



## wwPDB EM Validation Summary Report ⓘ

Jun 3, 2024 – 08:58 PM JST

PDB ID : 8XV9  
EMDB ID : EMD-38693  
Title : Fedratinib-bound human SLC19A3  
Authors : Dang, Y.; Wang, G.P.; Zhang, Z.  
Deposited on : 2024-01-14  
Resolution : 3.80 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis	: <b>FAILED</b>
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.36.2

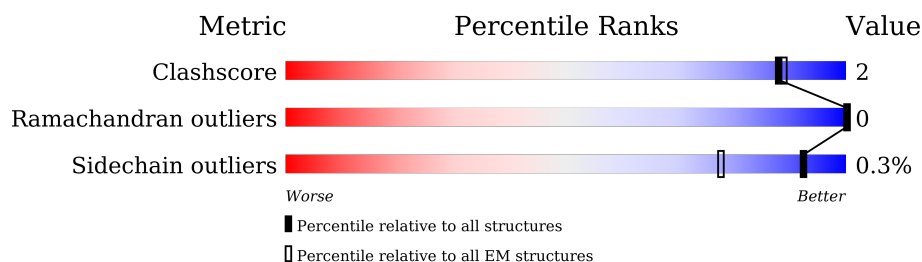
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	607	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3147 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Soluble cytochrome b562,Thiamine transporter 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	0	0
			3110	2100	466	528	16		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-107	LEU	-	expression tag	UNP P0ABE7
A	-106	GLU	-	expression tag	UNP P0ABE7
A	-105	VAL	-	expression tag	UNP P0ABE7
A	-104	LEU	-	expression tag	UNP P0ABE7
A	-103	PHE	-	expression tag	UNP P0ABE7
A	-102	GLN	-	expression tag	UNP P0ABE7
A	-101	GLY	-	expression tag	UNP P0ABE7
A	-100	PRO	-	expression tag	UNP P0ABE7
A	-99	SER	-	expression tag	UNP P0ABE7
A	-98	ARG	-	expression tag	UNP P0ABE7
A	-97	ALA	-	expression tag	UNP P0ABE7
A	-96	THR	-	expression tag	UNP P0ABE7
A	-89	TRP	MET	conflict	UNP P0ABE7
A	6	ILE	HIS	conflict	UNP P0ABE7
A	10	LEU	ARG	conflict	UNP P0ABE7
A	497	SER	-	expression tag	UNP Q9BZV2
A	498	ASN	-	expression tag	UNP Q9BZV2
A	499	SER	-	expression tag	UNP Q9BZV2

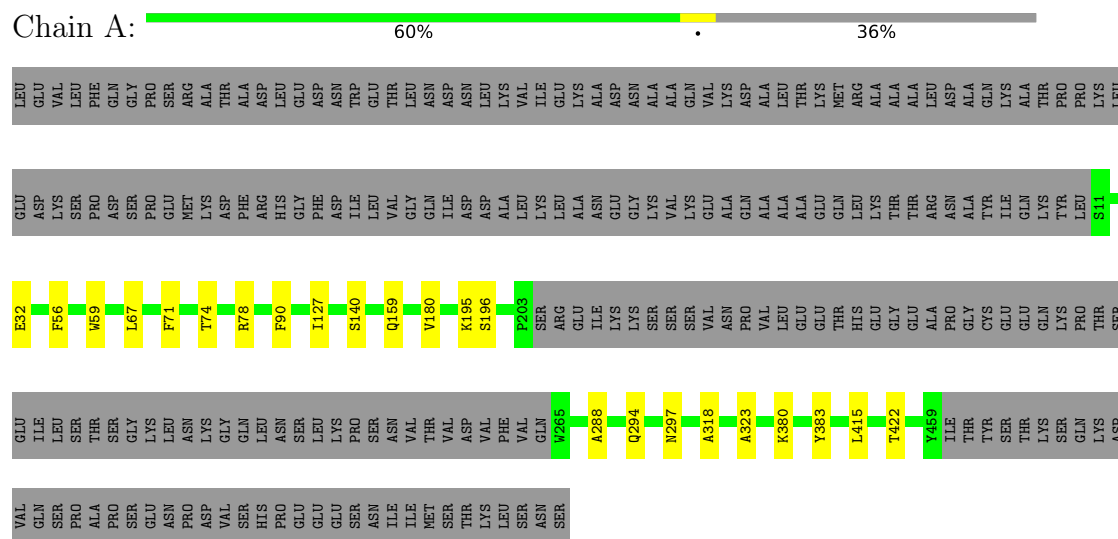
- Molecule 2 is N-tert-butyl-3-([5-methyl-2-({4-[2-(pyrrolidin-1-yl)ethoxy]phenyl}amino)pyrimidin-4-yl]amino}benzenesulfonamide (three-letter code: 2TA) (formula: C<sub>27</sub>H<sub>36</sub>N<sub>6</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 37	C 27	N 6	O 3	S 1	0



- Molecule 1: Soluble cytochrome b562, Thiamine transporter 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	416503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 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: 2TA

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	0.28	0/3206	0.49	0/4380

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	A	3110	0	3132	12	0
2	A	37	0	36	1	0
All	All	3147	0	3168	12	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 12 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:159:GLN:HG3	1:A:318:ALA:HB2	1.83	0.61
1:A:67:LEU:HD22	1:A:415:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ALA:HB1	1:A:380:LYS:HD3	1.92	0.52
1:A:32:GLU:OE1	2:A:501:2TA:NAW	2.40	0.51
1:A:127:ILE:HD13	1:A:140:SER:HA	1.96	0.47

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 PDB entries followed by that with respect to all EM entries.

