



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:12 PM UTC

PDB ID : 3LRB / pdb_00003lrb
Title : Structure of E. coli AdiC
Authors : Gao, X.; Lu, F.; Zhou, L.; Shi, Y.
Deposited on : 2010-02-10
Resolution : 3.61 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
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

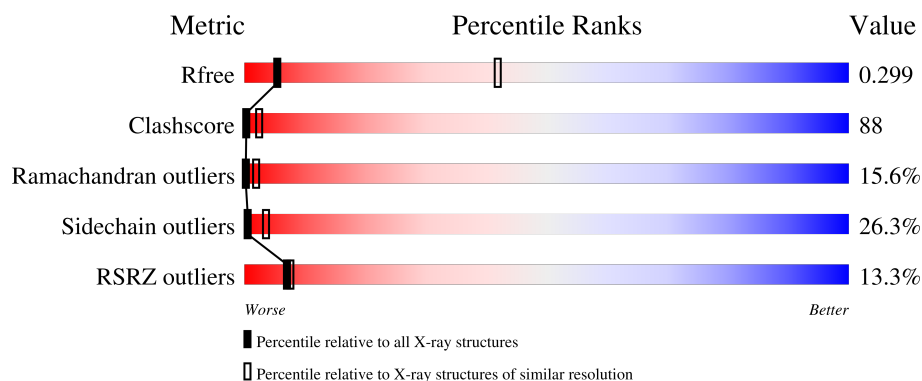
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	445	12% 16% 50% 22% 8%
1	B	445	13% 16% 49% 23% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6072 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.

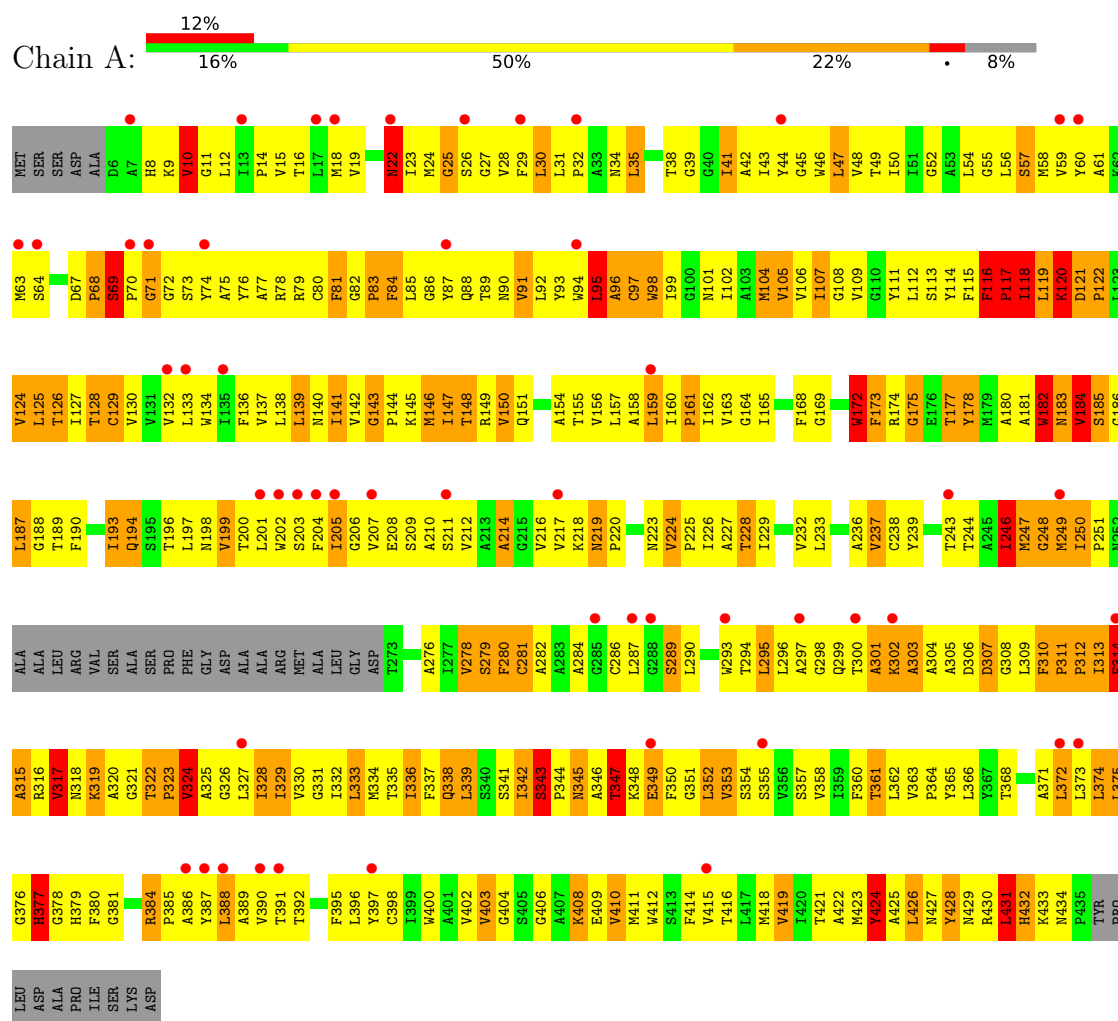
- Molecule 1 is a protein called Arginine/agmatine antiporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			
1	B	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			

