



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 1, 2023 – 11:08 PM EDT

PDB ID : 6ND3
Title : wild-type choline TMA lyase in complex with betaine aldehyde
Authors : Funk, M.A.; Drennan, C.L.
Deposited on : 2018-12-13
Resolution : 2.36 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 ⓘ 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 2.36 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 52117 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 Choline trimethylamine-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	795	6272	3975	1063	1189	45	0	1	0
1	B	794	6284	3982	1064	1192	46	0	3	0
1	C	795	6277	3978	1064	1190	45	0	1	0
1	D	796	6299	3991	1067	1195	46	0	3	0
1	E	795	6264	3971	1062	1186	45	0	0	0
1	F	794	6284	3982	1064	1192	46	0	3	0
1	G	795	6277	3978	1064	1190	45	0	1	0
1	H	796	6291	3987	1066	1192	46	0	2	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q30W70
A	-1	GLY	-	expression tag	UNP Q30W70
A	0	SER	-	expression tag	UNP Q30W70
A	1	SER	-	expression tag	UNP Q30W70
A	2	HIS	-	expression tag	UNP Q30W70
A	3	HIS	-	expression tag	UNP Q30W70
A	4	HIS	-	expression tag	UNP Q30W70
A	5	HIS	-	expression tag	UNP Q30W70
A	6	HIS	-	expression tag	UNP Q30W70
A	7	HIS	-	expression tag	UNP Q30W70
A	8	SER	-	expression tag	UNP Q30W70
A	9	SER	-	expression tag	UNP Q30W70
A	10	GLY	-	expression tag	UNP Q30W70

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	LEU	-	expression tag	UNP Q30W70
A	12	VAL	-	expression tag	UNP Q30W70
A	13	PRO	-	expression tag	UNP Q30W70
A	14	ARG	-	expression tag	UNP Q30W70
A	15	GLY	-	expression tag	UNP Q30W70
A	16	SER	-	expression tag	UNP Q30W70
A	17	HIS	-	expression tag	UNP Q30W70
A	18	MET	-	expression tag	UNP Q30W70
B	-2	MET	-	expression tag	UNP Q30W70
B	-1	GLY	-	expression tag	UNP Q30W70
B	0	SER	-	expression tag	UNP Q30W70
B	1	SER	-	expression tag	UNP Q30W70
B	2	HIS	-	expression tag	UNP Q30W70
B	3	HIS	-	expression tag	UNP Q30W70
B	4	HIS	-	expression tag	UNP Q30W70
B	5	HIS	-	expression tag	UNP Q30W70
B	6	HIS	-	expression tag	UNP Q30W70
B	7	HIS	-	expression tag	UNP Q30W70
B	8	SER	-	expression tag	UNP Q30W70
B	9	SER	-	expression tag	UNP Q30W70
B	10	GLY	-	expression tag	UNP Q30W70
B	11	LEU	-	expression tag	UNP Q30W70
B	12	VAL	-	expression tag	UNP Q30W70
B	13	PRO	-	expression tag	UNP Q30W70
B	14	ARG	-	expression tag	UNP Q30W70
B	15	GLY	-	expression tag	UNP Q30W70
B	16	SER	-	expression tag	UNP Q30W70
B	17	HIS	-	expression tag	UNP Q30W70
B	18	MET	-	expression tag	UNP Q30W70
C	-2	MET	-	expression tag	UNP Q30W70
C	-1	GLY	-	expression tag	UNP Q30W70
C	0	SER	-	expression tag	UNP Q30W70
C	1	SER	-	expression tag	UNP Q30W70
C	2	HIS	-	expression tag	UNP Q30W70
C	3	HIS	-	expression tag	UNP Q30W70
C	4	HIS	-	expression tag	UNP Q30W70
C	5	HIS	-	expression tag	UNP Q30W70
C	6	HIS	-	expression tag	UNP Q30W70
C	7	HIS	-	expression tag	UNP Q30W70
C	8	SER	-	expression tag	UNP Q30W70
C	9	SER	-	expression tag	UNP Q30W70
C	10	GLY	-	expression tag	UNP Q30W70

