



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:35 AM GMT

PDB ID : 3NXU  
Title : Crystal structure of human cytochrome P4503A4 bound to an inhibitor ritonavir  
Authors : Sevrioukova, I.F.; Poulos, T.L.  
Deposited on : 2010-07-14  
Resolution : 2.00 Å(reported)

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

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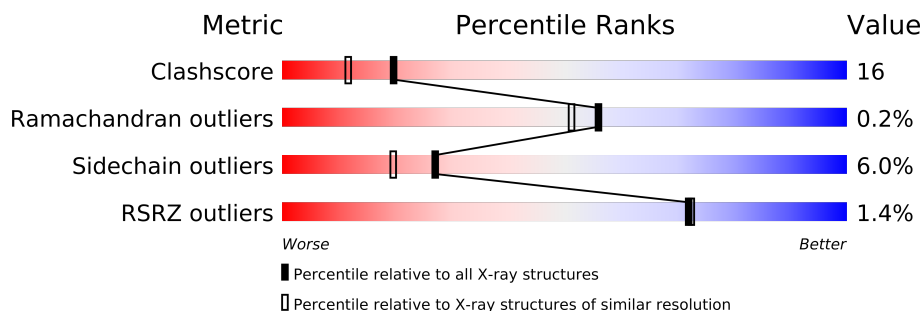
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	485	
1	B	485	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	DMS	A	703	-	X
2	DMS	B	705	-	X
4	RIT	B	600	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7955 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.

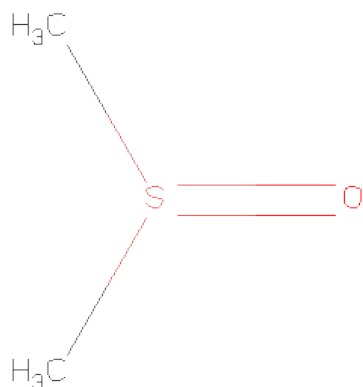
- Molecule 1 is a protein called Cytochrome P450 3A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3678	2394	603	657	24			
1	B	457	Total	C	N	O	S	0	0	0
			3678	2394	603	657	24			

There are 12 discrepancies between the modelled and reference sequences:

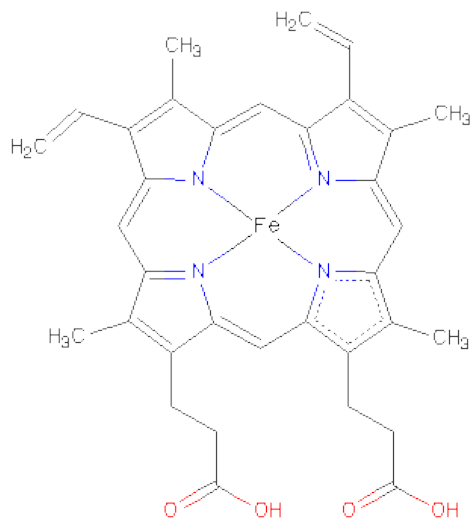
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	SEE REMARK 999	UNP P08684
A	24	ALA	-	SEE REMARK 999	UNP P08684
A	504	HIS	-	EXPRESSION TAG	UNP P08684
A	505	HIS	-	EXPRESSION TAG	UNP P08684
A	506	HIS	-	EXPRESSION TAG	UNP P08684
A	507	HIS	-	EXPRESSION TAG	UNP P08684
B	23	MET	-	SEE REMARK 999	UNP P08684
B	24	ALA	-	SEE REMARK 999	UNP P08684
B	504	HIS	-	EXPRESSION TAG	UNP P08684
B	505	HIS	-	EXPRESSION TAG	UNP P08684
B	506	HIS	-	EXPRESSION TAG	UNP P08684
B	507	HIS	-	EXPRESSION TAG	UNP P08684

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



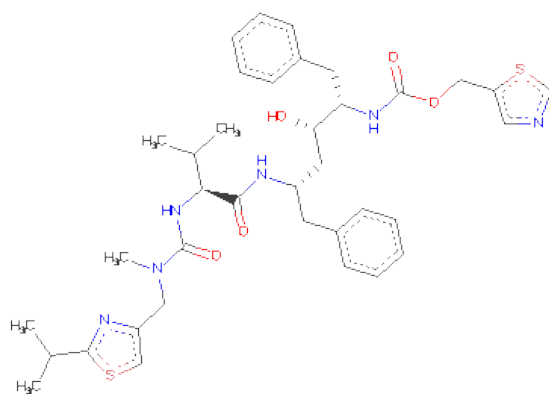
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is RITONAVIR (three-letter code: RIT) (formula:  $C_{37}H_{48}N_6O_5S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			50	37	6	5	2		
4	B	1	Total	C	N	O	S	0	0
			50	37	6	5	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total 217	O 217	0	0
5	B	172	Total 172	O 172	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.12Å 94.69Å 93.13Å 90.00° 124.25° 90.00°	Depositor
Resolution (Å)	40.40 – 2.00 77.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.40-2.00) 97.6 (77.33-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.262 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.4	EDS
Estimated twinning fraction	0.006 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1/2*h-1/2*k 0.003 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.009 for -h-k-l,l,k 0.016 for -h+k-l,-l,-k 0.003 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.005 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.010 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.016 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.012 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.015 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.018 for -h-2*l,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 76658 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

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



Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

## 5 Model quality

### 5.1 Standard geometry

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

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	0/3766	0.63	1/5094 (0.0%)
1	B	0.37	0/3766	0.61	0/5094
All	All	0.39	0/7532	0.62	1/10188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ARG	NE-CZ-NH2	-5.44	117.58	120.30

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	3678	0	3764	99	0
1	B	3678	0	3764	140	0
2	A	16	0	24	1	0
2	B	8	0	12	3	0
3	A	43	0	30	7	0
3	B	43	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	50	0	47	6	0
4	B	50	0	46	4	0
5	A	217	0	0	13	0
5	B	172	0	0	15	0
All	All	7955	0	7717	246	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 16.

