



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 12:02 am BST

PDB ID : 1IYL  
Title : Crystal Structure of Candida albicans N-myristoyltransferase with Non-peptidic Inhibitor  
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Deposited on : 2002-08-29  
Resolution : 3.20 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)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
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

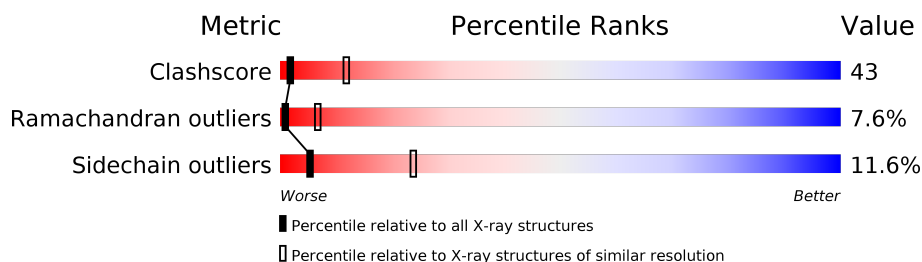
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	392	
1	B	392	
1	C	392	
1	D	392	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	R64	B	452	-	-	X	-

## 2 Entry composition [i](#)

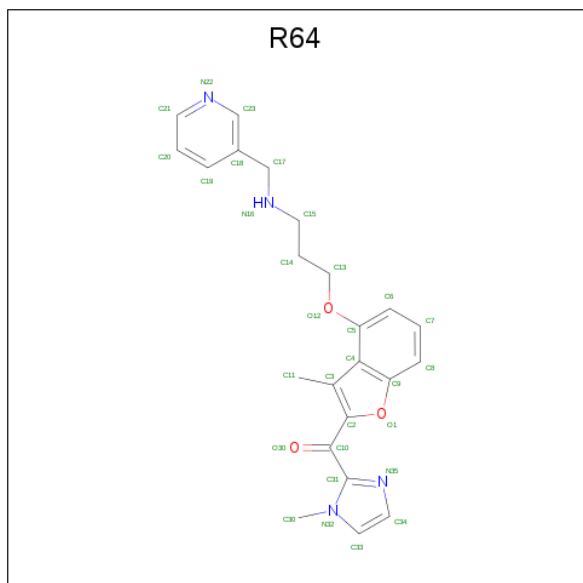
There are 2 unique types of molecules in this entry. The entry contains 12597 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myristoyl-CoA:Protein N-Myristoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3148	2039	514	586	9			
1	B	380	Total	C	N	O	S	0	0	0
			3117	2021	510	577	9			
1	C	381	Total	C	N	O	S	0	0	0
			3125	2025	511	580	9			
1	D	380	Total	C	N	O	S	0	0	0
			3117	2021	510	577	9			

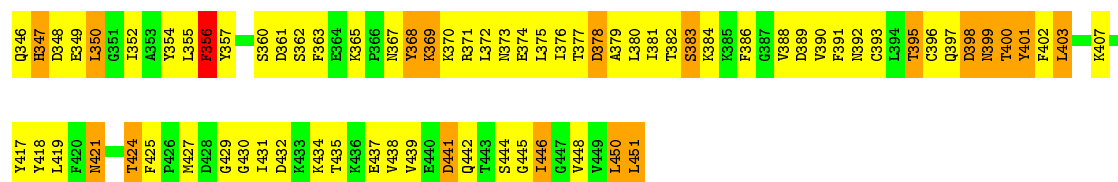
- Molecule 2 is (1-METHYL-1H-IMIDAZOL-2-YL)-(3-METHYL-4-{3-[(PYRIDIN-3-YLMETHYL)-AMINO]-PROPOXY}-BENZOFURAN-2-YL)-METHANONE (three-letter code: R64) (formula: C<sub>23</sub>H<sub>24</sub>N<sub>4</sub>O<sub>3</sub>).



