



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

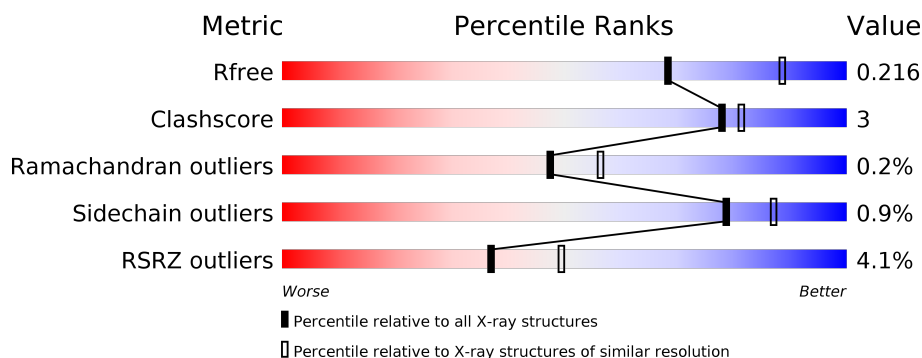
# 1 Overall quality at a glance

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  $\geq 3$ , 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>0%</div> <div>88% 5% 6%</div> </div>
1	B	849	<div> <div>7%</div> <div>85% 8% 6%</div> </div>
1	C	849	<div> <div>2%</div> <div>87% 6% 6%</div> </div>
1	D	849	<div> <div>2%</div> <div>85% 8% 6%</div> </div>
1	E	849	<div> <div>2%</div> <div>86% 7% 6%</div> </div>
1	F	849	<div> <div>13%</div> <div>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

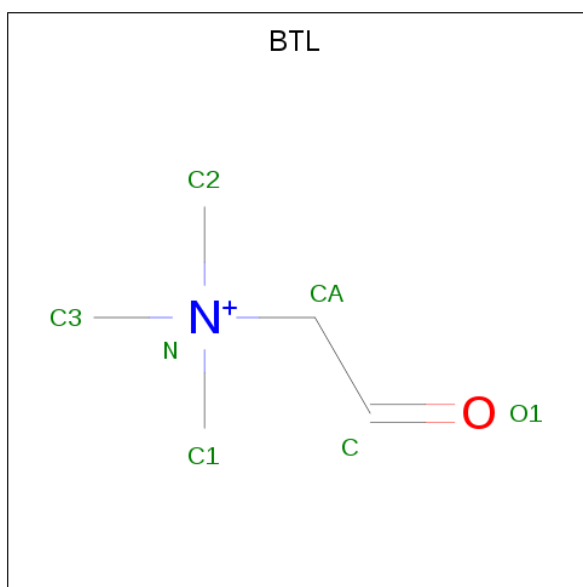
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Chain	Residue	Modelled	Actual	Comment	Reference
G	11	LEU	-	expression tag	UNP Q30W70
G	12	VAL	-	expression tag	UNP Q30W70
G	13	PRO	-	expression tag	UNP Q30W70
G	14	ARG	-	expression tag	UNP Q30W70
G	15	GLY	-	expression tag	UNP Q30W70
G	16	SER	-	expression 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: C<sub>5</sub>H<sub>12</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	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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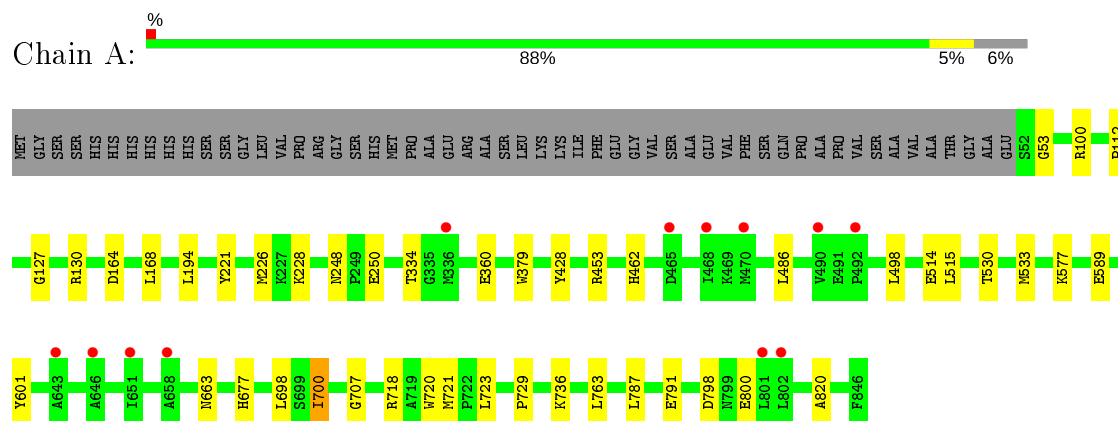
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	264	Total 264	O 264	0	0
3	F	81	Total 81	O 81	0	0
3	G	258	Total 258	O 258	0	0
3	H	206	Total 206	O 206	0	0

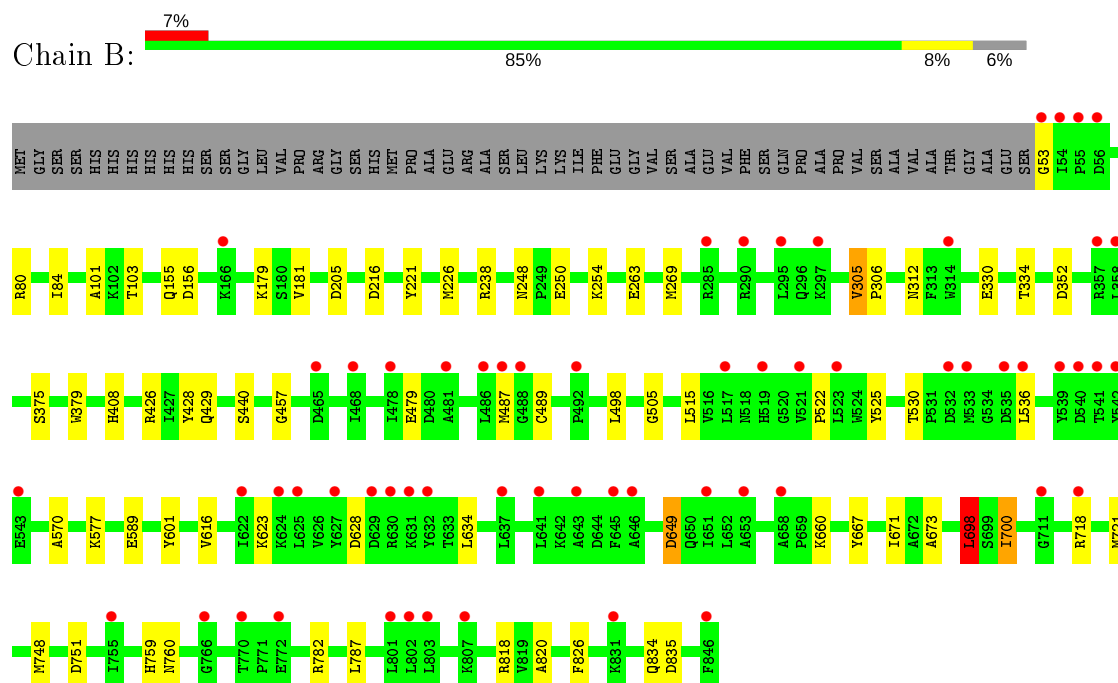
### 3 Residue-property plots

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

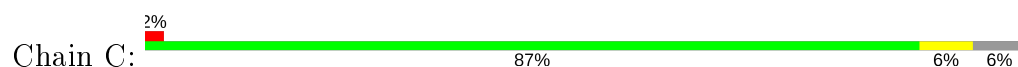
#### • Molecule 1: Choline trimethylamine-lyase

