



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 05:06 PM EDT

PDB ID : 4D2U
EMDB ID: : EMD-2557
Title : Negative-stain electron microscopy of E. coli ClpB (BAP form bound to ClpP)
Authors : Carroni, M.; Kummer, E.; Oguchi, Y.; Clare, D.K.; Wendler, P.; Sinning, I.;
Kopp, J.; Mogk, A.; Bukau, B.; Saibil, H.R.
Deposited on : unknown
Resolution : 17.00 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) : rb-20029824

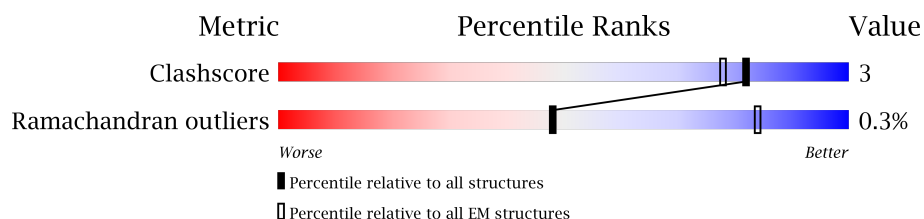
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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

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	858	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div> <div>90% • 8%</div>
1	B	858	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div> <div>90% • 8%</div>
1	C	858	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div> <div>90% • 8%</div>
1	D	858	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div> <div>90% • 8%</div>
1	E	858	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div> <div>90% • 8%</div>
1	F	858	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div> <div>90% • 8%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14202 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 CHAPERONE PROTEIN CLPB.

Mol	Chain	Residues	Atoms			AltConf	Trace
1	A	789	Total	C	N	0	0
			2367	1578	789		
1	B	789	Total	C	N	0	0
			2367	1578	789		
1	C	789	Total	C	N	0	0
			2367	1578	789		
1	D	789	Total	C	N	0	0
			2367	1578	789		
1	E	789	Total	C	N	0	0
			2367	1578	789		
1	F	789	Total	C	N	0	0
			2367	1578	789		

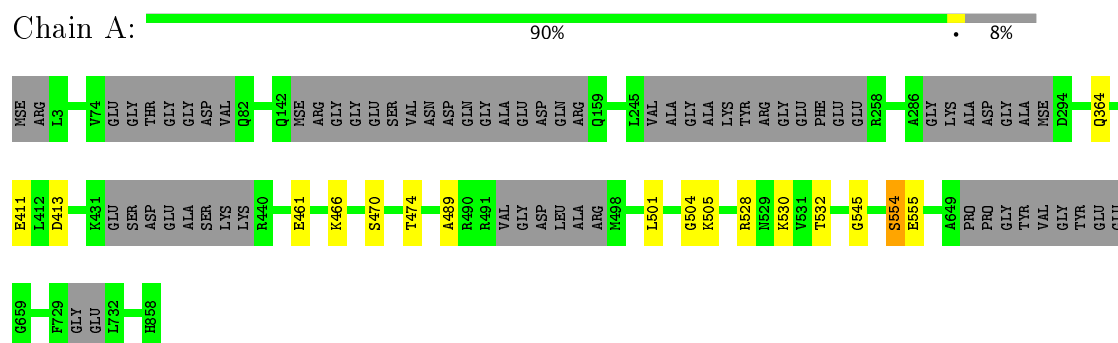
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	858	HIS	-	expression tag	UNP P63284
B	858	HIS	-	expression tag	UNP P63284
C	858	HIS	-	expression tag	UNP P63284
D	858	HIS	-	expression tag	UNP P63284
E	858	HIS	-	expression tag	UNP P63284
F	858	HIS	-	expression tag	UNP P63284

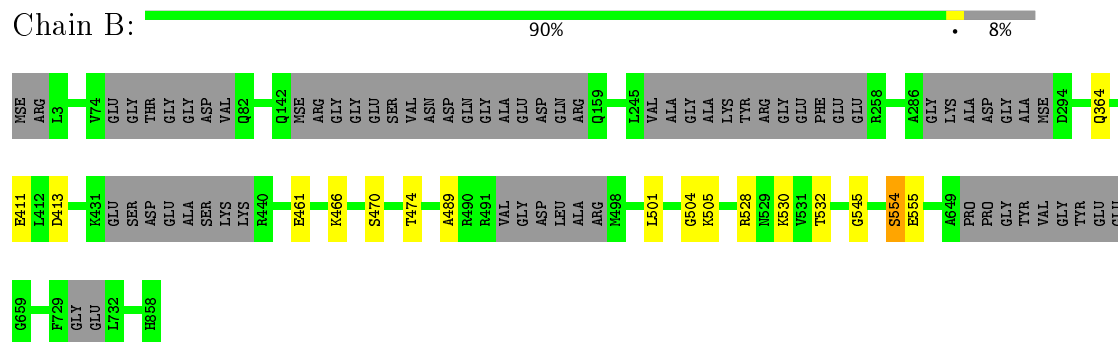
3 Residue-property plots [i](#)

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.

