



## wwPDB EM Map/Model Validation Report

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J83  
EMDB ID: : EMD-6120  
Title : Heptameric EspB Rosetta model guided by EM density  
Authors : Solomonson, M.; DiMaio, F.; Strynadka, N.C.J.  
Deposited on : 2014-09-30  
Resolution : 30.00 Å(reported)  
Based on PDB ID : 4WJ1

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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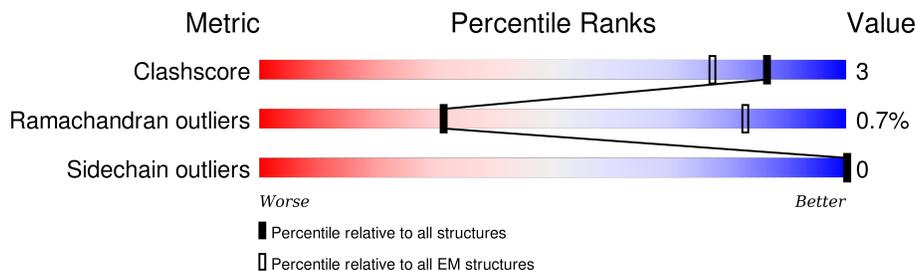
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 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 30.00 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
Sidechain outliers	111093	686

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  $\geq 3$ , 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	371	
1	B	371	
1	C	371	
1	D	371	
1	E	371	
1	F	371	
1	G	371	

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 29092 atoms, of which 14266 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 ESX-1 secretion-associated protein EspB.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	276	4156	1309	2038	376	426	7	0	0
1	B	276	4156	1309	2038	376	426	7	0	0
1	C	276	4156	1309	2038	376	426	7	0	0
1	D	276	4156	1309	2038	376	426	7	0	0
1	E	276	4156	1309	2038	376	426	7	0	0
1	F	276	4156	1309	2038	376	426	7	0	0
1	G	276	4156	1309	2038	376	426	7	0	0

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
A	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
A	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
A	-19	SER	-	EXPRESSION TAG	UNP P9WJD9
A	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
A	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
A	-7	SER	-	EXPRESSION TAG	UNP P9WJD9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
A	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
A	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
A	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
A	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
A	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
A	0	SER	-	EXPRESSION TAG	UNP P9WJD9
B	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
B	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
B	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
B	-19	SER	-	EXPRESSION TAG	UNP P9WJD9
B	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
B	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
B	-7	SER	-	EXPRESSION TAG	UNP P9WJD9
B	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
B	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
B	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
B	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
B	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
B	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
B	0	SER	-	EXPRESSION TAG	UNP P9WJD9
C	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
C	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
C	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
C	-19	SER	-	EXPRESSION TAG	UNP P9WJD9
C	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
C	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
C	-7	SER	-	EXPRESSION TAG	UNP P9WJD9
C	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
C	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
C	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
C	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
C	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
C	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
C	0	SER	-	EXPRESSION TAG	UNP P9WJD9
D	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
D	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
D	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
D	-19	SER	-	EXPRESSION TAG	UNP P9WJD9
D	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
D	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
D	-7	SER	-	EXPRESSION TAG	UNP P9WJD9
D	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
D	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
D	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
D	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
D	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
D	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
D	0	SER	-	EXPRESSION TAG	UNP P9WJD9
E	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
E	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
E	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
E	-19	SER	-	EXPRESSION TAG	UNP P9WJD9
E	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
E	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
E	-7	SER	-	EXPRESSION TAG	UNP P9WJD9
E	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
E	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
E	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
E	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
E	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
E	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
E	0	SER	-	EXPRESSION TAG	UNP P9WJD9
F	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
F	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
F	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
F	-19	SER	-	EXPRESSION TAG	UNP P9WJD9
F	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
F	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
F	-7	SER	-	EXPRESSION TAG	UNP P9WJD9
F	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
F	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
F	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
F	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
F	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
F	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
F	0	SER	-	EXPRESSION TAG	UNP P9WJD9
G	-22	MET	-	EXPRESSION TAG	UNP P9WJD9
G	-21	GLY	-	EXPRESSION TAG	UNP P9WJD9
G	-20	SER	-	EXPRESSION TAG	UNP P9WJD9
G	-19	SER	-	EXPRESSION TAG	UNP P9WJD9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-18	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-17	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-16	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-15	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-14	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-13	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-12	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-11	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-10	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-9	HIS	-	EXPRESSION TAG	UNP P9WJD9
G	-8	SER	-	EXPRESSION TAG	UNP P9WJD9
G	-7	SER	-	EXPRESSION TAG	UNP P9WJD9
G	-6	GLY	-	EXPRESSION TAG	UNP P9WJD9
G	-5	LEU	-	EXPRESSION TAG	UNP P9WJD9
G	-4	VAL	-	EXPRESSION TAG	UNP P9WJD9
G	-3	PRO	-	EXPRESSION TAG	UNP P9WJD9
G	-2	ALA	-	EXPRESSION TAG	UNP P9WJD9
G	-1	GLY	-	EXPRESSION TAG	UNP P9WJD9
G	0	SER	-	EXPRESSION TAG	UNP P9WJD9





