



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2017 – 11:13 AM EDT

PDB ID : 3FZ1  
Title : Crystal structure of a benzthiophene inhibitor bound to human Cyclin-dependent Kinase-2 (CDK-2)  
Authors : Kurumbail, R.G.; Caspers, N.  
Deposited on : unknown  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

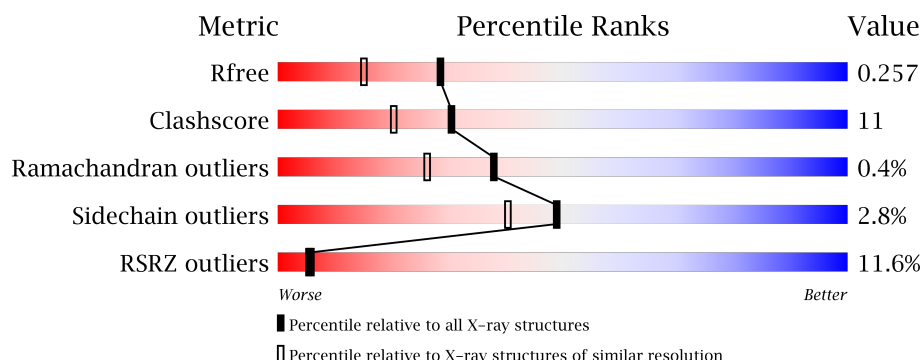
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	298	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition [i](#)

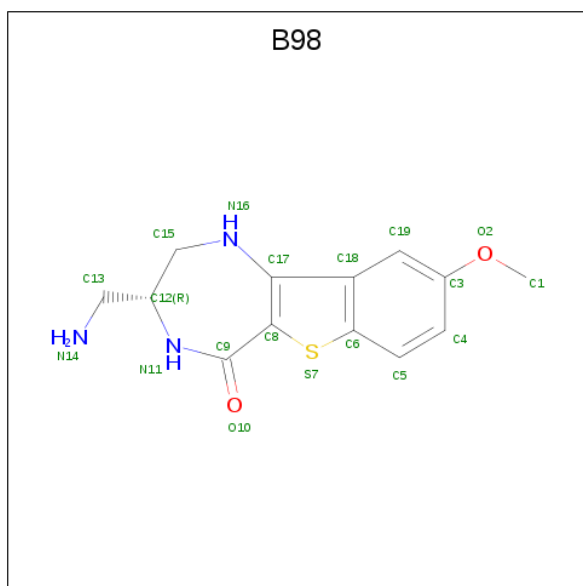
There are 3 unique types of molecules in this entry. The entry contains 2512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2282	1488	388	398	8			

- Molecule 2 is (3R)-3-(aminomethyl)-9-methoxy-1,2,3,4-tetrahydro-5H-[1]benzothieno[3,2-e][1,4]diazepin-5-one (three-letter code: B98) (formula: C<sub>13</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	13	3	2	1		

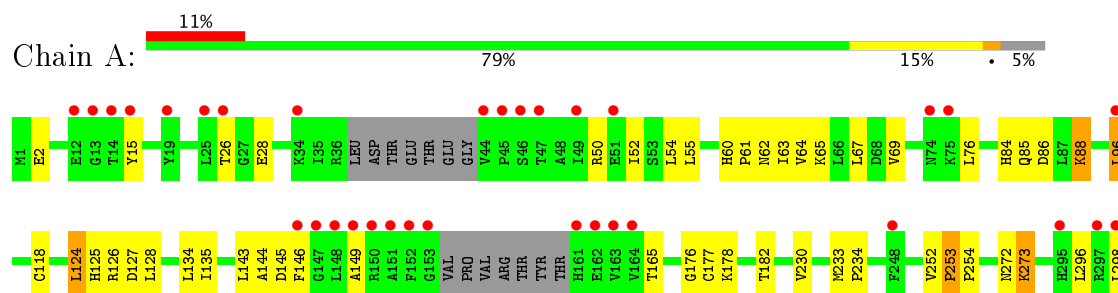
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		

### 3 Residue-property plots

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 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 ( $\text{RSRZ} > 2$ ). 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: Cell division protein kinase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.72Å 71.71Å 72.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.66 – 1.90 27.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (27.66-1.90) 99.0 (27.66-1.90)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.40 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.210 , 0.259 0.208 , 0.257	Depositor DCC
$R_{free}$ test set	1147 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: B98

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	0.44	0/2340	0.56	0/3170

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2282	0	2332	49	0
2	A	19	0	15	0	0
3	A	211	0	0	5	0
All	All	2512	0	2347	49	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 11.

