



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:42 AM UTC

PDB ID : 9E8P / pdb\_00009e8p  
Title : Crystal Structure of GABARAP-ATG3 conjugate  
Authors : Ohashi, K.; Otomo, T.  
Deposited on : 2024-11-05  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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>.

---

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

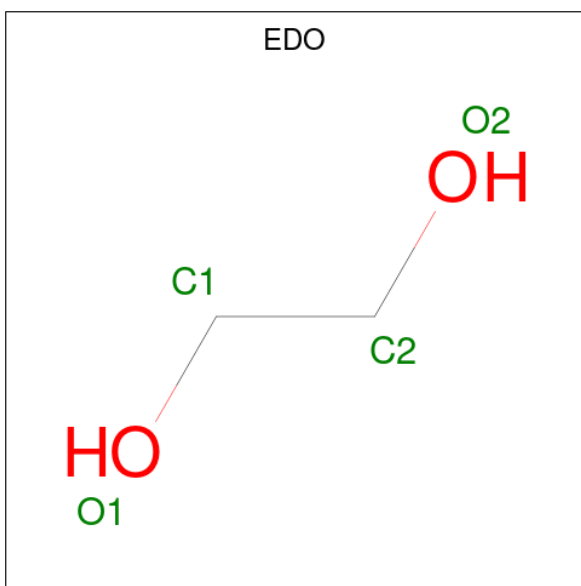






Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	3	Total	O	0	0
			3	3		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.39Å 97.39Å 166.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.33 – 2.70 38.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.33-2.70) 99.7 (38.33-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.218 , 0.249 0.218 , 0.247	Depositor DCC
$R_{free}$ test set	1995 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.4	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9955e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.





*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:GLU:OE1	2:D:15:ARG:NH2	2.54	0.40
2:C:45:ASP:OD1	2:C:45:ASP:N	2.49	0.40

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	172/223 (77%)	164 (95%)	8 (5%)	0	100	100
1	B	172/223 (77%)	161 (94%)	11 (6%)	0	100	100
2	C	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
2	D	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
All	All	570/682 (84%)	548 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	160/199 (80%)	158 (99%)	2 (1%)	61	83
1	B	160/199 (80%)	158 (99%)	2 (1%)	61	83
2	C	104/107 (97%)	104 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	104/107 (97%)	104 (100%)	0	100	100
All	All	528/612 (86%)	524 (99%)	4 (1%)	73	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	84	ARG
1	B	84	ARG
1	B	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	B	78	ASN
1	B	223	GLN
1	B	262	HIS
2	D	81	ASN
2	D	98	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	176/223 (78%)	-0.01	2 (1%) 78 76	51, 77, 103, 128	0
1	B	176/223 (78%)	0.02	4 (2%) 61 58	50, 81, 111, 135	0
2	C	115/118 (97%)	0.23	2 (1%) 69 67	67, 92, 143, 162	0
2	D	115/118 (97%)	0.34	1 (0%) 81 80	70, 96, 161, 181	0
All	All	582/682 (85%)	0.12	9 (1%) 72 70	50, 83, 138, 181	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	LYS	3.0
1	B	61	LEU	2.9
1	B	27	LYS	2.5
1	A	310	ARG	2.4
1	A	27	LYS	2.4
2	C	41	ILE	2.2
1	B	310	ARG	2.1
1	B	229	VAL	2.1
2	C	2	LYS	2.1

### 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	402	4/4	0.70	0.17	84,86,87,90	0
4	EDO	A	403	4/4	0.84	0.14	86,88,94,98	0
4	EDO	B	401	4/4	0.86	0.17	62,68,71,77	0
3	SO4	A	401	5/5	0.87	0.13	96,105,111,119	0
4	EDO	A	402	4/4	0.88	0.15	68,68,71,74	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.