



# wwPDB X-ray Structure Validation Summary Report

Jan 20, 2024 – 04:21 pm GMT

PDB ID : 7ANK  
Title : Crystal structure of sarcomeric protein FATZ-1 (d91-FATZ-1 construct) in complex with half dimer of alpha-actinin-2  
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Deposited on : 2020-10-12  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

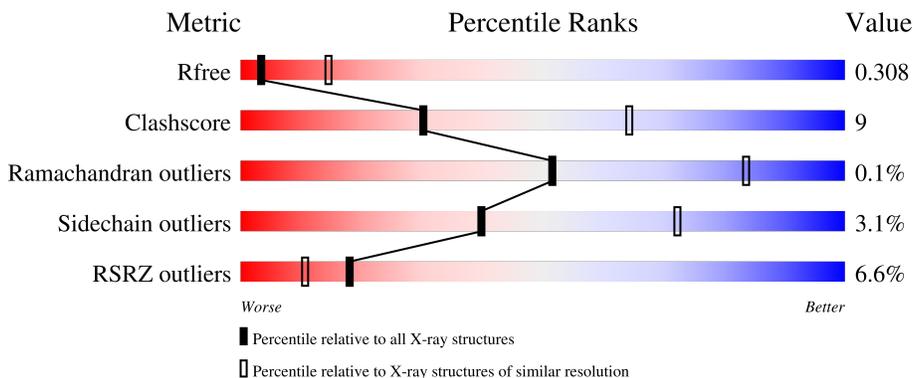
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	 8% 66% 22% 10%
2	B	389	 4% 80% 18%
3	C	209	 16% 82%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7319 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Alpha-actinin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3928	2463	716	728	21	71	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	SER	-	expression tag	UNP P35609
A	509	GLU	-	expression tag	UNP P35609
A	510	ARG	-	expression tag	UNP P35609
A	511	VAL	-	expression tag	UNP P35609
A	512	ARG	-	expression tag	UNP P35609
A	513	ASN	-	expression tag	UNP P35609
A	514	PHE	-	expression tag	UNP P35609
A	515	GLU	-	expression tag	UNP P35609
A	516	ASP	-	expression tag	UNP P35609
A	517	PRO	-	expression tag	UNP P35609
A	518	ALA	-	expression tag	UNP P35609
A	519	ALA	-	expression tag	UNP P35609
A	520	ASN	-	expression tag	UNP P35609
A	521	LYS	-	expression tag	UNP P35609
A	522	ALA	-	expression tag	UNP P35609
A	523	ARG	-	expression tag	UNP P35609
A	524	LYS	-	expression tag	UNP P35609
A	525	GLU	-	expression tag	UNP P35609
A	526	ALA	-	expression tag	UNP P35609
A	527	GLU	-	expression tag	UNP P35609
A	528	LEU	-	expression tag	UNP P35609
A	529	ALA	-	expression tag	UNP P35609
A	530	ALA	-	expression tag	UNP P35609
A	531	ALA	-	expression tag	UNP P35609
A	532	THR	-	expression tag	UNP P35609
A	533	ALA	-	expression tag	UNP P35609
A	534	GLU	-	expression tag	UNP P35609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	535	GLN	-	expression tag	UNP P35609

- Molecule 2 is a protein called Alpha-actinin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	382	3079	1926	538	599	16	36	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	GLY	-	expression tag	UNP P35609
B	507	SER	-	expression tag	UNP P35609
B	508	SER	-	expression tag	UNP P35609

- Molecule 3 is a protein called Myozenin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	38	312	201	52	57	2	0	0	0

