



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 06:41 AM EDT

PDB ID : 2GER / pdb_00002ger
Title : Crystal Structure and Oxidative Mechanism of Human Pyrroline-5-carboxylate Reductase
Authors : Meng, Z.; Lou, Z.; Liu, Z.; Rao, Z.
Deposited on : 2006-03-20
Resolution : 3.10 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 ⓘ 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
Xtrriage (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

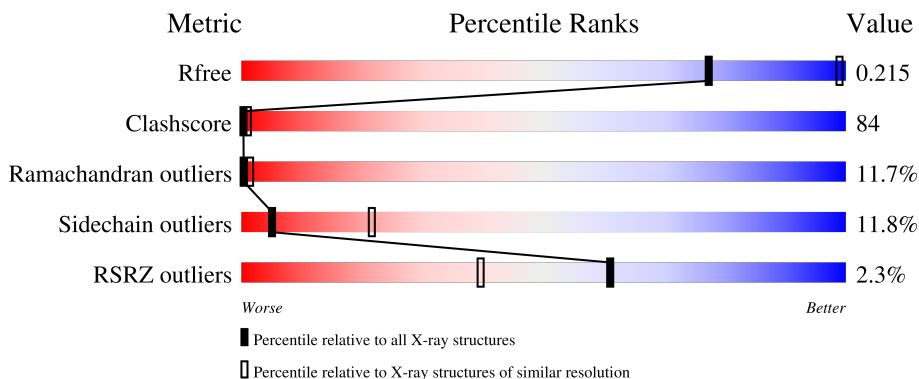
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	321	
1	B	321	
1	C	321	
1	D	321	
1	E	321	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10768 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 Pyrroline-5-carboxylate reductase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2038	1279	363	383	13	0	0	0
1	B	276	2025	1271	359	382	13	0	0	0
1	C	277	2032	1276	360	383	13	0	0	0
1	D	277	2038	1279	363	383	13	0	0	0
1	E	277	2038	1279	363	383	13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	cloning artifact	UNP P32322
A	0	ALA	-	cloning artifact	UNP P32322
B	-1	ARG	-	cloning artifact	UNP P32322
B	0	ALA	-	cloning artifact	UNP P32322
C	-1	ARG	-	cloning artifact	UNP P32322
C	0	ALA	-	cloning artifact	UNP P32322
D	-1	ARG	-	cloning artifact	UNP P32322
D	0	ALA	-	cloning artifact	UNP P32322
E	-1	ARG	-	cloning artifact	UNP P32322
E	0	ALA	-	cloning artifact	UNP P32322

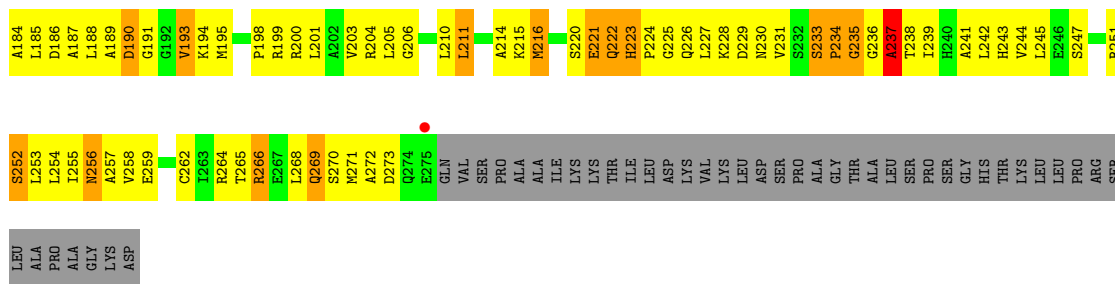
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	118	Total	O	0	0
			118	118		

