



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:49 PM UTC

PDB ID : 1WAB / pdb_00001wab
Title : PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE
Authors : Ho, Y.S.; Swenson, L.; Derewenda, U.; Serre, L.; Wei, Y.; Dauter, Z.; Hattori, M.; Aoki, J.; Arai, H.; Adachi, T.; Inoue, K.; Derewenda, Z.S.
Deposited on : 1996-10-30
Resolution : 1.70 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

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)	:	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

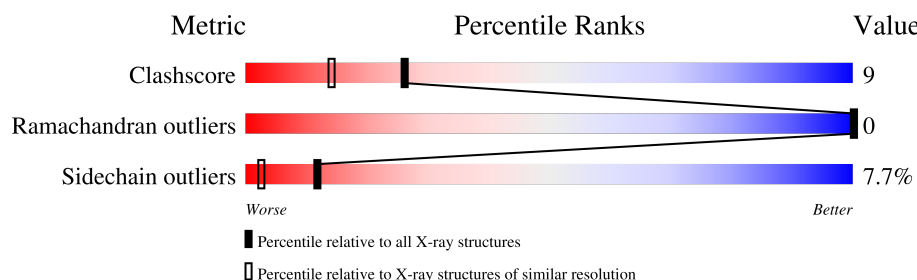
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	232	59% 24% 6% • 9%

2 Entry composition [i](#)

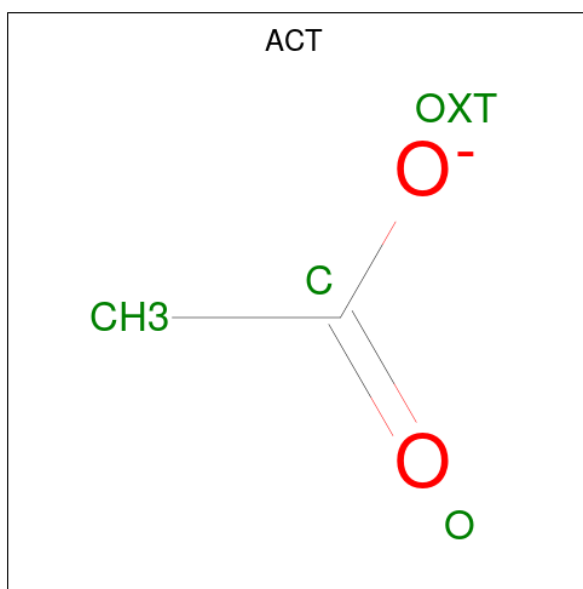
There are 3 unique types of molecules in this entry. The entry contains 1925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PLATELET-ACTIVATING FACTOR ACETYLHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	40	0	0
			1689	1066	321	297	5			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



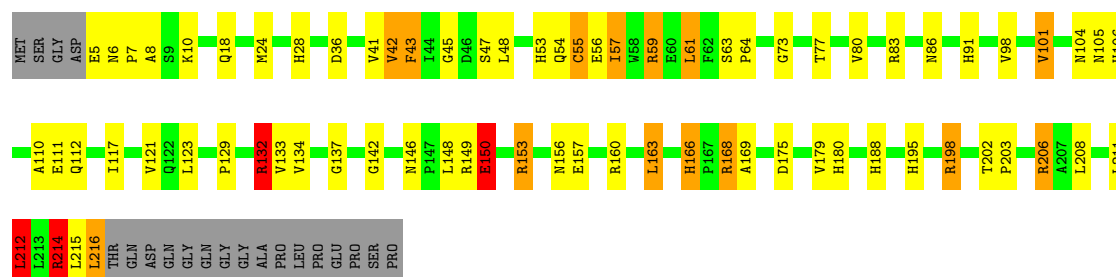
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	232	Total	O	0	0
			232	232		

Note EDS was not executed.

