



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:40 AM GMT

PDB ID : 2BDJ
Title : Src kinase in complex with inhibitor AP23464
Authors : Dalgarno, D.; Stehle, T.; Schelling, P.; Narula, S.; Sawyer, T.
Deposited on : 2005-10-20
Resolution : 2.50 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
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

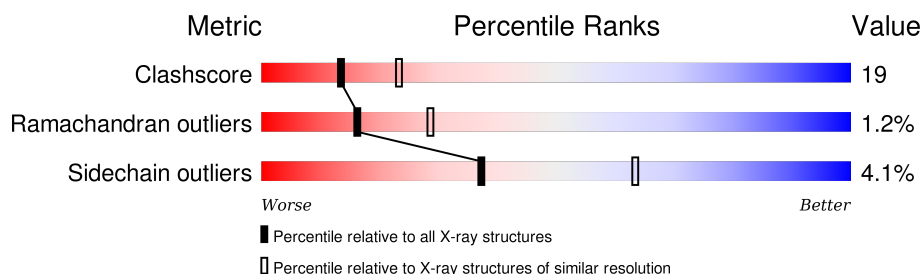
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	

2 Entry composition [i](#)

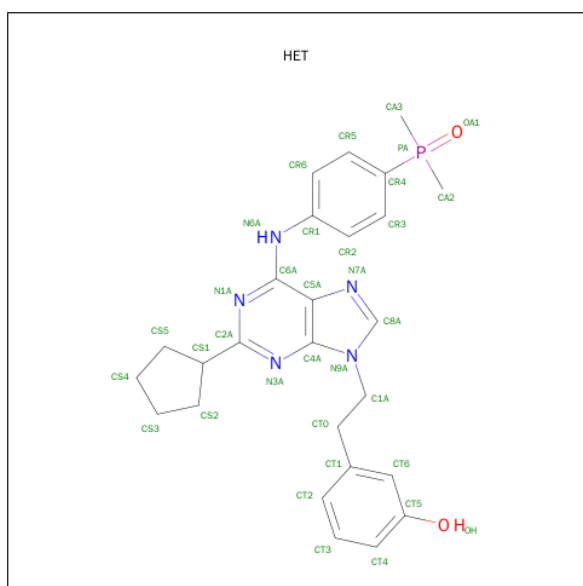
There are 3 unique types of molecules in this entry. The entry contains 2243 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			2048	1319	343	370	16			

- Molecule 2 is 3-[2-(2-CYCLOPENTYL-6-{[4-(DIMETHYLPHOSPHORYL)PHENYL]AMINO}-9H-PURIN-9-YL)ETHYL]PHENOL (three-letter code: HET) (formula: C₂₆H₃₀N₅O₂P).



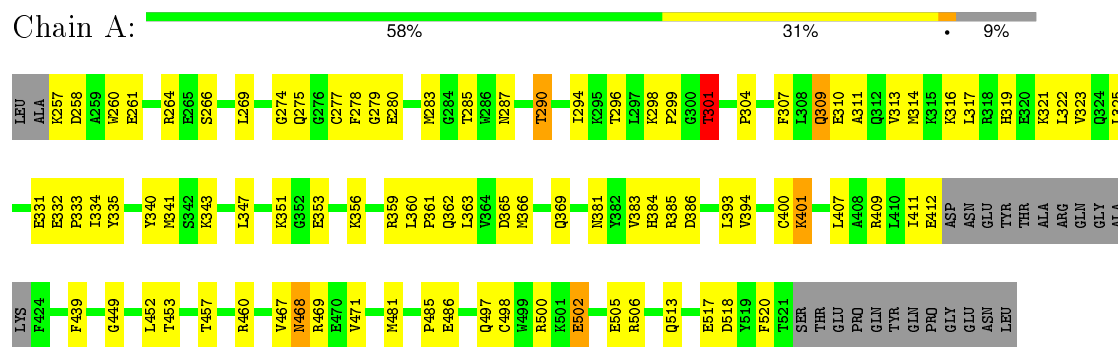
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			34	26	5	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		

Note EDS was not executed.

- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.10 Å 54.60 Å 69.00 Å 90.00° 99.97° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.158 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2243	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.42	0/2097	0.69	0/2838

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	2048	0	2052	75	0
2	A	34	0	28	5	0
3	A	161	0	0	14	0
All	All	2243	0	2080	78	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 19.

