

wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:58 PM BST

PDB ID : 4D2X
EMDB ID: : EMD-2559
Title : Negative-stain electron microscopy of E. coli ClpB of Y503D hyperactive mutant (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 : 2014-05-13
Resolution : 20.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

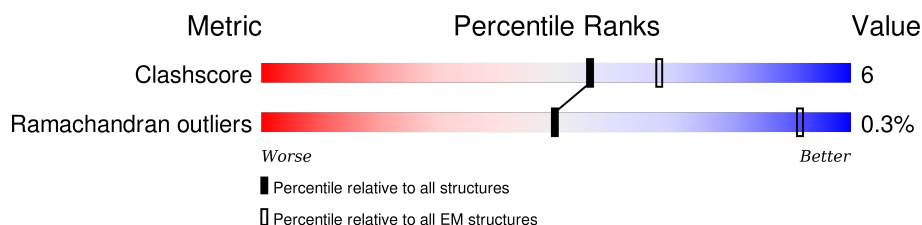
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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	114402	924
Ramachandran outliers	111179	726

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	■ 72% ■ ■ ■ ■ 26%
1	B	858	■ 74% ■ ■ ■ ■ 24%
1	C	858	■ 74% ■ ■ ■ ■ 24%
1	D	858	■ 74% ■ ■ ■ ■ 24%
1	E	858	■ 74% ■ ■ ■ ■ 24%
1	F	858	■ 74% ■ ■ ■ ■ 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11739 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	638	Total	C	N	0	0
			1914	1276	638		
1	B	655	Total	C	N	0	0
			1965	1310	655		
1	C	655	Total	C	N	0	0
			1965	1310	655		
1	D	655	Total	C	N	0	0
			1965	1310	655		
1	E	655	Total	C	N	0	0
			1965	1310	655		
1	F	655	Total	C	N	0	0
			1965	1310	655		

There are 6 discrepancies between the modelled and reference sequences:

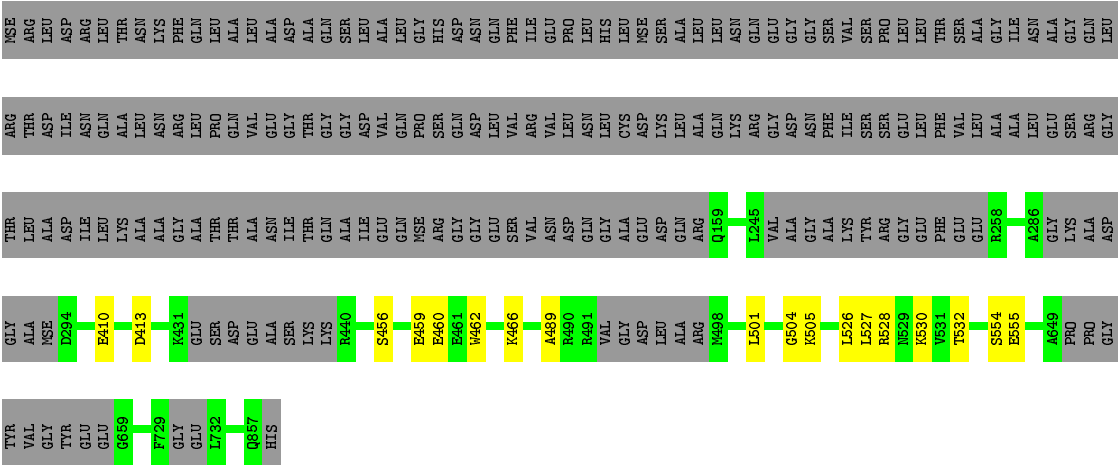
Chain	Residue	Modelled	Actual	Comment	Reference
A	858	HIS	-	EXPRESSION TAG	UNP P63284
B	858	HIS	-	EXPRESSION TAG	UNP P63284
C	858	HIS	-	EXPRESSION TAG	UNP P63284
D	858	HIS	-	EXPRESSION TAG	UNP P63284
E	858	HIS	-	EXPRESSION TAG	UNP P63284
F	858	HIS	-	EXPRESSION TAG	UNP P63284

