



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:09 AM GMT

PDB ID : 2A28  
Title : Atomic-resolution crystal structure of the second SH3 domain of yeast Bzz1 determined from a pseudomerohedrally twinned crystal  
Authors : Kursula, P.; Kursula, I.; Lehmann, F.; Zou, P.; Song, Y.H.; Wilmanns, M.  
Deposited on : 2005-06-22  
Resolution : 1.07 Å(reported)

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

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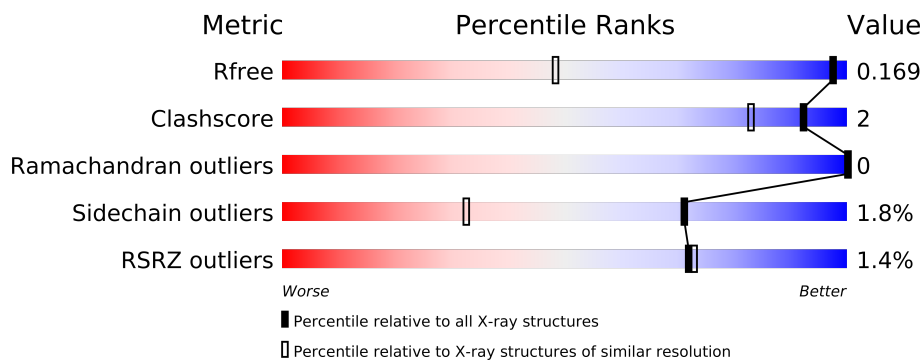
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.07 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	1099 (1.18-0.98)
Clashscore	79885	1084 (1.16-1.00)
Ramachandran outliers	78287	1025 (1.16-1.00)
Sidechain outliers	78261	1023 (1.16-1.00)
RSRZ outliers	66119	1099 (1.18-0.98)

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	54	
1	B	54	
1	C	54	
1	D	54	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2024 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 BZZ1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	54	Total	C	N	O	S	0	1	0
			409	255	61	90	3			
1	B	54	Total	C	N	O	S	0	2	0
			412	258	61	89	4			
1	C	54	Total	C	N	O	S	0	1	0
			409	255	61	90	3			
1	D	54	Total	C	N	O	S	0	0	0
			404	252	61	88	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P38822
A	2	ALA	-	CLONING ARTIFACT	UNP P38822
B	1	GLY	-	CLONING ARTIFACT	UNP P38822
B	2	ALA	-	CLONING ARTIFACT	UNP P38822
C	1	GLY	-	CLONING ARTIFACT	UNP P38822
C	2	ALA	-	CLONING ARTIFACT	UNP P38822
D	1	GLY	-	CLONING ARTIFACT	UNP P38822
D	2	ALA	-	CLONING ARTIFACT	UNP P38822

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		
2	B	116	Total	O	0	0
			116	116		
2	C	67	Total	O	0	0
			67	67		
2	D	99	Total	O	0	0
			99	99		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

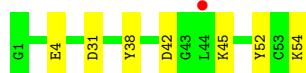
- Molecule 1: BZZ1 protein

Chain A: 



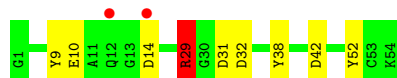
- Molecule 1: BZZ1 protein

Chain B: 



- Molecule 1: BZZ1 protein

Chain C: 



