



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2024 – 10:53 AM EDT

PDB ID : 2ZPA  
Title : Crystal Structure of tRNA(Met) Cytidine Acetyltransferase  
Authors : Chimnaronk, S.; Manita, T.; Yao, M.; Tanaka, I.  
Deposited on : 2008-07-08  
Resolution : 2.35 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

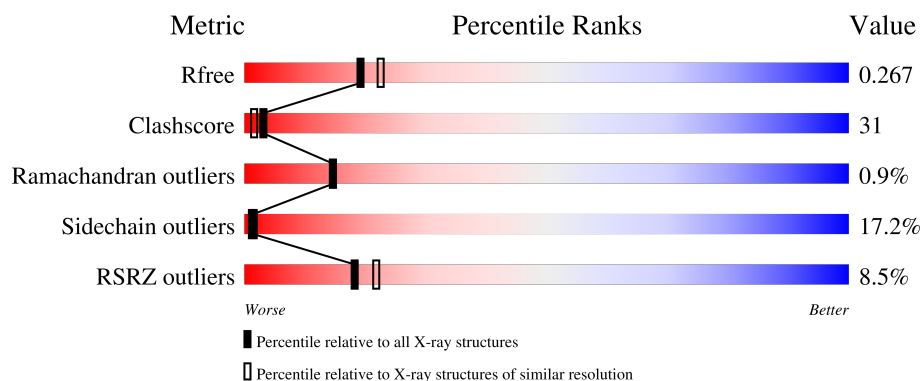
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (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 of 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	671	
1	B	671	

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	ACO	A	700	X	-	-	-
2	ACO	B	701	X	-	-	-

## 2 Entry composition [i](#)

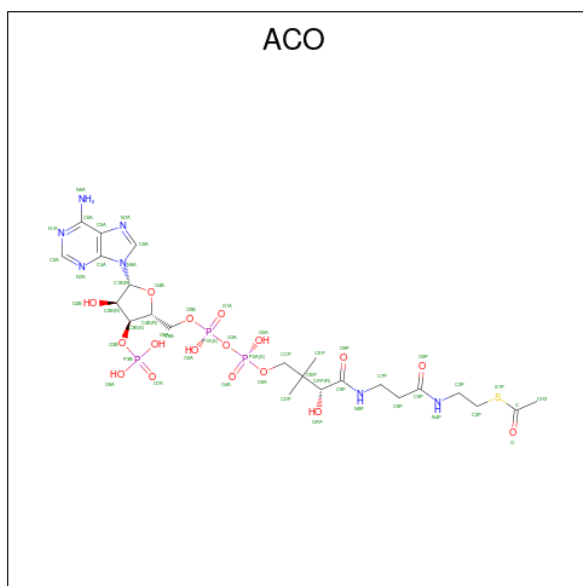
There are 5 unique types of molecules in this entry. The entry contains 10891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein ypfl.

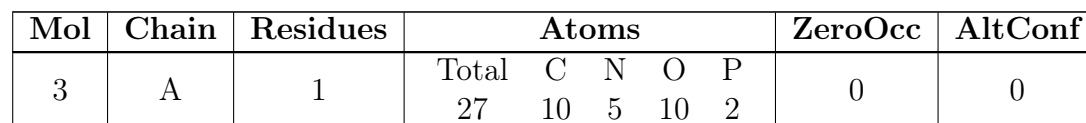
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	Se	0	0	0
			5189	3291	951	929	8	10			
1	B	662	Total	C	N	O	S	Se	0	0	0
			5218	3309	955	935	8	11			

