



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:48 pm BST

PDB ID : 1JNX
Title : Crystal structure of the BRCT repeat region from the breast cancer associated protein, BRCA1
Authors : Williams, R.S.; Green, R.; Glover, J.N.M.
Deposited on : 2001-07-26
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

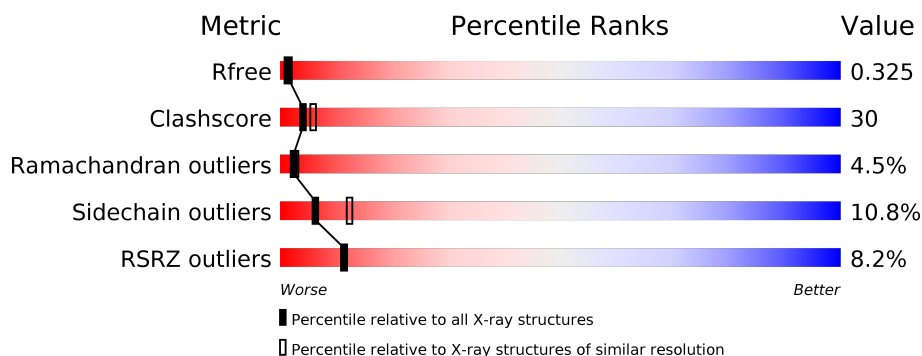
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 ≥ 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	X	214	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1660 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 BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	207	Total	C	N	O	S	0	0	0
			1544	996	253	281	14			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Ni	0	0
			1	1		

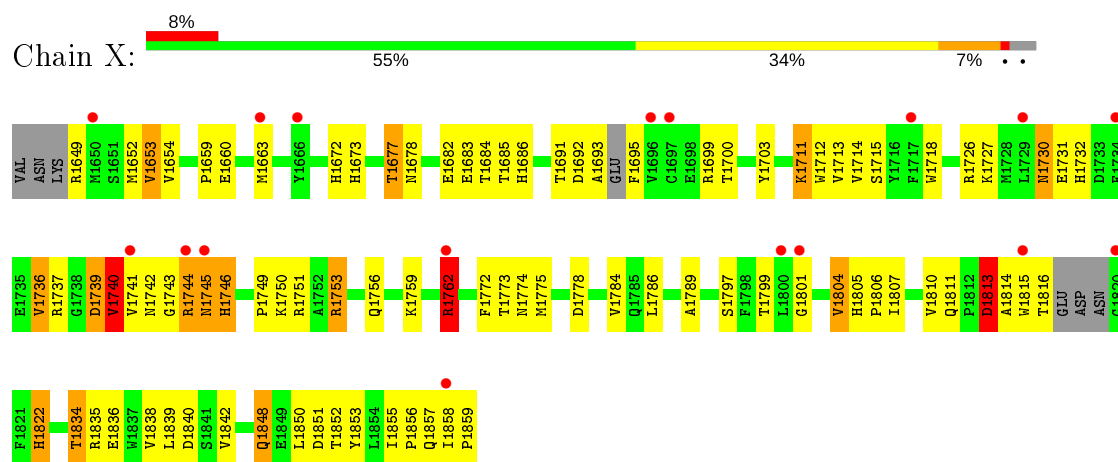
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	115	Total	O	0	0
			115	115		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: BREAST CANCER TYPE 1 SUSCEPTIBILITY PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.84Å 114.84Å 122.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 29.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 99.9 (29.18-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.76 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.259 , 0.302 0.281 , 0.325	Depositor DCC
R_{free} test set	826 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1660	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	X	0.74	0/1579	0.93	3/2153 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	X	1778	ASP	CB-CG-OD1	8.08	125.57	118.30
1	X	1813	ASP	CB-CG-OD2	6.75	124.37	118.30
1	X	1739	ASP	CB-CG-OD2	5.78	123.50	118.30

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	X	1544	0	1458	90	2
2	X	1	0	0	0	0
3	X	115	0	0	8	1
All	All	1660	0	1458	90	3

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 30.