All (49) 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:145:ASP:HB3	3:A:452:HOH:O	1.45	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HE2	1:A:88:LYS:HA	1.58	0.83
1:A:60:HIS:HD2	1:A:62:ASN:H	1.29	0.81
1:A:143:LEU:HD13	1:A:146:PHE:HE1	1.45	0.81
1:A:143:LEU:HD13	1:A:146:PHE:CE1	2.21	0.75
1:A:60:HIS:CD2	1:A:62:ASN:H	2.06	0.73
1:A:125:HIS:HD2	1:A:127:ASP:H	1.33	0.72
1:A:230:VAL:O	1:A:233:MET:HG3	1.96	0.65
1:A:84:HIS:HB3	1:A:298:LEU:HD22	1.79	0.65
1:A:88:LYS:HE3	3:A:379:HOH:O	1.97	0.64
1:A:118:CYS:SG	1:A:146:PHE:CZ	2.89	0.63
1:A:15:TYR:OH	1:A:149:ALA:HA	1.99	0.62
1:A:128:LEU:HD21	1:A:143:LEU:HD22	1.80	0.62
1:A:50:ARG:O	1:A:54:LEU:HG	2.02	0.59
1:A:88:LYS:CE	1:A:88:LYS:HA	2.32	0.59
1:A:124:LEU:HD22	1:A:182:THR:HG22	1.84	0.58
1:A:125:HIS:HE1	1:A:144:ALA:O	1.85	0.58
1:A:63:ILE:HD13	1:A:143:LEU:HB2	1.86	0.57
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.40	0.57
1:A:128:LEU:HD21	1:A:143:LEU:CD2	2.35	0.57
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.42	0.55
1:A:85:GLN:HG3	1:A:86:ASP:N	2.22	0.54
1:A:63:ILE:CD1	1:A:143:LEU:HD12	2.37	0.54
1:A:118:CYS:SG	1:A:146:PHE:CE2	3.04	0.50
1:A:176:GLY:O	1:A:234:PRO:HG2	2.12	0.48
1:A:273:LYS:HD2	1:A:273:LYS:N	2.26	0.48
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.95	0.48
1:A:63:ILE:HD13	1:A:143:LEU:HD12	1.96	0.48
1:A:60:HIS:HE1	3:A:382:HOH:O	1.96	0.47
1:A:143:LEU:HB3	1:A:146:PHE:HD1	1.79	0.47
1:A:85:GLN:HG2	1:A:135:ILE:HD11	1.95	0.47
1:A:165:THR:HG22	3:A:499:HOH:O	2.15	0.47
1:A:177:CYS:HB2	1:A:233:MET:CE	2.46	0.46
1:A:135:ILE:HD12	1:A:296:LEU:HD21	1.98	0.45
1:A:252:VAL:N	1:A:253:PRO:CD	2.81	0.44
1:A:26:THR:OG1	1:A:28:GLU:HB2	2.18	0.44
1:A:253:PRO:HB2	1:A:254:PRO:CD	2.47	0.44
1:A:69:VAL:HG13	1:A:76:LEU:HD11	2.00	0.44
1:A:178:LYS:HE2	3:A:343:HOH:O	2.17	0.43
1:A:96:LEU:HA	1:A:96:LEU:HD12	1.80	0.43
1:A:252:VAL:N	1:A:253:PRO:HD3	2.33	0.43
1:A:55:LEU:HD13	1:A:146:PHE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HD11	1:A:143:LEU:HD12	2.00	0.42
1:A:64:VAL:HG21	1:A:134:LEU:HD12	2.02	0.42
1:A:88:LYS:HE2	1:A:88:LYS:CA	2.32	0.41
1:A:65:LYS:HD3	1:A:67:LEU:CD2	2.50	0.41
1:A:52:ILE:HG22	1:A:69:VAL:HG21	2.03	0.41
1:A:252:VAL:C	1:A:254:PRO:HD2	2.41	0.40
1:A:88:LYS:CE	1:A:88:LYS:CA	2.97	0.40

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	A	278 / 298 (93%)	270 (97%)	7 (2%)	1 (0%)	38 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO

### 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	249 / 263 (95%)	242 (97%)	7 (3%)	49 40

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	88	LYS
1	A	96	LEU
1	A	124	LEU
1	A	126	ARG
1	A	272	ASN
1	A	273	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	59	ASN
1	A	60	HIS
1	A	121	HIS
1	A	125	HIS
1	A	268	HIS

### 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	B98	A	299	-	15,21,21	1.64	4 (26%)	12,30,30	3.45	4 (33%)

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	B98	A	299	-	-	0/2/17/17	0/2/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	299	B98	C12-N11	-2.49	1.43	1.47
2	A	299	B98	C5-C6	-2.18	1.37	1.40
2	A	299	B98	C17-N16	-2.02	1.36	1.40
2	A	299	B98	C9-N11	4.39	1.37	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	299	B98	C19-C18-C17	-9.41	130.02	135.54
2	A	299	B98	C1-O2-C3	-5.10	106.35	117.50
2	A	299	B98	O10-C9-N11	-2.42	118.12	121.60
2	A	299	B98	C17-C18-C6	3.66	111.63	107.49

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	284/298 (95%)	0.76	33 (11%) 5 6	13, 25, 53, 67	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	VAL	9.0
1	A	152	PHE	8.9
1	A	25	LEU	8.0
1	A	15	TYR	7.5
1	A	14	THR	7.0
1	A	164	VAL	6.8
1	A	151	ALA	6.7
1	A	162	GLU	6.6
1	A	146	PHE	6.6
1	A	45	PRO	6.2
1	A	148	LEU	5.5
1	A	13	GLY	5.5
1	A	49	ILE	5.3
1	A	74	ASN	5.1
1	A	96	LEU	5.1
1	A	297	ARG	4.8
1	A	46	SER	4.6
1	A	161	HIS	4.1
1	A	147	GLY	4.1
1	A	153	GLY	4.0
1	A	298	LEU	3.6
1	A	295	HIS	3.5
1	A	75	LYS	3.2
1	A	163	VAL	3.2
1	A	34	LYS	2.8
1	A	12	GLU	2.7
1	A	150	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	26	THR	2.5
1	A	248	PHE	2.4
1	A	47	THR	2.3
1	A	149	ALA	2.2
1	A	19	TYR	2.1
1	A	51	GLU	2.0

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	B98	A	299	19/19	0.83	0.17	-0.11	33,36,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.