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



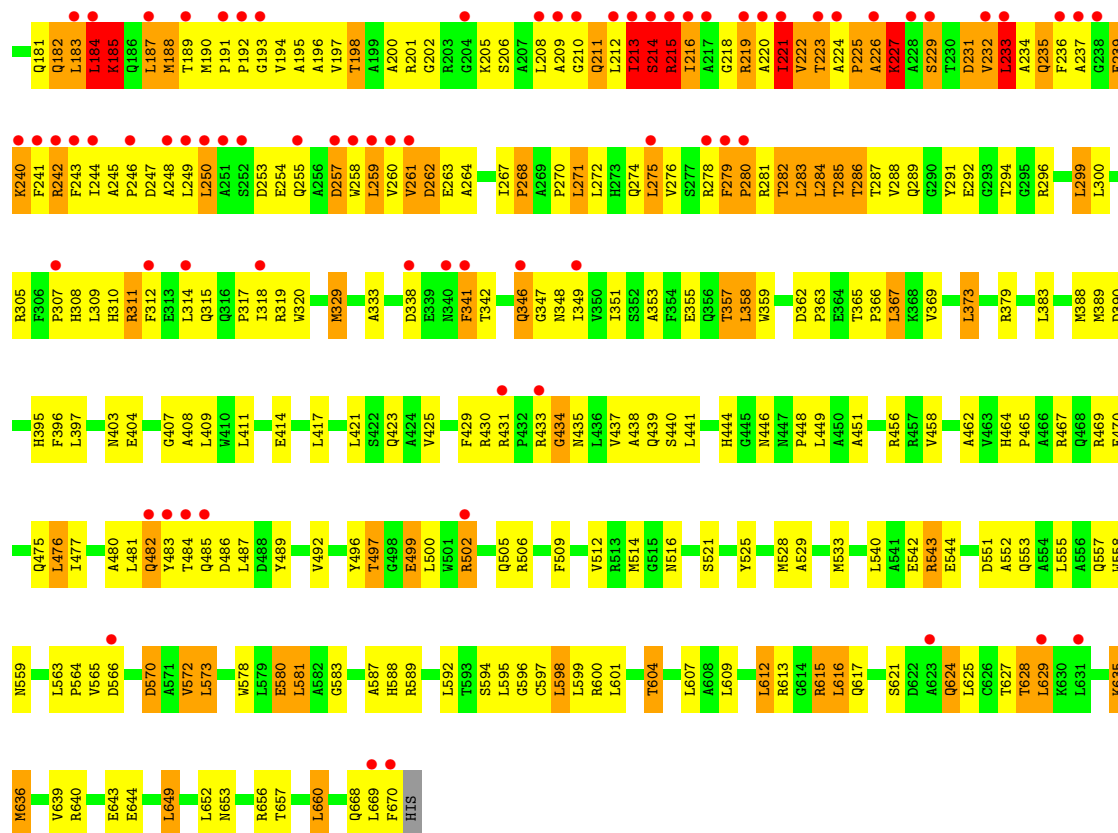
- 
- Diagram illustrating the Lewis structure of the sulfate ion ( $\text{SO}_4^{2-}$ ). The central sulfur atom (S) is bonded to four oxygen atoms (O). Two oxygen atoms are double-bonded to sulfur (top and bottom), and two are single-bonded (left and right). Each single-bonded oxygen has a negative charge ( $\text{O}^-$ ). The sulfur atom has a formal charge of +6, indicated by a green 'S' with a '+' sign. The oxygen atoms are labeled O1, O2, O3, and O4 in green. The overall charge is -2, indicated by a green '2-'.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	224	Total 224	O 224	0	0
5	B	126	Total 126	O 126	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.30Å 100.99Å 263.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.8 (20.00-2.35) 96.1 (20.00-2.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.49 (at 2.37Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.274 0.227 , 0.267	Depositor DCC
$R_{free}$ test set	5079 reflections (7.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ACO, SO4

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	0.48	0/5306	0.77	7/7197 (0.1%)
1	B	0.49	2/5335 (0.0%)	0.82	16/7236 (0.2%)
All	All	0.48	2/10641 (0.0%)	0.79	23/14433 (0.2%)

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	A	0	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLN	C-N	5.74	1.47	1.34
1	B	617	GLN	N-CA	5.51	1.57	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	CD-NE-CZ	14.20	143.47	123.60
1	A	66	GLN	C-N-CA	-10.02	96.65	121.70
1	B	49	TRP	N-CA-CB	9.03	126.86	110.60
1	B	187	LEU	N-CA-C	-8.68	87.57	111.00
1	A	226	ALA	N-CA-C	-8.12	89.08	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	TRP	Mainchain
1	B	48	LEU	Peptide
1	B	656	ARG	Sidechain

## 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	5189	0	5151	230	0
1	B	5218	0	5183	413	0
2	A	51	0	30	3	0
2	B	51	0	33	7	0
3	A	27	0	12	2	0
4	B	5	0	0	1	0
5	A	224	0	0	13	0
5	B	126	0	0	8	0
All	All	10891	0	10409	643	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 31.

