



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 02:12 PM JST

PDB ID : 8GW3  
Title : Crystal structure of human TAK1 kinase domain fused with TAB1  
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Deposited on : 2022-09-16  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

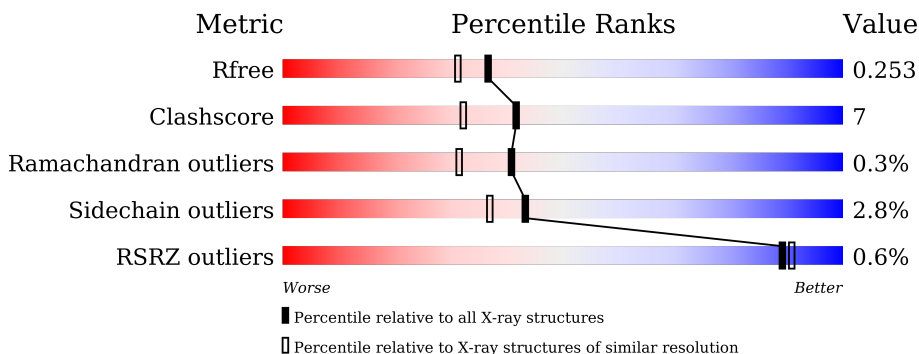
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	326	 78% 13% 8%
1	B	326	 77% 14% 8%
1	C	326	 78% 13% 9%
1	D	326	 71% 18% 10%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9458 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 Mitogen-activated protein kinase kinase kinase 7, TGF-beta-activated kinase 1 and MAP3K7-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	299	Total 2303	C 1490	N 388	O 405	S 20	0	0	0
1	B	299	Total 2270	C 1470	N 377	O 403	S 20	0	0	0
1	C	298	Total 2259	C 1469	N 377	O 394	S 19	0	0	0
1	D	294	Total 2207	C 1436	N 369	O 383	S 19	0	0	0


- Molecule 2 is water.

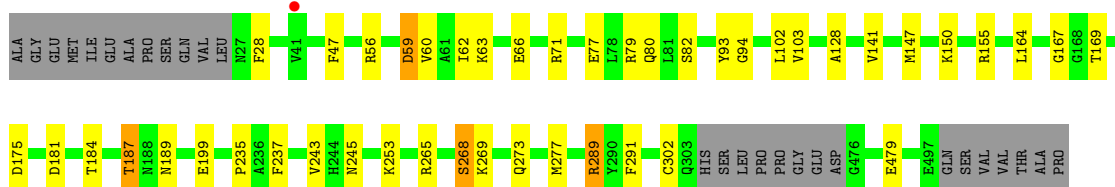
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total 146	O 146	0	0
2	B	116	Total 116	O 116	0	0
2	C	103	Total 103	O 103	0	0
2	D	54	Total 54	O 54	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

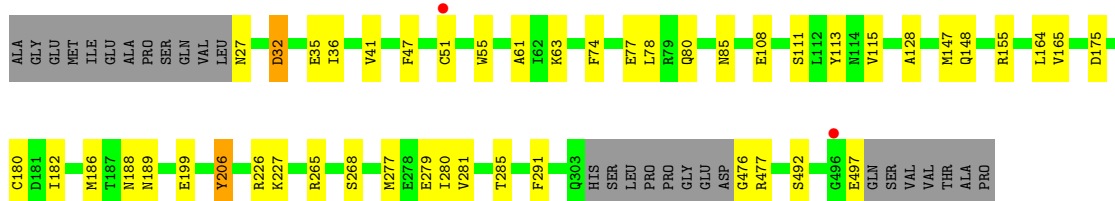
- Molecule 1: Mitogen-activated protein kinase kinase kinase 7, TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain A: 




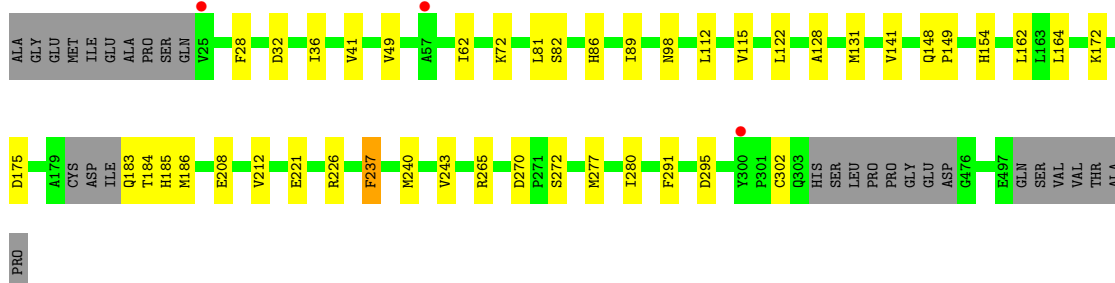
- Molecule 1: Mitogen-activated protein kinase kinase kinase 7, TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain B: 

