



wwPDB EM Validation Summary Report ⓘ

May 21, 2024 – 10:23 AM JST

PDB ID : 8IKA
EMDB ID : EMD-35507
Title : Cryo-EM structure of the encapsulin shell from Mycobacterium tuberculosis
Authors : Du, Z.; Lai, Y.; Gao, Y.; Rao, Z.; Gong, H.
Deposited on : 2023-02-28
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

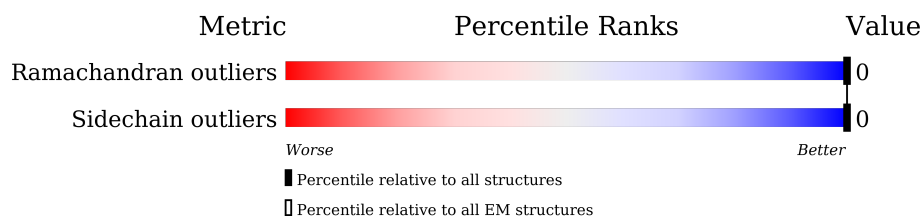
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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.



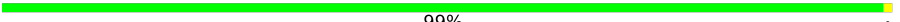
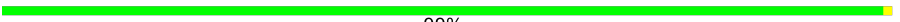
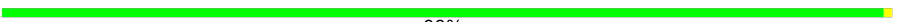












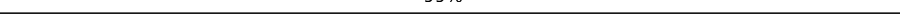
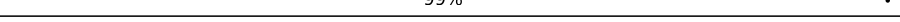
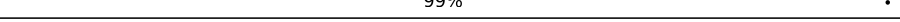
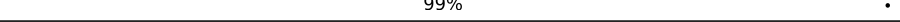
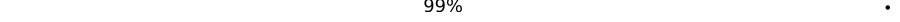
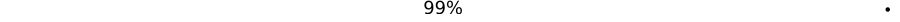
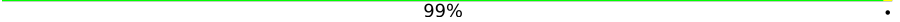
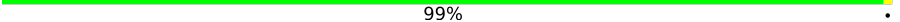
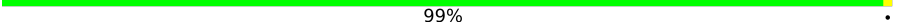
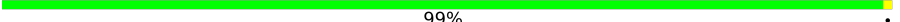
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A1	265	99% .
1	A2	265	99% .
1	A3	265	99% .
1	A4	265	99% .
1	A5	265	99% .
1	A6	265	99% .
1	A7	265	99% .
1	A8	265	99% .
1	A9	265	99% .
1	AA	265	99% .

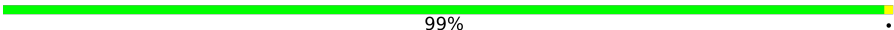
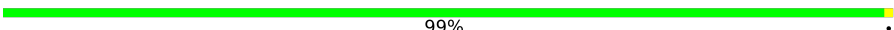
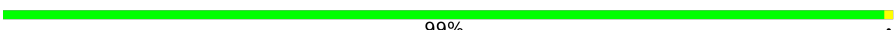
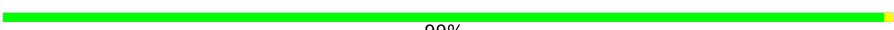
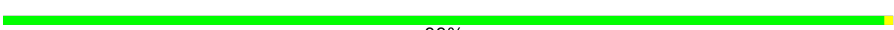





