



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:36 PM UTC

PDB ID : 9BWL / pdb\_00009bwl  
Title : Crystal structure of polyketoacyl-CoA thiolase from Burkholderia sp in complex with butyryl-coA  
Authors : Pereira, J.H.; Wang, Z.; Keasling, J.D.; Adams, P.D.  
Deposited on : 2024-05-21  
Resolution : 2.10 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.

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

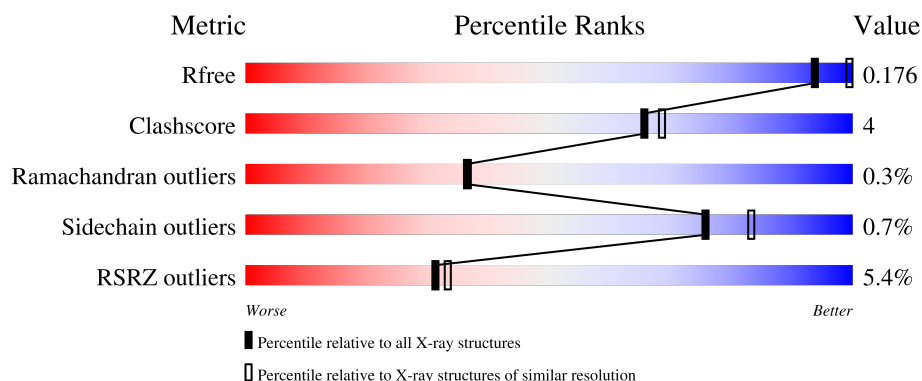
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	399	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6% ..</div> </div> </div>
1	B	399	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>8% ..</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12011 atoms, of which 5860 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.

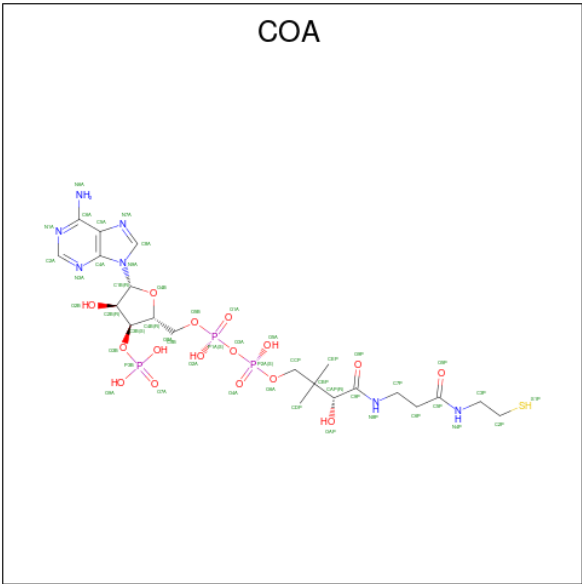
- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	394	Total	C	H	N	O	S	0	2	0
			5783	1799	2905	516	547	16			
1	B	393	Total	C	H	N	O	S	0	1	0
			5761	1792	2893	515	546	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0AAJ0LU93
A	2	HIS	-	expression tag	UNP A0AAJ0LU93
B	1	GLY	-	expression tag	UNP A0AAJ0LU93
B	2	HIS	-	expression tag	UNP A0AAJ0LU93

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			79	21	31	7	16	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			79	21	31	7	16	3	1		

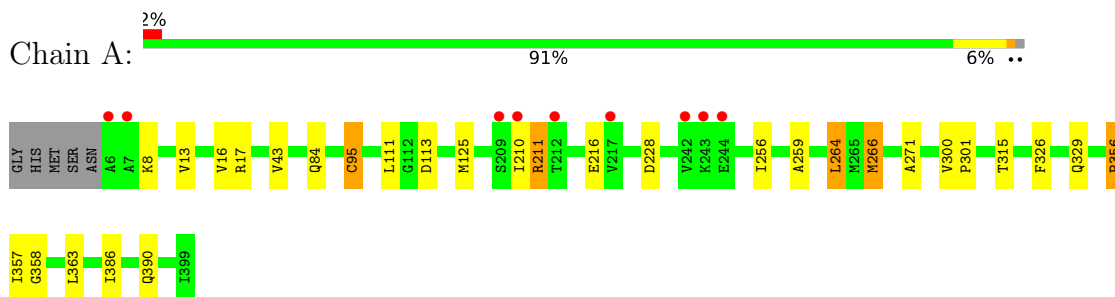
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		
3	B	111	Total	O	0	0
			111	111		

