



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1WUG / pdb_00001wug
Title : complex structure of PCAF bromodomain with small chemical ligand NP1
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Deposited on : 2004-12-07

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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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)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

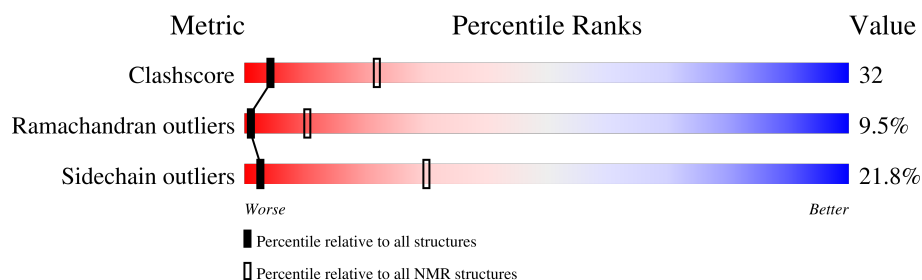
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	118	44% 41% 13% .

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2004 atoms, of which 1002 are hydrogens and 0 are deuteriums.

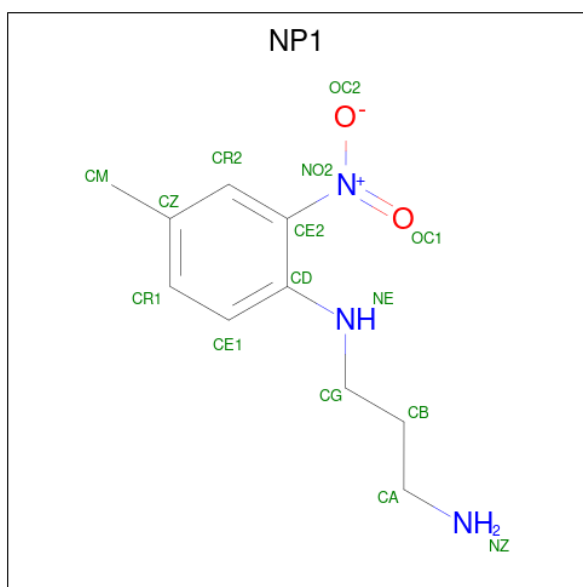
- Molecule 1 is a protein called Histone acetyltransferase PCAF.

Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1974	636	987	164	180	7	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	715	GLY	-	expression tag	UNP Q92831
A	716	SER	-	expression tag	UNP Q92831
A	717	HIS	-	expression tag	UNP Q92831
A	718	MET	-	expression tag	UNP Q92831
A	804	PRO	ALA	conflict	UNP Q92831
A	805	PRO	ALA	conflict	UNP Q92831

- Molecule 2 is N-(3-AMINOPROPYL)-4-METHYL-2-NITROBENZENAMINE (CCD ID: NP1) (formula: $C_{10}H_{15}N_3O_2$).

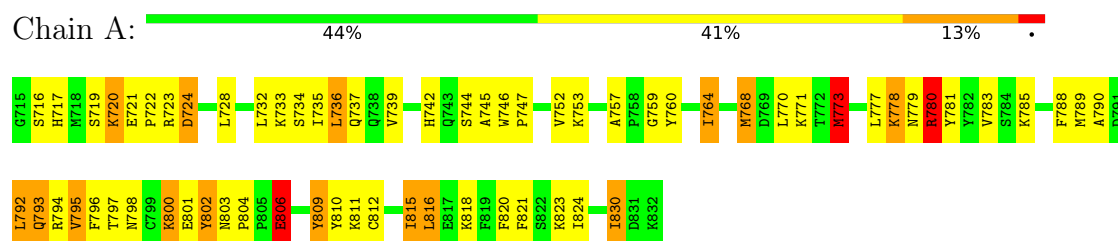


Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			30	10	15	3	2

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Histone acetyltransferase PCAF



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 200 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	3.851

