



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:24 AM UTC

PDB ID : 4MUP / pdb_00004mup
Title : Crystal structure of Agrobacterium tumefaciens ATU3138 (EFI target 505157), apo structure
Authors : Vetting, M.W.; Bouvier, J.T.; Groninger-Poe, F.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2013-09-23
Resolution : 1.60 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

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
Xtrriage (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

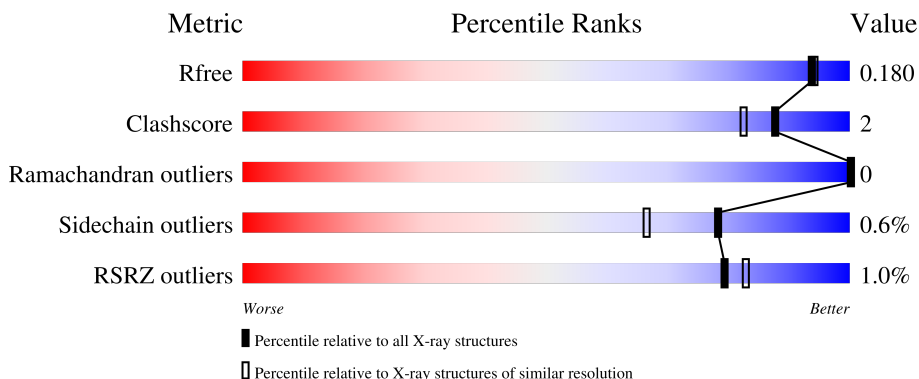
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	312	 85% 6% 9%
1	B	312	 87% 5% 8%
1	C	312	 83% 13%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 14024 atoms, of which 6425 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 AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	284	4359	1393	2163	398	396	9	0	0	0
1	B	286	4394	1404	2183	400	398	9	0	0	0
1	C	272	4198	1348	2079	381	381	9	0	2	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A9CEQ7
A	-18	GLY	-	expression tag	UNP A9CEQ7
A	-17	SER	-	expression tag	UNP A9CEQ7
A	-16	SER	-	expression tag	UNP A9CEQ7
A	-15	HIS	-	expression tag	UNP A9CEQ7
A	-14	HIS	-	expression tag	UNP A9CEQ7
A	-13	HIS	-	expression tag	UNP A9CEQ7
A	-12	HIS	-	expression tag	UNP A9CEQ7
A	-11	HIS	-	expression tag	UNP A9CEQ7
A	-10	HIS	-	expression tag	UNP A9CEQ7
A	-9	SER	-	expression tag	UNP A9CEQ7
A	-8	SER	-	expression tag	UNP A9CEQ7
A	-7	GLY	-	expression tag	UNP A9CEQ7
A	-6	LEU	-	expression tag	UNP A9CEQ7
A	-5	VAL	-	expression tag	UNP A9CEQ7
A	-4	PRO	-	expression tag	UNP A9CEQ7
A	-3	ARG	-	expression tag	UNP A9CEQ7
A	-2	GLY	-	expression tag	UNP A9CEQ7
A	-1	SER	-	expression tag	UNP A9CEQ7
A	0	HIS	-	expression tag	UNP A9CEQ7
B	-19	MET	-	expression tag	UNP A9CEQ7
B	-18	GLY	-	expression tag	UNP A9CEQ7
B	-17	SER	-	expression tag	UNP A9CEQ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP A9CEQ7
B	-15	HIS	-	expression tag	UNP A9CEQ7
B	-14	HIS	-	expression tag	UNP A9CEQ7
B	-13	HIS	-	expression tag	UNP A9CEQ7
B	-12	HIS	-	expression tag	UNP A9CEQ7
B	-11	HIS	-	expression tag	UNP A9CEQ7
B	-10	HIS	-	expression tag	UNP A9CEQ7
B	-9	SER	-	expression tag	UNP A9CEQ7
B	-8	SER	-	expression tag	UNP A9CEQ7
B	-7	GLY	-	expression tag	UNP A9CEQ7
B	-6	LEU	-	expression tag	UNP A9CEQ7
B	-5	VAL	-	expression tag	UNP A9CEQ7
B	-4	PRO	-	expression tag	UNP A9CEQ7
B	-3	ARG	-	expression tag	UNP A9CEQ7
B	-2	GLY	-	expression tag	UNP A9CEQ7
B	-1	SER	-	expression tag	UNP A9CEQ7
B	0	HIS	-	expression tag	UNP A9CEQ7
C	-19	MET	-	expression tag	UNP A9CEQ7
C	-18	GLY	-	expression tag	UNP A9CEQ7
C	-17	SER	-	expression tag	UNP A9CEQ7
C	-16	SER	-	expression tag	UNP A9CEQ7
C	-15	HIS	-	expression tag	UNP A9CEQ7
C	-14	HIS	-	expression tag	UNP A9CEQ7
C	-13	HIS	-	expression tag	UNP A9CEQ7
C	-12	HIS	-	expression tag	UNP A9CEQ7
C	-11	HIS	-	expression tag	UNP A9CEQ7
C	-10	HIS	-	expression tag	UNP A9CEQ7
C	-9	SER	-	expression tag	UNP A9CEQ7
C	-8	SER	-	expression tag	UNP A9CEQ7
C	-7	GLY	-	expression tag	UNP A9CEQ7
C	-6	LEU	-	expression tag	UNP A9CEQ7
C	-5	VAL	-	expression tag	UNP A9CEQ7
C	-4	PRO	-	expression tag	UNP A9CEQ7
C	-3	ARG	-	expression tag	UNP A9CEQ7
C	-2	GLY	-	expression tag	UNP A9CEQ7
C	-1	SER	-	expression tag	UNP A9CEQ7
C	0	HIS	-	expression tag	UNP A9CEQ7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	353	Total O 353 353	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	372	Total 372	O 372	0	0
2	C	348	Total 348	O 348	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.20Å 77.56Å 99.71Å 90.00° 95.49° 90.00°	Depositor
Resolution (Å)	31.60 – 1.60 31.60 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (31.60-1.60) 97.0 (31.60-1.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.147 , 0.181 0.149 , 0.180	Depositor DCC
R_{free} test set	5145 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14024	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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	0.61	0/2257	0.80	2/3075 (0.1%)
1	B	0.59	0/2272	0.81	2/3096 (0.1%)
1	C	0.60	0/2187	0.82	2/2978 (0.1%)
All	All	0.60	0/6716	0.81	6/9149 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	GLY	CA-C-N	6.33	126.88	120.04
1	A	39	GLY	C-N-CA	6.33	126.88	120.04
1	C	279	ASN	CA-C-N	-5.27	113.60	119.19
1	C	279	ASN	C-N-CA	-5.27	113.60	119.19
1	B	279	ASN	CA-C-N	-5.07	113.81	119.19