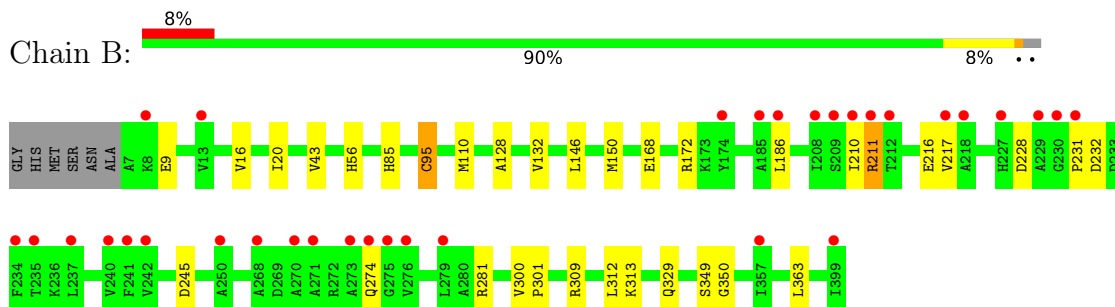
### 3 Residue-property plots [i](#)

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 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: Acetyl-CoA acetyltransferase



- Molecule 1: Acetyl-CoA acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.32Å 130.32Å 120.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 2.10 39.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.00-2.10) 99.8 (39.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.178 , 0.194 (Not available) , 0.176	Depositor DCC
$R_{free}$ test set	1998 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: COA, CY4

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	0.45	1/2915 (0.0%)	0.55	0/3946
1	B	0.33	0/2902	0.46	0/3929
All	All	0.39	1/5817 (0.0%)	0.51	0/7875

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	MET	SD-CE	-5.11	1.66	1.79

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356	PRO	Peptide

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2878	2905	2915	23	0
1	B	2868	2893	2901	24	0
2	A	48	31	32	3	0
2	B	48	31	32	2	0
3	A	198	0	0	3	0
3	B	111	0	0	2	0
All	All	6151	5860	5880	45	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 4.

