



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:42 AM GMT

PDB ID : 2D10  
Title : Crystal structure of the Radixin FERM domain complexed with the NHERF-1 C-terminal tail peptide  
Authors : Terawaki, S.; Maesaki, R.; Hakoshima, T.  
Deposited on : 2005-08-11  
Resolution : 2.50 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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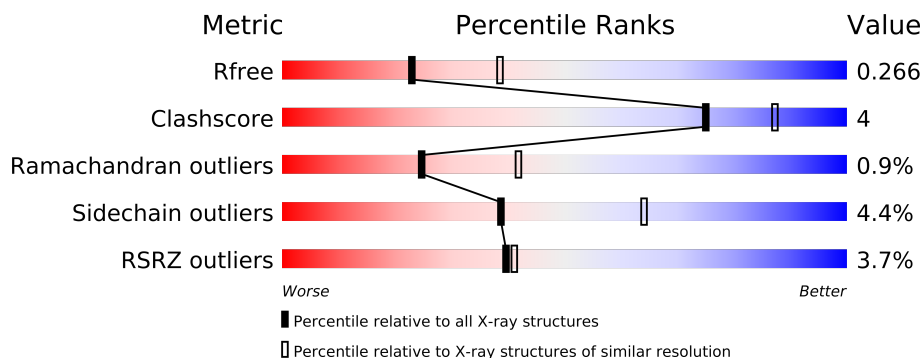
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	312	
1	B	312	
1	C	312	
1	D	312	
2	E	28	
2	F	28	
2	G	28	
2	H	28	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11025 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Radixin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2448	1582	415	442	9			
1	B	297	Total	C	N	O	S	0	0	0
			2456	1585	418	444	9			
1	C	297	Total	C	N	O	S	0	0	0
			2460	1588	419	444	9			
1	D	297	Total	C	N	O	S	0	0	0
			2456	1585	418	444	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP P26043
A	0	SER	-	CLONING ARTIFACT	UNP P26043
B	-1	GLY	-	CLONING ARTIFACT	UNP P26043
B	0	SER	-	CLONING ARTIFACT	UNP P26043
C	-1	GLY	-	CLONING ARTIFACT	UNP P26043
C	0	SER	-	CLONING ARTIFACT	UNP P26043
D	-1	GLY	-	CLONING ARTIFACT	UNP P26043
D	0	SER	-	CLONING ARTIFACT	UNP P26043

- Molecule 2 is a protein called Ezrin-radixin-moesin binding phosphoprotein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	S	0	0	0
			146	92	25	28	1			
2	F	20	Total	C	N	O	S	0	0	0
			150	94	25	30	1			
2	G	20	Total	C	N	O	S	0	0	0
			146	92	24	29	1			
2	H	20	Total	C	N	O	S	0	0	0
			146	92	25	28	1			

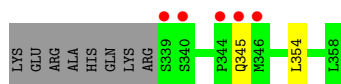
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total 160	O 160	0	0
3	B	168	Total 168	O 168	0	0
3	C	126	Total 126	O 126	0	0
3	D	153	Total 153	O 153	0	0
3	E	5	Total 5	O 5	0	0
3	F	1	Total 1	O 1	0	0
3	G	1	Total 1	O 1	0	0
3	H	3	Total 3	O 3	0	0



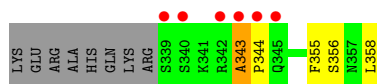
- Molecule 2: Ezrin-radixin-moesin binding phosphoprotein 50

Chain E: 



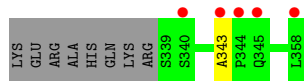
- Molecule 2: Ezrin-radixin-moesin binding phosphoprotein 50

Chain F: 



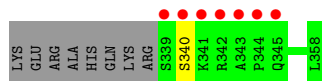
- Molecule 2: Ezrin-radixin-moesin binding phosphoprotein 50

Chain G: 



