wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 11:55 PM EDT

PDB ID	:	1U2J
Title	:	Crystal structure of the C-terminal domain from the catalase-peroxidase KatG of Escherichia coli (P21 21 21)
Authors	:	Carpena, X.; Melik-Adamyan, W.; Loewen, P.C.; Fita, I.
Deposited on	:	2004-07-19
Resolution	:	2.30 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

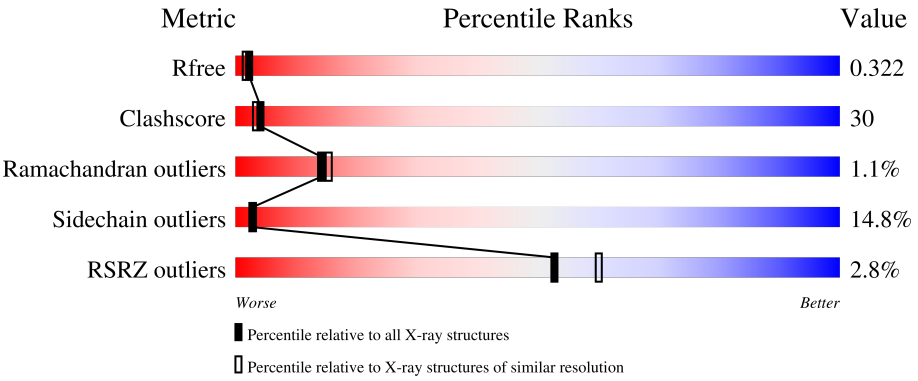
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	326	2% 49% 33% 8% • 10%
1	B	326	% 57% 27% 6% 10%
1	C	326	% 57% 29% 5% 10%
1	D	326	2% 51% 33% 6% 10%
1	E	326	3% 49% 33% 8% • 10%

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Mol	Chain	Length	Quality of chain
1	F	326	5% 41% 38% 11% 10%
1	G	326	4% 48% 34% 9% 10%
1	H	326	4% 44% 34% 11% 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18136 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	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	B	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	C	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	D	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	E	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	F	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	G	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			
1	H	295	Total	C	N	O	S	0	0	0
			2267	1435	391	435	6			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	MET	-	expression tag	UNP P13029
A	402	GLY	-	expression tag	UNP P13029
A	403	SER	-	expression tag	UNP P13029
A	404	SER	-	expression tag	UNP P13029
A	405	HIS	-	expression tag	UNP P13029
A	406	HIS	-	expression tag	UNP P13029
A	407	HIS	-	expression tag	UNP P13029
A	408	HIS	-	expression tag	UNP P13029
A	409	HIS	-	expression tag	UNP P13029
A	410	HIS	-	expression tag	UNP P13029
A	411	SER	-	expression tag	UNP P13029
A	412	SER	-	expression tag	UNP P13029
A	413	GLY	-	expression tag	UNP P13029

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Chain	Residue	Modelled	Actual	Comment	Reference
A	414	LEU	-	expression tag	UNP P13029
A	415	VAL	-	expression tag	UNP P13029
A	416	PRO	-	expression tag	UNP P13029
A	417	ARG	-	expression tag	UNP P13029
A	418	GLY	-	expression tag	UNP P13029
A	419	SER	-	expression tag	UNP P13029
A	420	HIS	-	expression tag	UNP P13029
A	421	MET	-	expression tag	UNP P13029
B	401	MET	-	expression tag	UNP P13029
B	402	GLY	-	expression tag	UNP P13029
B	403	SER	-	expression tag	UNP P13029
B	404	SER	-	expression tag	UNP P13029
B	405	HIS	-	expression tag	UNP P13029
B	406	HIS	-	expression tag	UNP P13029
B	407	HIS	-	expression tag	UNP P13029
B	408	HIS	-	expression tag	UNP P13029
B	409	HIS	-	expression tag	UNP P13029
B	410	HIS	-	expression tag	UNP P13029
B	411	SER	-	expression tag	UNP P13029
B	412	SER	-	expression tag	UNP P13029
B	413	GLY	-	expression tag	UNP P13029
B	414	LEU	-	expression tag	UNP P13029
B	415	VAL	-	expression tag	UNP P13029
B	416	PRO	-	expression tag	UNP P13029
B	417	ARG	-	expression tag	UNP P13029
B	418	GLY	-	expression tag	UNP P13029
B	419	SER	-	expression tag	UNP P13029
B	420	HIS	-	expression tag	UNP P13029
B	421	MET	-	expression tag	UNP P13029
C	401	MET	-	expression tag	UNP P13029
C	402	GLY	-	expression tag	UNP P13029
C	403	SER	-	expression tag	UNP P13029
C	404	SER	-	expression tag	UNP P13029
C	405	HIS	-	expression tag	UNP P13029
C	406	HIS	-	expression tag	UNP P13029
C	407	HIS	-	expression tag	UNP P13029
C	408	HIS	-	expression tag	UNP P13029
C	409	HIS	-	expression tag	UNP P13029
C	410	HIS	-	expression tag	UNP P13029
C	411	SER	-	expression tag	UNP P13029
C	412	SER	-	expression tag	UNP P13029
C	413	GLY	-	expression tag	UNP P13029

