



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID : 6AT1  
Title : STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE  
T STATE OF ASPARTATE CARBAMOYLTRANSFERASE. CRYSTAL  
STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-  
COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION  
Authors : Stevens, R.C.; Gouaux, J.E.; Lipscomb, W.N.  
Deposited on : 1990-04-26  
Resolution : 2.60 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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

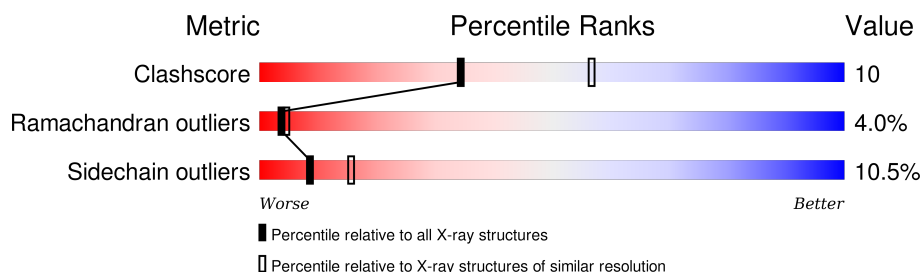
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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	310	 65%      28%      5% •
1	C	310	 63%      28%      8% •
2	B	153	 55%      35%      5% • 5%
2	D	153	 59%      31%      5% • 5%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7108 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 (T STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
C	60	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLU	GLN	CONFLICT	UNP P0A786
C	196	GLU	GLN	CONFLICT	UNP P0A786

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	CONFLICT	UNP P0A7F3
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

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

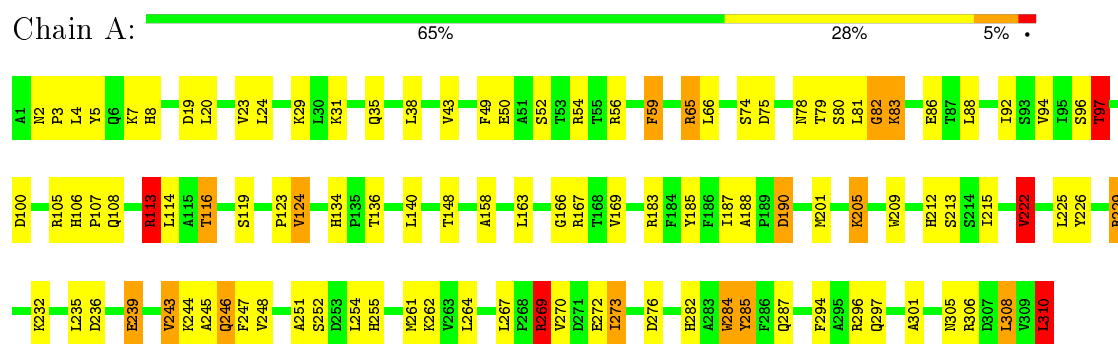
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

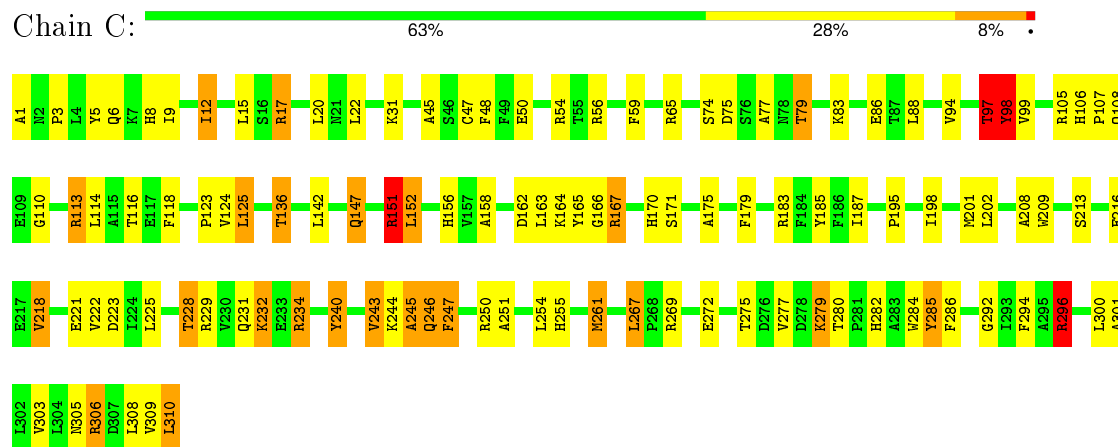
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

