



wwPDB EM Validation Summary Report ⓘ

Dec 13, 2022 – 12:22 AM EST

PDB ID : 3BYH
Title : Model of actin-fimbrin ABD2 complex
Authors : Galkin, V.E.; Orlova, A.; Cherepanova, O.; Lebart, M.C.; Egelman, E.H.
Deposited on : 2008-01-16
Resolution : 12.00 Å (reported)
Based on initial models : 2BTF, 1PXY

This is a wwPDB EM 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

<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>.

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

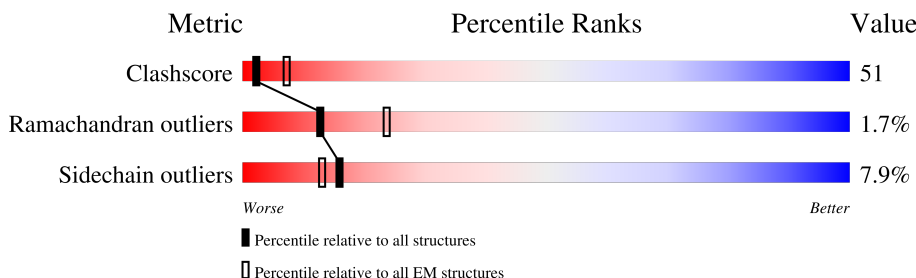
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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 ≥ 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	374	
2	B	231	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4795 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 Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		

- Molecule 2 is a protein called fimbrin ABD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	231	Total	C	N	O	S	0	0
			1878	1207	328	332	11		

4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 12.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-12.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4795	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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	1.00	0/2976	1.94	86/4022 (2.1%)
2	B	0.29	0/1912	0.50	0/2580
All	All	0.80	0/4888	1.55	86/6602 (1.3%)

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	1

There are no bond length outliers.

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	356	TRP	CD1-CG-CD2	13.46	117.06	106.30
1	A	5	ILE	CA-C-N	-11.79	91.26	117.20
1	A	210	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	356	TRP	CB-CG-CD1	-9.89	114.15	127.00
1	A	132	MET	CA-CB-CG	9.67	129.74	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ASP	Mainchain

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	2917	0	2863	321	0
2	B	1878	0	1933	212	0
All	All	4795	0	4796	485	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 51.

The worst 5 of 485 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:62:ARG:CG	1:A:204:ALA:HA	1.19	1.67
1:A:35:VAL:HB	1:A:70:PRO:CD	1.09	1.54
1:A:35:VAL:CB	1:A:70:PRO:HD3	1.09	1.54
2:B:498:MET:CE	2:B:610:LEU:HD22	1.13	1.54
2:B:498:MET:CG	2:B:610:LEU:HD13	1.31	1.54

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	364/374 (97%)	321 (88%)	33 (9%)	10 (3%)	5	31
2	B	227/231 (98%)	220 (97%)	7 (3%)	0	100	100
All	All	591/605 (98%)	541 (92%)	40 (7%)	10 (2%)	13	42

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	203	THR
1	A	233	SER
1	A	355	MET
1	A	5	ILE

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	317/317 (100%)	280 (88%)	37 (12%)	5	21
2	B	212/213 (100%)	207 (98%)	5 (2%)	49	69
All	All	529/530 (100%)	487 (92%)	42 (8%)	16	35

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	THR
1	A	368	SER
1	A	335	ARG
1	A	350	SER
2	B	437	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	458	GLN
2	B	465	GLN
2	B	605	ASN
2	B	492	GLN
2	B	403	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 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	4
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	335:ARG	C	336:LYS	N	7.03
1	A	145:SER	C	146:GLY	N	6.11
1	B	507:SER	C	513:GLU	N	5.94
1	A	69:TYR	C	70:PRO	N	5.40
1	A	33:SER	C	34:ILE	N	2.67