



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:34 PM GMT

PDB ID : 5DCA  
Title : Crystal structure of yeast full length Brr2 in complex with Prp8 Jab1 domain  
Authors : Absmeier, E.; Wollenhaupt, J.; Santos, K.F.; Wahl, M.C.  
Deposited on : 2015-08-23  
Resolution : 2.80 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

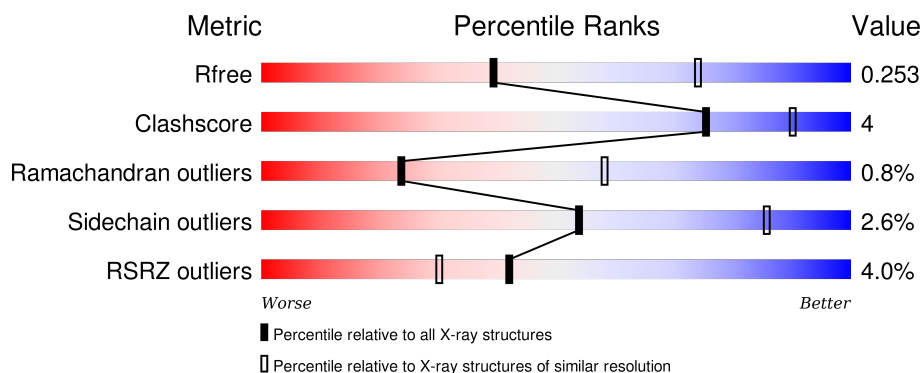
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	1948	
2	J	251	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17842 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 Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1948	Total	C	N	O	S	0	0	0
			15639	10006	2602	2973	58			

There are 103 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	HIS	deletion	UNP P32639
A	?	-	PRO	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ILE	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	MET	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ILE	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	TYR	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	HIS	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP P32639
A	?	-	ARG	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	LEU	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	PRO	deletion	UNP P32639
A	?	-	GLN	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	ARG	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	LYS	deletion	UNP P32639
A	?	-	PHE	deletion	UNP P32639
A	?	-	SER	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	THR	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	VAL	deletion	UNP P32639
A	?	-	ASN	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	GLY	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	ASP	deletion	UNP P32639
A	?	-	GLU	deletion	UNP P32639
A	?	-	ALA	deletion	UNP P32639

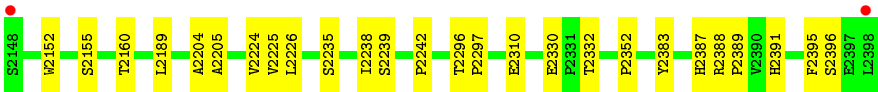
- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	251	Total	C	N	O	S	0	0	0
			2012	1298	325	383	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total 169	O 169	0	0
3	J	22	Total 22	O 22	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.85Å 178.85Å 181.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 178.85 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.80) 95.5 (178.85-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.202 , 0.255 0.205 , 0.253	Depositor DCC
$R_{free}$ test set	4257 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.5	EDS
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 89788 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17842	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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

### 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	0.32	0/15960	0.52	0/21620
2	J	0.32	0/2060	0.51	0/2792
All	All	0.32	0/18020	0.52	0/24412

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

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	15639	0	15665	123	0
2	J	2012	0	1972	17	0
3	A	169	0	0	3	0
3	J	22	0	0	0	0
All	All	17842	0	17637	136	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 4.

The worst 5 of 136 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:J:2387:HIS:C	2:J:2388:ARG:N	2.05	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:LEU:HA	1:A:1445:LEU:HD11	1.64	0.80
1:A:1555:GLU:C	1:A:1556:HIS:N	2.41	0.74
1:A:767:THR:O	1:A:771:THR:N	2.25	0.70
1:A:2121:LYS:O	1:A:2124:GLN:NE2	2.24	0.69

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	1937/1948 (99%)	1823 (94%)	97 (5%)	17 (1%)	21	55
2	J	247/251 (98%)	231 (94%)	16 (6%)	0	100	100
All	All	2184/2199 (99%)	2054 (94%)	113 (5%)	17 (1%)	24	58

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	A	498	SER
1	A	767	THR
1	A	172	GLU
1	A	321	GLU

### 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	1762/1762 (100%)	1714 (97%)	48 (3%)	52	85
2	J	223/223 (100%)	220 (99%)	3 (1%)	76	94
All	All	1985/1985 (100%)	1934 (97%)	51 (3%)	54	86

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1323	LEU
1	A	1460	ARG
1	A	2145	VAL
1	A	1428	LEU
1	A	1461	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	739	GLN
1	A	984	GLN
1	A	1426	ASN
1	A	676	ASN
1	A	1864	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
2	J	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	192:ILE	C	258:ASN	N	48.54
1	A	393:GLU	C	420:ASN	N	23.97
1	A	1828:GLU	C	1841:THR	N	9.71
1	A	1556:HIS	C	1557:ILE	N	2.56
1	A	1555:GLU	C	1556:HIS	N	2.41

## 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	1948/1948 (100%)	0.10	87 (4%) 37 26	57, 90, 184, 237	0
2	J	251/251 (100%)	-0.23	2 (0%) 87 81	59, 88, 151, 194	0
All	All	2199/2199 (100%)	0.06	89 (4%) 42 30	57, 89, 182, 237	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ASN	13.4
1	A	440	LEU	12.8
1	A	342	ASN	12.3
1	A	441	MET	12.1
1	A	173	LEU	9.2

### 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.