



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:58 AM UTC

PDB ID : 5A0U / pdb_00005a0u
Title : Structure of CutC choline lyase choline bound form from *Klebsiella pneumoniae*.
Authors : Kalnins, G.; Tars, K.
Deposited on : 2015-04-23
Resolution : 2.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

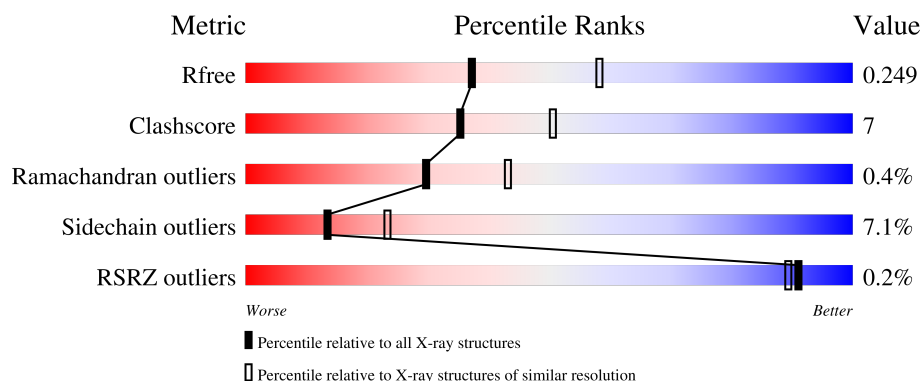
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	795	82% 15% .
1	B	795	82% 16% .
1	C	795	78% 20% .
1	D	795	81% 18% .
1	E	795	75% 21% .

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Mol	Chain	Length	Quality of chain
1	F	795	% 81% 16%
1	G	795	82% 16%
1	H	795	% 78% 20%

2 Entry composition

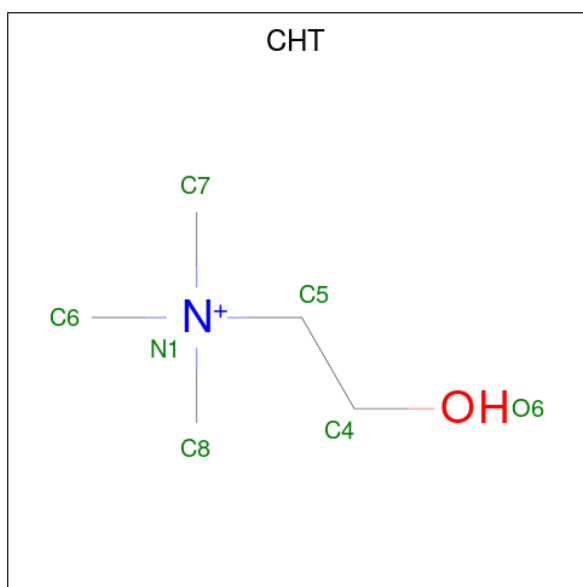
There are 3 unique types of molecules in this entry. The entry contains 52127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	792	Total	C	N	O	S	0	0	0
			6254	3954	1077	1181	42			
1	B	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	C	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	D	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	E	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	F	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	G	793	Total	C	N	O	S	0	0	0
			6261	3959	1078	1182	42			
1	H	795	Total	C	N	O	S	0	0	0
			6275	3968	1080	1185	42			

- Molecule 2 is CHOLINE ION (CCD ID: CHT) (formula: C₅H₁₄NO).



