



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2021 – 10:07 AM JST

PDB ID : 7VKM
Title : Crystal structure of TrkA (G595R) kinase domain
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Deposited on : 2021-09-30
Resolution : 2.55 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

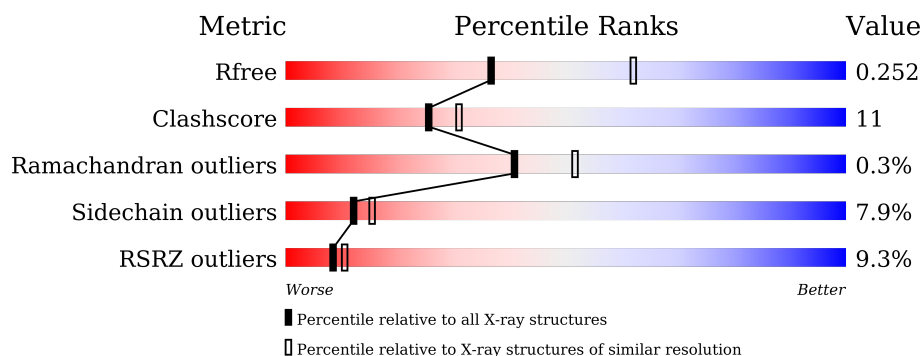
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 ≥ 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	<div> <div>9%</div> <div>68%</div> <div>21%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2463 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 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2410	1538	435	421	16	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	MET	-	initiating methionine	UNP J3KP20
A	472	SER	-	expression tag	UNP J3KP20
A	473	TYR	-	expression tag	UNP J3KP20
A	474	TYR	-	expression tag	UNP J3KP20
A	475	HIS	-	expression tag	UNP J3KP20
A	476	HIS	-	expression tag	UNP J3KP20
A	477	HIS	-	expression tag	UNP J3KP20
A	478	HIS	-	expression tag	UNP J3KP20
A	479	HIS	-	expression tag	UNP J3KP20
A	480	HIS	-	expression tag	UNP J3KP20
A	481	ASP	-	expression tag	UNP J3KP20
A	482	TYR	-	expression tag	UNP J3KP20
A	483	ASP	-	expression tag	UNP J3KP20
A	484	ILE	-	expression tag	UNP J3KP20
A	485	PRO	-	expression tag	UNP J3KP20
A	486	THR	-	expression tag	UNP J3KP20
A	487	THR	-	expression tag	UNP J3KP20
A	488	GLU	-	expression tag	UNP J3KP20
A	489	ASN	-	expression tag	UNP J3KP20
A	490	LEU	-	expression tag	UNP J3KP20
A	491	TYR	-	expression tag	UNP J3KP20
A	492	PHE	-	expression tag	UNP J3KP20
A	493	GLN	-	expression tag	UNP J3KP20
A	494	GLY	-	expression tag	UNP J3KP20
A	495	ALA	-	expression tag	UNP J3KP20
A	496	MET	-	expression tag	UNP J3KP20
A	497	GLY	-	expression tag	UNP J3KP20

