



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:18 AM GMT

PDB ID : 3E66  
Title : Crystal structure of the beta-finger domain of yeast Prp8  
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Deposited on : 2008-08-14  
Resolution : 2.05 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

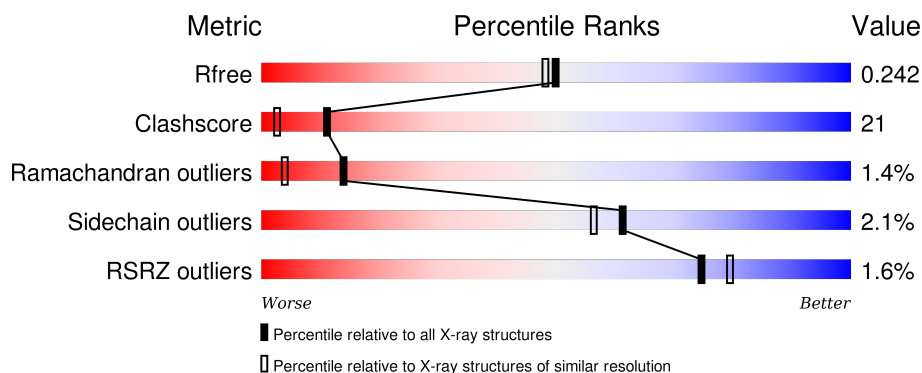
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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. 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	282	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 67%, green 22%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>67%</span> <span>22%</span> <span>10%</span> </div> </div>
1	B	282	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 60%, green 29%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>60%</span> <span>29%</span> <span>10%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4367 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 PRP8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2060	1326	344	382	8			
1	B	255	Total	C	N	O	S	0	0	0
			2060	1326	344	382	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1814	GLY	-	EXPRESSION TAG	UNP P33334
A	1815	PRO	-	EXPRESSION TAG	UNP P33334
A	1816	LEU	-	EXPRESSION TAG	UNP P33334
A	1817	GLY	-	EXPRESSION TAG	UNP P33334
A	1818	SER	-	EXPRESSION TAG	UNP P33334
A	1819	PRO	-	EXPRESSION TAG	UNP P33334
A	1820	GLU	-	EXPRESSION TAG	UNP P33334
A	1821	PHE	-	EXPRESSION TAG	UNP P33334
B	1814	GLY	-	EXPRESSION TAG	UNP P33334
B	1815	PRO	-	EXPRESSION TAG	UNP P33334
B	1816	LEU	-	EXPRESSION TAG	UNP P33334
B	1817	GLY	-	EXPRESSION TAG	UNP P33334
B	1818	SER	-	EXPRESSION TAG	UNP P33334
B	1819	PRO	-	EXPRESSION TAG	UNP P33334
B	1820	GLU	-	EXPRESSION TAG	UNP P33334
B	1821	PHE	-	EXPRESSION TAG	UNP P33334

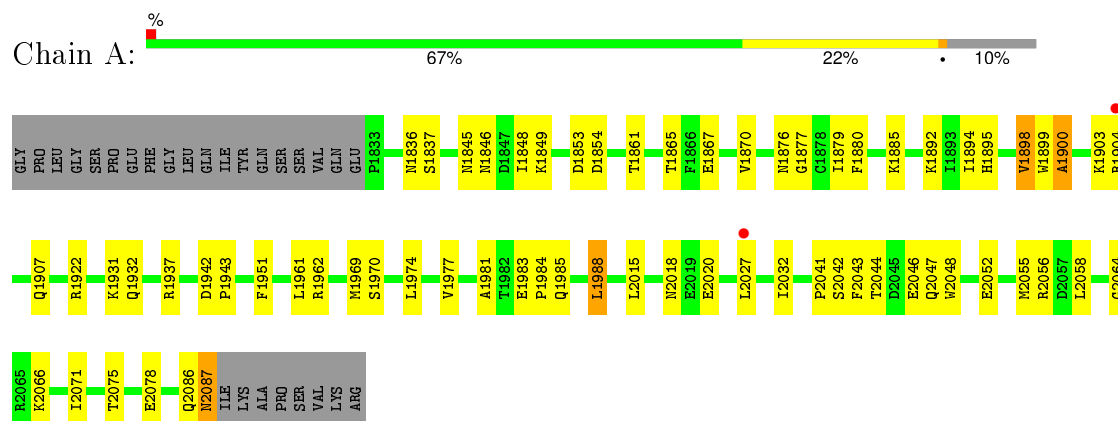
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	130	Total	O	0	0
			130	130		
2	B	117	Total	O	0	0
			117	117		