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	344	Total	O	0	0
			344	344		
3	B	294	Total	O	0	0
			294	294		
3	C	297	Total	O	0	0
			297	297		
3	D	307	Total	O	0	0
			307	307		

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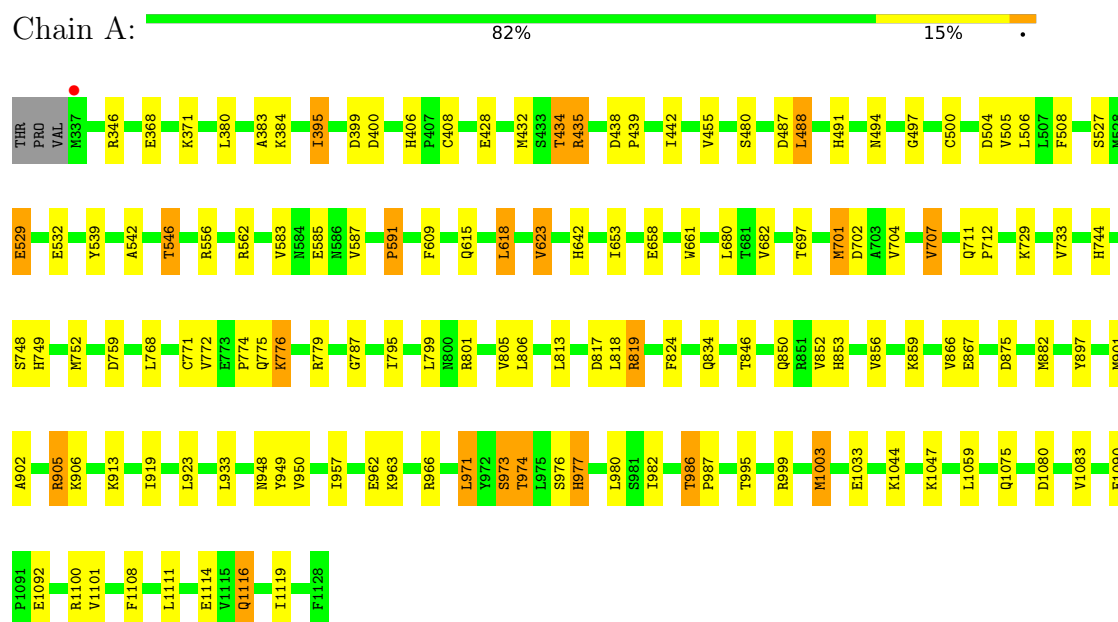
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	163	Total 163	O 163	0	0
3	F	152	Total 152	O 152	0	0
3	G	217	Total 217	O 217	0	0
3	H	202	Total 202	O 202	0	0

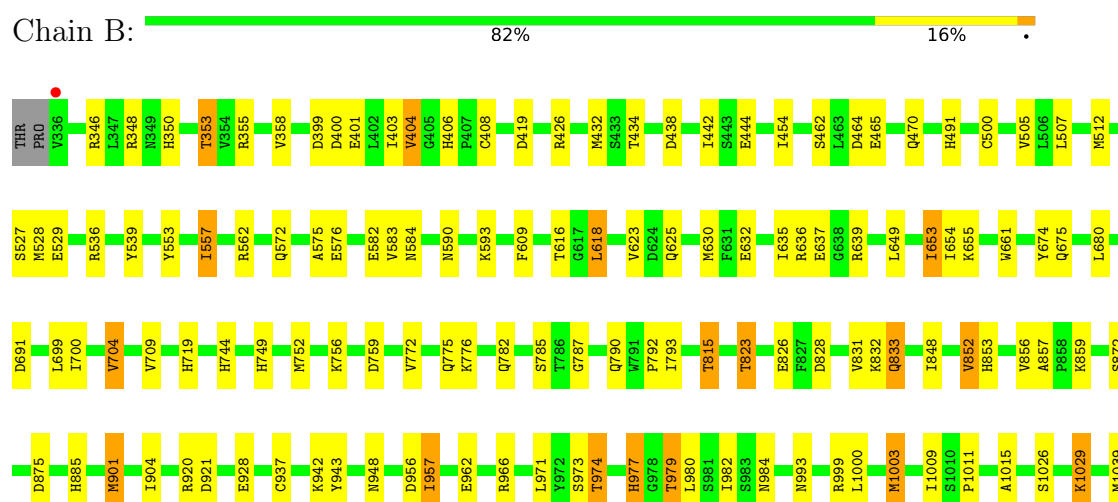
3 Residue-property plots

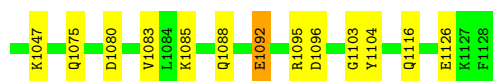
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CHOLINE TRIMETHYLAMINE LYASE



