



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:48 AM GMT

PDB ID : 4I3Q  
Title : Crystal structure of human CYP3A4 coordinated to a water molecule  
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Deposited on : 2012-11-26  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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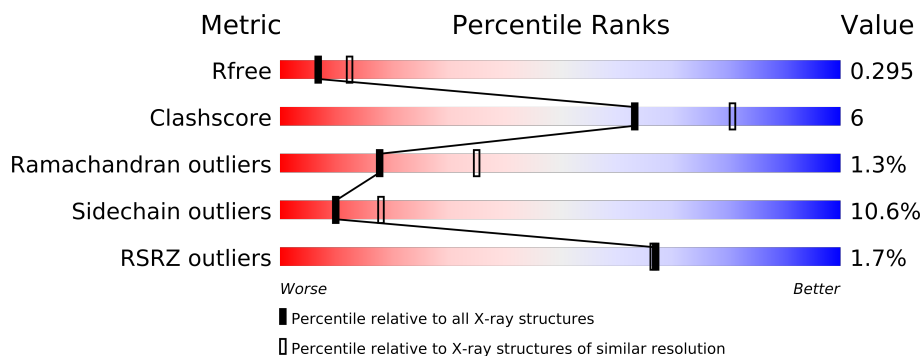
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	487	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3798 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	465	Total	C	N	O	S	0	0	0
			3749	2436	620	669	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	DELETION	UNP P08684
A	?	-	ILE	DELETION	UNP P08684
A	?	-	PRO	DELETION	UNP P08684
A	?	-	ASP	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	ALA	DELETION	UNP P08684
A	?	-	MET	DELETION	UNP P08684
A	?	-	GLU	DELETION	UNP P08684
A	?	-	THR	DELETION	UNP P08684
A	?	-	TRP	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	ALA	DELETION	UNP P08684
A	?	-	VAL	DELETION	UNP P08684
A	?	-	SER	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	VAL	DELETION	UNP P08684
A	?	-	LEU	DELETION	UNP P08684
A	?	-	LEU	DELETION	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 water.

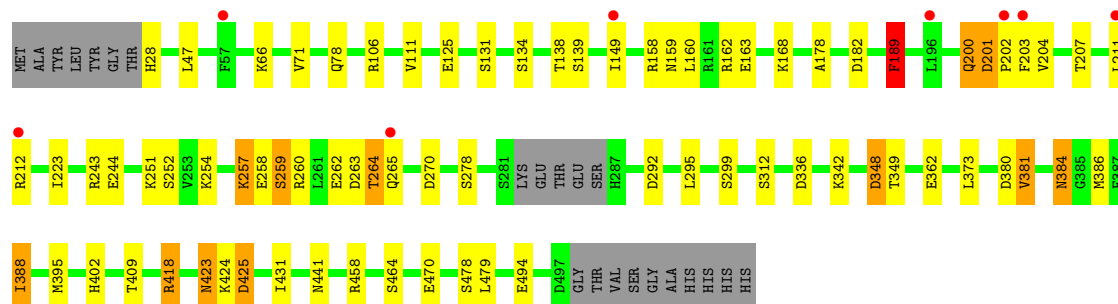
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	6	6	6	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Cytochrome P450 3A4

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.11Å 101.47Å 130.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.27 – 2.60 65.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (65.27-2.60) 98.4 (65.27-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.220 , 0.298 0.219 , 0.295	Depositor DCC
$R_{free}$ test set	819 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 16252 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

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	0.60	1/3841 (0.0%)	0.79	6/5195 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	ARG	CZ-NH1	5.81	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	GLN	N-CA-C	9.15	135.72	111.00
1	A	201	ASP	N-CA-CB	-8.64	95.04	110.60
1	A	200	GLN	CB-CA-C	-8.38	93.65	110.40
1	A	418	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	257	LYS	CB-CA-C	-6.33	97.75	110.40
1	A	336	ASP	CB-CG-OD1	5.17	122.96	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3749	0	0	21	0
2	A	43	0	0	0	0
3	A	6	0	0	1	0
All	All	3798	0	0	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:348:ASP:N	1:A:348:ASP:OD2	2.22	0.72
1:A:257:LYS:NZ	1:A:292:ASP:OD2	2.26	0.69
1:A:212:ARG:NH1	3:A:705:HOH:O	2.32	0.63
1:A:189:PHE:CD1	1:A:270:ASP:OD1	2.55	0.59
1:A:402:HIS:CD2	1:A:431:ILE:O	2.63	0.51
1:A:295:LEU:O	1:A:299:SER:OG	2.29	0.51
1:A:189:PHE:CA	1:A:270:ASP:OD1	2.60	0.50
1:A:423:ASN:O	1:A:425:ASP:N	2.45	0.49
1:A:381:VAL:O	1:A:388:ILE:N	2.46	0.49
1:A:138:THR:CG2	1:A:139:SER:N	2.77	0.47
1:A:159:ASN:OD1	1:A:162:ARG:NH1	2.48	0.47
1:A:178:ALA:O	1:A:182:ASP:OD2	2.34	0.45
1:A:258:GLU:O	1:A:260:ARG:N	2.49	0.45
1:A:201:ASP:O	1:A:202:PRO:C	2.53	0.44
1:A:470:GLU:CD	1:A:470:GLU:N	2.71	0.44
1:A:409:THR:O	1:A:418:ARG:NH1	2.52	0.42
1:A:264:THR:O	1:A:265:GLN:CB	2.66	0.42
1:A:203:PHE:O	1:A:207:THR:OG1	2.37	0.42
1:A:464:SER:N	1:A:494:GLU:O	2.53	0.41
1:A:270:ASP:O	1:A:270:ASP:OD2	2.38	0.41
1:A:395:MET:SD	1:A:395:MET:C	2.98	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	461/487 (95%)	410 (89%)	45 (10%)	6 (1%)	18	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	384	ASN
1	A	259	SER
1	A	342	LYS
1	A	424	LYS
1	A	189	PHE

