

Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 09:22 pm GMT

PDB ID : 5MHB

Title : Product-Complex of E.coli 5-Amino Laevulinic Acid Dehydratase Authors : Norton, E.; Erskine, P.T.; Shoolingin-Jordan, P.M.; Cooper, J.B.

Deposited on : 2016-11-23

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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

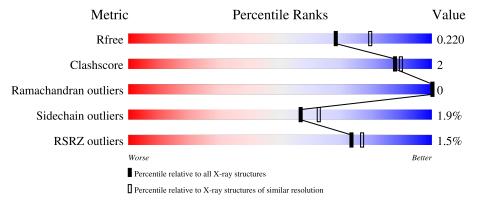
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.36 \end{tabular}$

1 Overall quality at a glance (i)

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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	· ·					
			2%						
1	A	324	88%	11%	•				



2 Entry composition (i)

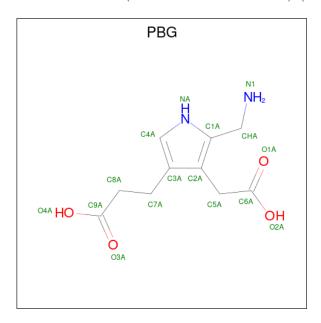
There are 5 unique types of molecules in this entry. The entry contains 2865 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Delta-aminolevulinic acid dehydratase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	323	Total	С	N	О	S	0	2	0
	11	020	2501	1564	440	478	19			

• Molecule 2 is 3-[5-(AMINOMETHYL)-4-(CARBOXYMETHYL)-1H-PYRROL-3-YL]PRO PANOIC ACID (three-letter code: PBG) (formula: C₁₀H₁₄N₂O₄).



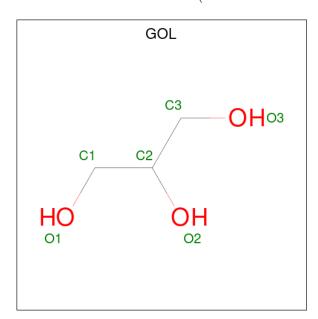
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 16	C 10	N 2	O 4	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Zn 3 3	0	0



• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

• Molecule 5 is water.

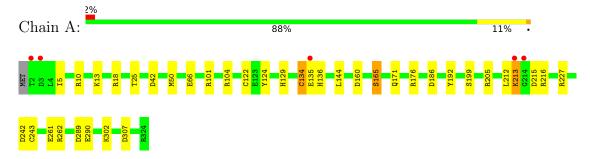
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	327	Total O 327 327	0	0



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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: Delta-aminolevulinic acid dehydratase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants	128.62Å 128.62Å 142.81Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.57 - 2.10	Depositor
Resolution (A)	36.67 - 2.10	EDS
% Data completeness	99.0 (95.57-2.10)	Depositor
(in resolution range)	99.0 (36.67-2.10)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
D D.	0.157 , 0.213	Depositor
R, R_{free}	0.169 , 0.220	DCC
R_{free} test set	1761 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 63.8	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2865	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: ZN, GOL, PBG

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	Boı	nd lengths	Bond angles		
		Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
	1	A	1.44	8/2543 (0.3%)	1.32	19/3424 (0.6%)	

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
1	A	290	GLU	CD-OE1	-8.90	1.15	1.25
1	A	124	TYR	CE1-CZ	8.11	1.49	1.38
1	A	243	CYS	CB-SG	7.07	1.94	1.82
1	A	165	SER	CB-OG	-6.98	1.33	1.42
1	A	261	GLU	CD-OE1	-6.26	1.18	1.25
1	A	199	SER	CB-OG	5.94	1.50	1.42
1	A	66	GLU	CD-OE2	5.75	1.31	1.25
1	A	242	ASP	CB-CG	5.07	1.62	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	289	ASP	CB-CG-OD1	10.50	127.75	118.30
1	A	176	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	A	186	ASP	CB-CG-OD2	-9.88	109.40	118.30
1	A	302	LYS	CD-CE-NZ	9.61	133.80	111.70
1	A	186	ASP	CB-CG-OD1	9.10	126.49	118.30
1	A	160	ASP	CB-CG-OD1	-7.62	111.44	118.30
1	A	307	ASP	CB-CG-OD1	-7.36	111.68	118.30
1	A	101	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	289	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	42	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	18	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	10	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	215	ASP	CB-CG-OD1	5.59	123.33	118.30



