



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:22 pm GMT

PDB ID : 1AGW  
Title : CRYSTAL STRUCTURE OF THE TYROSINE KINASE DOMAIN OF FIBROBLAST GROWTH FACTOR RECEPTOR 1 IN COMPLEX WITH SU4984 INHIBITOR  
Authors : Mohammadi, M.; Schlessinger, J.; Hubbard, S.R.  
Deposited on : 1997-03-25  
Resolution : 2.40 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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

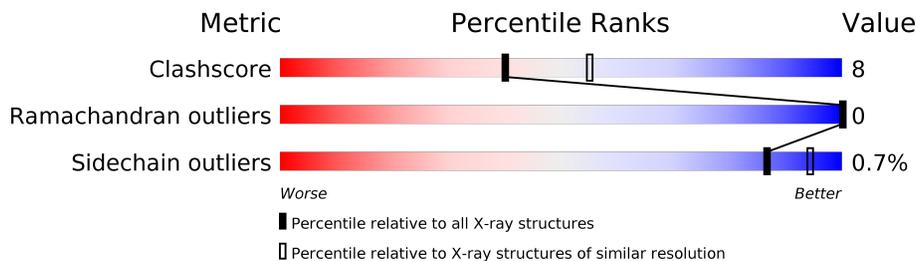
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	B	310	

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	SU2	A	1001	X	-	-	-
2	SU2	B	1000	X	-	-	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4607 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.

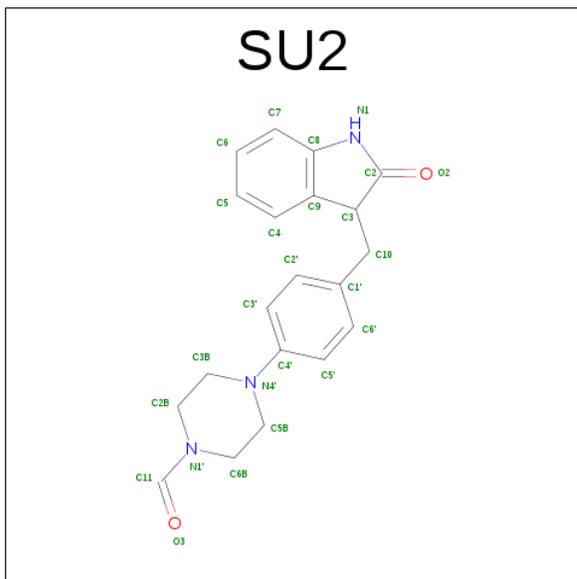
- Molecule 1 is a protein called FGF RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	278	2190	1400	381	391	18	0	1	0
1	B	272	2133	1364	364	386	19	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	VAL	LEU	CONFLICT	UNP P11362
A	488	ALA	CYS	CONFLICT	UNP P11362
A	584	SER	CYS	CONFLICT	UNP P11362
B	457	VAL	LEU	CONFLICT	UNP P11362
B	488	ALA	CYS	ENGINEERED	UNP P11362
B	584	SER	CYS	CONFLICT	UNP P11362

- Molecule 2 is 3-[4-(1-FORMYLPIPERAZIN-4-YL)-BENZYLIDENYL]-2-INDOLINONE (three-letter code: SU2) (formula: C<sub>20</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			25	20	3	2		
2	A	1	Total	C	N	O	0	0
			25	20	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	88	Total	O	0	0
			88	88		



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.36Å 57.08Å 65.53Å 90.00° 107.54° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	85.6 (6.00-2.40)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.44	Depositor
R, $R_{free}$	0.194 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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: SU2

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	0.40	0/2240	0.62	0/3028
1	B	0.38	0/2184	0.61	0/2949
All	All	0.39	0/4424	0.61	0/5977

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 [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	2190	0	2207	29	0
1	B	2133	0	2135	42	0
2	A	25	0	20	2	0
2	B	25	0	20	4	0
3	A	146	0	0	1	0
3	B	88	0	0	1	0
All	All	4607	0	4382	73	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 8.

