



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 12:59 AM EDT

PDB ID : 6UNL  
Title : CYP3A4 bound to an inhibitor  
Authors : Sevrioukova, I.  
Deposited on : 2019-10-12  
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](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.

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:

MolProbity : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.35.1

## 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.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3596 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 Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3509	2287	576	620	26	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

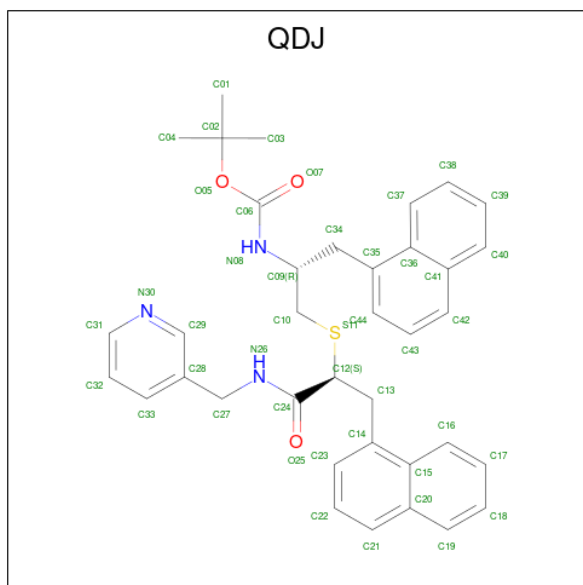
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP P08684
A	22	ALA	-	expression tag	UNP P08684
A	504	HIS	-	expression tag	UNP P08684
A	505	HIS	-	expression tag	UNP P08684
A	506	HIS	-	expression tag	UNP P08684
A	507	HIS	-	expression tag	UNP P08684

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is tert-butyl [(2R)-1-(naphthalen-1-yl)-3-{{(2S)-3-(naphthalen-1-yl)-1-oxo-1-{{(pyridin-3-yl)methyl}amino}propan-2-yl]sulfanyl}propan-2-yl]carbamate (three-letter code: QDJ) (formula: C<sub>37</sub>H<sub>39</sub>N<sub>3</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	44	37	3	3	1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.73Å 101.81Å 126.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.23 – 2.55	Depositor
% Data completeness (in resolution range)	95.8 (40.23-2.55)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.54Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.207 , 0.276	Depositor
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtrriage
Anisotropy	0.170	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

### 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 monosaccharides in this entry.

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

2 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
3	QDJ	A	602	2	47,48,48	4.92	25 (53%)	58,66,66	2.45	20 (34%)
2	HEM	A	601	1,3	41,50,50	1.66	6 (14%)	45,82,82	1.55	8 (17%)

