



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 30, 2020 – 02:03 am BST

PDB ID : 1N94  
Title : Aryl Tetrahydropyridine Inhibitors of Farnesyltransferase: Glycine, Phenylalanine and Histidine Derivates  
Authors : Gwaltney II, S.L.; O'Connor, S.J.; Nelson, L.T.; Sullivan, G.M.; Imade, H.; Wang, W.; Hasvold, L.; Li, Q.; Cohen, J.; Gu, W.Z.  
Deposited on : 2002-11-22  
Resolution : 3.50 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

PERCENTILES INFOmissingINFO

# 1 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5873 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.

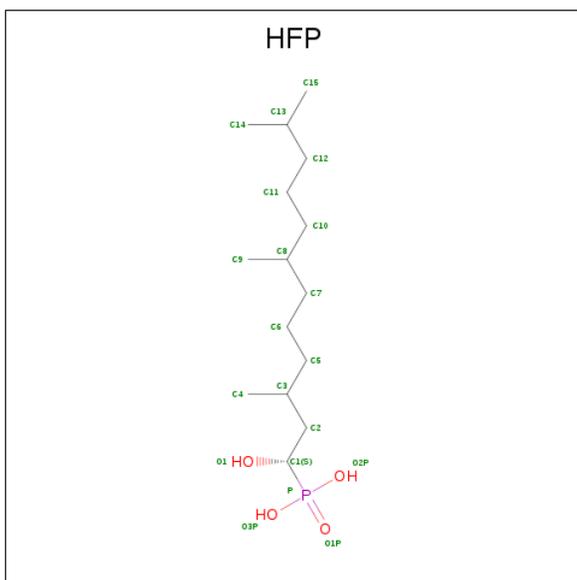
- Molecule 1 is a protein called Protein farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2689	1712	473	499	5	0	0	0

- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	397	3125	1995	539	568	23	0	0	0

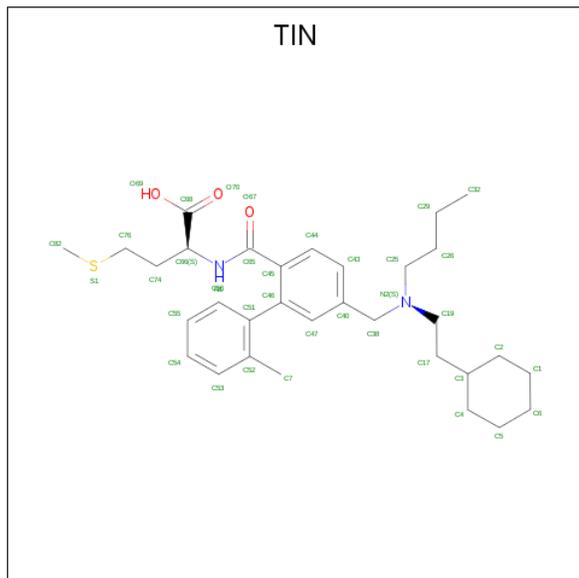
- Molecule 3 is ALPHA-HYDROXYFARNESYLPHOSPHONIC ACID (three-letter code: HFP) (formula: C<sub>15</sub>H<sub>33</sub>O<sub>4</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	20	15	4	1	0	0

- Molecule 4 is 2-{{(5-{{[BUTYL-(2-CYCLOHEXYL-ETHYL)-AMINO]-METHYL}}-2'-ME

THYL-BIPHENYL-2-CARBONYL)-AMINO]-4-METHYLSULFANYL-BUTYRIC ACID  
(three-letter code: TIN) (formula: C<sub>32</sub>H<sub>46</sub>N<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	38	32	2	3	1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	B	1	1	1	0	0



I311	H312	I315	H316	P321	A322	L323	H327	W328	M329	F330	H331	Q332	Q333	A334	L335	Q336	E337	Y338	I339	I340	M341	C342	C343	Q344	C345	G348	G349	D352	K353	P354	G355	K356	S357	R358	D359	F360	Y361	H362	T363	C364	Y365	C366	L370	A373	Q374	H375	F376	G377	S378	M381	L382
V386	M387	G388	V389	P390	E391	M392	V393	L394	Q395	P396	T397	H398	P399	V400	Y401	N402	I403	G404	P405	D406	K407	V408	A411	T412	T413	H414	F415	K418																							

