



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:20 am GMT

PDB ID : 3IKY
EMDB ID: : EMD-5129
Title : Structural model of ParM filament in the open state by 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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

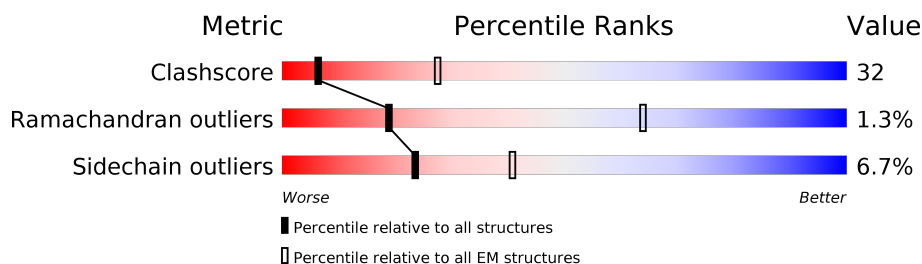
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	71% 27% .
1	B	320	70% 28% .
1	C	320	68% 28% .
1	D	320	69% 28% .
1	E	320	68% 28% .
1	F	320	69% 28% .
1	G	320	69% 28% .
1	H	320	69% 28% .
1	I	320	69% 28% .

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Mol	Chain	Length	Quality of chain
1	J	320	 69% 28% •
1	K	320	 72% 26% •
1	L	320	 72% 25% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30192 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	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	B	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	C	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	D	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	E	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	F	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	G	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	H	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	I	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	J	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	K	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		
1	L	320	Total	C	N	O	S	0	0
			2516	1586	425	497	8		

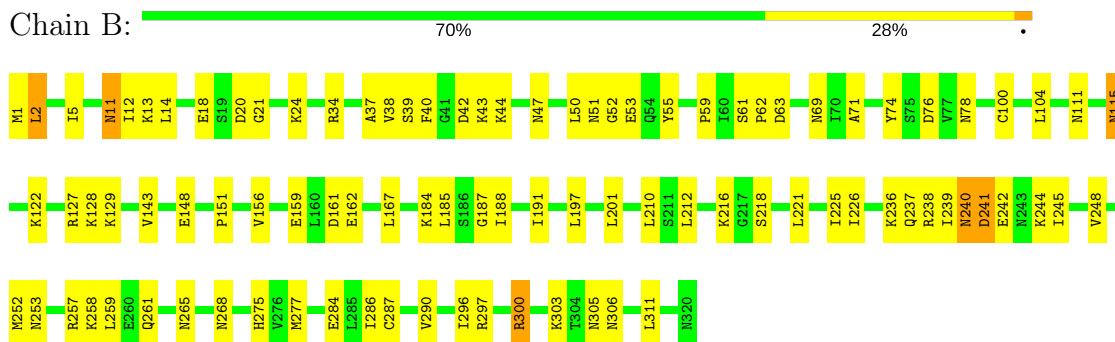
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



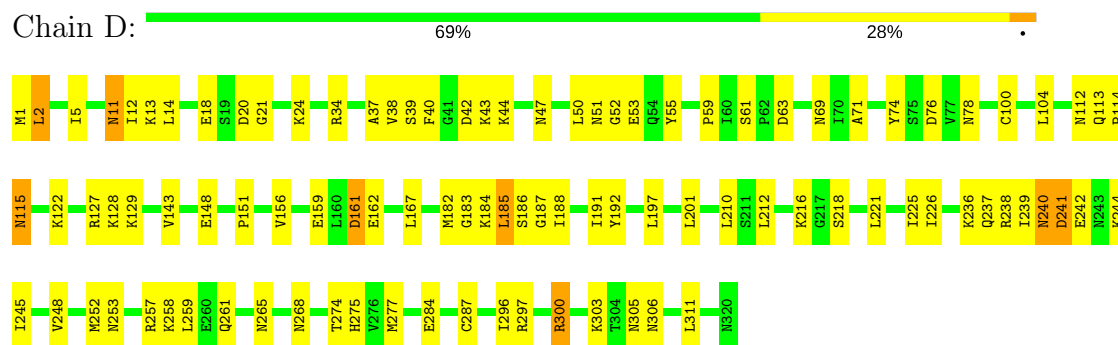
- Molecule 1: Plasmid segregation protein parM