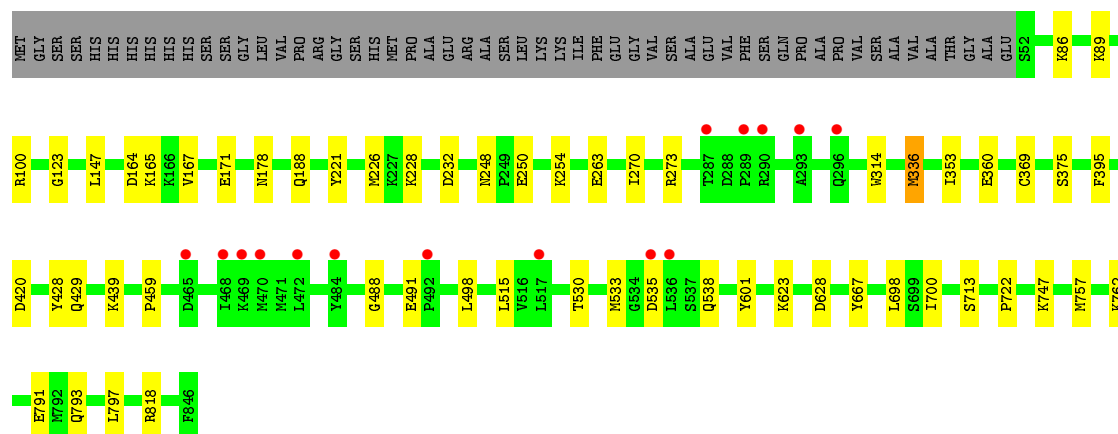


#### • Molecule 1: Choline trimethylamine-lyase

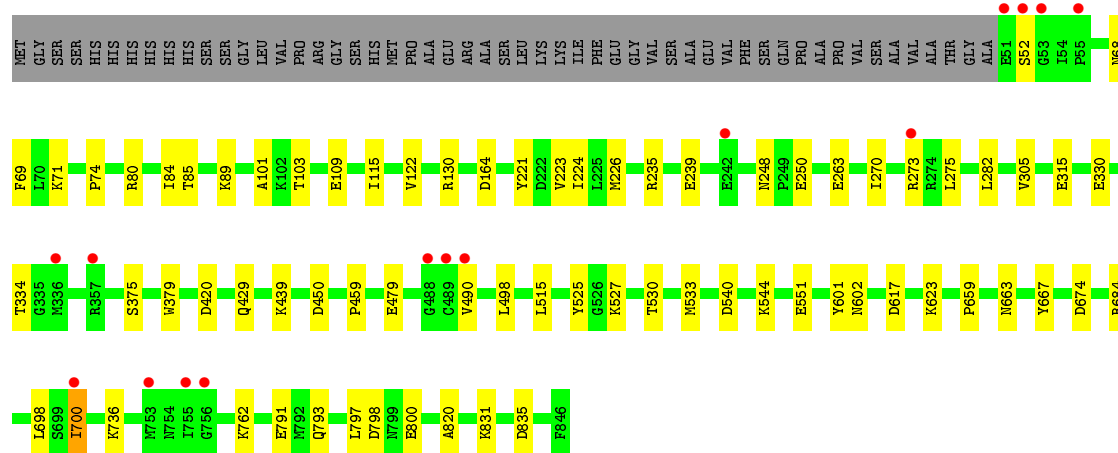
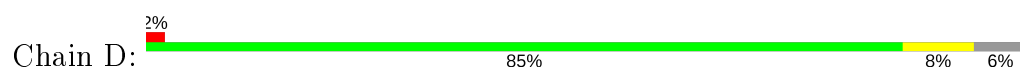


#### • Molecule 1: Choline trimethylamine-lyase

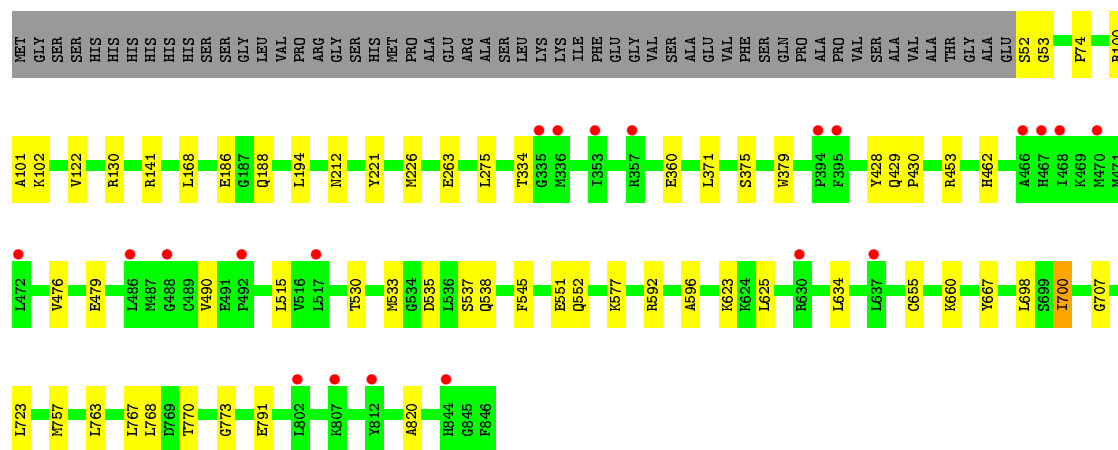
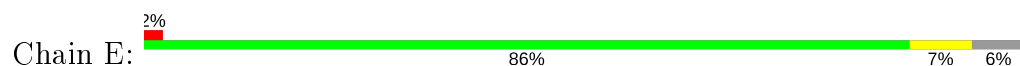




