



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 10:25 PM UTC

PDB ID : 9MPL / pdb\_00009mpl  
Title : BRD2-BD1 in complex with cyclic peptide 2.1C-W11A  
Authors : Patel, K.; Mackay, J.P.  
Deposited on : 2024-12-30  
Resolution : 3.11 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](mailto: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

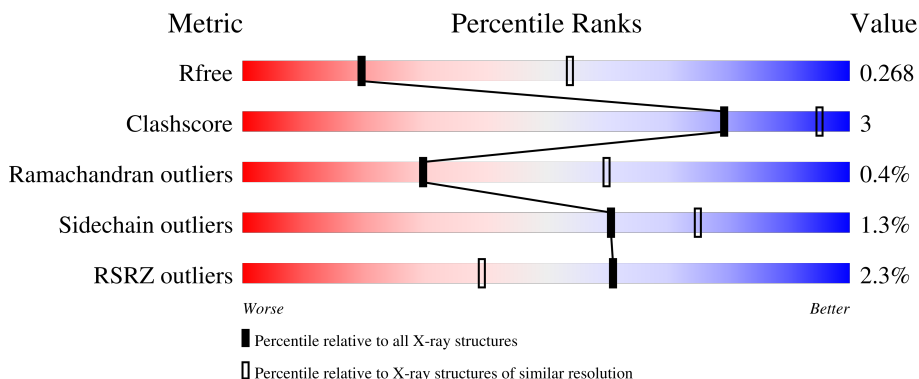
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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  $\geq 3$ , 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	135	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>79%</span> <span>7%</span> <span>14%</span> </div> </div>
1	B	135	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">3%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>79%</span> <span>7%</span> <span>14%</span> </div> </div>
2	C	15	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>87%</span> <span>13%</span> </div> </div>
2	G	15	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>80%</span> <span>13%</span> <span>7%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2168 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 Bromodomain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	36	0	0
			968	626	163	170	9			
1	B	116	Total	C	N	O	S	38	0	0
			968	626	163	170	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	-	expression tag	UNP P25440
A	61	PRO	-	expression tag	UNP P25440
A	62	LEU	-	expression tag	UNP P25440
A	63	GLY	-	expression tag	UNP P25440
A	64	SER	-	expression tag	UNP P25440
B	60	GLN	-	expression tag	UNP P25440
B	61	PRO	-	expression tag	UNP P25440
B	62	LEU	-	expression tag	UNP P25440
B	63	GLY	-	expression tag	UNP P25440
B	64	SER	-	expression tag	UNP P25440

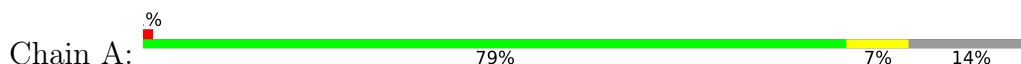
- Molecule 2 is a protein called 2.1C-W11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	S	0	0	1
			116	78	18	19	1			
2	C	15	Total	C	N	O	S	0	0	1
			116	78	18	19	1			

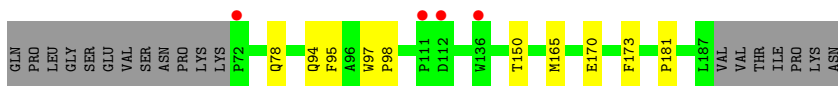
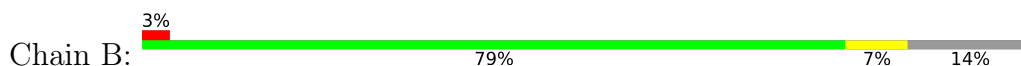
### 3 Residue-property plots [i](#)

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.

