54	ARG
1	T	58	VAL
1	U	54	ARG
1	U	58	VAL
1	V	54	ARG
1	V	58	VAL
1	W	54	ARG
1	W	58	VAL
1	X	54	ARG
1	X	58	VAL
1	Y	54	ARG
1	Y	58	VAL
1	Z	54	ARG
1	Z	58	VAL
1	AA	54	ARG
1	AA	58	VAL
1	BA	54	ARG
1	BA	58	VAL
1	CA	54	ARG
1	CA	58	VAL
1	DA	54	ARG
1	DA	58	VAL
1	EA	54	ARG
1	EA	58	VAL
1	FA	54	ARG
1	FA	58	VAL
1	GA	54	ARG
1	GA	58	VAL
1	HA	54	ARG
1	HA	58	VAL
1	IA	54	ARG
1	IA	58	VAL
1	JA	54	ARG
1	JA	58	VAL
1	KA	54	ARG
1	KA	58	VAL
1	LA	54	ARG

Continued on next page...

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Mol	Chain	Res	Type
1	LA	58	VAL
1	MA	54	ARG
1	MA	58	VAL
1	NA	54	ARG
1	NA	58	VAL
1	OA	54	ARG
1	OA	58	VAL
1	PA	54	ARG
1	PA	58	VAL
1	QA	54	ARG
1	QA	58	VAL
1	RA	54	ARG
1	RA	58	VAL
1	SA	54	ARG
1	SA	58	VAL
1	TA	54	ARG
1	TA	58	VAL
1	UA	54	ARG
1	UA	58	VAL
1	VA	54	ARG
1	VA	58	VAL
1	WA	54	ARG
1	WA	58	VAL
1	XA	54	ARG
1	XA	58	VAL
1	YA	54	ARG
1	YA	58	VAL
1	ZA	54	ARG
1	ZA	58	VAL
1	AB	54	ARG
1	AB	58	VAL
1	BB	54	ARG
1	BB	58	VAL
1	CB	54	ARG
1	CB	58	VAL
1	DB	54	ARG
1	DB	58	VAL
1	EB	54	ARG
1	EB	58	VAL
1	FB	54	ARG
1	FB	58	VAL
1	GB	54	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	GB	58	VAL
1	HB	54	ARG
1	HB	58	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	HIS
1	B	265	HIS
1	C	265	HIS
1	D	265	HIS
1	E	265	HIS
1	F	265	HIS
1	G	265	HIS
1	H	265	HIS
1	I	265	HIS
1	J	265	HIS
1	K	265	HIS
1	L	265	HIS
1	M	265	HIS
1	N	265	HIS
1	P	265	HIS
1	Q	265	HIS
1	R	265	HIS
1	S	265	HIS
1	T	265	HIS
1	U	265	HIS
1	V	265	HIS
1	W	265	HIS
1	X	265	HIS
1	Y	265	HIS
1	Z	265	HIS
1	AA	265	HIS
1	BA	265	HIS
1	CA	265	HIS
1	DA	265	HIS
1	EA	265	HIS
1	FA	265	HIS
1	GA	265	HIS
1	HA	265	HIS
1	IA	265	HIS
1	JA	265	HIS

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Mol	Chain	Res	Type
1	KA	265	HIS
1	LA	265	HIS
1	MA	265	HIS
1	OA	265	HIS
1	PA	265	HIS
1	QA	265	HIS
1	RA	265	HIS
1	SA	265	HIS
1	TA	265	HIS
1	UA	265	HIS
1	VA	265	HIS
1	WA	265	HIS
1	XA	265	HIS
1	YA	265	HIS
1	ZA	265	HIS
1	AB	265	HIS
1	BB	265	HIS
1	CB	265	HIS
1	DB	265	HIS
1	EB	265	HIS
1	FB	265	HIS
1	GB	265	HIS
1	HB	265	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.

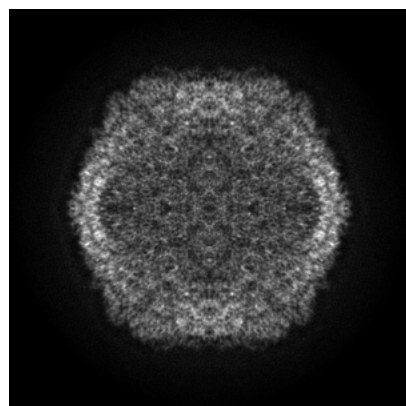
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13164. These allow visual inspection of the internal detail of the map and identification of artifacts.

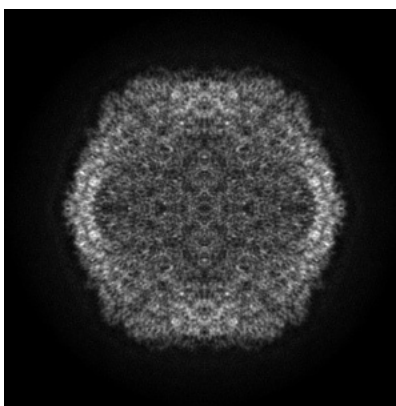
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