The worst 5 of 643 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:A:67:THR:CG2	1:A:71:ARG:HD3	1.36	1.51
1:B:185:LYS:HG3	1:B:215:ARG:NH2	1.51	1.25
1:B:274:GLN:HB3	1:B:278:ARG:NH2	1.62	1.14
1:B:221:ILE:HG23	1:B:259:LEU:HA	1.34	1.08
1:B:215:ARG:NH1	1:B:215:ARG:HG3	1.60	1.08

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	654/671 (98%)	633 (97%)	18 (3%)	3 (0%)	25	28
1	B	658/671 (98%)	605 (92%)	44 (7%)	9 (1%)	9	7
All	All	1312/1342 (98%)	1238 (94%)	62 (5%)	12 (1%)	14	14

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	LEU
1	B	227	LYS
1	B	215	ARG
1	B	232	VAL
1	A	225	PRO

### 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	532/532 (100%)	460 (86%)	72 (14%)	3	3
1	B	535/532 (101%)	424 (79%)	111 (21%)	1	0
All	All	1067/1064 (100%)	884 (83%)	183 (17%)	1	1

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	247	ASP

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Mol	Chain	Res	Type
1	B	348	ASN
1	B	255	GLN
1	B	283	LEU
1	B	433	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	371	GLN
1	B	419	GLN
1	B	446	ASN
1	A	444	HIS
1	A	423	GLN

### 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](#)

4 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	ACO	B	701	-	47,53,53	2.95	18 (38%)	60,79,79	4.65	31 (51%)
2	ACO	A	700	-	47,53,53	3.81	17 (36%)	60,79,79	5.40	31 (51%)
3	ADP	A	800	-	24,29,29	1.36	2 (8%)	29,45,45	1.79	5 (17%)
4	SO4	B	801	-	4,4,4	0.35	0	6,6,6	0.15	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	ACO	B	701	-	1/1/12/14	12/47/67/67	0/3/3/3
2	ACO	A	700	-	1/1/12/14	17/47/67/67	0/3/3/3
3	ADP	A	800	-	-	6/12/32/32	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ACO	O5P-C5P	17.50	1.58	1.23
2	B	701	ACO	O5P-C5P	8.20	1.39	1.23
2	A	700	ACO	O9P-C9P	7.31	1.37	1.23
2	B	701	ACO	P1A-O3A	-6.97	1.52	1.59
2	A	700	ACO	P1A-O3A	-6.38	1.52	1.59

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACO	C2P-C3P-N4P	16.47	146.81	112.41
2	A	700	ACO	CEP-CBP-CAP	15.46	135.13	108.77
2	A	700	ACO	O5P-C5P-C6P	-15.37	94.17	122.02
2	B	701	ACO	O5P-C5P-C6P	-15.24	94.41	122.02
2	B	701	ACO	C2P-C3P-N4P	14.14	141.94	112.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	700	ACO	C2B
2	B	701	ACO	C2B

5 of 35 torsion outliers are listed below:

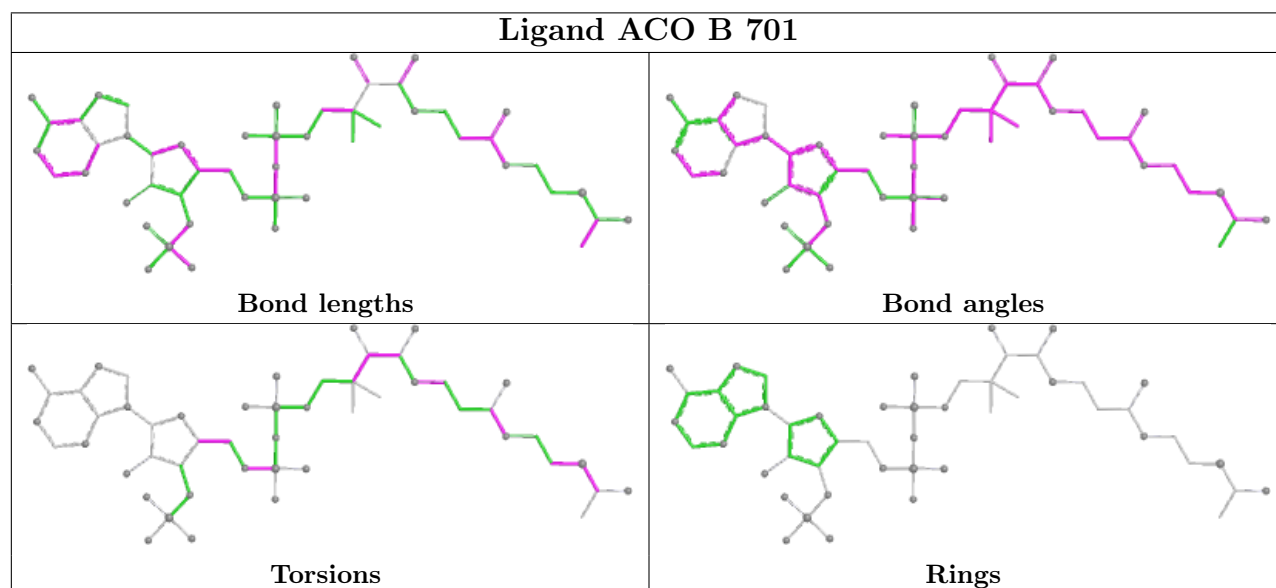
Mol	Chain	Res	Type	Atoms
2	A	700	ACO	O4B-C4B-C5B-O5B
2	A	700	ACO	C5B-O5B-P1A-O3A
2	A	700	ACO	CEP-CBP-CCP-O6A
2	A	700	ACO	C9P-CAP-CBP-CCP
2	A	700	ACO	C9P-CAP-CBP-CDP

