



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 07:35 AM EDT

PDB ID : 1TIQ  
Title : Crystal Structure of an Acetyltransferase (PaiA) in complex with CoA and DTT from *Bacillus subtilis*, Northeast Structural Genomics Target SR64.  
Authors : Forouhar, F.; Lee, I.; Shen, J.; Vorobiev, S.M.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2004-06-02  
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

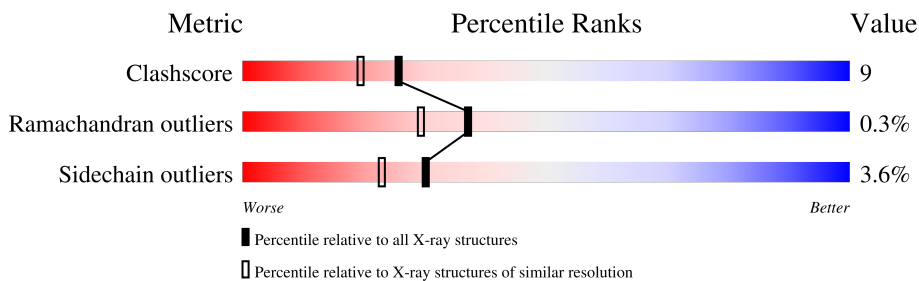
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	180	
1	B	180	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3203 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 Protease synthase and sporulation negative regulatory protein PAI 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	Se	0	0	0
			1414	899	231	276	1	7			
1	B	168	Total	C	N	O	S	Se	0	0	0
			1378	876	229	265	1	7			

There are 32 discrepancies between the modelled and reference sequences:

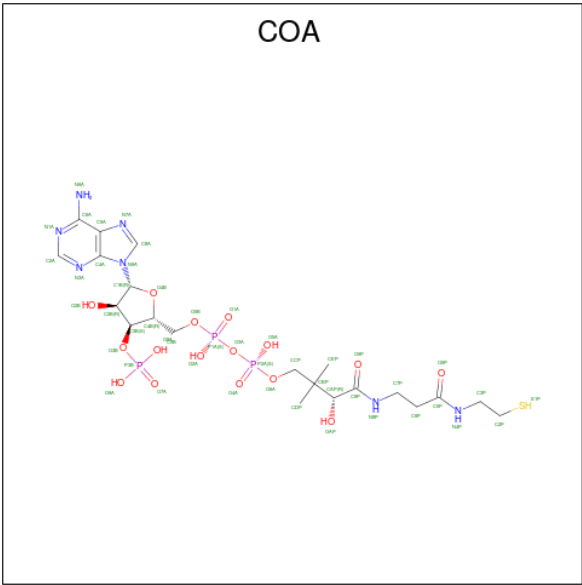
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P21340
A	5	MSE	MET	modified residue	UNP P21340
A	37	MSE	MET	modified residue	UNP P21340
A	57	MSE	MET	modified residue	UNP P21340
A	86	MSE	MET	modified residue	UNP P21340
A	145	MSE	MET	modified residue	UNP P21340
A	157	MSE	MET	modified residue	UNP P21340
A	167	MSE	MET	modified residue	UNP P21340
A	173	LEU	-	cloning artifact	UNP P21340
A	174	GLU	-	cloning artifact	UNP P21340
A	175	HIS	-	cloning artifact	UNP P21340
A	176	HIS	-	cloning artifact	UNP P21340
A	177	HIS	-	cloning artifact	UNP P21340
A	178	HIS	-	cloning artifact	UNP P21340
A	179	HIS	-	cloning artifact	UNP P21340
A	180	HIS	-	cloning artifact	UNP P21340
B	1	MET	-	initiating methionine	UNP P21340
B	5	MSE	MET	modified residue	UNP P21340
B	37	MSE	MET	modified residue	UNP P21340
B	57	MSE	MET	modified residue	UNP P21340
B	86	MSE	MET	modified residue	UNP P21340
B	145	MSE	MET	modified residue	UNP P21340
B	157	MSE	MET	modified residue	UNP P21340
B	167	MSE	MET	modified residue	UNP P21340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	173	LEU	-	cloning artifact	UNP P21340
B	174	GLU	-	cloning artifact	UNP P21340
B	175	HIS	-	cloning artifact	UNP P21340
B	176	HIS	-	cloning artifact	UNP P21340
B	177	HIS	-	cloning artifact	UNP P21340
B	178	HIS	-	cloning artifact	UNP P21340
B	179	HIS	-	cloning artifact	UNP P21340
B	180	HIS	-	cloning artifact	UNP P21340

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	A	1	Total	C	N	O	P	S	0	0
			22	11	2	7	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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	167	Total 167	O 167	0	0
5	B	105	Total 105	O 105	0	0

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

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

Note EDS was not executed.