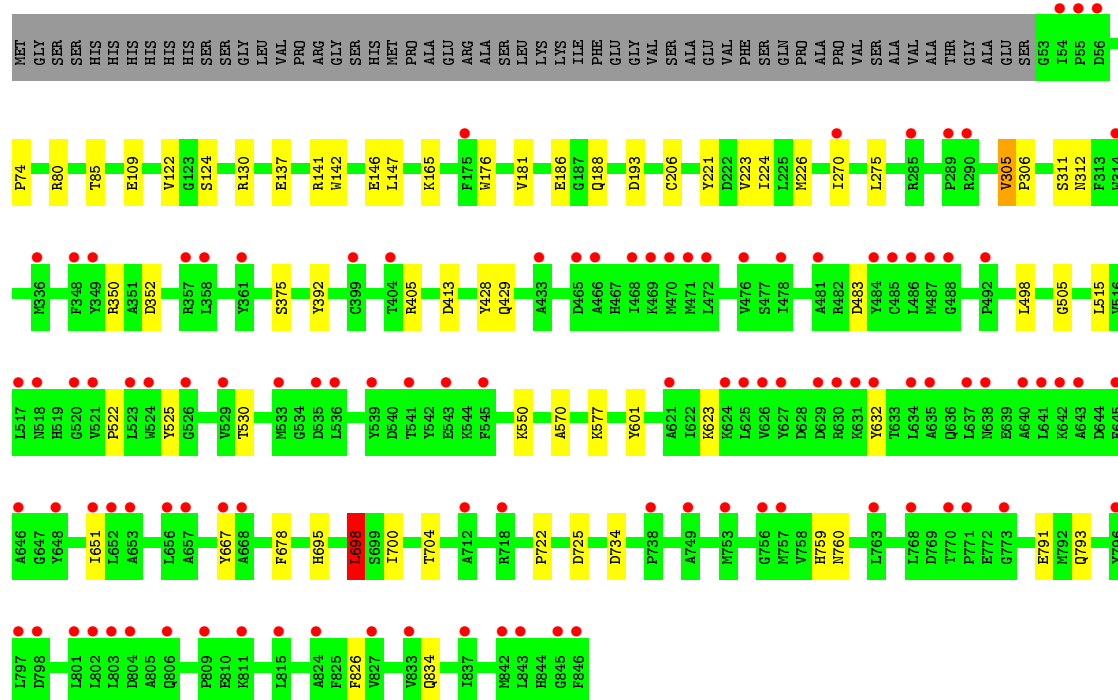
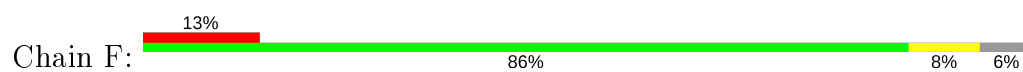
• Molecule 1: Choline trimethylamine-lyase



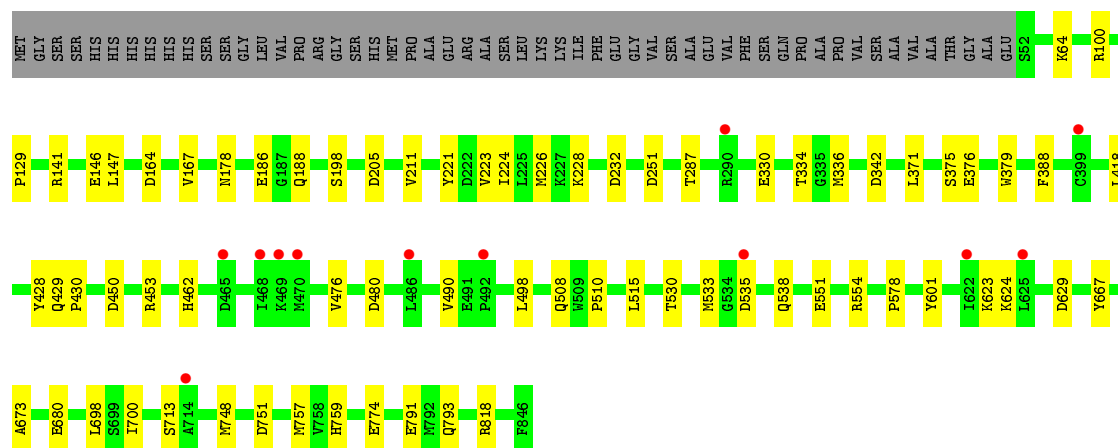
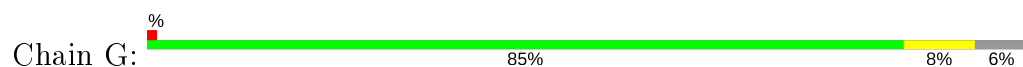
• Molecule 1: Choline trimethylamine-lyase



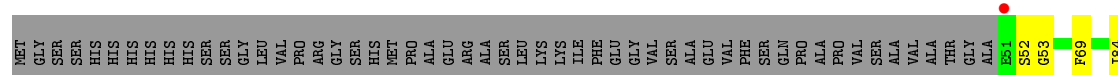
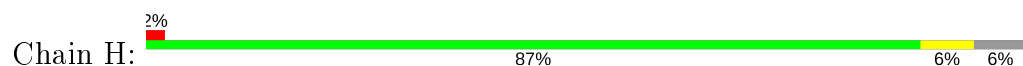
• Molecule 1: Choline trimethylamine-lyase

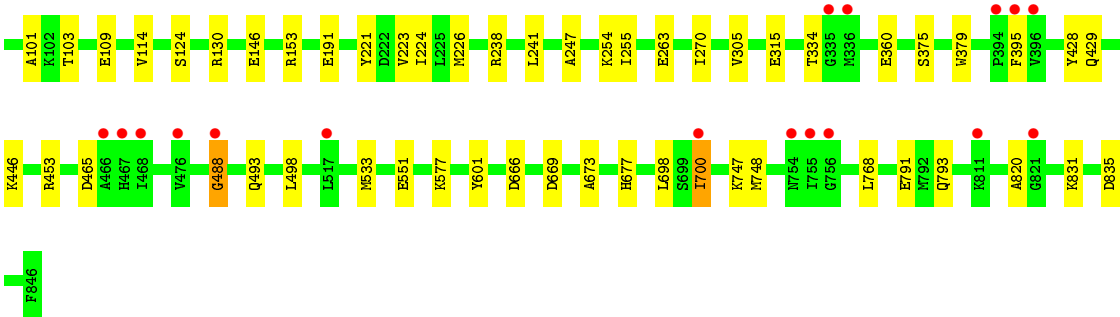


• Molecule 1: Choline trimethylamine-lyase



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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, 0.333 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.