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Chain	Residue	Modelled	Actual	Comment	Reference
C	414	LEU	-	expression tag	UNP P13029
C	415	VAL	-	expression tag	UNP P13029
C	416	PRO	-	expression tag	UNP P13029
C	417	ARG	-	expression tag	UNP P13029
C	418	GLY	-	expression tag	UNP P13029
C	419	SER	-	expression tag	UNP P13029
C	420	HIS	-	expression tag	UNP P13029
C	421	MET	-	expression tag	UNP P13029
D	401	MET	-	expression tag	UNP P13029
D	402	GLY	-	expression tag	UNP P13029
D	403	SER	-	expression tag	UNP P13029
D	404	SER	-	expression tag	UNP P13029
D	405	HIS	-	expression tag	UNP P13029
D	406	HIS	-	expression tag	UNP P13029
D	407	HIS	-	expression tag	UNP P13029
D	408	HIS	-	expression tag	UNP P13029
D	409	HIS	-	expression tag	UNP P13029
D	410	HIS	-	expression tag	UNP P13029
D	411	SER	-	expression tag	UNP P13029
D	412	SER	-	expression tag	UNP P13029
D	413	GLY	-	expression tag	UNP P13029
D	414	LEU	-	expression tag	UNP P13029
D	415	VAL	-	expression tag	UNP P13029
D	416	PRO	-	expression tag	UNP P13029
D	417	ARG	-	expression tag	UNP P13029
D	418	GLY	-	expression tag	UNP P13029
D	419	SER	-	expression tag	UNP P13029
D	420	HIS	-	expression tag	UNP P13029
D	421	MET	-	expression tag	UNP P13029
E	401	MET	-	expression tag	UNP P13029
E	402	GLY	-	expression tag	UNP P13029
E	403	SER	-	expression tag	UNP P13029
E	404	SER	-	expression tag	UNP P13029
E	405	HIS	-	expression tag	UNP P13029
E	406	HIS	-	expression tag	UNP P13029
E	407	HIS	-	expression tag	UNP P13029
E	408	HIS	-	expression tag	UNP P13029
E	409	HIS	-	expression tag	UNP P13029
E	410	HIS	-	expression tag	UNP P13029
E	411	SER	-	expression tag	UNP P13029
E	412	SER	-	expression tag	UNP P13029
E	413	GLY	-	expression tag	UNP P13029

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Chain	Residue	Modelled	Actual	Comment	Reference
E	414	LEU	-	expression tag	UNP P13029
E	415	VAL	-	expression tag	UNP P13029
E	416	PRO	-	expression tag	UNP P13029
E	417	ARG	-	expression tag	UNP P13029
E	418	GLY	-	expression tag	UNP P13029
E	419	SER	-	expression tag	UNP P13029
E	420	HIS	-	expression tag	UNP P13029
E	421	MET	-	expression tag	UNP P13029
F	401	MET	-	expression tag	UNP P13029
F	402	GLY	-	expression tag	UNP P13029
F	403	SER	-	expression tag	UNP P13029
F	404	SER	-	expression tag	UNP P13029
F	405	HIS	-	expression tag	UNP P13029
F	406	HIS	-	expression tag	UNP P13029
F	407	HIS	-	expression tag	UNP P13029
F	408	HIS	-	expression tag	UNP P13029
F	409	HIS	-	expression tag	UNP P13029
F	410	HIS	-	expression tag	UNP P13029
F	411	SER	-	expression tag	UNP P13029
F	412	SER	-	expression tag	UNP P13029
F	413	GLY	-	expression tag	UNP P13029
F	414	LEU	-	expression tag	UNP P13029
F	415	VAL	-	expression tag	UNP P13029
F	416	PRO	-	expression tag	UNP P13029
F	417	ARG	-	expression tag	UNP P13029
F	418	GLY	-	expression tag	UNP P13029
F	419	SER	-	expression tag	UNP P13029
F	420	HIS	-	expression tag	UNP P13029
F	421	MET	-	expression tag	UNP P13029
G	401	MET	-	expression tag	UNP P13029
G	402	GLY	-	expression tag	UNP P13029
G	403	SER	-	expression tag	UNP P13029
G	404	SER	-	expression tag	UNP P13029
G	405	HIS	-	expression tag	UNP P13029
G	406	HIS	-	expression tag	UNP P13029
G	407	HIS	-	expression tag	UNP P13029
G	408	HIS	-	expression tag	UNP P13029
G	409	HIS	-	expression tag	UNP P13029
G	410	HIS	-	expression tag	UNP P13029
G	411	SER	-	expression tag	UNP P13029
G	412	SER	-	expression tag	UNP P13029
G	413	GLY	-	expression tag	UNP P13029