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	LEU	-	expression tag	UNP Q30W70
C	12	VAL	-	expression tag	UNP Q30W70
C	13	PRO	-	expression tag	UNP Q30W70
C	14	ARG	-	expression tag	UNP Q30W70
C	15	GLY	-	expression tag	UNP Q30W70
C	16	SER	-	expression tag	UNP Q30W70
C	17	HIS	-	expression tag	UNP Q30W70
C	18	MET	-	expression tag	UNP Q30W70
D	-2	MET	-	expression tag	UNP Q30W70
D	-1	GLY	-	expression tag	UNP Q30W70
D	0	SER	-	expression tag	UNP Q30W70
D	1	SER	-	expression tag	UNP Q30W70
D	2	HIS	-	expression tag	UNP Q30W70
D	3	HIS	-	expression tag	UNP Q30W70
D	4	HIS	-	expression tag	UNP Q30W70
D	5	HIS	-	expression tag	UNP Q30W70
D	6	HIS	-	expression tag	UNP Q30W70
D	7	HIS	-	expression tag	UNP Q30W70
D	8	SER	-	expression tag	UNP Q30W70
D	9	SER	-	expression tag	UNP Q30W70
D	10	GLY	-	expression tag	UNP Q30W70
D	11	LEU	-	expression tag	UNP Q30W70
D	12	VAL	-	expression tag	UNP Q30W70
D	13	PRO	-	expression tag	UNP Q30W70
D	14	ARG	-	expression tag	UNP Q30W70
D	15	GLY	-	expression tag	UNP Q30W70
D	16	SER	-	expression tag	UNP Q30W70
D	17	HIS	-	expression tag	UNP Q30W70
D	18	MET	-	expression tag	UNP Q30W70
E	-2	MET	-	expression tag	UNP Q30W70
E	-1	GLY	-	expression tag	UNP Q30W70
E	0	SER	-	expression tag	UNP Q30W70
E	1	SER	-	expression tag	UNP Q30W70
E	2	HIS	-	expression tag	UNP Q30W70
E	3	HIS	-	expression tag	UNP Q30W70
E	4	HIS	-	expression tag	UNP Q30W70
E	5	HIS	-	expression tag	UNP Q30W70
E	6	HIS	-	expression tag	UNP Q30W70
E	7	HIS	-	expression tag	UNP Q30W70
E	8	SER	-	expression tag	UNP Q30W70
E	9	SER	-	expression tag	UNP Q30W70
E	10	GLY	-	expression tag	UNP Q30W70

Continued on next page...

Continued from previous page...