All (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
1:D:282:LEU:O	3:D:1002:HOH:O	1.92	0.86
1:D:164:ASP:OD2	3:D:1004:HOH:O	1.94	0.85
1:D:674:ASP:OD1	3:D:1005:HOH:O	1.97	0.81
1:H:465:ASP:OD2	3:H:1001:HOH:O	1.99	0.80
1:G:211:VAL:O	3:G:1001:HOH:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:ASP:OD1	3:B:1001:HOH:O	2.01	0.79
1:D:459:PRO:O	3:D:1006:HOH:O	1.99	0.79
1:D:479:GLU:OE1	3:D:1007:HOH:O	2.01	0.79
1:G:146:GLU:OE1	3:G:1003:HOH:O	2.03	0.77
1:B:269:MET:O	3:B:1002:HOH:O	2.03	0.76
1:A:453:ARG:NH2	3:A:1004:HOH:O	2.17	0.76
1:G:680:GLU:OE2	3:G:1004:HOH:O	2.03	0.76
1:G:205:ASP:OD2	3:G:1002:HOH:O	2.02	0.76
1:B:479:GLU:OE2	3:B:1005:HOH:O	2.04	0.74
1:B:179:LYS:O	3:B:1004:HOH:O	2.04	0.74
1:D:450:ASP:OD2	3:D:1010:HOH:O	2.06	0.74
1:B:628:ASP:OD2	1:B:667:TYR:OH	2.06	0.74
1:B:254:LYS:NZ	3:B:1008:HOH:O	2.22	0.73
1:D:659:PRO:O	3:D:1009:HOH:O	2.05	0.73
1:E:212:ASN:OD1	3:E:1002:HOH:O	2.06	0.73
1:C:459:PRO:O	3:C:1004:HOH:O	2.08	0.72
1:A:514:GLU:OE2	3:A:1001:HOH:O	2.07	0.72
1:C:263:GLU:OE1	3:C:1003:HOH:O	2.07	0.72
1:H:238:ARG:NH1	3:H:1003:HOH:O	2.13	0.70
1:F:188:GLN:OE1	3:F:1002:HOH:O	2.09	0.69
1:D:617:ASP:OD2	3:D:1011:HOH:O	2.10	0.69
1:E:537:SER:OG	3:E:1003:HOH:O	2.11	0.68
1:H:146:GLU:OE1	3:H:1002:HOH:O	2.11	0.68
1:G:188:GLN:OE1	3:G:1006:HOH:O	2.12	0.68
1:B:238:ARG:NH2	3:B:1003:HOH:O	2.04	0.67
1:G:198:SER:OG	3:G:1005:HOH:O	2.11	0.66
1:G:251:ASP:OD2	3:G:1007:HOH:O	2.13	0.66
1:A:729:PRO:O	3:A:1002:HOH:O	2.14	0.65
1:C:722:PRO:O	3:C:1006:HOH:O	2.15	0.64
1:H:247:ALA:O	3:H:1004:HOH:O	2.14	0.64
1:D:80:ARG:NH2	1:D:330:GLU:O	2.30	0.63
1:E:770:THR:OG1	3:E:1004:HOH:O	2.15	0.63
1:G:498:LEU:HA	1:G:601:TYR:HB2	1.82	0.62
1:E:53:GLY:HA2	1:E:360:GLU:HB2	1.80	0.61
1:C:188:GLN:OE1	3:C:1007:HOH:O	2.16	0.60
1:A:164:ASP:OD2	3:A:1003:HOH:O	2.16	0.60
1:A:228:LYS:NZ	3:A:1011:HOH:O	2.28	0.60
1:G:450:ASP:OD1	1:G:453:ARG:NH2	2.35	0.60
1:C:86:LYS:NZ	3:C:1014:HOH:O	2.34	0.59
1:B:440:SER:O	1:B:782:ARG:NH2	2.36	0.59
1:B:426:ARG:NH2	3:B:1012:HOH:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:SER:N	3:E:1017:HOH:O	2.34	0.58
1:G:223:VAL:HG23	1:G:224:ILE:HG13	1.84	0.58
1:E:533:MET:HE1	1:E:551:GLU:HB3	1.86	0.58
1:E:707:GLY:HA2	1:E:723:LEU:HD13	1.85	0.58
1:G:533:MET:HB2	3:G:1051:HOH:O	2.03	0.58
1:B:787:LEU:HD23	1:C:439:LYS:HD3	1.86	0.58
1:C:498:LEU:HA	1:C:601:TYR:HB2	1.86	0.58
1:A:798:ASP:OD2	1:A:800:GLU:HB2	2.04	0.57
1:G:450:ASP:OD1	3:G:1008:HOH:O	2.18	0.57
1:F:826:PHE:O	1:F:834:GLN:NE2	2.38	0.57
1:H:375:SER:HA	1:H:429:GLN:HB2	1.86	0.57
1:E:623:LYS:HE3	1:E:667:TYR:CZ	2.40	0.56
1:B:698:LEU:HD13	1:B:698:LEU:H	1.69	0.56
1:F:85:THR:HG1	1:F:176:TRP:HE1	1.53	0.56
1:C:164:ASP:OD2	3:C:1008:HOH:O	2.18	0.56
1:F:206:CYS:HA	1:F:505:GLY:HA2	1.88	0.55
1:H:498:LEU:HA	1:H:601:TYR:HB2	1.88	0.55
1:C:248:ASN:HB3	1:C:250:GLU:OE2	2.06	0.55
1:D:68:ASN:HA	1:D:71:LYS:HE2	1.86	0.55
1:A:248:ASN:HB3	1:A:250:GLU:OE2	2.07	0.54
1:A:130:ARG:HD2	3:A:1031:HOH:O	2.06	0.54
1:E:479:GLU:OE2	1:H:677:HIS:HE1	1.90	0.54
1:B:305:VAL:HG22	1:B:306:PRO:HA	1.89	0.54
1:C:89:LYS:NZ	1:C:171:GLU:OE2	2.36	0.54
1:B:760:ASN:O	3:B:1006:HOH:O	2.18	0.54
1:C:369:CYS:HB3	3:C:1239:HOH:O	2.08	0.54
1:F:522:PRO:HG2	1:F:525:TYR:HB3	1.89	0.54
1:A:707:GLY:HA2	1:A:723:LEU:HD13	1.90	0.53
1:E:592:ARG:NH1	1:E:596:ALA:O	2.41	0.53
1:D:109:GLU:HG2	1:D:270:ILE:HG21	1.90	0.53
1:C:533:MET:HB2	3:C:1009:HOH:O	2.08	0.53
1:D:85:THR:HG22	1:D:89:LYS:HE3	1.89	0.53
1:G:623:LYS:HE3	1:G:667:TYR:CZ	2.44	0.53
1:D:835:ASP:OD2	3:D:1012:HOH:O	2.18	0.53
1:D:101:ALA:HB1	1:D:263:GLU:HB3	1.90	0.53
1:B:155:GLN:NE2	1:B:156:ASP:OD1	2.39	0.52
1:C:791:GLU:OE2	1:C:793:GLN:NE2	2.43	0.52
1:E:130:ARG:HD2	3:E:1026:HOH:O	2.09	0.52
1:E:533:MET:HB2	3:E:1007:HOH:O	2.08	0.52
1:F:375:SER:HA	1:F:429:GLN:HB2	1.91	0.52
1:B:53:GLY:N	3:B:1014:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:624:LYS:NZ	1:G:629:ASP:OD2	2.30	0.51
1:A:53:GLY:HA2	1:A:360:GLU:HB2	1.92	0.51
1:D:221:TYR:O	1:D:226:MET:HG2	2.10	0.51
1:B:221:TYR:O	1:B:226:MET:HG2	2.11	0.51
1:D:798:ASP:OD2	1:D:800:GLU:HB2	2.10	0.51
1:F:623:LYS:HE3	1:F:667:TYR:CZ	2.46	0.51