All (45) 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:228:ASP:OD1	3:A:601:HOH:O	1.93	0.86
1:A:266:MET:CE	1:A:271:ALA:HA	2.24	0.67
1:A:95:CY4:HA22	2:A:500:COA:H32	1.82	0.61
1:A:95:CY4:HA23	2:A:500:COA:S1P	2.44	0.58
1:B:329:GLN:NE2	3:B:601:HOH:O	2.25	0.56
1:A:111:LEU:HD22	1:B:110:MET:HE2	1.86	0.56
1:A:386:ILE:HB	1:A:390:GLN:HB2	1.89	0.54
1:A:16:VAL:HG12	1:A:43:VAL:HG13	1.89	0.54
1:B:216:GLU:HA	1:B:216:GLU:OE1	2.07	0.54
1:A:266:MET:HE1	1:A:271:ALA:HA	1.89	0.54
1:B:172:ARG:NH2	1:B:245:ASP:O	2.40	0.53
1:B:95:CY4:HA23	2:B:500:COA:S1P	2.48	0.53
1:A:315:THR:OG1	3:A:602:HOH:O	2.19	0.52
1:B:228:ASP:OD1	1:B:228:ASP:N	2.43	0.52
1:A:326:PHE:H	1:A:329:GLN:HE21	1.58	0.52
1:B:312:LEU:O	1:B:313:LYS:HE2	2.11	0.51
1:A:125[B]:MET:HE3	1:A:256:ILE:HG23	1.93	0.51
1:B:132:VAL:HG22	1:B:146:LEU:HD12	1.92	0.50
1:B:186:LEU:HD22	1:B:231:PRO:HA	1.95	0.48
1:A:84:GLN:HG2	3:A:749:HOH:O	2.14	0.47
1:B:274:GLN:NE2	3:B:606:HOH:O	2.46	0.47
1:B:210:ILE:HG13	1:B:217:VAL:HG13	1.96	0.47
1:B:210:ILE:O	1:B:211:ARG:C	2.57	0.47
1:B:232:ASP:OD2	1:B:232:ASP:N	2.46	0.45
1:A:210:ILE:O	1:A:211:ARG:C	2.59	0.45
1:B:211:ARG:HA	1:B:216:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HB	1:A:301:PRO:CD	2.47	0.45
1:B:349:SER:OG	1:B:350:GLY:N	2.50	0.43
1:A:266:MET:CE	1:A:271:ALA:CA	2.94	0.43
1:B:20:ILE:HD11	1:B:363:LEU:HD11	2.00	0.43
1:B:9:GLU:OE1	1:B:281:ARG:NE	2.51	0.43
1:B:95:CY4:HA22	2:B:500:COA:H32	2.01	0.42
1:A:264:LEU:CD1	1:A:264:LEU:C	2.92	0.42
1:A:357:ILE:CG1	1:A:358:GLY:N	2.82	0.42
1:B:300:VAL:HB	1:B:301:PRO:CD	2.50	0.42
1:A:113:ASP:HA	1:B:309:ARG:HH22	1.84	0.42
1:A:259:ALA:HB3	1:A:356:PRO:HG3	2.01	0.41
1:B:128:ALA:CB	1:B:150:MET:HB2	2.51	0.41
1:B:168:GLU:O	1:B:172:ARG:HD3	2.20	0.41
1:A:8:LYS:HB3	1:A:8:LYS:HE2	1.92	0.41
1:A:17:ARG:HD2	1:A:363:LEU:HG	2.03	0.41
1:A:95:CY4:HA22	2:A:500:COA:C3P	2.50	0.41
1:A:211:ARG:HA	1:A:216:GLU:OE1	2.21	0.41
1:B:186:LEU:HD22	1:B:231:PRO:CA	2.51	0.41
1:B:16:VAL:HG12	1:B:43:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/399 (98%)	381 (97%)	11 (3%)	1 (0%)	36	36
1	B	391/399 (98%)	373 (95%)	17 (4%)	1 (0%)	36	36
All	All	784/798 (98%)	754 (96%)	28 (4%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	ARG
1	B	211	ARG

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/291 (99%)	287 (99%)	2 (1%)	76	83
1	B	288/291 (99%)	286 (99%)	2 (1%)	76	83
All	All	577/582 (99%)	573 (99%)	4 (1%)	76	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	264	LEU
1	B	56	HIS
1	B	85	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	159	GLN
1	A	304	GLN
1	A	329	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CY4	B	95	1	9,10,11	1.44	1 (11%)	7,11,13	6.82	3 (42%)
1	CY4	A	95	1	9,10,11	1.71	1 (11%)	7,11,13	4.51	1 (14%)

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
1	CY4	B	95	1	-	1/8/10/12	-
1	CY4	A	95	1	-	1/8/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	CY4	CA2-CA1	4.68	1.55	1.50
1	B	95	CY4	CA2-CA1	3.75	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	CY4	CA2-CA1-SG	-16.51	93.73	113.40
1	A	95	CY4	CA2-CA1-SG	-11.50	99.70	113.40
1	B	95	CY4	OA1-CA1-SG	5.10	129.17	122.68
1	B	95	CY4	CB-SG-CA1	-4.90	94.03	100.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	95	CY4	OA1-CA1-SG-CB
1	B	95	CY4	OA1-CA1-SG-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	95	CY4	2	0
1	A	95	CY4	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	COA	A	500	-	47,50,50	3.48	20 (42%)	69,75,75	1.62	13 (18%)
2	COA	B	500	-	47,50,50	3.36	21 (44%)	69,75,75	1.51	11 (15%)