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	2196	2163	2153	11	0
1	B	2211	2183	2173	7	0
1	C	2119	2079	2055	8	0
2	A	353	0	0	5	2
2	B	372	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	348	0	0	3	2
All	All	7599	6425	6381	26	2

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 26 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:133:ASP:OD2	2:A:584:HOH:O	2.13	0.67
1:A:56:LEU:HD22	1:A:241:TRP:CD1	2.35	0.60
1:A:45:GLY:HA2	1:A:46:ALA:C	2.28	0.59
1:B:84:VAL:HG21	1:B:93:ALA:HB2	1.86	0.58
1:C:84:VAL:HG21	1:C:93:ALA:HB2	1.86	0.58

All (2) 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:A:478:HOH:O	2:C:479:HOH:O[2_557]	1.97	0.23
2:A:404:HOH:O	2:C:414:HOH:O[2_557]	2.16	0.04

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	282/312 (90%)	277 (98%)	5 (2%)	0	100	100
1	B	284/312 (91%)	281 (99%)	3 (1%)	0	100	100
1	C	268/312 (86%)	264 (98%)	4 (2%)	0	100	100
All	All	834/936 (89%)	822 (99%)	12 (1%)	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	221/245 (90%)	219 (99%)	2 (1%)	70	55
1	B	223/245 (91%)	222 (100%)	1 (0%)	84	75
1	C	215/245 (88%)	214 (100%)	1 (0%)	81	70
All	All	659/735 (90%)	655 (99%)	4 (1%)	78	66

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

Mol	Chain	Res	Type
1	A	19	ARG
1	A	47	LEU
1	B	19	ARG
1	C	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	C	71	ASN

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 [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, 95th 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 ²)	Q<0.9
1	A	284/312 (91%)	-0.59	2 (0%) 84 87	8, 16, 38, 63	0
1	B	286/312 (91%)	-0.59	2 (0%) 84 87	7, 16, 40, 55	0
1	C	272/312 (87%)	-0.58	4 (1%) 72 76	8, 16, 38, 52	1 (0%)
All	All	842/936 (89%)	-0.59	8 (0%) 79 83	7, 16, 39, 63	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	PRO	3.3
1	A	45	GLY	3.0
1	A	44	PRO	3.0
1	C	46	ALA	3.0
1	B	289	VAL	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.