### 5.3.2 Protein sidechains ⓘ

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	426/443 (96%)	381 (89%)	45 (11%)	10	18

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	47	LEU
1	A	66	LYS
1	A	71	VAL
1	A	78	GLN
1	A	106	ARG
1	A	111	VAL
1	A	125	GLU
1	A	131	SER
1	A	134	SER
1	A	149	ILE
1	A	158	ARG
1	A	160	LEU
1	A	163	GLU
1	A	168	LYS
1	A	189	PHE
1	A	200	GLN

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Mol	Chain	Res	Type
1	A	204	VAL
1	A	211	LEU
1	A	223	ILE
1	A	243	ARG
1	A	244	GLU
1	A	251	LYS
1	A	252	SER
1	A	254	LYS
1	A	259	SER
1	A	262	GLU
1	A	264	THR
1	A	278	SER
1	A	312	SER
1	A	348	ASP
1	A	349	THR
1	A	362	GLU
1	A	373	LEU
1	A	380	ASP
1	A	381	VAL
1	A	384	ASN
1	A	386	MET
1	A	388	ILE
1	A	423	ASN
1	A	425	ASP
1	A	441	ASN
1	A	458	ARG
1	A	478	SER
1	A	479	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	HEM	A	601	1,3	49,50,50	5.48	24 (48%)	46,82,82	3.08	22 (47%)

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	HEM	A	601	1,3	-	0/14/114/114	0/0/8/8

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3D-C4D	21.13	1.49	1.44
2	A	601	HEM	C2D-C1D	19.36	1.49	1.44
2	A	601	HEM	C2B-C1B	13.23	1.47	1.44
2	A	601	HEM	C4A-C3A	7.30	1.49	1.40
2	A	601	HEM	CHB-C1B	6.56	1.45	1.35
2	A	601	HEM	CHA-C4D	6.42	1.45	1.35
2	A	601	HEM	C1C-NC	6.39	1.47	1.38
2	A	601	HEM	C4C-NC	6.05	1.46	1.38
2	A	601	HEM	C1A-NA	5.66	1.47	1.36
2	A	601	HEM	CHC-C1C	5.50	1.46	1.36
2	A	601	HEM	CHD-C4C	5.39	1.46	1.36
2	A	601	HEM	C4A-NA	4.60	1.45	1.36
2	A	601	HEM	FE-ND	4.18	2.13	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C4B	3.91	1.49	1.44
2	A	601	HEM	C1A-C2A	3.90	1.50	1.43
2	A	601	HEM	FE-NB	3.66	2.11	1.97
2	A	601	HEM	CHC-C4B	3.44	1.47	1.39
2	A	601	HEM	C2A-C3A	3.08	1.46	1.37
2	A	601	HEM	C3C-CAC	3.03	1.49	1.40
2	A	601	HEM	C3B-CAB	2.85	1.49	1.40
2	A	601	HEM	CHD-C1D	2.71	1.45	1.39
2	A	601	HEM	C1A-CHA	2.21	1.45	1.39
2	A	601	HEM	C2C-C1C	2.10	1.49	1.43
2	A	601	HEM	C1B-NB	-2.01	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3A-C4A-NA	8.98	116.19	109.41
2	A	601	HEM	C4C-NC-C1C	-6.60	98.68	105.53
2	A	601	HEM	C4A-NA-C1A	-6.24	98.55	106.76
2	A	601	HEM	C4D-ND-C1D	-5.65	99.38	105.16
2	A	601	HEM	CBD-CAD-C3D	-5.54	102.28	114.37
2	A	601	HEM	C2D-C1D-ND	4.79	118.59	112.93
2	A	601	HEM	C4A-CHB-C1B	-4.45	121.62	127.47
2	A	601	HEM	C2A-C1A-NA	4.02	115.31	109.73
2	A	601	HEM	C3A-C4A-CHB	-3.89	118.63	126.00
2	A	601	HEM	C2A-C1A-CHA	-3.64	119.09	126.00
2	A	601	HEM	C1A-CHA-C4D	-3.58	122.75	127.47
2	A	601	HEM	C1B-NB-C4B	-3.57	101.51	105.16
2	A	601	HEM	CHC-C1C-NC	-3.44	121.74	124.73
2	A	601	HEM	CHC-C4B-NB	-3.30	121.84	124.58
2	A	601	HEM	C4A-C3A-C2A	-3.27	104.72	107.00
2	A	601	HEM	CMB-C2B-C3B	2.72	132.58	126.16
2	A	601	HEM	C1A-C2A-C3A	-2.42	104.41	106.92
2	A	601	HEM	CAD-C3D-C4D	2.42	128.88	124.53
2	A	601	HEM	CHD-C1D-ND	-2.40	122.59	124.58
2	A	601	HEM	O1A-CGA-CBA	-2.39	114.80	123.03
2	A	601	HEM	CAA-CBA-CGA	-2.10	106.71	113.47
2	A	601	HEM	CMD-C2D-C3D	2.04	130.21	125.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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 <sup>2</sup> )	Q<0.9
1	A	465/487 (95%)	0.11	8 (1%) 67 66	59, 91, 137, 180	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	LEU	4.3
1	A	202	PRO	2.9
1	A	149	ILE	2.8
1	A	57	PHE	2.5
1	A	265	GLN	2.3
1	A	203	PHE	2.3
1	A	212	ARG	2.0
1	A	211	LEU	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	601	43/43	0.22	0.58	57,62,70,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.