



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 12:18 AM JST

PDB ID : 7DS4  
Title : Crystal structure of actin capping protein in complex with twinflin-1 C-terminus tail F323K mutant  
Authors : Takeda, S.  
Deposited on : 2020-12-30  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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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	:	2.18
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)	:	2.18



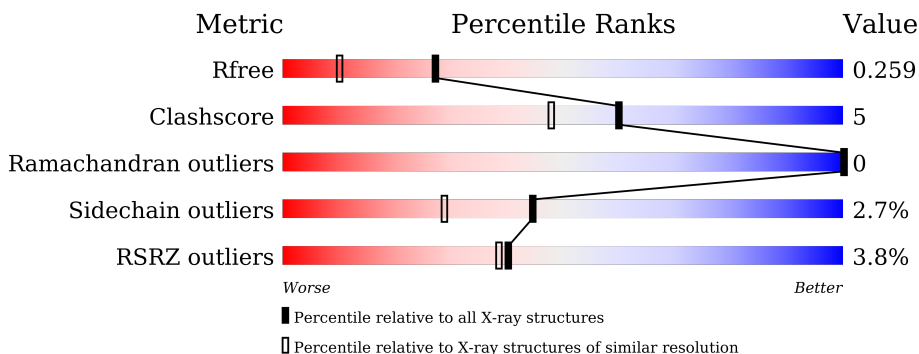
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	286	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>
2	B	244	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>.</div> </div> </div>
3	C	30	<div> <div>3%</div> <div> <div></div> <div>37%</div> <div>13%</div> <div>50%</div> </div> </div>



## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4578 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 F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	5	0
			2180	1375	378	422	5			

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	3	1
			1858	1162	318	368	10			

- Molecule 3 is a protein called Twinfilin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	0	0	0
			111	70	26	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	323	LYS	PHE	engineered mutation	UNP Q91YR1

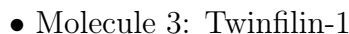
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	197	Total	O	0	9
			203	203		
4	B	207	Total	O	0	4
			209	209		
4	C	17	Total	O	0	0
			17	17		





- Molecule 1: F-actin-capping protein subunit alpha-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.45Å 66.72Å 164.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.22 – 1.85 44.22 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.22-1.85) 99.8 (44.22-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.18	Depositor
R, $R_{free}$	0.209 , 0.259 0.209 , 0.259	Depositor DCC
$R_{free}$ test set	2503 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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	0.34	0/2246	0.51	0/3055
2	B	0.36	0/1898	0.59	1/2566 (0.0%)
3	C	0.38	0/112	0.54	0/147
All	All	0.35	0/4256	0.55	1/5768 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	177	LEU	CA-CB-CG	5.12	127.06	115.30

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	2180	0	2054	23	0
2	B	1858	0	1810	20	0
3	C	111	0	127	4	0
4	A	203	0	0	2	0
4	B	209	0	0	0	0
4	C	17	0	0	1	0
All	All	4578	0	3991	37	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 5.