Chain A: 59% 24% 6% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.26Å 81.26Å 72.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.50 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (8.50-1.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, REFMAC, X-PLOR	Depositor
R, R_{free}	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1925	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: ACT

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	1.37	4/1734 (0.2%)	2.17	56/2358 (2.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ILE	C-N	-25.69	1.01	1.33
1	A	61	LEU	C-N	12.02	1.50	1.33
1	A	53	HIS	C-N	-6.81	1.23	1.33
1	A	137	GLY	CA-C	5.19	1.58	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ARG	CD-NE-CZ	23.52	157.34	124.40
1	A	57	ILE	CA-C-N	18.39	148.40	120.82
1	A	57	ILE	C-N-CA	18.39	148.40	120.82
1	A	166	HIS	CA-CB-CG	17.09	130.89	113.80
1	A	101	VAL	CB-CA-C	-15.43	89.65	111.40
1	A	160	ARG	CD-NE-CZ	14.81	145.14	124.40
1	A	214	ARG	CD-NE-CZ	14.62	144.87	124.40
1	A	57	ILE	CA-C-O	14.14	137.79	120.97
1	A	61	LEU	CA-C-N	-10.43	105.01	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LEU	C-N-CA	-10.43	105.01	122.11
1	A	175	ASP	O-C-N	8.70	128.71	121.31
1	A	150	GLU	CB-CG-CD	8.41	126.89	112.60
1	A	198	ARG	CD-NE-CZ	7.78	135.28	124.40
1	A	188	HIS	CA-CB-CG	-7.18	106.62	113.80
1	A	117	ILE	O-C-N	7.18	128.94	121.91
1	A	198	ARG	CG-CD-NE	7.09	127.61	112.00
1	A	156	ASN	OD1-CG-ND2	6.83	129.43	122.60
1	A	111	GLU	CB-CG-CD	6.81	124.17	112.60
1	A	43	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	214	ARG	N-CA-CB	6.66	119.94	109.82
1	A	41	VAL	CA-C-N	-6.49	114.64	123.14
1	A	41	VAL	C-N-CA	-6.49	114.64	123.14
1	A	106	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	98	VAL	O-C-N	6.18	129.66	123.18
1	A	59	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	132	ARG	O-C-N	6.15	129.91	122.96
1	A	117	ILE	CA-C-O	-6.04	114.77	121.17
1	A	149	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	A	59	ARG	CG-CD-NE	5.97	125.13	112.00
1	A	45	GLY	O-C-N	5.93	128.72	123.80
1	A	134	VAL	CA-C-O	-5.86	114.26	120.53
1	A	214	ARG	CG-CD-NE	5.71	124.56	112.00
1	A	104	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	18	GLN	N-CA-C	-5.57	105.52	112.93
1	A	168	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	179	VAL	O-C-N	5.46	128.95	122.83
1	A	206	ARG	CA-CB-CG	5.40	124.90	114.10
1	A	54	GLN	CA-C-N	5.39	130.57	121.14
1	A	54	GLN	C-N-CA	5.39	130.57	121.14
1	A	86	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	121	VAL	O-C-N	5.34	127.05	121.87
1	A	168	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	83	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	A	42	VAL	CA-CB-CG1	5.26	119.35	110.40
1	A	110	ALA	O-C-N	5.25	127.68	122.12
1	A	101	VAL	CA-CB-CG2	5.25	119.32	110.40
1	A	73	GLY	CA-C-O	5.21	125.99	121.41
1	A	132	ARG	CA-C-N	-5.19	116.41	123.10
1	A	132	ARG	C-N-CA	-5.19	116.41	123.10
1	A	175	ASP	CA-C-O	-5.16	115.49	119.46
1	A	91	HIS	CA-CB-CG	-5.15	108.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ILE	CB-CA-C	5.15	118.86	111.81
1	A	212	LEU	O-C-N	5.08	127.37	122.09
1	A	195	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	A	142	GLY	N-CA-C	-5.01	106.42	112.48
1	A	80	VAL	O-C-N	5.01	126.72	121.87

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	VAL	Mainchain
1	A	169	ALA	Mainchain
1	A	215	LEU	Mainchain
1	A	55	CYS	Peptide
1	A	57	ILE	Peptide

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	1689	0	1668	31	0
2	A	4	0	3	1	0
3	A	232	0	0	11	3
All	All	1925	0	1671	31	3

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 9.

