



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2020 – 07:32 am BST

PDB ID : 2G99  
Title : Structural basis for the specific recognition of methylated histone H3 lysine 4 by the WD-40 protein WDR5  
Authors : Chai, J.; Han, Z.; Wang, H.; Shen, Y.  
Deposited on : 2006-03-06  
Resolution : 1.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

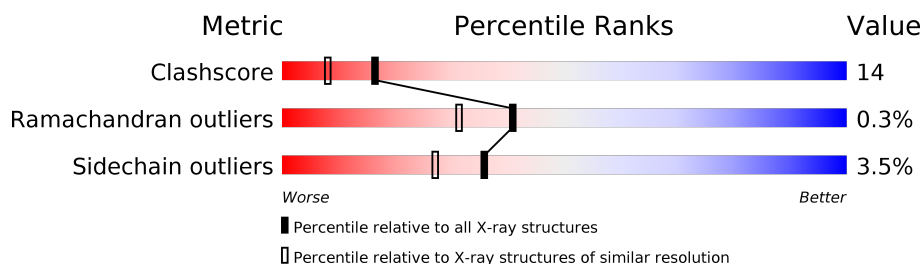
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	<div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	B	308	<div> <div>78%</div> <div>19%</div> <div>..</div> </div>
2	C	10	<div> <div>40%</div> <div>10%</div> <div>50%</div> </div>
2	D	10	<div> <div>20%</div> <div>30%</div> <div>50%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4800 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 WD-repeat protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2357	1505	393	450	9			
1	B	304	Total	C	N	O	S	0	0	0
			2357	1505	393	450	9			

- Molecule 2 is a protein called Histone H3.

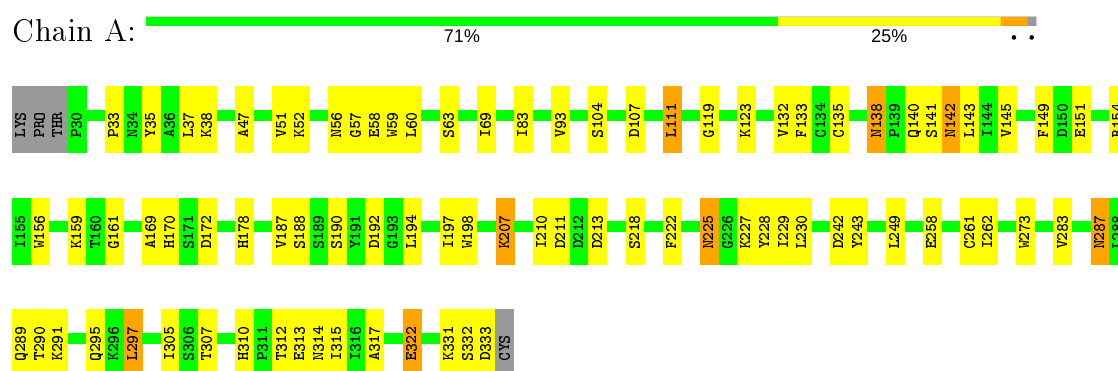
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			43	26	10	7			
2	D	5	Total	C	N	O	0	0	0
			43	26	10	7			

### 3 Residue-property plots

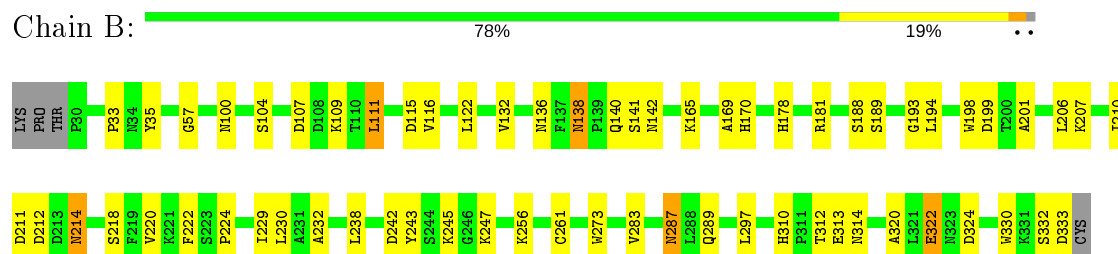
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