The worst 5 of 246 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:251:LYS:HG2	1:A:255:ARG:HH21	1.21	1.06
1:A:70:LYS:HD2	1:A:71:VAL:HG23	1.41	0.98
1:A:369:ILE:HG12	3:A:508:HEM:HMB1	1.52	0.90
1:B:472:GLN:HE21	1:B:476:LYS:H	1.16	0.90
1:A:370:ALA:HA	4:A:600:RIT:H50	1.50	0.90

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	451/485 (93%)	433 (96%)	17 (4%)	1 (0%)	56	51
1	B	451/485 (93%)	426 (94%)	24 (5%)	1 (0%)	56	51
All	All	902/970 (93%)	859 (95%)	41 (4%)	2 (0%)	56	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	424	LYS
1	A	405	PRO

### 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	418/441 (95%)	394 (94%)	24 (6%)	29	21
1	B	418/441 (95%)	392 (94%)	26 (6%)	26	18
All	All	836/882 (95%)	786 (94%)	50 (6%)	27	20

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	478	SER
1	B	78	GLN
1	B	451	ASN
1	A	485	PRO
1	B	59	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	GLN
1	B	65	HIS
1	B	384	ASN
1	A	461	GLN
1	B	352	GLN

### 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 ⓘ

10 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	HEM	A	508	1,4	49,50,50	2.76	12 (24%)	46,82,82	1.18	2 (4%)
4	RIT	A	600	3	53,53,53	6.29	35 (66%)	67,71,71	3.85	35 (52%)
2	DMS	A	700	-	3,3,3	0.96	0	3,3,3	0.80	0
2	DMS	A	701	-	3,3,3	0.83	0	3,3,3	0.88	0
2	DMS	A	702	-	3,3,3	0.76	0	3,3,3	0.87	0
2	DMS	A	703	-	3,3,3	0.75	0	3,3,3	0.80	0
3	HEM	B	508	1,4	49,50,50	2.64	13 (26%)	46,82,82	1.13	2 (4%)
4	RIT	B	600	3	53,53,53	6.64	37 (69%)	67,71,71	3.29	27 (40%)
2	DMS	B	704	-	3,3,3	2.08	2 (66%)	3,3,3	0.72	0
2	DMS	B	705	-	3,3,3	1.72	1 (33%)	3,3,3	0.91	0

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	HEM	A	508	1,4	-	0/14/114/114	0/0/8/8
4	RIT	A	600	3	-	0/50/53/53	0/4/4/4
2	DMS	A	700	-	-	0/0/0/0	0/0/0/0
2	DMS	A	701	-	-	0/0/0/0	0/0/0/0
2	DMS	A	702	-	-	0/0/0/0	0/0/0/0
2	DMS	A	703	-	-	0/0/0/0	0/0/0/0
3	HEM	B	508	1,4	-	0/14/114/114	0/0/8/8
4	RIT	B	600	3	-	0/50/53/53	0/4/4/4
2	DMS	B	704	-	-	0/0/0/0	0/0/0/0
2	DMS	B	705	-	-	0/0/0/0	0/0/0/0

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	RIT	C6-C2	-38.21	1.19	1.49
4	A	600	RIT	C6-C2	-30.57	1.25	1.49
4	A	600	RIT	C82-C85	12.95	1.61	1.51
4	A	600	RIT	O24-C10	11.01	1.43	1.21
3	B	508	HEM	C2D-C1D	10.64	1.47	1.44

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	RIT	C44-C15-N58	11.21	127.80	110.21
4	B	600	RIT	C44-C15-N58	10.53	126.73	110.21
4	A	600	RIT	C14-C13-C12	-10.33	99.74	113.43
4	A	600	RIT	C6-C2-C1	10.21	143.37	127.44
4	A	600	RIT	C26-C12-N11	9.26	121.00	110.20

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	457/485 (94%)	0.02	5 (1%) 77 78	24, 38, 64, 75	0
1	B	457/485 (94%)	0.09	8 (1%) 65 66	26, 46, 70, 83	0
All	All	914/970 (94%)	0.06	13 (1%) 72 72	24, 42, 68, 83	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	482	LEU	5.1
1	A	280	ASN	2.7
1	B	54	HIS	2.6
1	B	255	ARG	2.5
1	A	482	LEU	2.4

### 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	DMS	A	703	4/4	0.16	2.73	71,71,72,74	0
2	DMS	B	705	4/4	0.16	2.59	60,60,61,65	0
4	RIT	B	600	50/50	0.18	2.38	41,53,58,59	0
2	DMS	B	704	4/4	0.17	0.82	51,53,54,56	0
4	RIT	A	600	50/50	0.14	0.68	33,40,45,46	0
2	DMS	A	701	4/4	0.13	0.63	71,71,71,73	0
3	HEM	A	508	43/43	0.11	-0.14	23,26,29,31	0
2	DMS	A	702	4/4	0.12	-0.24	71,71,72,74	0
3	HEM	B	508	43/43	0.10	-0.26	30,32,34,36	0
2	DMS	A	700	4/4	0.12	-0.33	38,39,39,43	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.