1:H:221:TYR:O	1:H:226:MET:HG2	2.11	0.51
1:H:254:LYS:NZ	3:H:1018:HOH:O	2.44	0.51
1:B:660:LYS:O	3:B:1007:HOH:O	2.20	0.51
1:F:181:VAL:HG13	1:F:570:ALA:HB1	1.93	0.51
1:D:375:SER:HA	1:D:429:GLN:HB2	1.92	0.50
1:H:446:LYS:NZ	3:H:1020:HOH:O	2.44	0.50
1:B:673:ALA:HA	1:B:748:MET:HG2	1.91	0.50
1:F:791:GLU:OE2	1:F:793:GLN:NE2	2.41	0.50
1:C:623:LYS:HE3	1:C:667:TYR:CZ	2.46	0.50
1:G:64:LYS:NZ	3:G:1037:HOH:O	2.44	0.50
1:G:453:ARG:NH1	1:G:774:GLU:OE1	2.44	0.50
1:F:80:ARG:NH2	1:F:137:GLU:OE2	2.40	0.49
1:B:248:ASN:HB3	1:B:250:GLU:OE2	2.13	0.49
1:F:74:PRO:HG2	1:F:392:TYR:CZ	2.48	0.49
1:F:141:ARG:NH2	1:F:186:GLU:OE1	2.41	0.49
1:F:109:GLU:HG2	1:F:270:ILE:HG21	1.93	0.49
1:G:375:SER:HA	1:G:429:GLN:HB2	1.94	0.49
1:F:147:LEU:HD22	1:F:165:LYS:HG2	1.94	0.49
1:F:515:LEU:HD13	1:F:530:THR:HG21	1.95	0.49
1:G:388:PHE:HB3	3:G:1108:HOH:O	2.13	0.49
1:D:623:LYS:HE3	1:D:667:TYR:CZ	2.48	0.48
1:G:287:THR:N	3:G:1022:HOH:O	2.36	0.48
1:H:223:VAL:HG23	1:H:224:ILE:HG13	1.94	0.48
1:F:130:ARG:HG2	3:F:1003:HOH:O	2.14	0.48
1:H:101:ALA:HB1	1:H:263:GLU:HB3	1.95	0.48
1:H:305:VAL:HG11	1:H:315:GLU:HB3	1.94	0.48
1:B:522:PRO:HG2	1:B:525:TYR:HB3	1.95	0.48
1:D:533:MET:HE1	1:D:551[B]:GLU:HG3	1.94	0.48
1:E:188:GLN:OE1	3:E:1005:HOH:O	2.20	0.48
1:G:673:ALA:HA	1:G:748:MET:HG2	1.94	0.48
1:B:498:LEU:HA	1:B:601:TYR:HB2	1.96	0.48
1:B:623:LYS:HE3	1:B:667:TYR:CZ	2.49	0.48
1:C:221:TYR:O	1:C:226:MET:HG2	2.13	0.48
1:B:826:PHE:O	1:B:834:GLN:NE2	2.41	0.48
1:C:793:GLN:NE2	1:C:818:ARG:HH21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:GLU:HG2	1:H:270:ILE:HG21	1.96	0.48
1:F:122:VAL:HG23	1:F:275:LEU:HD21	1.96	0.47
1:G:141:ARG:NH2	1:G:186:GLU:OE1	2.45	0.47
1:B:312:ASN:HB2	1:B:352:ASP:OD2	2.14	0.47
1:D:334:THR:HB	1:D:379:TRP:CG	2.49	0.47
1:E:515:LEU:HD13	1:E:530:THR:HG21	1.96	0.47
1:B:80:ARG:NH2	1:B:330:GLU:O	2.46	0.47
1:D:498:LEU:HA	1:D:601:TYR:HB2	1.96	0.47
1:F:375:SER:O	3:F:1003:HOH:O	2.20	0.47
1:H:700:ILE:O	1:H:820:ALA:HB3	2.14	0.47
1:B:457:GLY:HA3	1:B:818:ARG:HB2	1.96	0.47
1:D:700:ILE:O	1:D:820:ALA:HB3	2.14	0.47
1:F:223:VAL:HG23	1:F:224:ILE:HG13	1.97	0.47
1:G:515:LEU:HD13	1:G:530:THR:HG21	1.98	0.47
1:H:334:THR:HB	1:H:379:TRP:CG	2.50	0.47
1:D:223:VAL:HG23	1:D:224:ILE:HG13	1.98	0.46
1:D:831:LYS:HE3	1:D:835:ASP:OD2	2.16	0.46
1:F:305:VAL:HG22	1:F:306:PRO:HA	1.97	0.46
1:A:677:HIS:HE1	1:D:479:GLU:OE2	1.98	0.46
1:A:718:ARG:HB2	1:A:721:MET:HG3	1.98	0.46
1:B:649:ASP:N	1:B:649:ASP:OD1	2.48	0.46
1:A:498:LEU:HA	1:A:601:TYR:HB2	1.98	0.46
1:H:53:GLY:HA2	1:H:360:GLU:HB2	1.98	0.46
1:H:153:ARG:NH2	3:H:1002:HOH:O	2.31	0.46
1:F:498:LEU:HA	1:F:601:TYR:HB2	1.98	0.46
1:E:453:ARG:NH1	1:E:768:LEU:O	2.48	0.45
1:F:350:ARG:NH2	1:F:413:ASP:OD2	2.49	0.45
1:C:270:ILE:HG12	1:C:273:ARG:HH11	1.80	0.45
1:D:74:PRO:HA	1:D:130:ARG:O	2.17	0.45
1:E:375:SER:HA	1:E:429:GLN:HB2	1.99	0.45
1:H:114:VAL:HB	1:H:124:SER:HB3	1.98	0.45
1:A:515:LEU:HD13	1:A:530:THR:HG21	1.99	0.45
1:E:700:ILE:O	1:E:820:ALA:HB3	2.16	0.45
1:G:221:TYR:O	1:G:226:MET:HG2	2.17	0.45
1:D:248:ASN:HB3	1:D:250:GLU:OE2	2.16	0.45
1:A:462:HIS:CE1	1:A:791:GLU:HG3	2.52	0.45
1:B:589:GLU:OE1	1:B:589:GLU:N	2.48	0.45
1:H:191:GLU:HB3	3:H:1025:HOH:O	2.17	0.45
1:H:791:GLU:OE2	1:H:793:GLN:NE2	2.49	0.45
1:A:112:PRO:HG2	1:A:127:GLY:HA2	1.99	0.45
1:C:254:LYS:NZ	3:C:1032:HOH:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:GLU:OE1	3:D:1013:HOH:O	2.21	0.45
1:E:141:ARG:NH2	1:E:186:GLU:OE1	2.46	0.45
1:E:533:MET:HE3	1:E:552:GLN:HG2	1.99	0.44
1:G:793:GLN:NE2	1:G:818:ARG:HH21	2.15	0.44
1:H:453:ARG:NH2	1:H:768:LEU:O	2.50	0.44
1:H:69:PHE:CE1	1:H:130:ARG:HD3	2.52	0.44
1:B:205:ASP:O	1:B:505:GLY:HA2	2.16	0.44
1:D:69:PHE:CE1	1:D:130:ARG:HD3	2.52	0.44
1:D:663:ASN:HB3	1:D:736:LYS:NZ	2.33	0.44
1:G:330:GLU:OE2	1:G:578:PRO:HD2	2.16	0.44
1:H:673:ALA:HA	1:H:748:MET:HG2	1.99	0.44
1:B:751:ASP:N	1:B:751:ASP:OD1	2.46	0.44
1:F:311:SER:OG	3:F:1004:HOH:O	2.21	0.44
1:G:551:GLU:OE2	1:G:554:ARG:NH1	2.51	0.44
1:D:762:LYS:HD2	1:D:797:LEU:HD11	1.99	0.44
1:E:462:HIS:CE1	1:E:791:GLU:HG3	2.52	0.44
1:C:336:MET:HG2	1:C:336:MET:H	1.47	0.44
1:D:305:VAL:HG11	1:D:315:GLU:HB3	2.00	0.44
