



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 06:45 PM GMT

PDB ID : 2JKQ
Title : FOCAL ADHESION KINASE CATALYTIC DOMAIN IN COMPLEX WITH
BIS-ANILINO PYRIMIDINE INHIBITOR
Authors : Lietha, D.; Eck, M.J.
Deposited on : 2008-08-29
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

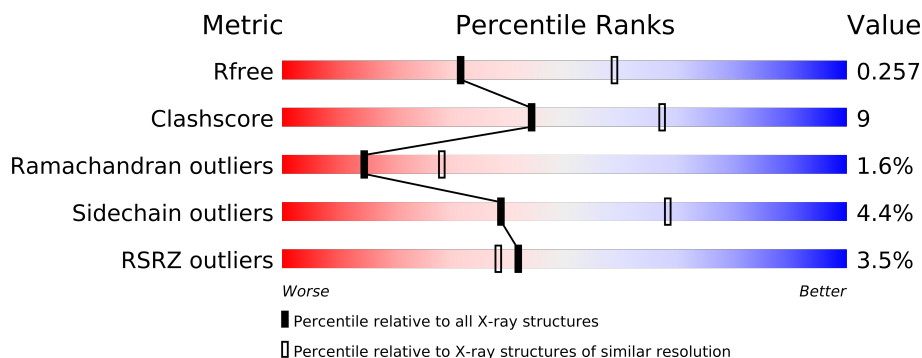
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	276	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2128 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.

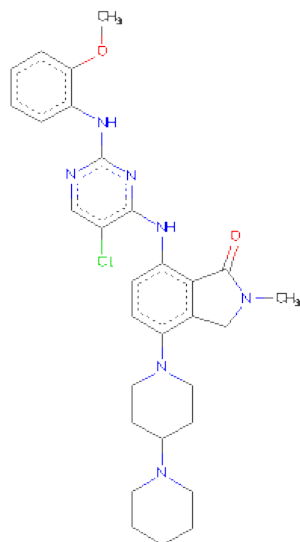
- Molecule 1 is a protein called FOCAL ADHESION KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2064	1318	357	372	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	LEU	MET	CONFLICT	UNP Q00944
A	516	TYR	PHE	CONFLICT	UNP Q00944
A	556	SER	ALA	CONFLICT	UNP Q00944
A	557	ASN	THR	CONFLICT	UNP Q00944

- Molecule 2 is 4-(1,4'-BIPIPERIDIN-1'-YL)-7-({5-CHLORO-2-[(2-METHOXYPHENYL) AMINO]PYRIMIDIN-4-YL} AMINO)-2-METHYL-2,3-DIHYDRO-1H-ISOINDOL-1-ONE (three-letter code: VG8) (formula: C₃₀H₃₆ClN₇O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			40	30	1	7	2		

- Molecule 3 is water.

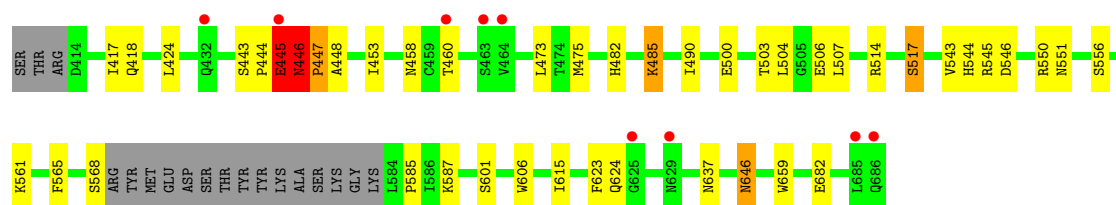
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		

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 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.

• Molecule 1: FOCAL ADHESION KINASE 1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.52Å 44.89Å 66.44Å 90.00° 95.42° 90.00°	Depositor
Resolution (Å)	33.08 – 2.60 33.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (33.08-2.60) 92.1 (33.07-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.262 0.209 , 0.257	Depositor DCC
R_{free} test set	339 reflections (4.69%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 13.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 7561 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2128	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VG8

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	0.75	8/2110 (0.4%)	0.65	3/2854 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	GLU	CD-OE1	19.73	1.47	1.25
1	A	446	ASN	CB-CG	9.02	1.71	1.51
1	A	445	GLU	C-N	8.67	1.53	1.34
1	A	446	ASN	CG-ND2	7.07	1.50	1.32
1	A	446	ASN	N-CA	-5.62	1.35	1.46
1	A	445	GLU	C-O	5.23	1.33	1.23
1	A	445	GLU	CA-C	5.15	1.66	1.52
1	A	446	ASN	CG-OD1	5.05	1.35	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	GLU	OE1-CD-OE2	8.57	133.59	123.30
1	A	446	ASN	CA-CB-CG	-6.09	100.00	113.40
1	A	446	ASN	N-CA-CB	5.92	121.26	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	445	GLU	Peptide
1	A	447	PRO	Peptide

