



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2X2N  
Title : X-ray structure of cyp51 from trypanosoma brucei in complex with posaconazole in two different conformations  
Authors : Chen, C.-K.; Leung, S.S.F.; Guilbert, C.; Jacobson, M.; Mckerrow, J.H.; Podust, L.M.  
Deposited on : 2010-01-14  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

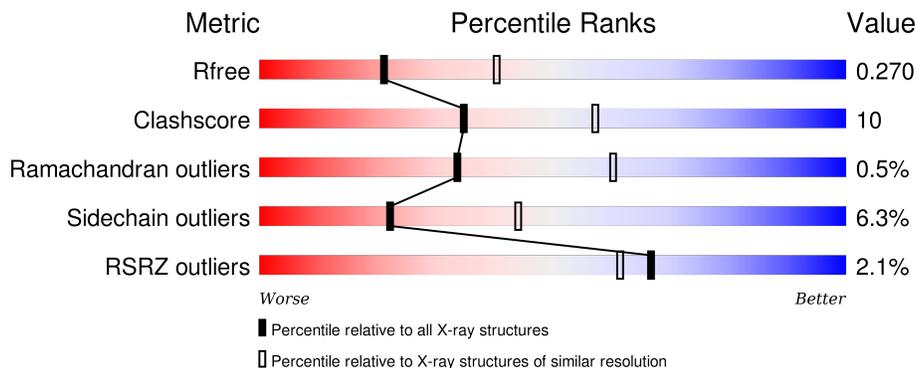
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	 2% 75% 17% • 6%
1	B	475	 3% 77% 14% • 7%
1	C	475	 % 71% 20% • 7%
1	D	475	 2% 68% 23% • 6%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14674 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 LANOSTEROL 14-ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	3534	2257	619	631	27	0	1	0
1	B	444	3493	2234	609	623	27	0	1	0
1	C	441	3488	2230	608	623	27	0	1	0
1	D	447	3533	2255	619	632	27	0	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
A	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
A	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
B	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
B	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
B	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
C	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
C	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
C	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
D	249	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
D	250	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8
D	251	ALA	GLU	ENGINEERED MUTATION	UNP Q385E8

- 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
3	A	1	Total	C	F	N	O	0	0
			51	37	2	8	4		
3	B	1	Total	C	F	N	O	0	0
			51	37	2	8	4		
3	C	1	Total	C	F	N	O	0	0
			51	37	2	8	4		
3	D	1	Total	C	F	N	O	0	0
			51	37	2	8	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	47	Total	O	0	0
			47	47		
4	C	69	Total	O	0	0
			69	69		
4	D	75	Total	O	0	0
			75	75		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.89Å 114.53Å 138.09Å 90.00° 131.83° 90.00°	Depositor
Resolution (Å)	102.90 – 2.60 21.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (102.90-2.60) 99.9 (21.25-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.191 , 0.264 0.204 , 0.270	Depositor DCC
$R_{free}$ test set	3572 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.1	EDS
Estimated twinning fraction	0.016 for -h-2*1,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 71152 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: HEM, X2N

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	0.72	2/3616 (0.1%)	0.81	7/4898 (0.1%)
1	B	0.71	0/3575	0.78	3/4844 (0.1%)
1	C	0.74	2/3569 (0.1%)	0.79	4/4833 (0.1%)
1	D	0.85	1/3614 (0.0%)	0.83	1/4897 (0.0%)
All	All	0.76	5/14374 (0.0%)	0.80	15/19472 (0.1%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	229	CYS	CB-SG	-7.06	1.70	1.82
1	A	101	GLU	CG-CD	6.37	1.61	1.51
1	D	256	SER	CA-CB	5.69	1.61	1.52
1	A	101	GLU	CB-CG	5.55	1.62	1.52
1	C	324	GLU	CG-CD	5.16	1.59	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH1	8.69	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	247	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	C	88	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	470	ARG	NE-CZ-NH1	6.38	123.49	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	273	GLY	Peptide
1	C	273	GLY	Peptide
1	D	273	GLY	Peptide

## 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	3534	0	3540	60	0
1	B	3493	0	3490	54	0
1	C	3488	0	3493	67	0
1	D	3533	0	3523	90	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
2	C	43	0	30	4	0
2	D	43	0	30	5	0
3	A	51	0	42	2	0
3	B	51	0	42	0	0
3	C	51	0	42	5	0
3	D	51	0	42	2	0
4	A	59	0	0	5	0
4	B	47	0	0	1	0
4	C	69	0	0	2	0
4	D	75	0	0	2	0
All	All	14674	0	14334	286	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 10.

The worst 5 of 286 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)
2:B:1478:HEM:HBC2	2:B:1478:HEM:HMC2	1.38	1.02
2:B:1478:HEM:CMC	2:B:1478:HEM:HBC2	1.95	0.94
2:A:1479:HEM:HMC2	2:A:1479:HEM:HBC2	1.48	0.92
1:B:192:LEU:HD11	1:B:239:ILE:HD13	1.52	0.91
1:D:205:GLU:OE2	1:D:294:HIS:CE1	2.24	0.91

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	445/475 (94%)	421 (95%)	20 (4%)	4 (1%)	21	42
1	B	441/475 (93%)	422 (96%)	18 (4%)	1 (0%)	52	77
1	C	438/475 (92%)	414 (94%)	23 (5%)	1 (0%)	52	77
1	D	446/475 (94%)	406 (91%)	38 (8%)	2 (0%)	39	65
All	All	1770/1900 (93%)	1663 (94%)	99 (6%)	8 (0%)	34	60