1:E:221:TYR:O	1:E:226:MET:HG2	2.18	0.44
1:C:395:PHE:O	1:C:488:GLY:HA2	2.17	0.44
1:D:273:ARG:HG3	3:D:1061:HOH:O	2.18	0.44
1:F:725:ASP:OD2	1:F:760:ASN:HB2	2.18	0.44
1:G:551:GLU:OE2	1:G:554:ARG:HD2	2.17	0.44
1:G:342:ASP:HB3	1:G:418:LEU:HD12	2.00	0.43
1:G:793:GLN:HE22	1:G:818:ARG:HH21	1.66	0.43
1:H:669:ASP:HB3	1:H:747:LYS:HD2	2.01	0.43
1:A:589:GLU:OE1	1:A:589:GLU:N	2.47	0.43
1:F:142:TRP:O	1:F:146[B]:GLU:HG2	2.18	0.43
1:G:462:HIS:CE1	1:G:791:GLU:HG3	2.54	0.43
1:B:375:SER:HA	1:B:429:GLN:HB2	2.00	0.43
1:D:115:ILE:HG12	1:D:122:VAL:HB	2.01	0.43
1:B:408:HIS:NE2	1:C:747:LYS:O	2.52	0.43
1:F:698:LEU:HD13	1:F:698:LEU:H	1.83	0.43
1:G:164:ASP:HA	1:G:167:VAL:HG12	2.01	0.43
1:G:228:LYS:HB2	1:G:232:ASP:HB2	1.99	0.43
1:D:122:VAL:HG23	1:D:275:LEU:HD21	2.00	0.43
1:F:312:ASN:HB2	1:F:352:ASP:OD2	2.17	0.43
1:F:550:LYS:HB3	1:F:678:PHE:CZ	2.54	0.43
1:G:751:ASP:OD1	1:G:751:ASP:N	2.47	0.43
1:A:700:ILE:O	1:A:820:ALA:HB3	2.19	0.43
1:C:535:ASP:O	1:C:538:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:ARG:HB2	1:B:721:MET:HG3	2.00	0.43
1:H:533:MET:HE1	1:H:551[B]:GLU:HG3	2.00	0.43
1:A:221:TYR:O	1:A:226:MET:HG2	2.18	0.43
1:H:493:GLN:HA	1:H:498:LEU:HD23	2.00	0.43
1:C:314:TRP:NE1	3:C:1005:HOH:O	2.12	0.42
1:D:525:TYR:CE2	1:D:527:LYS:HE2	2.54	0.42
1:E:655:CYS:O	1:E:660:LYS:NZ	2.45	0.42
1:F:704:THR:HG23	1:F:722:PRO:HG3	2.01	0.42
1:E:334:THR:HB	1:E:379:TRP:CG	2.54	0.42
1:F:221:TYR:O	1:F:226:MET:HG2	2.19	0.42
1:F:405:ARG:HG2	1:F:483:ASP:HB2	2.00	0.42
1:G:147:LEU:HD23	1:G:147:LEU:HA	1.94	0.42
1:A:533:MET:HB2	3:A:1021:HOH:O	2.18	0.42
1:C:228:LYS:HB2	1:C:232:ASP:HB2	2.01	0.42
1:C:375:SER:HA	1:C:429:GLN:HB2	2.01	0.42
1:D:84:ILE:HB	1:D:103:THR:HG21	2.00	0.42
1:E:767:LEU:O	1:E:773:GLY:HA3	2.18	0.42
1:D:540:ASP:OD1	1:D:544:LYS:HD2	2.20	0.42
1:E:545:PHE:CD1	1:E:634:LEU:HD11	2.55	0.42
1:C:515:LEU:HD13	1:C:530:THR:HG21	2.02	0.42
1:F:734:ASP:OD1	1:F:734:ASP:N	2.50	0.42
1:G:476:VAL:HG13	1:G:480:ASP:HB2	2.01	0.42
1:A:462:HIS:CE1	1:A:486:LEU:HD22	2.54	0.42
1:B:334:THR:HB	1:B:379:TRP:CG	2.55	0.42
1:C:147:LEU:HD22	1:C:165:LYS:HG2	2.02	0.42
1:G:508:GLN:HB2	1:G:510:PRO:HD2	2.00	0.42
1:H:666:ASP:OD1	1:H:747:LYS:NZ	2.40	0.42
1:B:101:ALA:HB1	1:B:263:GLU:HB3	2.02	0.42
1:C:491:GLU:N	1:C:491:GLU:OE1	2.53	0.42
1:D:663:ASN:HB3	1:D:736:LYS:HZ3	1.84	0.42
1:D:791:GLU:OE2	1:D:793:GLN:NE2	2.51	0.41
1:B:84:ILE:HB	1:B:103:THR:HG21	2.02	0.41
1:B:216:ASP:HA	1:B:487:MET:SD	2.60	0.41
1:E:535:ASP:O	1:E:538:GLN:HG2	2.21	0.41
1:H:241:LEU:HD11	1:H:255:ILE:HG23	2.01	0.41
1:A:334:THR:HB	1:A:379:TRP:CG	2.55	0.41
1:B:515:LEU:HD13	1:B:530:THR:HG21	2.01	0.41
1:H:395:PHE:O	1:H:488:GLY:HA2	2.21	0.41
1:D:623:LYS:NZ	3:D:1026:HOH:O	2.36	0.41
1:G:535:ASP:O	1:G:538:GLN:HG2	2.21	0.41
1:E:74:PRO:HA	1:E:130:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:HA	1:C:147:LEU:HD23	1.80	0.41
1:D:235:ARG:NH1	1:D:239:GLU:OE2	2.53	0.41
1:E:371:LEU:HD22	1:E:430:PRO:HD2	2.01	0.41
1:A:787:LEU:HD23	1:D:439:LYS:HD3	2.02	0.41
1:B:616:VAL:HG13	1:B:671:ILE:HB	2.03	0.41
1:D:515:LEU:HD13	1:D:530:THR:HG21	2.03	0.41
1:G:129:PRO:HB3	1:G:376:GLU:HG2	2.02	0.41
1:D:684:ARG:NH2	3:D:1059:HOH:O	2.54	0.41
1:F:698:LEU:CD1	1:F:698:LEU:H	2.34	0.41
1:G:334:THR:HB	1:G:379:TRP:CG	2.55	0.41
1:B:536:LEU:HD23	1:B:634:LEU:HB3	2.02	0.41
1:B:700:ILE:O	1:B:820:ALA:HB3	2.20	0.41
1:C:628:ASP:OD2	1:C:667:TYR:OH	2.20	0.41
1:C:762:LYS:HD2	1:C:797:LEU:HD11	2.03	0.41
1:E:479:GLU:OE2	1:H:677:HIS:CE1	2.72	0.41
1:F:632:TYR:CZ	1:F:651:ILE:HG12	2.56	0.41
1:C:123:GLY:HA3	3:C:1063:HOH:O	2.19	0.40
1:C:353:ILE:HD12	1:C:360:GLU:HG2	2.03	0.40
1:E:101:ALA:HB1	1:E:263:GLU:HB3	2.03	0.40
1:E:52:SER:N	3:E:1041:HOH:O	2.54	0.40
1:B:181:VAL:HG13	1:B:570:ALA:HB1	2.02	0.40
1:E:102:LYS:HE2	3:E:1231:HOH:O	2.21	0.40
1:G:371:LEU:HD22	1:G:430:PRO:HD2	2.02	0.40
1:A:663:ASN:HB3	1:A:736:LYS:HD2	2.03	0.40
1:A:720:TRP:O	3:A:1005:HOH:O	2.22	0.40
1:C:164:ASP:HA	1:C:167:VAL:HG12	2.02	0.40
1:F:74:PRO:HA	1:F:130:ARG:O	2.21	0.40
1:H:831:LYS:NZ	1:H:835:ASP:OD2	2.46	0.40
1:H:84:ILE:HB	1:H:103:THR:HG21	2.03	0.40
1:E:122:VAL:HG23	1:E:275:LEU:HD21	2.03	0.40

