



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2DEX / pdb\_00002dex  
Title : Crystal structure of human peptidylarginine deiminase 4 in complex with histone H3 N-terminal peptide including Arg17  
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Deposited on : 2006-02-18  
Resolution : 2.10 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.

The types of validation reports are described at

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

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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

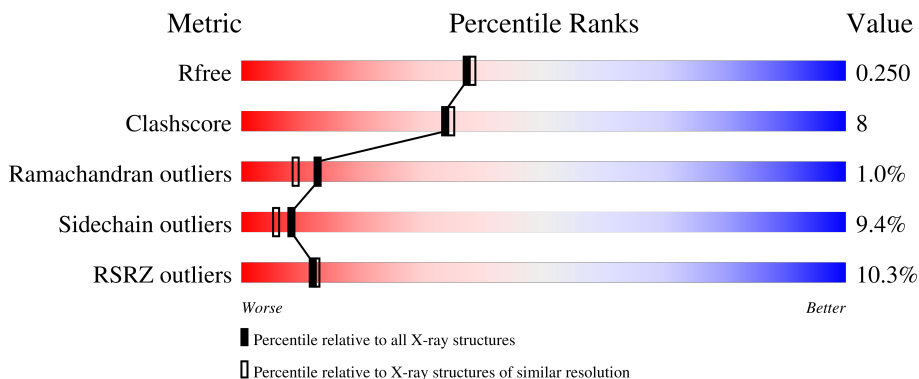
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	X	671	
2	A	10	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5190 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 Protein-arginine deiminase type IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	627	4937	3153	828	922	34	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-7	GLY	-	cloning artifact	UNP Q9UM07
X	-6	PRO	-	cloning artifact	UNP Q9UM07
X	-5	LEU	-	cloning artifact	UNP Q9UM07
X	-4	GLY	-	cloning artifact	UNP Q9UM07
X	-3	SER	-	cloning artifact	UNP Q9UM07
X	-2	PRO	-	cloning artifact	UNP Q9UM07
X	-1	GLU	-	cloning artifact	UNP Q9UM07
X	0	PHE	-	cloning artifact	UNP Q9UM07
X	645	ALA	CYS	engineered mutation	UNP Q9UM07

- Molecule 2 is a protein called 10-mer peptide from histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	A	5	41	25	10	6	0	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	X	5	5	5	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

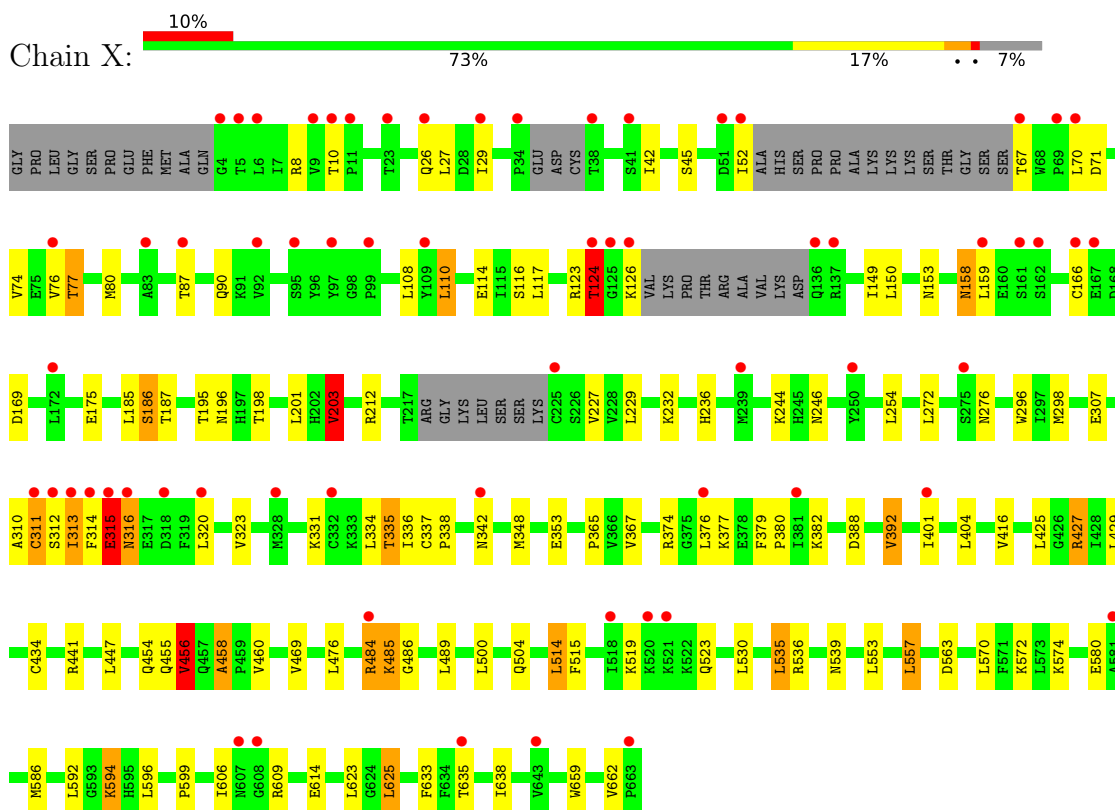
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	190	Total O 190 190	0	0
5	A	2	Total O 2 2	0	0