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NP1

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 (average) 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	1.37	0/1013 (0.0%)	1.50	4/1359 (0.3%)
All	All	1.37	0/1013 (0.0%)	1.50	4/1359 (0.3%)

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	764	ILE	N-CA-CB	-6.62	104.47	112.35
1	A	735	ILE	N-CA-CB	-5.30	104.84	110.62
1	A	815	ILE	N-CA-CB	-5.28	104.68	110.65
1	A	795	VAL	N-CA-CB	-5.06	104.63	110.55

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	987	987	984	63
2	A	15	15	15	7
All	All	1002	1002	999	64

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 32.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:739:VAL:HG13	1:A:816:LEU:HD21	0.90	1.43
1:A:744:SER:O	1:A:816:LEU:HD12	0.80	1.77
1:A:739:VAL:HG13	1:A:816:LEU:CD2	0.79	2.06
1:A:764:ILE:HD11	1:A:801:GLU:HB3	0.69	1.63
1:A:736:LEU:HD13	1:A:736:LEU:O	0.67	1.89
1:A:757:ALA:HA	2:A:201:NP1:HM1	0.62	1.71
1:A:812:CYS:HA	1:A:815:ILE:HD12	0.59	1.73
1:A:809:TYR:CE1	2:A:201:NP1:NO2	0.59	2.71
1:A:792:LEU:HD13	1:A:820:PHE:CE1	0.58	2.33
1:A:746:TRP:N	1:A:747:PRO:CD	0.58	2.67
1:A:809:TYR:CE1	2:A:201:NP1:OC2	0.56	2.58
1:A:809:TYR:CD1	2:A:201:NP1:OC2	0.55	2.59
1:A:752:VAL:HG13	2:A:201:NP1:CR1	0.55	2.31
1:A:793:GLN:O	1:A:797:THR:HG22	0.54	2.03
1:A:739:VAL:O	1:A:745:ALA:HB2	0.53	2.03
1:A:732:LEU:HD22	1:A:788:PHE:CG	0.53	2.39
1:A:800:LYS:CG	1:A:810:TYR:CE2	0.52	2.93
2:A:201:NP1:NE	2:A:201:NP1:OC1	0.51	2.43
1:A:800:LYS:CG	1:A:810:TYR:CD2	0.51	2.93
1:A:802:TYR:C	1:A:802:TYR:CD1	0.50	2.89
1:A:792:LEU:CD2	1:A:796:PHE:CZ	0.50	2.94
1:A:736:LEU:HD21	1:A:770:LEU:CD2	0.50	2.36
1:A:736:LEU:HD13	1:A:736:LEU:C	0.49	2.32
1:A:797:THR:HG23	1:A:798:ASN:N	0.48	2.24
1:A:810:TYR:CD1	1:A:810:TYR:C	0.47	2.92
1:A:778:LYS:CA	1:A:778:LYS:CE	0.46	2.92
1:A:764:ILE:HG21	1:A:798:ASN:ND2	0.46	2.25
1:A:746:TRP:CG	1:A:747:PRO:HD3	0.46	2.46
1:A:783:VAL:HG22	1:A:783:VAL:O	0.46	2.11
1:A:746:TRP:CE3	1:A:747:PRO:N	0.46	2.84
1:A:764:ILE:HD11	1:A:801:GLU:CB	0.46	2.38
1:A:824:ILE:HD12	1:A:830:ILE:HG12	0.45	1.86
1:A:773:MET:SD	1:A:788:PHE:CE1	0.45	3.10
1:A:747:PRO:HB3	1:A:809:TYR:CE1	0.45	2.47
1:A:800:LYS:HG2	1:A:810:TYR:CD2	0.44	2.47
1:A:802:TYR:CG	1:A:803:ASN:N	0.44	2.85
1:A:793:GLN:OE1	1:A:821:PHE:CZ	0.44	2.70
1:A:780:ARG:CD	1:A:780:ARG:O	0.43	2.66
1:A:792:LEU:HD23	1:A:796:PHE:CZ	0.43	2.48
1:A:722:PRO:O	1:A:724:ASP:N	0.43	2.52
1:A:746:TRP:N	1:A:747:PRO:HD3	0.43	2.27
1:A:778:LYS:CE	1:A:778:LYS:O	0.43	2.67