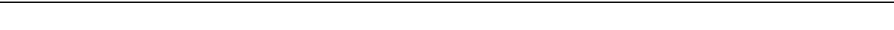

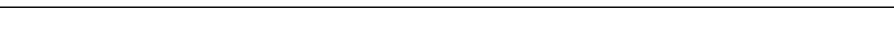
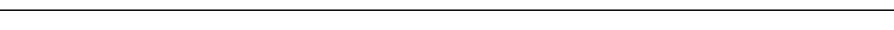
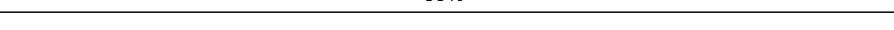
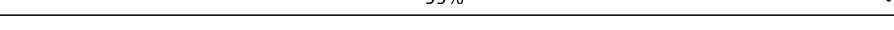
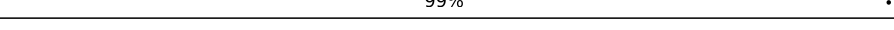
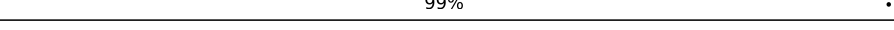
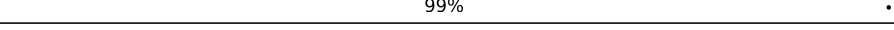
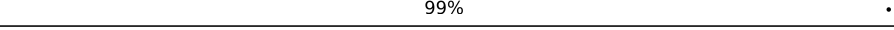
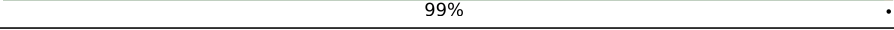
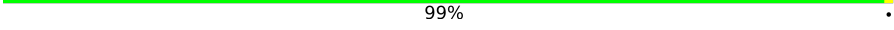
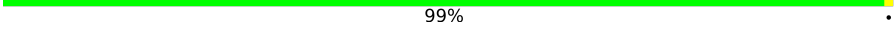
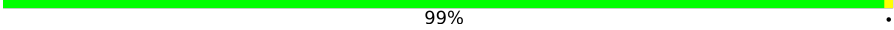
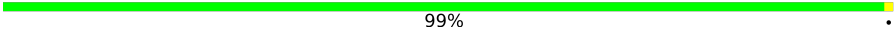
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Mol	Chain	Length	Quality of chain
1	AB	265	 99%
1	AC	265	 99%
1	AD	265	 99%
1	AE	265	 99%
1	AF	265	 99%
1	AG	265	 99%
1	AH	265	 99%
1	AI	265	 99%
1	AJ	265	 99%
1	AK	265	 99%
1	AL	265	 99%
1	AM	265	 99%
1	AN	265	 99%
1	AO	265	 99%
1	AP	265	 99%
1	AQ	265	 99%
1	AR	265	 99%
1	AS	265	 99%
1	AT	265	 99%
1	AU	265	 99%
1	AV	265	 99%
1	AW	265	 99%
1	AX	265	 99%
1	AY	265	 99%
1	AZ	265	 99%

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Mol	Chain	Length	Quality of chain
1	Aa	265	 99% .
1	Ab	265	 99% .
1	Ac	265	 99% .
1	Ad	265	 99% .
1	Ae	265	 99% .
1	Af	265	 99% .
1	Ag	265	 99% .
1	Ah	265	 99% .
1	Ai	265	 99% .
1	Aj	265	 99% .
1	Ak	265	 99% .
1	Al	265	 99% .
1	Am	265	 99% .
1	An	265	 99% .
1	Ao	265	 99% .
1	Ap	265	 99% .
1	Aq	265	 99% .
1	Ar	265	 99% .
1	As	265	 99% .
1	At	265	 99% .
1	Au	265	 99% .
1	Av	265	 99% .
1	Aw	265	 99% .
1	Ax	265	 99% .
1	Ay	265	 99% .

2 Entry composition

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 Type 1 encapsulin shell protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A2	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A3	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A4	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A5	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A6	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A7	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A8	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	A9	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AA	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AB	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AC	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AD	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AE	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AF	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AG	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		
1	AH	265	Total	C	N	O	S	0	0
			2034	1278	354	400	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AI	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AJ	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AK	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AL	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AM	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AN	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AO	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AP	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AQ	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AR	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AS	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AT	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AU	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AV	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AW	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AX	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AY	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	AZ	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	Ab	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ac	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ad	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ae	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Af	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ag	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ah	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ai	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Aj	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ak	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Al	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Am	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	An	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ao	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ap	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Aq	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ar	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	As	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	At	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Au	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Av	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Aw	265	Total 2034	C 1278	N 354	O 400	S 2	0	0
1	Ax	265	Total 2034	C 1278	N 354	O 400	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ay	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. 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. 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: Type 1 encapsulin shell protein

Chain A1:  99% .



