



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 03:29 PM EST

PDB ID : 3IKU  
EMDB ID : EMD-5128  
Title : Structural model of ParM filament in closed state from cryo-EM  
Authors : Galkin, V.E.; Orlova, A.; Rivera, C.; Mullins, R.D.; Egelman, E.H.  
Deposited on : 2009-08-06  
Resolution : 18.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

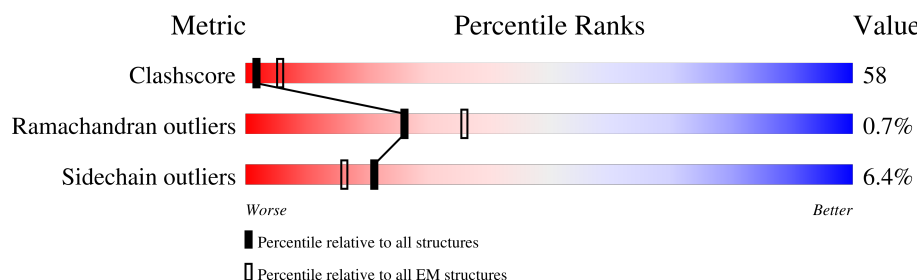
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 18.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	320	56% 39% ..
1	B	320	56% 40% ..
1	C	320	53% 43% ..
1	D	320	52% 43% ..
1	E	320	53% 42% ..
1	F	320	53% 43% ..
1	G	320	52% 43% ..
1	H	320	53% 42% ..
1	I	320	52% 44% ..

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Mol	Chain	Length	Quality of chain
1	J	320	<div><div></div><div>53%</div><div>43%</div><div>..</div></div>
1	K	320	<div><div></div><div>57%</div><div>39%</div><div>..</div></div>
1	L	320	<div><div></div><div>58%</div><div>38%</div><div>..</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29880 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.

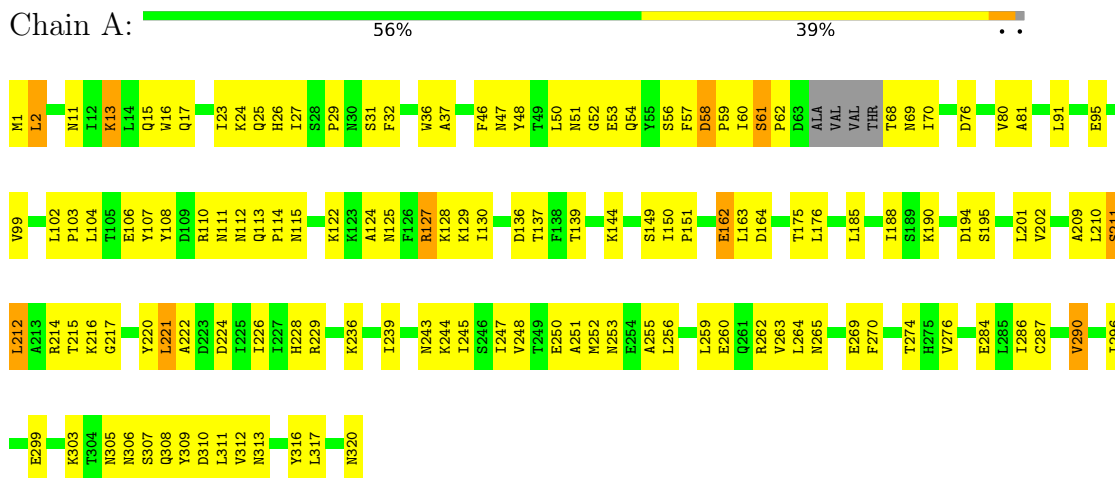
- Molecule 1 is a protein called Plasmid segregation protein parM.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	B	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	C	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	D	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	E	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	F	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	G	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	H	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	I	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	J	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	K	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		
1	L	316	Total	C	N	O	S	0	0
			2490	1569	421	492	8		

