Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:03 PM UTC

PDB ID	:	1U2K / pdb_00001u2k
Title	:	Crystal structure of the C-terminal domain from the catalase-peroxidase KatG of Escherichia coli (I41)
Authors	:	Carpena, X.; Melik-Adamyan, W.; Loewen, P.C.; Fita, I.
Deposited on	:	2004-07-19
Resolution	:	2.00 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*
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.

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

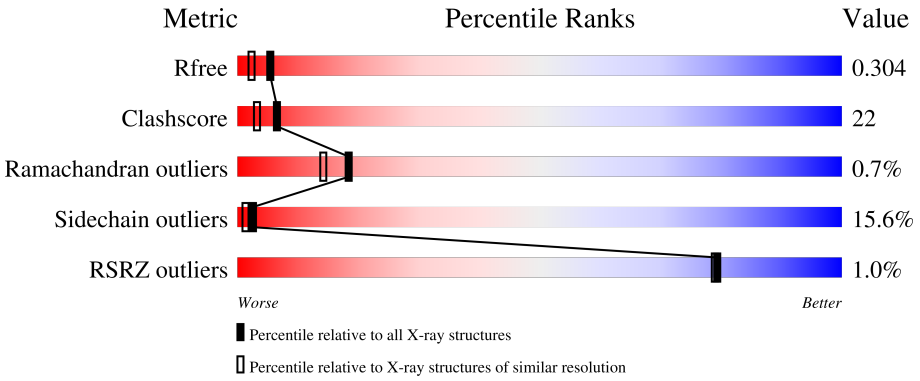
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	309	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2326 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 Peroxidase/catalase HPI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2233	1410	386	431	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	GLY	-	cloning artifact	UNP P13029
A	419	SER	-	cloning artifact	UNP P13029
A	420	HIS	-	cloning artifact	UNP P13029
A	421	MET	-	cloning artifact	UNP P13029

- Molecule 2 is water.

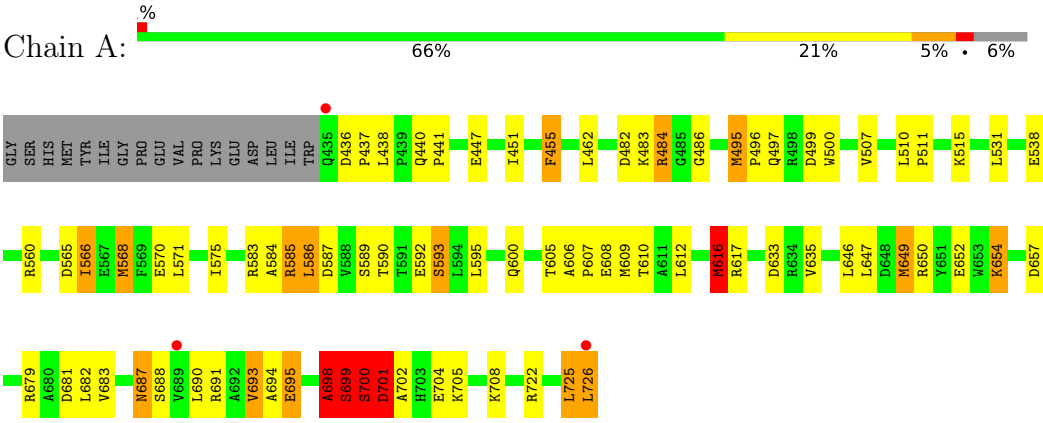
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	93	Total	O	0	0
			93	93		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Peroxidase/catalase HPI

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	59.23Å 59.23Å 160.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.00 18.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (18.00-2.00) 95.2 (18.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.189 , 0.249 (Not available) , 0.304	Depositor DCC
R_{free} test set	904 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.054 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2326	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.10	5/2271 (0.2%)	1.16	5/3077 (0.2%)

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	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	616	MET	SD-CE	7.56	1.98	1.79
1	A	495	MET	SD-CE	5.63	1.93	1.79
1	A	538	GLU	C-O	5.21	1.30	1.24
1	A	635	VAL	CA-CB	5.07	1.59	1.54
1	A	455	PHE	C-N	5.02	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	698	ALA	N-CA-C	6.11	120.47	113.19
1	A	486	GLY	N-CA-C	-5.77	104.92	111.85
1	A	699	SER	N-CA-C	5.43	122.36	110.80
1	A	586	LEU	N-CA-C	-5.33	102.16	110.10
1	A	695	GLU	N-CA-C	5.16	117.80	111.82

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	ASP	Peptide
1	A	586	LEU	Peptide
1	A	698	ALA	Peptide
1	A	699	SER	Peptide
1	A	700	SER	Peptide

5.2 Too-close contacts (i)

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	2233	0	2217	97	1
2	A	93	0	0	2	0
All	All	2326	0	2217	97	1

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 22.

