



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 09:08 am BST

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

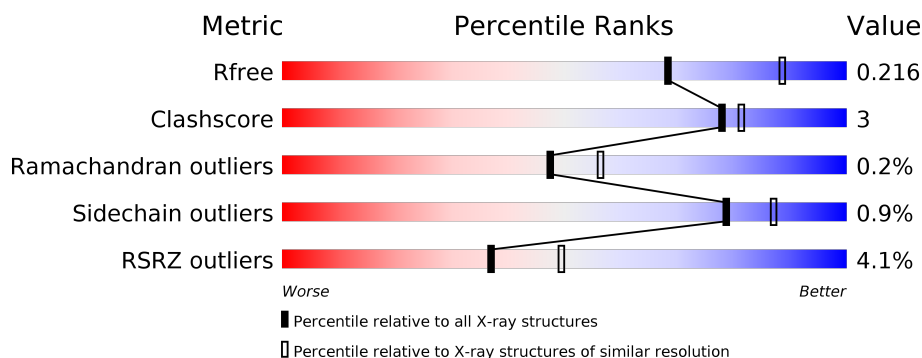
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 Å.

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))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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 $\leq 5\%$. 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
1	A	849	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 88%, yellow 88%, yellow 93%, grey 93%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 88% 5% 6% </div> </div>
1	B	849	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, orange 7%, orange 85%, yellow 85%, yellow 88%, grey 88%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 7% 85% 8% 6% </div> </div>
1	C	849	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 87%, yellow 87%, yellow 93%, grey 93%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 87% 6% 6% </div> </div>
1	D	849	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 85%, yellow 85%, yellow 88%, grey 88%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 85% 8% 6% </div> </div>
1	E	849	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 86%, yellow 86%, yellow 93%, grey 93%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 86% 7% 6% </div> </div>
1	F	849	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 13%, orange 13%, orange 86%, yellow 86%, yellow 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 13% 86% 8% 6% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	849	<div><div>%</div><div><div></div><div>85%</div><div>8%</div><div>6%</div></div></div>
1	H	849	<div><div>2%</div><div><div></div><div>87%</div><div>6%</div><div>6%</div></div></div>

2 Entry composition

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

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

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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

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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

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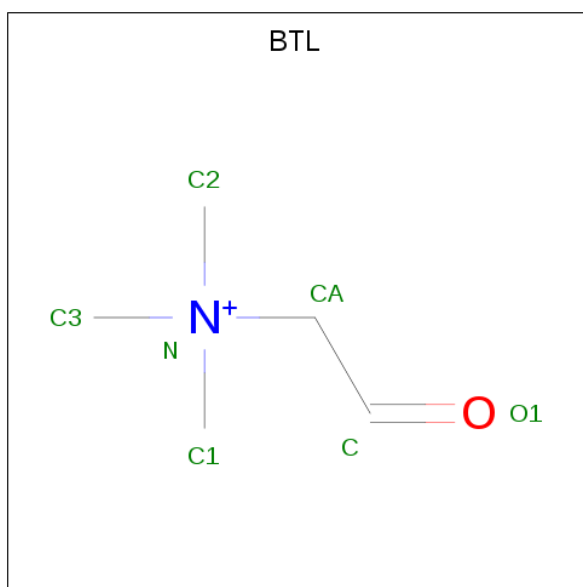
Chain	Residue	Modelled	Actual	Comment	Reference
E	11	LEU	-	expression tag	UNP Q30W70
E	12	VAL	-	expression tag	UNP Q30W70
E	13	PRO	-	expression tag	UNP Q30W70
E	14	ARG	-	expression tag	UNP Q30W70
E	15	GLY	-	expression tag	UNP Q30W70
E	16	SER	-	expression tag	UNP Q30W70
E	17	HIS	-	expression tag	UNP Q30W70
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

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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 BETAINES 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		