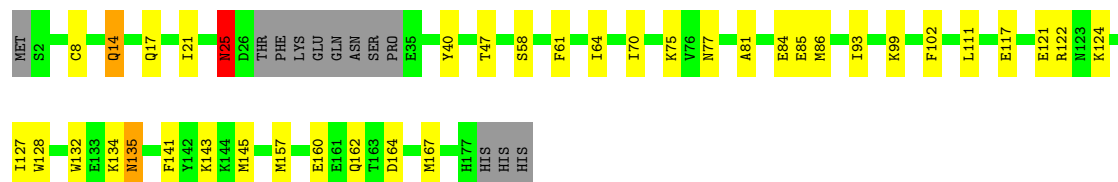
- Molecule 1: Protease synthase and sporulation negative regulatory protein PAI 1

Chain A: 



- Molecule 1: Protease synthase and sporulation negative regulatory protein PAI 1

Chain B: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.87Å 135.82Å 132.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 1.90	Depositor
% Data completeness (in resolution range)	96.0 (29.75-1.90)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3203	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

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

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	0.35	0/1432	0.55	0/1907
1	B	0.32	0/1396	0.50	0/1857
All	All	0.34	0/2828	0.52	0/3764

There are no bond length outliers.

There are no bond angle outliers.

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	1414	0	1382	30	0
1	B	1378	0	1341	25	0
2	A	70	0	51	2	0
2	B	48	0	32	0	0
3	A	16	0	16	0	0
4	B	5	0	0	0	0
5	A	167	0	0	7	1
5	B	105	0	0	3	1
All	All	3203	0	2822	54	2

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 9.

The worst 5 of 54 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:160:GLU:HG3	1:B:162:GLN:HE21	1.54	0.72
1:B:14:GLN:NE2	1:B:14:GLN:H	1.91	0.69
1:B:64:ILE:HB	1:B:111:LEU:HD21	1.75	0.68
1:B:75:LYS:HE2	1:B:77:ASN:HD21	1.64	0.61
1:A:64:ILE:HB	1:A:111:LEU:HD21	1.86	0.58

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1359:HOH:O	5:A:1359:HOH:O[4_566]	1.12	1.08
5:B:440:HOH:O	5:B:440:HOH:O[3_755]	2.06	0.14

## 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	171/180 (95%)	166 (97%)	5 (3%)	0	100	100
1	B	164/180 (91%)	156 (95%)	7 (4%)	1 (1%)	22	13
All	All	335/360 (93%)	322 (96%)	12 (4%)	1 (0%)	37	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	ASN

### 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	154/154 (100%)	148 (96%)	6 (4%)	27	20
1	B	149/154 (97%)	144 (97%)	5 (3%)	32	25
All	All	303/308 (98%)	292 (96%)	11 (4%)	30	23

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	ASN
1	B	86	MSE
1	B	164	ASP
1	B	135	ASN
1	A	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	149	GLN
1	B	135	ASN
1	B	18	GLN
1	B	100	ASN
1	B	17	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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$
4	SO4	B	401	-	4,4,4	0.34	0	6,6,6	0.11	0
3	DTT	A	1202	-	7,7,7	1.25	0	4,8,8	1.94	1 (25%)
2	COA	A	301	2	43,50,50	3.03	20 (46%)	56,75,75	2.92	17 (30%)
2	COA	A	303	2	18,21,50	2.54	8 (44%)	25,29,75	2.70	10 (40%)
2	COA	B	302	-	43,50,50	3.04	19 (44%)	56,75,75	2.77	18 (32%)
3	DTT	A	1201	-	7,7,7	1.29	0	4,8,8	1.99	2 (50%)

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	DTT	A	1202	-	-	0/8/8/8	-
2	COA	A	301	2	-	13/44/64/64	0/3/3/3
2	COA	A	303	2	-	4/27/27/64	-
2	COA	B	302	-	-	12/44/64/64	0/3/3/3
3	DTT	A	1201	-	-	0/8/8/8	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	COA	C2A-N3A	8.83	1.45	1.32
2	B	302	COA	C4A-N3A	8.70	1.47	1.35
2	A	301	COA	C4A-N3A	8.61	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	COA	C2A-N3A	8.49	1.45	1.32
2	B	302	COA	C2A-N1A	6.65	1.45	1.33

