



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 01:21 am BST

PDB ID : 3MBM  
Title : Crystal structure of 2C-methyl-D-erythritol 2,4-cyclodiphosphate synthase from Burkholderia pseudomallei with cytosine and FoL fragment 717, imidazole[2,1-b][1,3]thiazol-6-ylmethanol  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2010-03-25  
Resolution : 1.80 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

<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

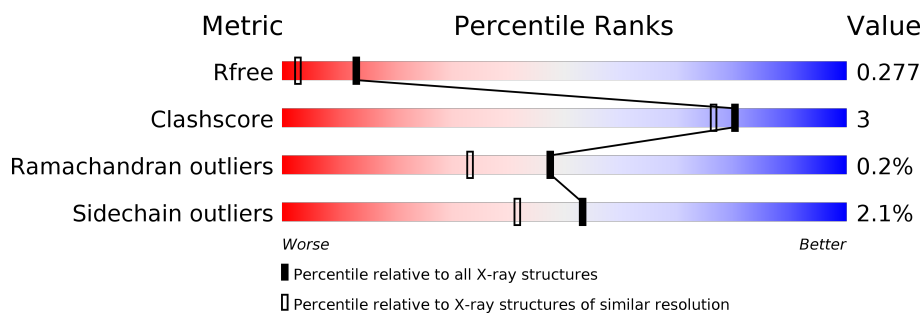
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	183	
1	B	183	
1	C	183	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3743 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	1	0
			1183	742	220	218	3			
1	B	154	Total	C	N	O	S	0	1	0
			1132	711	207	211	3			
1	C	151	Total	C	N	O	S	0	1	0
			1114	701	204	206	3			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q63T71
A	-19	ALA	-	EXPRESSION TAG	UNP Q63T71
A	-18	HIS	-	EXPRESSION TAG	UNP Q63T71
A	-17	HIS	-	EXPRESSION TAG	UNP Q63T71
A	-16	HIS	-	EXPRESSION TAG	UNP Q63T71
A	-15	HIS	-	EXPRESSION TAG	UNP Q63T71
A	-14	HIS	-	EXPRESSION TAG	UNP Q63T71
A	-13	HIS	-	EXPRESSION TAG	UNP Q63T71
A	-12	MET	-	EXPRESSION TAG	UNP Q63T71
A	-11	GLY	-	EXPRESSION TAG	UNP Q63T71
A	-10	THR	-	EXPRESSION TAG	UNP Q63T71
A	-9	LEU	-	EXPRESSION TAG	UNP Q63T71
A	-8	GLU	-	EXPRESSION TAG	UNP Q63T71
A	-7	ALA	-	EXPRESSION TAG	UNP Q63T71
A	-6	GLN	-	EXPRESSION TAG	UNP Q63T71
A	-5	THR	-	EXPRESSION TAG	UNP Q63T71
A	-4	GLN	-	EXPRESSION TAG	UNP Q63T71
A	-3	GLY	-	EXPRESSION TAG	UNP Q63T71
A	-2	PRO	-	EXPRESSION TAG	UNP Q63T71
A	-1	GLY	-	EXPRESSION TAG	UNP Q63T71
A	0	SER	-	EXPRESSION TAG	UNP Q63T71
B	-20	MET	-	EXPRESSION TAG	UNP Q63T71
B	-19	ALA	-	EXPRESSION TAG	UNP Q63T71