All (73) 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:B:545:ILE:HG21	2:B:1000:SU2:H7	1.53	0.89
2:B:1000:SU2:H6'	2:B:1000:SU2:O2	1.79	0.81
1:B:498:ILE:HG13	1:B:508:VAL:HG12	1.65	0.79
1:B:738:HIS:HD2	1:B:740:VAL:H	1.31	0.76
2:A:1001:SU2:O2	2:A:1001:SU2:H6'	1.86	0.74
1:B:727:ASN:O	1:B:731:MET:HG2	1.91	0.70
1:B:754:LEU:O	1:B:758:VAL:HG23	1.92	0.70
1:B:597:SER:O	1:B:601:VAL:HG23	1.92	0.68
1:A:705:PRO:HG2	1:A:708:GLU:HG2	1.77	0.66
1:B:489:PHE:N	1:B:517:LYS:HE2	2.11	0.66
1:A:754:LEU:O	1:A:758:VAL:HG23	1.98	0.64
1:B:489:PHE:H	1:B:517:LYS:HE2	1.65	0.62
1:B:747:PHE:O	1:B:751:VAL:HG23	1.99	0.62
1:B:494:LEU:HD11	1:B:510:LYS:HG3	1.82	0.61
1:B:474:PRO:HD2	1:B:477:ARG:HD3	1.83	0.60
1:B:738:HIS:HD2	1:B:740:VAL:N	2.00	0.59
1:B:565:SER:O	2:B:1000:SU2:H2'2	2.03	0.59
1:B:490:GLY:N	1:B:517:LYS:HG3	2.18	0.59
1:B:738:HIS:CD2	1:B:740:VAL:H	2.17	0.58
1:A:552:THR:HG22	1:A:557:LEU:CD1	2.33	0.58
1:A:551:CYS:HB2	1:A:558:TYR:HB2	1.86	0.58
1:A:738:HIS:HD2	1:A:740:VAL:H	1.50	0.57
1:A:649:HIS:CD2	1:A:675:ARG:HD3	2.40	0.56
1:A:564:ALA:O	2:A:1001:SU2:H5'	2.08	0.54
1:A:575:ALA:O	1:A:592:GLU:HA	2.07	0.53
1:B:723:SER:O	1:B:724:ASN:HB2	2.08	0.53
1:A:647:ASP:HB3	1:A:650:HIS:HB2	1.91	0.53
1:A:745:PRO:HB3	3:A:93:HOH:O	2.10	0.52
1:B:735:ASP:HB3	1:B:745:PRO:HD3	1.92	0.52
1:B:732:MET:O	1:B:735:ASP:HB2	2.10	0.50
1:A:656:LYS:HA	1:A:661:ARG:O	2.11	0.50
1:A:652:ASP:OD2	1:A:655:LYS:HB2	2.11	0.50
1:B:653:TYR:CZ	1:B:672:LEU:HD12	2.48	0.49
1:B:494:LEU:HD11	1:B:510:LYS:CG	2.43	0.48
1:B:605:TYR:O	1:B:609:ARG:HG3	2.13	0.48
1:A:576:ARG:HH11	1:A:576:ARG:HG3	1.78	0.47
1:B:477:ARG:HH21	1:B:499:GLY:HA3	1.79	0.47
1:B:489:PHE:CA	1:B:517:LYS:HE2	2.45	0.47
1:A:534:MET:HG2	1:A:643:GLY:HA2	1.97	0.46
1:B:654:TYR:N	1:B:654:TYR:CD1	2.82	0.46
1:B:663:PRO:HD2	3:B:110:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:721:LYS:HE3	1:B:725:CYS:O	2.15	0.46
1:B:705:PRO:HG2	1:B:708:GLU:HG2	1.98	0.46
1:B:701:TYR:HE1	1:B:717:HIS:CE1	2.34	0.46
1:A:618:LYS:N	1:A:618:LYS:HD2	2.31	0.46
1:A:649:HIS:HD2	1:A:675:ARG:NH1	2.14	0.46
1:A:482:LYS:HA	1:A:483:PRO:HD3	1.84	0.46
1:B:534[A]:MET:SD	1:B:643:GLY:HA2	2.56	0.45
1:A:610:GLY:HA3	1:A:639:ILE:HD12	1.99	0.45
1:B:498:ILE:CG1	1:B:508:VAL:HG12	2.42	0.45
1:A:477:ARG:HA	1:A:477:ARG:NE	2.30	0.45
1:A:534:MET:HG2	1:A:643:GLY:CA	2.47	0.45
1:B:477:ARG:NH2	1:B:499:GLY:O	2.50	0.45
1:B:730:TYR:CZ	1:B:734:ARG:HD3	2.52	0.44
1:B:489:PHE:HA	1:B:517:LYS:HE2	1.98	0.44
1:A:492:VAL:HG22	1:A:514:LYS:HG2	1.98	0.44
1:B:670:GLU:HG2	1:B:671:ALA:N	2.31	0.44
1:B:684:TRP:CE3	1:B:737:TRP:HA	2.53	0.43
1:B:674:ASP:O	1:B:676:ILE:HG13	2.19	0.42
1:A:474:PRO:HB2	1:A:477:ARG:HG2	2.00	0.42
1:A:552:THR:HG22	1:A:557:LEU:HD13	2.02	0.42
1:A:649:HIS:HD2	1:A:675:ARG:HH11	1.68	0.42
1:A:478:LEU:HD21	1:A:513:VAL:HG21	2.02	0.42
1:B:672:LEU:HD21	1:B:710:PHE:HE1	1.85	0.42
1:A:531:GLU:O	1:A:535:MET:HG3	2.19	0.41
1:B:498:ILE:HD12	1:B:498:ILE:N	2.35	0.41
1:B:676:ILE:O	1:B:676:ILE:HG22	2.21	0.41
1:B:605:TYR:CE2	1:B:609:ARG:HD2	2.57	0.40
1:B:545:ILE:HG21	2:B:1000:SU2:C7	2.38	0.40
1:B:699:SER:O	1:B:702:PRO:HD3	2.22	0.40
1:A:621:HIS:O	1:A:622:ARG:HB2	2.22	0.40
1:A:574:GLN:HG3	1:A:697:GLY:HA3	2.04	0.40
1:A:710:PHE:O	1:A:714:LYS:HG2	2.22	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	271/310 (87%)	262 (97%)	9 (3%)	0	100	100
1	B	264/310 (85%)	260 (98%)	4 (2%)	0	100	100
All	All	535/620 (86%)	522 (98%)	13 (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	Rotameric	Outliers	Percentiles	
1	A	236/271 (87%)	234 (99%)	2 (1%)	85	93
1	B	228/271 (84%)	227 (100%)	1 (0%)	93	97
All	All	464/542 (86%)	461 (99%)	3 (1%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	MET
1	A	618	LYS
1	B	510	LYS