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:728:LEU:CD2	1:A:783:VAL:C	0.43	2.92
1:A:794:ARG:O	1:A:798:ASN:CB	0.43	2.67
1:A:745:ALA:C	1:A:747:PRO:CD	0.42	2.92
1:A:779:ASN:O	1:A:780:ARG:C	0.42	2.62
1:A:804:PRO:O	1:A:806:GLU:N	0.42	2.52
1:A:790:ALA:O	1:A:794:ARG:N	0.42	2.53
1:A:736:LEU:C	1:A:736:LEU:CD1	0.42	2.92
1:A:779:ASN:O	1:A:781:TYR:N	0.42	2.53
1:A:739:VAL:O	1:A:745:ALA:CB	0.42	2.67
1:A:760:TYR:OH	1:A:798:ASN:ND2	0.42	2.53
1:A:788:PHE:CE2	1:A:792:LEU:HD12	0.42	2.49
1:A:719:SER:O	1:A:721:GLU:N	0.41	2.53
1:A:779:ASN:C	1:A:780:ARG:HG3	0.41	2.40
1:A:780:ARG:CD	1:A:780:ARG:C	0.41	2.94
1:A:802:TYR:CE2	1:A:809:TYR:CD2	0.41	3.08
1:A:752:VAL:HG22	2:A:201:NP1:HB2	0.41	1.91
1:A:746:TRP:CD2	1:A:747:PRO:CD	0.41	3.03
1:A:783:VAL:O	1:A:783:VAL:HG13	0.41	2.16
1:A:768:MET:O	1:A:795:VAL:HG22	0.41	2.16
1:A:728:LEU:HG	1:A:732:LEU:CD1	0.40	2.47
1:A:728:LEU:HD23	1:A:783:VAL:HA	0.40	1.92
1:A:796:PHE:CE1	1:A:816:LEU:HB3	0.40	2.52

6.3 Torsion angles

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	116/118 (98%)	92 (79%)	13 (11%)	11 (9%)	1	10
All	All	116/118 (98%)	92 (79%)	13 (11%)	11 (9%)	1	10

All 11 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	717	HIS

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Mol	Chain	Res	Type
1	A	720	LYS
1	A	723	ARG
1	A	742	HIS
1	A	759	GLY
1	A	773	MET
1	A	780	ARG
1	A	785	LYS
1	A	806	GLU
1	A	811	LYS
1	A	830	ILE

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	110/110 (100%)	86 (78%)	24 (22%)	2	30
All	All	110/110 (100%)	86 (78%)	24 (22%)	2	30

All 24 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	716	SER
1	A	720	LYS
1	A	724	ASP
1	A	733	LYS
1	A	734	SER
1	A	736	LEU
1	A	737	GLN
1	A	753	LYS
1	A	768	MET
1	A	771	LYS
1	A	773	MET
1	A	777	LEU
1	A	778	LYS
1	A	780	ARG
1	A	789	MET

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Mol	Chain	Res	Type
1	A	792	LEU
1	A	793	GLN
1	A	800	LYS
1	A	802	TYR
1	A	806	GLU
1	A	809	TYR
1	A	816	LEU
1	A	818	LYS
1	A	823	LYS

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	NP1	A	201	-	15,15,15	3.64	3 (20%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NP1	A	201	-	15,19,19	1.21	1 (6%)

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	NP1	A	201	-	-	0,7,9,9	0,1,1,1

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	NP1	OC1-NO2	11.44	1.42	1.22
2	A	201	NP1	CE2-NO2	6.76	1.33	1.45
2	A	201	NP1	CG-NE	2.07	1.50	1.45

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	NP1	CB-CG-NE	2.29	105.27	111.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided