



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:08 AM UTC

PDB ID : 1GRO / pdb_00001gro
Title : REGULATORY AND CATALYTIC MECHANISMS IN ESCHERICHIA COLI ISOCITRATE DEHYDROGENASE: MULTIPLE ROLES FOR N115
Authors : Grobler, J.A.; Hurley, J.H.
Deposited on : 1995-10-12
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

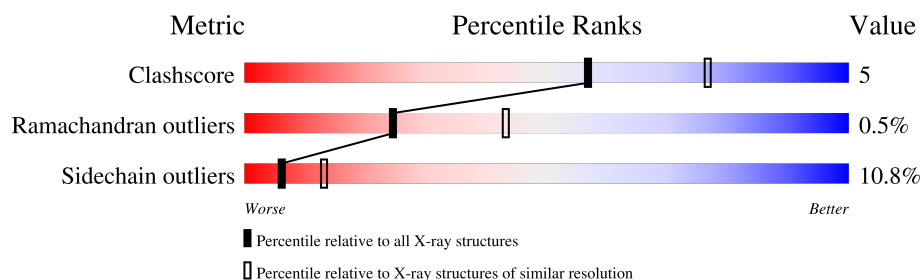
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	73% 20% 6% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3167 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3153	2013	530	592	18			

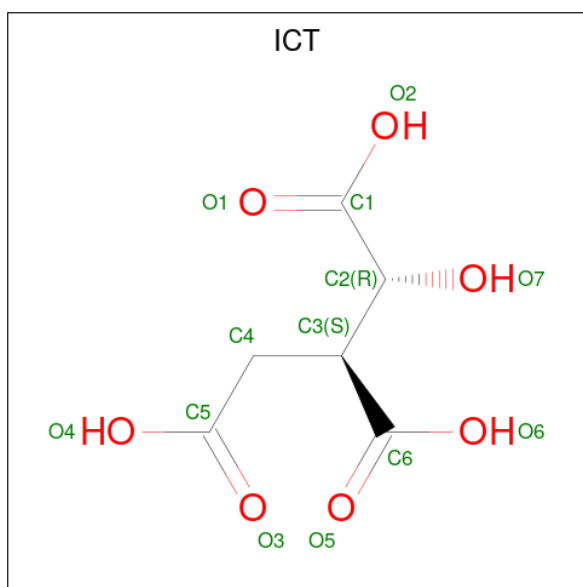
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLU	SER	engineered mutation	UNP P08200
A	115	LEU	ASN	engineered mutation	UNP P08200
A	192	ASP	GLU	conflict	UNP P08200

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

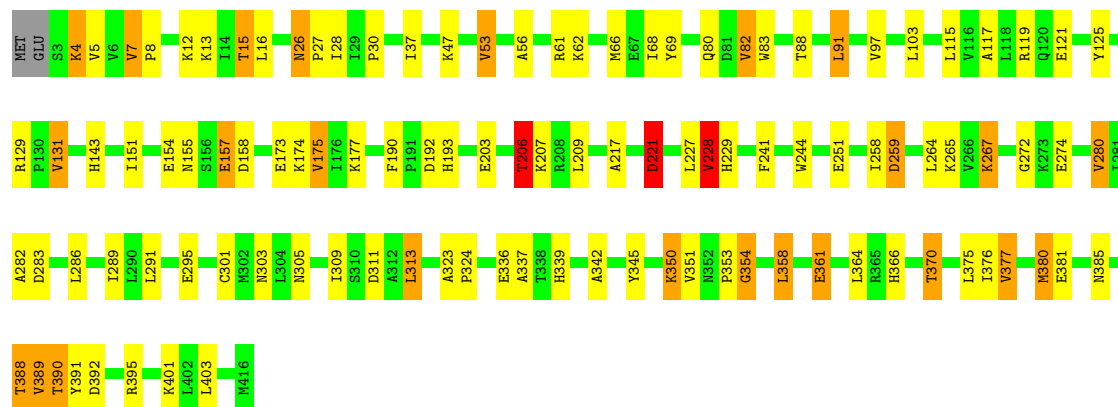
- Molecule 3 is ISOCITRIC ACID (CCD ID: ICT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

Note EDS was not executed.