- Molecule 1: CHAPERONE PROTEIN CLPB

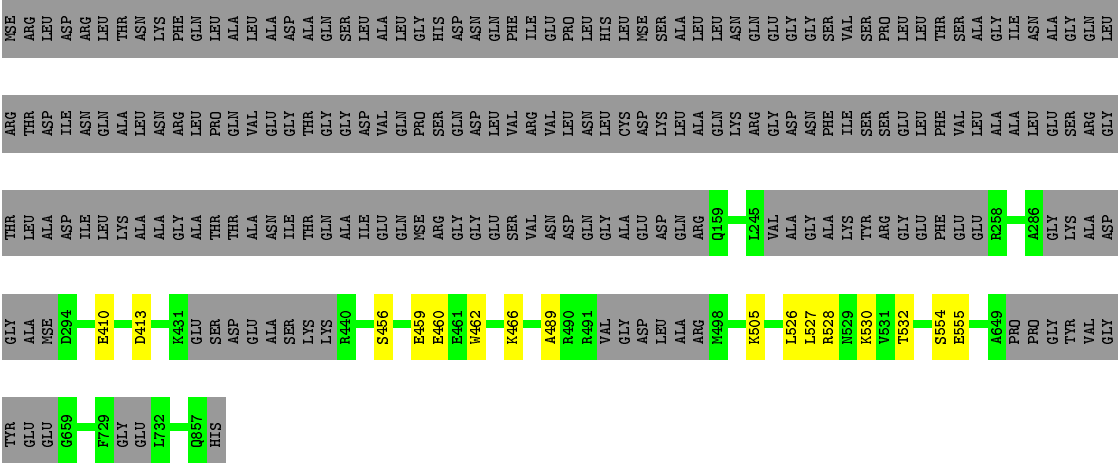
- Molecule 1: CHAPERONE PROTEIN CLPB

- Molecule 1: CHAPERONE PROTEIN CLPB

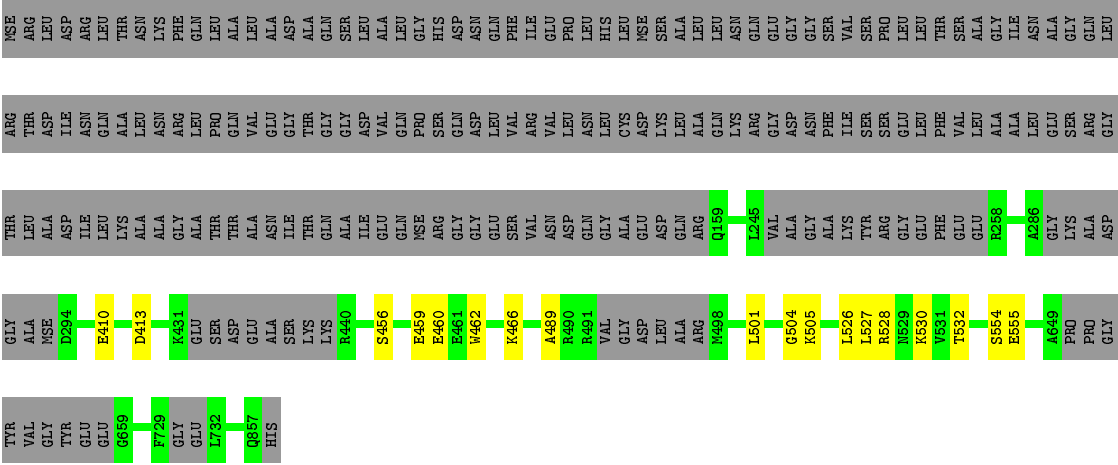


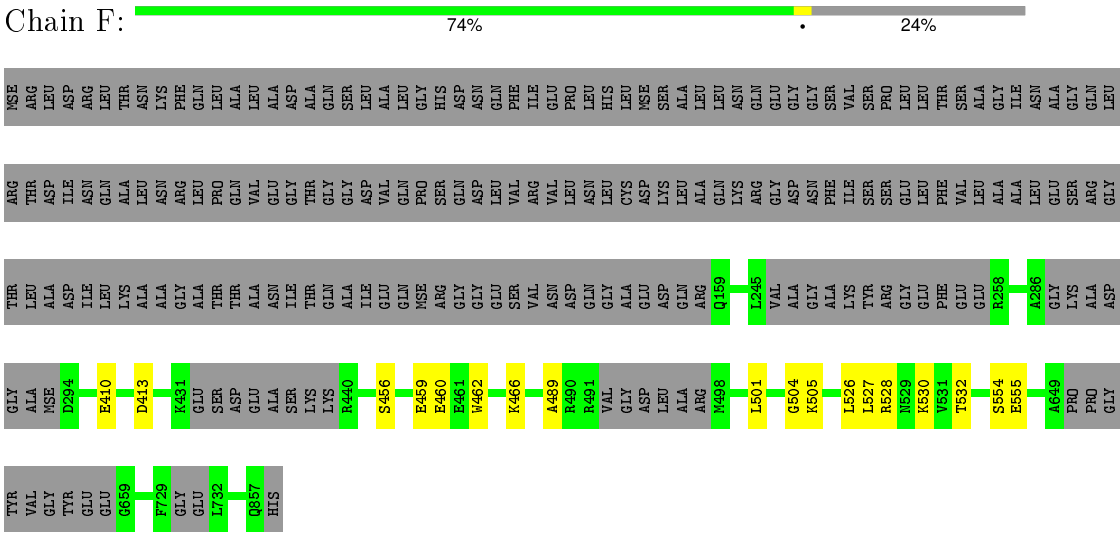
• Molecule 1: CHAPERONE PROTEIN CLPB



• Molecule 1: CHAPERONE PROTEIN CLPB



● Molecule 1: CHAPERONE PROTEIN CLPB



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	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	50000	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	0.37	0/1888	0.76	0/1862
1	B	0.37	0/1940	0.75	0/1915
1	C	0.37	0/1940	0.75	0/1915
1	D	0.37	0/1940	0.75	0/1915
1	E	0.37	0/1940	0.75	0/1915
1	F	0.37	0/1940	0.75	0/1915
All	All	0.37	0/11588	0.76	0/11437

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

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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	1914	0	684	17	0
1	B	1965	0	704	18	0
