



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 1MDR / pdb_00001mdr
Title : THE ROLE OF LYSINE 166 IN THE MECHANISM OF MANDELATE RACEMASE FROM PSEUDOMONAS PUTIDA: MECHANISTIC AND CRYSTALLOGRAPHIC EVIDENCE FOR STEREOSPECIFIC ALKYLATION BY (R)-ALPHA-PHENYLGLYCIDATE
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Deposited on : 1993-11-19
Resolution : 2.10 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

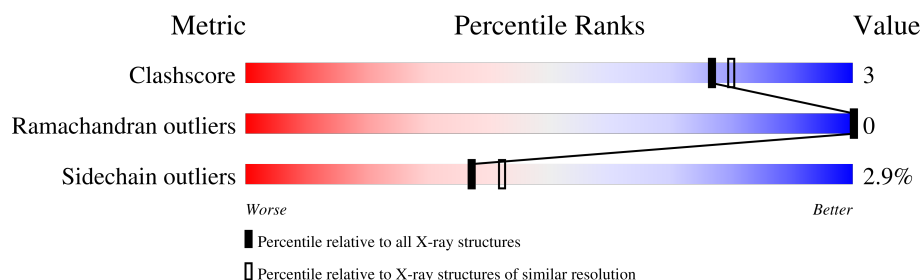
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	359	 84% 12% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2918 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.

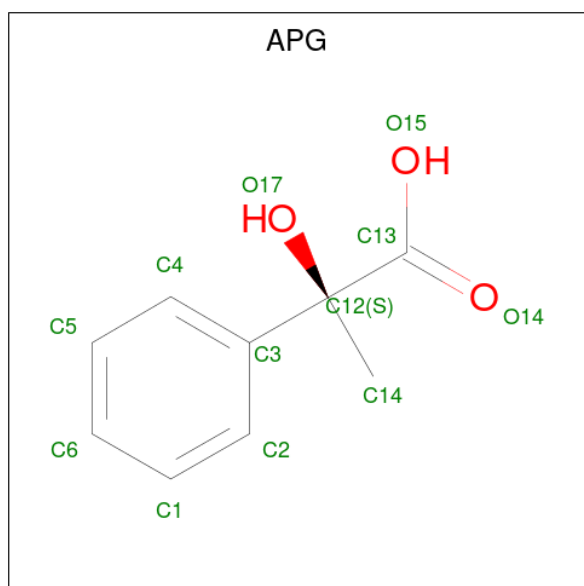
- Molecule 1 is a protein called MANDELATE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	357	2698	1727	462	496	13	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ATROLACTIC ACID (2-PHENYL-LACTIC ACID) (CCD ID: APG) (formula: C₉H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	9	3		

- Molecule 4 is water.

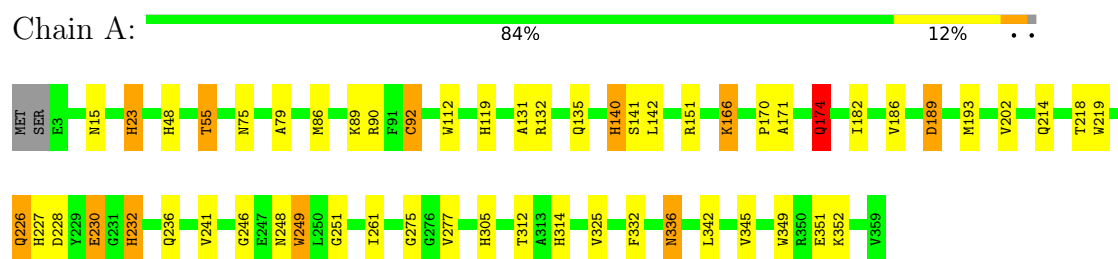
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	207	Total 207	O 207	0	0