5.2 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 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	2064	0	2063	31	0
2	A	40	0	36	6	0
3	A	24	0	0	3	0
All	All	2128	0	2099	36	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 9.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:506:GLU:OE1	2:A:1687:VG8:HBE2	1.58	1.04
1:A:444:PRO:O	1:A:445:GLU:HB2	1.72	0.85
1:A:544:HIS:HD2	1:A:546:ASP:H	1.34	0.74
1:A:514:ARG:HH11	1:A:517:SER:HB2	1.62	0.64
1:A:482:HIS:HA	1:A:561:LYS:HG2	1.78	0.63
2:A:1687:VG8:HBD1	2:A:1687:VG8:CAX	2.28	0.63
1:A:543:VAL:HG12	1:A:545:ARG:HG3	1.83	0.60
1:A:504:LEU:HD12	1:A:556:SER:HA	1.84	0.59
1:A:485:LYS:HB2	1:A:500:GLU:OE2	2.07	0.55
1:A:546:ASP:OD1	1:A:568:SER:C	2.46	0.54
1:A:475:MET:CE	1:A:565:PHE:HB2	2.38	0.54
1:A:475:MET:HE1	1:A:565:PHE:HB2	1.90	0.53
1:A:646:ASN:C	1:A:646:ASN:HD22	2.12	0.53
1:A:443:SER:HB3	3:A:2005:HOH:O	2.10	0.52
1:A:546:ASP:O	1:A:551:ASN:ND2	2.41	0.51
1:A:565:PHE:CD1	1:A:565:PHE:N	2.78	0.51
1:A:424:LEU:HD12	1:A:453:ILE:HD13	1.93	0.50
1:A:544:HIS:O	1:A:545:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:646:ASN:ND2	3:A:2023:HOH:O	2.45	0.48
1:A:544:HIS:CD2	1:A:546:ASP:H	2.24	0.47
2:A:1687:VG8:HAZ	2:A:1687:VG8:HBE1	1.67	0.46
2:A:1687:VG8:HBD1	2:A:1687:VG8:HAX1	1.97	0.46
1:A:444:PRO:O	1:A:445:GLU:CB	2.52	0.45
2:A:1687:VG8:CBD	2:A:1687:VG8:CAX	2.96	0.44
1:A:417:ILE:O	1:A:490:ILE:HG12	2.18	0.44
1:A:646:ASN:C	1:A:646:ASN:ND2	2.72	0.43
1:A:550:ARG:HH22	1:A:585:PRO:HB3	1.83	0.43
1:A:565:PHE:HD1	1:A:565:PHE:N	2.16	0.42
2:A:1687:VG8:HAW	2:A:1687:VG8:HAS2	1.72	0.42
1:A:458:ASN:C	1:A:460:THR:H	2.24	0.42
1:A:606:TRP:CE3	1:A:659:TRP:HA	2.56	0.41
1:A:445:GLU:N	1:A:446:ASN:HB2	2.34	0.41
1:A:544:HIS:HD2	1:A:546:ASP:N	2.09	0.40
1:A:507:LEU:HD21	1:A:615:ILE:HG12	2.02	0.40
1:A:587:LYS:HD3	1:A:623:PHE:HB2	2.04	0.40
1:A:485:LYS:HD2	3:A:2010:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	254/276 (92%)	244 (96%)	6 (2%)	4 (2%)	14 28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	GLU
1	A	447	PRO
1	A	448	ALA
1	A	446	ASN

5.3.2 Protein sidechains ⓘ

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	227/246 (92%)	217 (96%)	10 (4%)	39 68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	473	LEU
1	A	485	LYS
1	A	503	THR
1	A	517	SER
1	A	601	SER
1	A	624	GLN
1	A	637	ASN
1	A	646	ASN
1	A	682	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	A	437	HIS
1	A	470	GLN
1	A	544	HIS
1	A	624	GLN
1	A	637	ASN
1	A	646	ASN

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 ⓘ

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	VG8	A	1687	-	45,45,45	1.37	4 (8%)	64,64,64	2.17	18 (28%)

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	VG8	A	1687	-	-	0/18/48/48	1/4/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1687	VG8	CAN-CAM	-5.73	1.40	1.49
2	A	1687	VG8	CBE-NBC	2.71	1.50	1.46
2	A	1687	VG8	CAX-CAY	2.63	1.53	1.50
2	A	1687	VG8	CBL-CBJ	2.03	1.58	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1687	VG8	N1-C2-N3	-7.47	120.25	126.68
2	A	1687	VG8	CAN-CAM-NAU	6.70	112.57	106.36
2	A	1687	VG8	CAS-OAR-CAQ	-6.09	108.58	117.59
2	A	1687	VG8	OAR-CAQ-CAL	3.60	119.00	114.83
2	A	1687	VG8	CAJ-NAE-C4	-3.57	121.30	129.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1687	VG8	CBE-NBC-CBD	3.51	118.88	111.67
2	A	1687	VG8	CAY-CBB-NBC	3.30	123.96	118.88
2	A	1687	VG8	OAI-CAM-CAN	-3.19	124.84	128.89
2	A	1687	VG8	CBD-NBC-CBB	3.03	122.87	116.28
2	A	1687	VG8	CAX-NAU-CAM	-2.87	110.56	113.21
2	A	1687	VG8	C6-C5-C4	-2.76	118.34	120.25
2	A	1687	VG8	C2-N3-C4	2.69	122.57	116.97
2	A	1687	VG8	CAJ-CAN-CAM	2.63	133.44	129.18
2	A	1687	VG8	CAZ-CBB-NBC	-2.35	117.92	122.06
2	A	1687	VG8	OAR-CAQ-CAW	-2.19	120.76	124.37
2	A	1687	VG8	C6-N1-C2	2.14	120.18	116.02
2	A	1687	VG8	CBM-CBK-NBI	-2.06	107.45	111.11
2	A	1687	VG8	CAN-CAJ-NAE	2.02	122.70	120.58

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1687	VG8	CBD-CBE-CBF-CBG-CBH-NBC

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, 95th 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 ²)	Q<0.9
1	A	258/276 (93%)	0.24	9 (3%) 42 38	25, 33, 42, 53	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	GLN	5.5
1	A	685	LEU	5.2
1	A	625	GLY	3.7
1	A	432	GLN	2.9
1	A	445	GLU	2.8
1	A	629	ASN	2.6
1	A	460	THR	2.3
1	A	463	SER	2.2
1	A	464	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q < 0.9
2	VG8	A	1687	40/40	0.17	-0.48	26,30,45,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.