



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2ATC  
Title : CRYSTAL AND MOLECULAR STRUCTURES OF NATIVE AND CTP-LIGANDED ASPARTATE CARBAMOYLTRANSFERASE FROM ESCHERICHIA COLI  
Authors : Honzatko, R.B.; Crawford, J.L.; Monaco, H.L.; Ladner, J.E.; Edwards, B.F.P.; Evans, D.R.; Warren, S.G.; Wiley, D.C.; Ladner, R.C.; Lipscomb, W.N.  
Deposited on : 1982-03-24  
Resolution : 3.00 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](mailto: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)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

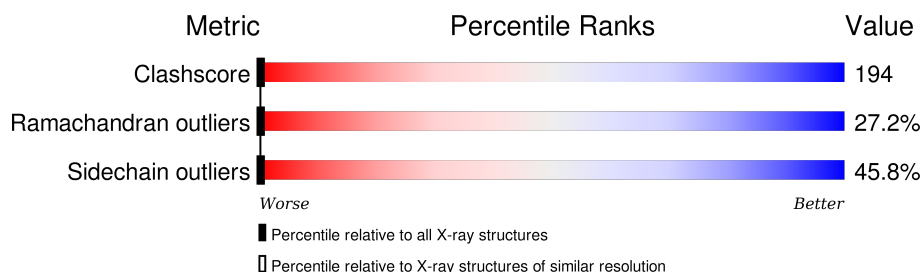
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	305	
2	B	152	

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	ZN	B	153	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3511 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 ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	X	0	0	0
			2362	1491	420	441	8	2			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	LYS	CONFLICT	UNP P0A786
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	86	GLN	GLU	CONFLICT	UNP P0A786
A	90	ASN	ASP	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	153	ASN	ASP	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
A	?	-	MET	DELETION	UNP P0A786
A	?	-	ALA	DELETION	UNP P0A786
A	?	-	GLU	DELETION	UNP P0A786
A	?	-	VAL	DELETION	UNP P0A786
A	?	-	ASP	DELETION	UNP P0A786
A	?	-	ILE	DELETION	UNP P0A786
A	?	-	LEU	DELETION	UNP P0A786
A	?	-	TYR	DELETION	UNP P0A786
A	234	ASX	ASN	CONFLICT	UNP P0A786
A	240	LEU	VAL	CONFLICT	UNP P0A786
A	241	VAL	LEU	CONFLICT	UNP P0A786
A	244	ASN	-	INSERTION	UNP P0A786
A	246	LEU	-	INSERTION	UNP P0A786
A	247	GLY	-	INSERTION	UNP P0A786
A	248	GLY	ASP	CONFLICT	UNP P0A786
A	254	MET	ALA	CONFLICT	UNP P0A786
A	256	ALA	MET	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1148	714	202	227	5			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ASN	ASP	CONFLICT	UNP P0A7F3
B	5	ASP	ASN	CONFLICT	UNP P0A7F3
B	10	ALA	GLU	CONFLICT	UNP P0A7F3
B	11	GLU	ALA	CONFLICT	UNP P0A7F3
B	19	ASN	ASP	CONFLICT	UNP P0A7F3
B	24	GLU	GLN	CONFLICT	UNP P0A7F3
B	39	GLN	ASP	CONFLICT	UNP P0A7F3
B	40	ASP	GLN	CONFLICT	UNP P0A7F3
B	70	GLU	GLN	CONFLICT	UNP P0A7F3
B	73	GLU	GLN	CONFLICT	UNP P0A7F3
B	87	ASN	ASP	CONFLICT	UNP P0A7F3
B	88	ASP	ASN	CONFLICT	UNP P0A7F3
B	103	ASN	-	INSERTION	UNP P0A7F3
B	?	-	ASN	DELETION	UNP P0A7F3
B	111	ASP	ASN	CONFLICT	UNP P0A7F3
B	?	-	LYS	DELETION	UNP P0A7F3
B	131	ASP	ASN	CONFLICT	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

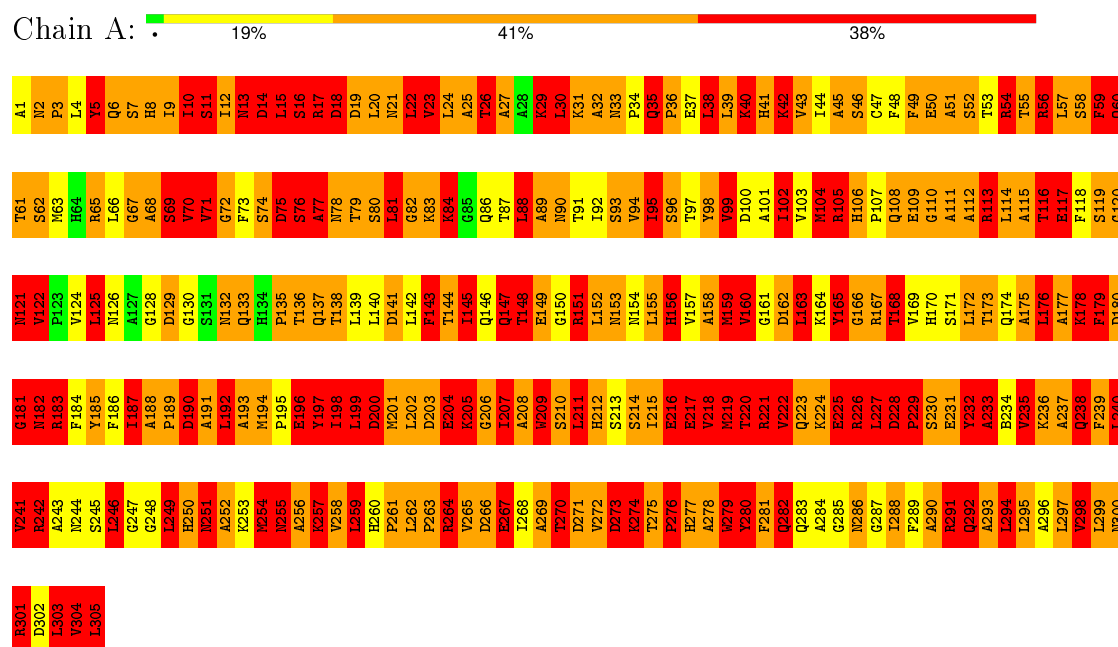
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