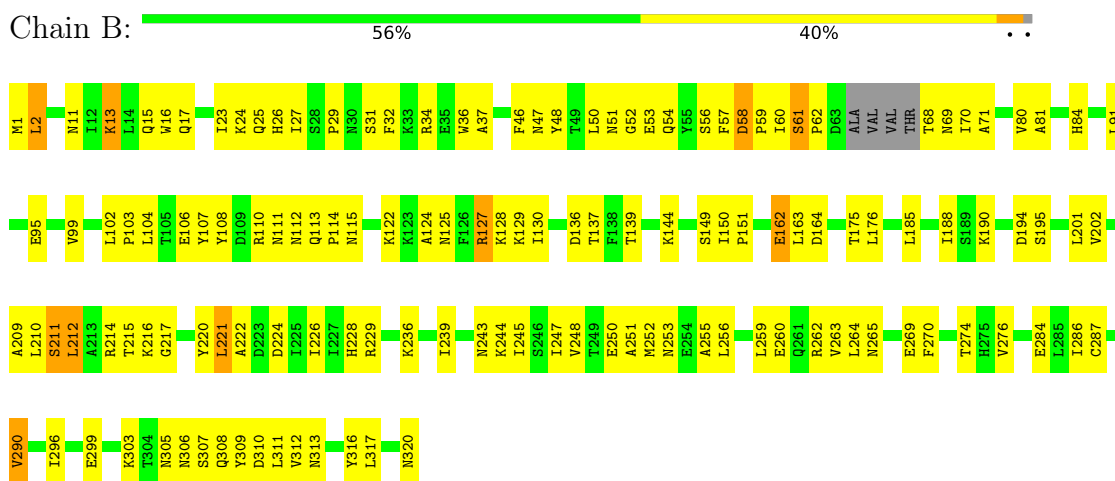
### 3 Residue-property plots

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.

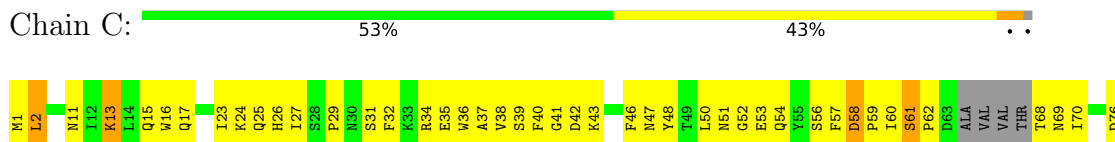
#### • Molecule 1: Plasmid segregation protein parM