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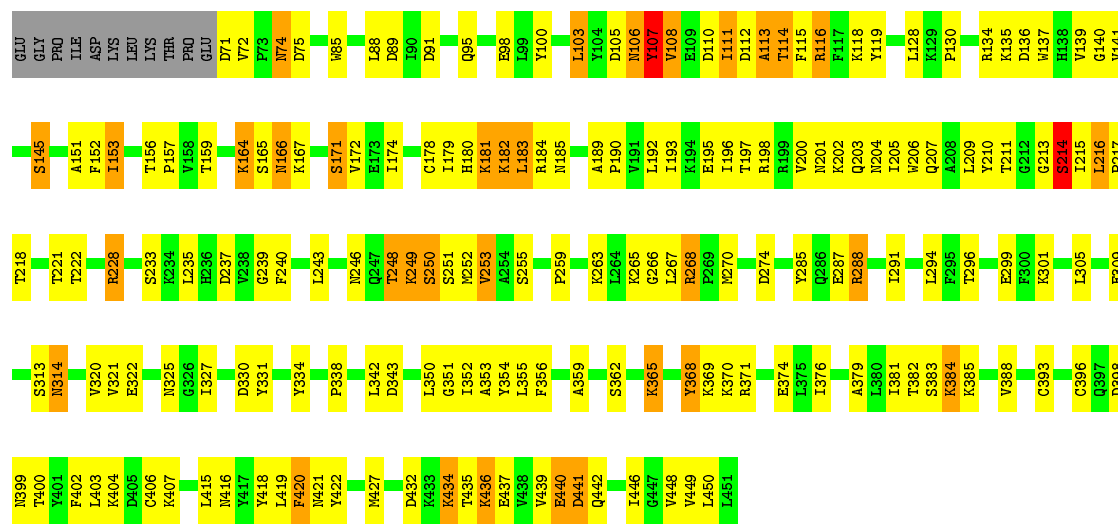
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			30	23	4	3		
2	C	1	Total	C	N	O	0	0
			30	23	4	3		





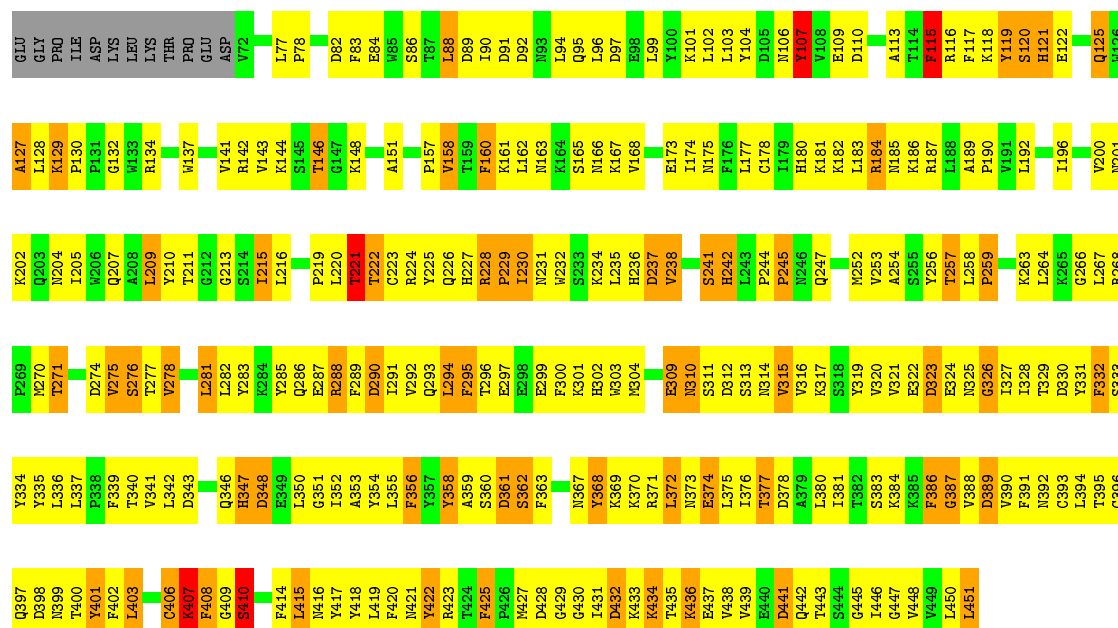
• Molecule 1: Myristoyl-CoA:Protein N-Myristoyltransferase

Chain C: 51% 38% 8% ..



