Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 03:38 PM EDT

PDB ID	:	1GRO
Title	:	REGULATORY AND CATALYTIC MECHANISMS IN ESCHERICHIA COLI ISOCITRATE DEHYDROGENASE: MULTIPLE ROLES FOR N115
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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 (i) symbol.

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

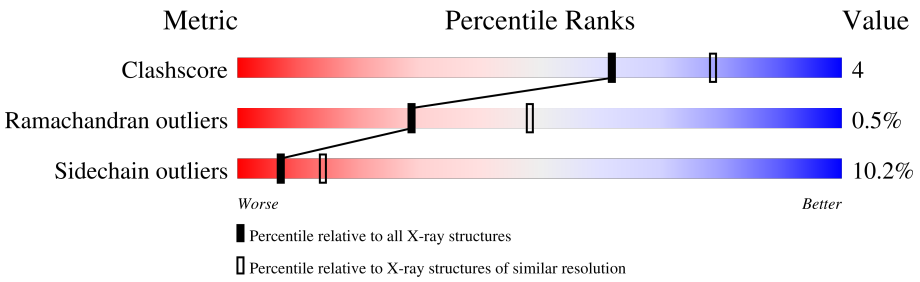
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	78% 18% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	414	3153	2013	530	592	18	0	0	0

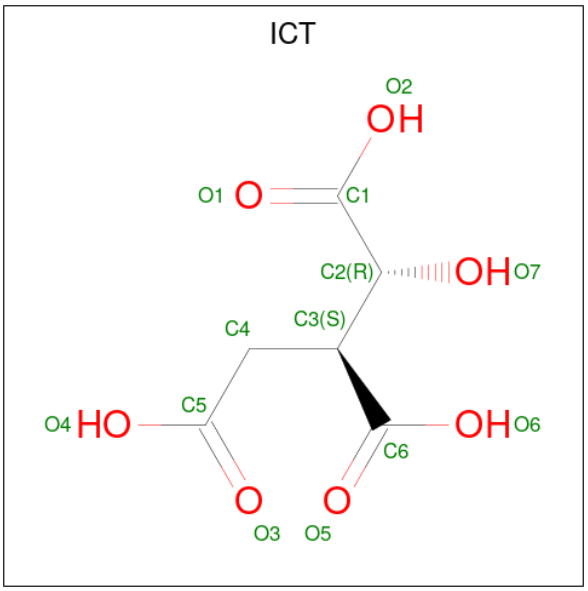
There are 3 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ISOCITRIC ACID (three-letter code: ICT) (formula: $C_6H_8O_7$).



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

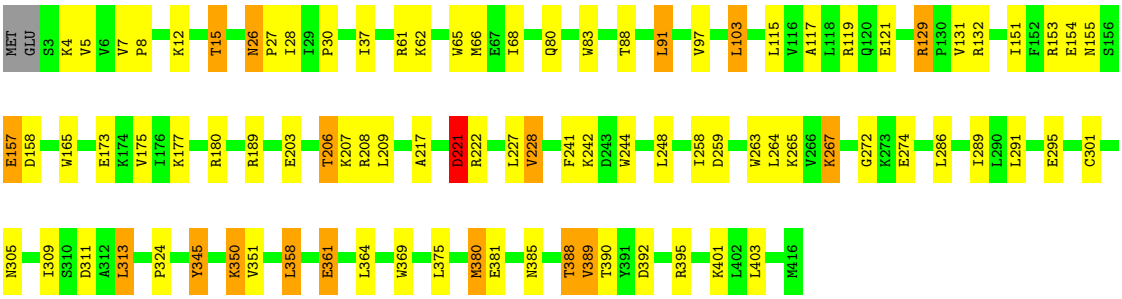
3 Residue-property plots (i)

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. 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. 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: ISOCITRATE DEHYDROGENASE

Chain A: 78% 18% •



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ICT, MG

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	0.74	0/3214	1.38	41/4355 (0.9%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	TRP	CD1-CG-CD2	8.96	113.46	106.30
1	A	165	TRP	CD1-CG-CD2	8.78	113.33	106.30
1	A	153	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	129	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	A	369	TRP	CD1-CG-CD2	7.97	112.67	106.30
1	A	83	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	A	244	TRP	CG-CD2-CE3	7.47	140.62	133.90
1	A	165	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	132	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	244	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	244	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	263	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	A	263	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	A	65	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	65	TRP	CD1-CG-CD2	6.71	111.67	106.30
1	A	380	MET	CG-SD-CE	-6.64	89.57	100.20
1	A	132	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	361	GLU	CA-CB-CG	6.48	127.66	113.40
1	A	369	TRP	CE2-CD2-CG	-6.42	102.16	107.30
1	A	15	THR	CA-CB-CG2	6.16	121.02	112.40
1	A	244	TRP	CB-CG-CD1	-6.13	119.03	127.00
1	A	61	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	208	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	389	VAL	N-CA-CB	-6.08	98.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	A	345	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	388	THR	N-CA-CB	-5.76	99.36	110.30
1	A	388	THR	CA-CB-CG2	5.74	120.44	112.40
1	A	189	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	180	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	258	ILE	N-CA-C	-5.64	95.78	111.00
1	A	165	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	395	ARG	CA-CB-CG	5.45	125.40	113.40
1	A	395	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	388	THR	CA-CB-OG1	-5.38	97.71	109.00
1	A	222	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	222	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	221	ASP	CA-C-N	-5.31	105.52	117.20
1	A	15	THR	CA-CB-OG1	-5.28	97.92	109.00
1	A	103	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	83	TRP	CG-CD2-CE3	5.26	138.63	133.90

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	3153	0	3150	28	0
2	A	1	0	0	0	0
3	A	13	0	5	0	0
All	All	3167	0	3155	28	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 4.

All (28) 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: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
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 (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	412/416 (99%)	397 (96%)	13 (3%)	2 (0%)	29 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP
1	A	259	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	324/338 (96%)	291 (90%)	33 (10%)	7 14

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	15	THR
1	A	26	ASN
1	A	80	GLN
1	A	91	LEU
1	A	97	VAL
1	A	103	LEU
1	A	131	VAL
1	A	155	ASN
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	242	LYS
1	A	248	LEU
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	267	LYS
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
1	A	375	LEU
1	A	380	MET
1	A	388	THR
1	A	389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	2,12,12	0.25	0	5,16,16	2.20	2 (40%)

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	-	1/6/16/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	418	ICT	C4-C3-C6	-3.70	107.69	112.70
3	A	418	ICT	C4-C3-C2	2.90	118.42	110.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	418	ICT	C2-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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.