



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SM2  
Title : Crystal structure of the phosphorylated Interleukin-2 tyrosine kinase catalytic domain  
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Deposited on : 2004-03-08  
Resolution : 2.30 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](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 (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

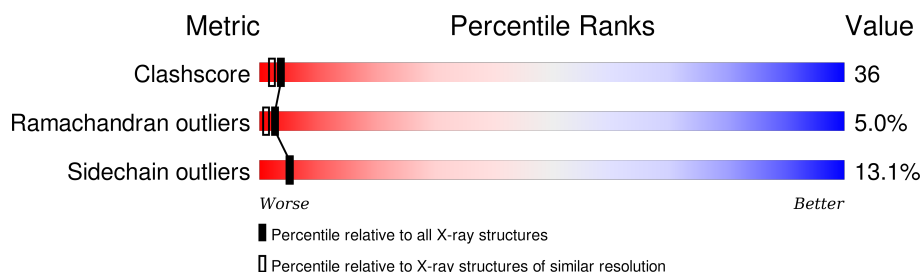
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	264	
1	B	264	

## 2 Entry composition [i](#)

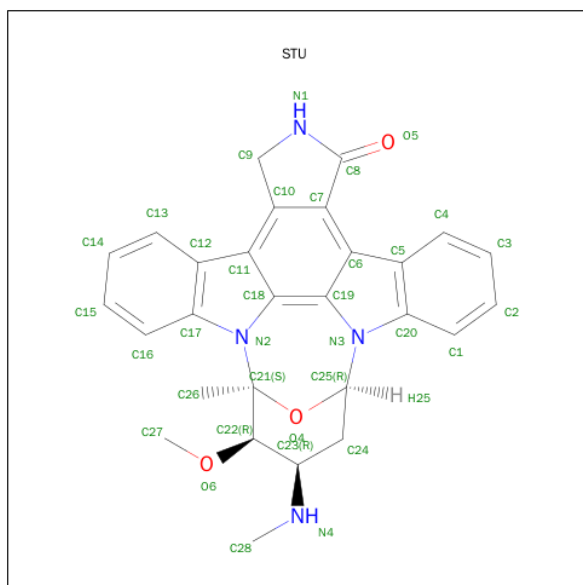
There are 3 unique types of molecules in this entry. The entry contains 4212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tyrosine-protein kinase ITK/TSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1956	1249	326	365	16			
1	B	241	Total	C	N	O	S	0	0	0
			1935	1237	322	360	16			

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula:  $C_{28}H_{26}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 3 is water.

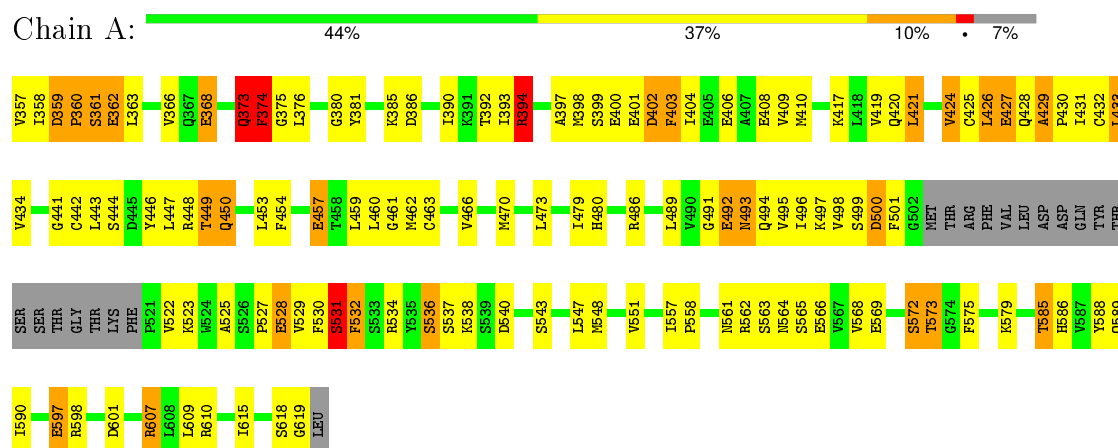
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total 144	O 144	0	0
3	B	107	Total 107	O 107	0	0

