



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 3, 2025 – 10:31 AM EDT

PDB ID : 3H66 / pdb\_00003h66  
Title : Catalytic domain of human Serine/Threonine Phosphatase 5 (PP5c) with two Zn<sup>2+</sup> atoms  
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Deposited on : 2009-04-23  
Resolution : 2.59 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 Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

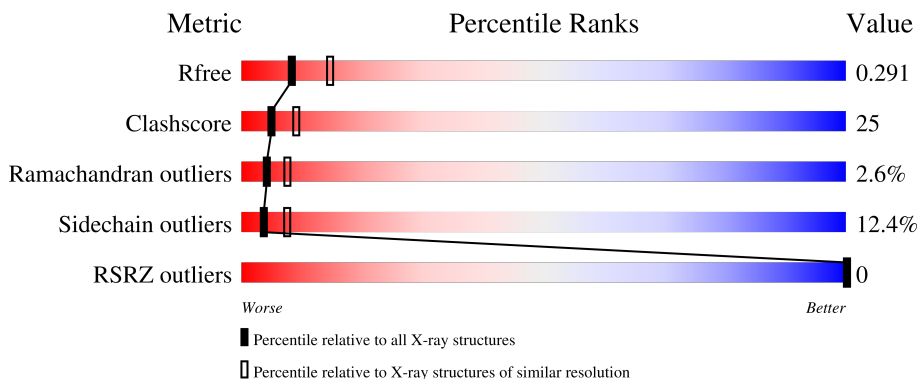
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	315	
1	B	315	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5116 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 Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			
1	B	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

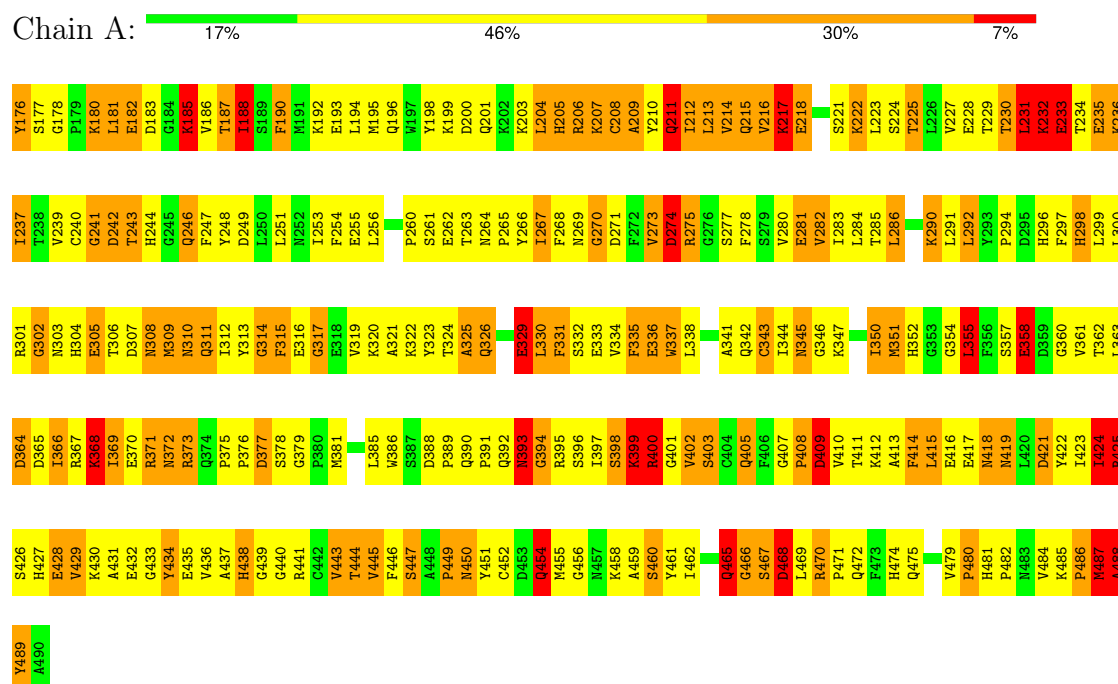
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	22	Total	O	0	0
			22	22		

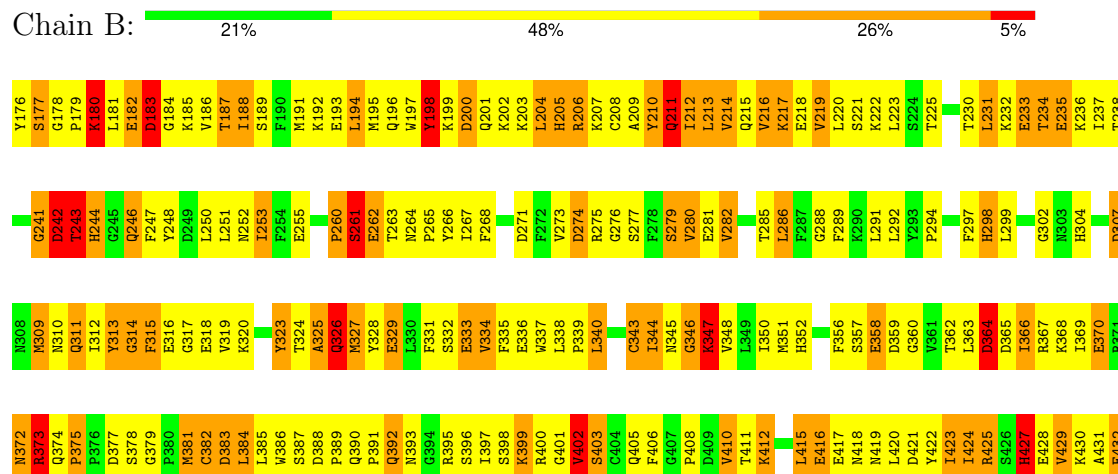
### 3 Residue-property plots

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: Serine/threonine-protein phosphatase 5