- Molecule 2: Ezrin-radixin-moesin binding phosphoprotein 50

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.39Å 146.28Å 177.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 2.50 29.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.93-2.50) 99.0 (29.69-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.91 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.229 , 0.268 0.229 , 0.266	Depositor DCC
$R_{free}$ test set	1593 reflections (2.60%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 62834 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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  >5	RMSZ	# Z  >5
1	A	0.37	0/2507	0.51	1/3387 (0.0%)
1	B	0.37	0/2515	0.53	1/3400 (0.0%)
1	C	0.35	0/2519	0.50	1/3404 (0.0%)
1	D	0.37	0/2515	0.51	1/3400 (0.0%)
2	E	0.33	0/149	0.43	0/201
2	F	0.39	0/153	0.50	0/206
2	G	0.36	0/149	0.44	0/201
2	H	0.37	0/149	0.46	0/201
All	All	0.37	0/10656	0.51	4/14400 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	297	PRO	N-CA-CB	6.28	110.83	103.30
1	C	297	PRO	N-CA-CB	6.26	110.81	103.30
1	A	297	PRO	N-CA-CB	6.19	110.72	103.30
1	B	297	PRO	N-CA-CB	5.79	110.25	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2448	0	2426	25	0
1	B	2456	0	2419	18	0
1	C	2460	0	2430	24	0
1	D	2456	0	2419	19	0
2	E	146	0	120	0	0
2	F	150	0	124	3	0
2	G	146	0	118	1	0
2	H	146	0	120	0	0
3	A	160	0	0	1	0
3	B	168	0	0	3	0
3	C	126	0	0	1	0
3	D	153	0	0	2	0
3	E	5	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	0	0
All	All	11025	0	10176	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 83 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:138:ASN:H	1:B:142:HIS:HD1	1.19	0.86
1:C:138:ASN:H	1:C:142:HIS:HD1	1.25	0.84
1:C:8:ARG:HH11	1:C:77:GLN:HE22	1.31	0.76
1:A:138:ASN:H	1:A:142:HIS:HD1	1.34	0.73
1:B:139:LYS:HD2	1:B:139:LYS:H	1.54	0.71

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	293/312 (94%)	284 (97%)	7 (2%)	2 (1%)	30 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	295/312 (95%)	287 (97%)	7 (2%)	1 (0%)	50	73
1	C	295/312 (95%)	284 (96%)	7 (2%)	4 (1%)	16	27
1	D	295/312 (95%)	289 (98%)	4 (1%)	2 (1%)	30	50
2	E	18/28 (64%)	18 (100%)	0	0	100	100
2	F	18/28 (64%)	15 (83%)	2 (11%)	1 (6%)	3	2
2	G	18/28 (64%)	18 (100%)	0	0	100	100
2	H	18/28 (64%)	17 (94%)	0	1 (6%)	3	2
All	All	1250/1360 (92%)	1212 (97%)	27 (2%)	11 (1%)	25	42

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ARG
1	B	180	ARG
1	C	180	ARG
1	C	296	LYS
1	C	297	PRO

### 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	262/282 (93%)	250 (95%)	12 (5%)	37	62
1	B	261/282 (93%)	248 (95%)	13 (5%)	34	58
1	C	262/282 (93%)	252 (96%)	10 (4%)	44	71
1	D	261/282 (93%)	250 (96%)	11 (4%)	40	66
2	E	13/26 (50%)	11 (85%)	2 (15%)	4	7
2	F	14/26 (54%)	14 (100%)	0	100	100
2	G	13/26 (50%)	13 (100%)	0	100	100
2	H	13/26 (50%)	13 (100%)	0	100	100
All	All	1099/1232 (89%)	1051 (96%)	48 (4%)	39	64

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	218	LEU
1	C	111	LEU
1	D	281	LEU
1	B	237	LYS
1	B	289	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	ASN
1	B	226	ASN
1	D	138	ASN
1	B	131	GLN
1	A	131	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	295/312 (94%)	-0.05	5 (1%) 67 69	20, 36, 49, 57	0
1	B	297/312 (95%)	-0.03	6 (2%) 62 64	21, 33, 52, 61	0
1	C	297/312 (95%)	0.21	9 (3%) 48 50	24, 40, 61, 65	0
1	D	297/312 (95%)	-0.09	4 (1%) 74 76	21, 33, 47, 59	0
2	E	20/28 (71%)	1.20	5 (25%) 1 1	57, 64, 79, 79	0
2	F	20/28 (71%)	1.51	6 (30%) 1 1	61, 68, 83, 84	0
2	G	20/28 (71%)	1.17	5 (25%) 1 1	73, 78, 87, 87	0
2	H	20/28 (71%)	1.40	7 (35%) 1 1	59, 68, 84, 84	0
All	All	1266/1360 (93%)	0.09	47 (3%) 39 41	20, 36, 63, 87	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	344	PRO	6.4
2	F	343	ALA	5.5
2	E	339	SER	5.3
2	F	339	SER	5.0
1	B	299	THR	5.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.