



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:57 AM GMT

PDB ID : 3CSU  
Title : CATALYTIC TRIMER OF ESCHERICHIA COLI ASPARTATE TRAN-  
SCARBAMOYLASE  
Authors : Beernink, P.T.; Endrizzi, J.A.; Alber, T.; Schachman, H.K.  
Deposited on : 1999-04-22  
Resolution : 1.88 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

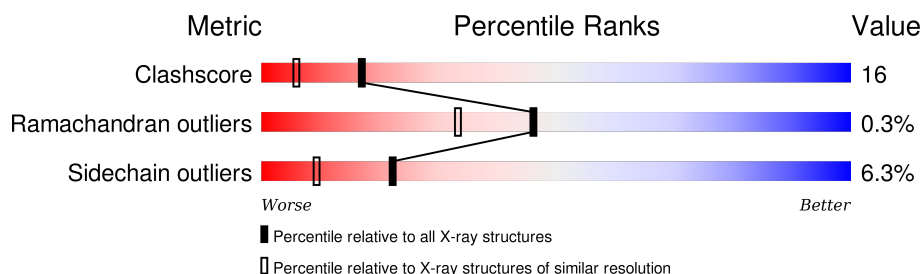
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)

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	
1	B	310	
1	C	310	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7601 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 PROTEIN (ASPARTATE CARBAMOYLTRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2225	1413	385	418	9			
1	B	288	Total	C	N	O	S	0	1	0
			2219	1409	384	417	9			
1	C	304	Total	C	N	O	S	0	0	0
			2366	1494	415	448	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

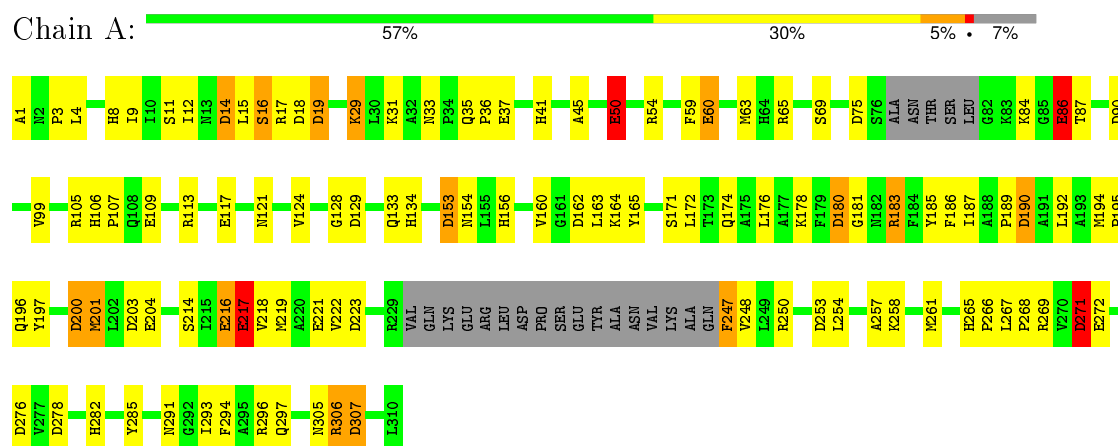
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O	0	0
			234	234		
3	B	233	Total	O	0	0
			233	233		
3	C	322	Total	O	0	0
			322	322		

### 3 Residue-property plots

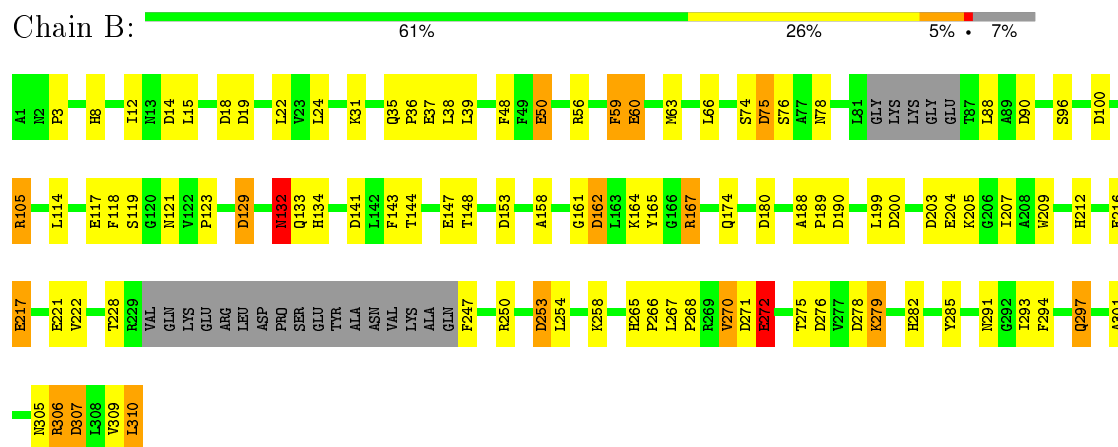
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