All (97) 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:590:THR:CG2	1:A:592:GLU:CD	1.89	1.42
1:A:647:LEU:HD12	1:A:698:ALA:CB	1.69	1.20
1:A:605:THR:HG22	1:A:607:PRO:HD2	1.20	1.19
1:A:590:THR:HG22	1:A:592:GLU:CD	1.70	1.14
1:A:590:THR:HG21	1:A:592:GLU:CD	1.64	1.09
1:A:590:THR:CG2	1:A:592:GLU:OE2	2.09	0.99
1:A:605:THR:CG2	1:A:607:PRO:HD2	1.93	0.98
1:A:590:THR:HG22	1:A:592:GLU:OE2	1.62	0.98
1:A:605:THR:HG22	1:A:607:PRO:CD	1.95	0.95
1:A:590:THR:HG21	1:A:592:GLU:OE1	1.66	0.93
1:A:698:ALA:O	1:A:699:SER:HB2	1.70	0.90
1:A:658:GLU:H	1:A:658:GLU:CD	1.77	0.90
1:A:647:LEU:HD12	1:A:698:ALA:HB2	1.52	0.90
1:A:495:MET:SD	1:A:499:ASP:OD2	2.32	0.87
1:A:725:LEU:O	1:A:726:LEU:HD12	1.73	0.86
1:A:495:MET:HB3	1:A:566:ILE:HD11	1.56	0.85
1:A:575:ILE:HG23	1:A:585:ARG:CD	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:THR:CG2	1:A:592:GLU:OE1	2.28	0.79
1:A:495:MET:CB	1:A:566:ILE:HD11	2.15	0.77
1:A:590:THR:CG2	1:A:592:GLU:CG	2.64	0.76
1:A:438:LEU:HD23	1:A:438:LEU:N	2.02	0.74
1:A:700:SER:C	1:A:702:ALA:H	1.95	0.74
1:A:605:THR:HG22	1:A:606:ALA:H	1.53	0.73
1:A:605:THR:HG22	1:A:606:ALA:N	2.04	0.73
1:A:647:LEU:HD12	1:A:698:ALA:HB3	1.68	0.73
1:A:590:THR:HG22	1:A:592:GLU:CG	2.19	0.72
1:A:658:GLU:CD	1:A:658:GLU:N	2.47	0.72
1:A:590:THR:HG23	1:A:592:GLU:CD	2.13	0.70
1:A:700:SER:CA	1:A:702:ALA:H	2.06	0.69
1:A:700:SER:HA	1:A:702:ALA:H	1.57	0.69
1:A:575:ILE:HG23	1:A:585:ARG:CG	2.22	0.69
1:A:612:LEU:O	1:A:616:MET:HG3	1.92	0.69
1:A:647:LEU:HD12	1:A:698:ALA:HB1	1.72	0.68
1:A:565:ASP:OD2	1:A:568:MET:HB2	1.93	0.68
1:A:700:SER:C	1:A:702:ALA:N	2.53	0.66
1:A:592:GLU:HG2	1:A:593:SER:N	2.11	0.66
1:A:590:THR:HG21	1:A:592:GLU:CG	2.26	0.65
1:A:725:LEU:O	1:A:726:LEU:CD1	2.45	0.65
1:A:654:LYS:HG3	2:A:2008:HOH:O	1.97	0.65
1:A:698:ALA:O	1:A:699:SER:CB	2.46	0.64
1:A:568:MET:HE3	1:A:571:LEU:HD12	1.81	0.62
1:A:590:THR:HG23	1:A:592:GLU:OE2	1.99	0.62
1:A:590:THR:HB	1:A:593:SER:HB3	1.81	0.61
1:A:455:PHE:CD2	1:A:455:PHE:C	2.78	0.61
1:A:606:ALA:HB3	1:A:607:PRO:HD3	1.82	0.61
1:A:437:PRO:HB2	1:A:438:LEU:HD23	1.83	0.61
1:A:440:GLN:HG3	1:A:441:PRO:HD2	1.82	0.61
1:A:612:LEU:O	1:A:616:MET:CG	2.50	0.60
1:A:605:THR:N	1:A:608:GLU:OE2	2.31	0.59
1:A:606:ALA:N	1:A:607:PRO:CD	2.67	0.58
1:A:575:ILE:HG23	1:A:585:ARG:HD2	1.86	0.57
1:A:647:LEU:CD1	1:A:698:ALA:HB2	2.31	0.55
1:A:691:ARG:HA	1:A:694:ALA:HB3	1.88	0.54
1:A:438:LEU:N	1:A:438:LEU:CD2	2.69	0.54
1:A:583:ARG:NH2	1:A:589:SER:O	2.41	0.54
1:A:701:ASP:OD1	1:A:701:ASP:C	2.51	0.53
1:A:725:LEU:O	1:A:726:LEU:CG	2.56	0.53
1:A:725:LEU:O	1:A:726:LEU:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ARG:O	1:A:683:VAL:HG23	2.10	0.52
1:A:605:THR:CG2	1:A:606:ALA:N	2.73	0.52
1:A:584:ALA:C	1:A:585:ARG:HG2	2.36	0.51
1:A:575:ILE:CG2	1:A:585:ARG:CG	2.89	0.51
1:A:482:ASP:OD2	1:A:484:ARG:HB2	2.10	0.51
1:A:647:LEU:CD1	1:A:698:ALA:CB	2.64	0.50
1:A:657:ASP:C	1:A:657:ASP:OD1	2.54	0.50
1:A:592:GLU:HG2	1:A:593:SER:H	1.74	0.50
1:A:447:GLU:O	1:A:451:ILE:HG12	2.12	0.49
1:A:484:ARG:NH1	1:A:568:MET:HG3	2.27	0.49
1:A:590:THR:CG2	1:A:592:GLU:HG2	2.39	0.49
1:A:610:THR:HG21	1:A:693:VAL:HG12	1.94	0.49
1:A:705:LYS:O	1:A:705:LYS:HG2	2.13	0.48
1:A:605:THR:CG2	1:A:606:ALA:H	2.22	0.48
1:A:646:LEU:O	1:A:646:LEU:HG	2.12	0.48
1:A:495:MET:HB3	1:A:566:ILE:CD1	2.37	0.48
1:A:649:MET:HE3	1:A:649:MET:H	1.79	0.48
1:A:704:GLU:HG2	2:A:2303:HOH:O	2.14	0.48
1:A:571:LEU:HD23	1:A:571:LEU:HA	1.52	0.47
1:A:647:LEU:HD11	1:A:695:GLU:HA	1.96	0.47
1:A:590:THR:HG22	1:A:592:GLU:HG2	1.95	0.46
1:A:496:PRO:HG3	1:A:570:GLU:HG2	1.96	0.46
1:A:617:ARG:NE	1:A:681:ASP:OD1	2.49	0.46
1:A:510:LEU:N	1:A:511:PRO:CD	2.78	0.45
1:A:575:ILE:CG2	1:A:585:ARG:CD	2.88	0.45
1:A:584:ALA:O	1:A:585:ARG:HG2	2.16	0.45
1:A:497:GLN:HG2	1:A:500:TRP:CH2	2.52	0.45
1:A:683:VAL:HG13	1:A:687:ASN:HB2	1.99	0.45
1:A:587:ASP:HB3	1:A:589:SER:H	1.82	0.44
1:A:687:ASN:O	1:A:688:SER:C	2.61	0.44
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.75	0.43
1:A:609:MET:HE2	1:A:609:MET:HB3	1.84	0.43
1:A:647:LEU:HD23	1:A:647:LEU:HA	1.64	0.42
1:A:484:ARG:HH11	1:A:568:MET:HG3	1.84	0.42
1:A:507:VAL:O	1:A:507:VAL:CG1	2.67	0.42
1:A:575:ILE:HG23	1:A:585:ARG:HG2	1.99	0.42
1:A:510:LEU:N	1:A:511:PRO:HD2	2.35	0.41
1:A:482:ASP:OD2	1:A:484:ARG:CB	2.69	0.41
1:A:647:LEU:CD1	1:A:695:GLU:HA	2.51	0.41