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	QDJ	A	602	2	-	11/31/31/31	0/5/5/5
2	HEM	A	601	1,3	-	1/12/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QDJ	C12-S11	23.03	2.07	1.83
3	A	602	QDJ	C10-S11	18.00	2.01	1.82
3	A	602	QDJ	C06-N08	6.50	1.50	1.34
2	A	601	HEM	C3C-C2C	-5.33	1.33	1.40
3	A	602	QDJ	C34-C09	4.92	1.64	1.53
3	A	602	QDJ	O05-C06	4.80	1.44	1.34
3	A	602	QDJ	C14-C15	4.28	1.52	1.42
2	A	601	HEM	C3C-CAC	3.24	1.54	1.47
3	A	602	QDJ	C24-N26	3.23	1.40	1.33
3	A	602	QDJ	C43-C44	3.16	1.45	1.38
3	A	602	QDJ	C36-C41	-3.06	1.37	1.43
3	A	602	QDJ	C23-C14	3.05	1.43	1.37
3	A	602	QDJ	C22-C23	3.04	1.45	1.38
2	A	601	HEM	CAB-C3B	2.97	1.55	1.47
2	A	601	HEM	FE-NB	2.96	2.11	1.96
3	A	602	QDJ	C44-C35	2.96	1.43	1.37
3	A	602	QDJ	C12-C24	2.88	1.56	1.52
3	A	602	QDJ	O05-C02	2.85	1.53	1.48
3	A	602	QDJ	C43-C42	2.83	1.43	1.36
3	A	602	QDJ	C35-C36	2.76	1.48	1.42
2	A	601	HEM	CMB-C2B	2.64	1.56	1.50
3	A	602	QDJ	C22-C21	2.63	1.42	1.36
3	A	602	QDJ	C03-C02	2.57	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	QDJ	C17-C16	2.57	1.42	1.36
3	A	602	QDJ	C13-C12	2.56	1.62	1.52
3	A	602	QDJ	C34-C35	2.51	1.58	1.51
3	A	602	QDJ	C18-C19	2.46	1.42	1.36
3	A	602	QDJ	C09-N08	2.41	1.51	1.46
3	A	602	QDJ	C38-C37	2.07	1.41	1.36
3	A	602	QDJ	C39-C40	2.03	1.41	1.36
2	A	601	HEM	CMA-C3A	2.02	1.55	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	QDJ	O05-C06-N08	9.78	126.45	110.02
3	A	602	QDJ	O25-C24-N26	-5.07	112.10	122.99
3	A	602	QDJ	C13-C14-C15	5.01	128.67	120.76
3	A	602	QDJ	O07-C06-N08	-4.89	116.83	124.85
3	A	602	QDJ	O05-C06-O07	-4.88	116.72	125.62
3	A	602	QDJ	C14-C13-C12	4.33	119.38	113.27
2	A	601	HEM	C4B-CHC-C1C	3.90	127.71	122.56
2	A	601	HEM	CBA-CAA-C2A	-3.84	106.06	112.62
3	A	602	QDJ	C35-C36-C41	3.50	123.33	118.98
3	A	602	QDJ	C09-N08-C06	3.44	127.60	122.30
3	A	602	QDJ	C21-C20-C19	-3.04	116.09	123.19
3	A	602	QDJ	C44-C35-C36	-3.03	114.77	119.08
2	A	601	HEM	C1B-NB-C4B	2.94	108.11	105.07
2	A	601	HEM	C4D-ND-C1D	2.84	108.00	105.07
2	A	601	HEM	CHD-C1D-ND	2.74	127.41	124.43
3	A	602	QDJ	C23-C14-C15	-2.68	115.27	119.08
2	A	601	HEM	CMA-C3A-C4A	-2.61	124.46	128.46
3	A	602	QDJ	C42-C41-C40	-2.42	117.54	123.19
3	A	602	QDJ	O25-C24-C12	-2.41	118.12	121.61
3	A	602	QDJ	C27-N26-C24	-2.34	118.97	122.34
3	A	602	QDJ	C37-C36-C35	-2.32	118.70	122.55
2	A	601	HEM	CMD-C2D-C1D	-2.29	121.55	125.04
3	A	602	QDJ	C13-C14-C23	-2.24	116.04	119.86
3	A	602	QDJ	C19-C20-C15	2.22	122.04	119.12
3	A	602	QDJ	C43-C42-C41	-2.17	117.06	120.44
3	A	602	QDJ	C21-C20-C15	2.09	121.88	119.12
3	A	602	QDJ	C34-C09-N08	2.01	114.25	110.39
2	A	601	HEM	C3D-C4D-ND	-2.00	107.94	110.17

There are no chirality outliers.