All (37) 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:243:ILE:HD13	2:B:187:MET:HE2	1.77	0.67
1:A:162:GLN:HG3	2:B:243:LEU:HD23	1.82	0.62
1:A:190:ALA:HB3	1:A:212:ILE:HB	1.87	0.57
2:B:66:ARG:O	3:C:332:LYS:HE2	2.05	0.56
1:A:247:TYR:CD1	2:B:233:PHE:HA	2.40	0.56
1:A:219:SER:OG	1:A:220:SER:N	2.42	0.52
2:B:18:PRO:O	2:B:21:ILE:HG13	2.09	0.52
1:A:165:PRO:HG3	4:A:351:HOH:O	2.11	0.51
2:B:19[A]:GLN:NE2	2:B:188:ASN:OD1	2.40	0.51
1:A:94:ILE:HG22	1:A:110:PRO:HA	1.92	0.50
1:A:120:TRP:HH2	1:A:218:VAL:HG23	1.77	0.50
2:B:227:THR:O	2:B:230:GLU:HG3	2.12	0.50
1:A:201:ASP:HB3	2:B:195:ARG:HH12	1.77	0.49
1:A:247:TYR:HD1	2:B:233:PHE:HA	1.76	0.49
3:C:333:ARG:NH1	4:C:401:HOH:O	2.46	0.48
1:A:192:LEU:O	1:A:209:HIS:HA	2.13	0.48
1:A:72:ASP:OD1	1:A:129:ARG:NH2	2.41	0.48
1:A:137:PRO:O	1:A:138[B]:ASN:ND2	2.48	0.46
1:A:177:TRP:CE3	1:A:190:ALA:HB2	2.51	0.46
1:A:170:ASN:HB2	4:A:314:HOH:O	2.18	0.44
2:B:86:GLY:O	2:B:88:MET:HG2	2.18	0.44
1:A:11[B]:GLU:H	1:A:11[B]:GLU:HG3	1.56	0.44
2:B:178:GLN:HA	2:B:187:MET:O	2.18	0.43
1:A:32:VAL:HG13	2:B:12:LEU:HD21	2.00	0.43
1:A:253:THR:OG1	1:A:254:THR:N	2.51	0.43
2:B:19[A]:GLN:OE1	2:B:188:ASN:ND2	2.48	0.43
1:A:120:TRP:CH2	1:A:218:VAL:HG23	2.54	0.43
2:B:63:ASP:O	3:C:332:LYS:HE3	2.19	0.42
1:A:216:VAL:HG11	1:A:228:PHE:HE1	1.84	0.42
2:B:17:PRO:HA	2:B:18:PRO:HD3	1.82	0.42
2:B:131:VAL:HA	2:B:152:HIS:O	2.20	0.41
2:B:155:GLU:HB2	3:C:326:PRO:HG3	2.01	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.83	0.41
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.86	0.41
2:B:135:LYS:HG3	2:B:149:ASP:OD1	2.21	0.41
2:B:197:MET:HG3	2:B:220:MET:CE	2.51	0.41
1:A:269:ILE:HD12	2:B:107:TYR:HD1	1.86	0.40

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 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	273/286 (96%)	261 (96%)	12 (4%)	0	100	100
2	B	232/244 (95%)	229 (99%)	3 (1%)	0	100	100
3	C	13/30 (43%)	12 (92%)	1 (8%)	0	100	100
All	All	518/560 (92%)	502 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	232/252 (92%)	227 (98%)	5 (2%)	52	36
2	B	206/216 (95%)	200 (97%)	6 (3%)	42	26
3	C	10/22 (46%)	9 (90%)	1 (10%)	7	1
All	All	448/490 (91%)	436 (97%)	12 (3%)	44	29

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	162	GLN
1	A	215	SER
1	A	218	VAL
1	A	254	THR

*Continued on next page...*



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Mol	Chain	Res	Type
2	B	105	ASP
2	B	148	TRP
2	B	164	THR
2	B	177	LEU
2	B	187	MET
2	B	230	GLU
3	C	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	196	GLN

### 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	270/286 (94%)	0.38	17 (6%) 20 19	20, 35, 67, 90	0
2	B	235/244 (96%)	0.13	2 (0%) 84 84	19, 28, 49, 67	0
3	C	15/30 (50%)	0.91	1 (6%) 17 17	29, 39, 60, 61	0
All	All	520/560 (92%)	0.28	20 (3%) 40 38	19, 32, 63, 90	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	144	ILE	6.2
1	A	112	ASP	4.8
1	A	120	TRP	4.4
1	A	276	SER	4.0
1	A	116	ALA	4.0
3	C	326	PRO	3.9
1	A	148	ILE	3.2
1	A	181	ILE	2.9
1	A	113	THR	2.8
1	A	218	VAL	2.5
1	A	114	GLU	2.5
1	A	221	ASP	2.5
1	A	201	ASP	2.4
1	A	84	ASN	2.3
2	B	231	ILE	2.3
1	A	216	VAL	2.2
1	A	253	THR	2.2
1	A	83	GLY	2.1
1	A	254	THR	2.1
1	A	251	SER	2.1



## 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.