All (31) 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:153:ARG:NH1	3:A:496:HOH:O	1.96	0.98
1:A:150:GLU:OE1	3:A:460:HOH:O	1.80	0.96
1:A:180:HIS:HD2	3:A:515:HOH:O	1.63	0.81
1:A:77:THR:H	1:A:105:ASN:HD21	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:HG2	3:A:402:HOH:O	1.85	0.76
1:A:214:ARG:HB2	1:A:214:ARG:HH11	1.51	0.74
1:A:47:SER:HB3	2:A:300:ACT:C	2.21	0.70
1:A:5:GLU:O	3:A:511:HOH:O	2.10	0.69
1:A:36:ASP:HB3	3:A:412:HOH:O	1.94	0.67
1:A:168:ARG:HD3	3:A:476:HOH:O	1.98	0.64
1:A:198:ARG:NH1	3:A:507:HOH:O	2.38	0.56
1:A:132:ARG:HH11	1:A:168:ARG:HG2	1.70	0.56
1:A:123:LEU:C	1:A:123:LEU:HD13	2.32	0.55
1:A:146:ASN:HD22	1:A:148:LEU:H	1.54	0.55
1:A:63:SER:HB2	1:A:64:PRO:HD3	1.93	0.51
1:A:180:HIS:CD2	3:A:515:HOH:O	2.49	0.50
1:A:129:PRO:O	1:A:168:ARG:NH2	2.45	0.50
1:A:24:MET:HG3	1:A:28:HIS:CE1	2.47	0.50
1:A:211:LEU:HA	1:A:214:ARG:HG3	1.94	0.50
1:A:150:GLU:HB3	3:A:496:HOH:O	2.13	0.49
1:A:163:LEU:HA	1:A:166:HIS:CD2	2.49	0.48
1:A:214:ARG:HH11	1:A:214:ARG:CB	2.24	0.47
1:A:153:ARG:O	1:A:157:GLU:HG3	2.15	0.46
1:A:6:ASN:ND2	1:A:8:ALA:H	2.14	0.45
1:A:48:LEU:HD12	3:A:397:HOH:O	2.16	0.45
1:A:212:LEU:O	1:A:216:LEU:HB2	2.18	0.44
1:A:168:ARG:CZ	1:A:168:ARG:HB2	2.48	0.43
1:A:6:ASN:HD21	1:A:112:GLN:HB3	1.84	0.43
1:A:6:ASN:HD22	1:A:7:PRO:HD2	1.84	0.42
1:A:43:PHE:HE2	1:A:208:LEU:HD21	1.85	0.42
1:A:202:THR:N	1:A:203:PRO:HD2	2.36	0.40

All (3) 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)
3:A:370:HOH:O	3:A:430:HOH:O[5_555]	1.89	0.31
3:A:312:HOH:O	3:A:381:HOH:O[5_555]	2.08	0.12
3:A:443:HOH:O	3:A:469:HOH:O[5_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	210/232 (90%)	200 (95%)	10 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	183/198 (92%)	169 (92%)	14 (8%)	12	2

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	42	VAL
1	A	55	CYS
1	A	56	GLU
1	A	59	ARG
1	A	61	LEU
1	A	101	VAL
1	A	132	ARG
1	A	150	GLU
1	A	163	LEU
1	A	206	ARG
1	A	212	LEU
1	A	214	ARG

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Mol	Chain	Res	Type
1	A	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	15	GLN
1	A	105	ASN
1	A	122	GLN
1	A	146	ASN
1	A	170	HIS
1	A	180	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	300	-	3,3,3	1.99	2 (66%)	3,3,3	1.14	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ACT	O-C	2.38	1.32	1.22
2	A	300	ACT	CH3-C	2.01	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	57:ILE	C	58:TRP	N	1.01

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.