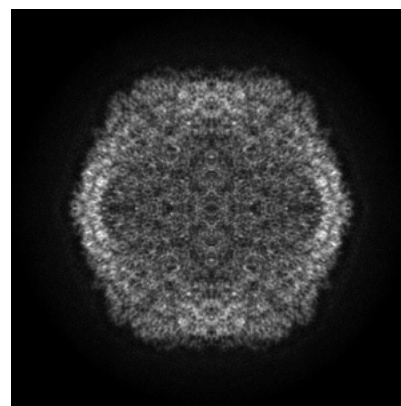
6.1.1 Primary map



X

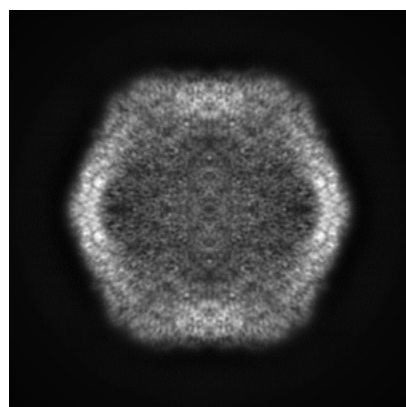


Y

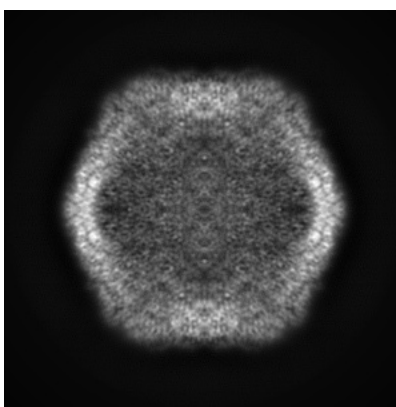


Z

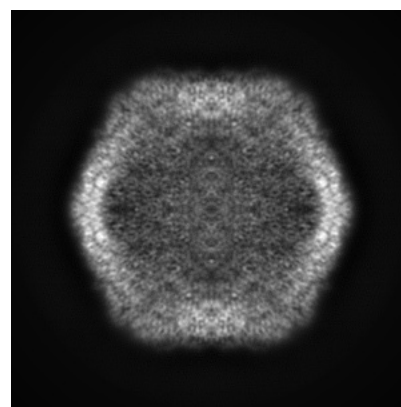
6.1.2 Raw map



X



Y

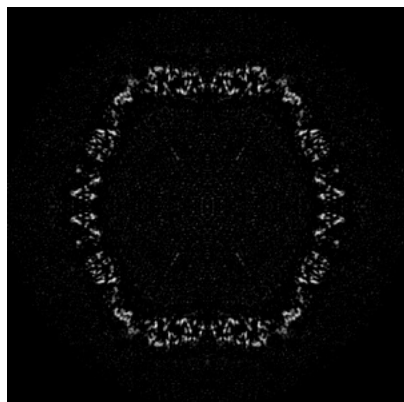


Z

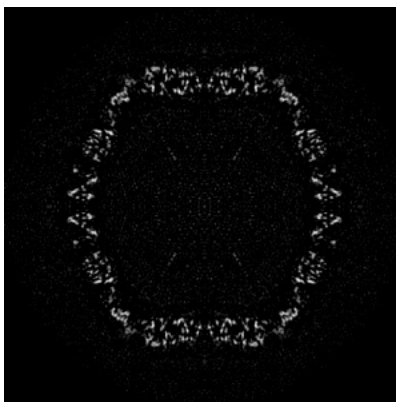
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

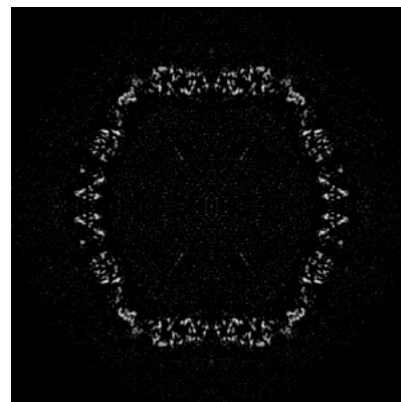
6.2.1 Primary map



X Index: 192

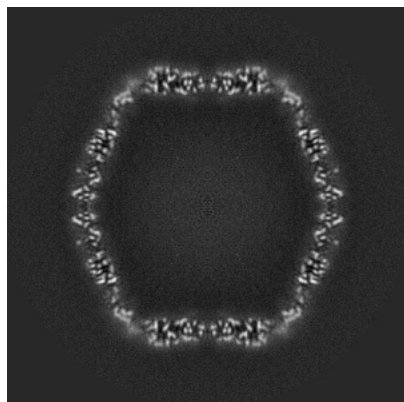


Y Index: 192

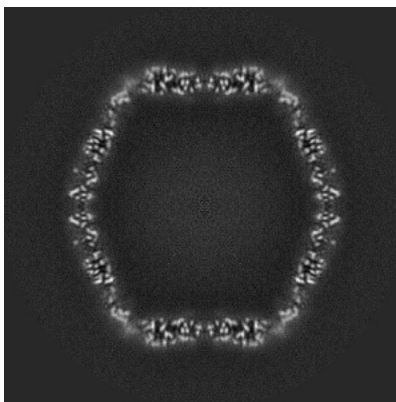


Z Index: 192

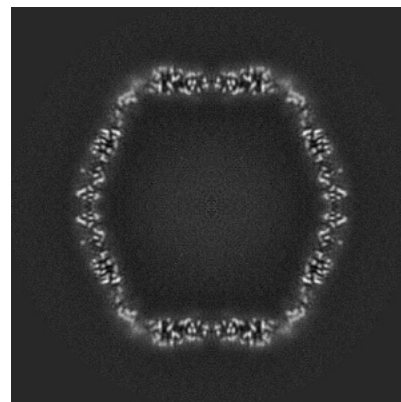
6.2.2 Raw map



X Index: 192



Y Index: 192

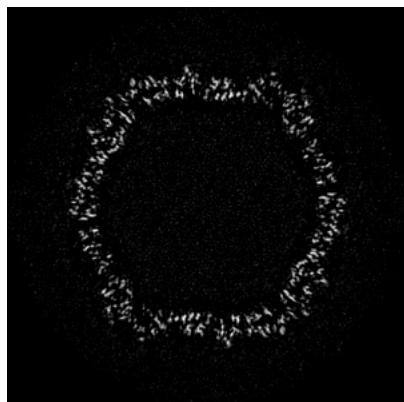


Z Index: 192

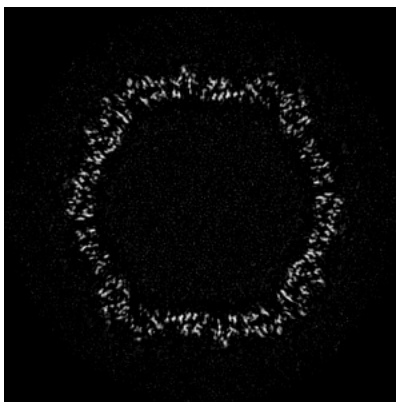
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