• Molecule 1: Myristoyl-CoA:Protein N-Myristoyltransferase

Chain D: 27% 52% 16% ..



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.28 Å 96.89 Å 269.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20	Depositor
% Data completeness (in resolution range)	98.8 (40.00-3.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.284 , 0.366	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12597	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 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: R64

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	0.59	1/3233 (0.0%)	0.70	3/4389 (0.1%)
1	B	0.54	1/3201 (0.0%)	0.65	1/4344 (0.0%)
1	C	0.52	1/3209 (0.0%)	0.68	1/4355 (0.0%)
1	D	0.55	0/3201	0.63	0/4344
All	All	0.55	3/12844 (0.0%)	0.67	5/17432 (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	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	TYR	C-N	-15.78	0.97	1.34
1	B	113	ALA	C-N	-7.78	1.16	1.34
1	C	113	ALA	C-N	-5.13	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ALA	O-C-N	-9.51	107.48	122.70
1	A	113	ALA	C-N-CA	8.64	143.29	121.70
1	C	107	TYR	CA-C-N	-6.40	103.11	117.20
1	B	107	TYR	O-C-N	5.96	132.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	113	ALA	CA-C-N	5.93	130.24	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	TYR	Mainchain
1	D	107	TYR	Mainchain

## 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	3148	0	3098	162	0
1	B	3117	0	3074	290	0
1	C	3125	0	3078	188	0
1	D	3117	0	3075	449	0
2	A	30	0	24	3	0
2	B	30	0	24	10	0
2	C	30	0	24	0	0
All	All	12597	0	12397	1070	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 43.

The worst 5 of 1070 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:D:228:ARG:HH11	1:D:380:LEU:HB3	1.09	1.16
1:D:184:ARG:HB2	1:D:184:ARG:HH11	1.06	1.12
1:D:451:LEU:HD12	1:D:451:LEU:H	1.23	1.03
1:D:264:LEU:HG	1:D:374:GLU:HB3	1.41	1.02
1:D:226:GLN:HA	1:D:410:SER:HA	1.41	1.00

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	382/392 (97%)	315 (82%)	49 (13%)	18 (5%)	2	17
1	B	378/392 (96%)	263 (70%)	78 (21%)	37 (10%)	0	3
1	C	379/392 (97%)	310 (82%)	48 (13%)	21 (6%)	2	14
1	D	378/392 (96%)	247 (65%)	91 (24%)	40 (11%)	0	2
All	All	1517/1568 (97%)	1135 (75%)	266 (18%)	116 (8%)	1	7

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	109	GLU
1	A	114	THR
1	A	246	ASN
1	A	342	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	353/360 (98%)	315 (89%)	38 (11%)	6	27
1	B	349/360 (97%)	314 (90%)	35 (10%)	7	30
1	C	350/360 (97%)	312 (89%)	38 (11%)	6	26
1	D	349/360 (97%)	297 (85%)	52 (15%)	3	14
All	All	1401/1440 (97%)	1238 (88%)	163 (12%)	5	24

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	71	ASP
1	C	243	LEU
1	D	403	LEU
1	C	75	ASP
1	C	159	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	307	HIS
1	C	106	ASN
1	D	236	HIS
1	B	373	ASN
1	C	166	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	R64	A	452	-	27,33,33	1.14	3 (11%)	30,45,45	1.53	7 (23%)
2	R64	B	452	-	27,33,33	1.19	4 (14%)	30,45,45	1.69	7 (23%)
2	R64	C	452	-	27,33,33	0.85	1 (3%)	30,45,45	1.19	4 (13%)