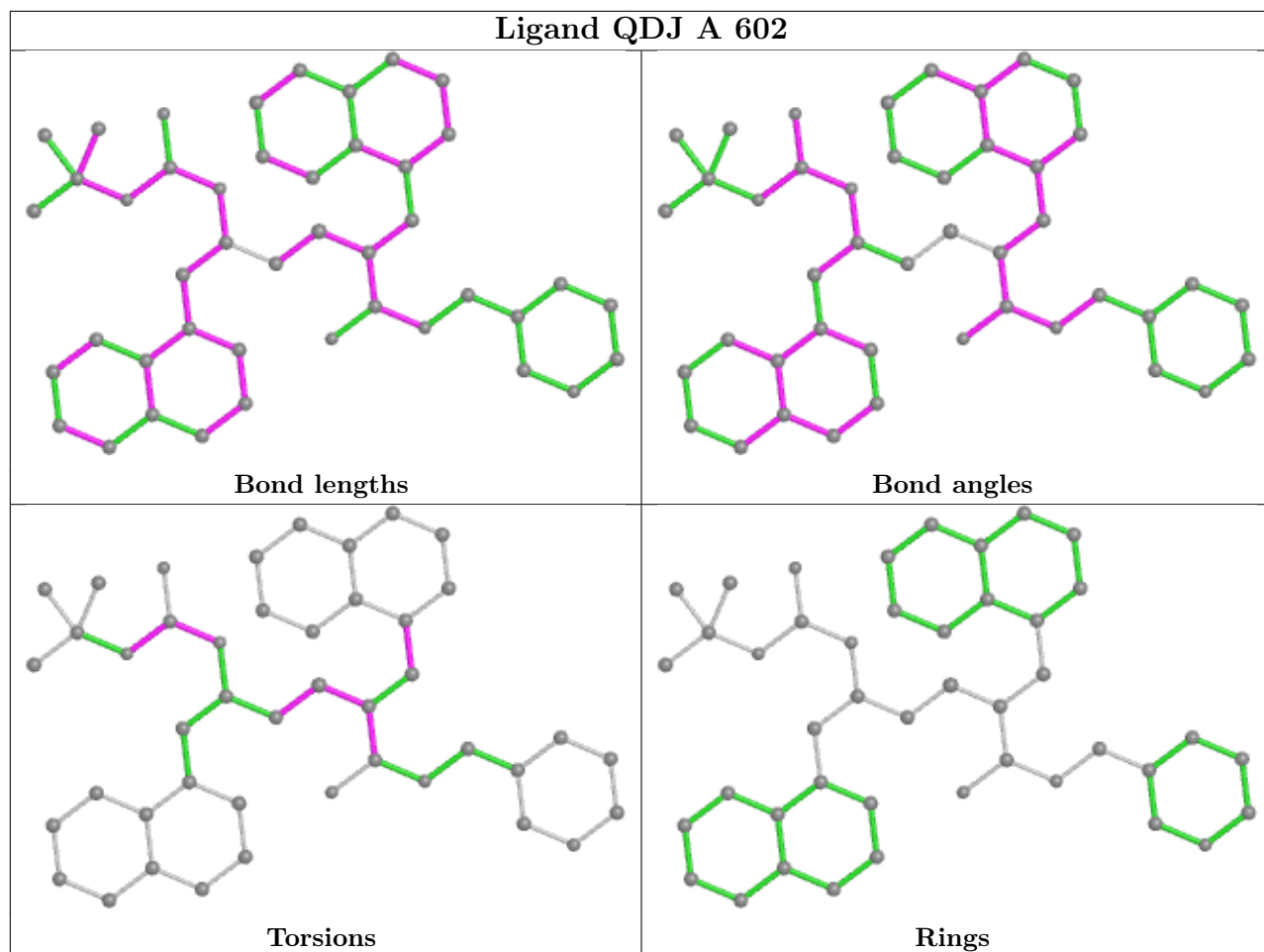
All (12) torsion outliers are listed below:

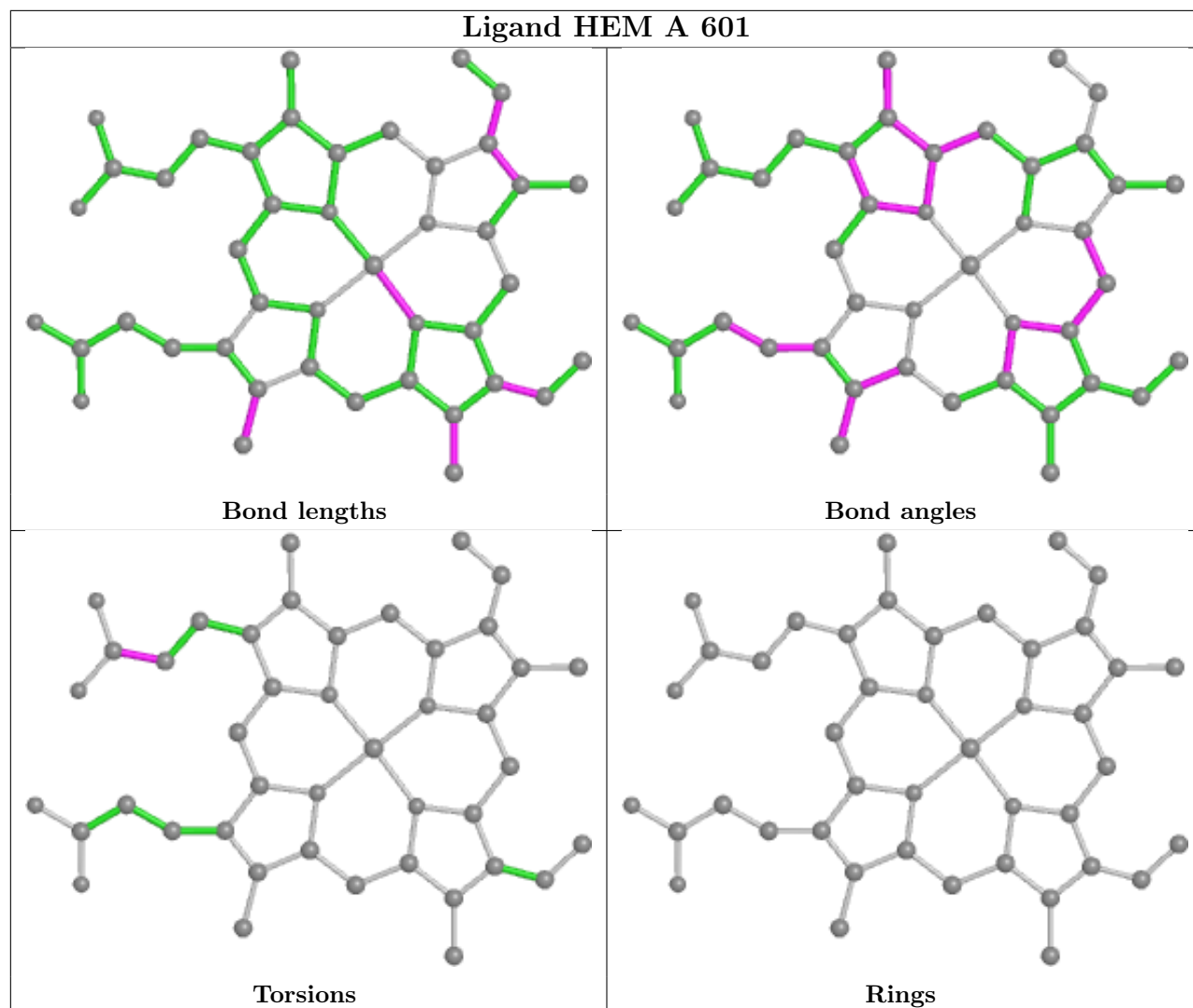
Mol	Chain	Res	Type	Atoms
3	A	602	QDJ	C09-C10-S11-C12
3	A	602	QDJ	C13-C12-S11-C10
3	A	602	QDJ	C24-C12-S11-C10
3	A	602	QDJ	C12-C13-C14-C15
3	A	602	QDJ	C12-C13-C14-C23
3	A	602	QDJ	C13-C12-C24-O25
3	A	602	QDJ	C13-C12-C24-N26
3	A	602	QDJ	N08-C06-O05-C02
3	A	602	QDJ	O07-C06-O05-C02
3	A	602	QDJ	O07-C06-N08-C09
3	A	602	QDJ	O05-C06-N08-C09
2	A	601	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

No monomer is involved in short contacts.

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers

EDS failed to run properly - this section is therefore empty.