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	COA	A	500	-	-	5/48/64/64	0/3/3/3
2	COA	B	500	-	-	7/48/64/64	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	COA	C2B-C3B	-11.72	1.27	1.53
2	B	500	COA	C2B-C3B	-11.65	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	COA	P2A-O3A	9.04	1.69	1.59
2	B	500	COA	P2A-O3A	8.00	1.68	1.59
2	A	500	COA	P1A-O3A	6.63	1.66	1.59
2	B	500	COA	C6A-N6A	6.12	1.49	1.34
2	A	500	COA	O4B-C4B	6.08	1.58	1.45
2	A	500	COA	C6A-N6A	5.91	1.49	1.34
2	B	500	COA	O4B-C4B	5.70	1.57	1.45
2	A	500	COA	O4B-C1B	-5.61	1.29	1.42
2	A	500	COA	C5P-N4P	5.58	1.46	1.33
2	B	500	COA	P1A-O3A	5.51	1.65	1.59
2	B	500	COA	C5P-N4P	5.50	1.46	1.33
2	B	500	COA	O4B-C1B	-5.49	1.29	1.42
2	A	500	COA	C2B-C1B	5.47	1.70	1.53
2	A	500	COA	C5B-C4B	-5.32	1.35	1.51
2	B	500	COA	C5B-C4B	-5.21	1.35	1.51
2	B	500	COA	C2B-C1B	5.16	1.69	1.53
2	B	500	COA	C9P-N8P	4.83	1.45	1.33
2	A	500	COA	C9P-N8P	4.70	1.44	1.33
2	B	500	COA	O9P-C9P	-3.41	1.16	1.23
2	B	500	COA	P3B-O3B	3.29	1.65	1.59
2	A	500	COA	P3B-O3B	3.24	1.65	1.59
2	A	500	COA	O9P-C9P	-2.99	1.17	1.23
2	A	500	COA	C3P-N4P	2.99	1.52	1.46
2	A	500	COA	CDP-CBP	2.95	1.59	1.53
2	B	500	COA	CDP-CBP	2.90	1.59	1.53
2	A	500	COA	C8A-N9A	-2.82	1.32	1.37
2	A	500	COA	P1A-O5B	2.80	1.70	1.59
2	B	500	COA	P1A-O5B	2.70	1.70	1.59
2	B	500	COA	CCP-CBP	2.67	1.57	1.52
2	B	500	COA	C8A-N9A	-2.60	1.33	1.37
2	B	500	COA	C3P-N4P	2.52	1.51	1.46
2	B	500	COA	P2A-O6A	2.51	1.69	1.59
2	A	500	COA	CCP-CBP	2.50	1.56	1.52
2	B	500	COA	C5A-N7A	-2.38	1.34	1.39
2	A	500	COA	C5A-N7A	-2.33	1.34	1.39
2	A	500	COA	P2A-O6A	2.29	1.68	1.59
2	A	500	COA	O3B-C3B	2.23	1.51	1.44
2	B	500	COA	O3B-C3B	2.22	1.51	1.44
2	B	500	COA	C3B-C4B	2.03	1.58	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	COA	C5A-C4A-N3A	-5.22	119.52	126.72
2	A	500	COA	C5A-C4A-N3A	-5.06	119.75	126.72
2	A	500	COA	N3A-C2A-N1A	-4.56	121.68	128.58
2	B	500	COA	N3A-C2A-N1A	-4.22	122.20	128.58
2	A	500	COA	N3A-C4A-N9A	4.00	133.97	127.17
2	B	500	COA	N3A-C4A-N9A	3.75	133.54	127.17
2	A	500	COA	C2A-N3A-C4A	3.61	120.64	111.83
2	B	500	COA	C2A-N3A-C4A	3.57	120.55	111.83
2	A	500	COA	N9A-C8A-N7A	-3.12	109.51	113.94
2	B	500	COA	C7P-C6P-C5P	3.07	117.50	112.39
2	B	500	COA	C4A-C5A-N7A	-2.98	107.18	110.58
2	B	500	COA	C5A-N7A-C8A	2.96	108.10	103.45
2	A	500	COA	C5A-N7A-C8A	2.95	108.09	103.45
2	B	500	COA	N9A-C8A-N7A	-2.93	109.78	113.94
2	A	500	COA	C4A-N9A-C8A	2.82	108.70	105.74
2	A	500	COA	C4A-C5A-N7A	-2.77	107.41	110.58
2	A	500	COA	C6P-C5P-N4P	2.69	121.25	116.34
2	A	500	COA	O4B-C1B-N9A	2.61	113.10	108.09
2	A	500	COA	O6A-CCP-CBP	-2.52	106.50	110.55
2	B	500	COA	O6A-CCP-CBP	-2.40	106.68	110.55
2	B	500	COA	C3B-C2B-C1B	2.34	105.04	99.89
2	A	500	COA	C7P-C6P-C5P	2.23	116.10	112.39
2	B	500	COA	C4A-N9A-C8A	2.16	108.00	105.74
2	A	500	COA	C2B-C1B-N9A	-2.14	107.99	113.30