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	R64	A	452	-	-	0/9/17/17	0/4/4/4
2	R64	B	452	-	-	1/9/17/17	0/4/4/4
2	R64	C	452	-	-	0/9/17/17	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	452	R64	C17-C18	-3.17	1.44	1.51
2	B	452	R64	C4-C9	-3.12	1.36	1.43
2	A	452	R64	C4-C9	-2.93	1.37	1.43
2	A	452	R64	C2-C10	-2.70	1.44	1.50
2	B	452	R64	C17-C18	-2.40	1.46	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	R64	C33-N32-C31	-3.87	104.15	108.56
2	B	452	R64	O30-C10-C2	3.61	125.04	118.58
2	A	452	R64	C33-N32-C31	-3.26	104.85	108.56
2	B	452	R64	O30-C10-C31	2.99	123.45	118.44
2	B	452	R64	C3-C4-C9	-2.99	105.43	110.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

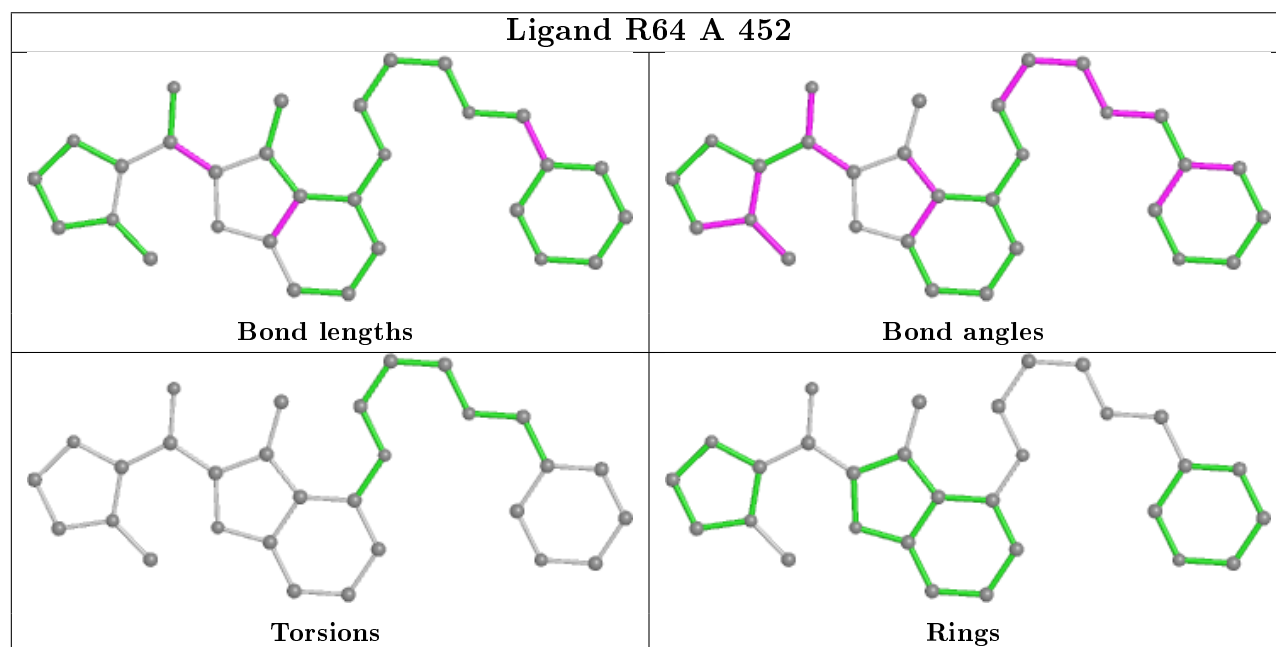
Mol	Chain	Res	Type	Atoms
2	B	452	R64	N16-C17-C18-C23