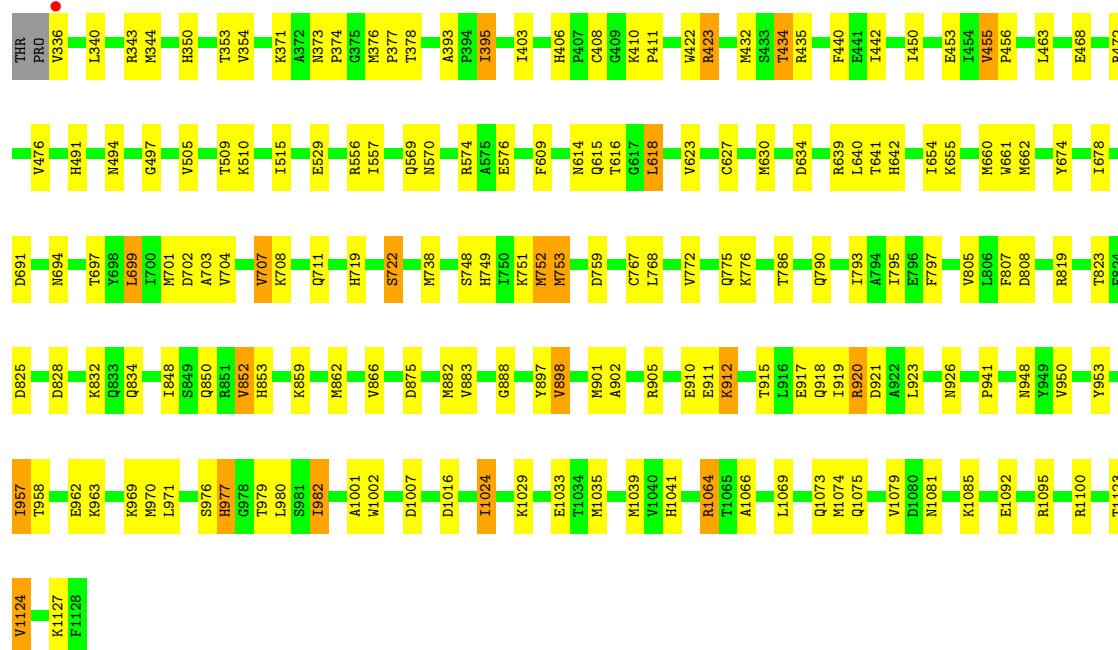
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE





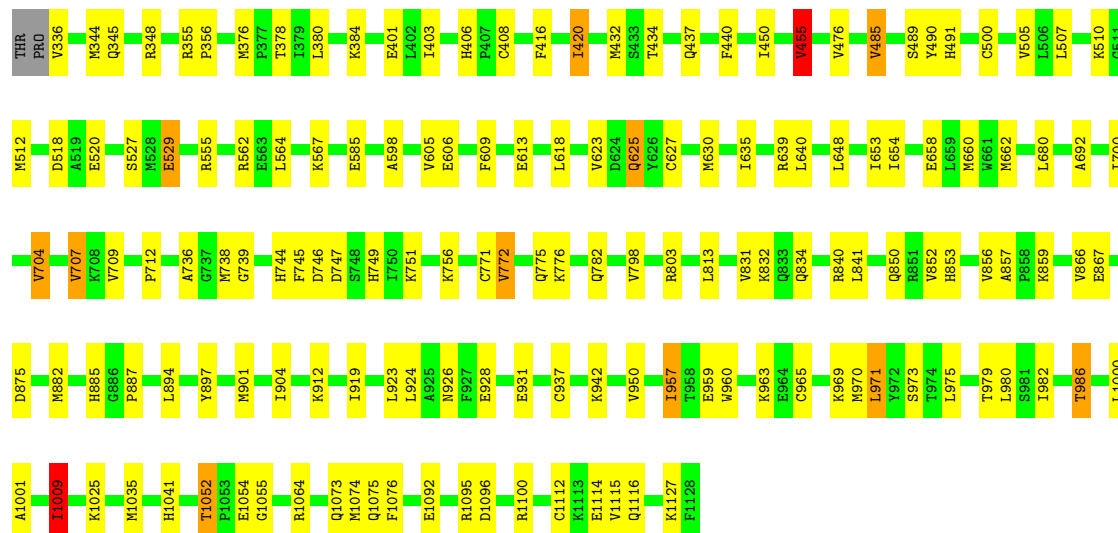
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain C: 78% 20%