All (90) 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:X:1813:ASP:O	1:X:1815:TRP:N	1.97	0.98
1:X:1739:ASP:OD1	1:X:1740:VAL:N	2.05	0.89
1:X:1749:PRO:O	1:X:1753:ARG:HG2	1.72	0.88
1:X:1753:ARG:NH1	1:X:1753:ARG:HB2	1.88	0.87
1:X:1822:HIS:HB3	1:X:1856:PRO:O	1.75	0.86
1:X:1750:LYS:HA	1:X:1753:ARG:CG	2.05	0.86
1:X:1759:LYS:O	1:X:1762:ARG:HD3	1.79	0.82
1:X:1682:GLU:H	1:X:1682:GLU:CD	1.83	0.81
1:X:1653:VAL:HG23	1:X:1677:THR:HG22	1.64	0.79
1:X:1726:ARG:O	1:X:1727:LYS:HG2	1.84	0.76
1:X:1750:LYS:HA	1:X:1753:ARG:HG2	1.67	0.75
1:X:1739:ASP:OD1	1:X:1741:VAL:N	2.19	0.75
1:X:1652:MET:HG2	1:X:1686:HIS:HB2	1.69	0.73
1:X:1692:ASP:O	1:X:1693:ALA:CB	2.35	0.73
1:X:1799:THR:HG22	1:X:1801:GLY:H	1.58	0.68
1:X:1753:ARG:HB2	1:X:1753:ARG:HH11	1.56	0.68
1:X:1695:PHE:N	3:X:2006:HOH:O	2.28	0.67
1:X:1743:GLY:HA3	3:X:2013:HOH:O	1.95	0.67
1:X:1753:ARG:CB	1:X:1753:ARG:HH11	2.08	0.67
1:X:1649:ARG:O	1:X:1685:THR:HG21	1.96	0.66
1:X:1737:ARG:O	1:X:1746:HIS:O	2.14	0.66
1:X:1822:HIS:N	1:X:1822:HIS:ND1	2.40	0.66
1:X:1692:ASP:O	1:X:1693:ALA:HB3	1.97	0.63
1:X:1739:ASP:CG	1:X:1740:VAL:H	2.00	0.63
1:X:1848:GLN:HG2	1:X:1853:TYR:HE1	1.64	0.62
1:X:1727:LYS:HE3	3:X:2102:HOH:O	1.99	0.62
1:X:1855:ILE:HG23	1:X:1856:PRO:HD2	1.82	0.62
1:X:1726:ARG:O	1:X:1727:LYS:CG	2.48	0.61
1:X:1848:GLN:HG2	1:X:1853:TYR:CE1	2.36	0.61
1:X:1804:VAL:HG22	1:X:1805:HIS:H	1.67	0.60
1:X:1813:ASP:C	1:X:1815:TRP:H	2.05	0.60
1:X:1784:VAL:HG13	1:X:1789:ALA:HB3	1.83	0.60
1:X:1699:ARG:HH21	1:X:1741:VAL:CG2	2.18	0.57
1:X:1732:HIS:ND1	3:X:2101:HOH:O	2.32	0.57
1:X:1699:ARG:HE	1:X:1741:VAL:CG2	2.19	0.55
1:X:1750:LYS:HA	1:X:1753:ARG:HG3	1.87	0.55
1:X:1745:ASN:O	1:X:1746:HIS:C	2.45	0.55
1:X:1713:VAL:HG12	1:X:1736:VAL:HG11	1.89	0.54
1:X:1750:LYS:O	1:X:1751:ARG:C	2.43	0.54
1:X:1699:ARG:HH21	1:X:1741:VAL:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1838:VAL:O	1:X:1842:VAL:HG23	2.09	0.52
1:X:1682:GLU:CD	1:X:1682:GLU:N	2.60	0.52
1:X:1859:PRO:HA	3:X:2073:HOH:O	2.10	0.52
1:X:1660:GLU:CD	1:X:1660:GLU:H	2.13	0.51
1:X:1806:PRO:C	1:X:1807:ILE:HG13	2.30	0.51
1:X:1822:HIS:CB	1:X:1856:PRO:O	2.56	0.50
1:X:1699:ARG:NH2	1:X:1741:VAL:HG22	2.26	0.50
1:X:1712:TRP:CE3	1:X:1731:GLU:HB3	2.47	0.50
1:X:1811:GLN:OE1	1:X:1835:ARG:NH2	2.45	0.49
1:X:1684:THR:O	1:X:1711:LYS:NZ	2.44	0.49
1:X:1743:GLY:O	1:X:1744:ARG:C	2.49	0.49
1:X:1822:HIS:O	1:X:1857:GLN:HA	2.12	0.49
1:X:1744:ARG:O	1:X:1745:ASN:C	2.50	0.49
1:X:1713:VAL:HG12	1:X:1736:VAL:CG1	2.43	0.49
1:X:1659:PRO:O	1:X:1663:MET:HG2	2.14	0.48
1:X:1736:VAL:CG2	1:X:1737:ARG:N	2.77	0.47
1:X:1684:THR:O	1:X:1711:LYS:CE	2.62	0.47
1:X:1773:THR:C	1:X:1775:MET:H	2.17	0.47
1:X:1737:ARG:O	1:X:1744:ARG:O	2.33	0.47
1:X:1835:ARG:HD3	1:X:1839:LEU:HD11	1.97	0.47
1:X:1730:ASN:OD1	1:X:1730:ASN:N	2.45	0.47
1:X:1855:ILE:CG2	1:X:1856:PRO:HD2	2.45	0.47
1:X:1714:VAL:HG12	1:X:1715:SER:N	2.30	0.47
1:X:1772:PHE:HD2	1:X:1835:ARG:HE	1.63	0.47
1:X:1773:THR:O	1:X:1775:MET:N	2.46	0.47
1:X:1736:VAL:HG23	1:X:1737:ARG:N	2.31	0.46
1:X:1672:HIS:O	1:X:1673:HIS:HB2	2.16	0.46
1:X:1714:VAL:CG1	1:X:1715:SER:N	2.79	0.45
1:X:1700:THR:O	1:X:1703:TYR:HB3	2.16	0.45
1:X:1742:ASN:OD1	1:X:1742:ASN:N	2.49	0.45
1:X:1805:HIS:HE1	3:X:2067:HOH:O	1.99	0.45
1:X:1714:VAL:HG12	1:X:1715:SER:O	2.17	0.45
1:X:1678:ASN:N	3:X:2004:HOH:O	2.27	0.43
1:X:1691:THR:HG21	1:X:1715:SER:HB2	2.01	0.43
1:X:1699:ARG:NH2	1:X:1840:ASP:OD1	2.51	0.43
1:X:1834:THR:HG23	1:X:1836:GLU:H	1.84	0.43
1:X:1695:PHE:HB3	1:X:1736:VAL:HA	2.01	0.43
1:X:1750:LYS:CA	1:X:1753:ARG:HG2	2.42	0.43
1:X:1682:GLU:OE1	1:X:1683:GLU:OE1	2.37	0.42
1:X:1739:ASP:CG	1:X:1740:VAL:N	2.58	0.42
1:X:1772:PHE:HA	1:X:1811:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1858:ILE:HA	1:X:1859:PRO:HD2	1.95	0.42
1:X:1714:VAL:HG11	1:X:1718:TRP:HB2	2.01	0.42
1:X:1815:TRP:O	1:X:1816:THR:CB	2.67	0.42
1:X:1804:VAL:HG22	1:X:1805:HIS:N	2.34	0.41
1:X:1850:LEU:O	1:X:1851:ASP:C	2.58	0.41
1:X:1835:ARG:CD	1:X:1839:LEU:HD11	2.50	0.41
1:X:1677:THR:HA	3:X:2004:HOH:O	2.21	0.41
1:X:1806:PRO:O	1:X:1807:ILE:HG13	2.20	0.41
1:X:1772:PHE:HB3	1:X:1835:ARG:HH21	1.84	0.41