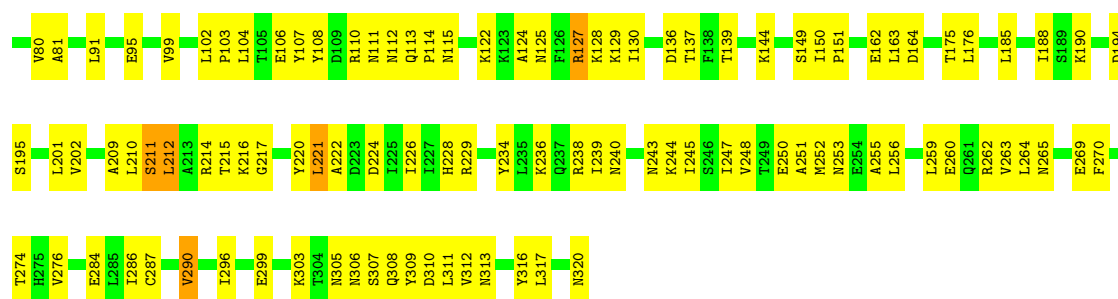


#### • Molecule 1: Plasmid segregation protein parM



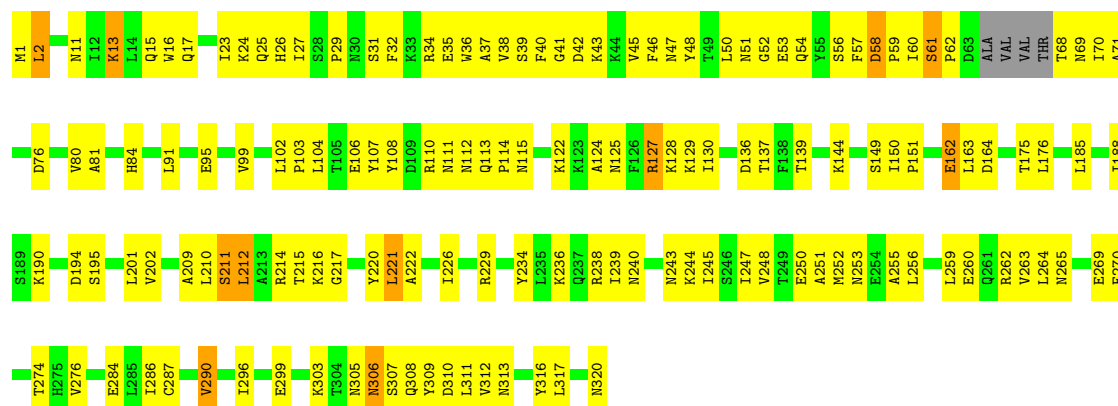
#### • Molecule 1: Plasmid segregation protein parM





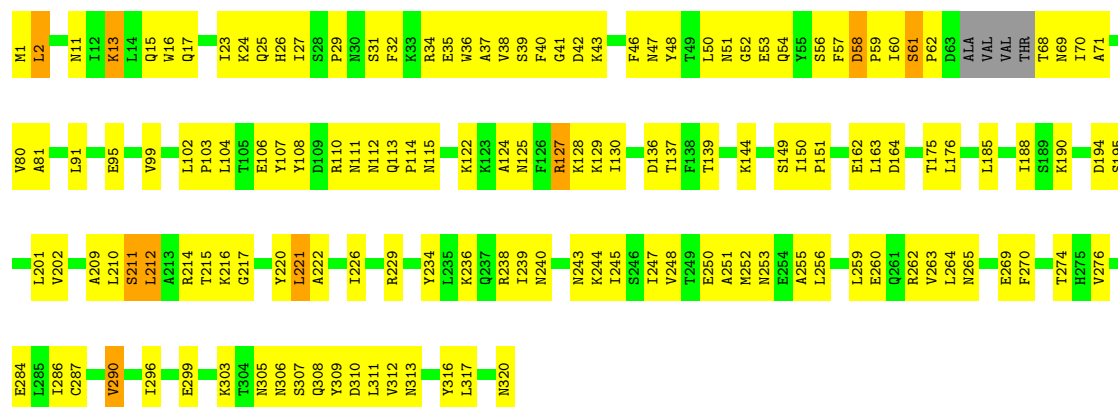
• Molecule 1: Plasmid segregation protein parM

Chain D: 52% 43% ..



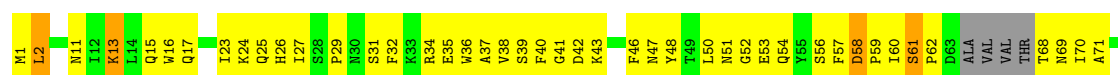
• Molecule 1: Plasmid segregation protein parM

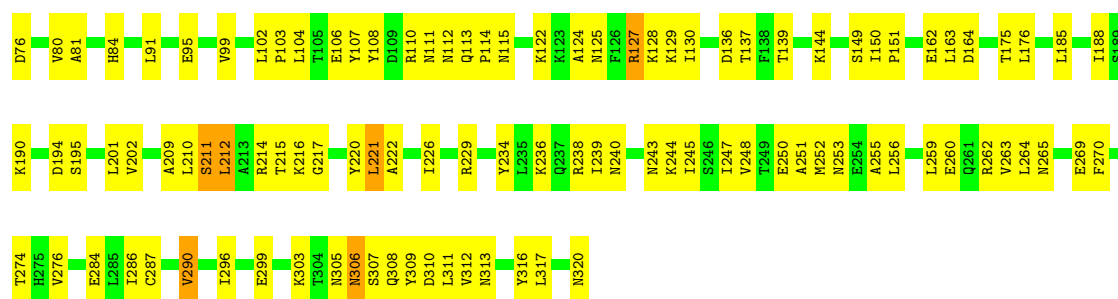
Chain E: 53% 42% ..



• Molecule 1: Plasmid segregation protein parM

Chain F: 53% 43% ..