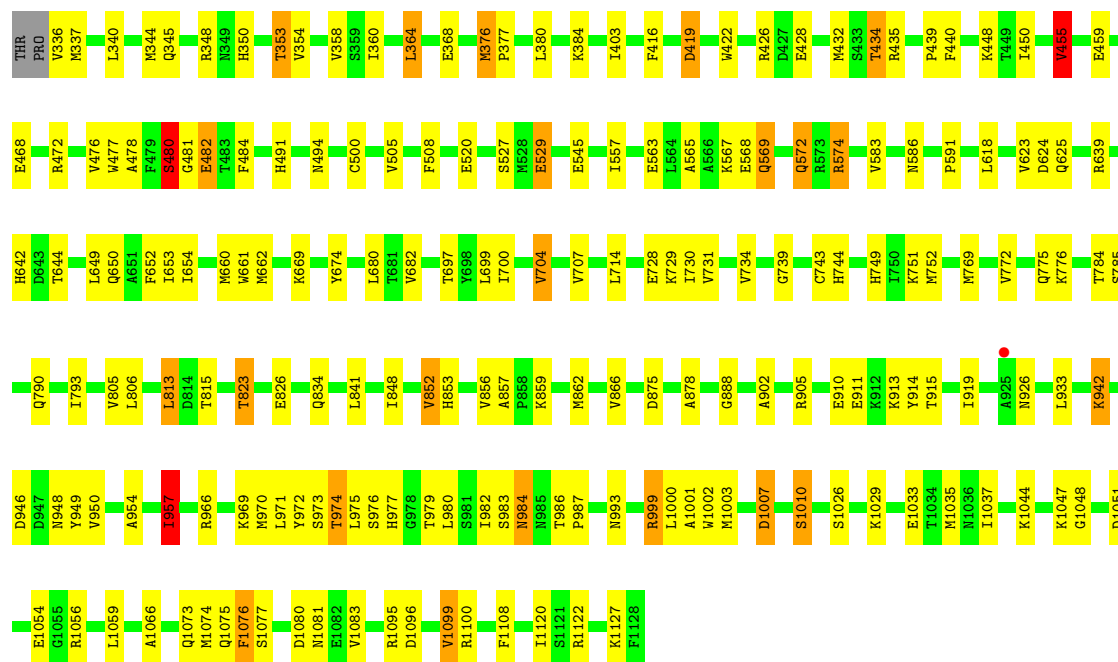
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain D: 81% 18%