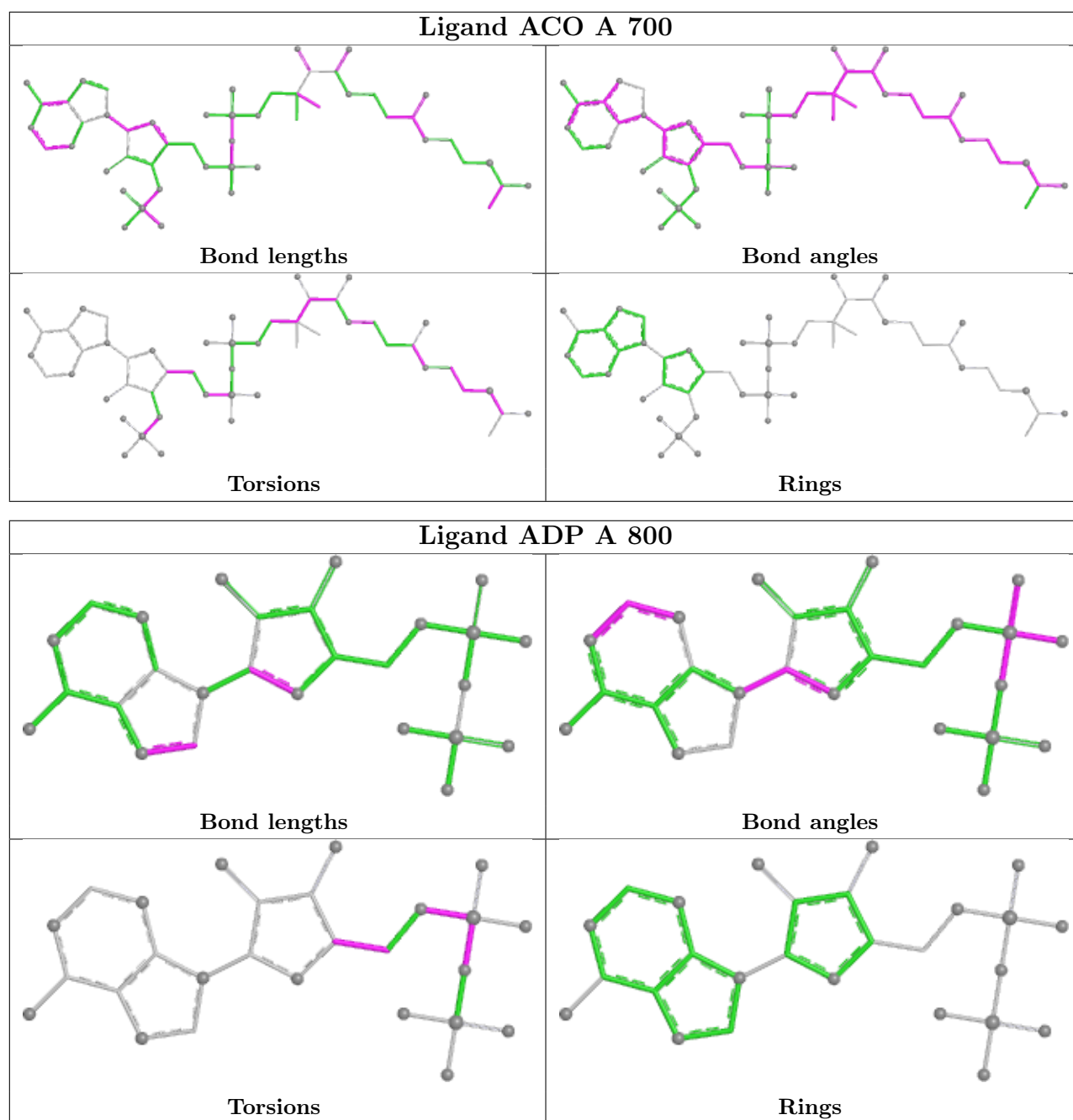
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ACO	7	0
2	A	700	ACO	3	0
3	A	800	ADP	2	0
4	B	801	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	648/671 (96%)	-0.03	23 (3%)	47	53	18, 35, 62, 90	0
1	B	651/671 (97%)	0.74	88 (13%)	8	10	22, 49, 99, 100	0
All	All	1299/1342 (96%)	0.36	111 (8%)	18	22	18, 42, 95, 100	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	PRO	6.3
1	B	258	TRP	5.7
1	A	54	PRO	5.4
1	B	65	LEU	5.2
1	B	217	ALA	4.7