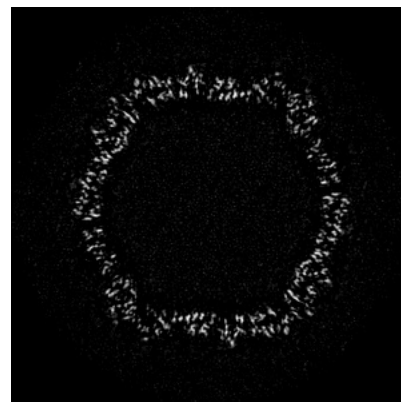
6.3.1 Primary map



X Index: 215

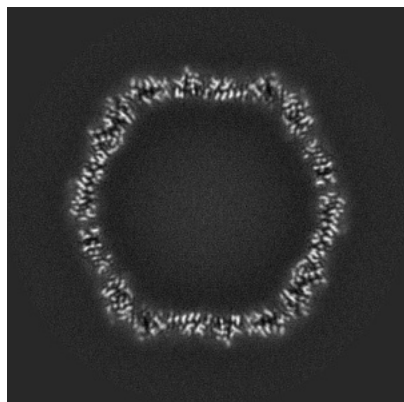


Y Index: 215

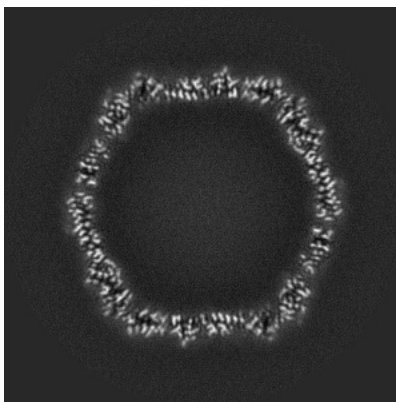


Z Index: 215

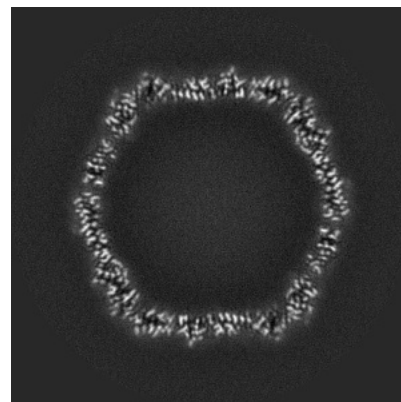
6.3.2 Raw map



X Index: 215



Y Index: 169

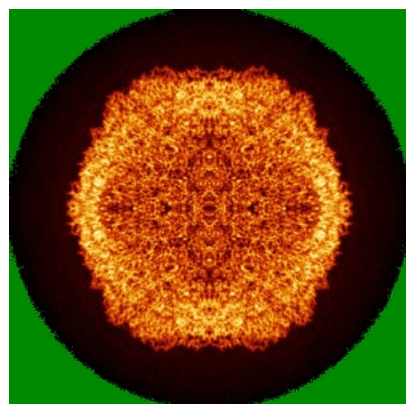


Z Index: 169

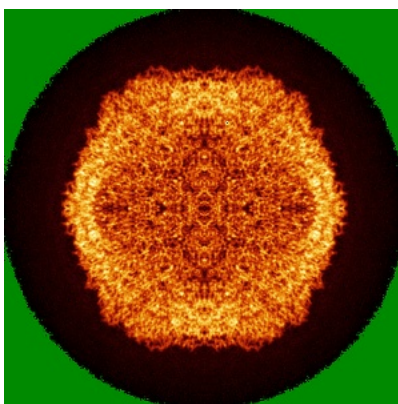
The images above show the largest variance slices of the map in three orthogonal directions.

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

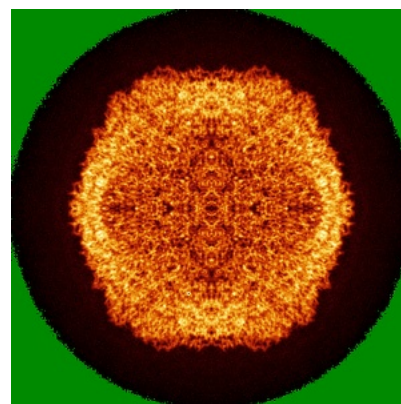
6.4.1 Primary map



X

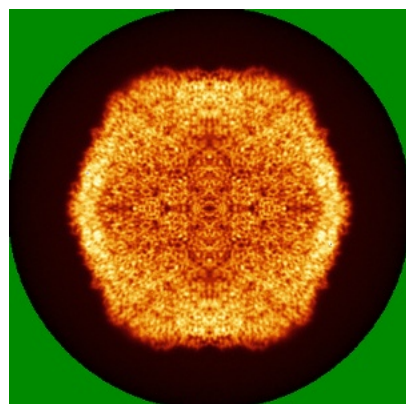


Y

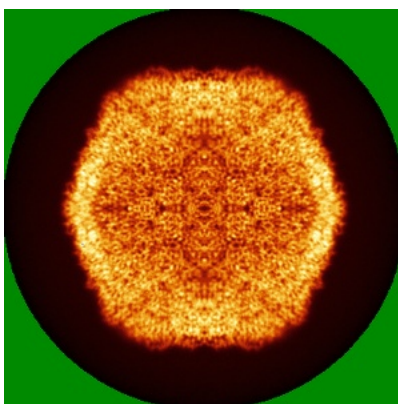


Z

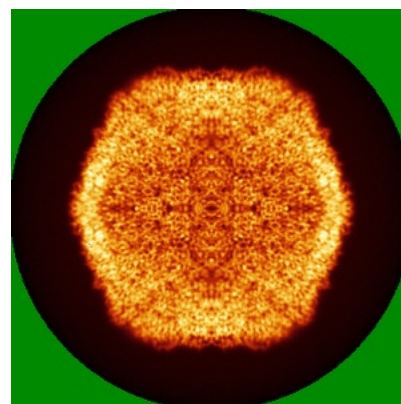
6.4.2 Raw map



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



X



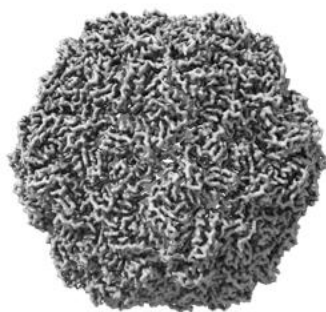
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