#### • Molecule 1: Serine/threonine-protein phosphatase 5



C433	Y434	E435	V436	A437	H438		R441	C442	V443	T444	V445	F446	S447	A448	P449	N450	Y451	C452	D453	Q454	N455		A459	S460	Y461	I462	H463	L464	Q465	G466	S467	D468	L469	R470	P471	Q472	F473	H474	Q475	F476	T477	A478	V479	P480	H481	P482	N483	V484	K485	P486	M487	A488	Y489	A490
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.25Å 41.68Å 106.09Å 90.00° 96.46° 90.00°	Depositor
Resolution (Å)	38.32 – 2.59 38.32 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.32-2.59) 92.4 (38.32-2.59)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, $R_{free}$	0.199 , 0.291 0.200 , 0.291	Depositor DCC
$R_{free}$ test set	1821 reflections (9.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	4.4	Xtriage
Anisotropy	1.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 28.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	3.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.02% 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

### 5.1 Standard geometry

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

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	3.03	255/2592 (9.8%)	2.41	150/3506 (4.3%)
1	B	2.85	207/2592 (8.0%)	2.25	133/3506 (3.8%)
All	All	2.94	462/5184 (8.9%)	2.33	283/7012 (4.0%)

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	A	0	2
1	B	0	2
All	All	0	4

The worst 5 of 462 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	VAL	C-O	14.03	1.39	1.24
1	A	390	GLN	C-O	-13.07	1.10	1.24
1	A	381	MET	C-O	-12.99	1.07	1.24
1	A	214	VAL	CA-CB	12.84	1.73	1.54
1	A	296	HIS	CA-C	12.61	1.69	1.52

The worst 5 of 283 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	HIS	CA-C-N	-13.33	107.32	120.52
1	A	481	HIS	C-N-CA	-13.33	107.32	120.52
1	B	367	ARG	N-CA-C	-13.03	97.06	111.14
1	A	358	GLU	N-CA-C	-11.33	92.13	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ALA	N-CA-C	-11.12	99.17	111.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	LEU	Peptide
1	A	454	GLN	Peptide
1	B	465	GLN	Peptide
1	B	477	THR	Peptide

## 5.2 Too-close contacts

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	2528	0	2462	131	0
1	B	2528	0	2462	115	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	34	0	0	12	1
3	B	22	0	0	6	0
All	All	5116	0	4924	246	1

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 25.

The worst 5 of 246 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:399:LYS:CD	1:A:399:LYS:CE	1.77	1.60
1:B:194:LEU:CD2	1:B:194:LEU:CG	1.79	1.59
1:A:330:LEU:CD1	1:A:330:LEU:CG	1.79	1.58
1:A:206:ARG:CD	1:A:206:ARG:CG	1.75	1.58
1:B:479:VAL:CB	1:B:479:VAL:CG1	1.79	1.56

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1:HOH:O	3:A:30:HOH:O[4_445]	2.09	0.11

## 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	313/315 (99%)	274 (88%)	33 (10%)	6 (2%)	6	13
1	B	313/315 (99%)	276 (88%)	27 (9%)	10 (3%)	3	5
All	All	626/630 (99%)	550 (88%)	60 (10%)	16 (3%)	4	7

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	ASP
1	B	393	ASN
1	B	450	ASN
1	B	468	ASP
1	A	377	ASP

### 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	279/279 (100%)	248 (89%)	31 (11%)	5	10
1	B	279/279 (100%)	241 (86%)	38 (14%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	558/558 (100%)	489 (88%)	69 (12%)	<b>4</b> <b>7</b>

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	398	SER
1	B	402	VAL
1	B	465	GLN
1	A	425	ARG
1	A	424	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	ASN
1	B	454	GLN
1	B	475	GLN
1	B	472	GLN
1	A	311	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	315/315 (100%)	-0.50	0 100 100	1, 2, 5, 17	4 (1%)
1	B	315/315 (100%)	-0.41	0 100 100	1, 2, 11, 24	4 (1%)
All	All	630/630 (100%)	-0.45	0 100 100	1, 2, 8, 24	8 (1%)

There are no RSRZ outliers to report.

### 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	ZN	B	501	1/1	0.98	0.03	25,25,25,25	0
2	ZN	A	501	1/1	0.99	0.03	8,8,8,8	0
2	ZN	B	500	1/1	0.99	0.02	2,2,2,2	0
2	ZN	A	500	1/1	0.99	0.02	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.