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

All (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
1	D	52	SER
1	D	700	ILE
1	H	52	SER
1	F	700	ILE
1	G	700	ILE
1	B	489	CYS
1	D	490	VAL
1	E	490	VAL
1	G	490	VAL
1	H	488	GLY

### 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
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

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	168	LEU
1	A	194	LEU
1	A	428	TYR
1	A	577	LYS
1	A	698	LEU
1	A	763	LEU
1	B	305	VAL
1	B	428	TYR
1	B	577	LYS
1	B	649	ASP
1	B	698	LEU
1	B	759	HIS
1	C	100	ARG
1	C	178	ASN
1	C	336	MET
1	C	428	TYR
1	C	698	LEU
1	C	713	SER
1	C	757	MET
1	D	698	LEU
1	E	100	ARG
1	E	168	LEU
1	E	194	LEU
1	E	428	TYR
1	E	476	VAL
1	E	577	LYS

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Mol	Chain	Res	Type
1	E	625	LEU
1	E	698	LEU
1	E	757	MET
1	E	763	LEU
1	F	124	SER
1	F	305	VAL
1	F	428	TYR
1	F	577	LYS
1	F	695	HIS
1	F	698	LEU
1	F	759	HIS
1	G	100	ARG
1	G	178	ASN
1	G	336	MET
1	G	428	TYR
1	G	698	LEU
1	G	713	SER
1	G	757	MET
1	G	759	HIS
1	H	428	TYR
1	H	577	LYS
1	H	698	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	677	HIS
1	B	68	ASN
1	B	218	ASN
1	B	248	ASN
1	B	677	HIS
1	B	708	GLN
1	B	806	GLN
1	C	759	HIS
1	D	559	ASN
1	D	677	HIS
1	E	188	GLN
1	E	243	GLN
1	E	806	GLN
1	F	248	ASN
1	F	806	GLN

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Mol	Chain	Res	Type
1	H	248	ASN
1	H	559	ASN
1	H	677	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 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	-

All (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
2	G	901	BTL	O1-C	3.84	1.41	1.19
2	F	901	BTL	O1-C	3.84	1.41	1.19
2	A	901	BTL	O1-C	3.81	1.41	1.19
2	C	901	BTL	CA-N	-2.22	1.47	1.52
2	B	901	BTL	CA-N	-2.20	1.47	1.52
2	E	901	BTL	CA-N	-2.19	1.47	1.52
2	H	901	BTL	CA-N	-2.19	1.47	1.52
2	F	901	BTL	CA-N	-2.19	1.47	1.52
2	F	901	BTL	C3-N	-2.13	1.43	1.50
2	A	901	BTL	CA-N	-2.13	1.47	1.52
2	E	901	BTL	C3-N	-2.12	1.43	1.50
2	B	901	BTL	C3-N	-2.11	1.43	1.50
2	C	901	BTL	C3-N	-2.11	1.43	1.50
2	G	901	BTL	C3-N	-2.11	1.43	1.50
2	D	901	BTL	C3-N	-2.10	1.43	1.50
2	G	901	BTL	CA-N	-2.08	1.47	1.52
2	H	901	BTL	C3-N	-2.07	1.44	1.50
2	D	901	BTL	CA-N	-2.01	1.47	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
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
2	E	901	BTL	O1-C-CA	-5.01	111.26	126.39
2	D	901	BTL	O1-C-CA	-4.78	111.97	126.39
2	C	901	BTL	O1-C-CA	-4.76	112.02	126.39

There are no chirality outliers.

All (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
2	F	901	BTL	C-CA-N-C2
2	E	901	BTL	C-CA-N-C2
2	H	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

### 6.1 Protein, DNA and RNA chains

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	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