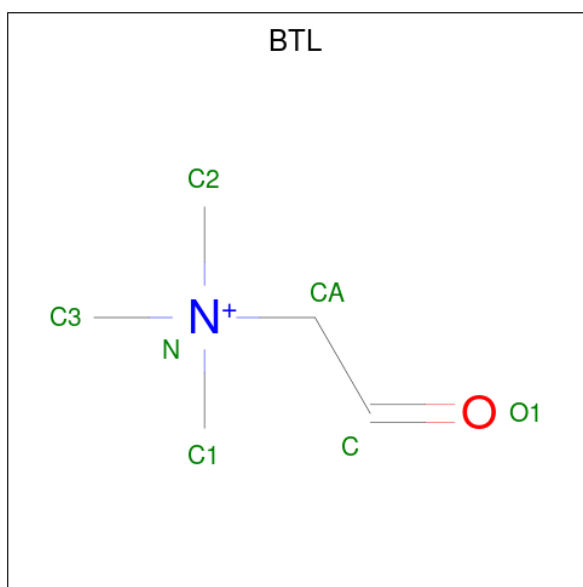
Chain	Residue	Modelled	Actual	Comment	Reference
E	11	LEU	-	expression tag	UNP Q30W70
E	12	VAL	-	expression tag	UNP Q30W70
E	13	PRO	-	expression tag	UNP Q30W70
E	14	ARG	-	expression tag	UNP Q30W70
E	15	GLY	-	expression tag	UNP Q30W70
E	16	SER	-	expression tag	UNP Q30W70
E	17	HIS	-	expression tag	UNP Q30W70
E	18	MET	-	expression tag	UNP Q30W70
F	-2	MET	-	expression tag	UNP Q30W70
F	-1	GLY	-	expression tag	UNP Q30W70
F	0	SER	-	expression tag	UNP Q30W70
F	1	SER	-	expression tag	UNP Q30W70
F	2	HIS	-	expression tag	UNP Q30W70
F	3	HIS	-	expression tag	UNP Q30W70
F	4	HIS	-	expression tag	UNP Q30W70
F	5	HIS	-	expression tag	UNP Q30W70
F	6	HIS	-	expression tag	UNP Q30W70
F	7	HIS	-	expression tag	UNP Q30W70
F	8	SER	-	expression tag	UNP Q30W70
F	9	SER	-	expression tag	UNP Q30W70
F	10	GLY	-	expression tag	UNP Q30W70
F	11	LEU	-	expression tag	UNP Q30W70
F	12	VAL	-	expression tag	UNP Q30W70
F	13	PRO	-	expression tag	UNP Q30W70
F	14	ARG	-	expression tag	UNP Q30W70
F	15	GLY	-	expression tag	UNP Q30W70
F	16	SER	-	expression tag	UNP Q30W70
F	17	HIS	-	expression tag	UNP Q30W70
F	18	MET	-	expression tag	UNP Q30W70
G	-2	MET	-	expression tag	UNP Q30W70
G	-1	GLY	-	expression tag	UNP Q30W70
G	0	SER	-	expression tag	UNP Q30W70
G	1	SER	-	expression tag	UNP Q30W70
G	2	HIS	-	expression tag	UNP Q30W70
G	3	HIS	-	expression tag	UNP Q30W70
G	4	HIS	-	expression tag	UNP Q30W70
G	5	HIS	-	expression tag	UNP Q30W70
G	6	HIS	-	expression tag	UNP Q30W70
G	7	HIS	-	expression tag	UNP Q30W70
G	8	SER	-	expression tag	UNP Q30W70
G	9	SER	-	expression tag	UNP Q30W70
G	10	GLY	-	expression tag	UNP Q30W70

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	11	LEU	-	expression tag	UNP Q30W70
G	12	VAL	-	expression tag	UNP Q30W70
G	13	PRO	-	expression tag	UNP Q30W70
G	14	ARG	-	expression tag	UNP Q30W70
G	15	GLY	-	expression tag	UNP Q30W70
G	16	SER	-	expression tag	UNP Q30W70
G	17	HIS	-	expression tag	UNP Q30W70
G	18	MET	-	expression tag	UNP Q30W70
H	-2	MET	-	expression tag	UNP Q30W70
H	-1	GLY	-	expression tag	UNP Q30W70
H	0	SER	-	expression tag	UNP Q30W70
H	1	SER	-	expression tag	UNP Q30W70
H	2	HIS	-	expression tag	UNP Q30W70
H	3	HIS	-	expression tag	UNP Q30W70
H	4	HIS	-	expression tag	UNP Q30W70
H	5	HIS	-	expression tag	UNP Q30W70
H	6	HIS	-	expression tag	UNP Q30W70
H	7	HIS	-	expression tag	UNP Q30W70
H	8	SER	-	expression tag	UNP Q30W70
H	9	SER	-	expression tag	UNP Q30W70
H	10	GLY	-	expression tag	UNP Q30W70
H	11	LEU	-	expression tag	UNP Q30W70
H	12	VAL	-	expression tag	UNP Q30W70
H	13	PRO	-	expression tag	UNP Q30W70
H	14	ARG	-	expression tag	UNP Q30W70
H	15	GLY	-	expression tag	UNP Q30W70
H	16	SER	-	expression tag	UNP Q30W70
H	17	HIS	-	expression tag	UNP Q30W70
H	18	MET	-	expression tag	UNP Q30W70

