

# wwPDB X-ray Structure Validation Summary Report (i)

Dec 14, 2023 - 03:37 am GMT

PDB ID : 2YA9

Title: Crystal structure of the autoinhibited form of mouse DAPK2

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Deposited on : 2011-02-18

Resolution : 2.30 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
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

al geometry (DNA, RNA) : Parkinson et al. (1996)

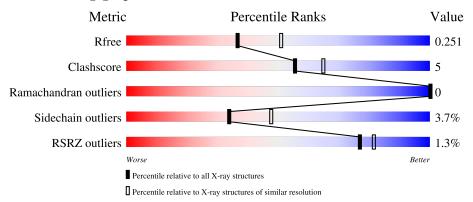
Ideal geometry (DNA, RNA) : Parkin Validation Pipeline (wwPDB-VP) : 2.36

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.30 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D1D	В	1302	_	_	X	_



### 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5357 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.

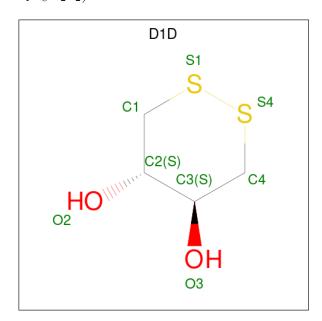
• Molecule 1 is a protein called DEATH-ASSOCIATED PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	299	Total	С	N	О	S	0	6	0
1	A	299	2481	1587	418	471	5	0	O	U
1	D	299	Total	С	N	О	S	0	2	0
1	D	<u> </u>	2446	1568	411	462	5	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

	Chain	Residue	Modelled	Actual	Comment	Reference
	Α	0	GLY	-	expression tag	UNP Q8VDF3
ĺ	В	0	GLY	-	expression tag	UNP Q8VDF3

• Molecule 2 is (4S,5S)-1,2-DITHIANE-4,5-DIOL (three-letter code: D1D) (formula:  $C_4H_8O_2S_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
2	A	1	Total 8	C 4	O 2	S 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	В	1	Total 8	C 4	O 2	S 2	0	0

• Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	207	Total O 207 207	0	0
4	В	206	Total O 206 206	0	0

 ${\tt SEQUENCE-PLOTS\ INFOmissing INFO}$ 



### 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	64.04Å 86.44Å 124.27Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.82 - 2.30	Depositor
rtesolution (A)	40.82 - 2.30	EDS
% Data completeness	97.2 (40.82-2.30)	Depositor
(in resolution range)	97.2 (40.82-2.30)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
D D.	0.206 , 0.261	Depositor
$R, R_{free}$	0.196 , $0.251$	DCC
$R_{free}$ test set	1525 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31 , 41.4	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5357	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 47.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0405e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 4 Model quality (i)

### 4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, D1D

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.34	0/2528	0.50	0/3411	
1	В	0.34	0/2492	0.48	0/3362	
All	All	0.34	0/5020	0.49	0/6773	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

#### 4.2 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	2481	0	2481	21	0
1	В	2446	0	2462	25	0
2	A	8	0	6	2	0
2	В	8	0	6	4	0
3	A	1	0	0	0	0
4	A	207	0	0	2	0
4	В	206	0	0	2	0
All	All	5357	0	4955	51	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 5.



The worst 5 of 51 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
2:A:1302:D1D:C3	2:A:1302:D1D:C4	1.80	1.57
2:B:1302:D1D:C3	2:B:1302:D1D:C4	1.80	1.52
1:A:47[A]:ARG:HG3	1:A:47[A]:ARG:HH11	1.10	1.11
1:A:47[B]:ARG:HG2	1:A:47[B]:ARG:HH11	1.14	1.08
1:B:26:ILE:HD11	1:B:28:LYS:HE3	1.62	0.82

There are no symmetry-related clashes.

#### 4.3 Torsion angles (i)

#### 4.3.1 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	Perce	$\mathbf{ntiles}$
1	A	303/361 (84%)	294 (97%)	9 (3%)	0	100	100
1	В	299/361~(83%)	293 (98%)	6 (2%)	0	100	100
All	All	602/722 (83%)	587 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 4.3.2 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	274/327 (84%)	264 (96%)	10 (4%)	35 49	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	В	270/327 (83%)	259 (96%)	11 (4%)	30 43	
All	All	544/654 (83%)	523 (96%)	21 (4%)	34 46	

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	58	ARG
1	В	170	ASP
1	В	293	LEU
1	В	261	ARG
1	В	118	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	107	GLN
1	A	223	GLN
1	В	223	GLN

#### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	Trme	Chain	Dag	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	D1D	A	1302	-	6,8,8	8.21	6 (100%)	6,10,10	1.79	2 (33%)
2	D1D	В	1302	-	6,8,8	8.17	5 (83%)	6,10,10	1.99	4 (66%)

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	D1D	A	1302	-	-	-	0/0/1/1
2	D1D	В	1302	-	-	-	0/0/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(A)	$Ideal(\AA)$
2	В	1302	D1D	C4-C3	14.35	1.80	1.52
2	A	1302	D1D	C4-C3	14.28	1.80	1.52
2	A	1302	D1D	C3-C2	11.17	1.69	1.52
2	В	1302	D1D	C3-C2	10.93	1.69	1.52
2	A	1302	D1D	C1-C2	6.41	1.65	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	1302	D1D	O3-C3-C4	2.66	114.49	109.91
2	В	1302	D1D	C1-C2-C3	2.46	117.32	112.45
2	A	1302	D1D	O2-C2-C1	2.36	113.98	109.91
2	В	1302	D1D	C4-C3-C2	2.25	116.89	112.45
2	В	1302	D1D	O2-C2-C1	2.23	113.75	109.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	D1D	2	0
2	В	1302	D1D	4	0

### 4.7 Other polymers (i)

There are no such residues in this entry.

### 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



### 5 Fit of model and data (i)

#### 5.1 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q<0.9
1	A	299/361~(82%)	-0.25	5 (1%) 70 7	6	10, 21, 50, 78	0
1	В	299/361 (82%)	-0.34	3 (1%) 82 8	6	12, 22, 46, 71	0
All	All	598/722 (82%)	-0.30	8 (1%) 77 8	1	10, 22, 47, 78	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	GLY	4.6
1	A	300	TYR	4.0
1	В	300	TYR	2.9
1	A	3	THR	2.9
1	В	3	THR	2.5

#### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

#### 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.4 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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
3	CA	A	1303	1/1	0.89	0.08	63,63,63,63	0
2	D1D	В	1302	8/8	0.94	0.10	21,38,43,43	0
2	D1D	A	1302	8/8	0.96	0.09	12,35,40,41	0

## 5.5 Other polymers (i)

There are no such residues in this entry.