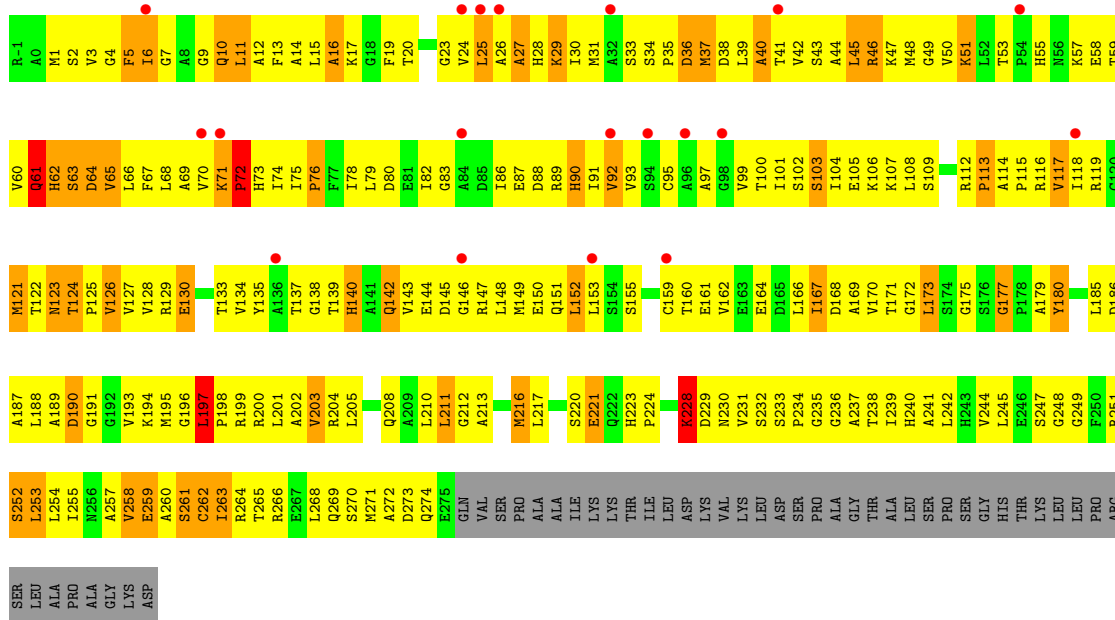
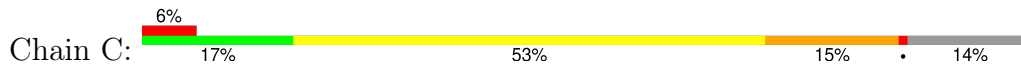
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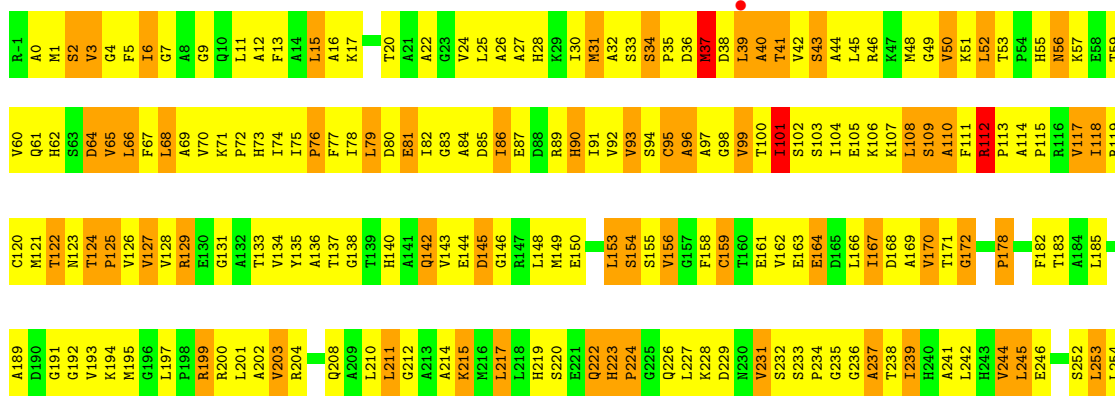
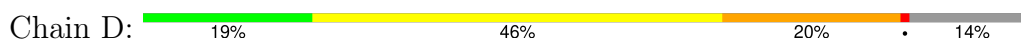
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	119	Total 119	O 119	0	0
2	D	126	Total 126	O 126	0	0
2	E	128	Total 128	O 128	0	0

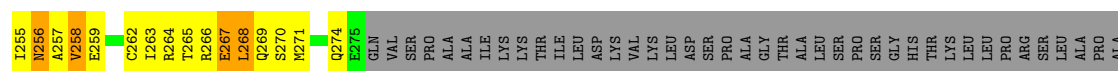


● Molecule 1: Pyrroline-5-carboxylate reductase 1



● Molecule 1: Pyrroline-5-carboxylate reductase 1

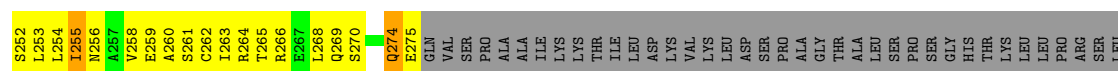
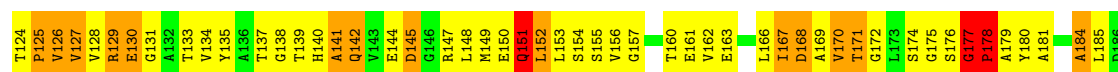
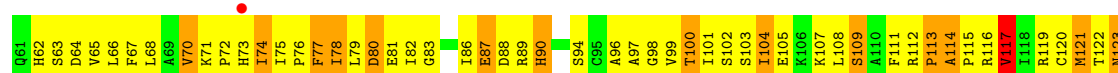
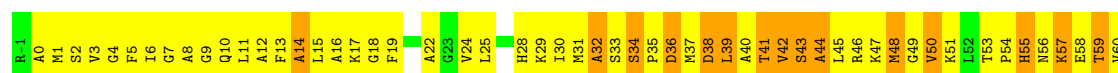