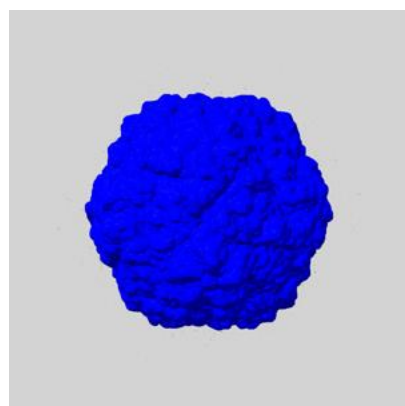
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

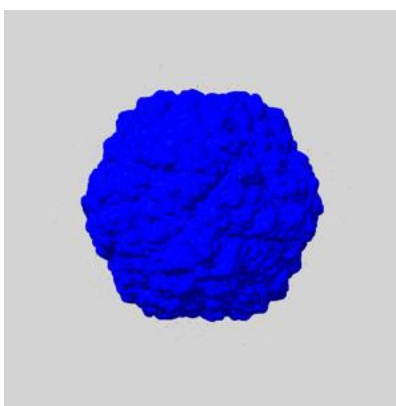
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

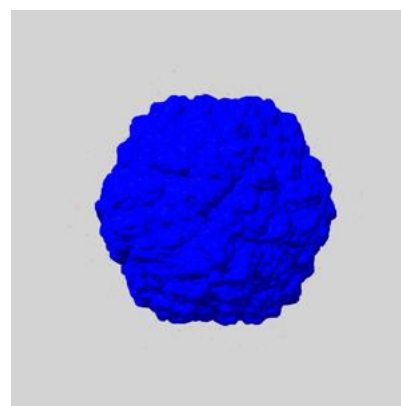
6.6.1 emd_13164_msk_1.map [i](#)