### 3 Residue-property plots

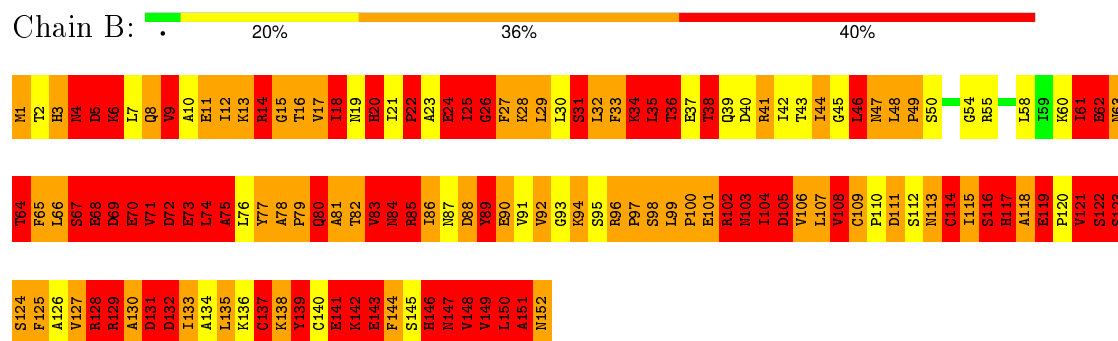
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN



#### • Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.70Å 131.70Å 199.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.270 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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: ZN

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	1.67	28/2399 (1.2%)	3.68	435/3256 (13.4%)
2	B	1.80	14/1165 (1.2%)	3.50	210/1575 (13.3%)
All	All	1.71	42/3564 (1.2%)	3.62	645/4831 (13.4%)

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	15
2	B	0	4
All	All	0	19

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	GLY	N-CA	13.06	1.65	1.46
2	B	119	GLU	CD-OE1	-8.62	1.16	1.25
1	A	230	SER	C-O	8.43	1.39	1.23
1	A	230	SER	N-CA	7.88	1.62	1.46
2	B	143	GLU	CG-CD	-7.51	1.40	1.51

The worst 5 of 645 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	ARG	CD-NE-CZ	26.04	160.05	123.60
1	A	242	ARG	NE-CZ-NH1	23.78	132.19	120.30
1	A	242	ARG	CD-NE-CZ	21.68	153.95	123.60
1	A	54	ARG	NE-CZ-NH2	-20.02	110.29	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	LEU	CA-CB-CG	19.93	161.14	115.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	ARG	Sidechain
1	A	35	GLN	Sidechain
1	A	54	ARG	Sidechain
1	A	56	ARG	Sidechain
1	A	65	ARG	Sidechain

## 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	2362	0	2360	840	6
2	B	1148	0	1114	518	10
3	B	1	0	0	2	0
All	All	3511	0	3474	1348	16

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 194.

The worst 5 of 1348 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)
2:B:66:LEU:H	2:B:66:LEU:CD1	1.34	1.38
2:B:9:VAL:CG1	2:B:14:ARG:HA	1.56	1.32
1:A:282:GLN:HE21	1:A:282:GLN:N	1.23	1.32
2:B:128:ARG:NH1	2:B:143:GLU:OE1	1.60	1.32
1:A:294:LEU:O	1:A:298:VAL:HG23	1.25	1.32

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:HIS:CB	2:B:4:ASN:O[6_555]	0.69	1.51
2:B:3:HIS:O	2:B:4:ASN:CB[6_555]	0.71	1.49
2:B:3:HIS:C	2:B:4:ASN:CA[6_555]	0.72	1.48
2:B:3:HIS:O	2:B:4:ASN:CA[6_555]	1.03	1.17
2:B:4:ASN:N	2:B:4:ASN:N[6_555]	1.46	0.74

## 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	302/305 (99%)	159 (53%)	71 (24%)	72 (24%)	0	0
2	B	150/152 (99%)	66 (44%)	33 (22%)	51 (34%)	0	0
All	All	452/457 (99%)	225 (50%)	104 (23%)	123 (27%)	0	0

5 of 123 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	6	GLN
1	A	10	ILE
1	A	11	SER
1	A	17	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	254/254 (100%)	136 (54%)	118 (46%)	0	0
2	B	126/136 (93%)	70 (56%)	56 (44%)	0	0
All	All	380/390 (97%)	206 (54%)	174 (46%)	0	0

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	GLU
1	A	255	ASN
2	B	122	SER
1	A	221	ARG
1	A	235	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	260	HIS
2	B	84	ASN
1	A	121	ASN
1	A	137	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.