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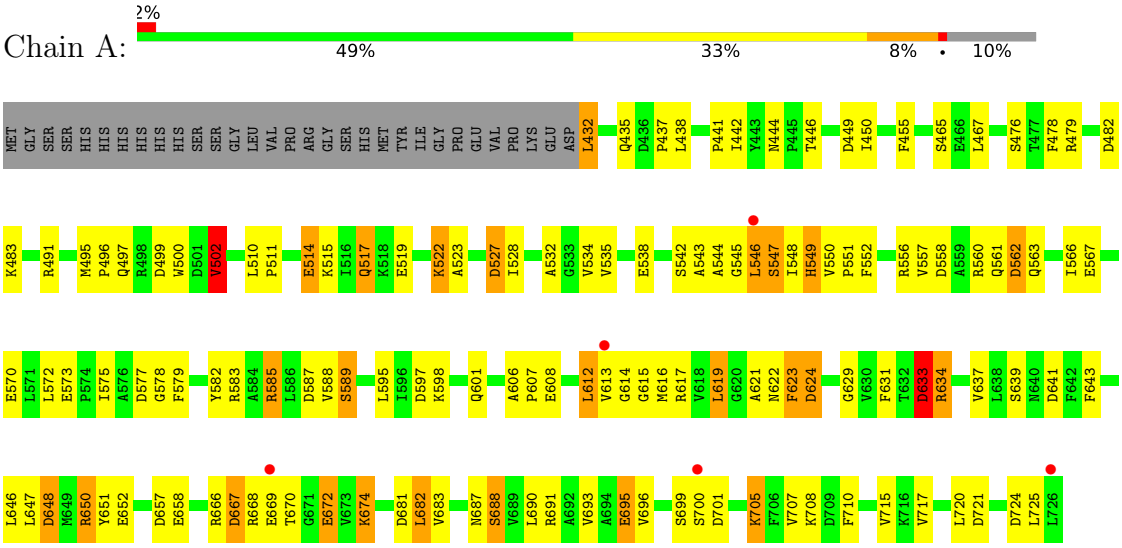
Chain	Residue	Modelled	Actual	Comment	Reference
G	414	LEU	-	expression tag	UNP P13029
G	415	VAL	-	expression tag	UNP P13029
G	416	PRO	-	expression tag	UNP P13029
G	417	ARG	-	expression tag	UNP P13029
G	418	GLY	-	expression tag	UNP P13029
G	419	SER	-	expression tag	UNP P13029
G	420	HIS	-	expression tag	UNP P13029
G	421	MET	-	expression tag	UNP P13029
H	401	MET	-	expression tag	UNP P13029
H	402	GLY	-	expression tag	UNP P13029
H	403	SER	-	expression tag	UNP P13029
H	404	SER	-	expression tag	UNP P13029
H	405	HIS	-	expression tag	UNP P13029
H	406	HIS	-	expression tag	UNP P13029
H	407	HIS	-	expression tag	UNP P13029
H	408	HIS	-	expression tag	UNP P13029
H	409	HIS	-	expression tag	UNP P13029
H	410	HIS	-	expression tag	UNP P13029
H	411	SER	-	expression tag	UNP P13029
H	412	SER	-	expression tag	UNP P13029
H	413	GLY	-	expression tag	UNP P13029
H	414	LEU	-	expression tag	UNP P13029
H	415	VAL	-	expression tag	UNP P13029
H	416	PRO	-	expression tag	UNP P13029
H	417	ARG	-	expression tag	UNP P13029
H	418	GLY	-	expression tag	UNP P13029
H	419	SER	-	expression tag	UNP P13029
H	420	HIS	-	expression tag	UNP P13029
H	421	MET	-	expression tag	UNP P13029

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.