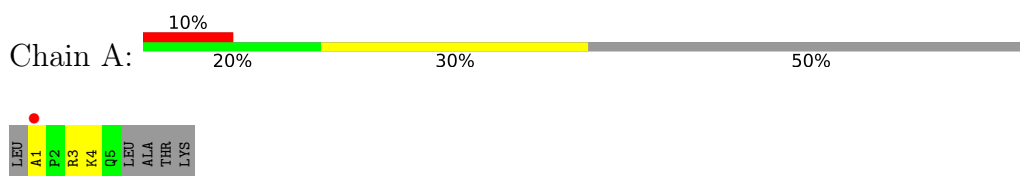
### 3 Residue-property plots [i](#)

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: Protein-arginine deiminase type IV



- Molecule 2: 10-mer peptide from histone H3



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.07Å 60.10Å 115.70Å 90.00° 124.32° 90.00°	Depositor
Resolution (Å)	33.13 – 2.10 33.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (33.13-2.10) 94.6 (33.13-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.203 , 0.247 0.210 , 0.250	Depositor DCC
$R_{free}$ test set	4628 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.4	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: SO4, CA

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	0.72	0/5056	0.88	9/6861 (0.1%)
2	A	0.73	0/41	1.06	1/53 (1.9%)
All	All	0.72	0/5097	0.88	10/6914 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	316	ASN	N-CA-C	8.23	122.68	108.76
1	X	456	VAL	N-CA-C	8.07	122.31	111.17
1	X	367	VAL	CB-CA-C	-7.70	101.64	110.96
1	X	203	VAL	CB-CA-C	-6.13	100.11	110.71
1	X	456	VAL	CB-CA-C	5.86	120.60	112.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	313	ILE	Peptide

## 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	4937	0	4900	76	0
2	A	41	0	48	2	0
3	X	5	0	0	0	0
4	X	15	0	0	0	0
5	A	2	0	0	1	0
5	X	190	0	0	7	0
All	All	5190	0	4948	77	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.

The worst 5 of 77 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:454:GLN:O	5:X:909:HOH:O	1.79	1.00
1:X:425:LEU:HD12	1:X:456:VAL:HG13	1.58	0.86
1:X:315:GLU:HG3	1:X:316:ASN:HD22	1.43	0.82
1:X:574:LYS:NZ	1:X:580:GLU:OE1	2.11	0.81
1:X:313:ILE:HB	1:X:338:PRO:HA	1.62	0.79

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	X	617/671 (92%)	591 (96%)	20 (3%)	6 (1%)	12   9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	3/10 (30%)	3 (100%)	0	0	100	100
All	All	620/681 (91%)	594 (96%)	20 (3%)	6 (1%)	12	9

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	484	ARG
1	X	124	THR
1	X	315	GLU
1	X	458	ALA
1	X	485	LYS

### 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	X	557/593 (94%)	504 (90%)	53 (10%)	8	5
2	A	4/8 (50%)	4 (100%)	0	100	100
All	All	561/601 (93%)	508 (91%)	53 (9%)	8	6

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	392	VAL
1	X	456	VAL
1	X	609	ARG
1	X	401	ILE
1	X	427	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	316	ASN
1	X	346	GLN

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Mol	Chain	Res	Type
1	X	538	HIS
1	X	504	GLN
1	X	505	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\# Z  > 2$
4	SO4	X	906	-	4,4,4	0.23	0	6,6,6	0.24	0
4	SO4	X	907	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	X	905	-	4,4,4	0.21	0	6,6,6	0.40	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 [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, 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	X	627/671 (93%)	0.91	64 (10%) 12 12	51, 63, 80, 95	0
2	A	5/10 (50%)	1.42	1 (20%) 3 3	67, 71, 75, 77	0
All	All	632/681 (92%)	0.92	65 (10%) 12 12	51, 63, 80, 95	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	312	SER	6.9
1	X	124	THR	5.8
1	X	313	ILE	5.4
1	X	125	GLY	4.7
1	X	314	PHE	4.6

### 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, 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	X	907	5/5	0.74	0.12	87,88,88,89	0
4	SO4	X	906	5/5	0.89	0.10	86,86,87,87	0
4	SO4	X	905	5/5	0.91	0.12	73,73,74,75	0
3	CA	X	904	1/1	0.96	0.13	62,62,62,62	0
3	CA	X	902	1/1	0.98	0.12	65,65,65,65	0
3	CA	X	903	1/1	0.98	0.15	62,62,62,62	0
3	CA	X	901	1/1	0.99	0.12	61,61,61,61	0
3	CA	X	900	1/1	1.00	0.09	53,53,53,53	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.