



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:35 PM GMT

PDB ID : 2X7F  
Title : CRYSTAL STRUCTURE OF THE KINASE DOMAIN OF HUMAN TRAF2-  
AND NCK-INTERACTING KINASE WITH WEE1CHK1 INHIBITOR  
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C.; Mahajan, P.; Pike, A.C.W.; Fedorov, O.; Chaikuad, A.; Von Delft, F.;  
Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Knapp, S.  
Deposited on : 2010-02-26  
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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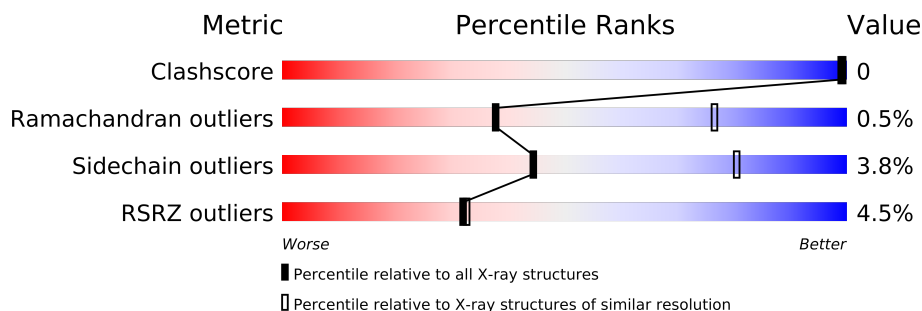
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.80 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	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. 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	326	
1	B	326	
1	C	326	
1	D	326	
1	E	326	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	824	B	500	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9367 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.

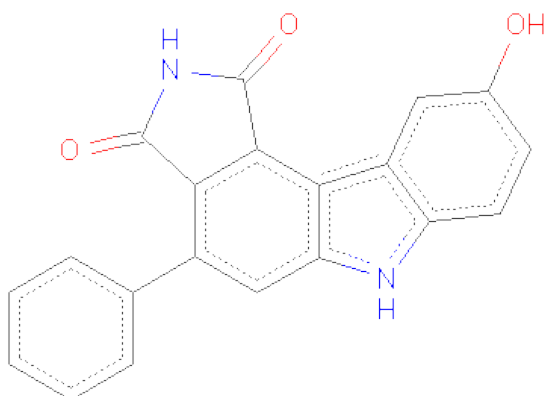
- Molecule 1 is a protein called TRAF2 AND NCK-INTERACTING PROTEIN KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			1924	1234	333	346	11			
1	B	288	Total	C	N	O	S	0	2	0
			2205	1408	387	395	15			
1	C	285	Total	C	N	O	S	0	0	0
			2069	1329	357	370	13			
1	D	236	Total	C	N	O	S	0	0	0
			1540	971	276	285	8			
1	E	251	Total	C	N	O	S	0	0	0
			1482	917	280	282	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q9UKE5
B	0	SER	-	EXPRESSION TAG	UNP Q9UKE5
C	0	SER	-	EXPRESSION TAG	UNP Q9UKE5
D	0	SER	-	EXPRESSION TAG	UNP Q9UKE5
E	0	SER	-	EXPRESSION TAG	UNP Q9UKE5

- Molecule 2 is 9-HYDROXY-4-PHENYLPYRROLO[3,4-C]CARBAZOLE-1,3(2H,6H)-DIONE (three-letter code: 824) (formula: C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>).



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

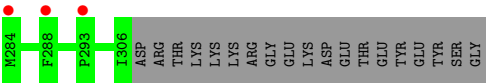
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

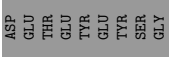
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	14	Total 14	O 14	0	0
4	C	3	Total 3	O 3	0	0





● Molecule 1: TRAF2 AND NCK-INTERACTING PROTEIN KINASE

Chain E:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.97Å 79.07Å 214.16Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	44.32 – 2.80 44.32 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.32-2.80) 99.8 (44.32-2.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT 2.8.0	Depositor
R, $R_{free}$	0.209 , 0.229 0.228 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 69.5	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 44023 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NA, 824

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	0.43	0/1967	0.64	0/2689
1	B	0.51	0/2265	0.68	0/3071
1	C	0.46	0/2118	0.66	0/2891
1	D	0.42	0/1574	0.62	0/2163
1	E	0.44	0/1507	0.63	0/2082
All	All	0.46	0/9431	0.65	0/12896

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1924	0	3	0	0
1	B	2205	0	4	1	0
1	C	2069	0	3	1	0
1	D	1540	0	0	0	0
1	E	1482	0	0	0	0
2	A	25	0	12	0	0
2	B	25	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	25	0	12	0	0
2	D	25	0	12	0	0
2	E	25	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	B	14	0	0	1	0
4	C	3	0	0	1	0
All	All	9367	0	70	2	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 0.