### 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](#)

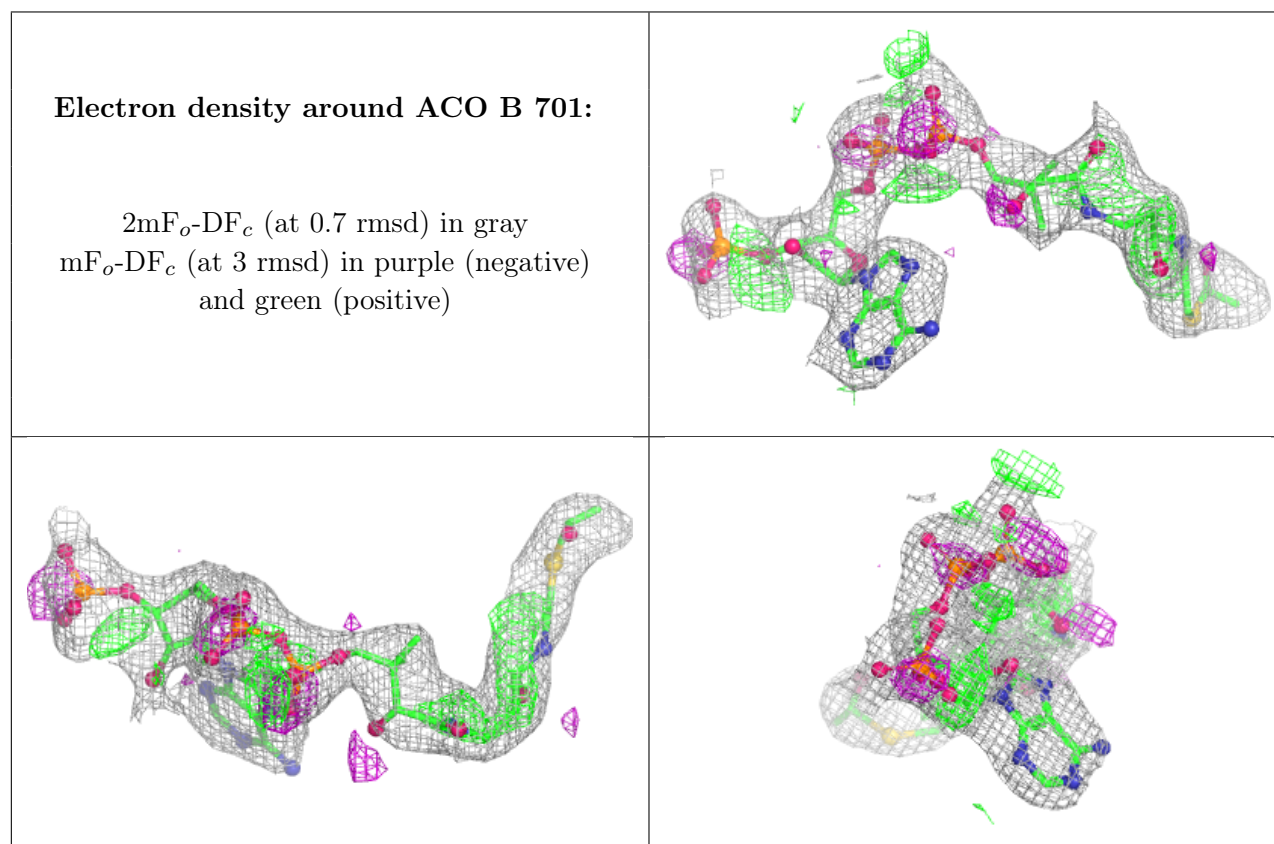
There are no monosaccharides in this entry.

