



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:35 PM GMT

PDB ID : 5A0U  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

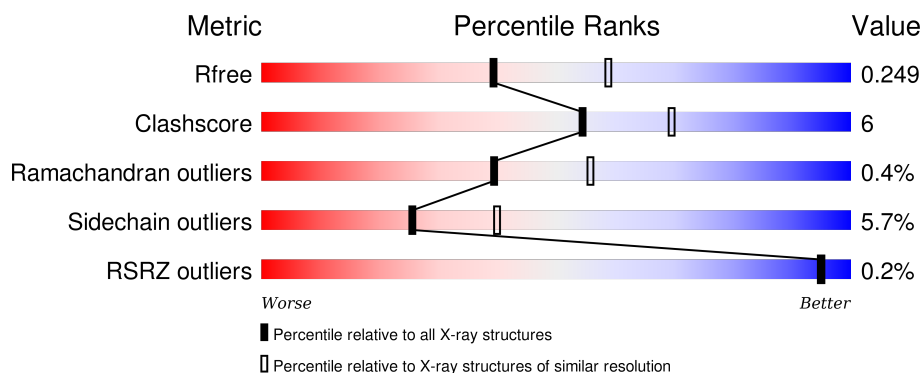
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	B	795	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	795	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	795	<div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	795	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	795	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div></div> </div> </div>
1	G	795	<div> <div></div> <div>85%</div> <div>13%</div> <div></div> </div>
1	H	795	<div> <div></div> <div>79%</div> <div>19%</div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CHT	D	2000	-	-	-	X
2	CHT	F	2000	-	-	-	X
2	CHT	H	2000	-	-	-	X

## 2 Entry composition

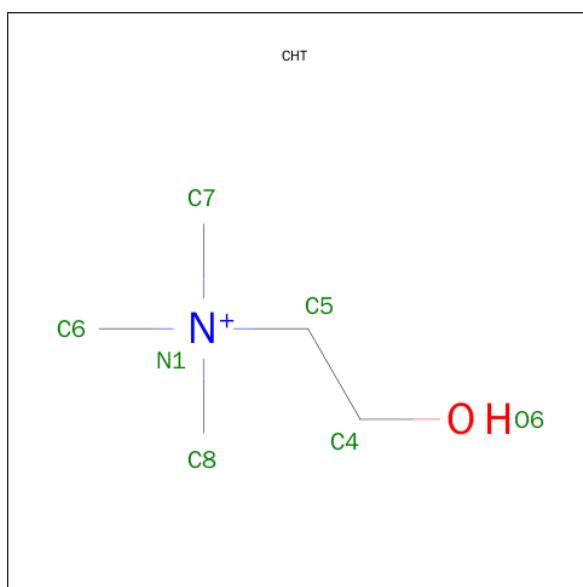
There are 3 unique types of molecules in this entry. The entry contains 52127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: CHT) (formula: C<sub>5</sub>H<sub>14</sub>NO).



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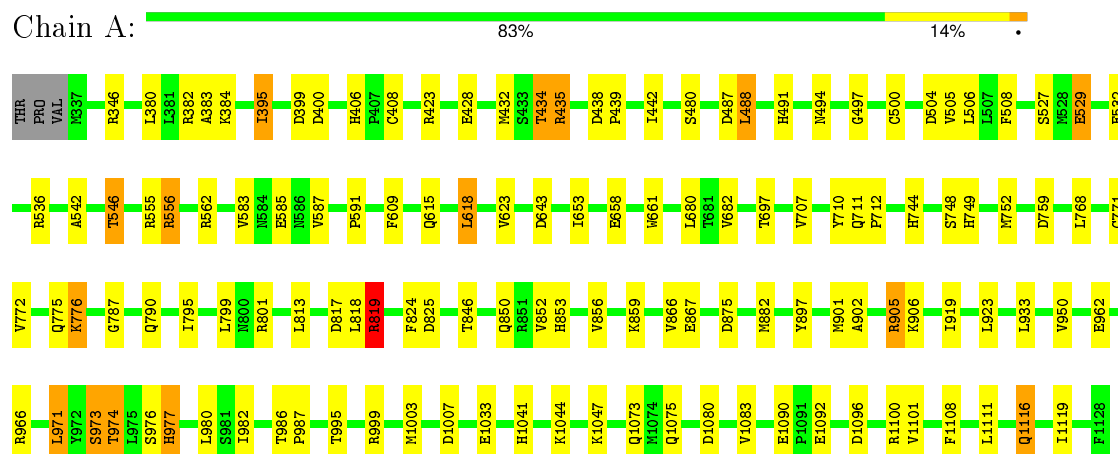
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	163	Total 163	O 163	0	0
3	F	152	Total 152	O 152	0	0
3	G	217	Total 217	O 217	0	0
3	H	202	Total 202	O 202	0	0