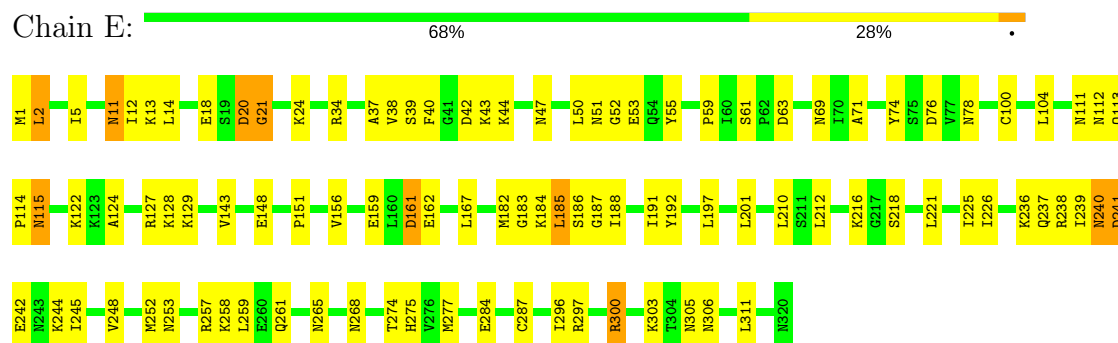
- Molecule 1: Plasmid segregation protein parM



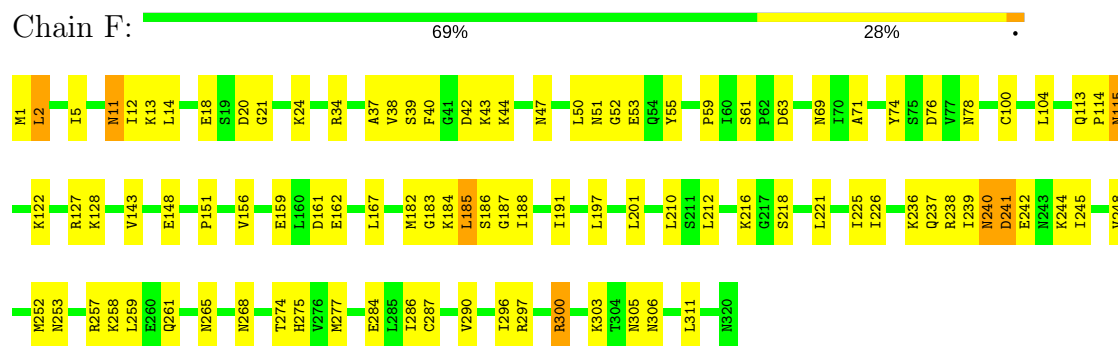
- Molecule 1: Plasmid segregation protein parM



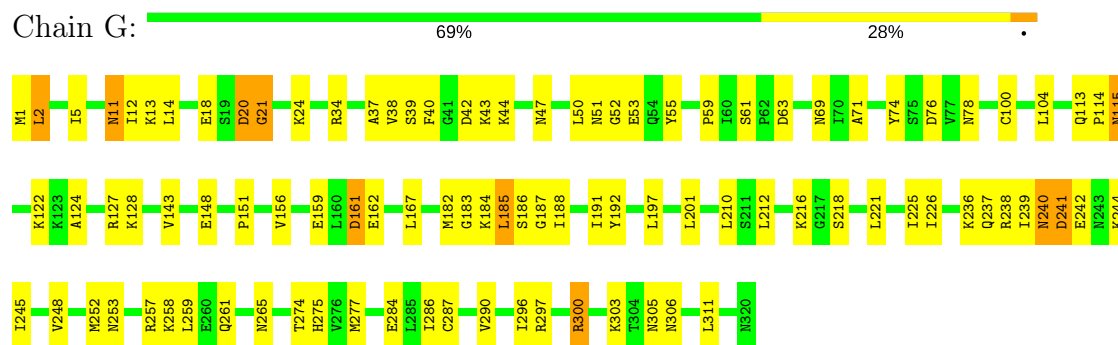
- Molecule 1: Plasmid segregation protein parM