- Molecule 1: Type 1 encapsulin shell protein

Chain A2:  99% .



- Molecule 1: Type 1 encapsulin shell protein

Chain A3:  99% .



- Molecule 1: Type 1 encapsulin shell protein

Chain A4:  99% .



- Molecule 1: Type 1 encapsulin shell protein

Chain A5:  99% .



- Molecule 1: Type 1 encapsulin shell protein

Chain A6:  99% .



- Molecule 1: Type 1 encapsulin shell protein

Chain A7:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain A8:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain A9:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AA:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AB:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AC:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AD:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AE: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AF: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AG: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AH: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AI: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AJ: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AK: 99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AL:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AM:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AN:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AO:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AP:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AQ:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AR:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AS:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AT:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AU:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AV:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AW:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AX:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain AY:  99%

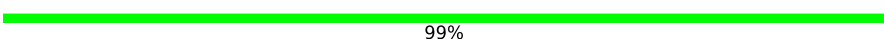


- Molecule 1: Type 1 encapsulin shell protein

Chain AZ:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Aa:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ab:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ac:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ad:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ae:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Af:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ag:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ah:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ai:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Aj:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ak:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Al:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Am:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain An:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ao:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ap:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Aq:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ar:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain As:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain At:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Au:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Av:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Aw:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ax:  99%



