



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2023 – 05:26 pm GMT

PDB ID : 4AD6  
Title : Synthesis and SAR of guanine based analogues for HPPK inhibitors  
Authors : Chhabra, S.; Peat, T.S.; Swarbrick, J.  
Deposited on : 2011-12-22  
Resolution : 1.85 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 : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.36

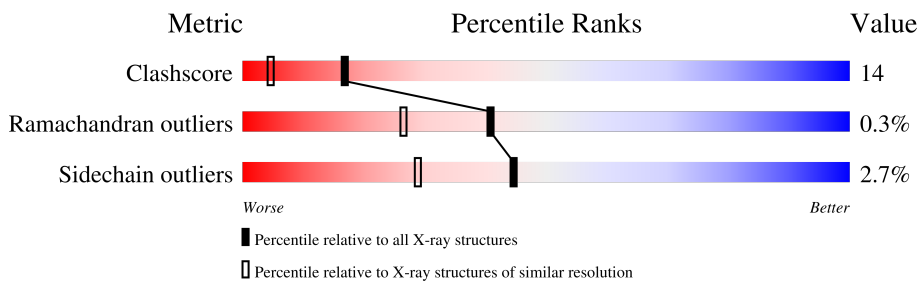
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.59Å 75.71Å 51.36Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85	Depositor
% Data completeness (in resolution range)	98.0 (30.00-1.85)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.264	Depositor
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtrriage
Anisotropy	0.063	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.10 % 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 9.3647e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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.

### 3 Model quality [i](#)

#### 3.1 Standard geometry [i](#)

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

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	0.91	1/1328 (0.1%)	1.04	7/1799 (0.4%)
1	B	0.90	2/1326 (0.2%)	0.99	0/1797
All	All	0.91	3/2654 (0.1%)	1.01	7/3596 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	TYR	CE1-CZ	6.19	1.46	1.38
1	A	89	TRP	CD2-CE2	5.45	1.47	1.41
1	B	89	TRP	CD2-CE2	5.06	1.47	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	92	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	142	LEU	CA-CB-CG	6.98	131.35	115.30
1	A	15	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	152	ASP	CB-CG-OD1	5.32	123.08	118.30

There are no chirality outliers.

There are no planarity outliers.

#### 3.2 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	1306	0	1336	39	0
1	B	1301	0	1326	37	0
2	A	15	0	9	1	0
2	B	15	0	9	0	0
3	A	89	0	0	7	0
3	B	78	0	0	3	0
All	All	2804	0	2680	75	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 75 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:43[B]:THR:HG23	1:A:154:VAL:HG22	1.43	1.00
1:B:25:ILE:HG22	1:B:29:TYR:HE2	1.30	0.97
1:B:25:ILE:HG22	1:B:29:TYR:CE2	2.05	0.92
1:A:115:HIS:HD2	1:A:117:ARG:H	1.09	0.91
1:A:43[B]:THR:HG21	1:A:123:PHE:HB3	1.54	0.89

There are no symmetry-related clashes.

### 3.3 Torsion angles [i](#)

#### 3.3.1 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	161/161 (100%)	159 (99%)	2 (1%)	0	100	100
1	B	161/161 (100%)	157 (98%)	3 (2%)	1 (1%)	25	12
All	All	322/322 (100%)	316 (98%)	5 (2%)	1 (0%)	41	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	TRP

### 3.3.2 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	150/147 (102%)	147 (98%)	3 (2%)	55	40
1	B	150/147 (102%)	145 (97%)	5 (3%)	38	21
All	All	300/294 (102%)	292 (97%)	8 (3%)	44	29

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	156	ARG
1	B	103	GLU
1	B	75	LEU
1	B	2	ILE
1	B	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
1	B	115	HIS
1	B	3	GLN
1	A	115	HIS
1	B	62	GLN

### 3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 3.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

2 ligands are modelled in this entry.

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.

### 3.7 Other polymers [i](#)

There are no such residues in this entry.

### 3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 4 Fit of model and data

### 4.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 4.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 4.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 4.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 4.5 Other polymers

EDS failed to run properly - this section is therefore empty.