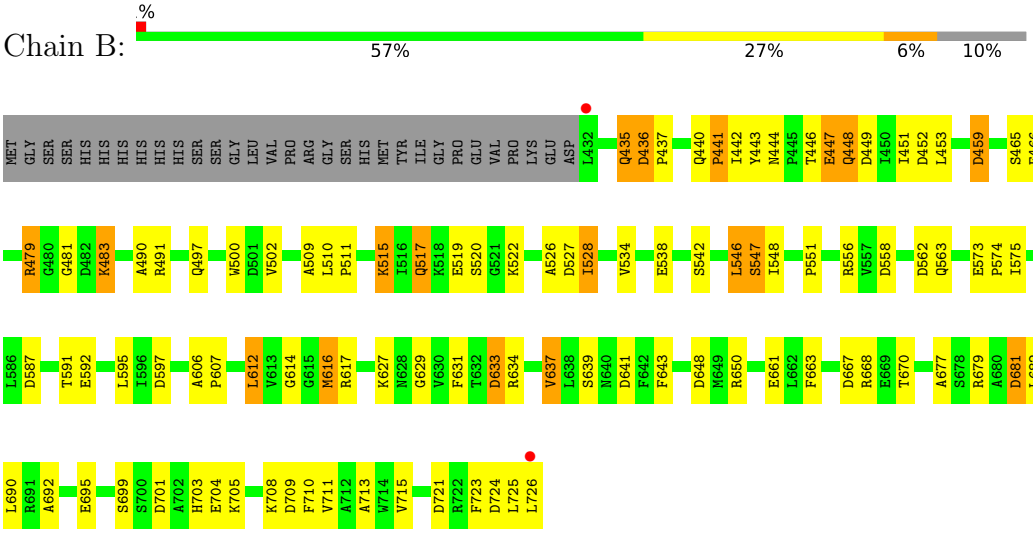
• Molecule 1: Peroxidase/catalase HPI

Chain A:



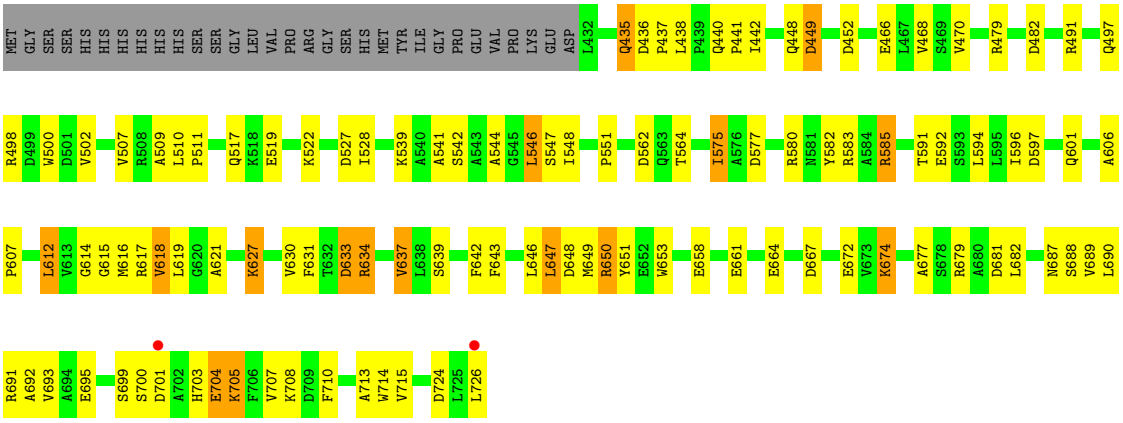
• Molecule 1: Peroxidase/catalase HPI

Chain B:



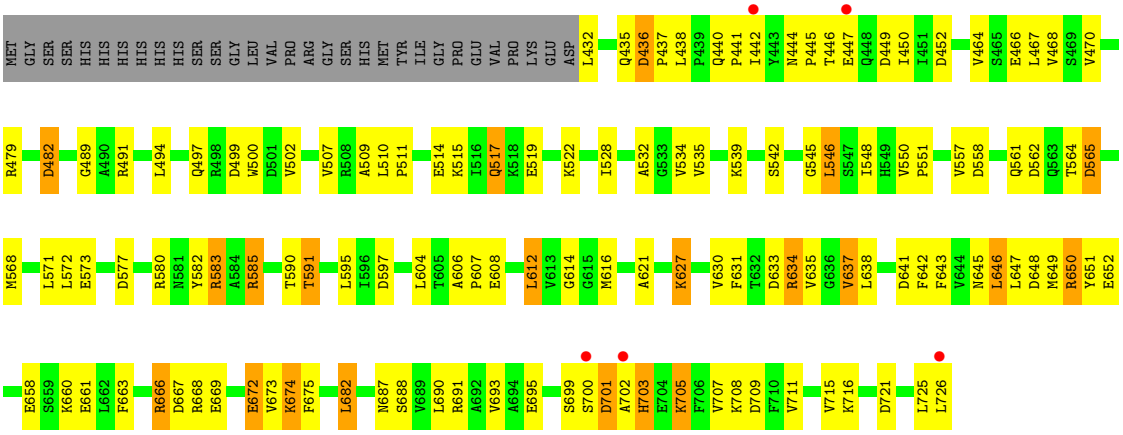
• Molecule 1: Peroxidase/catalase HPI

Chain C:



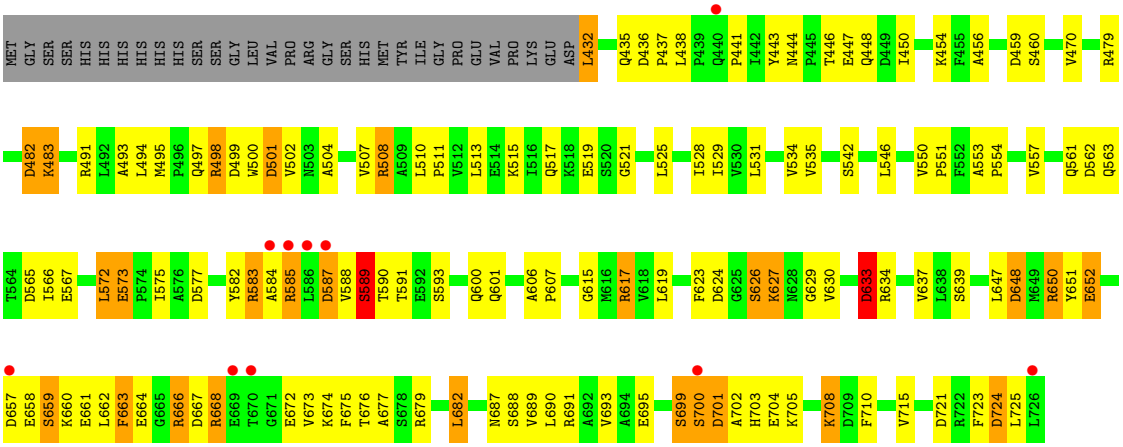
• Molecule 1: Peroxidase/catalase HPI

Chain D:

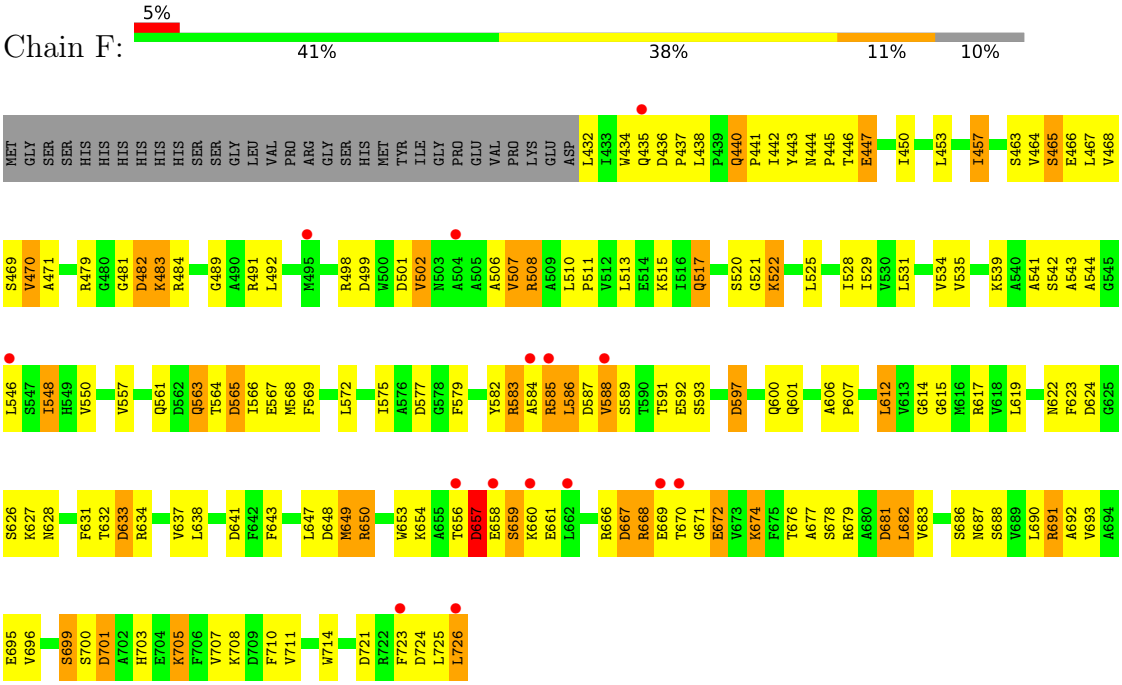


• Molecule 1: Peroxidase/catalase HPI

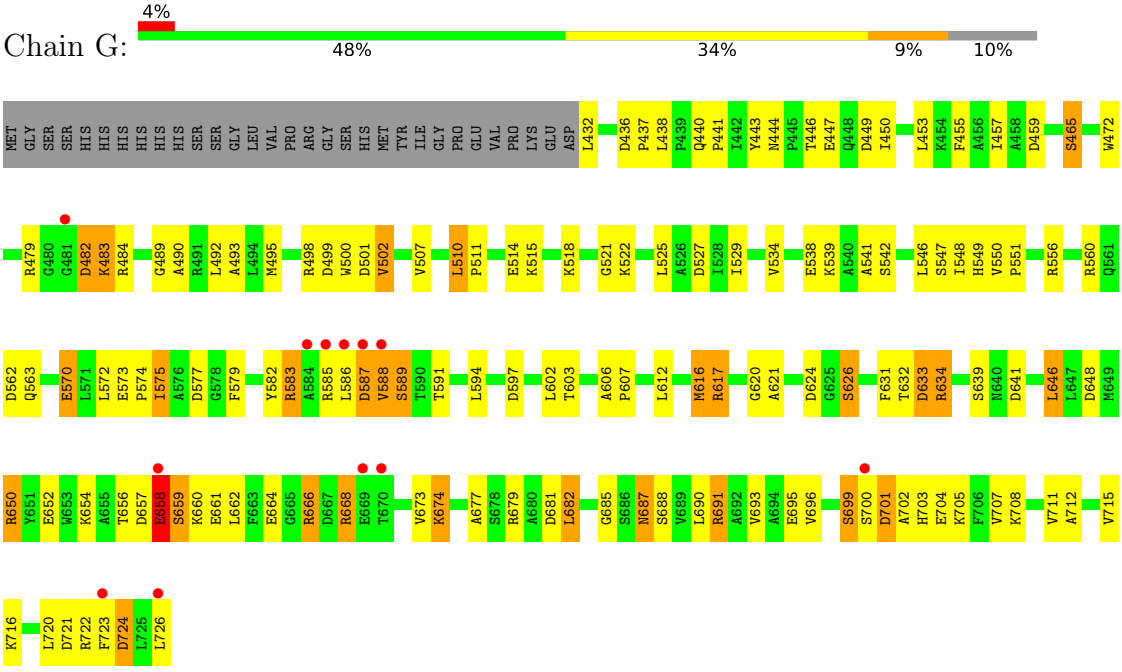
Chain E:



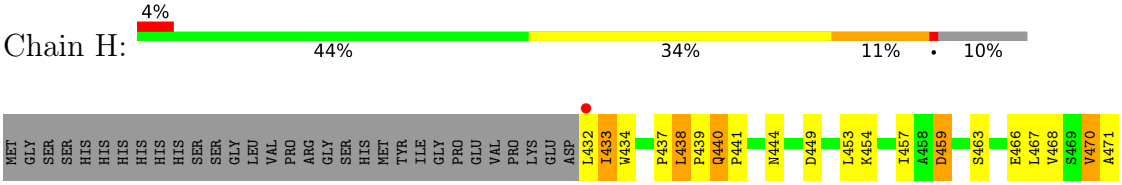
• Molecule 1: Peroxidase/catalase HPI

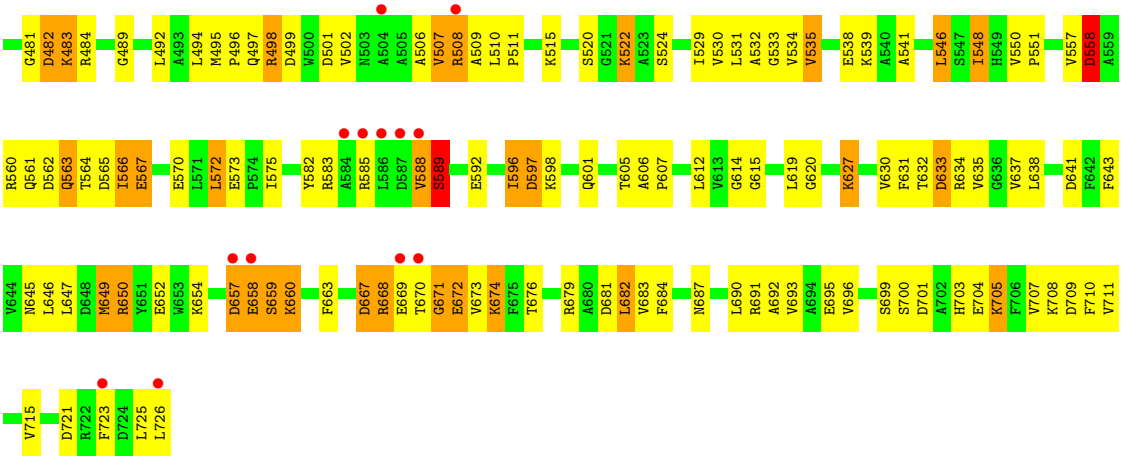


• Molecule 1: Peroxidase/catalase HPI



• Molecule 1: Peroxidase/catalase HPI




G481 D482 K483 R484 G489 L492 A493 L494 M495 P496 Q497 R498 D499 W500 D501 V502 N503 A504 A505 A506 V507 R508 A509 L510 P511 K515 S520 G521 K522 A523 S524 I529 V530 L531 A532 G533 V534 V535 E538 K539 A540 A541 L546 S547 I548 H549 V550 P551 V557 D558 A559
R560 Q561 D562 Q563 T564 D565 I566 E567 E570 L571 L572 E573 P574 I575 Y582 R583 A584 R585 L586 D587 V588 S589 E592 I596 D597 K598 Q601 T605 A606 P607 L612 V613 G614 G615 L619 G620 K627 V630 F631 T632 D633 R634 V635 G636 V637 L638 D641 F642 F643
V644 M645 L646 L647 D648 M649 R650 Y651 E652 W653 K654 D657 E658 S659 K660 F663 D667 R668 E669 T670 G671 E672 V673 K674 F675 T676 R679 A680 D681 L682 V683 F684 N687 L690 R691 A692 V693 A694 E695 V696 S699 S700 D701 A702 H703 E704 K705 F706 V707 K708 D709 F710 V711
V715 D721 R722 F723 D724 L725 L726

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.21Å 98.70Å 302.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.30 19.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-2.30) 91.4 (19.90-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.10 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.233 , 0.327 0.252 , 0.322	Depositor DCC
R_{free} test set	10340 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18136	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5185e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.60	0/2307	0.90	15/3127 (0.5%)
1	B	0.60	0/2307	0.86	10/3127 (0.3%)
1	C	0.63	0/2307	0.87	8/3127 (0.3%)
1	D	0.59	0/2307	0.89	15/3127 (0.5%)
1	E	0.59	0/2307	0.88	14/3127 (0.4%)
1	F	0.53	0/2307	0.84	12/3127 (0.4%)
1	G	0.55	0/2307	0.85	11/3127 (0.4%)
1	H	0.56	0/2307	0.82	11/3127 (0.4%)
All	All	0.58	0/18456	0.86	96/25016 (0.4%)