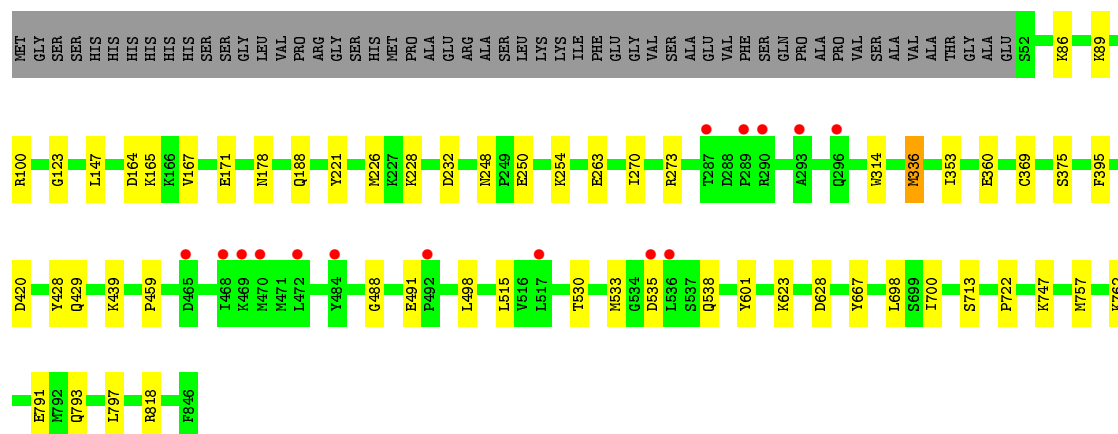
- Molecule 3 is water.

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		

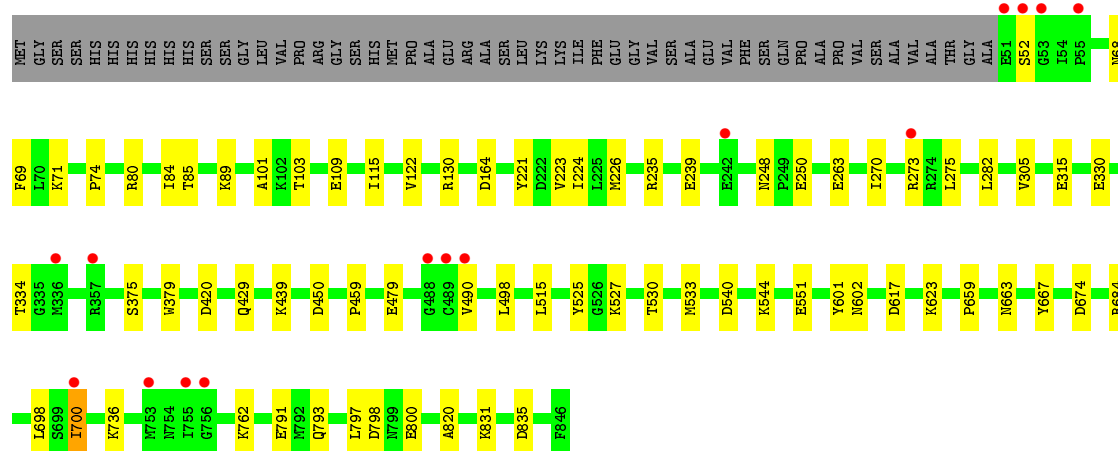
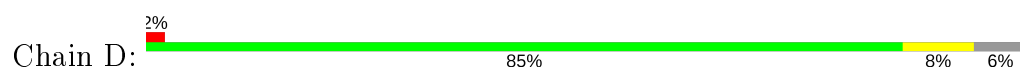
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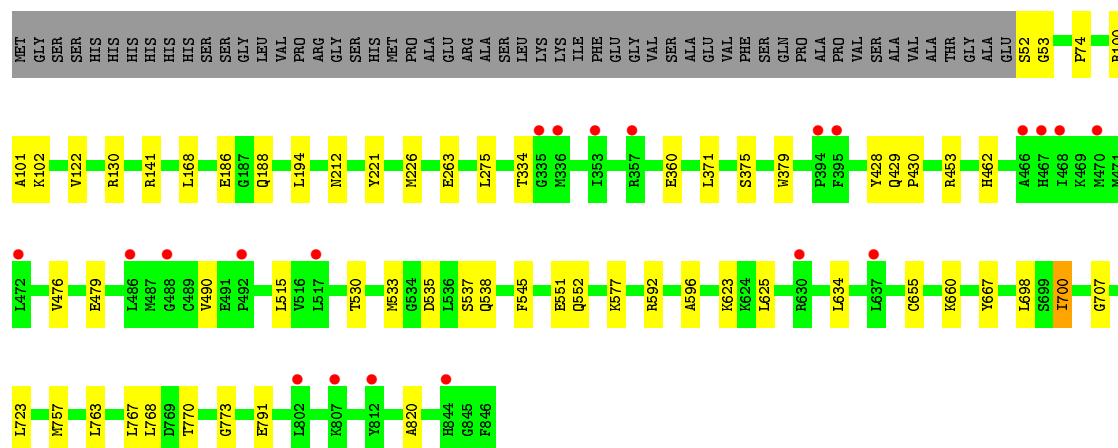
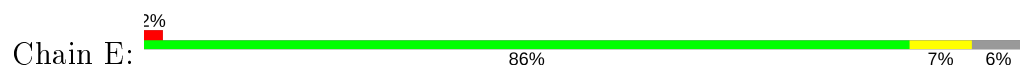
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	264	Total 264	O 264	0	0
3	F	81	Total 81	O 81	0	0
3	G	258	Total 258	O 258	0	0
3	H	206	Total 206	O 206	0	0