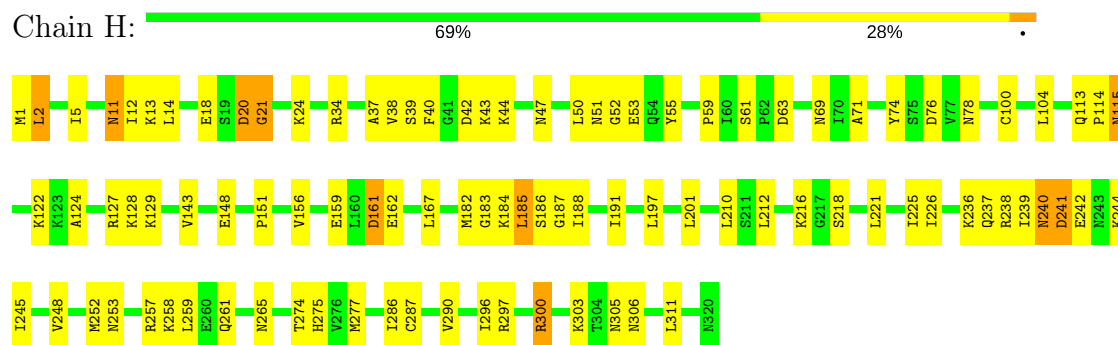
- Molecule 1: Plasmid segregation protein parM



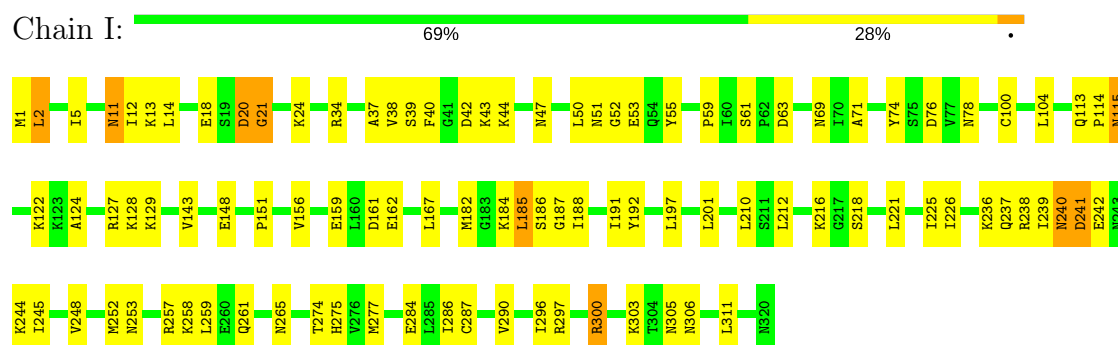
- Molecule 1: Plasmid segregation protein parM



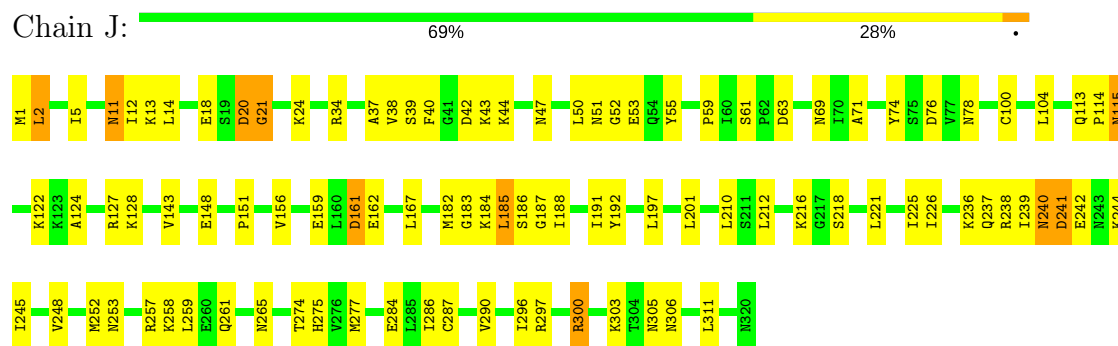
- Molecule 1: Plasmid segregation protein parM



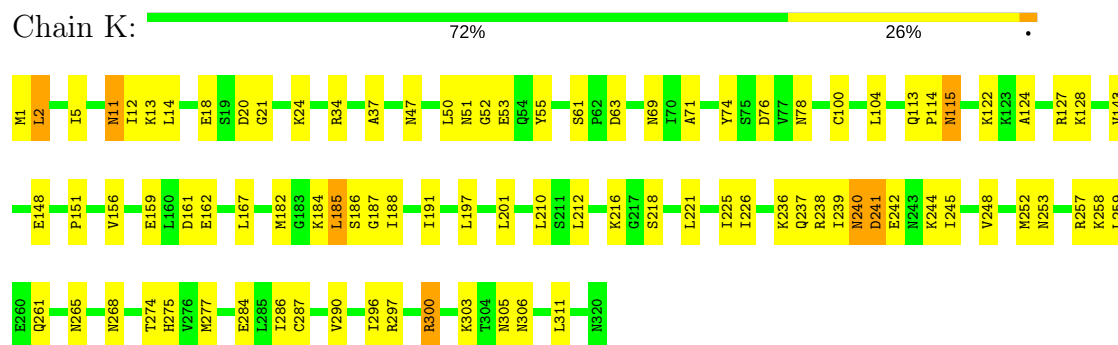
- Molecule 1: Plasmid segregation protein parM