### 3 Residue-property plots

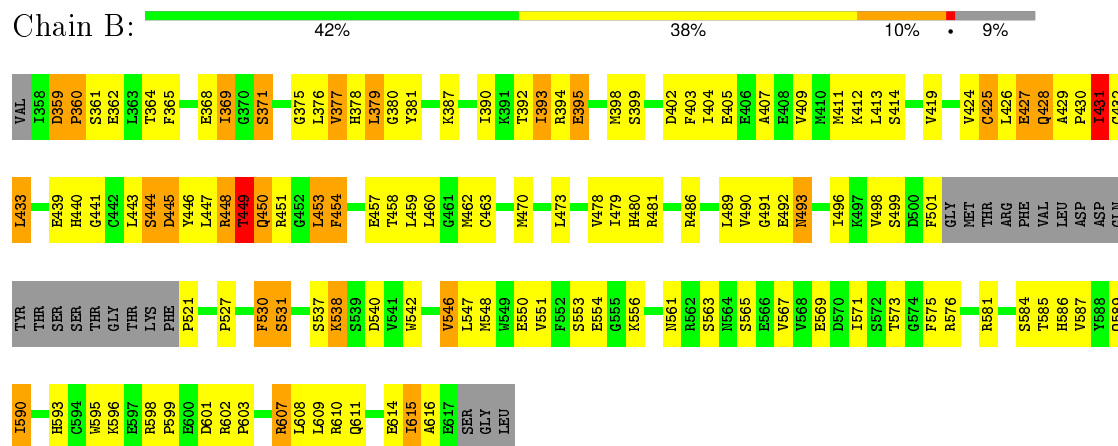
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Tyrosine-protein kinase ITK/TSK



#### • Molecule 1: Tyrosine-protein kinase ITK/TSK



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	125.10 Å   74.40 Å   78.90 Å 90.00°   93.90°   90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	70.0 (20.00-2.30)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNX	Depositor
R, $R_{free}$	0.214 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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: STU

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	0.77	3/2000 (0.1%)	0.72	2/2700 (0.1%)
1	B	0.75	2/1979 (0.1%)	0.74	1/2672 (0.0%)
All	All	0.76	5/3979 (0.1%)	0.73	3/5372 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	SER	CA-CB	-8.00	1.41	1.52
1	B	361	SER	CA-CB	-5.75	1.44	1.52
1	A	457	GLU	CA-CB	5.68	1.66	1.53
1	B	546	VAL	CA-CB	5.28	1.65	1.54
1	A	442	CYS	CB-SG	-5.23	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	PHE	N-CA-C	-6.09	94.56	111.00
1	B	530	PHE	CB-CA-C	-5.99	98.42	110.40
1	A	449	THR	N-CA-C	-5.36	96.52	111.00

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	1956	0	1913	139	0
1	B	1935	0	1893	137	0
2	A	35	0	26	3	0
2	B	35	0	26	3	0
3	A	144	0	0	29	0
3	B	107	0	0	23	0
All	All	4212	0	3858	279	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 36.

The worst 5 of 279 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:607:ARG:HB2	1:A:607:ARG:HH11	1.11	1.13
1:A:607:ARG:HB2	1:A:607:ARG:NH1	1.73	1.02
1:B:470:MET:HE3	1:B:498:VAL:HG21	1.42	1.01
1:B:593:HIS:HB2	3:B:10:HOH:O	1.67	0.94
1:B:590:ILE:O	3:B:10:HOH:O	1.94	0.86

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	241/264 (91%)	204 (85%)	26 (11%)	11 (5%)	3	1
1	B	237/264 (90%)	208 (88%)	16 (7%)	13 (6%)	2	1
All	All	478/528 (90%)	412 (86%)	42 (9%)	24 (5%)	3	1

5 of 24 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	361	SER
1	A	374	PHE
1	A	394	ARG
1	A	492	GLU
1	B	360	PRO

### 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	214/232 (92%)	184 (86%)	30 (14%)	4	4
1	B	212/232 (91%)	186 (88%)	26 (12%)	6	6
All	All	426/464 (92%)	370 (87%)	56 (13%)	5	5

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	THR
1	B	369	ILE
1	B	538	LYS
1	A	585	THR
1	A	607	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	586	HIS
1	A	589	GLN
1	B	428	GLN
1	A	564	ASN
1	B	378	HIS

### 5.3.3 RNA ⓘ

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	STU	A	301	-	27,42,42	2.16	12 (44%)	23,68,68	2.01	6 (26%)
2	STU	B	621	-	27,42,42	2.19	12 (44%)	23,68,68	2.13	9 (39%)

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	STU	A	301	-	-	0/4/42/42	0/0/8/8
2	STU	B	621	-	-	0/4/42/42	0/0/8/8

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	621	STU	C22-C23	-4.12	1.48	1.52
2	A	301	STU	C7-C6	-2.17	1.39	1.43
2	B	621	STU	C13-C12	2.02	1.45	1.41
2	B	621	STU	C14-C15	2.06	1.43	1.38
2	A	301	STU	C11-C18	2.11	1.45	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	STU	C6-C19-C18	-3.77	116.09	121.69
2	B	621	STU	C6-C19-C18	-2.87	117.42	121.69
2	B	621	STU	C15-C14-C13	-2.45	116.89	120.45
2	B	621	STU	C3-C2-C1	-2.45	116.89	120.45
2	B	621	STU	C1-C20-N3	-2.35	129.35	132.18

There are no chirality outliers.

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	301	STU	3	0
2	B	621	STU	3	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 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.