All (1) 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:554:PRO:O	1:A:722:ARG:NH2[6_565]	2.10	0.10

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	290/309 (94%)	273 (94%)	15 (5%)	2 (1%)	18 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	699	SER
1	A	701	ASP

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	199/250 (80%)	168 (84%)	31 (16%)	2 1

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	LYS
1	A	484	ARG
1	A	515	LYS
1	A	531	LEU

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Mol	Chain	Res	Type
1	A	548	ILE
1	A	560	ARG
1	A	566	ILE
1	A	568	MET
1	A	585	ARG
1	A	593	SER
1	A	595	LEU
1	A	600	GLN
1	A	616	MET
1	A	633	ASP
1	A	649	MET
1	A	650	ARG
1	A	652	GLU
1	A	654	LYS
1	A	658	GLU
1	A	659	SER
1	A	662	LEU
1	A	682	LEU
1	A	687	ASN
1	A	690	LEU
1	A	693	VAL
1	A	699	SER
1	A	700	SER
1	A	701	ASP
1	A	708	LYS
1	A	725	LEU
1	A	726	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	549	HIS
1	A	601	GLN
1	A	628	ASN
1	A	719	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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^2)	Q<0.9
1	A	292/309 (94%)	-0.16	3 (1%)	79	79	5, 20, 41, 56	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	GLN	2.6
1	A	689	VAL	2.6
1	A	726	LEU	2.2

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 oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.