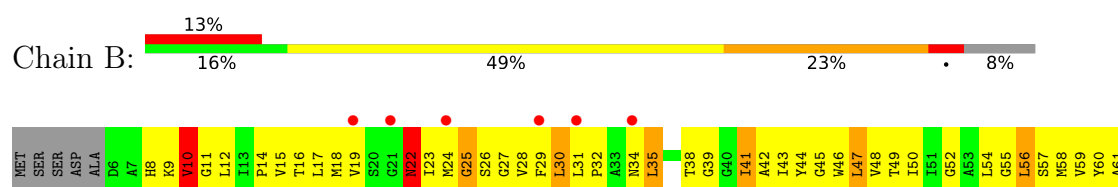
3 Residue-property plots

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: Arginine/agmatine antiporter



• Molecule 1: Arginine/agmatine antiporter



L431	H432	K433	N434	P435	TYR	PRO	LEU	ASP	R384	P385	A386	Y387	L388	A389	V390	T391	T392	F395	L396	Y397	C398	I399	W400	A401	V402	G403	G404	G405	G406	A407	K408	E409	V410	M411	W412	S413	F414	V415	T416	M418	V419	I420	T421	A422	M423	Y424	A425	L426	M427	Y428	M429	R430								
T368	G308	L309	F310	P311	L312	L313	F314	A315	R316	V317	N318	K319	A320	G321	T322	P323	V324	A325	G326	L327	I328	V329	V330	G331	I332	L333	M334	T335	I336	F337	Q338	L339	S340	I341	S343	P344	N345	A346	T347	K348	E349	F350	G351	L352	V353	S354	S355	V356	S357	V358	I359	F360	T361	L362	V363	P364	Y365	L366	Y367	
G247	N248	G248	M249	I250	P251	N252	ALA	ALA	LEU	ARG	VAL	SER	ALA	SER	PRO	PHE	GLY	ASP	ASP	ALA	ALA	ARG	MET	ALA	LEU	GLY	ASP	T273	A276	I277	V278	S279	F280	C281	A282	A283	A284	G285	C286	L287	G288	S289	L290	G291	G292	W293	T294	L295	L296	A297	G298	Q299	T300	A301	K302	A303	A304	A305	D306	D307
N183	V184	S185	G186	L187	G188	T189	F190	I193	Q194	S195	T196	L197	N198	V199	T200	L201	W202	S203	F204	G205	G206	P144	V207	E208	S209	A210	S211	V212	A213	A214	G215	V216	K218	N219	P220	N223	V224	P225	I226	A227	T228	I229	V232	L233	A236	V237	C238	Y239	V240	L241	S242	T243	T244	A245	I246					
P122	L123	V124	L125	T126	I127	T128	C129	V130	V131	V132	L133	W134	I135	F136	V137	L138	L139	N140	T141	V142	G143	K145	M146	T147	T148	R149	V150	Q151	A152	V153	A154	V155	T156	L157	A158	L159	I160	P161	I162	V163	G164	I165	A166	V167	F168	G169	M172	F173	R174	G175	E176	T177	Y178	M179	A180	A181	V182			
K62	M63	S64	F65	L66	D67	P68	S69	P70	G71	G72	S73	Y74	A75	Y76	A77	R78	R79	C80	F81	G82	P83	L85	G86	Y87	Q88	T89	N90	V91	L92	Y93	W94	L95	A96	C97	W98	I99	G100	M101	I102	A103	M104	V105	V106	I107	G108	V109	G110	Y111	L112	S113	Y114	F115	F116	P117	I118	L119	K120	D121		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.81Å 108.30Å 138.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.61 49.32 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.32-3.61) 99.8 (49.32-3.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.295 , 0.318 0.278 , 0.299	Depositor DCC
R_{free} test set	876 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	152.4	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 151.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6072	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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	0.63	0/3115	1.12	23/4264 (0.5%)
1	B	0.63	0/3115	1.12	23/4264 (0.5%)
All	All	0.63	0/6230	1.12	46/8528 (0.5%)