- Molecule 2 is BETAINE ALDEHYDE (three-letter code: BTL) (formula: C₅H₁₂NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		
2	C	1	Total	C	N	O	0	0
			7	5	1	1		
2	D	1	Total	C	N	O	0	0
			7	5	1	1		
2	E	1	Total	C	N	O	0	0
			7	5	1	1		
2	F	1	Total	C	N	O	0	0
			7	5	1	1		
2	G	1	Total	C	N	O	0	0
			7	5	1	1		
2	H	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	308	Total	O	0	0
			308	308		
3	B	118	Total	O	0	0
			118	118		
3	C	305	Total	O	0	0
			305	305		
3	D	273	Total	O	0	0
			273	273		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	264	Total 264	O 264	0	0
3	F	81	Total 81	O 81	0	0
3	G	258	Total 258	O 258	0	0
3	H	206	Total 206	O 206	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.22Å 234.70Å 159.02Å 90.00° 109.04° 90.00°	Depositor
Resolution (Å)	49.73 – 2.36	Depositor
% Data completeness (in resolution range)	98.8 (49.73-2.36)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.37Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.186 , 0.216	Depositor
Wilson B-factor (Å ²)	43.6	Xtrriage
Anisotropy	0.407	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
Total number of atoms	52117	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0658e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

8 ligands are 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	BTL	H	901	1	6,6,6	2.24	3 (50%)	4,8,8	2.53	1 (25%)
2	BTL	A	901	1	6,6,6	2.19	2 (33%)	4,8,8	2.58	1 (25%)
2	BTL	E	901	1	6,6,6	2.24	3 (50%)	4,8,8	2.53	1 (25%)
2	BTL	C	901	1	6,6,6	2.27	3 (50%)	4,8,8	2.40	1 (25%)
2	BTL	D	901	1	6,6,6	2.21	3 (50%)	4,8,8	2.41	1 (25%)
2	BTL	F	901	1	6,6,6	2.24	3 (50%)	4,8,8	2.61	1 (25%)
2	BTL	G	901	1	6,6,6	2.22	3 (50%)	4,8,8	2.53	1 (25%)
2	BTL	B	901	1	6,6,6	2.26	3 (50%)	4,8,8	2.59	1 (25%)

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
2	BTL	H	901	1	-	1/3/4/4	-
2	BTL	A	901	1	-	1/3/4/4	-
2	BTL	E	901	1	-	1/3/4/4	-
2	BTL	C	901	1	-	1/3/4/4	-
2	BTL	D	901	1	-	1/3/4/4	-
2	BTL	F	901	1	-	1/3/4/4	-
2	BTL	G	901	1	-	1/3/4/4	-
2	BTL	B	901	1	-	1/3/4/4	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	BTL	O1-C	3.91	1.42	1.19
2	B	901	BTL	O1-C	3.90	1.42	1.19
2	D	901	BTL	O1-C	3.86	1.41	1.19
2	H	901	BTL	O1-C	3.86	1.41	1.19
2	E	901	BTL	O1-C	3.86	1.41	1.19

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	BTL	O1-C-CA	-5.20	110.69	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	BTL	O1-C-CA	-5.16	110.81	126.39
2	A	901	BTL	O1-C-CA	-5.12	110.92	126.39
2	H	901	BTL	O1-C-CA	-5.05	111.16	126.39
2	G	901	BTL	O1-C-CA	-5.03	111.19	126.39

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	BTL	C-CA-N-C2
2	B	901	BTL	C-CA-N-C2
2	C	901	BTL	C-CA-N-C2
2	D	901	BTL	C-CA-N-C2
2	E	901	BTL	C-CA-N-C2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.