



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:27 am BST

PDB ID : 5M52
Title : Crystal structure of yeast Brr2 full-length in complex with Prp8 Jab1 domain
Authors : Wollenhaupt, J.; Absmeier, E.; Becke, C.; Santos, K.F.; Wahl, M.C.
Deposited on : 2016-10-20
Resolution : 3.40 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

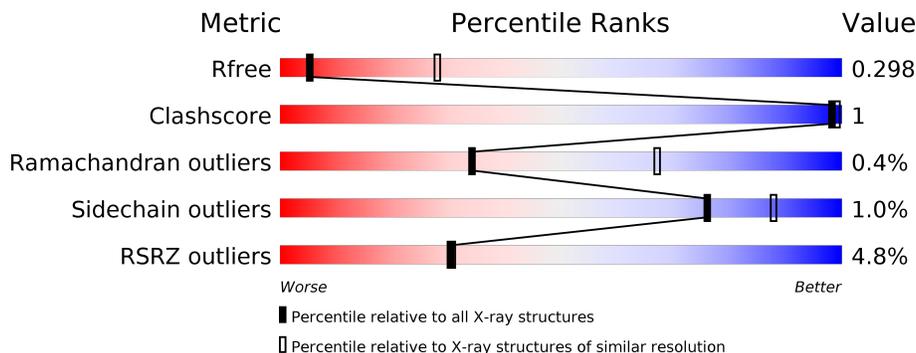
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 ≥ 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	2163	 4% 86% 12%
1	B	2163	 5% 83% 14%
2	C	270	 3% 97% ..
2	D	270	 % 96% ...

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 34522 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
			Total	C	N	O	S			
1	A	1910	Total 15320	C 9818	N 2546	O 2898	S 58	0	0	0
1	B	1862	Total 14927	C 9563	N 2476	O 2832	S 56	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	266	Total 2127	C 1368	N 341	O 412	S 6	0	0	0
2	D	268	Total 2138	C 1374	N 343	O 415	S 6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2144	GLY	-	expression tag	UNP P33334
C	2145	ALA	-	expression tag	UNP P33334
C	2146	MET	-	expression tag	UNP P33334
D	2144	GLY	-	expression tag	UNP P33334
D	2145	ALA	-	expression tag	UNP P33334
D	2146	MET	-	expression tag	UNP P33334

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	4	Total 4	O 4	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	179.34Å 181.16Å 210.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.40 48.72 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.72-3.40) 99.7 (48.72-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.252 , 0.296 0.252 , 0.298	Depositor DCC
R_{free} test set	2100 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.012 for k,h,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34522	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.36	0/15638	0.50	0/21190
1	B	0.36	0/15238	0.50	0/20653
2	C	0.35	0/2177	0.47	0/2952
2	D	0.35	0/2188	0.48	1/2966 (0.0%)
All	All	0.36	0/35241	0.49	1/47761 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

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	D	2398	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2133	PRO	Peptide

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	15320	0	15372	13	0
1	B	14927	0	14939	25	0
2	C	2127	0	2071	2	0
2	D	2138	0	2075	2	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
All	All	34522	0	34457	41	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 1.

The worst 5 of 41 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:B:1554:VAL:HG23	1:B:1557:ILE:HD11	1.73	0.70
2:C:2194:ILE:HD11	2:C:2293:ILE:HG21	1.74	0.69
1:B:557:ILE:HD11	1:B:604:VAL:HG22	1.81	0.62
1:A:1554:VAL:HG23	1:A:1557:ILE:HD11	1.84	0.59
1:A:1965:LEU:HD22	1:A:1972:ASN:HD22	1.68	0.59

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	1896/2163 (88%)	1780 (94%)	105 (6%)	11 (1%)	25 57
1	B	1846/2163 (85%)	1740 (94%)	101 (6%)	5 (0%)	41 72
2	C	264/270 (98%)	246 (93%)	17 (6%)	1 (0%)	34 67
2	D	266/270 (98%)	243 (91%)	21 (8%)	2 (1%)	19 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4272/4866 (88%)	4009 (94%)	244 (6%)	19 (0%)	34 67

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1612	VAL
2	C	2324	VAL
2	D	2401	ASP
1	A	1424	ILE
1	A	1609	MET

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	1726/1955 (88%)	1704 (99%)	22 (1%)	69 84
1	B	1681/1955 (86%)	1669 (99%)	12 (1%)	84 92
2	C	235/237 (99%)	234 (100%)	1 (0%)	91 95
2	D	235/237 (99%)	230 (98%)	5 (2%)	53 76
All	All	3877/4384 (88%)	3837 (99%)	40 (1%)	76 88

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1876	LEU
2	C	2296	THR
2	D	2296	THR
1	A	1990	VAL
1	B	311	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1972	ASN
1	A	2002	ASN
1	B	1701	ASN
1	A	1426	ASN
1	A	1435	ASN

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 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, 95th 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 ²)	Q<0.9
1	A	1910/2163 (88%)	0.28	82 (4%) 35 35	50, 91, 156, 200	0
1	B	1862/2163 (86%)	0.31	112 (6%) 21 23	48, 85, 158, 200	0
2	C	266/270 (98%)	0.26	8 (3%) 50 49	61, 93, 158, 170	0
2	D	268/270 (99%)	0.28	3 (1%) 80 79	63, 95, 137, 162	0
All	All	4306/4866 (88%)	0.29	205 (4%) 30 31	48, 89, 156, 200	0

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	ILE	6.9
1	B	121	GLU	6.5
1	A	366	THR	6.5
1	B	117	VAL	6.4
1	B	327	PRO	5.9

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.