wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	3LRB
Title	:	Structure of E. coli AdiC
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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 (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:

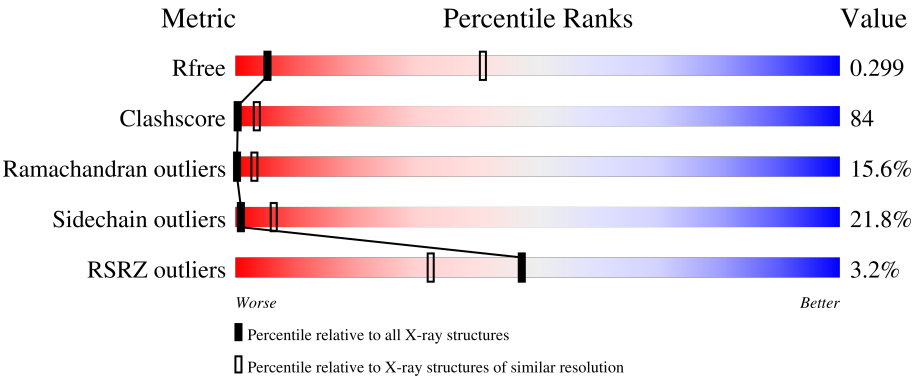
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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% 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	3% 18% 51% 20% · 8%
1	B	445	2% 18% 50% 20% · 8%

2 Entry composition (i)

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.

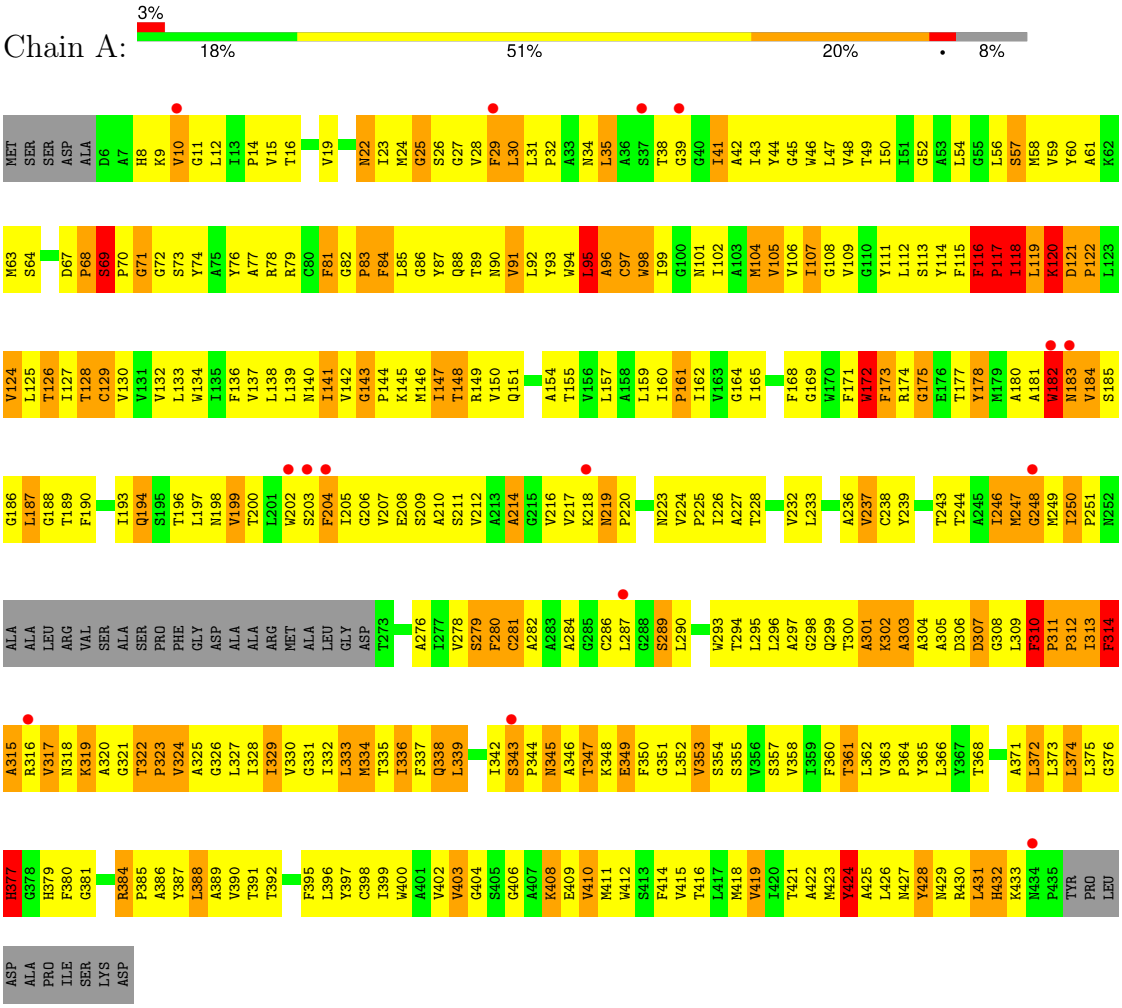
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			
1	B	410	Total	C	N	O	S	0	0	0
			3036	2020	481	514	21			

