



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:22 PM GMT

PDB ID : 4CAT  
Title : THREE-DIMENSIONAL STRUCTURE OF CATALASE FROM PENICILLIUM VITALE AT 2.0 ANGSTROMS RESOLUTION  
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Deposited on : 1983-02-24  
Resolution : 3.00 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

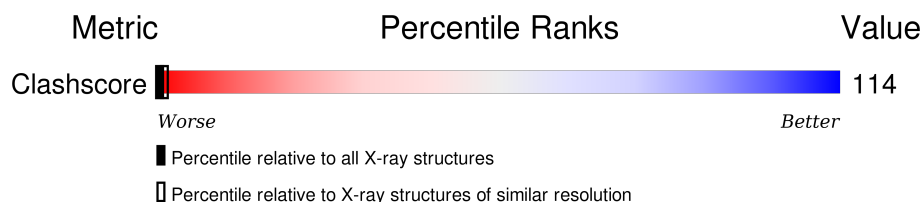
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	659	 51%                      48%                      .
1	B	659	 51%                      48%                      .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5360 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 CATALASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	0	0	0
			2637	1318	659	660			
1	B	659	Total	C	N	O	0	0	0
			2637	1318	659	660			

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



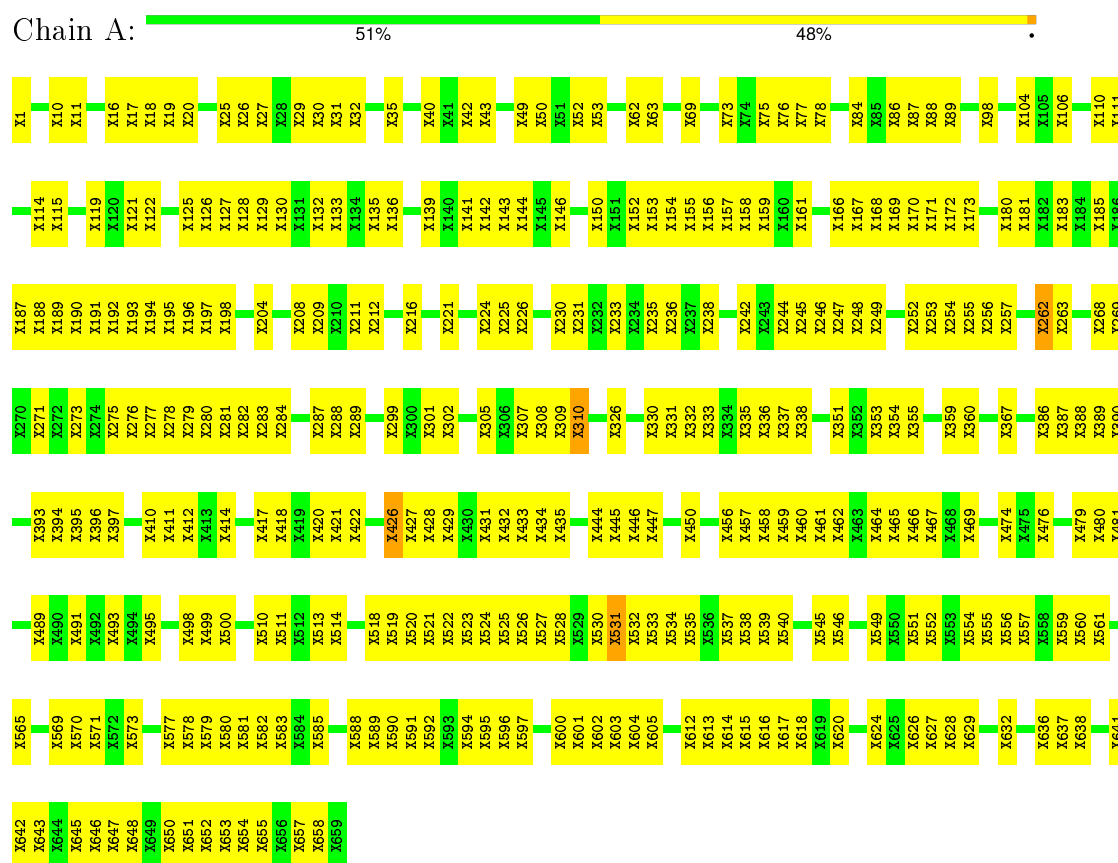
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