• Molecule 1: Choline trimethylamine-lyase



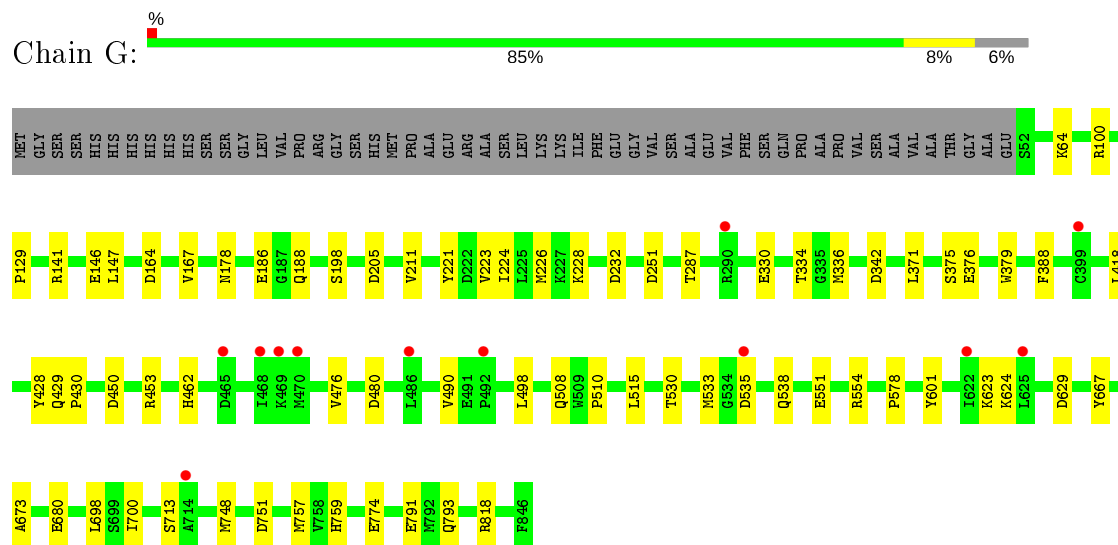
• Molecule 1: Choline trimethylamine-lyase



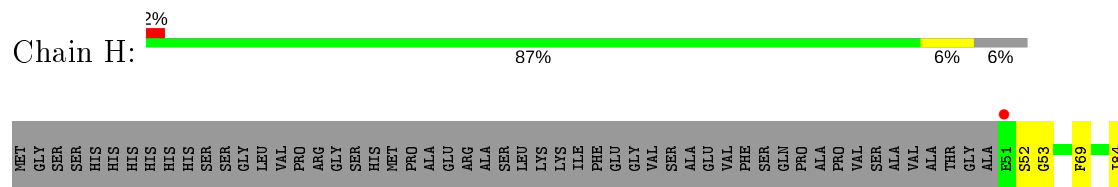
• Molecule 1: Choline trimethylamine-lyase