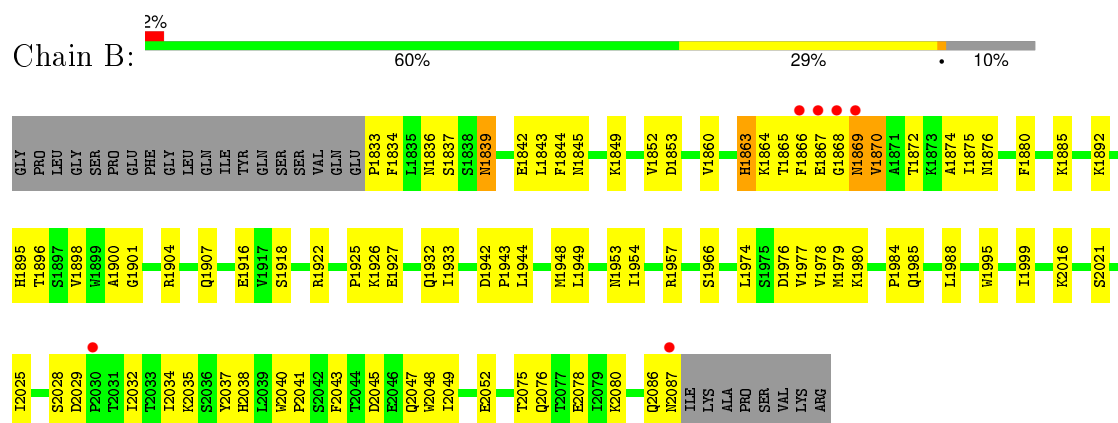
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: PRP8



#### • Molecule 1: PRP8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.17Å 84.81Å 94.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 49.04 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.0 (50.00-2.05) 92.6 (49.04-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.214 , 0.236 0.221 , 0.242	Depositor DCC
$R_{free}$ test set	3625 reflections (9.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70490 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4367	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 4.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/2103	0.61	0/2854
1	B	0.35	0/2103	0.60	0/2854
All	All	0.36	0/4206	0.60	0/5708

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	2060	0	2104	73	0
1	B	2060	0	2104	105	0
2	A	130	0	0	37	1
2	B	117	0	0	50	1
All	All	4367	0	4208	173	1

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 21.

The worst 5 of 173 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:1836:ASN:HA	2:A:202:HOH:O	1.38	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1842:GLU:HA	2:B:226:HOH:O	1.39	1.18
1:B:2049:ILE:HA	2:B:149:HOH:O	1.46	1.14
1:B:1852:VAL:HG22	2:B:228:HOH:O	1.44	1.13
1:B:1896:THR:HG22	2:B:224:HOH:O	1.45	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:123:HOH:O	2:B:184:HOH:O[4_556]	2.18	0.02

## 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	253/282 (90%)	241 (95%)	11 (4%)	1 (0%)	39	28
1	B	253/282 (90%)	239 (94%)	8 (3%)	6 (2%)	7	1
All	All	506/564 (90%)	480 (95%)	19 (4%)	7 (1%)	14	4

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1900	ALA
1	B	2028	SER
1	B	1865	THR
1	B	1869	ASN
1	B	1900	ALA

### 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	233 /256 (91%)	228 (98%)	5 (2%)	61	56
1	B	233 /256 (91%)	228 (98%)	5 (2%)	61	56
All	All	466 /512 (91%)	456 (98%)	10 (2%)	61	56

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2087	ASN
1	B	1839	ASN
1	B	1866	PHE
1	A	2055	MET
1	B	1863	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2087	ASN
1	B	1839	ASN
1	B	2054	GLN
1	A	2086	GLN
1	B	1932	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates 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	255/282 (90%)	-0.16	2 (0%) 87 90	18, 33, 61, 78	0
1	B	255/282 (90%)	0.00	6 (2%) 62 68	23, 38, 66, 99	0
All	All	510/564 (90%)	-0.08	8 (1%) 74 79	18, 35, 64, 99	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1866	PHE	5.3
1	B	1868	GLY	4.1
1	B	2087	ASN	3.1
1	B	1869	ASN	2.9
1	A	2027	LEU	2.4

### 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 carbohydrates 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.