### 3 Residue-property plots

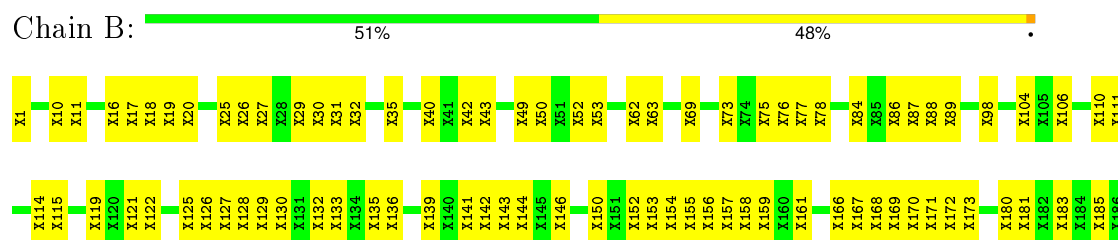
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: CATALASE



#### • Molecule 1: CATALASE



X637	X559	X269	X187
X638	X560	X270	X188
X641	X561	X271	X189
X642	X565	X272	X190
X643	X569	X273	X191
X644	X570	X274	X192
X645	X571	X275	X193
X646	X572	X276	X194
X647	X573	X277	X195
X648	X577	X278	X196
X649	X578	X279	X197
X650	X579	X280	X198
X651	X580	X281	X204
X652	X581	X282	X208
X653	X582	X283	X209
X654	X583	X284	X210
X655	X584	X287	X211
X656	X585	X288	X212
X657	X588	X299	X216
X658	X589	X300	X221
X659	X590	X301	X224
	X591	X302	X225
	X592	X305	X226
	X593	X306	X230
	X594	X307	X231
	X595	X308	X232
	X596	X309	X233
	X597	X310	X234
	X600	X326	X235
	X601	X330	X236
	X602	X331	X237
	X603	X332	X238
	X604	X333	X242
	X605	X334	X243
	X612	X335	X244
	X613	X336	X245
	X614	X337	X246
	X615	X338	X247
	X616	X351	X248
	X617	X352	X249
	X618	X353	X250
	X619	X354	X251
	X620	X355	X252
	X624	X359	X253
	X625	X360	X254
	X626	X367	X255
	X627	X386	X256
	X628	X387	X257
	X629	X388	X262
	X632	X389	X263
	X636		X268

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.40Å 144.40Å 133.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	A	0	14
1	B	0	14
All	All	0	28

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	UNK	Peptide
1	A	226	UNK	Mainchain
1	A	262	UNK	Peptide
1	A	263	UNK	Peptide
1	A	310	UNK	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	2637	0	99	316	6
1	B	2637	0	99	319	6
2	A	43	0	30	5	0
2	B	43	0	30	6	0
All	All	5360	0	258	638	6

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 114.

The worst 5 of 638 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:A:533:UNK:C	1:A:533:UNK:CA	1.76	1.64
1:B:533:UNK:CA	1:B:533:UNK:C	1.76	1.57
1:A:535:UNK:CA	1:A:535:UNK:N	1.69	1.55
1:A:534:UNK:N	1:A:534:UNK:CA	1.70	1.55
1:A:533:UNK:N	1:A:533:UNK:CA	1.72	1.51

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:UNK:O	1:B:53:UNK:O[4_555]	1.64	0.56
1:A:53:UNK:O	1:B:367:UNK:O[4_555]	1.64	0.56
1:A:367:UNK:O	1:B:53:UNK:C[4_555]	2.09	0.11
1:A:53:UNK:C	1:B:367:UNK:O[4_555]	2.09	0.11
1:A:367:UNK:O	1:B:53:UNK:CA[4_555]	2.12	0.08

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.



### 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 ⓘ

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$
2	HEM	A	660	-	30,50,50	2.11	4 (13%)	24,82,82	2.28	10 (41%)
2	HEM	B	660	-	30,50,50	2.11	4 (13%)	24,82,82	2.28	10 (41%)

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	660	-	-	0/10/54/54	0/0/8/8
2	HEM	B	660	-	-	0/10/54/54	0/0/8/8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	660	HEM	C2D-C3D	-6.70	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	660	HEM	C2D-C3D	-6.70	1.34	1.54
2	A	660	HEM	C3B-C4B	-6.14	1.46	1.51
2	B	660	HEM	C3B-C4B	-6.14	1.46	1.51
2	A	660	HEM	C3D-C4D	-3.99	1.46	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	660	HEM	C3C-CAC-CBC	-2.91	119.99	124.46
2	B	660	HEM	C3C-CAC-CBC	-2.91	119.99	124.46
2	A	660	HEM	C3B-CAB-CBB	-2.88	120.03	124.46
2	B	660	HEM	C3B-CAB-CBB	-2.88	120.03	124.46
2	A	660	HEM	CAA-CBA-CGA	-2.57	108.04	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	660	HEM	5	0
2	B	660	HEM	6	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.