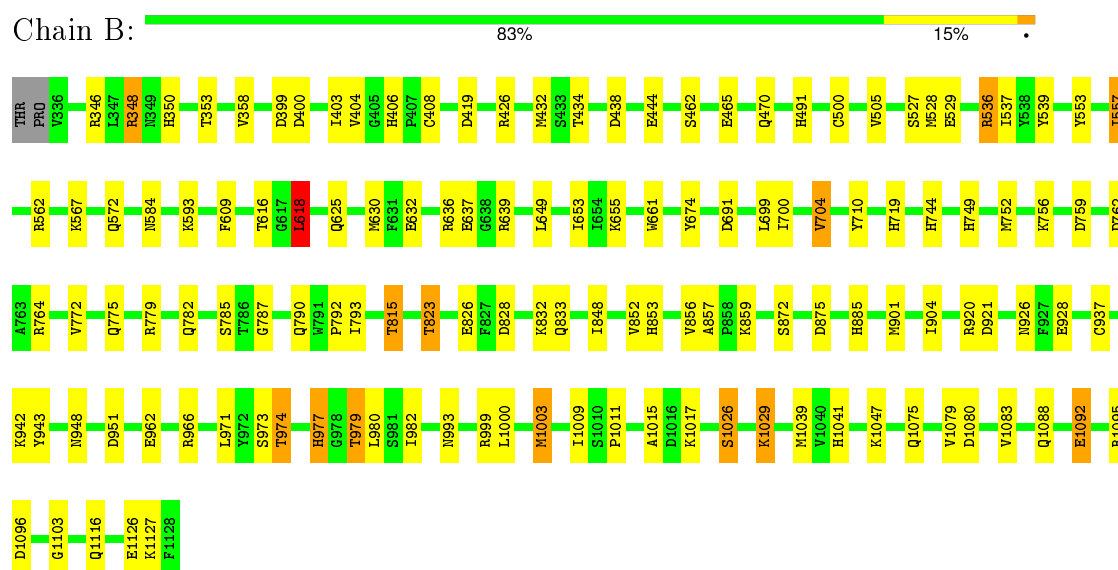
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

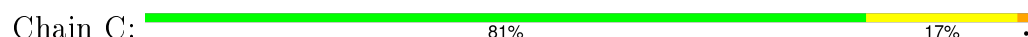
#### • Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

