

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 22, 2020 – 06:01 pm BST

PDB ID	:	4GT4
$\operatorname{Title}$	:	Structure of unliganded, inactive Ror2 kinase domain
Authors	:	Mendrola, J.M.; Lemmon, M.A.
Deposited on		
Resolution	:	2.41  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

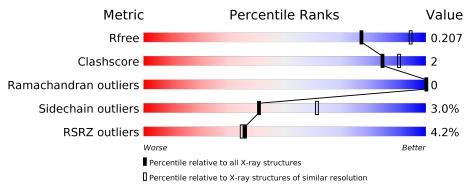
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathbf{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 <=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	А	308	83%	6%		11%
1	В	308	81%	7%	•	11%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4518 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	274	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
		214	2146	1395	360	376	15	0	L	0
1	р	072	Total	С	Ν	Ο	S	0	0	0
L	ГВ	273	2128	1386	359	368	15	U	0	

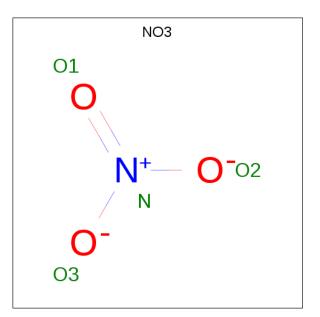
• Molecule 1 is a protein called Tyrosine-protein kinase transmembrane receptor ROR2.

Residue	Modelled	Actual	Comment	Reference
446	HIS	-	EXPRESSION TAG	UNP Q01974
447	HIS	-	EXPRESSION TAG	UNP Q01974
448	HIS	-	EXPRESSION TAG	UNP Q01974
449	HIS	-	EXPRESSION TAG	UNP Q01974
450	HIS	-	EXPRESSION TAG	UNP Q01974
451	HIS	-	EXPRESSION TAG	UNP Q01974
446	HIS	-	EXPRESSION TAG	UNP Q01974
447	HIS	-	EXPRESSION TAG	UNP Q01974
448	HIS	-	EXPRESSION TAG	UNP Q01974
449	HIS	-	EXPRESSION TAG	UNP Q01974
450	HIS	-	EXPRESSION TAG	UNP Q01974
451	HIS	-	EXPRESSION TAG	UNP Q01974
	$ \begin{array}{r}     446 \\     447 \\     448 \\     449 \\     450 \\     451 \\     446 \\     447 \\     448 \\     449 \\     450 \\     450 \\ \end{array} $	446         HIS           447         HIS           448         HIS           449         HIS           450         HIS           451         HIS           446         HIS           448         HIS           450         HIS           451         HIS           446         HIS           447         HIS           448         HIS           449         HIS           450         HIS	446       HIS       -         447       HIS       -         448       HIS       -         448       HIS       -         449       HIS       -         450       HIS       -         451       HIS       -         446       HIS       -         448       HIS       -         448       HIS       -         449       HIS       -         440       HIS       -         4450       HIS       -	446HIS-EXPRESSION TAG447HIS-EXPRESSION TAG448HIS-EXPRESSION TAG449HIS-EXPRESSION TAG450HIS-EXPRESSION TAG451HIS-EXPRESSION TAG446HIS-EXPRESSION TAG447HIS-EXPRESSION TAG448HIS-EXPRESSION TAG449HIS-EXPRESSION TAG450HIS-EXPRESSION TAG

There are 12 discrepancies between the modelled and reference sequences:

• Molecule 2 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total N O 4 1 3	0	0
2	А	1	TotalNO413	0	0
2	В	1	TotalNO413	0	0
2	В	1	Total N O 4 1 3	0	0

• Molecule 3 is water.

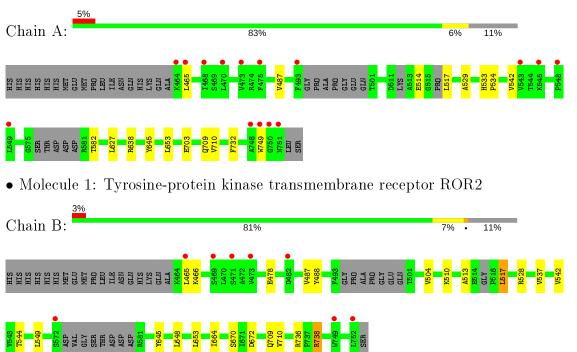
I	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	А	123	Total O 123 123	0	0
	3	В	105	Total O 105 105	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Tyrosine-protein kinase transmembrane receptor ROR2





