

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

#### May 22, 2020 – 05:16 pm BST

PDB ID	:	1W82
Title	:	p38 Kinase crystal structure in complex with small molecule inhibitor
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Deposited on		
$\operatorname{Resolution}$	:	2.20  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 following versions of software and data (see references (1)) were used in the production of this report:

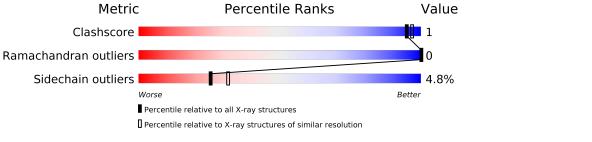
Xtriage (Phenix) EDS buster-report Percentile statistics Ideal geometry (proteins)	: : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996) 2.11

## 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 2.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503(2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	360	90%	7%	••



# 2 Entry composition (i)

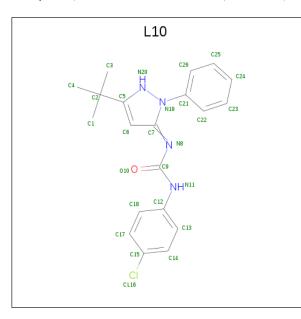
There are 3 unique types of molecules in this entry. The entry contains 3388 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MITOGEN-ACTIVATED PROTEIN KINASE 14.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	352	Total 2834	C 1813	N 484	O 524	S 13	0	0	1

• Molecule 2 is N-[(3Z)-5-TERT-BUTYL-2-PHENYL-1,2-DIHYDRO-3H-PYRAZOL-3-YLID ENE]-N'-(4-CHLOROPHENYL)UREA (three-letter code: L10) (formula: C<sub>20</sub>H<sub>21</sub>ClN<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	А	1	Total 26	C 20	Cl 1	N 4	0 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	528	Total O 528 528	0	0

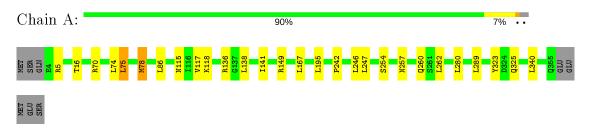


## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

• Molecule 1: MITOGEN-ACTIVATED PROTEIN KINASE 14





## 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	45.68Å 85.37Å 126.00Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	70.71 - 2.20	Depositor
% Data completeness	92.0 (70.71-2.20)	Depositor
(in resolution range)	52.0 (10.11 2.20)	Depositor
$R_{merge}$	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
Refinement program	REFMAC 5.2.0003A	Depositor
$R, R_{free}$	0.171 , $0.235$	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3388	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP



# 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:  ${\rm L10}$ 

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.57	0/2900	0.79	4/3939~(0.1%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	5	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	А	70	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	А	136	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	А	149	ARG	NE-CZ-NH1	5.35	122.97	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	А	2834	0	2821	7	0
2	А	26	0	21	0	0
3	А	528	0	0	1	0
All	All	3388	0	2842	7	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 1.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TYR:CE2	1:A:325:GLN:HG2	2.44	0.53
1:A:78:MET:HE2	1:A:141:ILE:HG12	1.91	0.52
1:A:115:ASN:ND2	3:A:2252:HOH:O	2.43	0.51
1:A:75:LEU:HB3	1:A:86:LEU:HG	1.98	0.44
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.99	0.43

The worst 5 of 7 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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	А	350/360~(97%)	342 (98%)	8 (2%)	0	100 100	

There are no Ramachandran outliers to report.

#### 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	nalysed Rotameric		Percentiles	
1	А	311/320~(97%)	296~(95%)	15~(5%)	25 32	

5 of 15 residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
1	А	138	LEU
1	А	167	LEU
1	А	280	LEU
1	А	118	LYS
1	А	262	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	80	HIS
1	А	201	ASN
1	А	260	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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	Chain Ros Lir		Res Link Bond lengths					Bond angles		
mor Type	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2		
2	L10	А	1356	-	24,28,28	1.90	2 (8%)	$32,\!40,\!40$	2.67	5 (15%)		



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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
2	L10	А	1356	-	-	4/16/18/18	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	1356	L10	C7-N8	8.52	1.39	1.28
2	А	1356	L10	C2-C5	-2.52	1.51	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
2	А	1356	L10	C21-N19-N20	9.75	125.63	117.75
2	А	1356	L10	C2-C5-N20	8.63	126.88	113.80
2	А	1356	L10	C5-C6-C7	4.08	107.65	102.62
2	А	1356	L10	N11-C9-N8	2.77	115.29	110.99
2	А	1356	L10	C3-C2-C5	-2.31	105.95	109.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	1356	L10	C4-C2-C5-N20
2	А	1356	L10	C3-C2-C5-N20
2	А	1356	L10	C1-C2-C5-N20
2	А	1356	L10	C4-C2-C5-C6

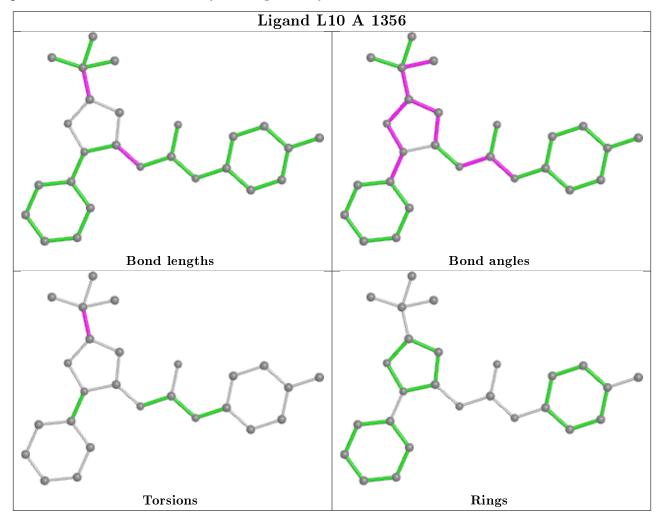
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and



any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



### 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

#### 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