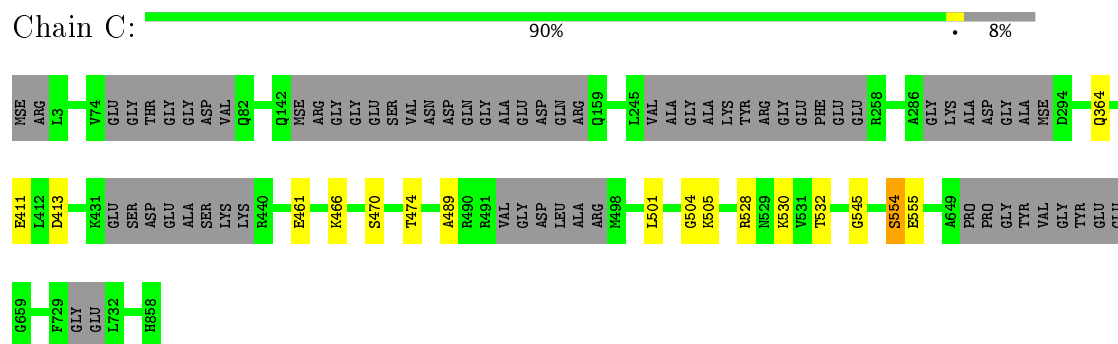
- Molecule 1: CHAPERONE PROTEIN CLPB



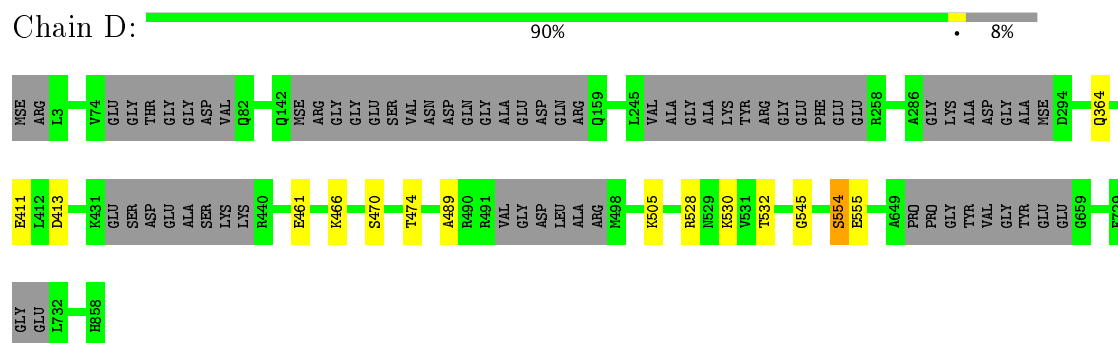
- Molecule 1: CHAPERONE PROTEIN CLPB



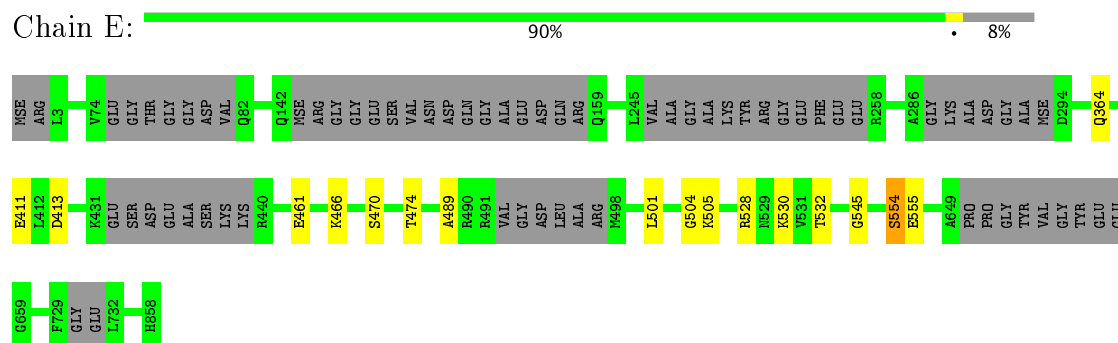
- Molecule 1: CHAPERONE PROTEIN CLPB



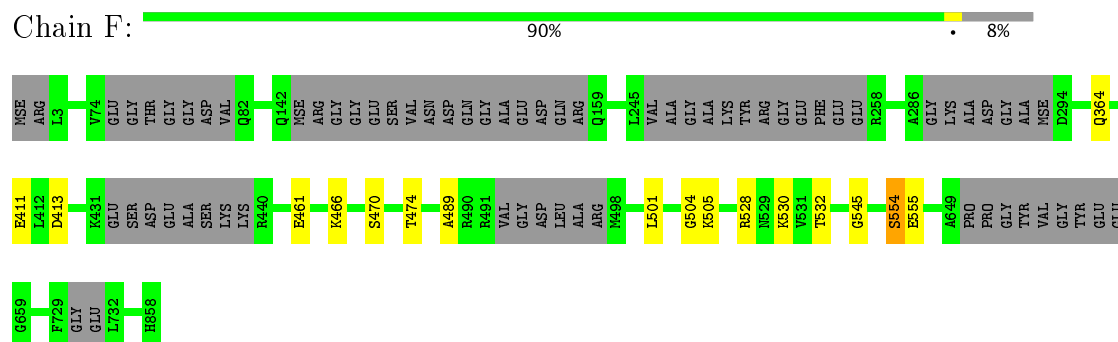
- Molecule 1: CHAPERONE PROTEIN CLPB



- Molecule 1: CHAPERONE PROTEIN CLPB



- Molecule 1: CHAPERONE PROTEIN CLPB



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	11568	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING ENTIRE FRAME	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	68000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k 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 >2	RMSZ	# Z >2
1	A	0.35	0/2339	0.73	0/2311
1	B	0.35	0/2339	0.73	0/2311
1	C	0.35	0/2339	0.73	0/2311
1	D	0.35	0/2339	0.73	0/2311
1	E	0.35	0/2339	0.73	0/2311
1	F	0.35	0/2339	0.73	0/2311
All	All	0.35	0/14034	0.73	0/13866

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	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
All	All	0	24

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	ASP	Peptide
1	A	489	ALA	Peptide
1	A	532	THR	Peptide
1	A	554	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	413	ASP	Peptide

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	2367	0	841	9	0
