wwPDB X-ray Structure Validation Summary Report (i)

Dec 6, 2023 – 01:23 pm GMT

PDB ID	:	1W56
Title	:	Stepwise introduction of zinc binding site into porphobilinogen synthase of Pseudomonas aeruginosa (mutations A129C and D131C)
Authors	:	Frere, F.; Reents, H.; Schubert, W.-D.; Heinz, D.W.; Jahn, D.
Deposited on	:	2004-08-05
Resolution	:	1.70 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 (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 (i)) were used in the production of this report:

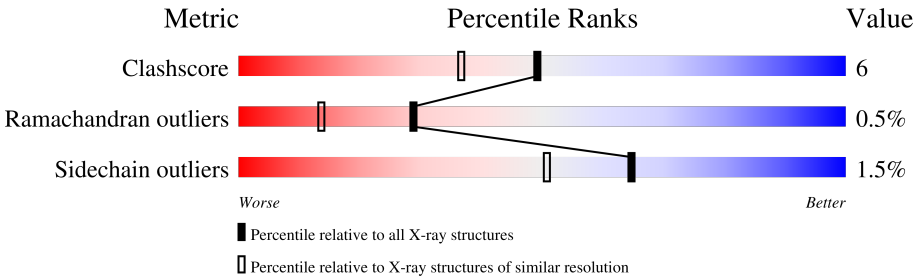
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	85% 12%
1	B	337	78% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6209 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.

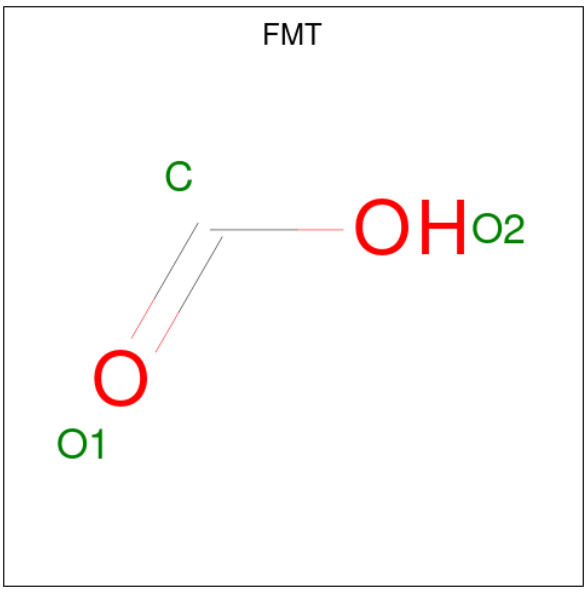
- Molecule 1 is a protein called DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	26	1
			2763	1731	495	520	17			
1	B	324	Total	C	N	O	S	0	28	1
			2740	1717	486	520	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	CYS	ALA	engineered mutation	UNP Q59643
A	131	CYS	ASP	engineered mutation	UNP Q59643
B	129	CYS	ALA	engineered mutation	UNP Q59643
B	131	CYS	ASP	engineered mutation	UNP Q59643
A	199	VAL	ILE	SEE REMARK 999	UNP Q59643
B	199	VAL	ILE	SEE REMARK 999	UNP Q59643

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	356	Total O 356 356	0	0
6	B	337	Total O 337 337	0	0

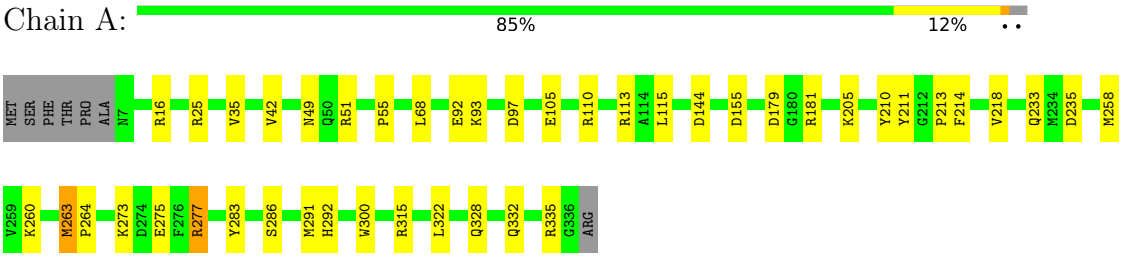
3 Residue-property plots (i)

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. 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.