Chain A: 73% 20% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 105.10Å 150.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3167	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: MG, ICT

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	0.93	14/3214 (0.4%)	1.66	54/4355 (1.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	HIS	CD2-NE2	-7.35	1.29	1.37
1	A	377	VAL	CA-CB	7.09	1.64	1.54
1	A	175	VAL	CA-CB	6.85	1.63	1.54
1	A	229	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	143	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	206	THR	CA-CB	6.20	1.63	1.53
1	A	82	VAL	CA-CB	6.03	1.60	1.53
1	A	193	HIS	CG-ND1	-5.92	1.31	1.38
1	A	131	VAL	CA-CB	5.85	1.61	1.54
1	A	366	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	339	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	280	VAL	CA-CB	5.33	1.62	1.54
1	A	228	VAL	CA-CB	5.33	1.61	1.54
1	A	53	VAL	CA-CB	5.02	1.60	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	8.99	121.59	112.60
1	A	258	ILE	N-CA-C	-8.08	95.78	107.98
1	A	283	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	388	THR	CA-CB-OG1	-7.93	97.71	109.60
1	A	15	THR	CA-CB-OG1	-7.79	97.92	109.60
1	A	389	VAL	N-CA-CB	-7.69	98.13	112.36
1	A	303	ASN	N-CA-C	7.44	119.08	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	GLU	N-CA-C	7.07	118.98	111.28
1	A	282	ALA	N-CA-C	6.96	118.87	111.28
1	A	391	TYR	N-CA-C	6.93	119.71	111.33
1	A	336	GLU	N-CA-C	6.87	119.61	108.76
1	A	361	GLU	CA-CB-CG	6.78	127.66	114.10
1	A	244	TRP	CG-CD2-CE3	6.72	140.62	133.90
1	A	390	THR	N-CA-CB	-6.34	101.38	110.44
1	A	15	THR	CA-CB-CG2	6.19	121.02	110.50
1	A	7	VAL	CA-C-N	6.16	126.48	119.83
1	A	7	VAL	C-N-CA	6.16	126.48	119.83
1	A	342	ALA	CA-C-N	6.15	126.04	119.28
1	A	342	ALA	C-N-CA	6.15	126.04	119.28
1	A	26	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	388	THR	N-CA-CB	-6.02	99.36	110.56
1	A	389	VAL	N-CA-C	5.91	118.70	108.90
1	A	193	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	388	THR	CA-CB-CG2	5.84	120.44	110.50
1	A	125	TYR	N-CA-C	5.82	120.22	113.18
1	A	376	ILE	CA-C-O	-5.77	115.05	121.17
1	A	47	LYS	CA-C-O	-5.74	114.78	120.70
1	A	366	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	A	354	GLY	N-CA-C	5.69	119.77	112.83
1	A	395	ARG	CA-CB-CG	5.65	125.40	114.10
1	A	370	THR	N-CA-CB	-5.65	101.82	110.12
1	A	388	THR	CB-CA-C	5.60	120.93	111.41
1	A	395	ARG	CB-CA-C	-5.60	101.17	110.68
1	A	353	PRO	CA-C-N	5.55	126.25	120.03
1	A	353	PRO	C-N-CA	5.55	126.25	120.03
1	A	26	ASN	CB-CG-ND2	5.41	124.51	116.40
1	A	174	LYS	CA-C-O	-5.35	115.19	120.70
1	A	4	LYS	CA-CB-CG	-5.34	103.42	114.10
1	A	69	TYR	N-CA-C	5.30	117.71	108.76
1	A	339	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	A	192	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	259	ASP	N-CA-C	5.25	121.98	110.80
1	A	244	TRP	CB-CG-CD1	-5.24	119.03	126.90
1	A	143	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	155	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	337	ALA	N-CA-C	-5.20	102.16	109.96
1	A	190	PHE	CA-C-N	5.19	124.86	119.56
1	A	190	PHE	C-N-CA	5.19	124.86	119.56
1	A	56	ALA	N-CA-C	5.17	117.00	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	MET	CG-SD-CE	-5.15	89.57	100.90
1	A	13	LYS	CB-CA-C	-5.06	101.00	109.65
1	A	83	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	A	323	ALA	CA-C-N	5.03	125.24	120.31
1	A	323	ALA	C-N-CA	5.03	125.24	120.31

There are no chirality outliers.