- Molecule 1: Type 1 encapsulin shell protein

Chain Ay:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251715	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	A1	0.43	0/2074	0.69	1/2828 (0.0%)
1	A2	0.43	0/2074	0.69	1/2828 (0.0%)
1	A3	0.43	0/2074	0.69	1/2828 (0.0%)
1	A4	0.43	0/2074	0.69	1/2828 (0.0%)
1	A5	0.43	0/2074	0.69	1/2828 (0.0%)
1	A6	0.43	0/2074	0.69	1/2828 (0.0%)
1	A7	0.43	0/2074	0.69	1/2828 (0.0%)
1	A8	0.43	0/2074	0.69	1/2828 (0.0%)
1	A9	0.43	0/2074	0.69	1/2828 (0.0%)
1	AA	0.43	0/2074	0.69	1/2828 (0.0%)
1	AB	0.43	0/2074	0.69	1/2828 (0.0%)
1	AC	0.43	0/2074	0.69	1/2828 (0.0%)
1	AD	0.43	0/2074	0.69	1/2828 (0.0%)
1	AE	0.43	0/2074	0.69	1/2828 (0.0%)
1	AF	0.43	0/2074	0.69	1/2828 (0.0%)
1	AG	0.43	0/2074	0.69	1/2828 (0.0%)
1	AH	0.43	0/2074	0.69	1/2828 (0.0%)
1	AI	0.43	0/2074	0.69	1/2828 (0.0%)
1	AJ	0.43	0/2074	0.69	1/2828 (0.0%)
1	AK	0.43	0/2074	0.69	1/2828 (0.0%)
1	AL	0.43	0/2074	0.69	1/2828 (0.0%)
1	AM	0.43	0/2074	0.69	1/2828 (0.0%)
1	AN	0.43	0/2074	0.69	1/2828 (0.0%)
1	AO	0.43	0/2074	0.69	1/2828 (0.0%)
1	AP	0.43	0/2074	0.69	1/2828 (0.0%)
1	AQ	0.43	0/2074	0.69	1/2828 (0.0%)
1	AR	0.43	0/2074	0.69	1/2828 (0.0%)
1	AS	0.43	0/2074	0.69	1/2828 (0.0%)
1	AT	0.43	0/2074	0.69	1/2828 (0.0%)
1	AU	0.43	0/2074	0.69	1/2828 (0.0%)
1	AV	0.43	0/2074	0.69	1/2828 (0.0%)
1	AW	0.43	0/2074	0.69	1/2828 (0.0%)
1	AX	0.43	0/2074	0.69	1/2828 (0.0%)
1	AY	0.43	0/2074	0.69	1/2828 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AZ	0.43	0/2074	0.69	1/2828 (0.0%)
1	Aa	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ab	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ac	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ad	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ae	0.43	0/2074	0.69	1/2828 (0.0%)
1	Af	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ag	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ah	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ai	0.43	0/2074	0.69	1/2828 (0.0%)
1	Aj	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ak	0.43	0/2074	0.69	1/2828 (0.0%)
1	Al	0.43	0/2074	0.69	1/2828 (0.0%)
1	Am	0.43	0/2074	0.69	1/2828 (0.0%)
1	An	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ao	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ap	0.43	0/2074	0.69	1/2828 (0.0%)
1	Aq	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ar	0.43	0/2074	0.69	1/2828 (0.0%)
1	As	0.43	0/2074	0.69	1/2828 (0.0%)
1	At	0.43	0/2074	0.69	1/2828 (0.0%)
1	Au	0.43	0/2074	0.69	1/2828 (0.0%)
1	Av	0.43	0/2074	0.69	1/2828 (0.0%)
1	Aw	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ax	0.43	0/2074	0.69	1/2828 (0.0%)
1	Ay	0.43	0/2074	0.69	1/2828 (0.0%)
All	All	0.43	0/124440	0.69	60/169680 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	1
1	A2	0	1
1	A3	0	1
1	A4	0	1
1	A5	0	1
1	A6	0	1
1	A7	0	1
1	A8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A9	0	1
1	AA	0	1
1	AB	0	1
1	AC	0	1
1	AD	0	1
1	AE	0	1
1	AF	0	1
1	AG	0	1
1	AH	0	1
1	AI	0	1
1	AJ	0	1
1	AK	0	1
1	AL	0	1
1	AM	0	1
1	AN	0	1
1	AO	0	1
1	AP	0	1
1	AQ	0	1
1	AR	0	1
1	AS	0	1
1	AT	0	1
1	AU	0	1
1	AV	0	1
1	AW	0	1
1	AX	0	1
1	AY	0	1
1	AZ	0	1
1	Aa	0	1
1	Ab	0	1
1	Ac	0	1
1	Ad	0	1
1	Ae	0	1
1	Af	0	1
1	Ag	0	1
1	Ah	0	1
1	Ai	0	1
1	Aj	0	1
1	Ak	0	1
1	Al	0	1
1	Am	0	1
1	An	0	1
1	Ao	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Ap	0	1
1	Aq	0	1
1	Ar	0	1
1	As	0	1
1	At	0	1
1	Au	0	1
1	Av	0	1
1	Aw	0	1
1	Ax	0	1
1	Ay	0	1
All	All	0	60

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AC	54	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	AH	54	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	AK	54	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	AN	54	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	AR	54	ARG	NE-CZ-NH2	5.17	122.88	120.30