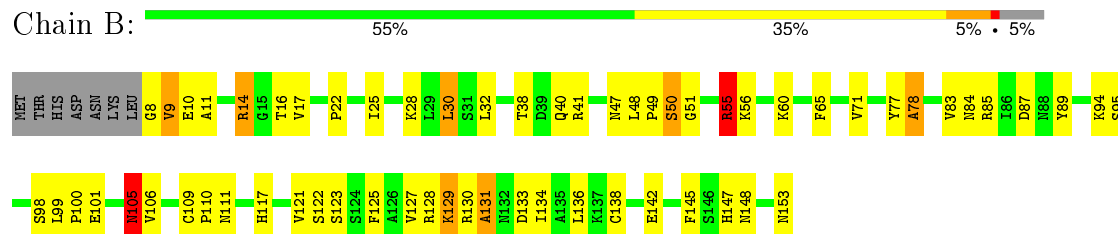
#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



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



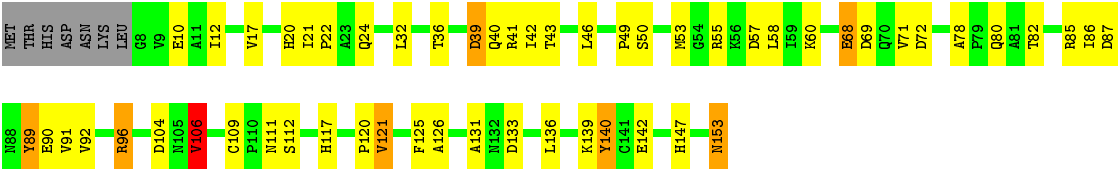
● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D: 

59%

31%

5% • 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.00 Å   122.00 Å   142.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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	0.87	0/2461	1.61	25/3339 (0.7%)
1	C	0.88	0/2461	1.69	43/3339 (1.3%)
2	B	0.81	0/1155	1.55	13/1561 (0.8%)
2	D	0.77	0/1155	1.52	10/1561 (0.6%)
All	All	0.85	0/7232	1.61	91/9800 (0.9%)

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	2
1	C	0	7
2	B	0	2
2	D	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH2	14.40	127.50	120.30
1	A	269	ARG	NE-CZ-NH2	12.95	126.77	120.30
1	C	113	ARG	NE-CZ-NH1	-11.59	114.50	120.30
1	A	56	ARG	NE-CZ-NH2	11.03	125.82	120.30
1	A	56	ARG	NE-CZ-NH1	-10.05	115.28	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	A	285	TYR	Sidechain
2	B	78	ALA	Peptide
2	B	89	TYR	Sidechain
1	C	98	TYR	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	2415	0	2422	50	0
1	C	2415	0	2422	48	0
2	B	1138	0	1154	28	0
2	D	1138	0	1154	18	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	7108	0	7152	142	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 10.

The worst 5 of 142 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:136:THR:HB	1:A:296:ARG:NH2	1.95	0.80
1:C:251:ALA:HA	1:C:254:LEU:HD12	1.67	0.74
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.67	0.73
2:B:14:ARG:HG3	2:B:87:ASP:HA	1.70	0.71
2:B:48:LEU:O	2:B:55:ARG:HA	1.90	0.71

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	308/310 (99%)	286 (93%)	13 (4%)	9 (3%)	6	9
1	C	308/310 (99%)	278 (90%)	19 (6%)	11 (4%)	4	6
2	B	144/153 (94%)	125 (87%)	11 (8%)	8 (6%)	2	2
2	D	144/153 (94%)	122 (85%)	14 (10%)	8 (6%)	2	2
All	All	904/926 (98%)	811 (90%)	57 (6%)	36 (4%)	4	4

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	190	ASP
1	A	246	GLN
2	B	105	ASN
2	B	129	LYS

### 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	261/261 (100%)	235 (90%)	26 (10%)	9	18
1	C	261/261 (100%)	233 (89%)	28 (11%)	8	15
2	B	129/136 (95%)	119 (92%)	10 (8%)	16	30
2	D	129/136 (95%)	111 (86%)	18 (14%)	4	7
All	All	780/794 (98%)	698 (90%)	82 (10%)	8	16

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	9	ILE
1	C	116	THR
2	D	82	THR
1	C	12	ILE
1	C	79	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	305	ASN
1	C	170	HIS
1	A	287	GLN
1	C	282	HIS

### 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 2 ligands modelled in this entry, 2 are 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

### 6.1 Protein, DNA and RNA chains

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

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

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

### 6.4 Ligands

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

### 6.5 Other polymers

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