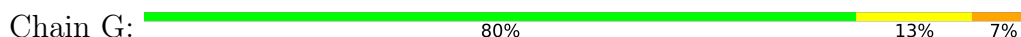
- Molecule 1: Bromodomain-containing protein 2



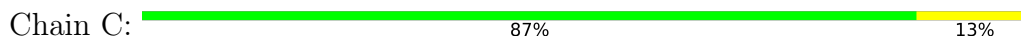
- Molecule 1: Bromodomain-containing protein 2



- Molecule 2: 2.1C-W11A



- Molecule 2: 2.1C-W11A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.99Å 77.99Å 57.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 3.11 46.31 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.31-3.11) 99.6 (46.31-3.11)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.210 , 0.268 0.211 , 0.268	Depositor DCC
$R_{free}$ test set	323 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, 0.333 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: ALY, NH2, ACE

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	0.08	0/994	0.23	0/1344
1	B	0.07	0/994	0.22	0/1344
2	C	0.08	0/105	0.25	0/144
2	G	0.08	0/105	0.24	0/144
All	All	0.08	0/2198	0.23	0/2976

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	968	0	965	4	0
1	B	968	0	965	5	0
2	C	116	0	104	1	0
2	G	116	0	104	2	0
All	All	2168	0	2138	11	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 3.

All (11) 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:150:THR:HG23	2:G:12:LEU:HD23	1.84	0.59
1:B:78:GLN:NE2	1:B:181:PRO:O	2.40	0.52
2:C:0:ACE:H3	2:C:13:CYS:HA	1.90	0.48
1:B:97:TRP:CG	1:B:98:PRO:HD3	2.52	0.44
1:A:152:CYS:SG	1:A:162:ILE:HG13	2.60	0.42
1:A:91:TRP:CZ2	1:A:100:ARG:HD3	2.55	0.42
1:A:148:MET:HE2	1:A:148:MET:HB3	1.94	0.41
1:A:97:TRP:CG	1:A:98:PRO:HD3	2.56	0.41
2:G:0:ACE:H3	2:G:13:CYS:HA	2.00	0.41
1:B:95:PHE:HB3	1:B:165:MET:HB3	2.04	0.40
1:B:170:GLU:HA	1:B:173:PHE:HB3	2.04	0.40

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	114/135 (84%)	113 (99%)	1 (1%)	0	100	100
1	B	114/135 (84%)	112 (98%)	2 (2%)	0	100	100
2	C	12/15 (80%)	12 (100%)	0	0	100	100
2	G	12/15 (80%)	11 (92%)	0	1 (8%)	0	3
All	All	252/300 (84%)	248 (98%)	3 (1%)	1 (0%)	30	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	13	CYS

### 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	106/124 (86%)	104 (98%)	2 (2%)	50	71
1	B	106/124 (86%)	105 (99%)	1 (1%)	70	78
2	C	10/10 (100%)	10 (100%)	0	100	100
2	G	10/10 (100%)	10 (100%)	0	100	100
All	All	232/268 (87%)	229 (99%)	3 (1%)	61	75

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	157	LYS
1	B	94	GLN

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

Mol	Chain	Res	Type
1	A	83	HIS
1	B	146	ASN
1	B	167	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
2	ALY	G	7	2	10,11,12	0.87	0	7,12,14	0.60	0
2	ALY	C	7	2	10,11,12	0.87	0	7,12,14	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALY	G	7	2	-	4/9/10/12	-
2	ALY	C	7	2	-	4/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	7	ALY	O-C-CA-CB
2	C	7	ALY	C-CA-CB-CG
2	G	7	ALY	CE-CD-CG-CB
2	C	7	ALY	CG-CD-CE-NZ
2	G	7	ALY	C-CA-CB-CG
2	C	7	ALY	CA-CB-CG-CD
2	C	7	ALY	CE-CD-CG-CB
2	G	7	ALY	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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 [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	116/135 (85%)	0.09	2 (1%) 69 48	22, 44, 71, 86	10 (8%)
1	B	116/135 (85%)	0.25	4 (3%) 48 28	25, 53, 86, 128	8 (6%)
2	C	12/15 (80%)	-0.12	0 100 100	39, 42, 49, 58	0
2	G	12/15 (80%)	0.02	0 100 100	41, 44, 47, 51	0
All	All	256/300 (85%)	0.15	6 (2%) 61 39	22, 48, 84, 128	18 (7%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	TRP	3.1
1	B	112	ASP	2.7
1	A	72	PRO	2.6
1	B	72	PRO	2.5
1	A	111	PRO	2.1
1	B	111	PRO	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	ALY	C	7	12/13	0.90	0.12	34,37,39,40	0
2	ALY	G	7	12/13	0.94	0.10	39,40,44,45	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.