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	384/607 (63%)	363 (94%)	21 (6%)	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 PDB entries followed by that with respect to all EM entries.

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	333/524 (64%)	332 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LYS

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	173	ASN
1	A	294	GLN
1	A	297	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](#)

1 ligand is 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	2TA	A	501	-	39,40,40	3.29	14 (35%)	55,57,57	2.25	12 (21%)

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	2TA	A	501	-	-	18/26/33/33	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2TA	CAT-NAP	-9.92	1.28	1.47
2	A	501	2TA	SBD-NBE	9.81	1.76	1.61
2	A	501	2TA	CAQ-NAP	5.90	1.58	1.47
2	A	501	2TA	C4-NAW	5.75	1.46	1.36
2	A	501	2TA	C2-NAF	5.62	1.48	1.36

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	2TA	OBK-SBD-OBJ	-8.48	109.12	119.55
2	A	501	2TA	C5-C6-N1	-6.84	118.12	125.11
2	A	501	2TA	C5-C4-N3	-5.38	117.23	123.37
2	A	501	2TA	CAG-NAF-C2	-5.10	114.42	129.23
2	A	501	2TA	N1-C2-N3	-4.85	121.95	126.55

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	2TA	CAN-CAO-NAP-CAQ
2	A	501	2TA	N1-C2-NAF-CAG
2	A	501	2TA	N3-C2-NAF-CAG
2	A	501	2TA	CBA-CBB-SBD-OBJ
2	A	501	2TA	CBC-CBB-SBD-OBJ

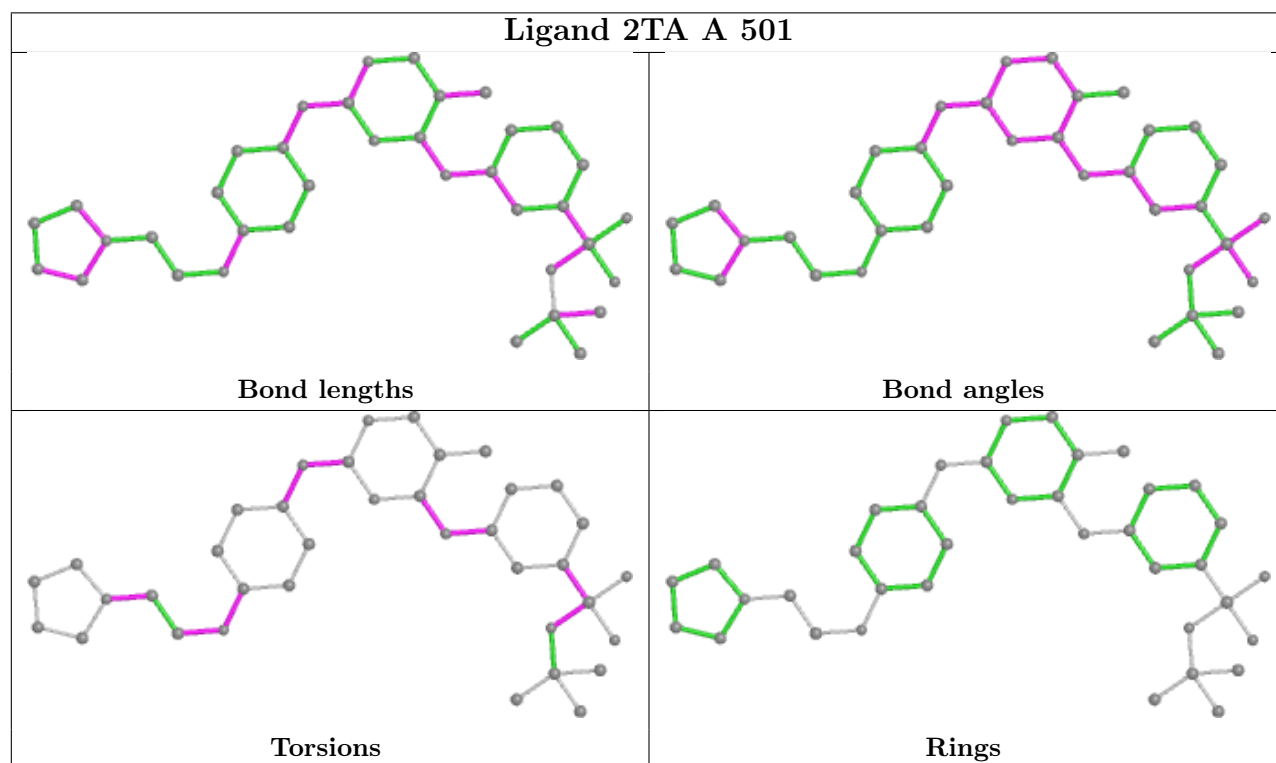
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	2TA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.