There are no planarity outliers.

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	3153	0	3150	29	0
2	A	1	0	0	0	0
3	A	13	0	5	0	0
All	All	3167	0	3155	29	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 5.

All (29) 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:206:THR:HB	1:A:241:PHE:CD1	2.25	0.71
1:A:305:ASN:O	1:A:309:ILE:HG12	1.97	0.65
1:A:345:TYR:CD1	1:A:350:LYS:HD2	2.38	0.58
1:A:26:ASN:HA	1:A:62:LYS:O	2.05	0.56
1:A:117:ALA:O	1:A:121:GLU:HB2	2.06	0.56
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.90	0.54
1:A:354:GLY:HA2	1:A:380:MET:HE1	1.90	0.53
1:A:68:ILE:HD12	1:A:88:THR:HG23	1.92	0.52
1:A:267:LYS:HE2	1:A:272:GLY:HA2	1.93	0.49
1:A:401:LYS:HE3	1:A:403:LEU:HD11	1.95	0.48
1:A:30:PRO:HA	1:A:66:MET:O	2.13	0.48
1:A:309:ILE:O	1:A:313:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.84	0.45
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.98	0.45
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.98	0.45
1:A:8:PRO:HD2	1:A:28:ILE:HD13	1.99	0.44
1:A:129:ARG:HB2	1:A:151:ILE:HB	1.99	0.44
1:A:228:VAL:HG22	1:A:301:CYS:HB3	2.00	0.44
1:A:157:GLU:HB2	1:A:158:ASP:H	1.64	0.43
1:A:12:LYS:O	1:A:27:PRO:HA	2.19	0.43
1:A:390:THR:HG23	1:A:392:ASP:OD1	2.18	0.43
1:A:115:LEU:HD21	1:A:119:ARG:NH2	2.34	0.43
1:A:115:LEU:O	1:A:119:ARG:HG3	2.18	0.42
1:A:289:ILE:HD12	1:A:313:LEU:HD13	2.00	0.42
1:A:381:GLU:O	1:A:385:ASN:HB2	2.19	0.42
1:A:203:GLU:O	1:A:207:LYS:HG2	2.20	0.41
1:A:217:ALA:O	1:A:221:ASP:HA	2.20	0.41
1:A:265:LYS:HG2	1:A:274:GLU:HB3	2.02	0.41
1:A:5:VAL:HG21	1:A:91:LEU:HD21	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	412/416 (99%)	397 (96%)	13 (3%)	2 (0%)	24	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP
1	A	259	ASP

5.3.2 Protein sidechains ⓘ

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	324/338 (96%)	289 (89%)	35 (11%)	6 13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	15	THR
1	A	16	LEU
1	A	53	VAL
1	A	61	ARG
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	97	VAL
1	A	103	LEU
1	A	131	VAL
1	A	157	GLU
1	A	173	GLU
1	A	175	VAL
1	A	177	LYS
1	A	206	THR
1	A	227	LEU
1	A	228	VAL
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	286	LEU
1	A	291	LEU
1	A	295	GLU
1	A	311	ASP
1	A	313	LEU
1	A	350	LYS
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU

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Mol	Chain	Res	Type
1	A	370	THR
1	A	375	LEU
1	A	377	VAL
1	A	388	THR
1	A	389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	A	348	GLN

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	ICT	A	418	2	12,12,12	1.36	3 (25%)	13,16,16	1.56	2 (15%)

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
3	ICT	A	418	2	-	1/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	ICT	O2-C1	-2.39	1.23	1.30
3	A	418	ICT	O6-C6	-2.24	1.23	1.30
3	A	418	ICT	O4-C5	-2.13	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	418	ICT	O2-C1-C2	2.79	121.05	113.31
3	A	418	ICT	C4-C3-C6	-2.24	107.69	111.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	418	ICT	C6-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.