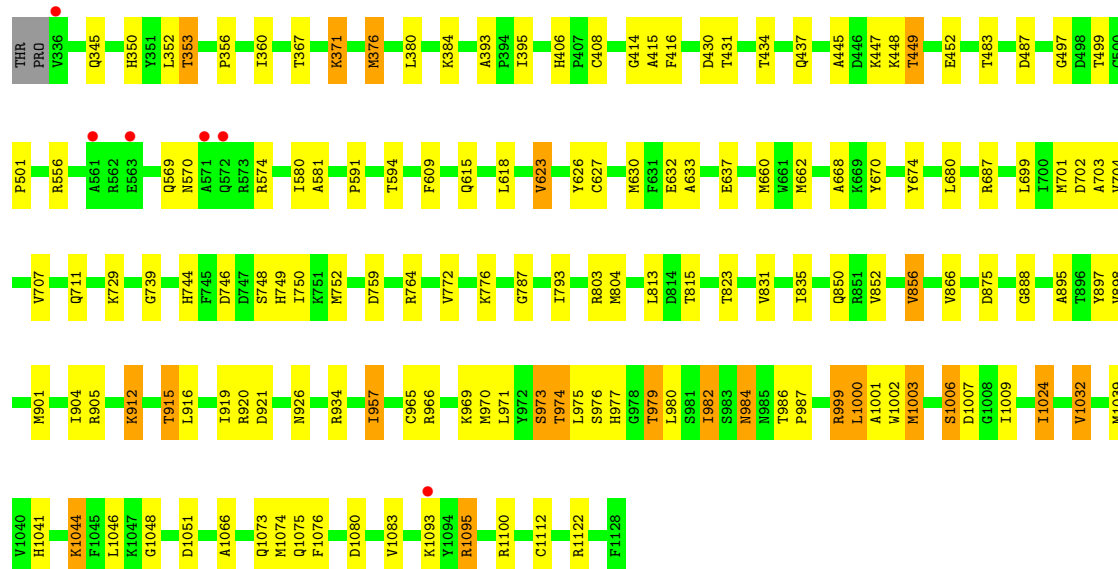
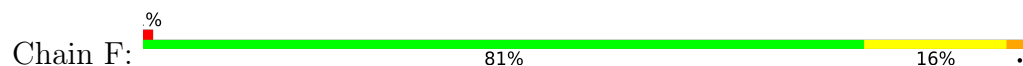


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

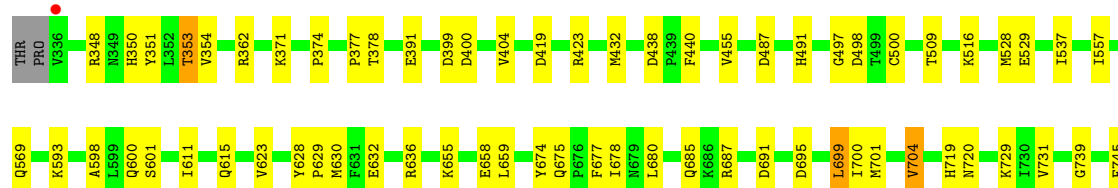
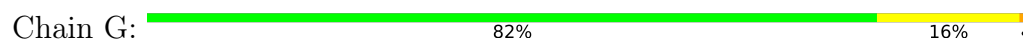
Chain E: 75% 21%