All (78) 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)
2:A:800:HET:HR6	2:A:800:HET:N1A	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:PRO:HB3	1:A:334:ILE:HD11	1.61	0.82
1:A:319:HIS:HB3	1:A:322:LEU:HG	1.69	0.74
1:A:411:ILE:HA	3:A:98:HOH:O	1.91	0.71
1:A:500:ARG:O	1:A:506:ARG:HD2	1.96	0.65
1:A:309:GLN:O	1:A:313:VAL:HG23	1.96	0.65
1:A:363:LEU:HA	1:A:366:MET:HE2	1.78	0.65
1:A:311:ALA:HA	1:A:314:MET:HE2	1.80	0.64
1:A:369:GLN:HB2	3:A:129:HOH:O	1.98	0.63
1:A:323:VAL:HG21	1:A:393:LEU:HD12	1.81	0.62
1:A:360:LEU:HB3	1:A:361:PRO:HD3	1.81	0.62
1:A:279:GLY:O	1:A:280:GLU:HG3	2.01	0.61
1:A:383:VAL:HG13	1:A:385:ARG:HD2	1.84	0.60
1:A:513:GLN:O	1:A:517:GLU:HG3	2.02	0.58
1:A:386:ASP:HB2	1:A:407:LEU:HD12	1.84	0.58
1:A:307:PHE:HB2	3:A:80:HOH:O	2.02	0.58
1:A:502:GLU:HB3	1:A:505:GLU:HG3	1.86	0.58
1:A:359:ARG:HG2	1:A:359:ARG:HH11	1.68	0.57
1:A:366:MET:HA	3:A:129:HOH:O	2.04	0.57
1:A:279:GLY:HA2	1:A:298:LYS:HG3	1.86	0.56
1:A:468:ASN:HB2	3:A:96:HOH:O	2.05	0.56
1:A:457:THR:O	1:A:460:ARG:HG2	2.05	0.56
1:A:309:GLN:HG3	1:A:310:GLU:N	2.22	0.55
1:A:385:ARG:HD3	1:A:407:LEU:O	2.06	0.55
1:A:412:GLU:HG3	3:A:78:HOH:O	2.07	0.55
2:A:800:HET:CR6	2:A:800:HET:N1A	2.63	0.54
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.42	0.54
1:A:363:LEU:HA	1:A:366:MET:CE	2.38	0.54
1:A:353:GLU:O	1:A:356:LYS:HG2	2.07	0.54
1:A:266:SER:HB2	1:A:287:ASN:ND2	2.23	0.53
1:A:274:GLY:HA3	2:A:800:HET:HS42	1.91	0.52
1:A:313:VAL:HG12	1:A:317:LEU:HD12	1.91	0.52
1:A:296:THR:HG22	1:A:335:TYR:CD1	2.44	0.52
1:A:498:CYS:O	1:A:506:ARG:HG2	2.08	0.52
1:A:385:ARG:NH1	1:A:409:ARG:HB2	2.25	0.52
1:A:460:ARG:HB3	3:A:121:HOH:O	2.11	0.51
1:A:467:VAL:O	1:A:471:VAL:HG23	2.10	0.51
1:A:258:ASP:OD1	1:A:260:TRP:HD1	1.94	0.51
1:A:383:VAL:HG22	1:A:385:ARG:HG3	1.94	0.50
1:A:257:LYS:CG	1:A:261:GLU:HG3	2.42	0.50
1:A:332:GLU:HA	1:A:334:ILE:N	2.26	0.50
1:A:275:GLN:NE2	1:A:298:LYS:NZ	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLU:HA	1:A:333:PRO:C	2.34	0.48
1:A:400:CYS:HB2	3:A:129:HOH:O	2.13	0.47
1:A:257:LYS:HG2	1:A:261:GLU:HG3	1.96	0.47
1:A:264:ARG:NH2	1:A:331:GLU:HB3	2.30	0.47
1:A:453:THR:O	1:A:457:THR:HG23	2.14	0.47
1:A:316:LYS:HB3	3:A:145:HOH:O	2.15	0.47
1:A:385:ARG:HH11	1:A:409:ARG:HB2	1.80	0.47
1:A:449:GLY:O	1:A:452:LEU:HB2	2.15	0.46
1:A:481:MET:HG2	3:A:36:HOH:O	2.15	0.46
1:A:257:LYS:HG2	1:A:258:ASP:H	1.79	0.46
1:A:341:MET:HG3	1:A:393:LEU:HB3	1.97	0.46
1:A:384:HIS:O	1:A:385:ARG:HB2	2.17	0.45
1:A:269:LEU:HD22	1:A:294:ILE:HD13	1.99	0.45
1:A:285:THR:HA	1:A:290:THR:O	2.17	0.44
1:A:279:GLY:HA3	1:A:296:THR:O	2.18	0.44
1:A:381:ASN:ND2	3:A:89:HOH:O	2.50	0.44
1:A:485:PRO:O	1:A:486:GLU:CB	2.65	0.44
1:A:365:ASP:O	1:A:369:GLN:HG3	2.17	0.43
1:A:497:GLN:O	1:A:506:ARG:HG3	2.18	0.43
1:A:385:ARG:HG2	1:A:439:PHE:CD1	2.53	0.43
1:A:359:ARG:HG2	1:A:359:ARG:NH1	2.33	0.42
1:A:359:ARG:H	1:A:362:GLN:NE2	2.17	0.42
1:A:278:PHE:CD1	1:A:301:THR:HG22	2.54	0.42
1:A:275:GLN:NE2	1:A:298:LYS:HZ1	2.18	0.42
1:A:341:MET:HG3	1:A:393:LEU:CB	2.50	0.42
1:A:485:PRO:O	1:A:486:GLU:HB2	2.19	0.41
1:A:274:GLY:HA3	2:A:800:HET:CS4	2.50	0.41
1:A:353:GLU:HA	1:A:356:LYS:HD3	2.02	0.41
1:A:343:LYS:HB2	1:A:394:VAL:HB	2.02	0.41
1:A:321:LYS:HA	1:A:321:LYS:HD3	1.86	0.41
2:A:800:HET:HT6	3:A:45:HOH:O	2.21	0.41
1:A:411:ILE:HD12	3:A:153:HOH:O	2.21	0.41
1:A:341:MET:HE2	1:A:401:LYS:HB2	2.03	0.41
1:A:314:MET:HE3	1:A:325:LEU:HD13	2.03	0.40
1:A:520:PHE:HA	3:A:122:HOH:O	2.21	0.40
1:A:351:LYS:HB3	1:A:351:LYS:HE2	1.88	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	250/279 (90%)	227 (91%)	20 (8%)	3 (1%)	16	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	THR
1	A	468	ASN
1	A	299	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	220/240 (92%)	211 (96%)	9 (4%)	37	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	CYS
1	A	290	THR
1	A	301	THR
1	A	309	GLN
1	A	347	LEU
1	A	401	LYS
1	A	469	ARG
1	A	502	GLU

