



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:28 PM UTC

PDB ID : 9QS7 / pdb_00009qs7
Title : AcuB, Acetoin utilization protein
Authors : Zheng, L.J.; Bange, G.
Deposited on : 2025-04-04
Resolution : 2.41 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

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	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	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

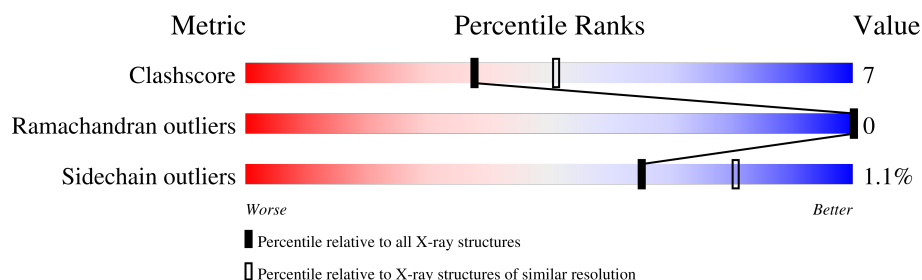
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	215	
1	B	215	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3304 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.

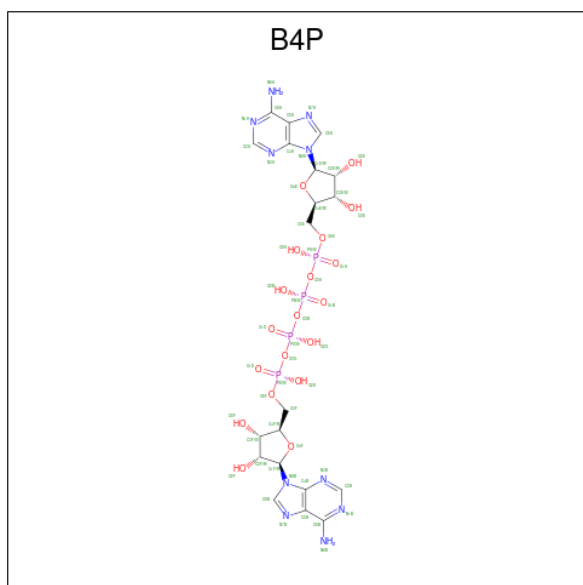
- Molecule 1 is a protein called Acetoin utilization protein AcuB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1597	1021	278	289	9			
1	B	202	Total	C	N	O	S	0	0	0
			1599	1028	274	288	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P39066
A	1	GLY	-	expression tag	UNP P39066
B	0	MET	-	initiating methionine	UNP P39066
B	1	GLY	-	expression tag	UNP P39066

- Molecule 2 is BIS(ADENOSINE)-5'-TETRAPHOSPHATE (CCD ID: B4P) (formula: $C_{20}H_{28}N_{10}O_{19}P_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
2	B	1	Total	C	N	O	P	0	0
			53	20	10	19	4		

- Molecule 3 is water.

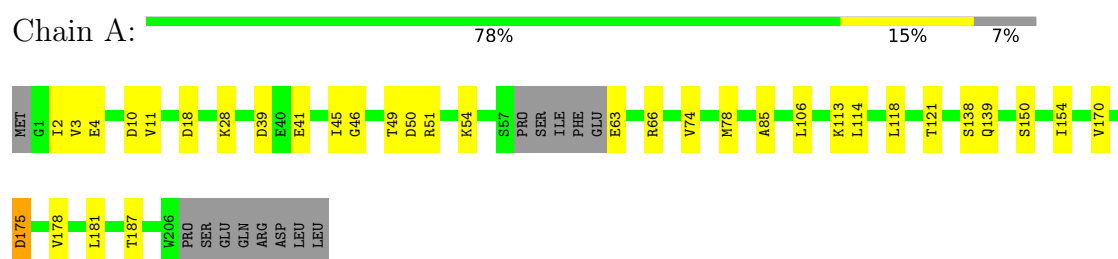
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