### 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.

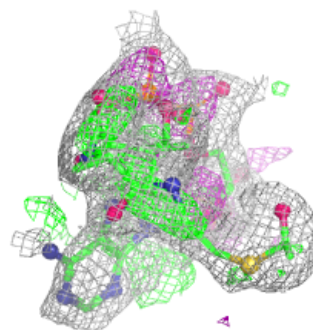
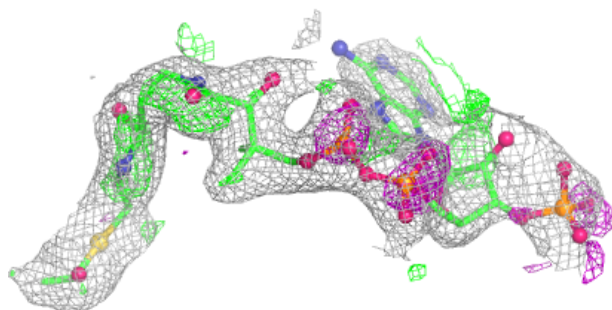
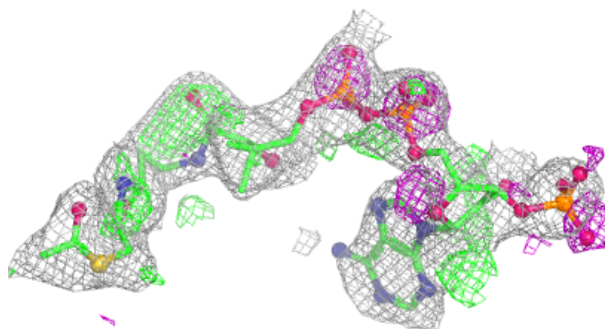
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	801	5/5	0.76	0.12	77,78,78,79	0
2	ACO	B	701	51/51	0.87	0.18	24,50,93,95	0
2	ACO	A	700	51/51	0.88	0.19	18,66,88,89	0
3	ADP	A	800	27/27	0.94	0.09	29,38,39,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

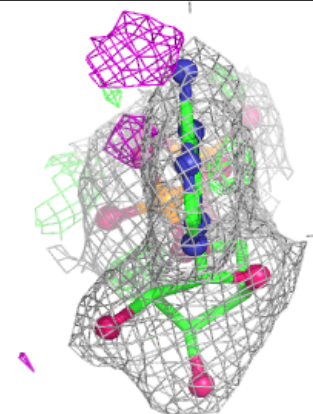
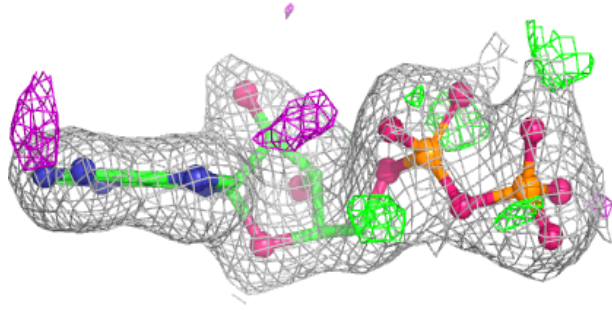
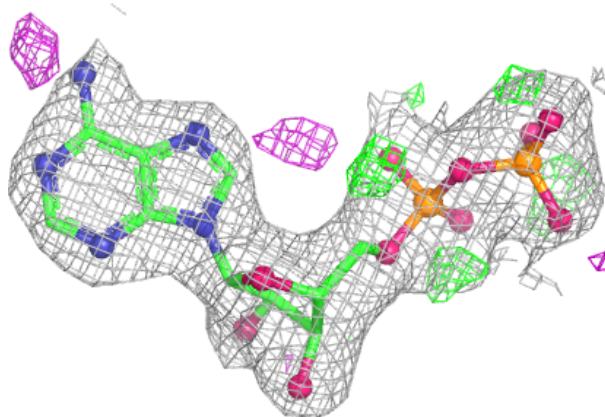


**Electron density around ACO A 700:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP A 800:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.