There are no chirality outliers.

All (12) torsion outliers are listed below:

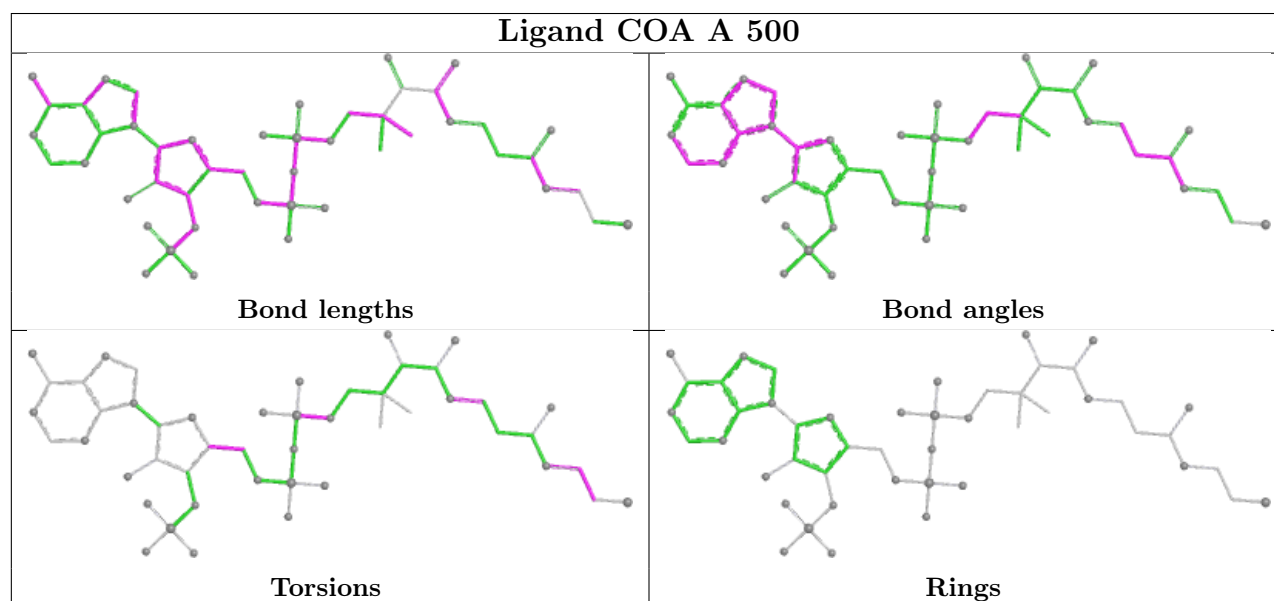
Mol	Chain	Res	Type	Atoms
2	A	500	COA	C2P-C3P-N4P-C5P
2	B	500	COA	P2A-O3A-P1A-O5B
2	B	500	COA	C2P-C3P-N4P-C5P
2	B	500	COA	S1P-C2P-C3P-N4P
2	A	500	COA	O4B-C4B-C5B-O5B
2	B	500	COA	O4B-C4B-C5B-O5B
2	B	500	COA	CDP-CBP-CCP-O6A
2	A	500	COA	C6P-C7P-N8P-C9P
2	A	500	COA	S1P-C2P-C3P-N4P
2	B	500	COA	CAP-CBP-CCP-O6A
2	A	500	COA	CCP-O6A-P2A-O4A
2	B	500	COA	CEP-CBP-CCP-O6A