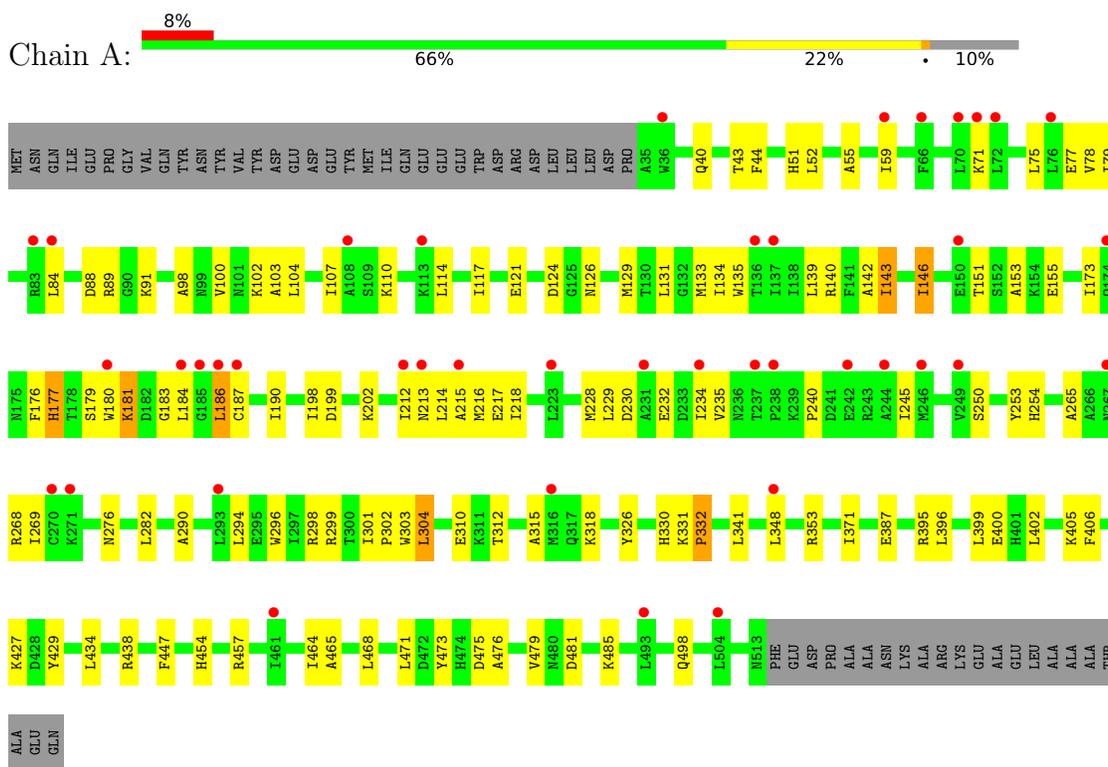
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	91	GLY	-	expression tag	UNP Q9NP98

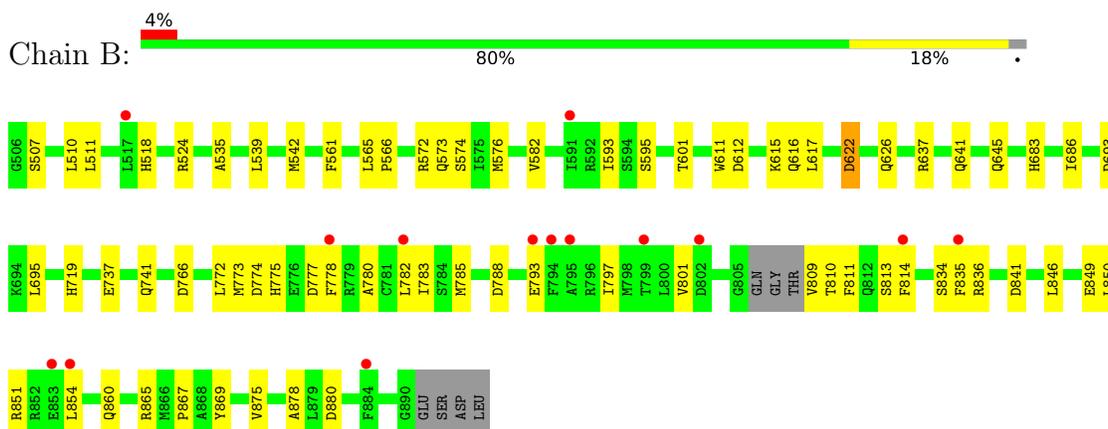
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Alpha-actinin-2