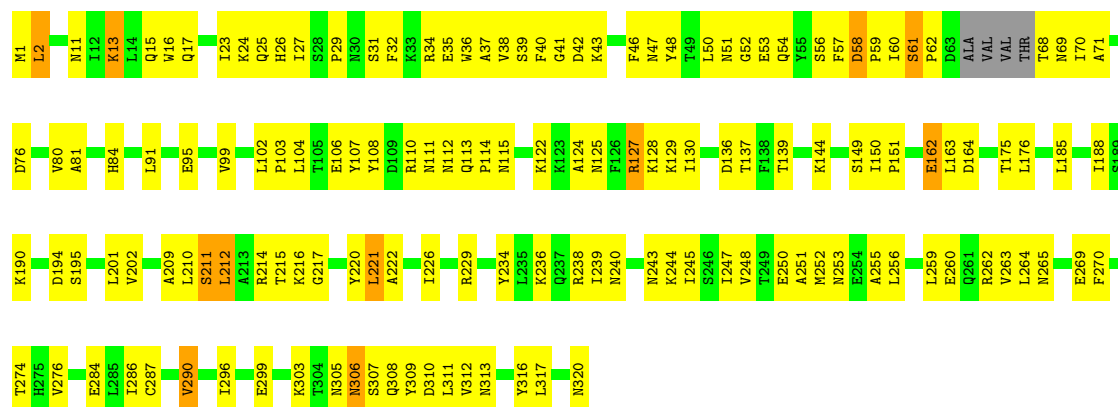
• Molecule 1: Plasmid segregation protein parM

Chain G: 52% 43% ..



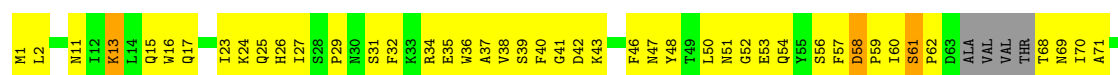
• Molecule 1: Plasmid segregation protein parM

Chain H: 53% 42% ..



• Molecule 1: Plasmid segregation protein parM

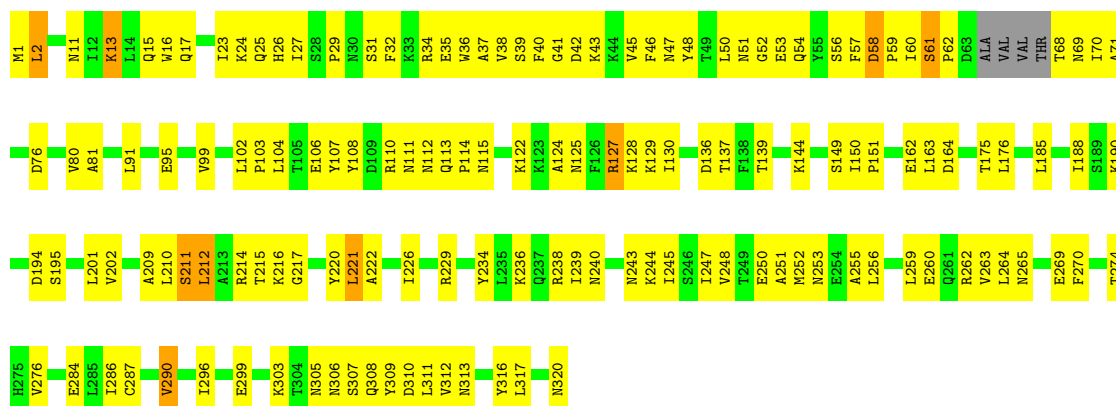
Chain I: 52% 44% ..





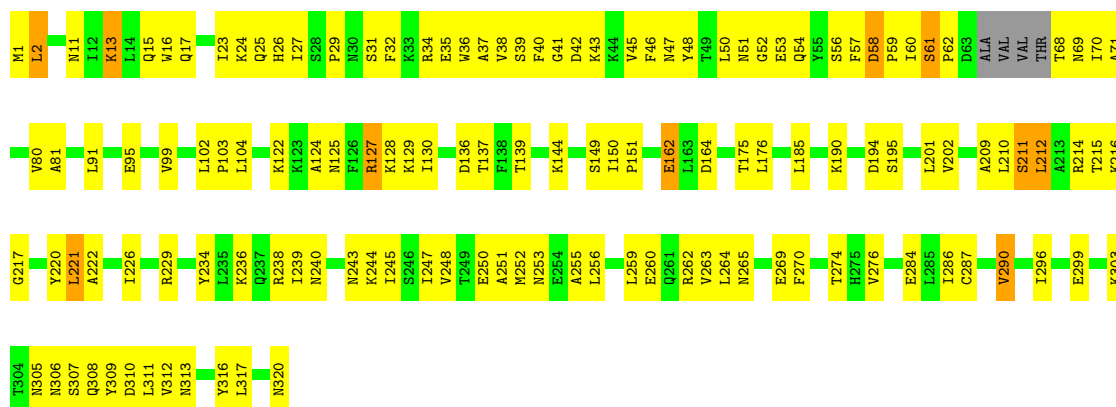
• Molecule 1: Plasmid segregation protein parM