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	COA	N3A-C2A-N1A	-11.23	113.42	128.67
2	A	301	COA	CDP-CBP-CCP	-11.08	89.93	108.22
2	B	302	COA	N3A-C2A-N1A	-11.00	113.74	128.67
2	B	302	COA	CDP-CBP-CCP	-10.70	90.56	108.22
2	A	303	COA	CEP-CBP-CCP	-9.41	92.69	108.22

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

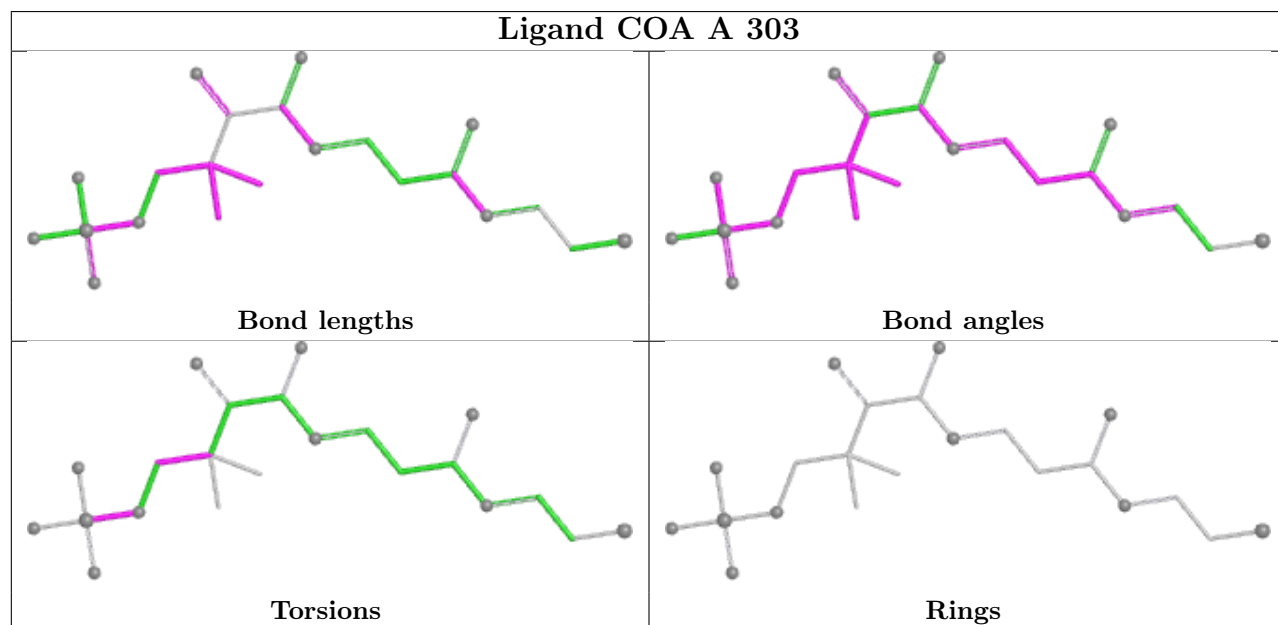
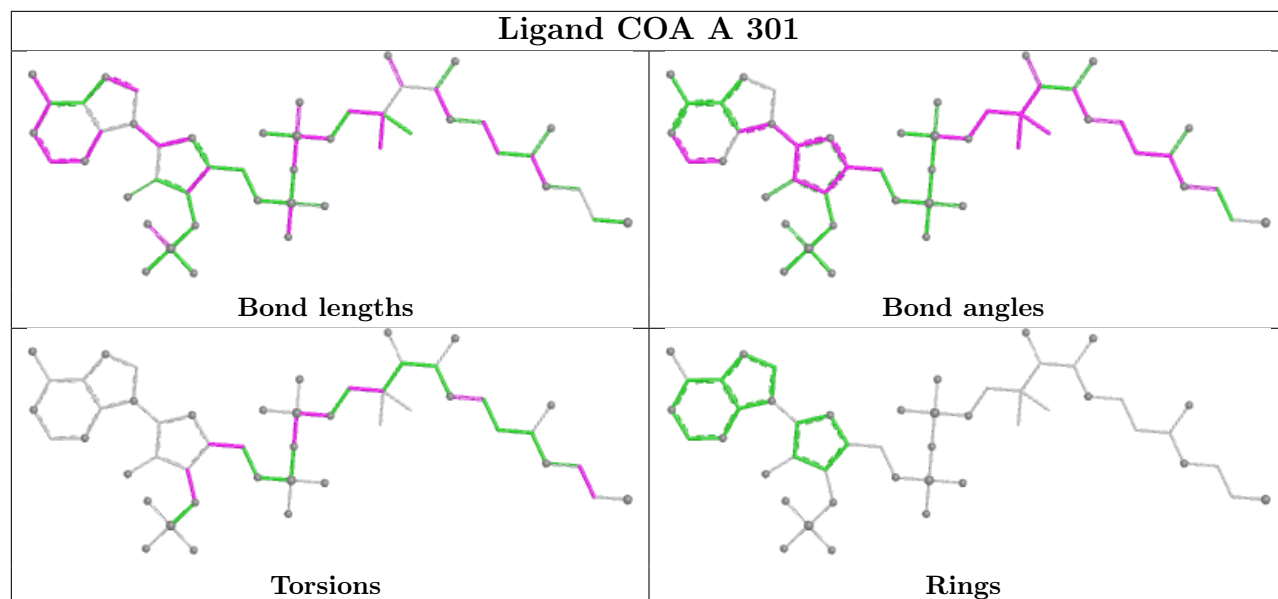
Mol	Chain	Res	Type	Atoms
2	A	301	COA	O4B-C4B-C5B-O5B
2	A	301	COA	CCP-O6A-P2A-O3A
2	A	301	COA	CCP-O6A-P2A-O4A
2	A	301	COA	CCP-O6A-P2A-O5A
2	A	301	COA	CDP-CBP-CCP-O6A