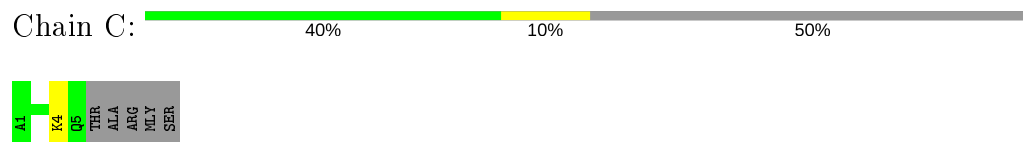
- Molecule 1: WD-repeat protein 5



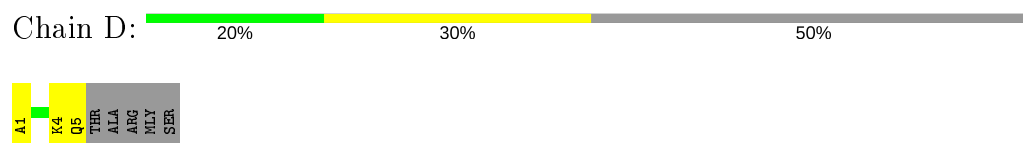
- Molecule 1: WD-repeat protein 5



- Molecule 2: Histone H3



- Molecule 2: Histone H3



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.19Å 46.89Å 112.31Å 90.00° 117.40° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 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: MLY

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	0.35	0/2414	0.70	1/3275 (0.0%)
1	B	0.34	0/2414	0.71	1/3275 (0.0%)
2	C	0.27	0/31	0.59	0/40
2	D	0.34	0/31	1.25	0/40
All	All	0.35	0/4890	0.71	2/6630 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASP	N-CA-C	-5.07	97.31	111.00
1	A	242	ASP	N-CA-C	-5.04	97.39	111.00

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	2357	0	2342	80	0
1	B	2357	0	2342	54	0
2	C	43	0	50	1	0
2	D	43	0	50	4	0
All	All	4800	0	4784	137	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 14.

The worst 5 of 137 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:A:225:ASN:HD22	1:A:227:LYS:HG2	1.28	0.96
1:A:207:LYS:HZ3	1:A:243:TYR:HD1	1.17	0.89
1:A:142:ASN:H	1:A:142:ASN:HD22	1.20	0.88
1:B:115:ASP:HB2	1:B:122:LEU:HD11	1.58	0.86
1:A:187:VAL:HG22	1:A:197:ILE:HG13	1.59	0.84

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	302/308 (98%)	289 (96%)	12 (4%)	1 (0%)	41	31
1	B	302/308 (98%)	291 (96%)	10 (3%)	1 (0%)	41	31
2	C	2/10 (20%)	2 (100%)	0	0	100	100
2	D	2/10 (20%)	1 (50%)	1 (50%)	0	100	100
All	All	608/636 (96%)	583 (96%)	23 (4%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	GLU
1	B	322	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	266 / 270 (98%)	254 (96%)	12 (4%)	27	18
1	B	266 / 270 (98%)	259 (97%)	7 (3%)	46	39
2	C	3 / 6 (50%)	3 (100%)	0	100	100
2	D	3 / 6 (50%)	3 (100%)	0	100	100
All	All	538 / 552 (98%)	519 (96%)	19 (4%)	36	27

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	A	289	GLN
1	B	194	LEU
1	A	249	LEU
1	B	214	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	ASN
1	A	310	HIS
1	B	178	HIS
1	A	265	ASN
1	B	265	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](#)

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	MLY	D	4	2	9,10,11	0.85	0	6,11,13	2.39	4 (66%)
2	MLY	C	4	2	9,10,11	0.74	0	6,11,13	1.62	1 (16%)

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	MLY	D	4	2	-	2/8/9/11	-
2	MLY	C	4	2	-	4/8/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	4	MLY	CD-CE-NZ	3.26	122.61	113.79
2	D	4	MLY	CH1-NZ-CE	3.09	122.97	110.74
2	D	4	MLY	CH2-NZ-CE	2.80	121.82	110.74
2	C	4	MLY	CH2-NZ-CE	2.43	120.38	110.74
2	D	4	MLY	CH2-NZ-CH1	-2.35	103.65	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4	MLY	C-CA-CB-CG
2	C	4	MLY	N-CA-CB-CG
2	C	4	MLY	C-CA-CB-CG
2	C	4	MLY	CA-CB-CG-CD
2	C	4	MLY	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	MLY	3	0
2	C	4	MLY	1	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.