- Molecule 1: Plasmid segregation protein parM

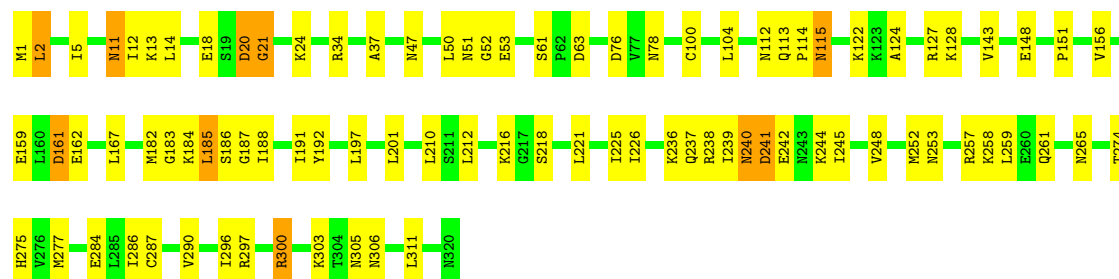


- Molecule 1: Plasmid segregation protein parM



- Molecule 1: Plasmid segregation protein parM

Chain L:



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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 >2	RMSZ	# Z >2
1	A	0.35	0/2557	0.61	0/3463
1	B	0.35	0/2557	0.61	0/3463
1	C	0.35	0/2557	0.61	0/3463
1	D	0.35	0/2557	0.61	0/3463
1	E	0.35	0/2557	0.61	0/3463
1	F	0.35	0/2557	0.61	0/3463
1	G	0.35	0/2557	0.61	0/3463
1	H	0.35	0/2557	0.61	0/3463
1	I	0.35	0/2557	0.61	0/3463
1	J	0.35	0/2557	0.61	0/3463
1	K	0.35	0/2557	0.61	0/3463
1	L	0.35	0/2557	0.61	0/3463
All	All	0.35	0/30684	0.61	0/41556

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	2516	0	2509	177	0
1	B	2516	0	2509	220	0
1	C	2516	0	2504	291	0
1	D	2516	0	2504	286	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2516	0	2504	289	0
1	F	2516	0	2504	284	0
1	G	2516	0	2504	285	0
1	H	2516	0	2504	291	0
1	I	2516	0	2504	290	0
1	J	2516	0	2504	292	0
1	K	2516	0	2505	219	0
1	L	2516	0	2505	175	0
All	All	30192	0	30060	1910	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 32.

The worst 5 of 1910 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:C:38:VAL:CG2	1:E:113:GLN:CA	1.88	1.52
1:E:38:VAL:CG2	1:G:113:GLN:CA	1.88	1.51
1:J:38:VAL:CG2	1:L:113:GLN:CA	1.88	1.51
1:D:38:VAL:CG2	1:F:113:GLN:CA	1.88	1.51
1:H:38:VAL:CG2	1:J:113:GLN:CA	1.88	1.50

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	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	B	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	C	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	E	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	F	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	G	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	H	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	I	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	J	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	K	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
1	L	318/320 (99%)	302 (95%)	12 (4%)	4 (1%)	14	56
All	All	3816/3840 (99%)	3624 (95%)	144 (4%)	48 (1%)	19	56

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	52	GLY
1	A	241	ASP
1	B	20	ASP
1	B	52	GLY

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	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	B	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	C	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	D	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	E	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	F	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	G	284/284 (100%)	265 (93%)	19 (7%)	19	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	I	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	J	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	K	284/284 (100%)	265 (93%)	19 (7%)	19	51
1	L	284/284 (100%)	265 (93%)	19 (7%)	19	51
All	All	3408/3408 (100%)	3180 (93%)	228 (7%)	23	51

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	185	LEU
1	G	240	ASN
1	L	11	ASN
1	F	237	GLN
1	G	11	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 212 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	111	ASN
1	G	240	ASN
1	L	25	GLN
1	F	228	HIS
1	G	25	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 carbohydrates 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.