3 Residue-property plots

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: MANDELATE RACEMASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.15Å 125.15Å 105.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2918	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.07	12/2754 (0.4%)	1.68	40/3750 (1.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	HIS	CD2-NE2	-7.29	1.29	1.37
1	A	23	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	241	VAL	CA-CB	6.32	1.62	1.54
1	A	232	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	325	VAL	CA-CB	6.17	1.62	1.54
1	A	305	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	119	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	227	HIS	CG-ND1	-5.68	1.31	1.38
1	A	345	VAL	CA-CB	5.61	1.61	1.54
1	A	314	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	140	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	312	THR	CA-CB	5.40	1.60	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	GLN	OE1-CD-NE2	-9.16	113.44	122.60
1	A	48	HIS	CB-CG-CD2	-8.78	119.79	131.20
1	A	248	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	A	132	ARG	O-C-N	-7.68	116.80	121.71
1	A	15	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	A	174	GLN	OE1-CD-NE2	-7.36	115.24	122.60
1	A	351	GLU	N-CA-C	7.01	119.82	111.33
1	A	232	HIS	CB-CG-CD2	-6.98	122.12	131.20
1	A	336	ASN	OD1-CG-ND2	-6.98	115.62	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	A	119	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	A	23	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	A	214	GLN	CB-CG-CD	6.10	122.98	112.60
1	A	342	LEU	CA-C-N	6.02	126.04	119.90
1	A	342	LEU	C-N-CA	6.02	126.04	119.90
1	A	131	ALA	O-C-N	-5.93	115.63	122.93
1	A	249	TRP	CG-CD2-CE3	5.86	139.76	133.90
1	A	226	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	202	VAL	N-CA-CB	-5.72	105.99	110.45
1	A	251	GLY	CA-C-N	5.63	125.30	119.56
1	A	251	GLY	C-N-CA	5.63	125.30	119.56
1	A	48	HIS	CB-CG-ND1	5.58	131.06	122.70
1	A	349	TRP	CE2-CD2-CG	-5.56	100.53	107.20
1	A	132	ARG	CA-C-O	-5.45	115.48	120.50
1	A	79	ALA	CA-C-N	5.43	125.51	119.32
1	A	79	ALA	C-N-CA	5.43	125.51	119.32
1	A	189	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	219	TRP	CA-CB-CG	5.32	123.71	113.60
1	A	332	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	75	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	55	THR	CA-C-N	5.21	124.88	119.56
1	A	55	THR	C-N-CA	5.21	124.88	119.56
1	A	345	VAL	CG1-CB-CG2	-5.21	99.34	110.80
1	A	275	GLY	O-C-N	-5.19	116.73	122.55
1	A	119	HIS	CB-CG-ND1	5.18	130.48	122.70
1	A	214	GLN	CG-CD-NE2	5.17	124.15	116.40
1	A	349	TRP	CB-CG-CD1	-5.09	119.27	126.90
1	A	248	ASN	CB-CG-ND2	5.07	124.01	116.40
1	A	261	ILE	CB-CG1-CD1	-5.07	103.15	113.80
1	A	336	ASN	CB-CG-ND2	5.03	123.94	116.40

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	2698	0	2748	16	0
2	A	1	0	0	0	0
3	A	12	0	8	0	0
4	A	207	0	0	1	0
All	All	2918	0	2756	16	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 3.

All (16) 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:135:GLN:HA	1:A:336:ASN:HD22	1.57	0.69
1:A:89:LYS:O	1:A:92:CYS:HB2	2.03	0.59
1:A:112:TRP:CD1	1:A:277:VAL:HB	2.42	0.55
1:A:142:LEU:N	1:A:166:LYS:HB2	2.23	0.54
1:A:171:ALA:HB3	1:A:174:GLN:NE2	2.24	0.53
1:A:193:MET:HG3	1:A:218:THR:HB	1.91	0.52
1:A:228:ASP:O	1:A:232:HIS:HD2	1.92	0.52
1:A:86:MET:O	1:A:90:ARG:HG2	2.12	0.50
1:A:230:GLU:HB3	4:A:573:HOH:O	2.15	0.46
1:A:246:GLY:HA2	1:A:249:TRP:CD2	2.52	0.45
1:A:141:SER:C	1:A:166:LYS:HB2	2.42	0.45
1:A:170:PRO:HD2	1:A:174:GLN:OE1	2.18	0.43
1:A:140:HIS:HD2	1:A:151:ARG:NH2	2.15	0.43
1:A:140:HIS:CD2	1:A:151:ARG:NH2	2.87	0.43
1:A:23:HIS:O	1:A:141:SER:HB2	2.20	0.41
1:A:182:ILE:O	1:A:186:VAL:HG22	2.21	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	355/359 (99%)	343 (97%)	12 (3%)	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	280/282 (99%)	272 (97%)	8 (3%)	37	42

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	92	CYS
1	A	166	LYS
1	A	174	GLN
1	A	189	ASP
1	A	226	GLN
1	A	230	GLU
1	A	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	214	GLN
1	A	232	HIS
1	A	336	ASN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	APG	A	399	2	11,12,12	1.96	3 (27%)	12,17,17	1.47	4 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	APG	A	399	2	-	4/12/12/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	399	APG	C12-C3	5.15	1.56	1.53
3	A	399	APG	O15-C13	-2.33	1.22	1.30
3	A	399	APG	C14-C12	2.09	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	APG	O17-C12-C3	2.49	113.39	108.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	399	APG	C4-C3-C12	-2.37	118.05	120.83
3	A	399	APG	C14-C12-C3	-2.24	107.57	111.96
3	A	399	APG	C2-C3-C12	2.09	123.28	120.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	399	APG	C3-C12-C13-O14
3	A	399	APG	C3-C12-C13-O15
3	A	399	APG	O17-C12-C13-O14
3	A	399	APG	O17-C12-C13-O15

There are no ring outliers.

No monomer is involved in short contacts.

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.