### 3 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.11Å 172.11Å 69.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.94 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (33.94-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.18Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.295 , 0.296	Depositor
Wilson B-factor (Å <sup>2</sup> )	59.8	Xtrriage
Anisotropy	0.118	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtrriage
Total number of atoms	5873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HFP, ZN, TIN

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	0.40	0/2755	0.65	0/3738
2	B	0.42	0/3208	0.70	0/4353
All	All	0.41	0/5963	0.68	0/8091

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	93	TYR	Sidechain

### 4.2 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	2689	0	2614	282	0
2	B	3125	0	3058	287	0
3	A	20	0	28	20	0
4	A	38	0	45	10	0
5	B	1	0	0	0	0
All	All	5873	0	5745	552	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 48.

The worst 5 of 552 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:164:LYS:HD3	3:A:501:HFP:O1P	1.18	1.30
1:A:200:TYR:CB	3:A:501:HFP:H43	1.86	1.04
1:A:200:TYR:CG	3:A:501:HFP:H43	1.93	1.03
2:B:280:ARG:HH12	2:B:292:CYS:HA	1.21	1.00
1:A:165:ASN:ND2	1:A:168:VAL:H	1.61	0.99

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 4.3.2 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	294/294 (100%)	285 (97%)	9 (3%)	40	70
2	B	335/335 (100%)	324 (97%)	11 (3%)	38	68
All	All	629/629 (100%)	609 (97%)	20 (3%)	39	69

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	29	GLU
2	B	64	PHE
2	B	243	PRO
1	A	287	ARG
1	A	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
2	B	120	GLN
2	B	344	GLN
2	B	48	GLN
2	B	134	GLN

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

#### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

#### 4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	HFP	A	501	1	17,19,19	1.75	5 (29%)	22,25,25	2.26	7 (31%)
4	TIN	A	1	-	37,40,40	1.56	7 (18%)	46,52,52	1.91	5 (10%)

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
3	HFP	A	501	1	2/2/5/5	8/22/22/22	-
4	TIN	A	1	-	-	13/29/41/41	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HFP	C2-C3	-4.64	1.34	1.53
3	A	501	HFP	C7-C8	-3.33	1.35	1.52
4	A	1	TIN	C38-N2	3.05	1.53	1.47
4	A	1	TIN	C45-C46	3.01	1.45	1.40
4	A	1	TIN	C44-C45	2.80	1.44	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	TIN	C66-N1-C65	10.15	135.42	122.34
3	A	501	HFP	C3-C2-C1	7.51	122.82	115.21
4	A	1	TIN	C7-C52-C53	-3.89	112.72	120.31
4	A	1	TIN	C7-C52-C51	3.15	127.70	122.33
3	A	501	HFP	C4-C3-C2	3.04	120.58	110.89

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	HFP	C3
3	A	501	HFP	C8

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HFP	P-C1-C2-C3
3	A	501	HFP	O1-C1-C2-C3

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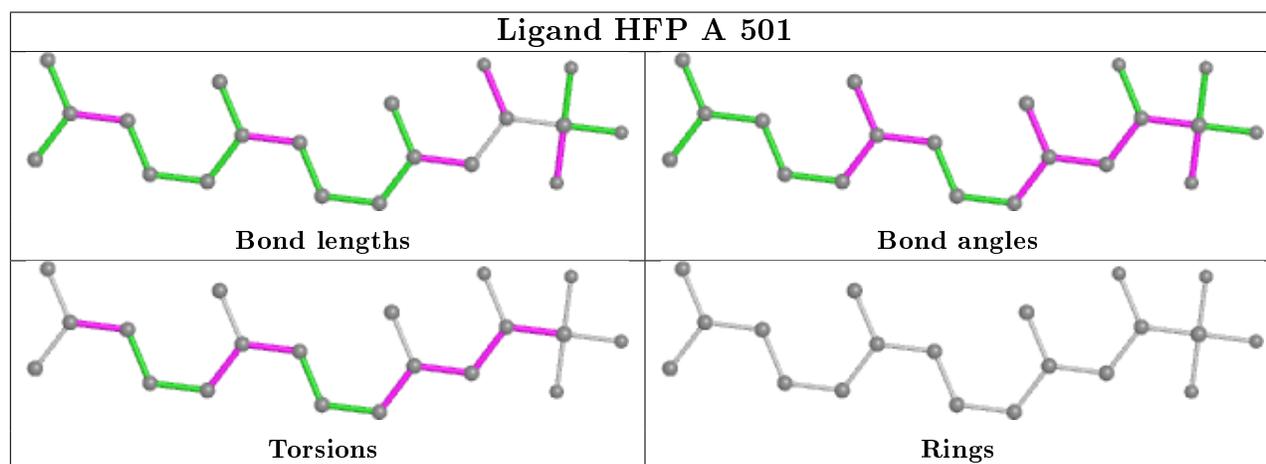
Mol	Chain	Res	Type	Atoms
4	A	1	TIN	C45-C65-N1-C66
4	A	1	TIN	O67-C65-N1-C66
4	A	1	TIN	C74-C66-N1-C65