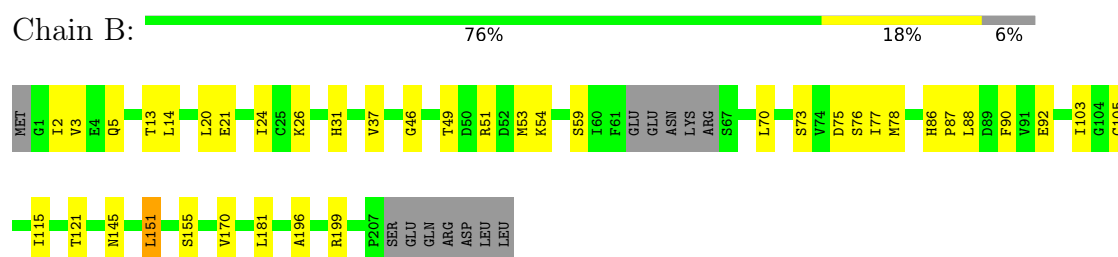
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Acetoin utilization protein AcuB



• Molecule 1: Acetoin utilization protein AcuB



4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	81.55Å 81.55Å 338.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.62 – 2.41	Depositor
% Data completeness (in resolution range)	100.0 (70.62-2.41)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.238 , 0.283	Depositor
Wilson B-factor (Å ²)	82.4	Xtriage
Anisotropy	0.218	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3304	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B4P

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	0.10	0/1624	0.26	0/2196
1	B	0.12	0/1629	0.32	0/2207
All	All	0.11	0/3253	0.29	0/4403

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1597	0	1665	26	0
1	B	1599	0	1666	27	0
2	A	53	0	24	2	0
2	B	53	0	24	4	0
3	B	2	0	0	0	0
All	All	3304	0	3379	47	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 7.

All (47) 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:39:ASP:HB3	1:A:45:ILE:HD11	1.69	0.75
1:B:14:LEU:HB2	1:B:37:VAL:HG12	1.73	0.71
1:A:28:LYS:HE2	1:B:59:SER:HA	1.76	0.68
1:A:51:ARG:HD2	1:B:31:HIS:CD2	2.31	0.66
1:A:85:ALA:HB2	1:A:106:LEU:HD12	1.81	0.62
1:B:53:MET:HE1	1:B:77:ILE:HG21	1.81	0.61
1:B:87:PRO:HG3	1:B:115:ILE:HD11	1.82	0.61
1:A:63:GLU:HG2	1:A:66:ARG:HD3	1.86	0.58
1:B:2:ILE:HG22	1:B:5:GLN:HG3	1.86	0.57
1:B:75:ASP:HA	1:B:78:MET:HE3	1.86	0.57
1:B:73:SER:O	1:B:76:SER:OG	2.22	0.57
1:A:63:GLU:OE1	1:A:66:ARG:NH1	2.38	0.56
1:B:151:LEU:O	1:B:155:SER:OG	2.23	0.54
1:A:3:VAL:HG13	1:A:118:LEU:HD11	1.92	0.52
1:A:139:GLN:HE22	1:B:90:PHE:HB3	1.75	0.51
1:A:46:GLY:HA3	1:A:78:MET:HE3	1.93	0.51
1:A:121:THR:HG21	2:B:301:B4P:H51B	1.92	0.51
2:A:301:B4P:H51A	1:B:121:THR:HG21	1.94	0.50
1:B:86:HIS:CG	1:B:87:PRO:HD2	2.47	0.49
1:A:51:ARG:HD2	1:B:31:HIS:HD2	1.78	0.49
1:B:49:THR:HG21	2:B:301:B4P:H2E	1.94	0.49
1:B:170:VAL:HG22	1:B:181:LEU:HD12	1.94	0.48
1:A:51:ARG:HH11	1:B:31:HIS:HD2	1.62	0.48
1:A:11:VAL:HG11	1:A:114:LEU:HD21	1.94	0.48
1:B:21:GLU:HA	1:B:70:LEU:HD22	1.95	0.48
1:A:28:LYS:HA	1:B:54:LYS:HD3	1.96	0.47
1:A:50:ASP:O	1:A:54:LYS:HG3	2.14	0.47
1:A:170:VAL:HG12	1:A:181:LEU:HD12	1.96	0.47
1:A:41:GLU:O	1:A:113:LYS:NZ	2.49	0.46
1:A:139:GLN:NE2	1:B:92:GLU:HB2	2.31	0.46
2:B:301:B4P:O1A	2:B:301:B4P:H8A	2.17	0.45
1:A:49:THR:HG21	2:A:301:B4P:H2F	1.98	0.45
1:B:51:ARG:HE	1:B:51:ARG:HB2	1.61	0.45
1:A:18:ASP:O	1:A:74:VAL:HG13	2.17	0.44
1:B:21:GLU:HB2	1:B:70:LEU:HB3	1.99	0.44
1:B:46:GLY:HA3	1:B:78:MET:SD	2.57	0.43
1:A:150:SER:O	1:A:154:ILE:HD12	2.18	0.43
1:A:138:SER:OG	1:A:187:THR:O	2.23	0.43
1:B:13:THR:O	1:B:26:LYS:NZ	2.50	0.42
1:B:20:LEU:O	1:B:24:ILE:HG13	2.19	0.42
1:A:10:ASP:O	2:B:301:B4P:H2B	2.20	0.41
1:B:103:ILE:HD12	1:B:105:CYS:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:O	1:A:78:MET:HB3	2.20	0.41
1:B:196:ALA:HA	1:B:199:ARG:HB2	2.03	0.41
1:A:175:ASP:HB2	1:A:178:VAL:CG1	2.50	0.41
1:B:145:ASN:N	1:B:145:ASN:HD22	2.19	0.40
1:A:2:ILE:HD12	1:A:4:GLU:HB3	2.04	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	197/215 (92%)	192 (98%)	5 (2%)	0	100	100
1	B	198/215 (92%)	193 (98%)	5 (2%)	0	100	100
All	All	395/430 (92%)	385 (98%)	10 (2%)	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	185/199 (93%)	184 (100%)	1 (0%)	81	90
1	B	186/199 (94%)	183 (98%)	3 (2%)	55	74
All	All	371/398 (93%)	367 (99%)	4 (1%)	65	81