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	649	HIS
1	B	680	GLN
1	B	738	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](#)

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	SU2	A	1001	-	26,28,28	1.51	6 (23%)	33,39,39	2.72	9 (27%)
2	SU2	B	1000	-	26,28,28	1.55	6 (23%)	33,39,39	2.81	10 (30%)

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	SU2	A	1001	-	1/1/4/6	0/10/32/32	0/4/4/4
2	SU2	B	1000	-	1/1/4/6	0/10/32/32	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	SU2	C9-C3	-4.26	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SU2	C9-C3	-3.77	1.44	1.51
2	B	1000	SU2	C8-C9	2.12	1.41	1.39
2	B	1000	SU2	C5B-N4'	2.24	1.50	1.46
2	B	1000	SU2	C2-N1	2.25	1.37	1.35
2	A	1001	SU2	C8-C9	2.32	1.41	1.39
2	A	1001	SU2	C2B-N1'	2.33	1.50	1.46
2	A	1001	SU2	C5B-N4'	2.57	1.50	1.46
2	A	1001	SU2	C2-N1	2.57	1.37	1.35
2	A	1001	SU2	C6B-N1'	2.98	1.51	1.46
2	B	1000	SU2	C2B-N1'	3.12	1.51	1.46
2	B	1000	SU2	C6B-N1'	3.15	1.51	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	SU2	O2-C2-N1	-6.18	120.32	125.81
2	A	1001	SU2	O2-C2-N1	-6.13	120.36	125.81
2	B	1000	SU2	C8-N1-C2	-5.08	108.83	111.84
2	A	1001	SU2	C8-N1-C2	-4.68	109.06	111.84
2	A	1001	SU2	C9-C8-N1	-3.82	107.51	109.30
2	B	1000	SU2	C9-C8-N1	-3.46	107.68	109.30
2	B	1000	SU2	C2B-N1'-C11	-3.17	119.99	122.63
2	A	1001	SU2	C2B-N1'-C11	-2.79	120.30	122.63
2	B	1000	SU2	C6B-N1'-C11	-2.22	120.78	122.63
2	B	1000	SU2	C2B-C3B-N4'	2.03	114.67	110.68
2	B	1000	SU2	C6B-C5B-N4'	2.15	114.92	110.68
2	A	1001	SU2	C2B-C3B-N4'	2.32	115.25	110.68
2	A	1001	SU2	C6B-C5B-N4'	2.67	115.94	110.68
2	B	1000	SU2	C10-C3-C9	5.30	124.85	112.83
2	A	1001	SU2	C10-C3-C9	5.35	124.95	112.83
2	A	1001	SU2	C3B-C2B-N1'	6.99	116.12	110.35
2	A	1001	SU2	C5B-C6B-N1'	7.39	116.45	110.35
2	B	1000	SU2	C5B-C6B-N1'	7.58	116.61	110.35
2	B	1000	SU2	C3B-C2B-N1'	7.73	116.74	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1000	SU2	C3
2	A	1001	SU2	C3

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	1001	SU2	2	0
2	B	1000	SU2	4	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.