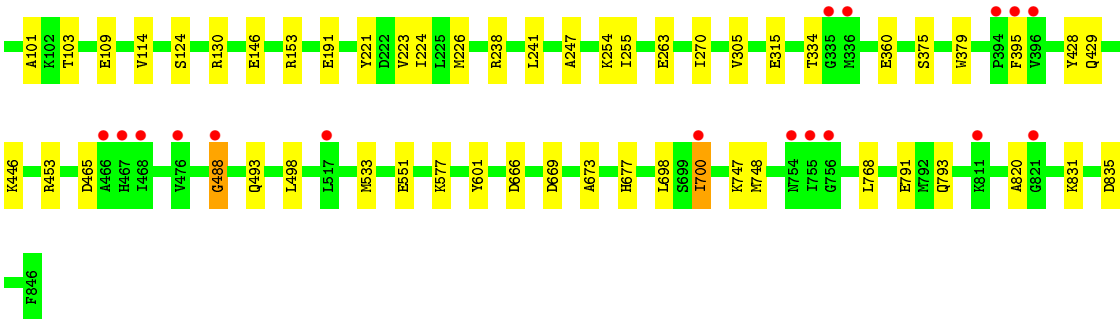


- Molecule 1: Choline trimethylamine-lyase



- Molecule 1: Choline trimethylamine-lyase





4 Data and refinement statistics

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 49.73 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.73-2.36) 98.8 (49.73-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.186 , 0.216 0.186 , 0.216	Depositor DCC
R_{free} test set	8775 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52117	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage'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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	0/6417	0.43	0/8692
1	B	0.25	0/6429	0.41	1/8707 (0.0%)
1	C	0.26	0/6422	0.42	0/8697
1	D	0.25	0/6444	0.42	0/8726
1	E	0.25	0/6409	0.42	0/8681
1	F	0.25	0/6429	0.41	1/8707 (0.0%)
1	G	0.25	0/6422	0.41	0/8697
1	H	0.25	0/6436	0.41	0/8715
All	All	0.25	0/51408	0.42	2/69622 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	LEU	CA-CB-CG	6.34	129.87	115.30
1	F	698	LEU	CA-CB-CG	6.14	129.42	115.30

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	6272	0	6130	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6284	0	6141	42	0
1	C	6277	0	6144	36	0
1	D	6299	0	6159	47	0
1	E	6264	0	6127	33	0
1	F	6284	0	6141	36	0
1	G	6277	0	6144	40	0
1	H	6291	0	6156	33	0
2	A	7	0	11	0	0
2	B	7	0	11	0	0
2	C	7	0	11	0	0
2	D	7	0	11	0	0
2	E	7	0	11	0	0
2	F	7	0	11	0	0
2	G	7	0	11	0	0
2	H	7	0	11	0	0
3	A	308	0	0	8	0
3	B	118	0	0	10	0
3	C	305	0	0	13	0
3	D	273	0	0	15	0
3	E	264	0	0	9	0
3	F	81	0	0	5	0
3	G	258	0	0	12	0
3	H	206	0	0	8	0
All	All	52117	0	49230	286	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.

The worst 5 of 286 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:F:193:ASP:O	3:F:1001:HOH:O	1.80	1.00
1:C:250:GLU:O	3:C:1001:HOH:O	1.80	1.00
1:D:420:ASP:OD2	3:D:1001:HOH:O	1.86	0.94
1:C:420:ASP:OD2	3:C:1002:HOH:O	1.85	0.93
1:D:602:ASN:O	3:D:1003:HOH:O	1.93	0.86

There are no symmetry-related clashes.

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	794/849 (94%)	769 (97%)	24 (3%)	1 (0%)	51	63
1	B	795/849 (94%)	762 (96%)	31 (4%)	2 (0%)	41	47
1	C	794/849 (94%)	766 (96%)	27 (3%)	1 (0%)	51	63
1	D	797/849 (94%)	771 (97%)	23 (3%)	3 (0%)	34	38
1	E	793/849 (93%)	772 (97%)	19 (2%)	2 (0%)	41	47
1	F	795/849 (94%)	767 (96%)	27 (3%)	1 (0%)	51	63
1	G	794/849 (94%)	769 (97%)	23 (3%)	2 (0%)	41	47
1	H	796/849 (94%)	771 (97%)	22 (3%)	3 (0%)	34	38
All	All	6358/6792 (94%)	6147 (97%)	196 (3%)	15 (0%)	47	56

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	700	ILE
1	H	700	ILE
1	A	700	ILE
1	B	700	ILE
1	C	700	ILE