All (3) 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)
1:X:1663:MET:SD	1:X:1663:MET:SD[10_665]	2.05	0.15
3:X:2036:HOH:O	3:X:2036:HOH:O[11_555]	2.06	0.14
1:X:1663:MET:CE	1:X:1663:MET:CE[10_665]	2.19	0.01

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	X	201/214 (94%)	180 (90%)	12 (6%)	9 (4%)	2 3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	1740	VAL
1	X	1744	ARG
1	X	1745	ASN
1	X	1762	ARG
1	X	1774	ASN

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Mol	Chain	Res	Type
1	X	1814	ALA
1	X	1746	HIS
1	X	1756	GLN
1	X	1813	ASP

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	X	158/191 (83%)	141 (89%)	17 (11%)	6 12

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1653	VAL
1	X	1654	VAL
1	X	1677	THR
1	X	1711	LYS
1	X	1730	ASN
1	X	1736	VAL
1	X	1740	VAL
1	X	1753	ARG
1	X	1762	ARG
1	X	1786	LEU
1	X	1797	SER
1	X	1804	VAL
1	X	1810	VAL
1	X	1822	HIS
1	X	1834	THR
1	X	1848	GLN
1	X	1852	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	1721	GLN
1	X	1779	GLN
1	X	1848	GLN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	X	207/214 (96%)	0.65	17 (8%) 11 11	20, 37, 56, 63	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1696	VAL	4.6
1	X	1820	GLY	4.5
1	X	1650	MET	4.3
1	X	1729	LEU	4.2
1	X	1858	ILE	4.0
1	X	1800	LEU	3.3
1	X	1744	ARG	3.1
1	X	1697	CYS	3.0
1	X	1745	ASN	2.7
1	X	1815	TRP	2.7
1	X	1663	MET	2.7
1	X	1762	ARG	2.5
1	X	1734	PHE	2.4
1	X	1801	GLY	2.3
1	X	1741	VAL	2.2
1	X	1717	PHE	2.1
1	X	1666	TYR	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	X	1901	1/1	0.94	0.12	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.