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LEU	D200	M201	L202	D203	E204	R205	G206						E216	E217	E221	V222	D223						M227						Q231	R232	E233	R234	L235	D236	P237	S238	E239						V243	N256						M261						H265	P266						R269	V270	D271	E272						T275	D276	V277	D278	K279						H282						Y285						R296						L299						R306	D307	L308	VAL
	R105	H106	P107	Q108	E109	G110	A111	A112	R113	L114	T116	E117	F118						M121	V122	P123	V124	L125						D129	G130	S131	N132	Q133						D141	L142	Q146	E147						L152	D153	N154	L155						D162	L163	K164	Y165	G166	R167						S171	Q174	A175						D180	G181	N182	R183						D190	A191	L192						P195																

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.12Å 82.54Å 210.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.88	Depositor
% Data completeness (in resolution range)	94.6 (20.00-1.88)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.190 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.77	10/2267 (0.4%)	1.22	33/3078 (1.1%)
1	B	0.76	9/2266 (0.4%)	1.22	34/3081 (1.1%)
1	C	0.79	13/2410 (0.5%)	1.25	39/3272 (1.2%)
All	All	0.77	32/6943 (0.5%)	1.23	106/9431 (1.1%)

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLU	CD-OE2	8.20	1.34	1.25
1	B	50	GLU	CD-OE2	7.18	1.33	1.25
1	B	117	GLU	CD-OE2	6.36	1.32	1.25
1	C	147	GLU	CD-OE2	6.25	1.32	1.25
1	C	216	GLU	CD-OE2	6.18	1.32	1.25

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	B	90	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	19	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	B	162	ASP	CB-CG-OD1	7.82	125.34	118.30
1	A	19	ASP	CB-CG-OD1	7.69	125.22	118.30

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	2225	0	2213	89	0
1	B	2219	0	2207	64	0
1	C	2366	0	2362	70	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	234	0	0	16	0
3	B	233	0	0	7	0
3	C	322	0	0	11	0
All	All	7601	0	6782	222	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 16.

The worst 5 of 222 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:C:8:HIS:HD2	1:C:124:VAL:H	1.11	0.95
1:C:47:CYS:HB3	1:C:73:PHE:CZ	2.05	0.92
1:B:114:LEU:HD11	1:B:118:PHE:HE2	1.32	0.91
1:C:114:LEU:HD11	1:C:118:PHE:HE2	1.42	0.84
1:A:8:HIS:HD2	1:A:124:VAL:H	1.22	0.83

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	282/310 (91%)	268 (95%)	14 (5%)	0	100	100
1	B	283/310 (91%)	269 (95%)	12 (4%)	2 (1%)	26	13
1	C	300/310 (97%)	290 (97%)	9 (3%)	1 (0%)	46	33
All	All	865/930 (93%)	827 (96%)	35 (4%)	3 (0%)	46	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	B	270	VAL
1	C	270	VAL

### 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	238/261 (91%)	219 (92%)	19 (8%)	15	5
1	B	239/261 (92%)	227 (95%)	12 (5%)	30	16
1	C	256/261 (98%)	241 (94%)	15 (6%)	24	11
All	All	733/783 (94%)	687 (94%)	46 (6%)	22	9

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	132	ASN
1	B	272	GLU
1	C	271	ASP
1	B	134	HIS
1	B	167	ARG

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	C	13	ASN
1	C	64	HIS
1	C	231	GLN
1	B	305	ASN
1	C	8	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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.