1	B	2367	0	841	9	0
1	C	2367	0	841	10	0
1	D	2367	0	841	9	0
1	E	2367	0	841	9	0
1	F	2367	0	841	9	0
All	All	14202	0	5046	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 55 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:A:470:SER:CA	1:A:530:LYS:N	1.67	1.46
1:F:470:SER:CA	1:F:530:LYS:N	1.67	1.41
1:B:470:SER:CA	1:B:530:LYS:N	1.67	1.39
1:C:470:SER:CA	1:C:530:LYS:N	1.67	1.36
1:E:470:SER:CA	1:E:530:LYS:N	1.67	1.35

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	767/858 (89%)	736 (96%)	29 (4%)	2 (0%)	44	81
1	B	767/858 (89%)	736 (96%)	29 (4%)	2 (0%)	44	81
1	C	767/858 (89%)	736 (96%)	29 (4%)	2 (0%)	44	81
1	D	767/858 (89%)	736 (96%)	29 (4%)	2 (0%)	44	81
1	E	767/858 (89%)	736 (96%)	29 (4%)	2 (0%)	44	81
1	F	767/858 (89%)	736 (96%)	29 (4%)	2 (0%)	44	81
All	All	4602/5148 (89%)	4416 (96%)	174 (4%)	12 (0%)	48	81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	555	GLU
1	B	555	GLU
1	C	555	GLU
1	D	555	GLU
1	E	555	GLU

5.3.2 Protein sidechains [i](#)

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

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	E	3
1	B	3
1	C	3
1	A	3
1	F	3

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	552:MSE	C	553:GLU	N	15.46
1	B	552:MSE	C	553:GLU	N	15.46
1	C	552:MSE	C	553:GLU	N	15.46
1	D	552:MSE	C	553:GLU	N	15.46
1	E	552:MSE	C	553:GLU	N	15.46