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Mol	Chain	Res	Type
1	A	518	ASP

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	275	GLN
1	A	287	ASN
1	A	312	GLN
1	A	362	GLN
1	A	391	ASN
1	A	497	GLN
1	A	513	GLN

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	HET	A	800	-	34,38,38	5.67	13 (38%)	36,55,55	2.26	7 (19%)

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	HET	A	800	-	-	0/15/26/26	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	HET	PA-CA3	-23.24	1.50	1.80
2	A	800	HET	PA-CA2	-19.06	1.55	1.80
2	A	800	HET	CR1-N6A	-7.20	1.25	1.40
2	A	800	HET	C1A-CT0	-2.85	1.46	1.52
2	A	800	HET	CT4-CT5	2.61	1.44	1.38
2	A	800	HET	CT2-CT1	2.84	1.44	1.38
2	A	800	HET	CT3-CT4	2.92	1.44	1.38
2	A	800	HET	CT3-CT2	2.95	1.45	1.38
2	A	800	HET	CT6-CT5	2.99	1.43	1.39
2	A	800	HET	CR6-CR1	3.10	1.44	1.39
2	A	800	HET	PA-OA1	4.01	1.55	1.48
2	A	800	HET	CT6-CT1	4.13	1.46	1.39
2	A	800	HET	C5A-C4A	4.95	1.51	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HET	C4A-C5A-N7A	-7.90	102.22	109.48
2	A	800	HET	N3A-C2A-N1A	-5.24	118.55	126.17
2	A	800	HET	C5A-C6A-N1A	-2.68	117.72	120.48
2	A	800	HET	CS2-CS1-C2A	-2.56	109.11	114.47
2	A	800	HET	CR6-CR1-N6A	-2.19	113.50	120.66
2	A	800	HET	CR1-N6A-C6A	2.36	133.61	128.40
2	A	800	HET	C2A-N3A-C4A	6.74	121.17	115.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	HET	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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