1	C	1965	0	704	17	0
1	D	1965	0	704	16	0
1	E	1965	0	704	17	0
1	F	1965	0	704	17	0
All	All	11739	0	4204	102	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 6.

The worst 5 of 102 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:D:460:GLU:CA	1:D:527:LEU:C	1.89	1.41
1:C:460:GLU:CA	1:C:527:LEU:C	1.89	1.41
1:B:460:GLU:CA	1:B:527:LEU:C	1.89	1.39
1:E:460:GLU:CA	1:E:527:LEU:C	1.89	1.39
1:F:460:GLU:CA	1:F:527:LEU:C	1.89	1.39

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	618/858 (72%)	588 (95%)	28 (4%)	2 (0%)	46	83
1	B	637/858 (74%)	607 (95%)	28 (4%)	2 (0%)	46	83
1	C	637/858 (74%)	607 (95%)	28 (4%)	2 (0%)	46	83
1	D	637/858 (74%)	607 (95%)	28 (4%)	2 (0%)	46	83
1	E	637/858 (74%)	607 (95%)	28 (4%)	2 (0%)	46	83
1	F	637/858 (74%)	607 (95%)	28 (4%)	2 (0%)	46	83
All	All	3803/5148 (74%)	3623 (95%)	168 (4%)	12 (0%)	50	83

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](#)

There are no chain breaks in this entry.