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	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	PRO	CA-C-N	10.20	132.59	119.84
1	A	311	PRO	C-N-CA	10.20	132.59	119.84
1	B	311	PRO	CA-C-N	9.81	132.10	119.84
1	B	311	PRO	C-N-CA	9.81	132.10	119.84
1	A	116	PHE	CA-C-N	-8.50	109.21	119.84

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	PHE	Peptide
1	A	377	HIS	Peptide
1	A	424	TYR	Peptide
1	B	116	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	B	377	HIS	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	3036	0	3141	561	0
1	B	3036	0	3141	562	0
All	All	6072	0	6282	1090	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 88.

The worst 5 of 1090 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:315:ALA:HB1	1:A:316:ARG:HA	1.19	1.16
1:A:430:ARG:HG2	1:B:374:LEU:HD23	1.28	1.15
1:B:38:THR:HB	1:B:39:GLY:HA3	1.18	1.14
1:B:315:ALA:HB1	1:B:316:ARG:HA	1.15	1.14
1:A:38:THR:HB	1:A:39:GLY:HA3	1.19	1.12

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	406/445 (91%)	261 (64%)	82 (20%)	63 (16%)	0	2
1	B	406/445 (91%)	262 (64%)	80 (20%)	64 (16%)	0	2
All	All	812/890 (91%)	523 (64%)	162 (20%)	127 (16%)	0	2

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	68	PRO
1	A	83	PRO
1	A	116	PHE
1	A	117	PRO

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	314/343 (92%)	230 (73%)	84 (27%)	0	3
1	B	314/343 (92%)	233 (74%)	81 (26%)	0	4
All	All	628/686 (92%)	463 (74%)	165 (26%)	0	3

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	163	VAL
1	B	329	ILE
1	B	178	TYR
1	B	229	ILE
1	B	354	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	8	HIS

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Mol	Chain	Res	Type
1	B	22	ASN
1	B	379	HIS
1	B	219	ASN
1	B	223	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 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	410/445 (92%)	0.80	52 (12%) 8 8	109, 173, 311, 406	0
1	B	410/445 (92%)	0.85	57 (13%) 6 7	108, 172, 311, 406	0
All	All	820/890 (92%)	0.83	109 (13%) 7 7	108, 172, 313, 406	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	TRP	10.6
1	A	287	LEU	6.6
1	B	287	LEU	6.2
1	A	205	ILE	5.8
1	A	13	ILE	5.2

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.