3 Residue-property plots (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.

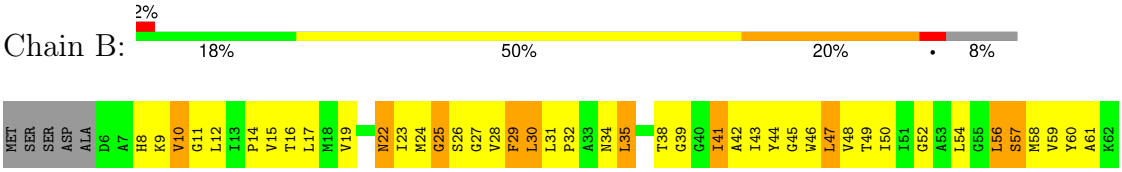
• Molecule 1: Arginine/agmatine antiporter

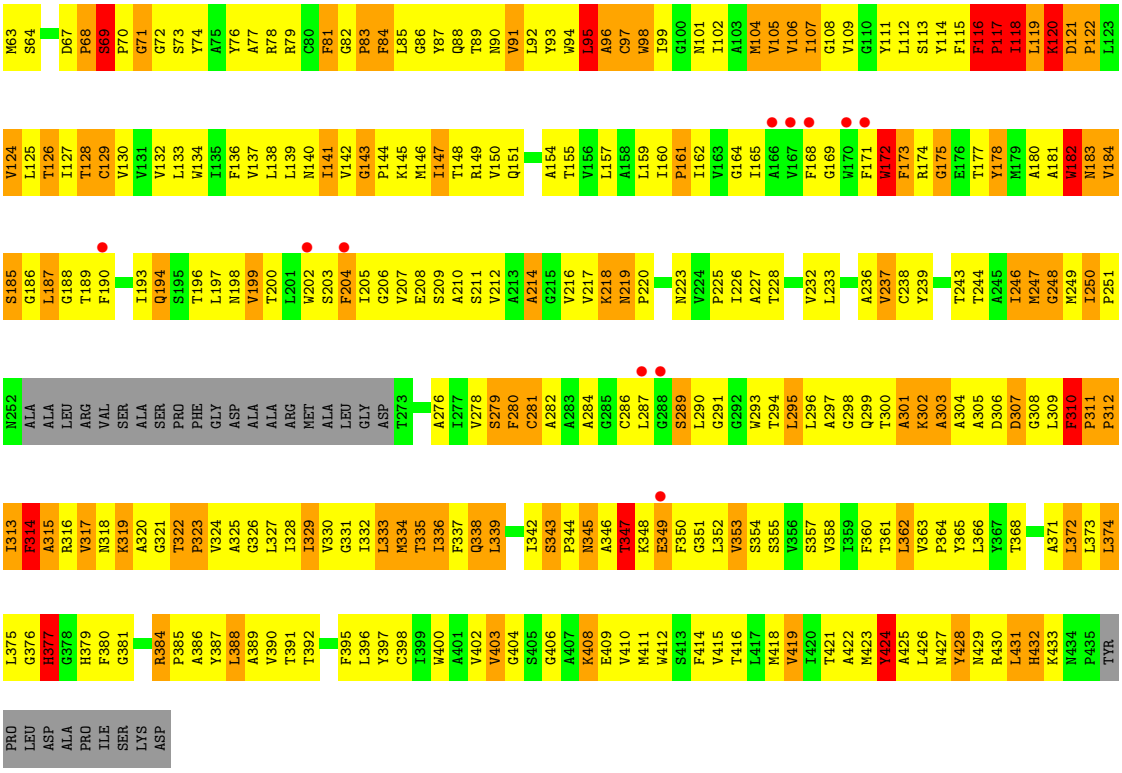
Chain A:



• Molecule 1: Arginine/agmatine antiporter

Chain B:




M63 S64 D67 P68 S69 P70 G71 G72 S73 Y74 A75 Y76 A77 R78 R79 C80 F81 G82 P83 F84 L85 G86 Y87 Q88 T89 N90 V91 L92 Y93 W94 L95 A96 C97 W98 I99 G100 N101 I102 A103 M104 V105 V106 I107 G108 V109 G110 Y111 L112 S113 Y114 F115 F116 P117 I118 L119 K120 D121 P122 L123
V124 L125 T126 I127 T128 C129 V130 V131 V132 L133 W134 I135 F136 V137 L138 L139 N140 I141 V142 G143 P144 K145 M146 I147 T148 R149 V150 Q151 A154 T155 V156 L157 A158 L159 I160 P161 I162 V163 G164 I165 A166 V167 F168 G169 W170 F171 W172 F173 R174 G175 E176 T177 Y178 M179 A180 A181 W182 N183 V184
S185 G186 L187 G188 T189 F190 I193 Q194 S195 T196 L197 N198 V199 T200 L201 W202 S203 F204 I205 G206 V207 E208 S209 A210 S211 V212 A213 A214 G215 V216 V217 K218 N219 P220 N223 V224 P225 I226 A227 T228 V232 L233 A236 V237 C238 Y239 T243 T244 A245 I246 M247 G248 M249 I250 P251
N252 ALA ALA LEU ARG VAL SER ALA SER PRO PHE GLY 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 G308 L309 F310 P311 P312
I313 F314 A315 R316 V317 N318 K319 A320 G321 T322 P323 V324 A325 G326 L327 I328 I329 V330 G331 I332 L333 M334 T335 I336 F337 Q338 L339 I342 S343 P344 N345 A346 I347 K348 E349 F350 G351 L352 V353 S354 S355 V356 S357 V358 I359 F360 T361 L362 V363 P364 Y365 L366 Y367 T368 A371 L372 L373 L374
L375 G376 H377 G378 H379 F380 G381 R384 P385 A386 Y387 L388 A389 V390 T391 T392 F395 L396 Y397 C398 I399 W400 A401 V402 V403 G404 S405 G406 A407 K408 E409 V410 M411 W412 S413 F414 V415 T416 L417 M418 V419 I420 T421 A422 M423 Y424 A425 L426 N427 Y428 N429 R430 L431 H432 K433 N434 P435 TYR
PRO LEU ASP ALA PRO ILE SER LYS ASP

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.25 , 132.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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	0.48	0/3115	0.74	2/4264 (0.0%)
1	B	0.48	0/3115	0.74	2/4264 (0.0%)
All	All	0.48	0/6230	0.74	4/8528 (0.0%)

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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	PRO	C-N-CD	-6.25	106.85	120.60
1	B	311	PRO	C-N-CD	-5.78	107.89	120.60
1	A	432	HIS	N-CA-C	5.72	126.45	111.00
1	B	432	HIS	N-CA-C	5.38	125.52	111.00

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
1	B	377	HIS	Peptide

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	3036	0	3141	537	0
1	B	3036	0	3141	538	0
All	All	6072	0	6282	1040	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 1040 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

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	406/445 (91%)	261 (64%)	82 (20%)	63 (16%)	0 3
1	B	406/445 (91%)	262 (64%)	80 (20%)	64 (16%)	0 3
All	All	812/890 (91%)	523 (64%)	162 (20%)	127 (16%)	0 3

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 (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	314/343 (92%)	246 (78%)	68 (22%)	1 6
1	B	314/343 (92%)	245 (78%)	69 (22%)	1 6
All	All	628/686 (92%)	491 (78%)	137 (22%)	1 6

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	302	LYS
1	B	329	ILE
1	B	388	LEU
1	A	314	PHE
1	A	310	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	223	ASN
1	B	379	HIS
1	A	338	GLN
1	A	379	HIS
1	B	22	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	410/445 (92%)	-0.08	15 (3%)	41	27	109, 173, 311, 406	0
1	B	410/445 (92%)	-0.20	11 (2%)	54	39	108, 172, 311, 406	0
All	All	820/890 (92%)	-0.14	26 (3%)	47	32	108, 172, 313, 406	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	ALA	7.2
1	A	248	GLY	4.1
1	A	37	SER	4.0
1	B	170	TRP	3.8
1	A	287	LEU	3.4

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.