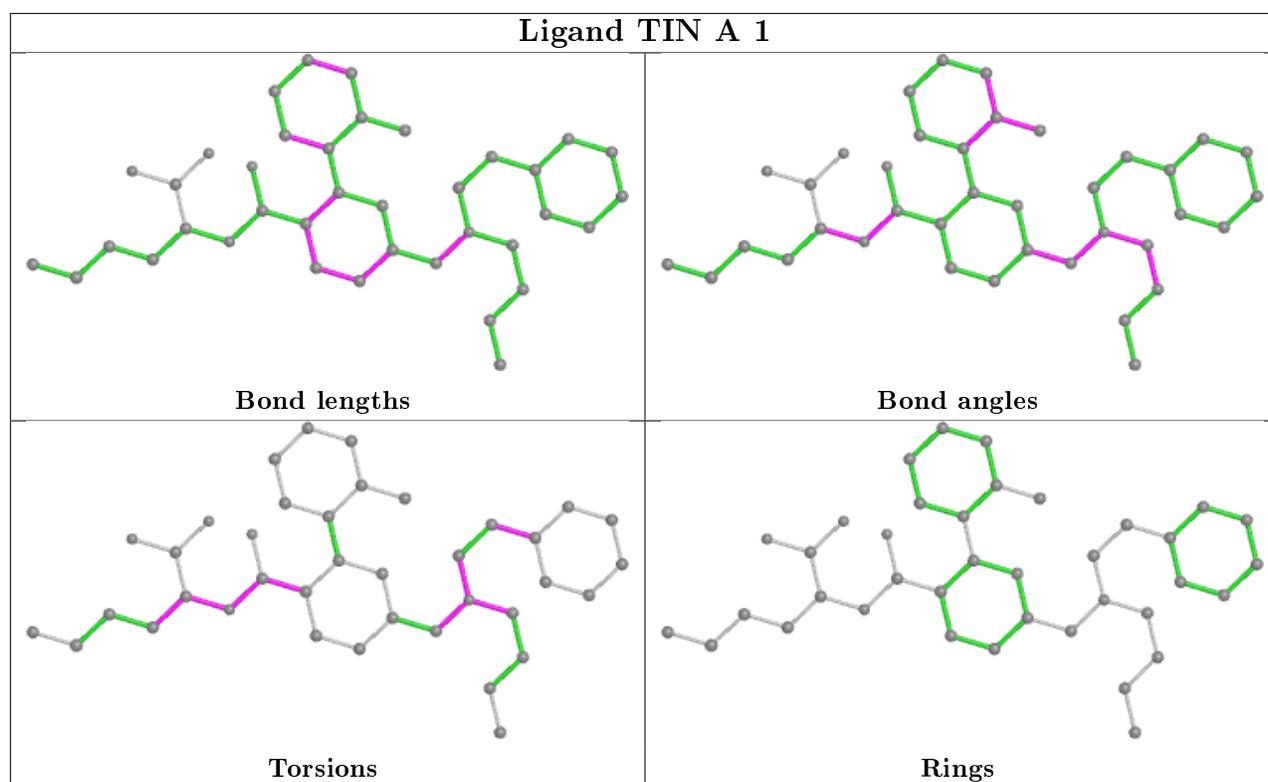
There are no ring outliers.

2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HFP	20	0
4	A	1	TIN	10	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.





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 5.4 Ligands

EDS was not executed - this section is therefore empty.

### 5.5 Other polymers

EDS was not executed - this section is therefore empty.