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	1455	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	49000	Depositor
Image detector	FEI EAGLE (4k x 4k)	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	0.84	0/2159	1.04	12/2938 (0.4%)
1	B	0.84	0/2159	1.04	11/2938 (0.4%)
1	C	0.84	0/2159	1.04	12/2938 (0.4%)
1	D	0.84	0/2159	1.04	11/2938 (0.4%)
1	E	0.84	0/2159	1.04	11/2938 (0.4%)
1	F	0.84	0/2159	1.04	11/2938 (0.4%)
1	G	0.84	0/2159	1.04	11/2938 (0.4%)
All	All	0.84	0/15113	1.04	79/20566 (0.4%)

There are no bond length outliers.

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	177	GLU	C-N-CA	12.77	149.11	122.30
1	E	177	GLU	C-N-CA	12.76	149.09	122.30
1	B	177	GLU	C-N-CA	12.76	149.09	122.30
1	C	177	GLU	C-N-CA	12.74	149.06	122.30
1	D	177	GLU	C-N-CA	12.74	149.05	122.30

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	2118	2038	2035	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2118	2038	2035	10	0
1	C	2118	2038	2035	10	0
1	D	2118	2038	2035	11	0
1	E	2118	2038	2035	12	0
1	F	2118	2038	2035	10	0
1	G	2118	2038	2035	12	0
All	All	14826	14266	14245	74	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 74 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:245:GLN:C	1:A:248:PRO:HD2	2.14	0.68
1:B:245:GLN:C	1:B:248:PRO:HD2	2.14	0.68
1:E:245:GLN:C	1:E:248:PRO:HD2	2.14	0.68
1:D:245:GLN:C	1:D:248:PRO:HD2	2.14	0.68
1:G:245:GLN:C	1:G:248:PRO:HD2	2.14	0.68

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	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26 71
1	B	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26 71
1	C	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26 71
1	D	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26 71
1	E	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26	71
1	G	274/371 (74%)	265 (97%)	7 (3%)	2 (1%)	26	71
All	All	1918/2597 (74%)	1855 (97%)	49 (3%)	14 (1%)	31	71

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	B	99	THR
1	C	99	THR
1	D	99	THR
1	E	99	THR

### 5.3.2 Protein sidechains [i](#)

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	215/286 (75%)	215 (100%)	0	100	100
1	B	215/286 (75%)	215 (100%)	0	100	100
1	C	215/286 (75%)	215 (100%)	0	100	100
1	D	215/286 (75%)	215 (100%)	0	100	100
1	E	215/286 (75%)	215 (100%)	0	100	100
1	F	215/286 (75%)	215 (100%)	0	100	100
1	G	215/286 (75%)	215 (100%)	0	100	100
All	All	1505/2002 (75%)	1505 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	274	ASN

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Mol	Chain	Res	Type
1	G	274	ASN
1	E	274	ASN
1	B	274	ASN
1	F	274	ASN

### 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.