- Molecule 1: BZZ1 protein

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	32.84Å 51.74Å 59.94Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	20.00 – 1.07 19.98 – 1.07	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-1.07) 95.3 (19.98-1.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 1.07Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.111 , 0.166 0.119 , 0.169	Depositor DCC
$R_{free}$ test set	694 reflections (0.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.6	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.3	EDS
Estimated twinning fraction	0.366 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 84808 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	2024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.79	0/421	1.38	6/568 (1.1%)
1	B	0.77	0/428	1.44	7/578 (1.2%)
1	C	0.71	0/421	1.77	15/568 (2.6%)
1	D	0.78	0/412	1.46	5/556 (0.9%)
All	All	0.76	0/1682	1.52	33/2270 (1.5%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	32	ASP	CB-CG-OD1	10.02	127.31	118.30
1	C	29	ARG	NE-CZ-NH2	9.13	124.86	120.30
1	C	29	ARG	NE-CZ-NH1	-8.53	116.04	120.30
1	B	4[A]	GLU	OE1-CD-OE2	-8.07	113.61	123.30
1	B	4[B]	GLU	OE1-CD-OE2	-8.07	113.61	123.30
1	D	29	ARG	CD-NE-CZ	7.84	134.58	123.60
1	C	29	ARG	CD-NE-CZ	7.55	134.17	123.60
1	A	7	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	D	15	ASP	CB-CG-OD1	-7.42	111.63	118.30
1	C	38	TYR	CG-CD1-CE1	7.17	127.04	121.30
1	C	10	GLU	OE1-CD-OE2	-6.99	114.91	123.30
1	C	38	TYR	CZ-CE2-CD2	6.98	126.08	119.80
1	C	38	TYR	CB-CG-CD1	6.58	124.94	121.00
1	A	31	ASP	CB-CG-OD1	6.53	124.17	118.30
1	C	38	TYR	CG-CD2-CE2	-6.47	116.12	121.30
1	C	52	TYR	CB-CG-CD1	6.44	124.86	121.00
1	D	29	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	29	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	9	TYR	CB-CG-CD2	6.24	124.75	121.00
1	C	31	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	C	31	ASP	CB-CG-OD1	6.06	123.76	118.30
1	C	38	TYR	CD1-CE1-CZ	-6.00	114.40	119.80
1	B	52	TYR	CD1-CE1-CZ	5.65	124.89	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	20	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	9	TYR	CB-CG-CD2	5.53	124.32	121.00
1	C	42	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	7	TYR	CB-CG-CD2	5.44	124.27	121.00
1	B	38	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	40[A]	GLU	CA-CB-CG	5.26	124.97	113.40
1	A	40[B]	GLU	CA-CB-CG	5.26	124.97	113.40
1	B	45	LYS	CA-CB-CG	5.22	124.89	113.40
1	B	31	ASP	CB-CG-OD2	5.03	122.83	118.30

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	409	0	0	0	0
1	B	412	0	0	2	0
1	C	409	0	0	2	0
1	D	404	0	0	1	0
2	A	108	0	0	0	0
2	B	116	0	0	0	0
2	C	67	0	0	0	0
2	D	99	0	0	1	0
All	All	2024	0	0	3	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 2.

All (3) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:42:ASP:O	1:C:29:ARG:NE	2.46	0.48
1:D:12:GLN:NE2	2:D:138:HOH:O	2.49	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:42:ASP:O	1:C:29:ARG:NH2	2.53	0.41

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	53/54 (98%)	53 (100%)	0	0	100	100
1	B	54/54 (100%)	54 (100%)	0	0	100	100
1	C	53/54 (98%)	52 (98%)	1 (2%)	0	100	100
1	D	52/54 (96%)	52 (100%)	0	0	100	100
All	All	212/216 (98%)	211 (100%)	1 (0%)	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	42/41 (102%)	42 (100%)	0	100	100
1	B	43/41 (105%)	42 (98%)	1 (2%)	63	21
1	C	42/41 (102%)	40 (95%)	2 (5%)	35	5
1	D	41/41 (100%)	41 (100%)	0	100	100
All	All	168/164 (102%)	165 (98%)	3 (2%)	71	32

All (3) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	54	LYS
1	C	14	ASP
1	C	29	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	54/54 (100%)	0.04	0 100 100	6, 9, 16, 23	0
1	B	54/54 (100%)	0.20	1 (1%) 64 64	7, 10, 22, 26	0
1	C	54/54 (100%)	0.32	2 (3%) 39 41	10, 12, 28, 35	0
1	D	54/54 (100%)	0.12	0 100 100	7, 11, 23, 28	0
All	All	216/216 (100%)	0.17	3 (1%) 72 73	6, 11, 25, 35	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	GLN	3.2
1	C	14	ASP	3.2
1	B	44	LEU	2.4

### 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.