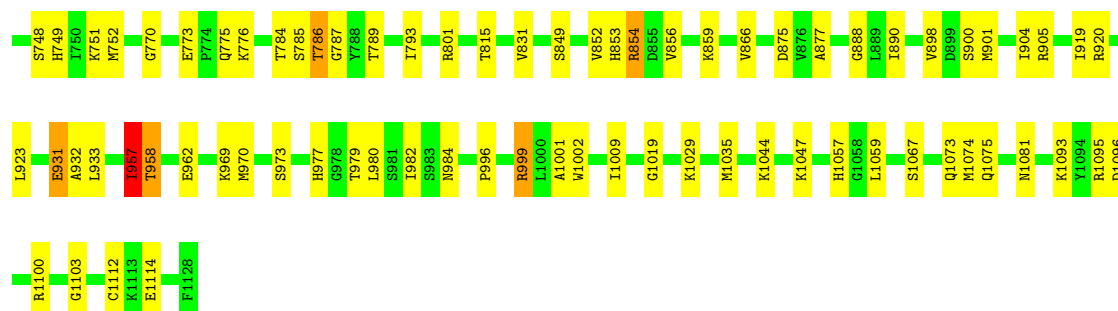


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

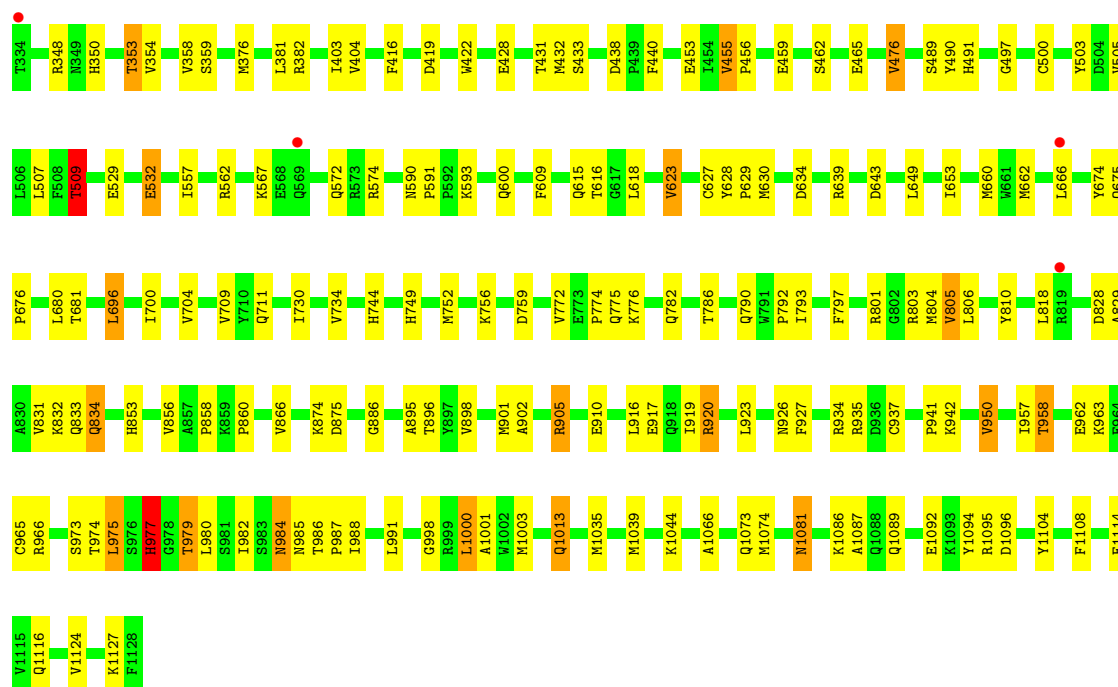
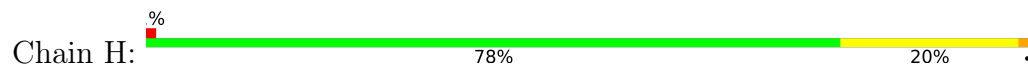


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE





• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.41Å 221.87Å 419.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	209.74 – 2.40 209.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (209.74-2.40) 93.6 (209.74-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.188 , 0.247 0.194 , 0.249	Depositor DCC
R_{free} test set	15197 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	52127	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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: CHT

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	0.88	1/6385 (0.0%)	1.02	7/8640 (0.1%)
1	B	0.83	0/6392	1.02	6/8650 (0.1%)
1	C	0.85	0/6392	1.02	11/8650 (0.1%)
1	D	0.89	0/6392	1.02	6/8650 (0.1%)
1	E	0.78	2/6392 (0.0%)	1.00	6/8650 (0.1%)
1	F	0.79	0/6392	0.98	3/8650 (0.0%)
1	G	0.81	1/6392 (0.0%)	1.00	6/8650 (0.1%)
1	H	0.83	1/6407 (0.0%)	1.01	8/8672 (0.1%)
All	All	0.83	5/51144 (0.0%)	1.01	53/69212 (0.1%)