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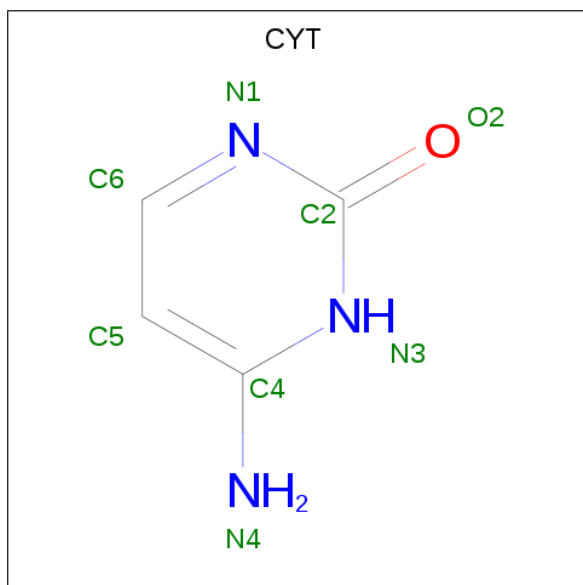
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	EXPRESSION TAG	UNP Q63T71
B	-17	HIS	-	EXPRESSION TAG	UNP Q63T71
B	-16	HIS	-	EXPRESSION TAG	UNP Q63T71
B	-15	HIS	-	EXPRESSION TAG	UNP Q63T71
B	-14	HIS	-	EXPRESSION TAG	UNP Q63T71
B	-13	HIS	-	EXPRESSION TAG	UNP Q63T71
B	-12	MET	-	EXPRESSION TAG	UNP Q63T71
B	-11	GLY	-	EXPRESSION TAG	UNP Q63T71
B	-10	THR	-	EXPRESSION TAG	UNP Q63T71
B	-9	LEU	-	EXPRESSION TAG	UNP Q63T71
B	-8	GLU	-	EXPRESSION TAG	UNP Q63T71
B	-7	ALA	-	EXPRESSION TAG	UNP Q63T71
B	-6	GLN	-	EXPRESSION TAG	UNP Q63T71
B	-5	THR	-	EXPRESSION TAG	UNP Q63T71
B	-4	GLN	-	EXPRESSION TAG	UNP Q63T71
B	-3	GLY	-	EXPRESSION TAG	UNP Q63T71
B	-2	PRO	-	EXPRESSION TAG	UNP Q63T71
B	-1	GLY	-	EXPRESSION TAG	UNP Q63T71
B	0	SER	-	EXPRESSION TAG	UNP Q63T71
C	-20	MET	-	EXPRESSION TAG	UNP Q63T71
C	-19	ALA	-	EXPRESSION TAG	UNP Q63T71
C	-18	HIS	-	EXPRESSION TAG	UNP Q63T71
C	-17	HIS	-	EXPRESSION TAG	UNP Q63T71
C	-16	HIS	-	EXPRESSION TAG	UNP Q63T71
C	-15	HIS	-	EXPRESSION TAG	UNP Q63T71
C	-14	HIS	-	EXPRESSION TAG	UNP Q63T71
C	-13	HIS	-	EXPRESSION TAG	UNP Q63T71
C	-12	MET	-	EXPRESSION TAG	UNP Q63T71
C	-11	GLY	-	EXPRESSION TAG	UNP Q63T71
C	-10	THR	-	EXPRESSION TAG	UNP Q63T71
C	-9	LEU	-	EXPRESSION TAG	UNP Q63T71
C	-8	GLU	-	EXPRESSION TAG	UNP Q63T71
C	-7	ALA	-	EXPRESSION TAG	UNP Q63T71
C	-6	GLN	-	EXPRESSION TAG	UNP Q63T71
C	-5	THR	-	EXPRESSION TAG	UNP Q63T71
C	-4	GLN	-	EXPRESSION TAG	UNP Q63T71
C	-3	GLY	-	EXPRESSION TAG	UNP Q63T71
C	-2	PRO	-	EXPRESSION TAG	UNP Q63T71
C	-1	GLY	-	EXPRESSION TAG	UNP Q63T71
C	0	SER	-	EXPRESSION TAG	UNP Q63T71

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

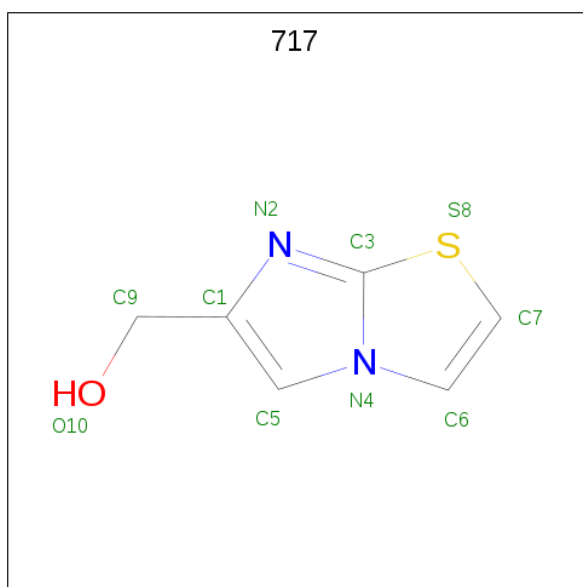
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 6-AMINOPYRIMIDIN-2(1H)-ONE (three-letter code: CYT) (formula:  $C_4H_5N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	3	1		
3	B	1	Total	C	N	O	0	0
			8	4	3	1		
3	C	1	Total	C	N	O	0	0
			8	4	3	1		

- Molecule 4 is imidazo[2,1-b][1,3]thiazol-6-ylmethanol (three-letter code: 717) (formula:  $C_6H_6N_2OS$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			10	6	2	1	1		
4	B	1	Total	C	N	O	S	0	0
			10	6	2	1	1		
4	C	1	Total	C	N	O	S	0	0
			10	6	2	1	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			16	8	2	6		


- Molecule 6 is water.

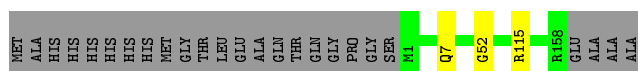
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	133	Total	O	0	0
			133	133		
6	B	45	Total	O	0	0
			45	45		
6	C	63	Total	O	0	0
			63	63		

### 3 Residue-property plots [i](#)

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. 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. 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.