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	192	ARG	Sidechain
1	A2	192	ARG	Sidechain
1	A3	192	ARG	Sidechain
1	A4	192	ARG	Sidechain
1	A5	192	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A2	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A3	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A4	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A5	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A6	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A7	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A8	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	A9	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	AC	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AD	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AE	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AF	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AG	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AH	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AI	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AJ	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AK	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AL	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AM	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AN	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AO	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AP	263/265 (99%)	259 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AQ	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AR	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AS	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AT	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AU	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AV	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AW	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AX	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AY	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	AZ	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	Ac	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ad	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ae	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Af	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ag	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ah	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ai	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Aj	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ak	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Al	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Am	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	An	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ao	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ap	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Aq	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ar	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	As	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	At	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Au	263/265 (99%)	259 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Av	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Aw	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ax	263/265 (99%)	259 (98%)	4 (2%)	0	100	100
1	Ay	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	A1	218/218 (100%)	218 (100%)	0	100	100
1	A2	218/218 (100%)	218 (100%)	0	100	100
1	A3	218/218 (100%)	218 (100%)	0	100	100
1	A4	218/218 (100%)	218 (100%)	0	100	100
1	A5	218/218 (100%)	218 (100%)	0	100	100
1	A6	218/218 (100%)	218 (100%)	0	100	100
1	A7	218/218 (100%)	218 (100%)	0	100	100
1	A8	218/218 (100%)	218 (100%)	0	100	100
1	A9	218/218 (100%)	218 (100%)	0	100	100
1	AA	218/218 (100%)	218 (100%)	0	100	100
1	AB	218/218 (100%)	218 (100%)	0	100	100
1	AC	218/218 (100%)	218 (100%)	0	100	100
1	AD	218/218 (100%)	218 (100%)	0	100	100
1	AE	218/218 (100%)	218 (100%)	0	100	100
1	AF	218/218 (100%)	218 (100%)	0	100	100
1	AG	218/218 (100%)	218 (100%)	0	100	100
1	AH	218/218 (100%)	218 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AI	218/218 (100%)	218 (100%)	0	100	100
1	AJ	218/218 (100%)	218 (100%)	0	100	100
1	AK	218/218 (100%)	218 (100%)	0	100	100
1	AL	218/218 (100%)	218 (100%)	0	100	100
1	AM	218/218 (100%)	218 (100%)	0	100	100
1	AN	218/218 (100%)	218 (100%)	0	100	100
1	AO	218/218 (100%)	218 (100%)	0	100	100
1	AP	218/218 (100%)	218 (100%)	0	100	100
1	AQ	218/218 (100%)	218 (100%)	0	100	100
1	AR	218/218 (100%)	218 (100%)	0	100	100
1	AS	218/218 (100%)	218 (100%)	0	100	100
1	AT	218/218 (100%)	218 (100%)	0	100	100
1	AU	218/218 (100%)	218 (100%)	0	100	100
1	AV	218/218 (100%)	218 (100%)	0	100	100
1	AW	218/218 (100%)	218 (100%)	0	100	100
1	AX	218/218 (100%)	218 (100%)	0	100	100
1	AY	218/218 (100%)	218 (100%)	0	100	100
1	AZ	218/218 (100%)	218 (100%)	0	100	100
1	Aa	218/218 (100%)	218 (100%)	0	100	100
1	Ab	218/218 (100%)	218 (100%)	0	100	100
1	Ac	218/218 (100%)	218 (100%)	0	100	100
1	Ad	218/218 (100%)	218 (100%)	0	100	100
1	Ae	218/218 (100%)	218 (100%)	0	100	100
1	Af	218/218 (100%)	218 (100%)	0	100	100
1	Ag	218/218 (100%)	218 (100%)	0	100	100
1	Ah	218/218 (100%)	218 (100%)	0	100	100
1	Ai	218/218 (100%)	218 (100%)	0	100	100
1	Aj	218/218 (100%)	218 (100%)	0	100	100
1	Ak	218/218 (100%)	218 (100%)	0	100	100
1	Al	218/218 (100%)	218 (100%)	0	100	100
1	Am	218/218 (100%)	218 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	An	218/218 (100%)	218 (100%)	0	100	100
1	Ao	218/218 (100%)	218 (100%)	0	100	100
1	Ap	218/218 (100%)	218 (100%)	0	100	100
1	Aq	218/218 (100%)	218 (100%)	0	100	100
1	Ar	218/218 (100%)	218 (100%)	0	100	100
1	As	218/218 (100%)	218 (100%)	0	100	100
1	At	218/218 (100%)	218 (100%)	0	100	100
1	Au	218/218 (100%)	218 (100%)	0	100	100
1	Av	218/218 (100%)	218 (100%)	0	100	100
1	Aw	218/218 (100%)	218 (100%)	0	100	100
1	Ax	218/218 (100%)	218 (100%)	0	100	100
1	Ay	218/218 (100%)	218 (100%)	0	100	100
All	All	13080/13080 (100%)	13080 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
1	AT	247	GLN
1	Au	247	GLN
1	Aa	247	GLN
1	At	247	GLN
1	Ay	247	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.