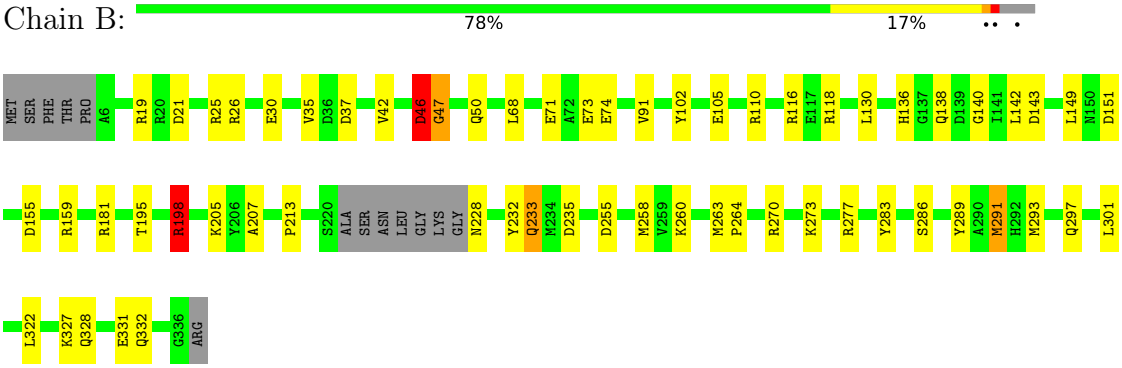
• Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE

Chain A:



• Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.32Å 126.32Å 85.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 1.70	Depositor
% Data completeness (in resolution range)	98.5 (87.71-1.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.138 , 0.182	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6209	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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: K, ZN, MG, FMT

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	1.16	2/2810 (0.1%)	1.17	15/3805 (0.4%)
1	B	1.19	4/2786 (0.1%)	1.22	17/3774 (0.5%)
All	All	1.18	6/5596 (0.1%)	1.19	32/7579 (0.4%)

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	B	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	GLU	CD-OE2	6.22	1.32	1.25
1	B	102	TYR	CE1-CZ	-6.05	1.30	1.38
1	B	233	GLN	CD-OE1	5.78	1.36	1.24
1	A	92	GLU	CD-OE1	5.49	1.31	1.25
1	B	71	GLU	CD-OE2	-5.43	1.19	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	16	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	51	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	97	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	47	GLY	N-CA-C	8.03	133.18	113.10
1	A	51	ARG	NE-CZ-NH2	-8.03	116.29	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	46[B]	ASP	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	2763	0	2735	35	0
1	B	2740	0	2696	35	0
2	A	3	0	1	0	0
2	B	3	0	1	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	356	0	0	19	0
6	B	337	0	0	5	0
All	All	6209	0	5433	65	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 6.

The worst 5 of 65 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:263[B]:MET:HE3	6:A:2339:HOH:O	1.38	1.19
1:A:275[B]:GLU:HG2	6:A:2314:HOH:O	1.44	1.15
1:A:277[A]:ARG:NH1	6:A:2317:HOH:O	1.89	1.03
1:A:263[B]:MET:CE	6:A:2339:HOH:O	1.96	1.03
1:A:263[A]:MET:HE3	1:B:263[A]:MET:HG2	1.40	1.03

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	354/337 (105%)	348 (98%)	5 (1%)	1 (0%)	41 24
1	B	348/337 (103%)	335 (96%)	10 (3%)	3 (1%)	17 5
All	All	702/674 (104%)	683 (97%)	15 (2%)	4 (1%)	29 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ARG
1	B	47	GLY
1	B	46[A]	ASP
1	B	46[B]	ASP

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	290/270 (107%)	287 (99%)	3 (1%)	76 67
1	B	288/270 (107%)	282 (98%)	6 (2%)	53 36
All	All	578/540 (107%)	569 (98%)	9 (2%)	65 48

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	291[A]	MET
1	B	291[B]	MET

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Mol	Chain	Res	Type
1	B	181	ARG
1	B	198	ARG
1	B	228	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	233	GLN
1	B	297	GLN
1	B	332	GLN
1	A	332	GLN
1	A	7	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	FMT	B	1337	-	2,2,2	0.89	0	1,1,1	0.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMT	A	1337	-	2,2,2	0.76	0	1,1,1	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.