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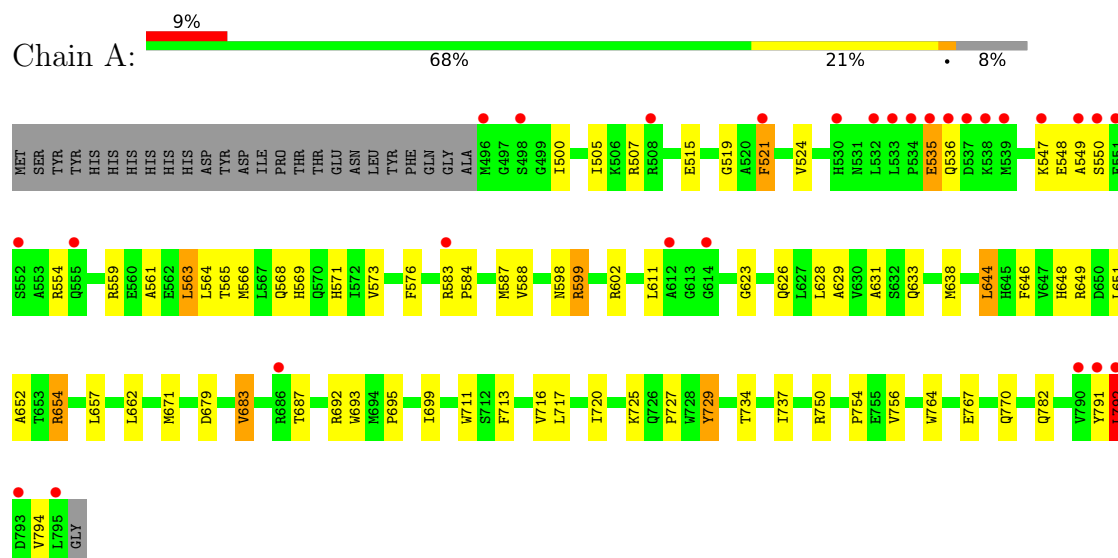
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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	SER	-	expression tag	UNP J3KP20
A	499	GLY	-	expression tag	UNP J3KP20
A	500	ILE	-	expression tag	UNP J3KP20
A	501	ARG	-	expression tag	UNP J3KP20
A	595	ARG	GLY	engineered mutation	UNP J3KP20

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	53	Total O 53 53	0	0

- Molecule 1: Tyrosine-protein kinase receptor



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	105.42Å 105.42Å 203.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.69 – 2.55 41.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.69-2.55) 99.9 (41.66-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.08 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.199 , 0.257 0.202 , 0.252	Depositor DCC
R_{free} test set	724 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2463	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

5.1 Standard geometry

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	0.69	0/2469	0.87	1/3340 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	ARG	NE-CZ-NH1	-6.01	117.29	120.30

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	2410	0	2407	51	1
2	A	53	0	0	0	0
All	All	2463	0	2407	51	1

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 11.