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	E	0	1
1	G	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	480	SER	CA-C	7.53	1.58	1.52
1	E	455	VAL	CA-CB	6.79	1.58	1.53
1	A	986	THR	N-CA	-5.56	1.43	1.46
1	G	957	ILE	N-CA	5.27	1.53	1.46
1	H	975	LEU	CA-C	5.15	1.59	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	455	VAL	N-CA-CB	11.38	117.67	110.50
1	E	455	VAL	N-CA-CB	11.18	117.55	110.50
1	D	1009	ILE	N-CA-C	-9.11	104.15	112.90
1	E	480	SER	N-CA-C	7.70	122.82	111.34
1	H	455	VAL	N-CA-CB	7.15	115.01	110.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	480	SER	Peptide
1	G	377	PRO	Peptide
1	G	789	THR	Peptide

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	6254	0	6171	83	0
1	B	6261	0	6180	84	0
1	C	6261	0	6180	108	0
1	D	6261	0	6180	89	0
1	E	6261	0	6180	102	0
1	F	6261	0	6180	97	0
1	G	6261	0	6180	74	0
1	H	6275	0	6194	97	0
2	A	7	0	14	1	0
2	B	7	0	14	0	0
2	C	7	0	14	1	0
2	D	7	0	14	0	0
2	E	7	0	14	0	0
2	F	7	0	14	0	0
2	G	7	0	14	2	0
2	H	7	0	14	0	0
3	A	344	0	0	5	0
3	B	294	0	0	8	0
3	C	297	0	0	4	0
3	D	307	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	163	0	0	1	0
3	F	152	0	0	11	0
3	G	217	0	0	6	0
3	H	202	0	0	4	0
All	All	52127	0	49557	734	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 7.

The worst 5 of 734 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:G:979:THR:HG21	1:G:1009:ILE:HD11	1.44	0.97
1:D:376:MET:HE1	1:D:380:LEU:HG	1.46	0.94
1:C:722:SER:O	1:C:1064:ARG:NH2	2.01	0.92
1:E:999:ARG:NH2	1:E:1003:MET:O	2.03	0.92
1:F:999:ARG:NH1	1:F:1003:MET:O	2.02	0.91

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	790/795 (99%)	761 (96%)	24 (3%)	5 (1%)	21	32
1	B	791/795 (100%)	756 (96%)	32 (4%)	3 (0%)	30	43
1	C	791/795 (100%)	756 (96%)	33 (4%)	2 (0%)	36	50
1	D	791/795 (100%)	761 (96%)	28 (4%)	2 (0%)	36	50
1	E	791/795 (100%)	755 (95%)	33 (4%)	3 (0%)	30	43
1	F	791/795 (100%)	750 (95%)	36 (5%)	5 (1%)	21	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	791/795 (100%)	760 (96%)	28 (4%)	3 (0%)	30	43
1	H	793/795 (100%)	765 (96%)	26 (3%)	2 (0%)	36	50
All	All	6329/6360 (100%)	6064 (96%)	240 (4%)	25 (0%)	30	43

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	772	VAL
1	F	1112	CYS
1	G	982	ILE
1	H	772	VAL
1	A	435	ARG

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	668/671 (100%)	626 (94%)	42 (6%)	16	29
1	B	669/671 (100%)	626 (94%)	43 (6%)	16	28
1	C	669/671 (100%)	623 (93%)	46 (7%)	14	24
1	D	669/671 (100%)	626 (94%)	43 (6%)	16	28
1	E	669/671 (100%)	604 (90%)	65 (10%)	8	12
1	F	669/671 (100%)	617 (92%)	52 (8%)	11	20
1	G	669/671 (100%)	629 (94%)	40 (6%)	17	31
1	H	671/671 (100%)	621 (92%)	50 (8%)	12	21
All	All	5353/5368 (100%)	4972 (93%)	381 (7%)	13	23

