



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 05:50 AM GMT

PDB ID : 3C4F  
Title : FGFR TYROSINE KINASE DOMAIN IN COMPLEX WITH 3-(3-methoxy  
benzyl)-7-azaindole  
Authors : Zhang, K.Y.J.; Wang, W.  
Deposited on : 2008-01-29  
Resolution : 2.07 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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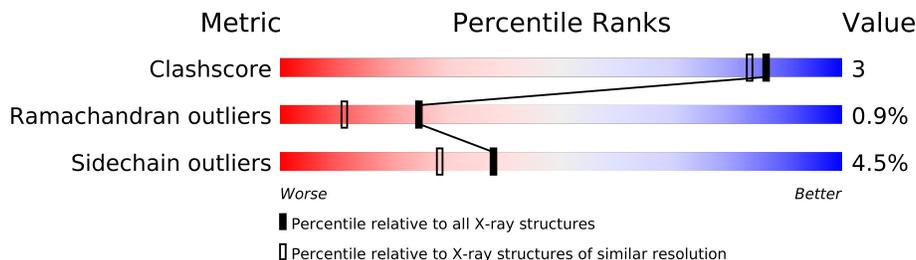
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.07 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	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	302	
1	B	302	

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5031 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

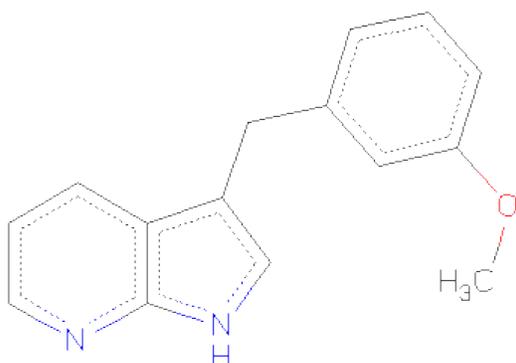
- Molecule 1 is a protein called Basic fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2320	1472	401	429	18	0	1	0
1	B	290	2319	1472	401	429	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	ALA	CYS	ENGINEERED	UNP P11362
B	488	ALA	CYS	ENGINEERED	UNP P11362

- Molecule 2 is 3-(3-METHOXYBENZYL)-1H-PYRROLO[2,3-B]PYRIDINE (three-letter code: C4F) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	18	15	2	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	18	15	2	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	213	213	213	0	0
3	B	143	143	143	0	0

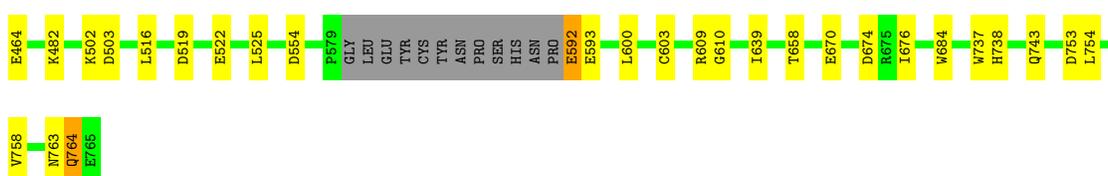
### 3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

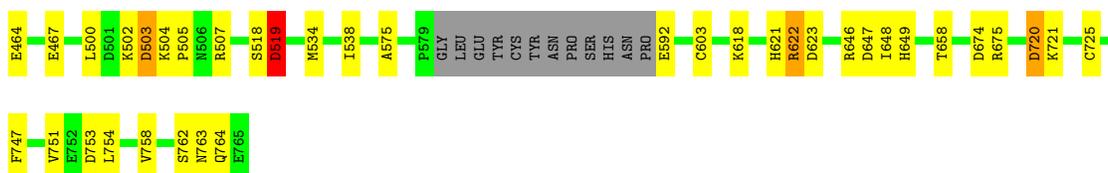
- Molecule 1: Basic fibroblast growth factor receptor 1

Chain A:



- Molecule 1: Basic fibroblast growth factor receptor 1

Chain B:



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.19Å 57.62Å 65.37Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	50.00 – 2.07	Depositor
% Data completeness (in resolution range)	94.5 (50.00-2.07)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.211 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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: C4F