X



Y

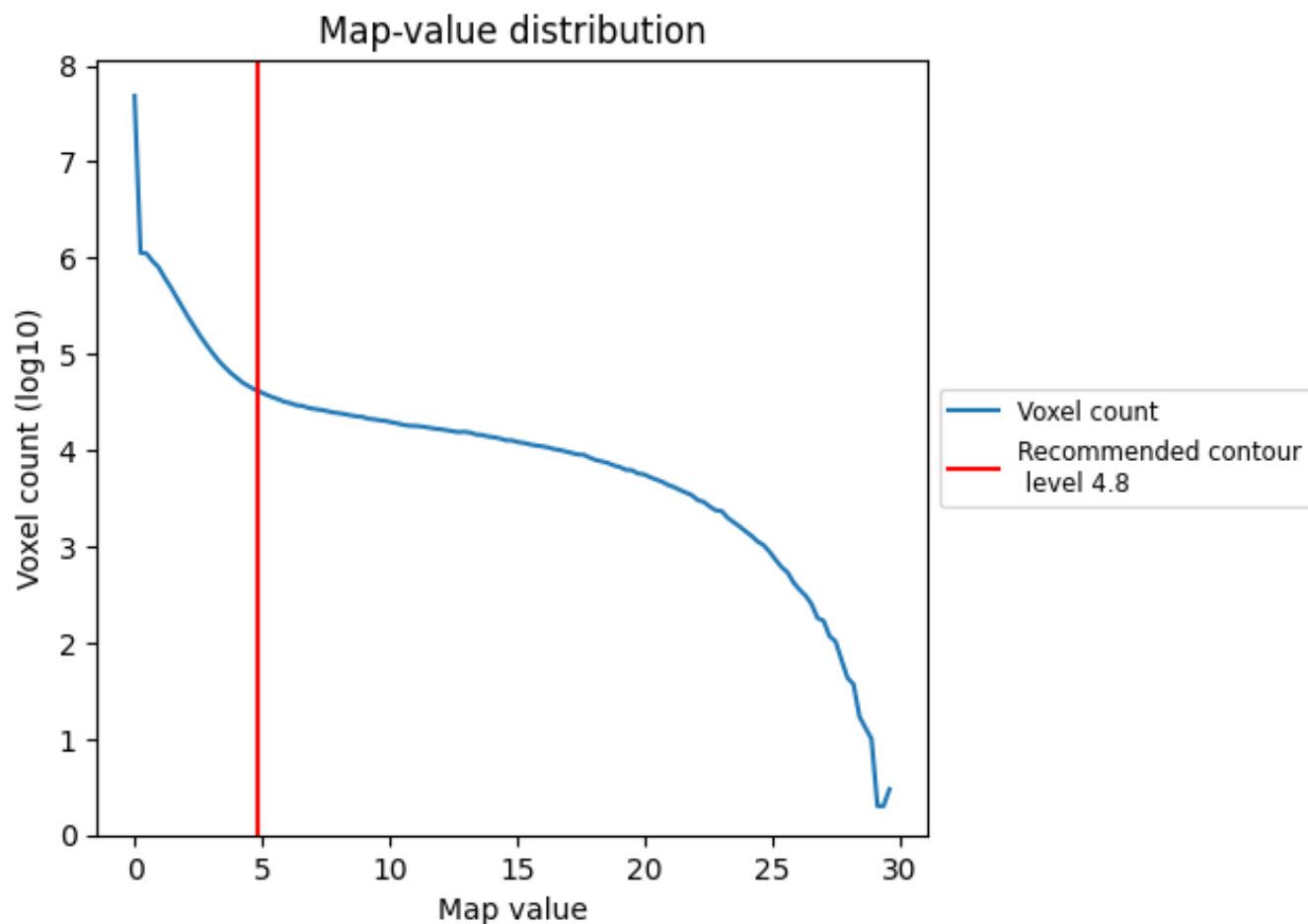


Z

7 Map analysis [i](#)

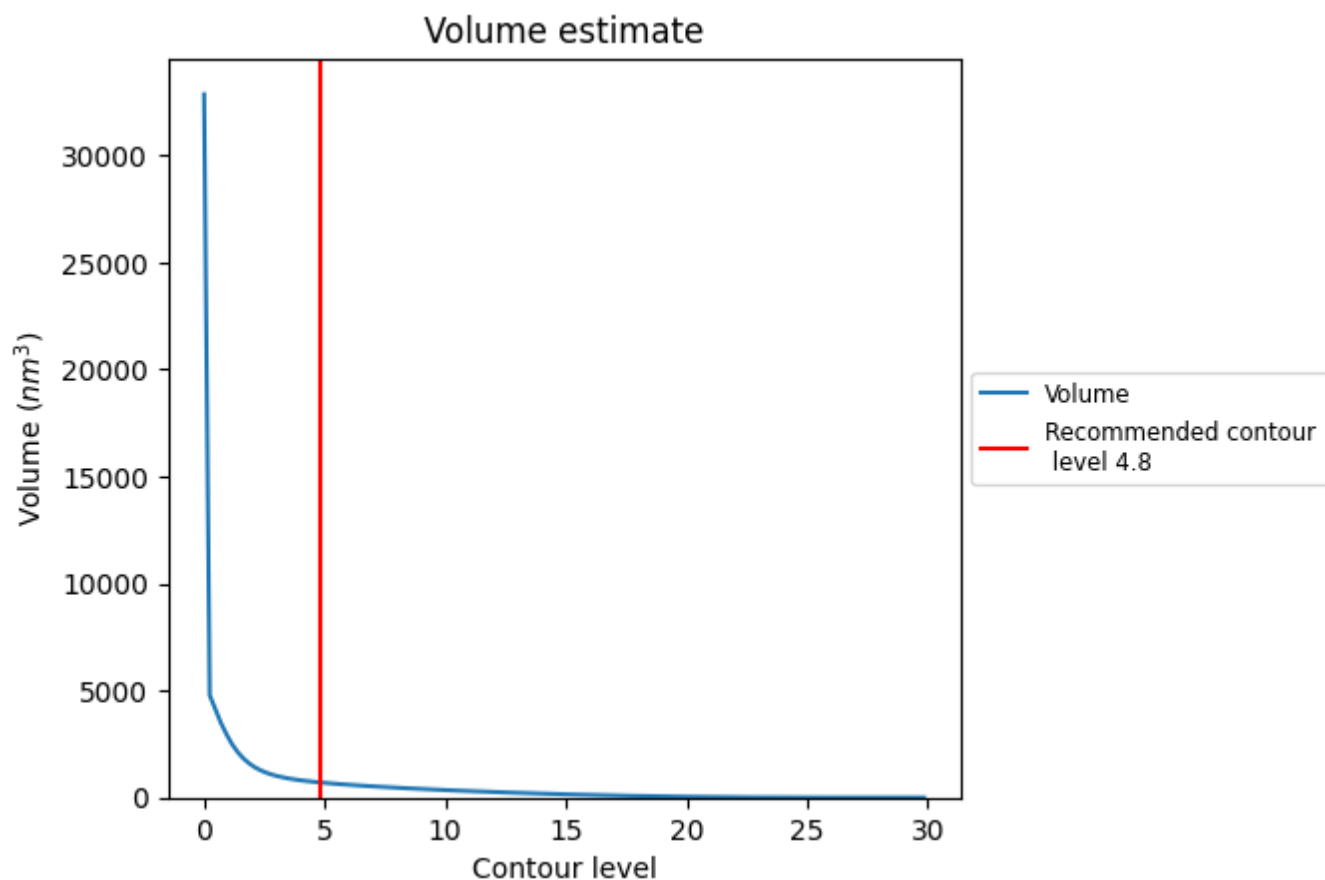
This section contains the results of statistical analysis of the map.

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.