GLY
LYS
ASP

• Molecule 1: Pyrroline-5-carboxylate reductase 1

Chain E: 17% 50% 18% 14%



ALA
PRO
ALA
GLY
LYS
ASP

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.61Å 123.81Å 120.79Å 90.00° 121.76° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 50.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 98.6 (50.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.11Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.261 0.221 , 0.215	Depositor DCC
R_{free} test set	2346 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtrriage
Anisotropy	0.391	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 126.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.028 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.036 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.88	0/2069	1.32	34/2800 (1.2%)
1	B	0.77	0/2055	1.24	20/2781 (0.7%)
1	C	0.82	0/2063	1.31	28/2793 (1.0%)
1	D	0.91	1/2069 (0.0%)	1.32	25/2800 (0.9%)
1	E	0.84	0/2069	1.34	28/2800 (1.0%)
All	All	0.84	1/10325 (0.0%)	1.31	135/13974 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	6	ILE	CA-CB	-5.47	1.47	1.54

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	39	LEU	N-CA-C	-13.02	97.39	113.28
1	D	101	ILE	N-CA-C	-10.67	100.47	110.82
1	B	193	VAL	N-CA-C	-10.47	100.14	110.72
1	B	1	MET	N-CA-C	9.35	119.24	108.49
1	A	0	ALA	N-CA-C	-9.31	101.85	113.02

There are no chirality outliers.

There are no planarity outliers.

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	2038	0	2082	339	0
1	B	2025	0	2063	376	0
1	C	2032	0	2071	375	0
1	D	2038	0	2082	318	0
1	E	2038	0	2082	336	0
2	A	106	0	0	48	0
2	B	118	0	0	53	0
2	C	119	0	0	55	0
2	D	126	0	0	49	0
2	E	128	0	0	63	0
All	All	10768	0	10380	1726	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 84.

The worst 5 of 1726 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:D:239:ILE:HD12	1:D:239:ILE:H	1.08	1.16
1:C:75:ILE:HD12	1:C:99:VAL:HG21	1.27	1.16
1:B:75:ILE:HB	1:B:76:PRO:HD3	1.22	1.14
1:E:101:ILE:HD11	1:E:138:GLY:HA2	1.28	1.14
1:C:86:ILE:HD11	1:C:108:LEU:HD22	1.34	1.09

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	275/321 (86%)	182 (66%)	60 (22%)	33 (12%)	0 1
1	B	272/321 (85%)	168 (62%)	68 (25%)	36 (13%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	275/321 (86%)	183 (66%)	60 (22%)	32 (12%)	0	1
1	D	275/321 (86%)	183 (66%)	68 (25%)	24 (9%)	0	4
1	E	275/321 (86%)	183 (66%)	57 (21%)	35 (13%)	0	1
All	All	1372/1605 (86%)	899 (66%)	313 (23%)	160 (12%)	0	1

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	10	GLN
1	A	11	LEU
1	A	36	ASP
1	A	37	MET

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	215/250 (86%)	177 (82%)	38 (18%)	2	9
1	B	213/250 (85%)	196 (92%)	17 (8%)	11	37
1	C	214/250 (86%)	196 (92%)	18 (8%)	10	35
1	D	215/250 (86%)	181 (84%)	34 (16%)	2	12
1	E	215/250 (86%)	195 (91%)	20 (9%)	8	31
All	All	1072/1250 (86%)	945 (88%)	127 (12%)	5	21

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
1	E	77	PHE
1	C	247	SER
1	E	70	VAL
1	E	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	240	HIS
1	D	28	HIS
1	E	274	GLN
1	C	269	GLN
1	D	140	HIS

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 oligosaccharides 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 [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, 95th 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	277/321 (86%)	-0.16	1 (0%) 88 76	27, 79, 115, 154	0
1	B	276/321 (85%)	0.23	10 (3%) 46 26	26, 120, 172, 187	0
1	C	277/321 (86%)	0.28	19 (6%) 23 12	23, 117, 169, 183	0
1	D	277/321 (86%)	-0.23	1 (0%) 88 76	24, 70, 117, 163	0
1	E	277/321 (86%)	-0.19	1 (0%) 88 76	23, 78, 126, 156	0
All	All	1384/1605 (86%)	-0.01	32 (2%) 61 39	23, 82, 160, 187	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	ALA	3.9
1	B	136	ALA	3.6
1	B	75	ILE	3.6
1	B	92	VAL	3.5
1	E	73	HIS	2.8

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.