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	0.65	0/2373	0.87	4/3204 (0.1%)
1	B	0.58	0/2367	0.83	6/3196 (0.2%)
All	All	0.61	0/4740	0.85	10/6400 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	753	ASP	CB-CG-OD2	6.99	124.59	118.30
1	B	647	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	519	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	623	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	674	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	554	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	753	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	674	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	519	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	503	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2320	0	2335	13	0
1	B	2319	0	2334	11	0
2	A	18	0	14	0	0
2	B	18	0	14	0	0
3	A	213	0	0	3	0
3	B	143	0	0	4	0
All	All	5031	0	4697	24	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:738:HIS:CD2	1:A:743:GLN:HB2	2.11	0.85
1:B:518:SER:O	3:B:332:HOH:O	2.13	0.67
1:A:738:HIS:HD2	1:A:743:GLN:HB2	1.65	0.58
1:A:763:ASN:O	1:A:764:GLN:HB2	2.04	0.58
1:B:464:GLU:OE1	3:B:78:HOH:O	2.18	0.56
1:B:649:HIS:HA	1:B:675:ARG:NH1	2.22	0.54
1:B:754:LEU:O	1:B:758:VAL:HG23	2.08	0.53
1:B:747:PHE:O	1:B:751:VAL:HG23	2.09	0.52
1:B:519:ASP:OD1	3:B:326:HOH:O	2.19	0.52
1:A:610:GLY:HA3	1:A:639:ILE:HD12	1.92	0.52
1:B:534:MET:HG3	1:B:538:ILE:HD12	1.95	0.49
1:A:684:TRP:CD1	1:A:684:TRP:C	2.86	0.48
1:A:670:GLU:OE1	3:A:785:HOH:O	2.20	0.48
1:A:670:GLU:HG3	3:A:770:HOH:O	2.14	0.47
1:B:721:LYS:NZ	1:B:725:CYS:O	2.46	0.46
1:B:621:HIS:O	1:B:622:ARG:HB2	2.15	0.46
1:A:754:LEU:O	1:A:758:VAL:HG23	2.17	0.45
1:A:592:GLU:O	1:A:593:GLU:C	2.57	0.43
1:A:516:LEU:HD11	1:A:525:LEU:HD13	2.01	0.42
1:A:684:TRP:CE3	1:A:737:TRP:HA	2.54	0.42
1:B:575:ALA:HB2	3:B:161:HOH:O	2.19	0.42
1:B:720:ASP:OD1	1:B:720:ASP:N	2.53	0.42
1:A:676:ILE:HD13	3:A:935:HOH:O	2.19	0.41
1:A:600:LEU:O	1:A:603[A]:CYS:HB3	2.20	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 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	287/302 (95%)	280 (98%)	6 (2%)	1 (0%)	50	39
1	B	286/302 (95%)	276 (96%)	6 (2%)	4 (1%)	16	5
All	All	573/604 (95%)	556 (97%)	12 (2%)	5 (1%)	25	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	764	GLN
1	B	764	GLN
1	B	500	LEU
1	B	622	ARG
1	B	505	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	255/265 (96%)	247 (97%)	8 (3%)	52	45
1	B	254/265 (96%)	239 (94%)	15 (6%)	28	17
All	All	509/530 (96%)	486 (96%)	23 (4%)	38	28

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	GLU
1	A	482	LYS
1	A	502	LYS
1	A	503	ASP

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Mol	Chain	Res	Type
1	A	522	GLU
1	A	592	GLU
1	A	609	ARG
1	A	658	THR
1	B	467	GLU
1	B	502	LYS
1	B	503	ASP
1	B	504	LYS
1	B	507	ARG
1	B	519	ASP
1	B	592	GLU
1	B	603	CYS
1	B	618	LYS
1	B	646	ARG
1	B	648	ILE
1	B	658	THR
1	B	720	ASP
1	B	762	SER
1	B	763	ASN

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

Mol	Chain	Res	Type
1	A	738	HIS
1	A	749	GLN
1	B	680	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

2 ligands are 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	C4F	A	1	-	20,20,20	1.51	4 (20%)	27,27,27	1.53	5 (18%)
2	C4F	B	2	-	20,20,20	1.65	3 (15%)	27,27,27	1.34	5 (18%)

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	C4F	A	1	-	-	0/6/6/6	0/1/3/3
2	C4F	B	2	-	-	0/6/6/6	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	C4F	C8-N7	-4.93	1.28	1.37
2	A	1	C4F	C8-N7	-4.35	1.29	1.37
2	B	2	C4F	C1-C6	-2.93	1.35	1.43
2	A	1	C4F	C1-C6	-2.87	1.36	1.43
2	A	1	C4F	C8-C9	-2.36	1.34	1.37
2	B	2	C4F	C9-C1	2.15	1.49	1.42
2	A	1	C4F	C2-C1	-2.15	1.37	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	C4F	C3-C2-C1	-3.83	115.30	120.88
2	A	1	C4F	C8-C9-C1	-3.32	103.19	107.29
2	B	2	C4F	C8-C9-C1	-3.22	103.32	107.29
2	A	1	C4F	C9-C8-N7	2.95	112.93	107.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	C4F	C3-C2-C1	-2.70	116.95	120.88
2	A	1	C4F	C9-C10-C11	-2.67	107.50	114.14
2	B	2	C4F	C9-C8-N7	2.51	112.18	107.94
2	B	2	C4F	N7-C6-N5	2.14	129.14	125.34
2	B	2	C4F	C3-C4-N5	-2.07	120.75	123.89
2	A	1	C4F	N7-C6-N5	2.02	128.93	125.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.