All (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
1	F	641	LEU	5.6
1	F	802	LEU	5.4
1	F	632	TYR	5.4
1	B	517	LEU	5.2
1	F	845	GLY	5.0
1	F	536	LEU	4.8
1	B	53	GLY	4.5
1	F	465[A]	ASP	4.5
1	F	488	GLY	4.5
1	B	627	TYR	4.3
1	F	358	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	763	LEU	4.3
1	B	358	LEU	4.2
1	B	632	TYR	4.0
1	B	802	LEU	3.9
1	F	630	ARG	3.9
1	F	646	ALA	3.9
1	F	640	ALA	3.8
1	B	285	ARG	3.7
1	F	533	MET	3.7
1	F	803	LEU	3.7
1	B	536	LEU	3.7
1	F	517	LEU	3.6
1	F	486	LEU	3.6
1	F	797	LEU	3.6
1	F	357	ARG	3.6
1	G	468	ILE	3.6
1	F	270	ILE	3.6
1	F	642	LYS	3.5
1	B	645	PHE	3.5
1	F	521	VAL	3.5
1	F	627	TYR	3.5
1	F	637	LEU	3.5
1	F	361	TYR	3.5
1	B	630	ARG	3.4
1	F	466	ALA	3.4
1	B	465[A]	ASP	3.4
1	F	804	ASP	3.4
1	F	545	PHE	3.3
1	D	51	GLU	3.3
1	B	539	TYR	3.2
1	F	523	LEU	3.2
1	F	56	ASP	3.2
1	F	635	ALA	3.2
1	C	289	PRO	3.2
1	E	807	LYS	3.2
1	F	827	VAL	3.2
1	F	842	MET	3.2
1	G	465[A]	ASP	3.1
1	F	757[A]	MET	3.1
1	F	524	TRP	3.1
1	C	465[A]	ASP	3.1
1	H	755	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	481	ALA	3.1
1	H	51	GLU	3.1
1	B	290	ARG	3.1
1	B	295	LEU	3.1
1	B	357	ARG	3.1
1	F	543	GLU	3.0
1	F	843	LEU	3.0
1	G	622	ILE	3.0
1	B	56	ASP	3.0
1	F	643	ALA	3.0
1	B	55	PRO	3.0
1	B	625	LEU	3.0
1	E	492	PRO	3.0
1	C	468	ILE	3.0
1	F	833	VAL	3.0
1	B	803	LEU	3.0
1	B	807	LYS	3.0
1	C	287	THR	3.0
1	F	472	LEU	3.0
1	G	535	ASP	2.9
1	F	399	CYS	2.9
1	F	846	PHE	2.9
1	B	658	ALA	2.9
1	F	668	ALA	2.9
1	F	54	ILE	2.9
1	B	541	THR	2.9
1	F	529	VAL	2.9
1	B	486	LEU	2.9
1	C	492	PRO	2.9
1	B	629	ASP	2.9
1	H	468	ILE	2.9
1	B	624	LYS	2.8
1	F	624	LYS	2.8
1	B	533	MET	2.8
1	C	293	ALA	2.8
1	A	492	PRO	2.8
1	F	712	ALA	2.8
1	F	631	LYS	2.8
1	F	798	ASP	2.8
1	A	658	ALA	2.7
1	F	541	THR	2.7
1	E	637	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	166	LYS	2.7
1	F	468	ILE	2.7
1	G	714	ALA	2.7
1	B	637	LEU	2.7
1	F	476	VAL	2.7
1	F	809	PRO	2.7
1	B	297	LYS	2.7
1	C	470	MET	2.7
1	B	492	PRO	2.6
1	B	651	ILE	2.6
1	A	643	ALA	2.6
1	F	433	ALA	2.6
1	F	651	ILE	2.6
1	F	815	LEU	2.6
1	H	396	VAL	2.6
1	B	521	VAL	2.6
1	F	773	GLY	2.6
1	H	488	GLY	2.6
1	F	806	GLN	2.6
1	A	465[A]	ASP	2.6
1	G	469	LYS	2.6
1	C	535	ASP	2.6
1	A	646	ALA	2.6
1	D	755	ILE	2.6
1	D	52	SER	2.5
1	A	490	VAL	2.5
1	E	335	GLY	2.5
1	F	518	ASN	2.5
1	B	488	GLY	2.5
1	D	273	ARG	2.5
1	F	484	TYR	2.5
1	F	478	ILE	2.5
1	F	492	PRO	2.5
1	F	738	PRO	2.5
1	H	395	PHE	2.5
1	B	646	ALA	2.5
1	B	468	ILE	2.5
1	G	492	PRO	2.5
1	F	626	VAL	2.5
1	B	535	ASP	2.5
1	F	535	ASP	2.5
1	B	772	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	517	LEU	2.5
1	D	336	MET	2.5
1	F	470	MET	2.5
1	F	485	CYS	2.5
1	A	801	LEU	2.5
1	C	517	LEU	2.4
1	D	242	GLU	2.4
1	C	296	GLN	2.4
1	B	801	LEU	2.4
1	B	643	ALA	2.4
1	F	653	ALA	2.4
1	F	289	PRO	2.4
1	E	357	ARG	2.4
1	C	472	LEU	2.4
1	F	768	LEU	2.4
1	G	486	LEU	2.4
1	C	469	LYS	2.4
1	E	472	LEU	2.4
1	G	625	LEU	2.4
1	B	631	LYS	2.4
1	F	629	ASP	2.4
1	H	336	MET	2.4
1	B	846	PHE	2.4
1	F	404	THR	2.4
1	B	314	TRP	2.4
1	C	536	LEU	2.4
1	F	657	ALA	2.4
1	H	466	ALA	2.4
1	F	348	PHE	2.4
1	F	638	ASN	2.4
1	A	468	ILE	2.3
1	E	488	GLY	2.3
1	H	821	GLY	2.3
1	E	394	PRO	2.3
1	F	771	PRO	2.3
1	F	796	TYR	2.3
1	A	802	LEU	2.3
1	B	831	LYS	2.3
1	F	336	MET	2.3
1	F	756	GLY	2.3
1	B	519	HIS	2.3
1	E	467	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	837	ILE	2.3
1	B	540	ASP	2.3
1	D	488	GLY	2.3
1	E	844	HIS	2.3
1	A	651	ILE	2.3
1	D	700	ILE	2.3
1	B	542	TYR	2.3
1	B	478	ILE	2.3
1	B	641	LEU	2.3
1	B	770	THR	2.3
1	F	648	TYR	2.3
1	F	520	GLY	2.3
1	F	753	MET	2.3
1	F	285	ARG	2.3
1	D	490	VAL	2.3
1	F	314	TRP	2.3
1	B	755	ILE	2.3
1	E	466	ALA	2.3
1	E	468	ILE	2.3
1	F	749	ALA	2.3
1	F	290	ARG	2.2
1	F	175	PHE	2.2
1	H	700	ILE	2.2
1	F	656	LEU	2.2
1	F	801	LEU	2.2
1	F	349	TYR	2.2
1	E	395	PHE	2.2
1	B	622	ILE	2.2
1	H	756	GLY	2.2
1	C	484	TYR	2.2
1	C	290	ARG	2.2
1	G	399	CYS	2.2
1	E	802	LEU	2.2
1	D	357	ARG	2.2
1	F	718	ARG	2.2
1	G	470	MET	2.2
1	B	532	ASP	2.2
1	D	489	CYS	2.2
1	F	770	THR	2.2
1	H	467	HIS	2.2
1	B	487	MET	2.2
1	D	753	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	812	TYR	2.2
1	F	621	ALA	2.2
1	F	811	LYS	2.2
1	E	630	ARG	2.1
1	H	476	VAL	2.1
1	E	353	ILE	2.1
1	B	523	LEU	2.1
1	E	486	LEU	2.1
1	F	652	LEU	2.1
1	F	55	PRO	2.1
1	B	766	GLY	2.1
1	D	53	GLY	2.1
1	B	653	ALA	2.1
1	D	756	GLY	2.1
1	F	471	MET	2.1
1	B	711	GLY	2.1
1	F	526	GLY	2.1
1	F	667	TYR	2.1
1	H	517	LEU	2.1
1	B	543	GLU	2.1
1	E	336	MET	2.1
1	B	481	ALA	2.1
1	D	55	PRO	2.1
1	A	470	MET	2.0
1	F	469	LYS	2.0
1	H	754	ASN	2.0
1	H	394	PRO	2.0
1	G	290	ARG	2.0
1	F	487	MET	2.0
1	H	811	LYS	2.0
1	A	336	MET	2.0
1	E	470	MET	2.0
1	H	335	GLY	2.0
1	B	718	ARG	2.0
1	F	824	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	B-factors( $\text{\AA}^2$ )	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.