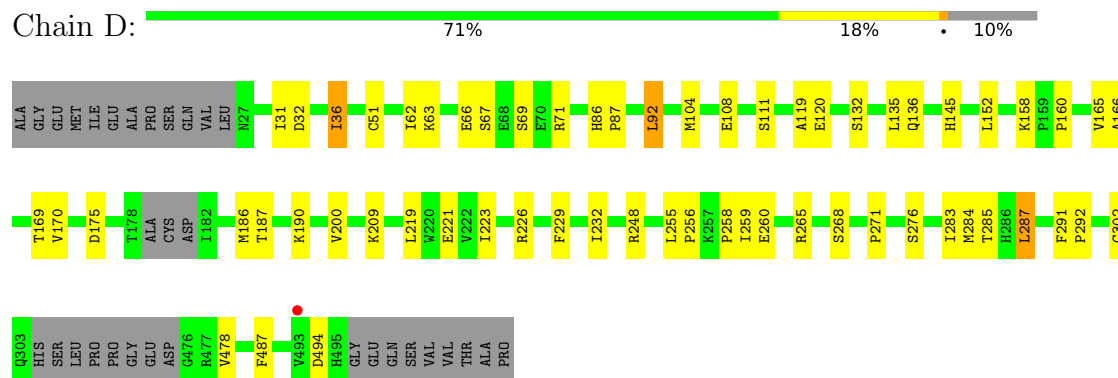


- Molecule 1: Mitogen-activated protein kinase kinase kinase 7, TGF-beta-activated kinase 1 and MAP3K7-binding protein 1

Chain C: 



- Molecule 1: Mitogen-activated protein kinase kinase kinase 7, TGF-beta-activated kinase 1 and MAP3K7-binding protein 1



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.81Å 196.46Å 72.42Å 90.00° 115.24° 90.00°	Depositor
Resolution (Å)	58.63 – 2.05 65.50 – 2.05	Depositor EDS
% Data completeness (in resolution range)	69.2 (58.63-2.05) 69.3 (65.50-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.05Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.221 , 0.258 0.218 , 0.253	Depositor DCC
$R_{free}$ test set	3546 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.50	0/2369	0.67	0/3225
1	B	0.45	1/2336 (0.0%)	0.65	1/3189 (0.0%)
1	C	0.46	0/2323	0.65	0/3167
1	D	0.44	0/2270	0.68	2/3097 (0.1%)
All	All	0.46	1/9298 (0.0%)	0.66	3/12678 (0.0%)

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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	CYS	CB-SG	-5.34	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	ASP	CB-CG-OD2	-16.09	103.82	118.30
1	D	32	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	32	ASP	CB-CG-OD1	-5.81	113.07	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	119	ALA	Peptide

## 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	2303	0	2210	33	0
1	B	2270	0	2139	31	0
1	C	2259	0	2156	29	0
1	D	2207	0	2088	32	0
2	A	146	0	0	16	0
2	B	116	0	0	11	0
2	C	103	0	0	10	0
2	D	54	0	0	5	0
All	All	9458	0	8593	123	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 7.

The worst 5 of 123 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:147:MET:O	2:A:601:HOH:O	1.85	0.92
1:A:77:GLU:OE2	2:A:602:HOH:O	1.87	0.91
1:B:32:ASP:HB3	1:B:35:GLU:HG3	1.58	0.85
1:B:199:GLU:OE2	2:B:602:HOH:O	1.94	0.85
1:A:59:ASP:O	2:A:603:HOH:O	1.94	0.84

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	295/326 (90%)	282 (96%)	12 (4%)	1 (0%)	41	31
1	B	295/326 (90%)	282 (96%)	13 (4%)	0	100	100
1	C	292/326 (90%)	277 (95%)	14 (5%)	1 (0%)	41	31
1	D	288/326 (88%)	274 (95%)	12 (4%)	2 (1%)	22	12
All	All	1170/1304 (90%)	1115 (95%)	51 (4%)	4 (0%)	41	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	120	GLU
1	C	185	HIS
1	A	189	ASN
1	D	190	LYS

### 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	233/279 (84%)	227 (97%)	6 (3%)	46	39
1	B	226/279 (81%)	224 (99%)	2 (1%)	78	79
1	C	224/279 (80%)	219 (98%)	5 (2%)	52	46
1	D	215/279 (77%)	203 (94%)	12 (6%)	21	12
All	All	898/1116 (80%)	873 (97%)	25 (3%)	43	37

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	51	CYS
1	D	111	SER
1	D	494	ASP
1	D	92	LEU
1	D	145	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	B	148	GLN
1	C	98	ASN
1	C	254	ASN

### 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 monosaccharides 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, 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	299/326 (91%)	-0.16	1 (0%) 94 94	26, 39, 60, 66	0
1	B	299/326 (91%)	-0.13	2 (0%) 87 89	29, 44, 68, 77	0
1	C	298/326 (91%)	-0.18	3 (1%) 82 84	28, 44, 65, 74	0
1	D	294/326 (90%)	0.03	1 (0%) 94 94	38, 56, 72, 86	0
All	All	1190/1304 (91%)	-0.11	7 (0%) 89 91	26, 46, 68, 86	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	57	ALA	5.5
1	A	41	VAL	3.8
1	B	51	CYS	3.3
1	B	496	GLY	2.8
1	C	300	TYR	2.8

### 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 monosaccharides 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.