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	1
1	B	0	1
1	F	0	2
1	G	0	1
1	H	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	482	ASP	CB-CG-OD2	7.75	125.28	118.30
1	C	577	ASP	CB-CG-OD2	7.65	125.18	118.30
1	D	558	ASP	CB-CG-OD2	7.59	125.13	118.30
1	D	577	ASP	CB-CG-OD2	7.59	125.13	118.30
1	D	721	ASP	CB-CG-OD2	7.54	125.09	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PHE	Peptide
1	B	724	ASP	Peptide
1	F	443	TYR	Peptide
1	F	724	ASP	Peptide
1	G	574	PRO	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	2267	0	2255	124	0
1	B	2267	0	2255	91	0
1	C	2267	0	2255	122	0
1	D	2267	0	2255	125	1
1	E	2267	0	2255	148	0
1	F	2267	0	2255	176	0
1	G	2267	0	2255	161	0
1	H	2267	0	2255	154	1
All	All	18136	0	18040	1075	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 30.

The worst 5 of 1075 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:E:437:PRO:C	1:E:438:LEU:HD22	1.22	1.43
1:E:502:VAL:CG2	1:E:582:TYR:CE2	2.09	1.34
1:E:502:VAL:HG22	1:E:582:TYR:CE2	1.67	1.28
1:F:624:ASP:OD2	1:F:626:SER:HB2	1.26	1.28
1:H:502:VAL:CG2	1:H:582:TYR:CE2	2.18	1.26

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:D:590:THR:OG1	1:H:567:GLU:OE2[3_755]	2.08	0.12

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	293/326 (90%)	276 (94%)	15 (5%)	2 (1%)	22 26
1	B	293/326 (90%)	269 (92%)	23 (8%)	1 (0%)	41 50
1	C	293/326 (90%)	277 (94%)	16 (6%)	0	100 100
1	D	293/326 (90%)	274 (94%)	18 (6%)	1 (0%)	41 50
1	E	293/326 (90%)	271 (92%)	19 (6%)	3 (1%)	15 17
1	F	293/326 (90%)	260 (89%)	23 (8%)	10 (3%)	3 2
1	G	293/326 (90%)	267 (91%)	21 (7%)	5 (2%)	9 8
1	H	293/326 (90%)	271 (92%)	19 (6%)	3 (1%)	15 17
All	All	2344/2608 (90%)	2165 (92%)	154 (7%)	25 (1%)	14 15

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	700	SER
1	E	589	SER
1	F	586	LEU
1	F	671	GLY
1	F	705	LYS

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	238/265 (90%)	201 (84%)	37 (16%)	2	2
1	B	238/265 (90%)	207 (87%)	31 (13%)	4	4
1	C	238/265 (90%)	211 (89%)	27 (11%)	6	6
1	D	238/265 (90%)	207 (87%)	31 (13%)	4	4
1	E	238/265 (90%)	204 (86%)	34 (14%)	3	3
1	F	238/265 (90%)	195 (82%)	43 (18%)	1	1
1	G	238/265 (90%)	204 (86%)	34 (14%)	3	3
1	H	238/265 (90%)	193 (81%)	45 (19%)	1	1
All	All	1904/2120 (90%)	1622 (85%)	282 (15%)	3	3

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	691	ARG
1	H	433	ILE
1	H	572	LEU
1	D	442	ILE
1	C	726	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	687	ASN
1	H	687	ASN
1	E	687	ASN
1	G	600	GLN
1	E	444	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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	295/326 (90%)	-0.08	5 (1%)	70	76	9, 22, 41, 64	0
1	B	295/326 (90%)	-0.10	2 (0%)	87	91	12, 21, 41, 70	0
1	C	295/326 (90%)	-0.18	2 (0%)	87	91	7, 19, 39, 55	0
1	D	295/326 (90%)	-0.15	5 (1%)	70	76	9, 20, 41, 51	0
1	E	295/326 (90%)	0.04	10 (3%)	45	52	7, 23, 49, 73	0
1	F	295/326 (90%)	0.19	15 (5%)	28	35	12, 30, 56, 76	0
1	G	295/326 (90%)	0.12	12 (4%)	37	44	10, 25, 51, 81	0
1	H	295/326 (90%)	0.13	14 (4%)	31	38	10, 27, 54, 71	0
All	All	2360/2608 (90%)	-0.00	65 (2%)	53	60	7, 23, 47, 81	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	726	LEU	7.9
1	F	726	LEU	7.7
1	H	585	ARG	5.7
1	F	584	ALA	5.6
1	E	726	LEU	5.5

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 monosaccharides 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.