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	669/712 (94%)	662 (99%)	7 (1%)	76	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	671/712 (94%)	665 (99%)	6 (1%)	78	87
1	C	671/712 (94%)	664 (99%)	7 (1%)	76	85
1	D	673/712 (94%)	672 (100%)	1 (0%)	93	97
1	E	668/712 (94%)	658 (98%)	10 (2%)	65	76
1	F	671/712 (94%)	664 (99%)	7 (1%)	76	85
1	G	671/712 (94%)	663 (99%)	8 (1%)	71	82
1	H	672/712 (94%)	669 (100%)	3 (0%)	91	95
All	All	5366/5696 (94%)	5317 (99%)	49 (1%)	78	87

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	168	LEU
1	E	625	LEU
1	G	759	HIS
1	E	428	TYR
1	E	698	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	759	HIS
1	D	677	HIS
1	F	806	GLN
1	B	806	GLN
1	H	248	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 [i](#)

There are no carbohydrates in this entry.

5.6 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	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%)
2	BTL	A	901	1	6,6,6	2.19	2 (33%)	4,8,8	2.58	1 (25%)
2	BTL	D	901	1	6,6,6	2.21	3 (50%)	4,8,8	2.41	1 (25%)
2	BTL	C	901	1	6,6,6	2.27	3 (50%)	4,8,8	2.40	1 (25%)
2	BTL	F	901	1	6,6,6	2.24	3 (50%)	4,8,8	2.61	1 (25%)
2	BTL	E	901	1	6,6,6	2.24	3 (50%)	4,8,8	2.53	1 (25%)
2	BTL	H	901	1	6,6,6	2.24	3 (50%)	4,8,8	2.53	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	G	901	1	-	1/3/4/4	-
2	BTL	B	901	1	-	1/3/4/4	-
2	BTL	A	901	1	-	1/3/4/4	-
2	BTL	D	901	1	-	1/3/4/4	-
2	BTL	C	901	1	-	1/3/4/4	-
2	BTL	F	901	1	-	1/3/4/4	-
2	BTL	E	901	1	-	1/3/4/4	-
2	BTL	H	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
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	G	901	BTL	C-CA-N-C2
2	B	901	BTL	C-CA-N-C2
2	A	901	BTL	C-CA-N-C2
2	D	901	BTL	C-CA-N-C2
2	C	901	BTL	C-CA-N-C2

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 [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, 95th 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	795/849 (93%)	0.02	12 (1%) 73 81	29, 43, 68, 95	0
1	B	794/849 (93%)	0.42	61 (7%) 13 20	36, 63, 89, 116	0
1	C	795/849 (93%)	-0.01	15 (1%) 66 76	30, 45, 68, 95	0
1	D	796/849 (93%)	0.01	15 (1%) 66 76	32, 48, 73, 99	0
1	E	795/849 (93%)	0.14	21 (2%) 56 65	30, 49, 67, 101	0
1	F	794/849 (93%)	0.75	107 (13%) 3 4	43, 75, 109, 130	0
1	G	795/849 (93%)	0.13	12 (1%) 73 81	34, 53, 79, 100	0
1	H	796/849 (93%)	0.12	18 (2%) 60 70	35, 55, 76, 102	0
All	All	6360/6792 (93%)	0.20	261 (4%) 37 49	29, 53, 86, 130	0

The worst 5 of 261 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ILE	7.3
1	F	645	PHE	7.3
1	F	539	TYR	6.4
1	F	625	LEU	5.9
1	F	634	LEU	5.8

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 carbohydrates 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, 95th 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	B-factors(Å ²)	Q<0.9
2	BTL	B	901	7/7	0.91	0.22	49,51,54,55	0
2	BTL	F	901	7/7	0.94	0.21	57,60,61,61	0
2	BTL	E	901	7/7	0.96	0.27	41,42,45,48	0
2	BTL	H	901	7/7	0.97	0.26	45,47,48,49	0
2	BTL	G	901	7/7	0.98	0.19	34,38,42,42	0
2	BTL	A	901	7/7	0.98	0.24	30,32,37,38	0
2	BTL	D	901	7/7	0.98	0.27	37,41,42,43	0
2	BTL	C	901	7/7	0.99	0.19	35,36,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.