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	102.83Å $112.92$ Å $114.76$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	45.80 - 2.41	Depositor
Resolution (A)	46.92 - 2.41	EDS
% Data completeness	99.9 (45.80-2.41)	Depositor
(in resolution range)	99.9 (46.92 - 2.41)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.26 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1108)	Depositor
D D	0.177 , $0.205$	Depositor
$R, R_{free}$	0.179 , $0.207$	DCC
$R_{free}$ test set	1330 reflections $(5.07\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	28.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , $60.5$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4518	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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:  $\rm NO3$ 

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.21	0/2201	0.37	0/2988	
1	В	0.21	0/2184	0.37	0/2968	
All	All	0.21	0/4385	0.37	0/5956	

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 (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	А	2146	0	2048	8	0
1	В	2128	0	2037	12	0
2	А	8	0	0	0	0
2	В	8	0	0	0	0
3	А	123	0	0	2	0
3	В	105	0	0	0	0
All	All	4518	0	4085	19	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 2.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ASP:OD1	1:B:738:ARG:NH2	2.24	0.71
1:B:736:ARG:O	1:B:738:ARG:NH1	2.33	0.62
1:B:528:ARG:NH2	1:B:537:VAL:O	2.36	0.56
1:A:582:THR:HG22	1:B:670:SER:HB3	1.88	0.54
1:B:645:TYR:HB3	1:B:653:LEU:HB3	1.91	0.52

clash magnitude.

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	Perce	ntiles
1	А	265/308~(86%)	$257 \ (97\%)$	8 (3%)	0	100	100
1	В	265/308~(86%)	260~(98%)	5 (2%)	0	100	100
All	All	530/616~(86%)	517 (98%)	13~(2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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		Outliers	Percentiles	
1	А	218/271~(80%)	212~(97%)	6(3%)	43 63	
1	В	215/271 (79%)	208~(97%)	7(3%)	38 57	

Continued on next page...



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Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles	
All	All	433/542~(80%)	420 (97%)	13 (3%)	41 61	

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	749	TRP
1	В	466	LYS
1	В	709	GLN
1	А	732	PHE
1	В	517	LEU

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

#### 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)

4 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		Res Link	Bond lengths			Bond angles		
	Type	Cham	nes L		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	NO3	А	802	-	1,3,3	3.56	1 (100%)	$0,\!3,\!3$	0.00	-
2	NO3	А	801	-	1,3,3	3.56	1 (100%)	$0,\!3,\!3$	0.00	-
2	NO3	В	802	-	1,3,3	<mark>3.58</mark>	1 (100%)	$0,\!3,\!3$	0.00	-
2	NO3	В	801	-	1,3,3	<mark>3.58</mark>	1 (100%)	$0,\!3,\!3$	0.00	-

All (4) bond length outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	801	NO3	O1-N	3.58	1.40	1.24
2	В	802	NO3	O1-N	3.58	1.40	1.24
2	А	802	NO3	O1-N	3.56	1.40	1.24
2	А	801	NO3	O1-N	3.56	1.40	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	$OWAB(Å^2)$	Q<0.9
1	А	274/308~(88%)	-0.03	15 (5%) 25 24	13, 33, 79, 97	0
1	В	273/308~(88%)	-0.08	8 (2%) 51 50	16, 36, 76, 89	0
All	All	547/616 (88%)	-0.05	23 (4%) 36 35	13, 34, 78, 97	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	471	SER	3.9
1	А	749	TRP	3.7
1	А	464	LYS	3.6
1	А	465	LEU	3.5
1	А	751	ASN	3.1

### 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 carbohydrates in this entry.

## 6.4 Ligands (i)

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. The B-factors column lists the minimum, median,  $95^{th}$  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	RSCC	$\mathbf{RSR}$	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$\mathbf{Q}{<}0.9$
2	NO3	А	802	4/4	0.79	0.18	$55,\!61,\!61,\!63$	0
2	NO3	В	801	4/4	0.85	0.18	$39,\!44,\!44,\!50$	0
2	NO3	В	802	4/4	0.94	0.11	$62,\!64,\!65,\!67$	0
2	NO3	А	801	4/4	0.99	0.15	$23,\!26,\!27,\!35$	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