5 of 381 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1026	SER
1	F	1044	LYS

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Mol	Chain	Res	Type
1	E	1127	LYS
1	F	815	THR
1	G	623	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 195 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	853	HIS
1	G	350	HIS
1	E	1041	HIS
1	F	625	GLN
1	G	560	HIS

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 oligosaccharides 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	CHT	D	2000	-	6,6,6	1.24	1 (16%)	8,8,8	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CHT	H	2000	-	6,6,6	0.65	0	8,8,8	0.68	0
2	CHT	A	2000	-	6,6,6	0.60	0	8,8,8	0.56	0
2	CHT	E	2000	-	6,6,6	0.76	0	8,8,8	0.48	0
2	CHT	F	2000	-	6,6,6	0.68	0	8,8,8	0.82	0
2	CHT	B	2000	-	6,6,6	0.77	0	8,8,8	0.48	0
2	CHT	C	2000	-	6,6,6	0.78	0	8,8,8	0.58	0
2	CHT	G	2000	-	6,6,6	0.71	0	8,8,8	0.80	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
2	CHT	D	2000	-	-	1/4/4/4	-
2	CHT	H	2000	-	-	3/4/4/4	-
2	CHT	A	2000	-	-	0/4/4/4	-
2	CHT	E	2000	-	-	0/4/4/4	-
2	CHT	F	2000	-	-	4/4/4/4	-
2	CHT	B	2000	-	-	3/4/4/4	-
2	CHT	C	2000	-	-	0/4/4/4	-
2	CHT	G	2000	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	CHT	C5-N1	-2.04	1.45	1.51

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2000	CHT	O6-C4-C5-N1
2	F	2000	CHT	O6-C4-C5-N1
2	H	2000	CHT	C4-C5-N1-C6
2	H	2000	CHT	C4-C5-N1-C7
2	H	2000	CHT	C4-C5-N1-C8

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	CHT	1	0
2	C	2000	CHT	1	0
2	G	2000	CHT	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, 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	792/795 (99%)	-0.61	1 (0%) 92 90	12, 20, 34, 67	0
1	B	793/795 (99%)	-0.48	1 (0%) 92 90	15, 24, 39, 59	0
1	C	793/795 (99%)	-0.44	1 (0%) 92 90	13, 24, 42, 73	0
1	D	793/795 (99%)	-0.58	0 100 100	12, 21, 34, 50	0
1	E	793/795 (99%)	-0.13	1 (0%) 92 90	18, 32, 52, 71	0
1	F	793/795 (99%)	-0.01	6 (0%) 82 80	18, 34, 55, 84	0
1	G	793/795 (99%)	-0.38	1 (0%) 92 90	15, 27, 45, 65	0
1	H	795/795 (100%)	-0.31	4 (0%) 87 85	16, 28, 46, 77	0
All	All	6345/6360 (99%)	-0.37	15 (0%) 91 89	12, 26, 46, 84	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	334	THR	4.2
1	C	336	VAL	3.5
1	G	336	VAL	3.1
1	F	571	ALA	3.0
1	F	336	VAL	3.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CHT	F	2000	7/7	0.89	0.15	42,45,47,48	0
2	CHT	D	2000	7/7	0.92	0.12	25,29,30,33	0
2	CHT	H	2000	7/7	0.94	0.10	27,30,30,33	0
2	CHT	E	2000	7/7	0.95	0.09	30,31,32,32	0
2	CHT	G	2000	7/7	0.96	0.08	24,24,25,27	0
2	CHT	C	2000	7/7	0.97	0.07	17,18,18,18	0
2	CHT	A	2000	7/7	0.98	0.05	14,14,15,16	0
2	CHT	B	2000	7/7	0.99	0.05	19,19,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.