



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:38 PM UTC

PDB ID : 1N5O / pdb_00001n5o
Title : Structural consequences of a cancer-causing BRCA1-BRCT missense mutation
Authors : Williams, R.S.; Glover, J.N.M.
Deposited on : 2002-11-06
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

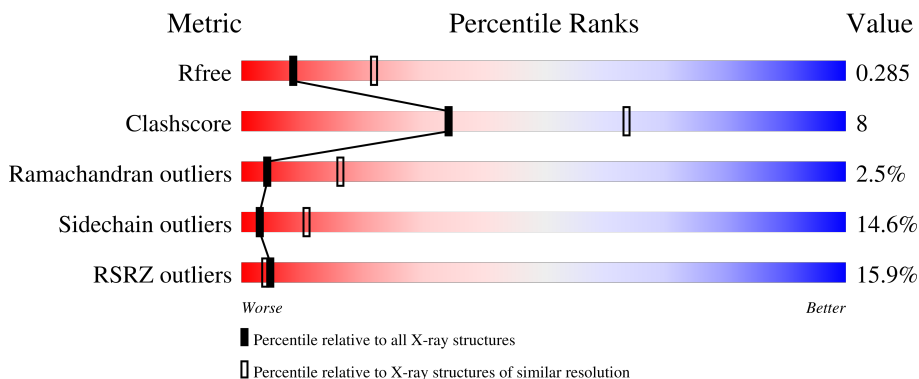
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of 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	15% 70% 21% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1618 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
			1548	997	256	282	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1775	ARG	MET	engineered mutation	UNP P38398

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		

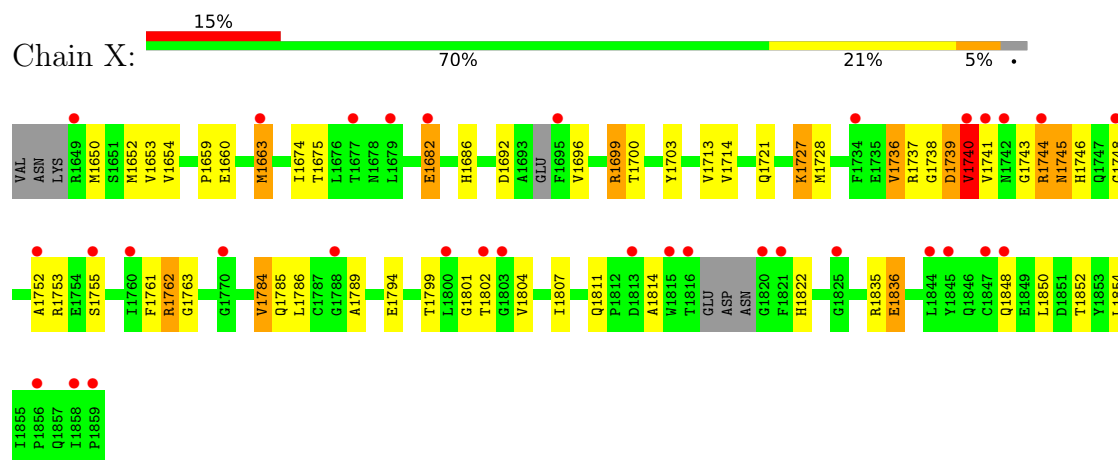
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	59	Total	O	0	0
			59	59		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ($RSRZ > 2$). 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	114.53Å 114.53Å 121.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.80) 99.0 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.0, CNS	Depositor
R, R_{free}	0.274 , 0.298 0.274 , 0.285	Depositor DCC
R_{free} test set	828 reflections (6.90%)	wwPDB-VP
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	1618	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, SO4

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	0.78	1/1583 (0.1%)	1.31	11/2157 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1663	MET	SD-CE	10.24	2.05	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1745	ASN	N-CA-C	12.95	125.47	111.36
1	X	1741	VAL	N-CA-C	-9.59	101.42	111.58
1	X	1738	GLY	N-CA-C	6.63	119.82	110.74
1	X	1736	VAL	N-CA-C	5.54	116.72	109.58
1	X	1822	HIS	N-CA-C	-5.51	106.14	112.92
1	X	1814	ALA	N-CA-C	5.45	119.03	112.38
1	X	1699	ARG	CB-CA-C	-5.44	102.41	110.67
1	X	1713	VAL	N-CA-C	-5.41	98.66	106.88
1	X	1752	ALA	N-CA-C	5.35	116.92	111.14
1	X	1802	THR	N-CA-C	5.26	118.48	111.75
1	X	1692	ASP	N-CA-C	-5.20	102.33	110.17

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	X	1548	0	1462	23	0
2	X	1	0	0	0	0
3	X	10	0	0	0	0
4	X	59	0	0	1	0
All	All	1618	0	1462	23	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 8.