All (2) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:247:ARG:NH1	4:C:2003:HOH:O	2.37	0.57
1:B:168:LYS:NZ	4:B:2008:HOH:O	2.53	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	268/326 (82%)	255 (95%)	12 (4%)	1 (0%)	43 80
1	B	284/326 (87%)	275 (97%)	7 (2%)	2 (1%)	30 69
1	C	279/326 (86%)	271 (97%)	7 (2%)	1 (0%)	43 80
1	D	224/326 (69%)	215 (96%)	8 (4%)	1 (0%)	43 80
1	E	237/326 (73%)	227 (96%)	8 (3%)	2 (1%)	27 65
All	All	1292/1630 (79%)	1243 (96%)	42 (3%)	7 (0%)	38 76

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	171	ASP
1	D	171	ASP
1	E	171	ASP
1	A	171	ASP
1	B	171	ASP

### 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	153/284 (54%)	149 (97%)	4 (3%)	59	90
1	B	219/284 (77%)	208 (95%)	11 (5%)	34	70
1	C	186/284 (66%)	177 (95%)	9 (5%)	35	72
1	D	105/284 (37%)	102 (97%)	3 (3%)	55	88
1	E	69/284 (24%)	68 (99%)	1 (1%)	78	96
All	All	732/1420 (52%)	704 (96%)	28 (4%)	44	80

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	267	GLU
1	C	135	ARG
1	D	244	LEU
1	B	280	THR
1	B	284	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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	824	A	500	-	29,29,29	3.48	13 (44%)	39,44,44	4.25	19 (48%)
2	824	B	500	-	29,29,29	3.72	15 (51%)	39,44,44	4.65	19 (48%)
2	824	C	500	-	29,29,29	3.53	12 (41%)	39,44,44	4.20	17 (43%)
2	824	D	500	-	29,29,29	3.42	13 (44%)	39,44,44	4.33	19 (48%)
2	824	E	500	-	29,29,29	3.61	15 (51%)	39,44,44	3.98	17 (43%)

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	824	A	500	-	-	0/4/4/4	0/1/5/5
2	824	B	500	-	-	0/4/4/4	0/1/5/5
2	824	C	500	-	-	0/4/4/4	0/1/5/5
2	824	D	500	-	-	0/4/4/4	0/1/5/5
2	824	E	500	-	-	0/4/4/4	0/1/5/5

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	824	C15-C16	9.10	1.57	1.41
2	B	500	824	C17-C19	8.75	1.55	1.37
2	C	500	824	C15-C16	8.66	1.56	1.41
2	E	500	824	C17-C19	8.49	1.54	1.37
2	B	500	824	O1-C5	-8.48	1.07	1.24

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	824	C19-C17-C15	-16.53	110.49	120.49
2	D	500	824	C19-C17-C15	-15.86	110.90	120.49
2	B	500	824	C6-N1-C5	-13.85	102.73	109.98
2	C	500	824	C6-N1-C5	-13.72	102.80	109.98
2	A	500	824	C6-N1-C5	-13.38	102.98	109.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	276/326 (84%)	0.14	13 (4%) 30 30	59, 99, 164, 196	0
1	B	288/326 (88%)	0.02	3 (1%) 79 79	33, 57, 102, 172	0
1	C	285/326 (87%)	0.09	7 (2%) 54 55	51, 85, 133, 189	0
1	D	236/326 (72%)	0.15	18 (7%) 14 12	68, 113, 165, 207	0
1	E	251/326 (76%)	0.08	19 (7%) 14 12	95, 127, 170, 214	0
All	All	1336/1630 (81%)	0.09	60 (4%) 32 33	33, 98, 161, 214	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	88	ALA	6.2
1	D	130	ILE	4.7
1	E	110	ALA	4.6
1	D	42	GLY	4.4
1	D	99	ASP	4.2

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	824	E	500	25/25	0.28	0.47	96,101,104,105	0
2	824	C	500	25/25	0.24	0.23	48,57,61,63	0
2	824	A	500	25/25	0.19	-0.15	53,62,67,70	0
2	824	B	500	25/25	0.18	-0.42	25,30,37,38	0
2	824	D	500	25/25	0.19	-0.69	87,91,94,95	0
3	NA	A	1315	1/1	0.14	-1.07	70,70,70,70	0
3	NA	E	1311	1/1	0.07	-1.91	83,83,83,83	0
3	NA	C	1315	1/1	0.13	-1.99	68,68,68,68	0
3	NA	D	1308	1/1	0.06	-2.28	94,94,94,94	0
3	NA	B	1315	1/1	0.08	-6.08	56,56,56,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.