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	372	TYR
1	D	40	PRO
1	B	372	TYR
1	A	371	SER
1	D	475	ARG

### 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	381/410 (93%)	358 (94%)	23 (6%)	24	47
1	B	375/410 (92%)	355 (95%)	20 (5%)	28	53
1	C	376/410 (92%)	356 (95%)	20 (5%)	28	53
1	D	379/410 (92%)	347 (92%)	32 (8%)	14	26
All	All	1511/1640 (92%)	1416 (94%)	95 (6%)	22	44

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	421	LYS
1	C	234	THR
1	D	358	MET
1	C	61	ARG
1	C	152	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	GLN
1	C	166	ASN
1	D	331	ASN
1	B	431	GLN
1	C	71	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	HEM	A	1479	1,3	30,50,50	2.58	6 (20%)	24,82,82	2.57	12 (50%)
3	X2N	A	1480	2	46,57,57	1.71	4 (8%)	51,82,82	2.26	15 (29%)
2	HEM	B	1478	1,3	30,50,50	2.43	4 (13%)	24,82,82	2.73	9 (37%)
3	X2N	B	1479	2	46,57,57	1.76	5 (10%)	51,82,82	2.47	16 (31%)
2	HEM	C	1478	1,3	30,50,50	2.48	5 (16%)	24,82,82	2.19	8 (33%)
3	X2N	C	1479	2	46,57,57	1.91	4 (8%)	51,82,82	2.63	17 (33%)
2	HEM	D	1478	1,3	30,50,50	2.22	5 (16%)	24,82,82	2.24	8 (33%)
3	X2N	D	1479	2	46,57,57	1.81	6 (13%)	51,82,82	2.40	17 (33%)

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	1479	1,3	-	0/10/54/54	0/0/8/8
3	X2N	A	1480	2	-	1/34/59/59	1/7/7/7
2	HEM	B	1478	1,3	-	0/10/54/54	0/0/8/8
3	X2N	B	1479	2	-	1/34/59/59	1/7/7/7
2	HEM	C	1478	1,3	-	0/10/54/54	0/0/8/8
3	X2N	C	1479	2	-	1/34/59/59	1/7/7/7
2	HEM	D	1478	1,3	-	0/10/54/54	0/0/8/8
3	X2N	D	1479	2	-	0/34/59/59	0/7/7/7

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1479	HEM	C3B-C4B	-10.86	1.42	1.51
2	B	1478	HEM	C3B-C4B	-9.67	1.43	1.51
2	C	1478	HEM	C3B-C4B	-9.21	1.43	1.51
3	C	1479	X2N	CBN-NBW	-8.40	1.34	1.44
3	B	1479	X2N	CBN-NBW	-8.08	1.34	1.44

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1478	HEM	C3C-CAC-CBC	-6.43	114.60	124.46
3	C	1479	X2N	CAY-NBU-CBM	-5.53	103.09	117.92
3	D	1479	X2N	CAX-CAZ-NBU	-5.34	100.05	110.63
3	B	1479	X2N	CAJ-CBL-NBT	-4.88	114.82	121.38
3	A	1480	X2N	CAY-NBU-CBM	-4.81	105.02	117.92

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1479	X2N	C2-CBC-NBV-CAS
3	A	1480	X2N	C2-CBC-NBV-CAS
3	B	1479	X2N	C2-CBC-NBV-CAS

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1479	X2N	CAW-CAX-CAY-CAZ-NBT-NBU
3	A	1480	X2N	CAW-CAX-CAY-CAZ-NBT-NBU
3	B	1479	X2N	CAW-CAX-CAY-CAZ-NBT-NBU

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1479	HEM	4	0
3	A	1480	X2N	2	0
2	B	1478	HEM	7	0
2	C	1478	HEM	4	0
3	C	1479	X2N	5	0
2	D	1478	HEM	5	0
3	D	1479	X2N	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	448/475 (94%)	-0.13	10 (2%) 65 59	43, 53, 67, 74	0
1	B	444/475 (93%)	-0.15	13 (2%) 55 48	43, 54, 67, 74	0
1	C	441/475 (92%)	-0.19	6 (1%) 78 74	43, 53, 67, 74	0
1	D	447/475 (94%)	-0.19	8 (1%) 71 66	44, 54, 68, 76	0
All	All	1780/1900 (93%)	-0.16	37 (2%) 67 61	43, 54, 68, 76	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	257	SER	5.8
1	A	257	SER	3.9
1	A	478	ALA	3.7
1	D	258	THR	3.7
1	C	258	THR	3.7

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	X2N	C	1479	51/51	0.84	0.21	1.49	21,44,78,78	0
3	X2N	D	1479	51/51	0.86	0.19	0.87	28,44,75,76	0
3	X2N	A	1480	51/51	0.87	0.20	0.46	17,41,72,73	0
2	HEM	D	1478	43/43	0.97	0.16	0.19	38,45,51,56	0
2	HEM	B	1478	43/43	0.98	0.15	0.10	46,52,59,62	0
3	X2N	B	1479	51/51	0.90	0.15	-0.18	35,47,73,73	0
2	HEM	C	1478	43/43	0.98	0.14	-0.35	47,49,54,57	0
2	HEM	A	1479	43/43	0.98	0.14	-0.35	38,44,47,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.