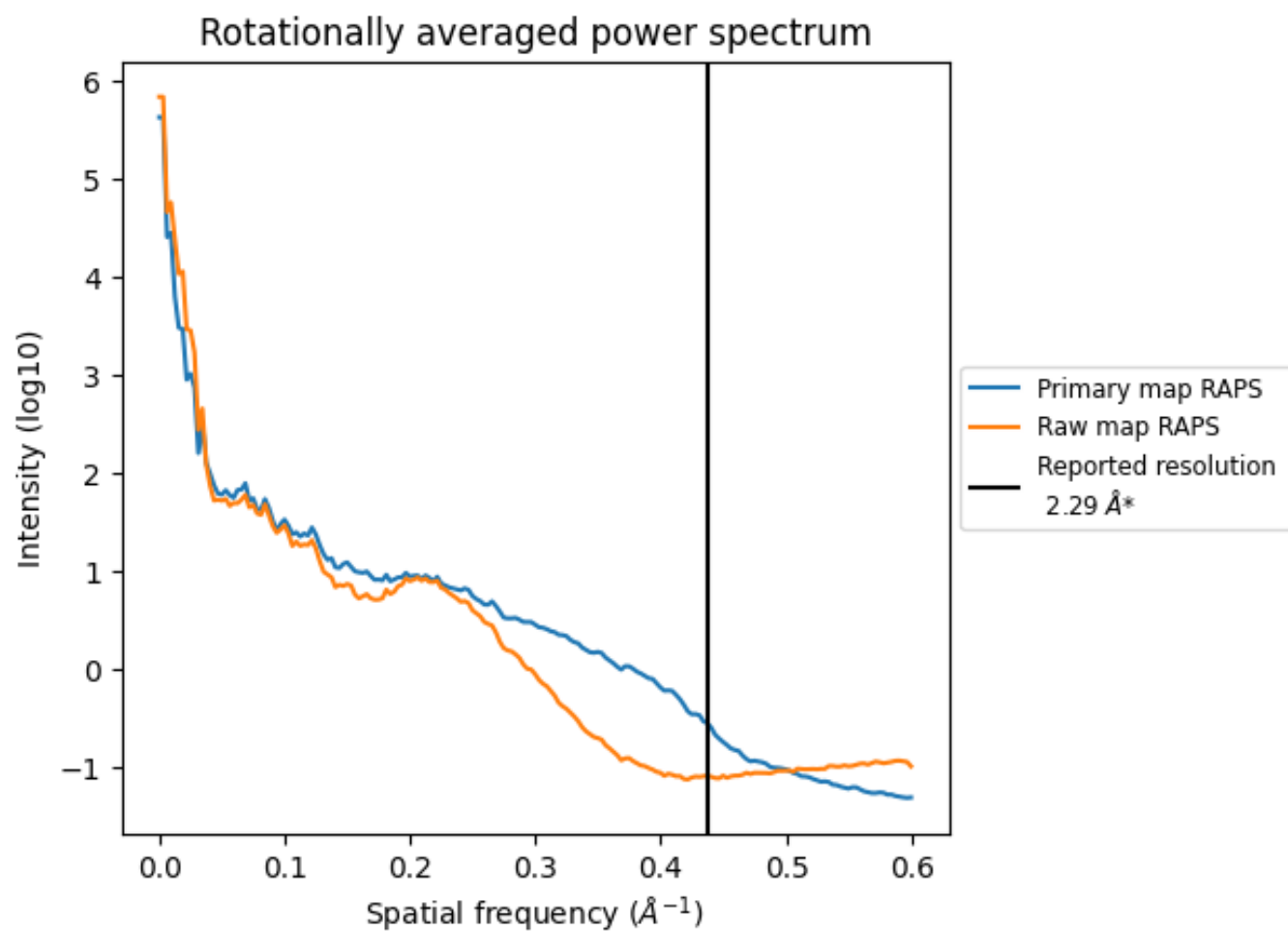
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 706 nm^3 ; this corresponds to an approximate mass of 638 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 ⓘ

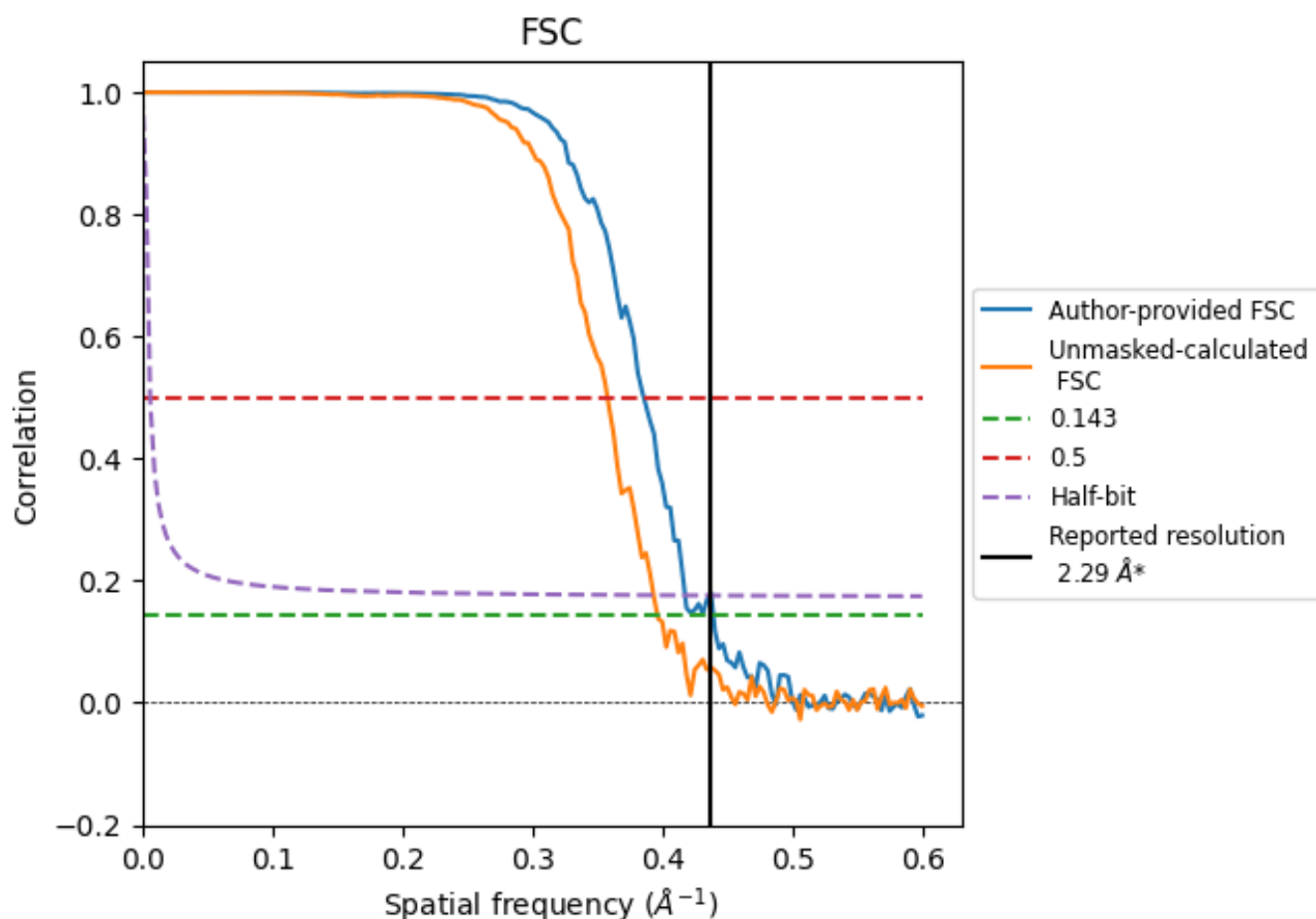


*Reported resolution corresponds to spatial frequency of 0.437 Å⁻¹

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 0.437 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