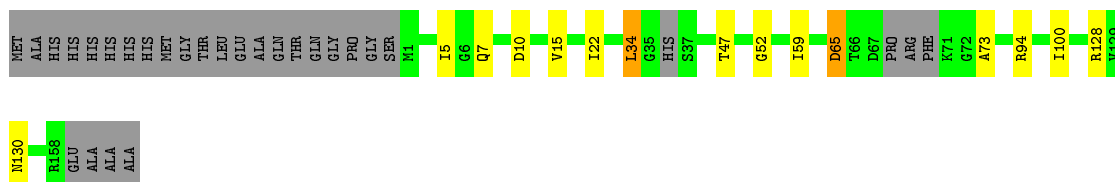
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain A: 




- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain B: 



- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain C: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.54Å 67.57Å 60.03Å 90.00° 96.12° 90.00°	Depositor
Resolution (Å)	25.50 – 1.80 25.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (25.50-1.80) 96.0 (25.50-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.188 , 0.217 0.250 , 0.277	Depositor DCC
$R_{free}$ test set	2090 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 717, ZN, TRS, CYT

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	0.68	0/1205	0.75	0/1633
1	B	0.55	0/1149	0.70	1/1556 (0.1%)
1	C	0.62	0/1132	0.73	0/1535
All	All	0.62	0/3486	0.73	1/4724 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ASP	CB-CG-OD1	6.45	124.10	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1183	0	1193	2	0
1	B	1132	0	1135	16	0
1	C	1114	0	1125	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	8	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	4	0	0
3	C	8	0	4	0	0
4	A	10	0	6	0	0
4	B	10	0	6	0	0
4	C	10	0	6	0	0
5	A	16	0	24	0	0
6	A	133	0	0	1	0
6	B	45	0	0	0	0
6	C	63	0	0	0	0
All	All	3743	0	3507	19	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 19 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:B:15:VAL:HG22	1:B:34:LEU:HD21	1.37	1.03
1:B:15:VAL:CG2	1:B:34:LEU:HD21	2.23	0.61
1:C:42:LEU:HD22	1:C:100:ILE:HD11	1.85	0.58
1:B:34:LEU:HD23	1:B:34:LEU:N	2.21	0.55
1:B:5[B]:ILE:CD1	1:C:5:ILE:CD1	2.86	0.54

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	157/183 (86%)	155 (99%)	2 (1%)	0	100	100
1	B	149/183 (81%)	146 (98%)	2 (1%)	1 (1%)	22	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	148/183 (81%)	144 (97%)	4 (3%)	0	100	100
All	All	454/549 (83%)	445 (98%)	8 (2%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	ALA

### 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	117/135 (87%)	116 (99%)	1 (1%)	78	75
1	B	110/135 (82%)	107 (97%)	3 (3%)	44	31
1	C	109/135 (81%)	106 (97%)	3 (3%)	43	30
All	All	336/405 (83%)	329 (98%)	7 (2%)	53	42

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	ASP
1	C	95	ASN
1	C	1	MET
1	B	7	GLN
1	C	7	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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$
3	CYT	C	165	-	7,8,8	1.35	1 (14%)	8,10,10	5.18	5 (62%)
4	717	C	163	2	6,11,11	2.82	2 (33%)	3,15,15	2.26	1 (33%)
4	717	A	165	2	6,11,11	1.95	2 (33%)	3,15,15	1.80	1 (33%)
3	CYT	B	164	-	7,8,8	0.99	0	8,10,10	6.79	3 (37%)
5	TRS	A	166[B]	-	7,7,7	0.34	0	9,9,9	0.52	0
5	TRS	A	166[A]	-	7,7,7	0.21	0	9,9,9	0.48	0
4	717	B	165	2	6,11,11	2.31	2 (33%)	3,15,15	1.64	1 (33%)
3	CYT	A	164	-	7,8,8	1.24	1 (14%)	8,10,10	6.36	3 (37%)

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
3	CYT	C	165	-	-	-	0/1/1/1
4	717	C	163	2	-	0/0/2/2	0/2/2/2
4	717	A	165	2	-	0/0/2/2	0/2/2/2
3	CYT	B	164	-	-	-	0/1/1/1
5	TRS	A	166[B]	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TRS	A	166[A]	-	-	4/9/9/9	-
4	717	B	165	2	-	0/0/2/2	0/2/2/2
3	CYT	A	164	-	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	163	717	C3-N2	5.82	1.41	1.33
4	B	165	717	C3-N2	3.96	1.39	1.33
4	B	165	717	C5-C1	3.84	1.41	1.36
4	A	165	717	C5-C1	3.60	1.41	1.36
4	C	163	717	C5-C1	3.54	1.41	1.36

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	164	CYT	N1-C2-N3	-13.61	117.61	128.43
3	A	164	CYT	N1-C2-N3	-12.52	118.48	128.43
3	B	164	CYT	C6-N1-C2	11.97	120.32	114.42
3	A	164	CYT	C6-N1-C2	11.86	120.27	114.42
3	C	165	CYT	N1-C2-N3	-9.97	120.51	128.43

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	166[B]	TRS	C1-C-C3-O3
5	A	166[B]	TRS	C2-C-C3-O3
5	A	166[B]	TRS	N-C-C3-O3
5	A	166[A]	TRS	C1-C-C3-O3
5	A	166[A]	TRS	C2-C-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.