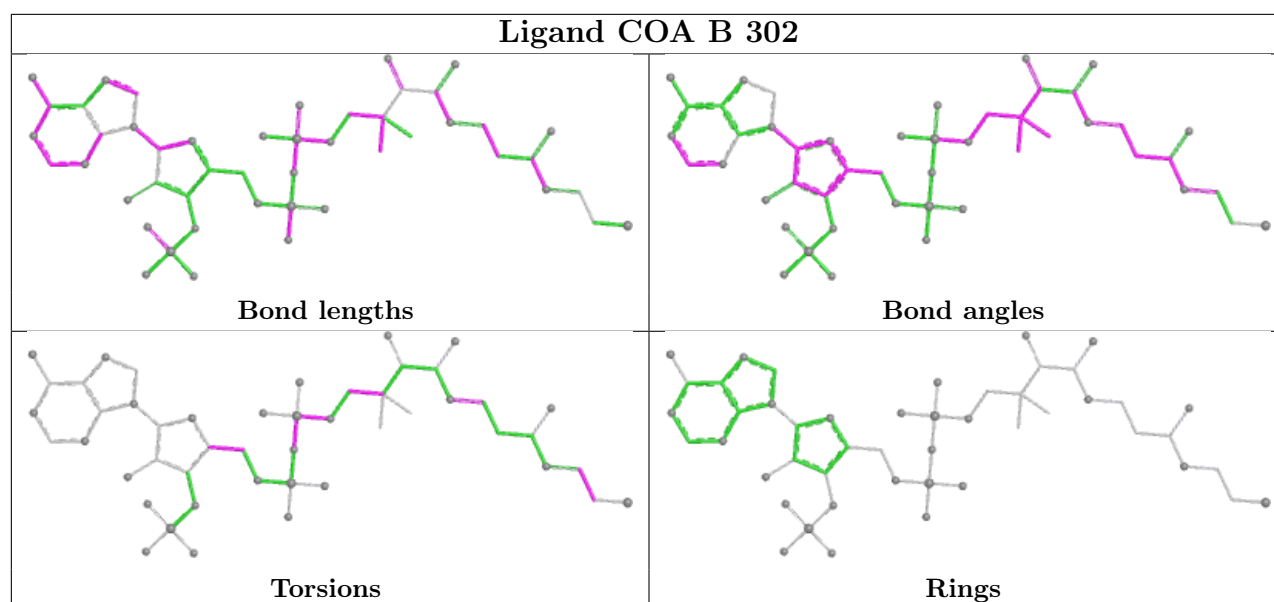
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	COA	2	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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.