

wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2023 – 06:42 AM EDT

PDB ID : 3C1I

Title: Substrate binding, deprotonation and selectivity at the periplasmic entrance

of the E. coli ammonia channel AmtB

Authors: Lupo, D.; Winkler, F.K.

Deposited on : 2008-01-23

Resolution : 2.30 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

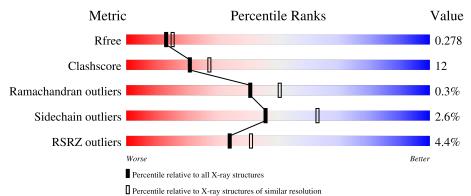
Validation Pipeline (wwPDB-VP) : 2.36

Overall quality at a glance (i) 1

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



Whole archive Similar resolution Metric (#Entries) (#Entries, resolution range(Å)) R_{free} 5042 (2.30-2.30) 130704 Clashscore 141614 5643 (2.30-2.30) Ramachandran outliers 138981 5575 (2.30-2.30) Sidechain outliers 138945 5575 (2.30-2.30)

RSRZ outliers 127900 4938 (2.30-2.30)

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			
			4%			
1	A	424	66%	20%	14%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LDA	A	426	-	-	X	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2801 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 Ammonia channel.

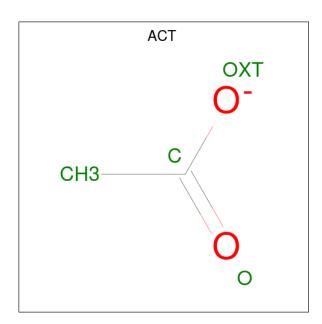
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	366	Total	С	N	О	S	0	0	0
_	11	330	2657	1757	426	455	19			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	ALA	PHE	engineered mutation	UNP P69681
A	407	ASP	-	expression tag	UNP P69681
A	408	GLN	-	expression tag	UNP P69681
A	409	ALA	-	expression tag	UNP P69681
A	410	GLN	-	expression tag	UNP P69681
A	411	GLN	-	expression tag	UNP P69681
A	412	PRO	-	expression tag	UNP P69681
A	413	ALA	-	expression tag	UNP P69681
A	414	GLN	-	expression tag	UNP P69681
A	415	ALA	-	expression tag	UNP P69681
A	416	ASP	-	expression tag	UNP P69681
A	417	LEU	-	expression tag	UNP P69681
A	418	GLU	-	expression tag	UNP P69681
A	419	HIS	-	expression tag	UNP P69681
A	420	HIS	-	expression tag	UNP P69681
A	421	HIS		expression tag	UNP P69681
A	422	HIS	-	expression tag	UNP P69681
A	423	HIS	-	expression tag	UNP P69681
Α	424	HIS	_	expression tag	UNP P69681

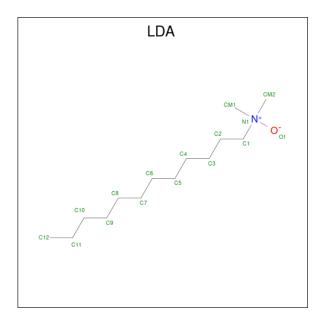
• Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total 4	C 2	O 2	0	0

 \bullet Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 16	C 14	N 1	O 1	0	0

• Molecule 4 is water.



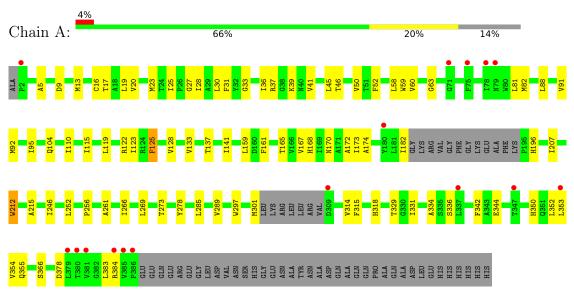
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	124	Total O 124 124	0	0



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 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.







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants	109.22Å 109.22Å 84.44Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 - 2.30	Depositor
Resolution (A)	14.91 - 2.30	EDS
% Data completeness	97.9 (15.00-2.30)	Depositor
(in resolution range)	97.9 (14.91-2.30)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) > 1$	2.48 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.213 , 0.246	Depositor
R, R_{free}	0.257 , 0.278	DCC
R_{free} test set	1252 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35 , 76.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.065 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2801	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: ACT, LDA

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).

Mal	Chain	Bond	lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.53	0/2718	0.58	1/3708 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	A	88	LEU	CA-CB-CG	5.62	128.22	115.30

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	2657	0	2723	66	0
2	A	4	0	3	0	0
3	A	16	0	31	15	0
4	A	124	0	0	13	0
All	All	2801	0	2757	66	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 12.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:45:LEU:HB2	4:A:533:HOH:O	1.36	1.25
1:A:17:THR:HA	4:A:539:HOH:O	1.54	1.05
1:A:37:ARG:HD2	4:A:472:HOH:O	1.74	0.87
1:A:168:HIS:CE1	3:A:426:LDA:H81	2.09	0.87
1:A:23:MET:HA	4:A:536:HOH:O	1.74	0.85

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	360/424 (85%)	342 (95%)	17 (5%)	1 (0%)	41 50	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ARG

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	$265/311 \ (85\%)$	258 (97%)	7 (3%)	46 63	

5 of 7 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	212	TRP
1	A	252	LEU
1	A	353	LEU
1	A	336	SER
1	A	125	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	350	HIS
1	A	351	GLN
1	A	355	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	Bo	ond leng	an ths	В	ond ang	les
MIOI	туре			LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	425	-	3,3,3	0.76	0	3,3,3	1.43	0



7	Mol Typ		Chain	Res	s Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Counts		RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
	3	LDA	A	426	-	12,15,15	2.08	1 (8%)	14,17,17	0.72	1 (7%)

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	LDA	A	426	-	-	8/13/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	$\operatorname{Ideal}(ext{\AA})$
3	A	426	LDA	O1-N1	-7.02	1.25	1.42

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	426	LDA	CM1-N1-C1	2.41	115.30	110.23

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	426	LDA	C2-C1-N1-O1
3	A	426	LDA	C2-C1-N1-CM1
3	A	426	LDA	C3-C4-C5-C6
3	A	426	LDA	C6-C7-C8-C9
3	A	426	LDA	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	426	LDA	15	0

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, 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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9
1	A	366/424 (86%)	0.11	16 (4%) 3	84 41	12, 23, 41, 57	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	TYR	4.1
1	A	386	PRO	3.8
1	A	384	ARG	3.3
1	A	309	ASP	3.2
1	A	2	PRO	3.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
2	ACT	A	425	4/4	0.88	0.25	55,56,57,57	0
3	LDA	A	426	16/16	0.91	0.14	2,15,58,62	0



6.5 Other polymers (i)

There are no such residues in this entry.