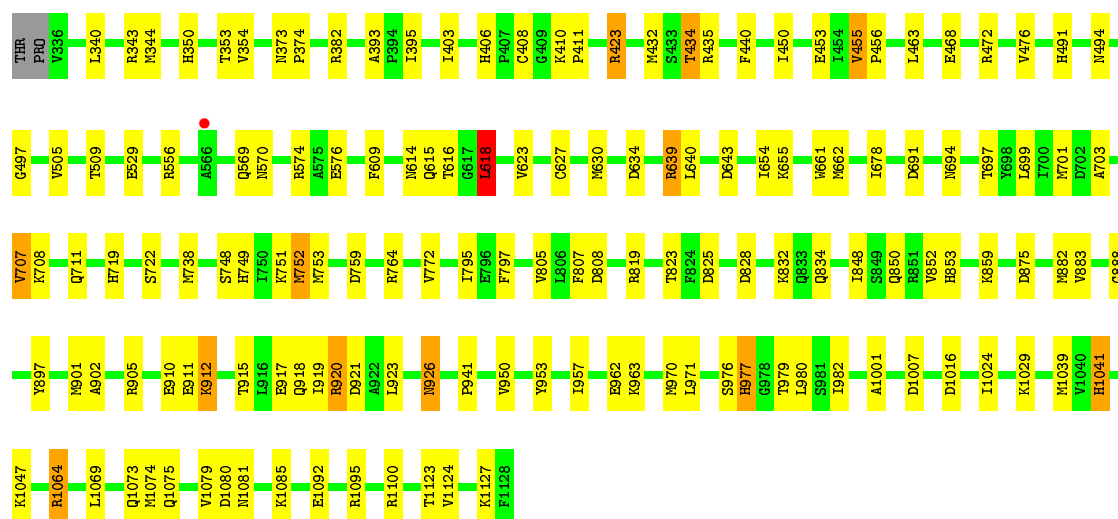


#### • Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



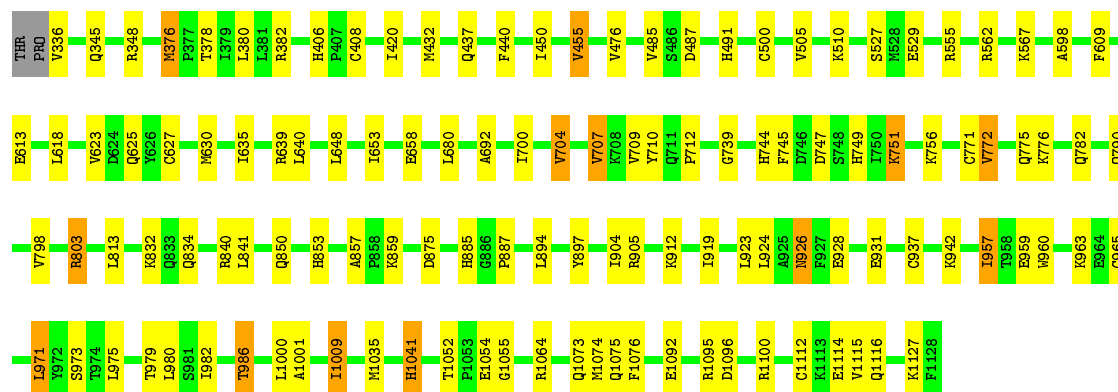
#### • Molecule 1: CHOLINE TRIMETHYLAMINE LYASE





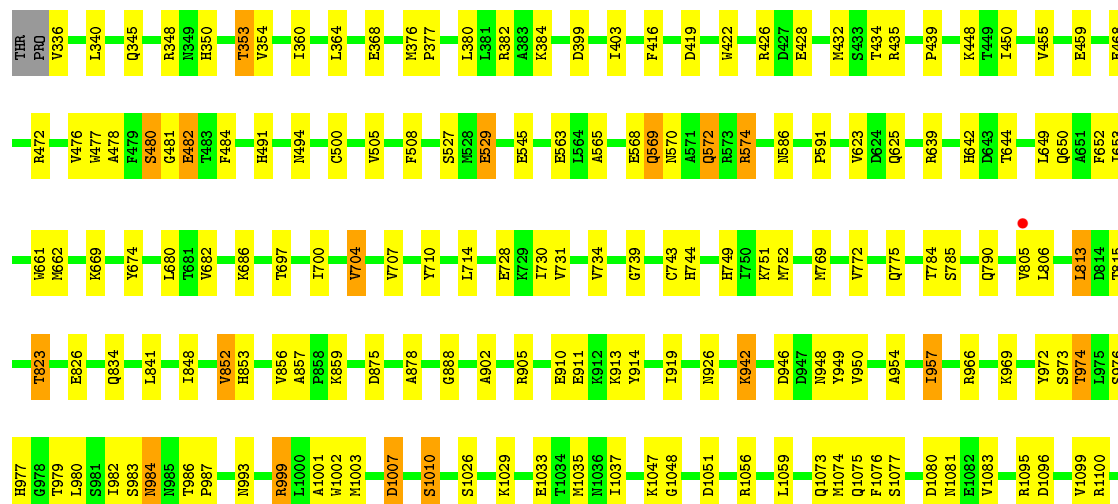
### • Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain D: 84% 14%



### • Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

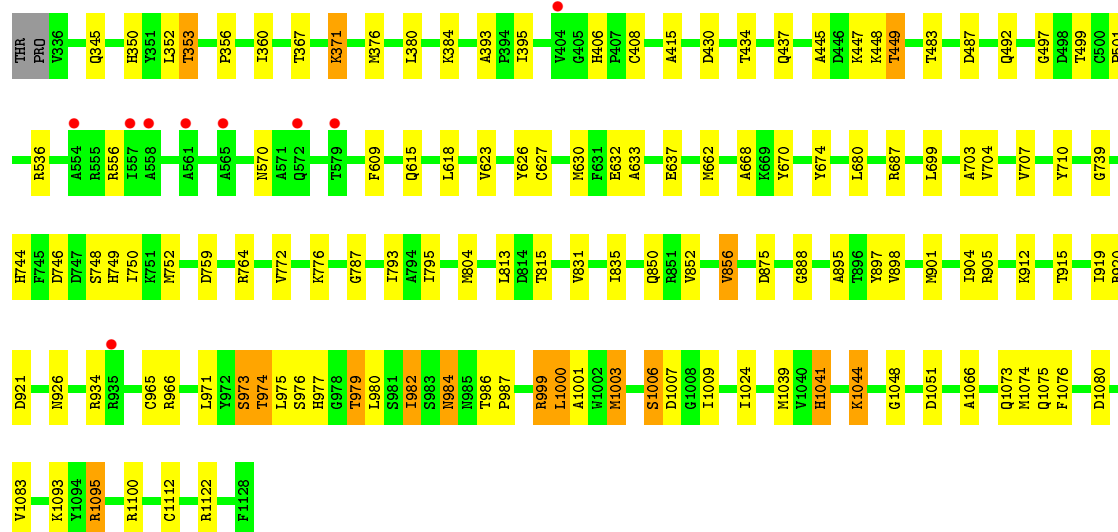
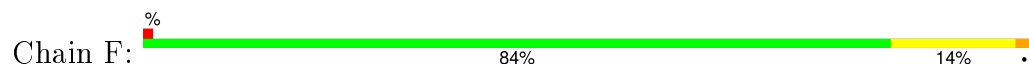
Chain E: 78% 19%



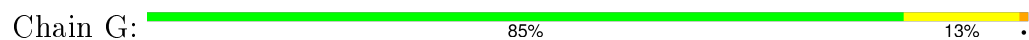




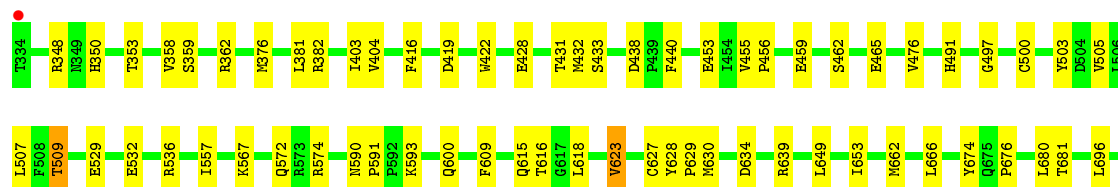
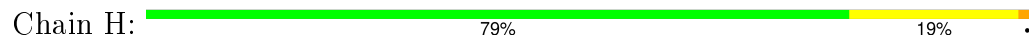
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE



• 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, $\alpha$ , $\beta$ , $\gamma$	89.41Å 221.87Å 419.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	209.74 – 2.40 76.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (209.74-2.40) 93.6 (76.21-2.40)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 304460 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	52127	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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: 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	0.65	0/6385	0.84	10/8640 (0.1%)
1	B	0.61	0/6392	0.80	7/8650 (0.1%)
1	C	0.62	0/6392	0.82	7/8650 (0.1%)
1	D	0.65	0/6392	0.82	6/8650 (0.1%)
1	E	0.57	0/6392	0.76	1/8650 (0.0%)
1	F	0.58	0/6392	0.75	1/8650 (0.0%)
1	G	0.59	0/6392	0.78	6/8650 (0.1%)
1	H	0.60	0/6407	0.77	3/8672 (0.0%)
All	All	0.61	0/51144	0.79	41/69212 (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

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	764	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	A	382	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	764	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	382	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	C	753	MET	CG-SD-CE	-7.57	88.08	100.20

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	73	0
1	B	6261	0	6180	75	0
1	C	6261	0	6180	94	0
1	D	6261	0	6180	71	0
1	E	6261	0	6180	88	0
1	F	6261	0	6180	85	0
1	G	6261	0	6180	66	0
1	H	6275	0	6194	90	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	7	0
3	C	297	0	0	4	0
3	D	307	0	0	6	0
3	E	163	0	0	1	0
3	F	152	0	0	10	0
3	G	217	0	0	6	0
3	H	202	0	0	4	0
All	All	52127	0	49557	642	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 642 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: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
1:E:568:GLU:O	1:E:574:ARG:NH1	2.04	0.89

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%)	30	43
1	B	791/795 (100%)	756 (96%)	32 (4%)	3 (0%)	39	56
1	C	791/795 (100%)	756 (96%)	33 (4%)	2 (0%)	46	63
1	D	791/795 (100%)	761 (96%)	28 (4%)	2 (0%)	46	63
1	E	791/795 (100%)	755 (95%)	33 (4%)	3 (0%)	39	56
1	F	791/795 (100%)	750 (95%)	36 (5%)	5 (1%)	30	43
1	G	791/795 (100%)	760 (96%)	28 (4%)	3 (0%)	39	56
1	H	793/795 (100%)	765 (96%)	26 (3%)	2 (0%)	46	63
All	All	6329/6360 (100%)	6064 (96%)	240 (4%)	25 (0%)	39	56

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	772	VAL
1	F	1112	CYS
1	G	982	ILE

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Mol	Chain	Res	Type
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%)	631 (94%)	37 (6%)	27	42
1	B	669/671 (100%)	632 (94%)	37 (6%)	27	42
1	C	669/671 (100%)	633 (95%)	36 (5%)	27	43
1	D	669/671 (100%)	633 (95%)	36 (5%)	27	43
1	E	669/671 (100%)	619 (92%)	50 (8%)	17	26
1	F	669/671 (100%)	632 (94%)	37 (6%)	27	42
1	G	669/671 (100%)	641 (96%)	28 (4%)	36	56
1	H	671/671 (100%)	627 (93%)	44 (7%)	21	32
All	All	5353/5368 (100%)	5048 (94%)	305 (6%)	25	40

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	980	LEU
1	E	813	LEU
1	H	875	ASP
1	D	1092	GLU
1	E	529	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	790	GLN
1	E	625	GLN
1	H	749	HIS

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Mol	Chain	Res	Type
1	D	853	HIS
1	E	406	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	2000	-	6,6,6	0.58	0	8,8,8	0.56	0
2	CHT	B	2000	-	6,6,6	0.75	0	8,8,8	0.48	0
2	CHT	C	2000	-	6,6,6	0.75	0	8,8,8	0.57	0
2	CHT	D	2000	-	6,6,6	1.20	0	8,8,8	1.05	0
2	CHT	E	2000	-	6,6,6	0.75	0	8,8,8	0.48	0
2	CHT	F	2000	-	6,6,6	0.66	0	8,8,8	0.81	0
2	CHT	G	2000	-	6,6,6	0.70	0	8,8,8	0.79	0
2	CHT	H	2000	-	6,6,6	0.62	0	8,8,8	0.68	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	A	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	B	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	C	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	D	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	E	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	F	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	G	2000	-	-	0/4/4/4	0/0/0/0
2	CHT	H	2000	-	-	0/4/4/4	0/0/0/0

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.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	792/795 (99%)	-0.69	0 100 100	12, 20, 34, 67	0
1	B	793/795 (99%)	-0.67	0 100 100	15, 24, 39, 59	0
1	C	793/795 (99%)	-0.59	1 (0%) 95 95	13, 24, 42, 73	0
1	D	793/795 (99%)	-0.67	0 100 100	12, 21, 34, 50	0
1	E	793/795 (99%)	-0.43	1 (0%) 95 95	18, 32, 52, 71	0
1	F	793/795 (99%)	-0.35	9 (1%) 82 82	18, 34, 55, 84	0
1	G	793/795 (99%)	-0.58	0 100 100	15, 27, 45, 65	0
1	H	795/795 (100%)	-0.56	2 (0%) 94 94	16, 28, 46, 77	0
All	All	6345/6360 (99%)	-0.57	13 (0%) 95 95	12, 26, 46, 84	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	819	ARG	3.1
1	F	561	ALA	2.9
1	F	572	GLN	2.5
1	H	334	THR	2.5
1	F	557	ILE	2.5

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CHT	F	2000	7/7	0.92	0.20	5.35	42,45,47,48	0
2	CHT	D	2000	7/7	0.94	0.18	3.92	25,29,30,33	0
2	CHT	H	2000	7/7	0.95	0.14	2.92	27,30,30,33	0
2	CHT	E	2000	7/7	0.96	0.13	0.49	30,31,32,32	0
2	CHT	B	2000	7/7	0.98	0.11	0.25	19,19,20,20	0
2	CHT	A	2000	7/7	0.98	0.12	0.16	14,14,15,16	0
2	CHT	C	2000	7/7	0.97	0.11	0.13	17,18,18,18	0
2	CHT	G	2000	7/7	0.97	0.11	-0.11	24,24,25,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.