



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2ADV / pdb\_00002adv  
Title : Crystal Structures Of Glutaryl 7-Aminocephalosporanic Acid Acylase: mutational study of activation mechanism  
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Deposited on : 2005-07-21  
Resolution : 2.24 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49



## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5746 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 Glutaryl 7- Aminocephalosporanic Acid Acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	161	1255	798	220	236	1	0	0	0

- Molecule 2 is a protein called Glutaryl 7- Aminocephalosporanic Acid Acylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	28	208	131	38	39	0	0	0

- Molecule 3 is a protein called Glutaryl 7- Aminocephalosporanic Acid Acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	494	3909	2472	689	737	11	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	11	Total	O	0	0
			11	11		
4	C	260	Total	O	0	0
			260	260		



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.78Å 73.78Å 384.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.24	Depositor
% Data completeness (in resolution range)	94.6 (48.22-2.24)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.183 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.79	1/1297 (0.1%)	0.90	0/1777
2	B	0.62	0/214	0.83	0/295
3	C	0.71	0/4016	0.83	2/5478 (0.0%)
All	All	0.73	1/5527 (0.0%)	0.85	2/7550 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	VAL	CA-CB	8.21	1.58	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	437	VAL	N-CA-C	5.66	116.03	108.11
3	C	47	GLY	N-CA-C	5.51	117.44	110.38

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	1255	0	1167	2	0
2	B	208	0	203	1	0
3	C	3909	0	3754	16	0
4	A	103	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	11	0	0	0	0
4	C	260	0	0	4	0
All	All	5746	0	5124	19	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 2.

The worst 5 of 19 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)
3:C:31:PHE:CD2	4:C:783:HOH:O	2.48	0.65
3:C:50:GLN:HE22	3:C:57:ARG:HH11	1.56	0.51
3:C:300:HIS:HE1	4:C:762:HOH:O	1.94	0.51
2:B:27:THR:O	2:B:27:THR:HG23	2.10	0.51
3:C:31:PHE:HD2	4:C:783:HOH:O	1.88	0.50

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	159/166 (96%)	150 (94%)	7 (4%)	2 (1%)	9	5
2	B	26/28 (93%)	25 (96%)	1 (4%)	0	100	100
3	C	492/500 (98%)	479 (97%)	12 (2%)	1 (0%)	43	48
All	All	677/694 (98%)	654 (97%)	20 (3%)	3 (0%)	30	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO

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Mol	Chain	Res	Type
3	C	177	PHE
1	A	7	GLN

### 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	123/128 (96%)	120 (98%)	3 (2%)	43	51
2	B	22/22 (100%)	22 (100%)	0	100	100
3	C	409/415 (99%)	397 (97%)	12 (3%)	37	44
All	All	554/565 (98%)	539 (97%)	15 (3%)	39	47

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	83	LEU
3	C	475	TYR
3	C	105	ARG
3	C	479	ARG
3	C	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	297	GLN
3	C	300	HIS
3	C	485	HIS
1	A	117	GLN
1	A	128	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 oligosaccharides 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.