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

Mol	Chain	Res	Type
1	A	175	ASP
1	B	3	VAL
1	B	88	LEU
1	B	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	139	GLN
1	A	162	GLN
1	B	31	HIS
1	B	145	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](#)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

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.

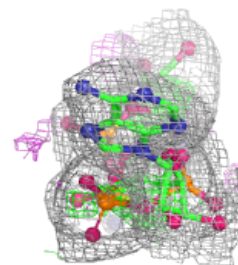
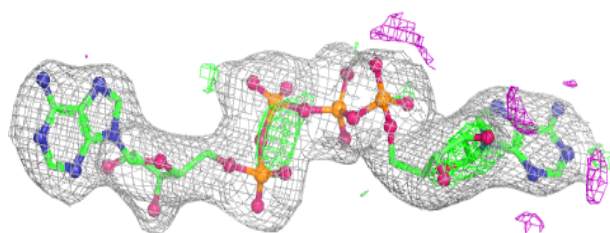
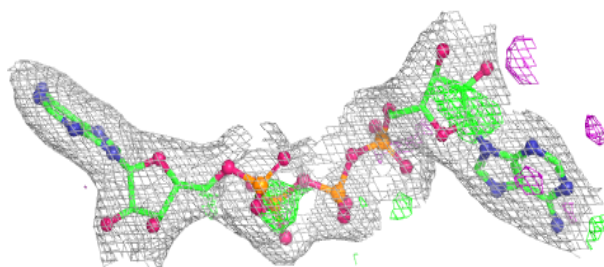
6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

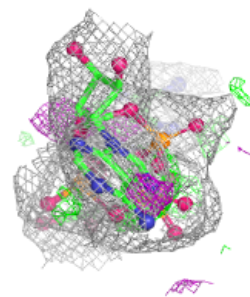
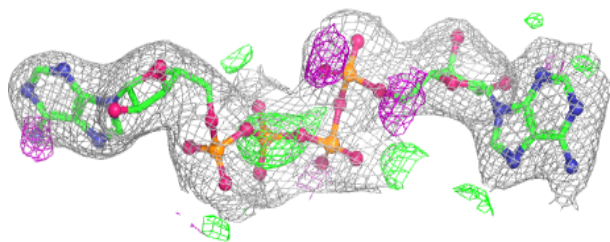
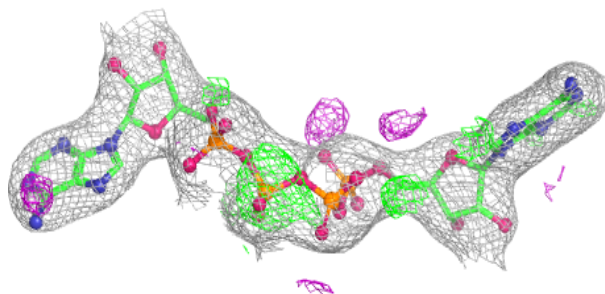
Electron density around B4P A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B4P B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.