- Molecule 2: Alpha-actinin-2



● Molecule 3: Myozenin-1



GLY PRO THR VAL GLY GLN LEU GLY THR ALA GLY GLY PHE TYR SER LYS SER ASN GLY ARG GLY SER GLN ALA GLY TYR SER GLY ALA GLN TYR GLY TYR GLY ASP GLN HIS LEU LEU GLY GLY GLY GLY ALA GLY THR GLY GLY PRO ALA GLN

ALA GLY ARG GLY ALA ALA GLY THR ALA GLY VAL GLY GLU THR LYS SER GLY ASP GLN ALA ALA GLY GLU GLY LYS HIS ILE THR VAL PHE LYS T183 Y184 W188 F189 R190 A191 M192 Q197 Q198 LYS MET GLU LEU LEU GLY ILE ASP LEU LEU ALA TYR VAL GLY ALA R212 L215

P227 Y231 E232 K233 ALA SER LYS ARG MET THR PHE GLN MET PRO LYS PHE ASP LEU GLY PRO ALA LEU LEU SER GLU PRO LEU VAL ILE THR TYR ASN GLN ASN LEU SER ASN ARG PRO SER PHE ASN ARG THR PRO ILE PRO TRP LEU SER SER GLY PRO VAL ASP TVR ASN VAL ASP ILE

GLY ILE LEU ASP GLU THR GLU LEU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.60Å 56.92Å 209.38Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	46.94 – 3.20 46.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.94-3.20) 98.9 (46.94-3.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 3.19Å)	Xtrriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, $R_{free}$	0.255 , 0.284 0.282 , 0.308	Depositor DCC
$R_{free}$ test set	1288 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	127.5	Xtrriage
Anisotropy	0.516	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 154.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	206.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.35	0/3999	0.52	0/5386
2	B	0.33	0/3134	0.49	0/4232
3	C	0.27	0/321	0.47	0/431
All	All	0.34	0/7454	0.51	0/10049

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	3928	0	3937	85	0
2	B	3079	0	3001	54	0
3	C	312	0	300	4	0
All	All	7319	0	7238	134	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 9.

The worst 5 of 134 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)
2:B:611:TRP:HE1	2:B:615:LYS:HE2	1.22	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:772:LEU:HB2	2:B:811:PHE:HA	1.42	0.99
1:A:139:LEU:HA	1:A:143:ILE:HG13	1.53	0.88
1:A:282:LEU:HB3	1:A:348:LEU:HD21	1.54	0.87
2:B:810:THR:HB	2:B:813:SER:HB3	1.57	0.86

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 X-ray entries followed by that with respect to entries of similar resolution.

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	477/535 (89%)	467 (98%)	10 (2%)	0	100	100
2	B	378/389 (97%)	359 (95%)	18 (5%)	1 (0%)	41	74
3	C	34/209 (16%)	32 (94%)	2 (6%)	0	100	100
All	All	889/1133 (78%)	858 (96%)	30 (3%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	788	ASP

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	420/467 (90%)	402 (96%)	18 (4%)	29	64
2	B	332/338 (98%)	327 (98%)	5 (2%)	65	85
3	C	32/151 (21%)	31 (97%)	1 (3%)	40	72
All	All	784/956 (82%)	760 (97%)	24 (3%)	40	72

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	PRO
1	A	498	GLN
1	A	395	ARG
2	B	511	LEU
1	A	181	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	632	GLN
2	B	684	ASN
2	B	860	GLN
1	A	444	HIS
1	A	276	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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	470/535 (87%)	0.54	41 (8%) 10 5	134, 206, 270, 286	0
2	B	377/389 (96%)	0.24	14 (3%) 41 26	145, 191, 288, 295	0
3	C	38/209 (18%)	0.21	3 (7%) 12 6	186, 222, 241, 246	0
All	All	885/1133 (78%)	0.40	58 (6%) 18 11	134, 196, 277, 295	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	TRP	5.8
2	B	778	PHE	5.6
1	A	185	GLY	5.2
1	A	212	ILE	5.0
1	A	66	PHE	4.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.