All (51) 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:549:ALA:CB	1:A:583:ARG:HD2	1.86	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ALA:HB3	1:A:583:ARG:HD2	1.47	0.95
1:A:754:PRO:CD	1:A:792:LEU:HD11	2.13	0.77
1:A:549:ALA:HB2	1:A:583:ARG:HD2	1.71	0.72
1:A:767:GLU:HG3	1:A:770:GLN:HE21	1.63	0.64
1:A:519:GLY:N	1:A:671:MET:HE1	2.12	0.64
1:A:629:ALA:O	1:A:633:GLN:HG3	2.01	0.61
1:A:654:ARG:NH1	1:A:693:TRP:CH2	2.68	0.61
1:A:519:GLY:N	1:A:671:MET:CE	2.66	0.58
1:A:750:ARG:O	1:A:791:TYR:HE2	1.86	0.58
1:A:576:PHE:HB2	1:A:588:VAL:HG22	1.86	0.58
1:A:638:MET:HE1	1:A:651:LEU:HD21	1.85	0.58
1:A:573:VAL:HG21	1:A:657:LEU:HD12	1.86	0.57
1:A:791:TYR:O	1:A:792:LEU:O	2.23	0.57
1:A:644:LEU:N	1:A:644:LEU:HD23	2.20	0.57
1:A:750:ARG:O	1:A:791:TYR:CE2	2.58	0.56
1:A:563:LEU:HD21	1:A:646:PHE:HE2	1.72	0.53
1:A:569:HIS:HD2	1:A:571:HIS:H	1.57	0.53
1:A:754:PRO:HD3	1:A:792:LEU:HD11	1.90	0.53
1:A:628:LEU:HD21	1:A:756:VAL:HG21	1.91	0.51
1:A:716:VAL:O	1:A:720:ILE:HG13	2.10	0.51
1:A:648:HIS:O	1:A:649:ARG:HB2	2.11	0.51
1:A:754:PRO:CG	1:A:792:LEU:HD11	2.41	0.51
1:A:598:ASN:OD1	1:A:602:ARG:HD2	2.12	0.50
1:A:550:SER:O	1:A:554:ARG:HG3	2.12	0.49
1:A:692:ARG:HD3	1:A:727:PRO:O	2.13	0.48
1:A:638:MET:CE	1:A:713:PHE:CD1	2.97	0.47
1:A:654:ARG:NH1	1:A:693:TRP:CZ3	2.83	0.47
1:A:725:LYS:HE2	1:A:729:TYR:CD2	2.50	0.47
1:A:535:GLU:HG2	1:A:536:GLN:HG2	1.98	0.46
1:A:683:VAL:HG12	1:A:687:THR:HB	1.98	0.46
1:A:569:HIS:CD2	1:A:571:HIS:H	2.34	0.45
1:A:631:ALA:HB1	1:A:717:LEU:HD21	1.98	0.45
1:A:519:GLY:HA3	1:A:671:MET:HE3	1.99	0.45
1:A:725:LYS:HE2	1:A:729:TYR:HD2	1.81	0.44
1:A:654:ARG:NH1	1:A:679:ASP:HB3	2.32	0.44
1:A:699:ILE:HG21	1:A:737:ILE:HG23	2.00	0.44
1:A:519:GLY:HA3	1:A:671:MET:CE	2.49	0.43
1:A:521:PHE:CZ	1:A:548[A]:GLU:HG2	2.53	0.43
1:A:638:MET:HE1	1:A:651:LEU:CD2	2.48	0.43
1:A:564:LEU:HD12	1:A:587:MET:HE1	2.01	0.43
1:A:652:ALA:HA	1:A:716:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:PRO:HB3	1:A:711:TRP:CG	2.54	0.43
1:A:561:ALA:O	1:A:565:THR:OG1	2.31	0.42
1:A:638:MET:HE1	1:A:713:PHE:CD1	2.54	0.42
1:A:583:ARG:CG	1:A:584:PRO:HA	2.49	0.41
1:A:767:GLU:HB2	1:A:770:GLN:HB2	2.02	0.41
1:A:524:VAL:HG23	1:A:671:MET:SD	2.61	0.41
1:A:623:GLY:O	1:A:626:GLN:N	2.53	0.41
1:A:711:TRP:CE3	1:A:764:TRP:HA	2.56	0.41
1:A:638:MET:HE1	1:A:713:PHE:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:NH1	1:A:611:LEU:O[4_555]	1.99	0.21

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	299/326 (92%)	285 (95%)	13 (4%)	1 (0%)	41 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	792	LEU

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	253/275 (92%)	233 (92%)	20 (8%)	12	15

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	ILE
1	A	505	ILE
1	A	507	ARG
1	A	515	GLU
1	A	521	PHE
1	A	535	GLU
1	A	547	LYS
1	A	559	ARG
1	A	563	LEU
1	A	566	MET
1	A	568	GLN
1	A	599	ARG
1	A	644	LEU
1	A	662	LEU
1	A	683	VAL
1	A	729	TYR
1	A	734	THR
1	A	782	GLN
1	A	792	LEU
1	A	794	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	HIS
1	A	570	GLN
1	A	770	GLN

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 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

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, 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	300/326 (92%)	0.37	28 (9%) 8 10	33, 58, 113, 136	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	791	TYR	5.8
1	A	521	PHE	4.8
1	A	793	ASP	4.3
1	A	535	GLU	4.3
1	A	551	GLU	4.3
1	A	538	LYS	4.1
1	A	534	PRO	4.1
1	A	496	MET	4.0
1	A	795	LEU	3.8
1	A	537	ASP	3.6
1	A	792	LEU	3.3
1	A	549	ALA	3.3
1	A	536	GLN	3.0
1	A	533	LEU	2.8
1	A	790	VAL	2.6
1	A	498	SER	2.5
1	A	550	SER	2.4
1	A	614	GLY	2.4
1	A	583	ARG	2.2
1	A	552	SER	2.2
1	A	530	HIS	2.2
1	A	686	ARG	2.2
1	A	547	LYS	2.1
1	A	539	MET	2.1
1	A	612	ALA	2.1
1	A	508	ARG	2.1
1	A	532	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	555	GLN	2.0

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.