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	101	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	50	MET	CG-SD-CE	-5.36	91.62	100.20
1	A	216	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	262	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	18	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	104	ARG	CG-CD-NE	5.02	122.33	111.80

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	2501	0	2496	9	0
2	A	16	0	11	2	0
3	A	3	0	0	0	0
4	A	18	0	24	0	0
5	A	327	0	0	3	1
All	All	2865	0	2531	10	1

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.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:25:THR:HG22	5:A:617:HOH:O	2.02	0.59
1:A:13:LYS:NZ	5:A:504:HOH:O	2.44	0.50
1:A:129:HIS:CE1	1:A:212:LEU:HD11	2.49	0.48
1:A:134:CYS:SG	1:A:136:HIS:CE1	3.08	0.46
2:A:401:PBG:HHA1	2:A:401:PBG:O2A	2.17	0.44
1:A:122:CYS:SG	2:A:401:PBG:HHA2	2.59	0.43
1:A:213:LYS:HD3	1:A:213:LYS:N	2.34	0.43
1:A:227[B]:ARG:HD3	5:A:675:HOH:O	2.18	0.42
1:A:165:SER:HB3	1:A:192:TYR:CE1	2.54	0.42



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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:144:LEU:HD22	1:A:171:GLN:HA	2.01	0.42

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
5:A:689:HOH:O	5:A:739:HOH:O[5_555]	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	323/324 (100%)	315 (98%)	8 (2%)	0	100 1	.00

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	260/259 (100%)	255 (98%)	5 (2%)	57 63	

All (5) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	5	ILE
1	A	134	CYS
1	A	135	GLU
1	A	205	ARG
1	A	213	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	136	HIS
1	A	271	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	Pog	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
WIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	407	-	5,5,5	0.62	0	5,5,5	0.73	0



Mol	Mol Type Chain Re		Res	Link	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PBG	A	401	3	15,16,16	3.68	6 (40%)	15,21,21	2.32	5 (33%)
4	GOL	A	406	-	5,5,5	0.27	0	5,5,5	0.79	0
4	GOL	A	405	-	5,5,5	1.00	0	5,5,5	1.27	0

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
4	GOL	A	407	-	-	2/4/4/4	-
2	PBG	A	401	3	-	3/9/11/11	0/1/1/1
4	GOL	A	406	-	-	0/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
2	A	401	PBG	CHA-C1A	-10.59	1.39	1.51
2	A	401	PBG	C5A-C2A	-6.30	1.38	1.51
2	A	401	PBG	C7A-C3A	4.61	1.60	1.51
2	A	401	PBG	C5A-C6A	-2.60	1.45	1.51
2	A	401	PBG	C8A-C9A	2.37	1.56	1.50
2	A	401	PBG	O2A-C6A	-2.22	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	401	PBG	CHA-C1A-C2A	-5.08	120.30	130.00
2	A	401	PBG	C2A-C5A-C6A	4.95	120.14	114.21
2	A	401	PBG	C7A-C8A-C9A	-2.76	106.01	113.76
2	A	401	PBG	O3A-C9A-C8A	-2.33	115.59	123.08
2	A	401	PBG	O4A-C9A-C8A	2.02	120.51	114.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PBG	C2A-C3A-C7A-C8A
4	A	405	GOL	C1-C2-C3-O3



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Mol	Chain	Res	Type	Atoms
4	A	405	GOL	O2-C2-C3-O3
4	A	407	GOL	C1-C2-C3-O3
4	A	407	GOL	O2-C2-C3-O3
2	A	401	PBG	C2A-C5A-C6A-O2A
2	A	401	PBG	C2A-C5A-C6A-O1A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PBG	2	0

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^{th} 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	323/324 (99%)	-0.41	5 (1%) 73 77	15, 32, 56, 93	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	LYS	3.6
1	A	2	THR	2.4
1	A	135	GLU	2.4
1	A	3	ASP	2.4
1	A	214	GLY	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 monosaccharides 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	GOL	A	407	6/6	0.79	0.22	55,80,82,83	0
4	GOL	A	405	6/6	0.80	0.22	55,60,60,63	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	GOL	A	406	6/6	0.85	0.20	57,62,66,70	0
2	PBG	A	401	16/16	0.97	0.12	22,33,39,47	0
3	ZN	A	403	1/1	0.99	0.04	31,31,31,31	0
3	ZN	A	404	1/1	1.00	0.02	33,33,33,33	0
3	ZN	A	402	1/1	1.00	0.01	42,42,42,42	1

6.5 Other polymers (i)

There are no such residues in this entry.