All (23) 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:1663:MET:SD	1:X:1663:MET:CE	2.05	1.45
1:X:1659:PRO:O	1:X:1663:MET:HG2	1.85	0.77
1:X:1682:GLU:H	1:X:1682:GLU:CD	2.06	0.62
1:X:1663:MET:CE	1:X:1663:MET:CG	2.78	0.61
1:X:1652:MET:HG2	1:X:1686:HIS:HB2	1.85	0.58
1:X:1663:MET:HB3	1:X:1663:MET:HE3	1.88	0.54
1:X:1811:GLN:HG3	1:X:1835:ARG:HD3	1.90	0.52
1:X:1799:THR:HG22	1:X:1801:GLY:H	1.74	0.52
1:X:1700:THR:H	1:X:1703:TYR:HB3	1.80	0.47
1:X:1737:ARG:O	1:X:1746:HIS:O	2.33	0.47
1:X:1784:VAL:HG13	1:X:1789:ALA:HB3	1.96	0.46
1:X:1663:MET:CE	1:X:1663:MET:HB3	2.46	0.46
1:X:1850:LEU:O	1:X:1854:LEU:HG	2.16	0.45
1:X:1739:ASP:OD1	1:X:1740:VAL:N	2.42	0.45
1:X:1696:VAL:HG13	1:X:1739:ASP:HA	1.99	0.45
1:X:1762:ARG:HB3	1:X:1763:GLY:H	1.75	0.42
1:X:1727:LYS:HD3	1:X:1727:LYS:HA	1.53	0.42
1:X:1745:ASN:O	1:X:1746:HIS:C	2.62	0.42
1:X:1761:PHE:HB3	1:X:1789:ALA:HB2	2.02	0.41
1:X:1743:GLY:O	1:X:1744:ARG:C	2.64	0.41
1:X:1836:GLU:HG3	4:X:37:HOH:O	2.20	0.41
1:X:1663:MET:CE	1:X:1663:MET:CB	2.99	0.40
1:X:1650:MET:HB3	1:X:1674:ILE:HG23	2.03	0.40

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	X	201/214 (94%)	180 (90%)	16 (8%)	5 (2%)	4	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	1744	ARG
1	X	1762	ARG
1	X	1740	VAL
1	X	1739	ASP
1	X	1748	GLY

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%)	135 (85%)	23 (15%)	3	11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1653	VAL
1	X	1654	VAL
1	X	1660	GLU
1	X	1675	THR
1	X	1682	GLU
1	X	1699	ARG

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Mol	Chain	Res	Type
1	X	1714	VAL
1	X	1721	GLN
1	X	1727	LYS
1	X	1728	MET
1	X	1736	VAL
1	X	1740	VAL
1	X	1753	ARG
1	X	1755	SER
1	X	1784	VAL
1	X	1785	GLN
1	X	1786	LEU
1	X	1794	GLU
1	X	1804	VAL
1	X	1807	ILE
1	X	1836	GLU
1	X	1848	GLN
1	X	1852	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	1721	GLN
1	X	1732	HIS
1	X	1779	GLN
1	X	1785	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	X	201	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	X	202	-	4,4,4	0.23	0	6,6,6	0.23	0

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

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, 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%)	0.95	33 (15%) 5 4	19, 29, 39, 44	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1816	THR	7.0
1	X	1800	LEU	7.0
1	X	1820	GLY	5.5
1	X	1859	PRO	4.8
1	X	1815	TRP	4.6
1	X	1663	MET	4.5
1	X	1748	GLY	4.4
1	X	1858	ILE	4.2
1	X	1821	PHE	3.8
1	X	1649	ARG	3.1
1	X	1856	PRO	2.8
1	X	1755	SER	2.8
1	X	1848	GLN	2.8
1	X	1847	CYS	2.8
1	X	1752	ALA	2.8
1	X	1742	ASN	2.7
1	X	1803	GLY	2.7
1	X	1844	LEU	2.6
1	X	1760	ILE	2.6
1	X	1845	TYR	2.5
1	X	1734	PHE	2.5
1	X	1695	PHE	2.4
1	X	1744	ARG	2.3
1	X	1825	GLY	2.3
1	X	1740	VAL	2.2
1	X	1813	ASP	2.1
1	X	1741	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	1770	GLY	2.1
1	X	1802	THR	2.1
1	X	1679	LEU	2.1
1	X	1788	GLY	2.1
1	X	1682	GLU	2.0
1	X	1677	THR	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	X	202	5/5	0.74	0.15	69,69,70,71	0
3	SO4	X	201	5/5	0.76	0.14	125,125,125,125	0
2	CO	X	301	1/1	0.94	0.12	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.