



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:46 AM GMT

PDB ID : 2IMO
Title : Crystal structure of allantoate amidohydrolase from Escherichia coli at pH 4.6
Authors : Agarwal, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center
for Structural Genomics (NYSGXRC)
Deposited on : 2006-10-04
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

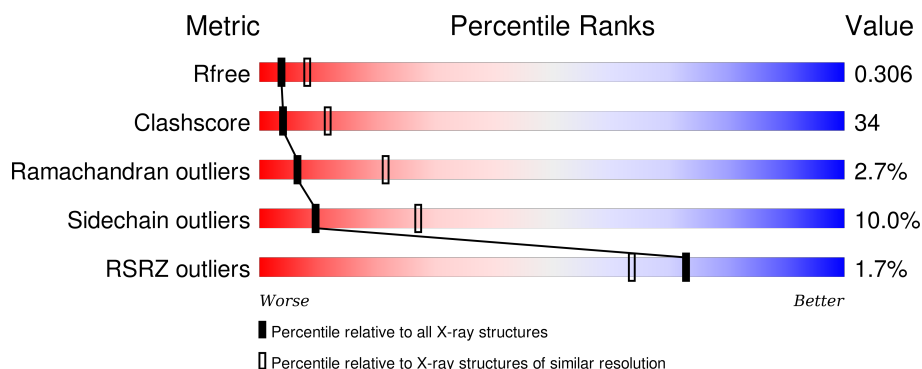
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	423	<div> <div>2%</div> <div>50% 37% 7% • 6%</div> </div>
1	B	423	<div> <div>2%</div> <div>39% 44% 9% • 7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6265 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 Allantoate amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	Se	0	0	0
			3128	1975	541	592	7	13			
1	B	394	Total	C	N	O	S	Se	0	0	0
			3080	1946	535	579	7	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP P77425
A	2	SER	-	CLONING ARTIFACT	UNP P77425
A	3	LEU	-	CLONING ARTIFACT	UNP P77425
A	29	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	49	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	125	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	167	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	234	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	258	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	308	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	315	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	325	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	332	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	354	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	373	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	405	MSE	MET	MODIFIED RESIDUE	UNP P77425
A	414	GLU	-	EXPRESSION TAG	UNP P77425
A	415	GLY	-	EXPRESSION TAG	UNP P77425
A	416	GLY	-	EXPRESSION TAG	UNP P77425
A	417	SER	-	EXPRESSION TAG	UNP P77425
A	418	HIS	-	EXPRESSION TAG	UNP P77425
A	419	HIS	-	EXPRESSION TAG	UNP P77425
A	420	HIS	-	EXPRESSION TAG	UNP P77425
A	421	HIS	-	EXPRESSION TAG	UNP P77425
A	422	HIS	-	EXPRESSION TAG	UNP P77425

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	HIS	-	EXPRESSION TAG	UNP P77425
B	1	MSE	-	CLONING ARTIFACT	UNP P77425
B	2	SER	-	CLONING ARTIFACT	UNP P77425
B	3	LEU	-	CLONING ARTIFACT	UNP P77425
B	29	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	49	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	125	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	167	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	234	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	258	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	308	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	315	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	325	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	332	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	354	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	373	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	405	MSE	MET	MODIFIED RESIDUE	UNP P77425
B	414	GLU	-	EXPRESSION TAG	UNP P77425
B	415	GLY	-	EXPRESSION TAG	UNP P77425
B	416	GLY	-	EXPRESSION TAG	UNP P77425
B	417	SER	-	EXPRESSION TAG	UNP P77425
B	418	HIS	-	EXPRESSION TAG	UNP P77425
B	419	HIS	-	EXPRESSION TAG	UNP P77425
B	420	HIS	-	EXPRESSION TAG	UNP P77425
B	421	HIS	-	EXPRESSION TAG	UNP P77425
B	422	HIS	-	EXPRESSION TAG	UNP P77425
B	423	HIS	-	EXPRESSION TAG	UNP P77425

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	20	Total O 20 20	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.75Å 183.92Å 48.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.78 – 2.80 48.78 – 2.77	Depositor EDS
% Data completeness (in resolution range)	90.0 (48.78-2.80) 88.5 (48.78-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.302 0.264 , 0.306	Depositor DCC
R_{free} test set	578 reflections (2.94%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 21933 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6265	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	2/3183 (0.1%)	0.74	3/4302 (0.1%)
1	B	0.54	4/3136 (0.1%)	0.71	1/4239 (0.0%)
All	All	0.55	6/6319 (0.1%)	0.72	4/8541 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	MSE	CG-SE	-5.50	1.76	1.95
1	B	29	MSE	CG-SE	-5.45	1.76	1.95
1	B	354	MSE	CG-SE	-5.08	1.78	1.95
1	B	125	MSE	CG-SE	-5.07	1.78	1.95
1	A	49	MSE	CG-SE	-5.05	1.78	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LEU	CA-CB-CG	6.11	129.36	115.30
1	B	66	GLY	N-CA-C	-5.41	99.57	113.10
1	A	343	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	68	LEU	N-CA-C	-5.30	96.69	111.00

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	3128	0	3064	180	0
1	B	3080	0	3028	247	0
2	A	37	0	0	6	0
2	B	20	0	0	3	0
All	All	6265	0	6092	419	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 34.

The worst 5 of 419 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:B:344:CYS:HA	1:B:349:LEU:HD12	1.42	1.02
1:A:365:PHE:HB3	1:A:371:THR:HG21	1.49	0.94
1:A:379:ILE:HD11	1:A:389:ARG:HB2	1.49	0.94
1:B:209:VAL:HG11	1:B:373:MSE:HE3	1.49	0.93
1:A:208:VAL:HG13	1:A:340:LEU:HD23	1.51	0.92

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	393/423 (93%)	350 (89%)	35 (9%)	8 (2%)	9	30
1	B	390/423 (92%)	328 (84%)	49 (13%)	13 (3%)	5	16
All	All	783/846 (93%)	678 (87%)	84 (11%)	21 (3%)	6	21

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	34	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	36	PRO
1	B	320	ASP
1	B	379	ILE
1	A	129	GLU

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	338/341 (99%)	306 (90%)	32 (10%)	11	30
1	B	331/341 (97%)	296 (89%)	35 (11%)	8	24
All	All	669/682 (98%)	602 (90%)	67 (10%)	9	27

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ARG
1	B	44	GLN
1	B	378	SER
1	A	393	THR
1	B	14	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	ASN
1	B	92	ASN
1	B	384	HIS
1	B	75	GLN
1	A	202	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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	386/423 (91%)	-0.14	3 (0%) 87 81	26, 45, 66, 84	0
1	B	381/423 (90%)	0.12	10 (2%) 59 47	32, 59, 91, 99	0
All	All	767/846 (90%)	-0.01	13 (1%) 73 63	26, 51, 84, 99	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	5.7
1	B	26	ALA	5.2
1	B	175	PRO	4.1
1	B	27	GLY	3.2
1	B	129	GLU	2.9

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 carbohydrates 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.