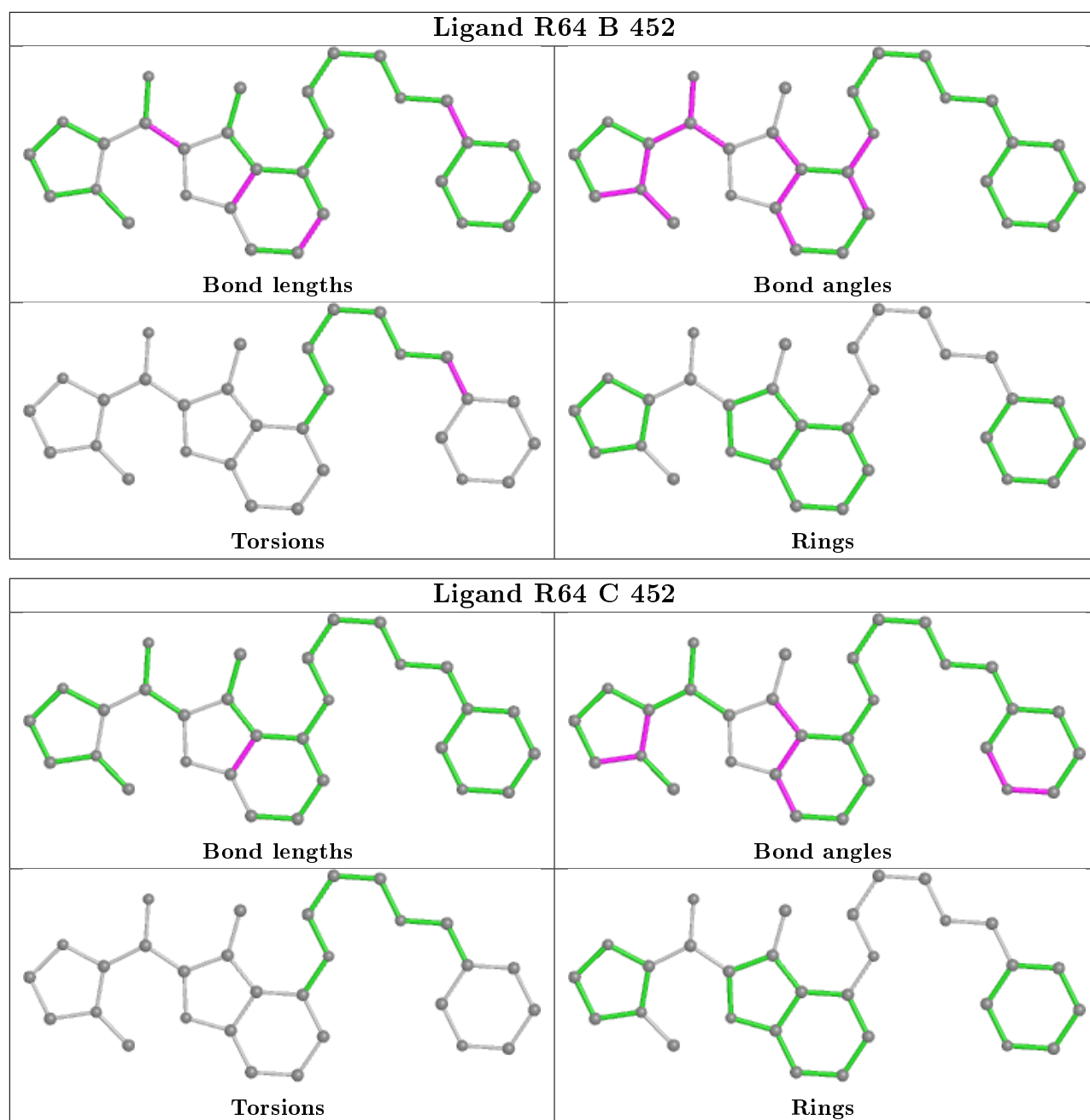
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	452	R64	3	0
2	B	452	R64	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

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Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	113:ALA	C	114:THR	N	1.16
1	A	107:TYR	C	108:VAL	N	0.97

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.