Chain J: 53% 43% ..



• Molecule 1: Plasmid segregation protein parM

Chain K: 57% 39% ..





## 4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	The micrographs were multiplied by the CTF to correct phases	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	

## 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	0.40	0/2527	0.67	0/3413
1	B	0.40	0/2527	0.67	0/3413
1	C	0.40	0/2527	0.67	0/3413
1	D	0.40	0/2527	0.67	0/3413
1	E	0.40	0/2527	0.67	0/3413
1	F	0.40	0/2527	0.67	0/3413
1	G	0.40	0/2527	0.67	0/3413
1	H	0.40	0/2527	0.67	0/3413
1	I	0.40	0/2527	0.67	0/3413
1	J	0.40	0/2527	0.67	0/3413
1	K	0.40	0/2527	0.67	0/3413
1	L	0.40	0/2527	0.67	0/3413
All	All	0.40	0/30324	0.67	0/40956

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2490	0	2467	304	0
1	B	2490	0	2466	315	0
1	C	2490	0	2464	411	0
1	D	2490	0	2464	412	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2490	0	2464	407	0
1	F	2490	0	2464	408	0
1	G	2490	0	2464	412	0
1	H	2490	0	2464	416	0
1	I	2490	0	2464	413	0
1	J	2490	0	2464	412	0
1	K	2490	0	2468	314	0
1	L	2490	0	2468	299	0
All	All	29880	0	29581	3422	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 58.

The worst 5 of 3422 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:G:112:ASN:HB3	1:I:43:LYS:CE	1.24	1.66
1:A:112:ASN:HB3	1:C:43:LYS:CE	1.24	1.65
1:E:112:ASN:HB3	1:G:43:LYS:CE	1.24	1.65
1:F:112:ASN:HB3	1:H:43:LYS:CE	1.24	1.61
1:H:112:ASN:HB3	1:J:43:LYS:CE	1.24	1.59

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22 63
1	B	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22 63
1	C	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	E	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	F	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	G	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	H	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	I	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	J	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	K	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
1	L	306/320 (96%)	290 (95%)	14 (5%)	2 (1%)	22	63
All	All	3672/3840 (96%)	3480 (95%)	168 (5%)	24 (1%)	26	63

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	B	211	SER
1	C	211	SER
1	D	211	SER
1	E	211	SER

### 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	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	B	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	C	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	D	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	E	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	F	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	G	281/284 (99%)	263 (94%)	18 (6%)	17	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	I	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	J	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	K	281/284 (99%)	263 (94%)	18 (6%)	17	42
1	L	281/284 (99%)	263 (94%)	18 (6%)	17	42
All	All	3372/3408 (99%)	3156 (94%)	216 (6%)	21	42

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	127	ARG
1	H	311	LEU
1	L	13	LYS
1	G	212	LEU
1	H	53	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	265	ASN
1	J	240	ASN
1	I	47	ASN
1	I	265	ASN
1	K	51	ASN

### 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	3
1	C	3
1	D	3
1	E	3
1	F	3
1	G	3
1	H	3
1	I	3
1	J	3
1	K	3
1	L	3

The worst 5 of 36 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	115:ASN	C	116:THR	N	5.17
1	B	115:ASN	C	116:THR	N	5.17
1	C	115:ASN	C	116:THR	N	5.17
1	D	115:ASN	C	116:THR	N	5.17
1	E	115:ASN	C	116:THR	N	5.17

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5128. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.