



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 09:49 am GMT

PDB ID : 1K05
Title : Crystal structure of the Focal Adhesion Targeting Domain of Focal Adhesion Kinase
Authors : Arold, S.T.; Hoellerer, M.K.; Noble, M.E.M.
Deposited on : 2001-09-18
Resolution : 2.90 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

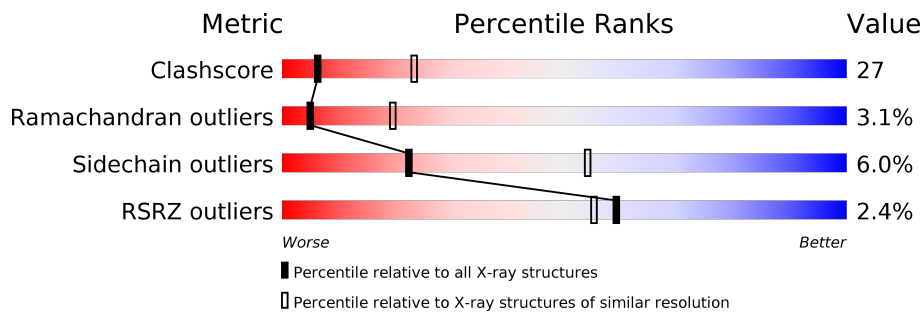
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 ≥ 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	162	<div> <div>44%</div> <div>35%</div> <div>5%</div> <div>17%</div> </div>
1	B	162	<div> <div>49%</div> <div>33%</div> <div>6%</div> <div>12%</div> </div>
1	C	162	<div> <div>44%</div> <div>38%</div> <div>5%</div> <div>12%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3257 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 FOCAL ADHESION KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1053	664	180	202	7			
1	B	142	Total	C	N	O	S	0	0	0
			1098	695	184	212	7			
1	C	142	Total	C	N	O	S	0	0	0
			1100	695	185	213	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	C	5	Total	O	0	0
			5	5		

- Molecule 1: FOCAL ADHESION KINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	87.48Å 222.10Å 97.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.30 – 2.90 31.31 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.9 (31.30-2.90) 96.1 (31.31-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.285 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3257	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0/1064	0.64	0/1438
1	B	0.46	0/1113	0.66	0/1509
1	C	0.42	0/1114	0.64	0/1510
All	All	0.44	0/3291	0.65	0/4457

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	1053	0	1106	52	0
1	B	1098	0	1149	62	0
1	C	1100	0	1149	71	0
2	A	1	0	0	0	0
2	C	5	0	0	0	0
All	All	3257	0	3404	179	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 27.

The worst 5 of 179 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:976:PRO:HD3	1:A:1045:MET:HG2	1.43	1.01
1:A:1049:THR:HG22	1:A:1050:ARG:H	1.33	0.92
1:C:943:GLN:HB2	1:C:944:PRO:HD3	1.53	0.88
1:A:1013:GLN:HG3	1:A:1014:GLN:H	1.38	0.87
1:A:1013:GLN:HG3	1:A:1014:GLN:N	1.89	0.87

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	133/162 (82%)	113 (85%)	17 (13%)	3 (2%)	7	27
1	B	140/162 (86%)	127 (91%)	9 (6%)	4 (3%)	5	21
1	C	140/162 (86%)	117 (84%)	17 (12%)	6 (4%)	3	12
All	All	413/486 (85%)	357 (86%)	43 (10%)	13 (3%)	5	19

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1008	VAL
1	C	942	ILE
1	C	944	PRO
1	A	980	HIS
1	B	944	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	118/142 (83%)	111 (94%)	7 (6%)	23	55
1	B	124/142 (87%)	114 (92%)	10 (8%)	14	38
1	C	124/142 (87%)	119 (96%)	5 (4%)	36	71
All	All	366/426 (86%)	344 (94%)	22 (6%)	22	54

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	937	GLU
1	B	992	SER
1	C	948	GLU
1	B	942	ILE
1	B	985	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	927	ASN
1	C	1013	GLN
1	C	927	ASN
1	B	921	ASN
1	B	980	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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](#)

There are no ligands in this entry.

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](#)

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	135/162 (83%)	-0.24	2 (1%) 74 72	47, 72, 95, 113	0
1	B	142/162 (87%)	-0.27	3 (2%) 64 60	45, 69, 87, 123	0
1	C	142/162 (87%)	-0.12	5 (3%) 44 38	62, 82, 115, 128	0
All	All	419/486 (86%)	-0.21	10 (2%) 59 55	45, 74, 108, 128	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	906	PRO	4.8
1	B	907	GLN	3.1
1	C	1009	MET	2.7
1	C	1048	GLN	2.7
1	C	950	TYR	2.5

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.