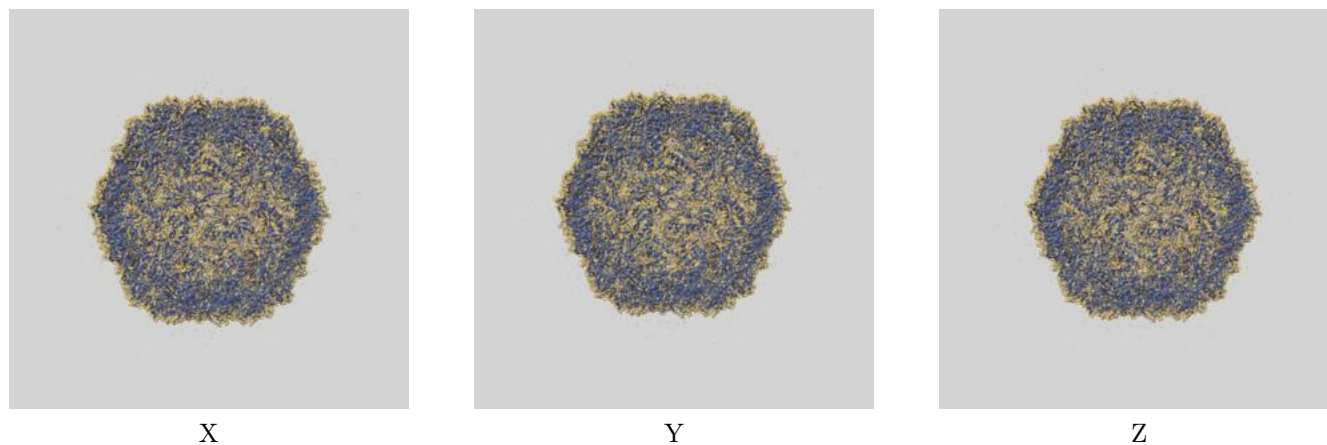
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.29	-	-
Author-provided FSC curve	2.28	2.59	2.40
Unmasked-calculated*	2.52	2.80	2.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.52 differs from the reported value 2.29 by more than 10 %

9 Map-model fit [i](#)

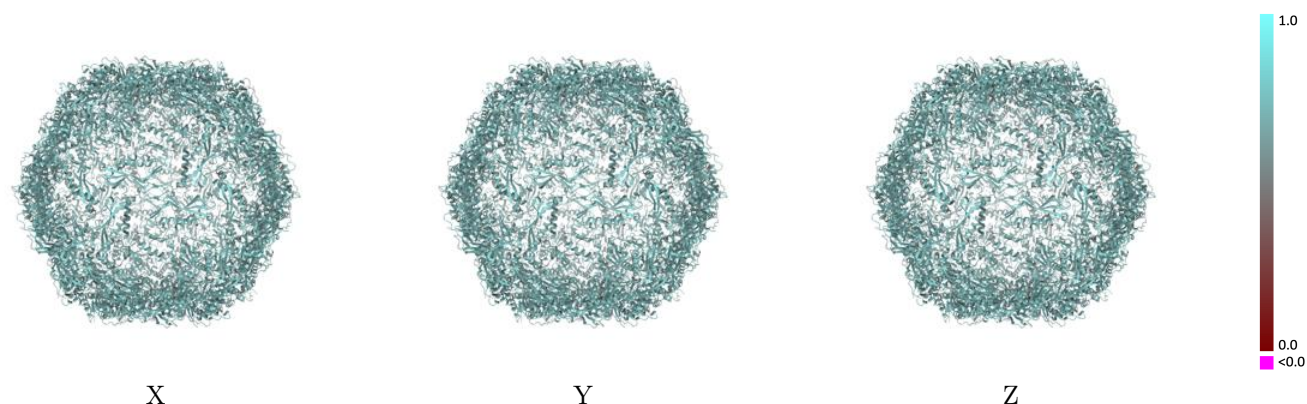
This section contains information regarding the fit between EMDB map EMD-13164 and PDB model 7P1T. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



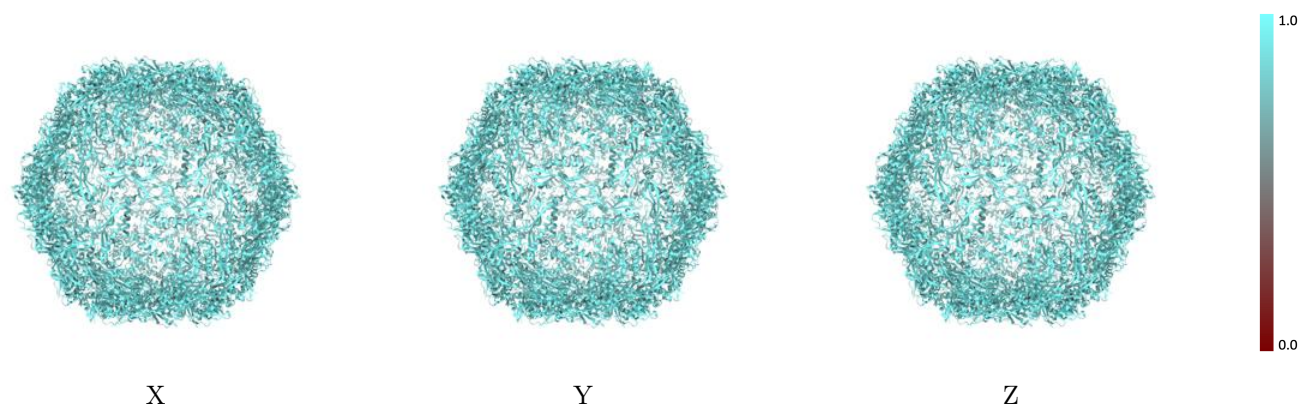
The images above show the 3D surface view of the map at the recommended contour level 4.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



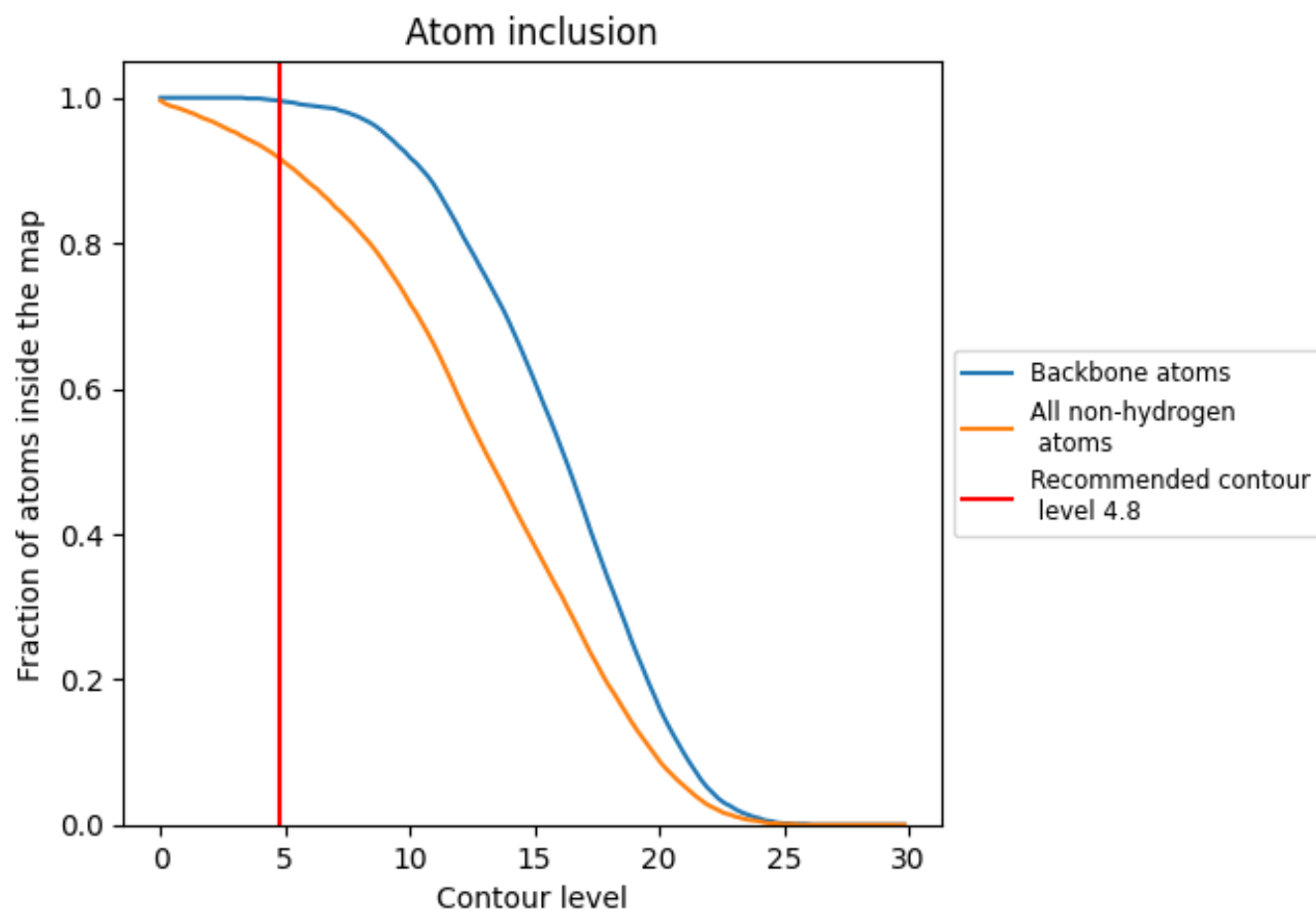
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 92% 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 (4.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.6690
A	 0.9170	 0.6690
AA	 0.9150	 0.6690
AB	 0.9160	 0.6720
B	 0.9130	 0.6680
BA	 0.9180	 0.6740
BB	 0.9180	 0.6680
C	 0.9170	 0.6730
CA	 0.9150	 0.6660
CB	 0.9140	 0.6670
D	 0.9160	 0.6700
DA	 0.9130	 0.6660
DB	 0.9190	 0.6710
E	 0.9140	 0.6690
EA	 0.9130	 0.6690
EB	 0.9160	 0.6680
F	 0.9140	 0.6690
FA	 0.9170	 0.6700
FB	 0.9210	 0.6730
G	 0.9120	 0.6650
GA	 0.9200	 0.6710
GB	 0.9170	 0.6670
H	 0.9190	 0.6720
HA	 0.9160	 0.6650
HB	 0.9140	 0.6670
I	 0.9150	 0.6680
IA	 0.9140	 0.6680
J	 0.9170	 0.6670
JA	 0.9140	 0.6690
K	 0.9140	 0.6680
KA	 0.9160	 0.6690
L	 0.9140	 0.6680
LA	 0.9180	 0.6720
M	 0.9190	 0.6720
MA	 0.9170	 0.6650



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Chain	Atom inclusion	Q-score
N	 0.9170	 0.6690
NA	 0.9150	 0.6710
O	 0.9160	 0.6650
OA	 0.9170	 0.6700
P	 0.9160	 0.6700
PA	 0.9150	 0.6680
Q	 0.9160	 0.6670
QA	 0.9170	 0.6750
R	 0.9160	 0.6710
RA	 0.9170	 0.6680
S	 0.9150	 0.6690
SA	 0.9150	 0.6670
T	 0.9130	 0.6690
TA	 0.9190	 0.6710
U	 0.9180	 0.6710
UA	 0.9140	 0.6680
V	 0.9140	 0.6700
VA	 0.9200	 0.6760
W	 0.9190	 0.6750
WA	 0.9160	 0.6680
X	 0.9170	 0.6670
XA	 0.9130	 0.6660
Y	 0.9120	 0.6670
YA	 0.9170	 0.6710
Z	 0.9180	 0.6710
ZA	 0.9140	 0.6690