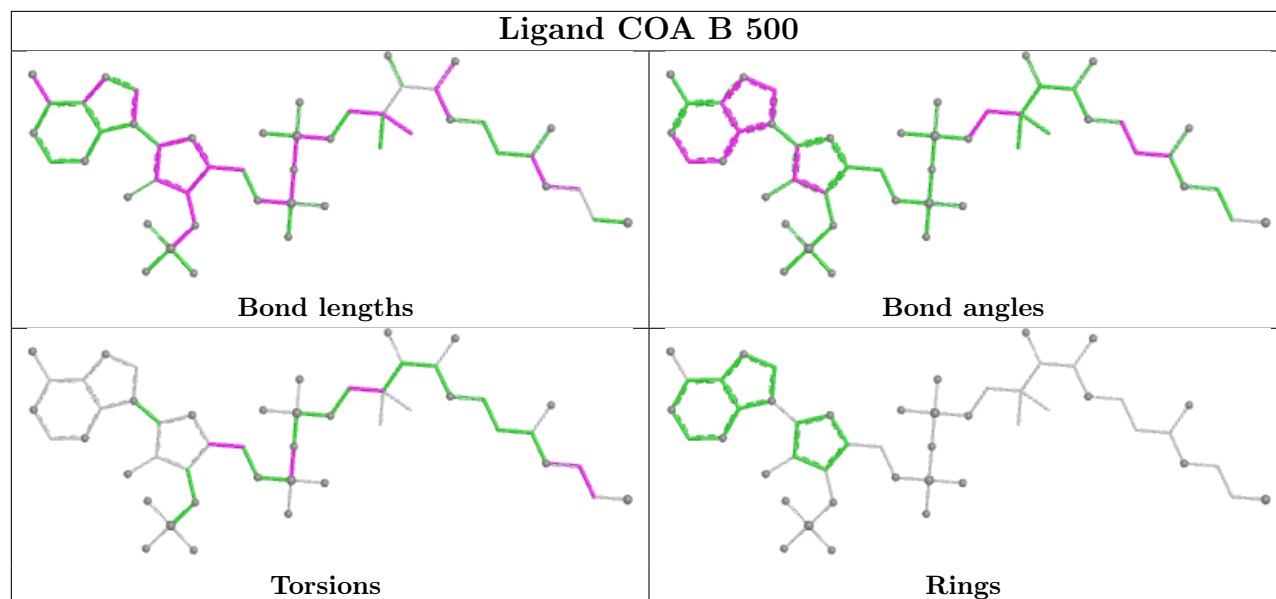
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	COA	3	0
2	B	500	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

### 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	393/399 (98%)	-0.26	9 (2%) 61 64	33, 55, 85, 184	2 (0%)
1	B	392/399 (98%)	0.40	33 (8%) 17 18	43, 74, 145, 201	1 (0%)
All	All	785/798 (98%)	0.07	42 (5%) 31 33	33, 61, 125, 201	3 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	ILE	5.5
1	A	217	VAL	4.7
1	A	210	ILE	4.4
1	B	242	VAL	3.9
1	B	275	GLY	3.7
1	B	231	PRO	3.6
1	B	208	ILE	3.6
1	B	276	VAL	3.5
1	B	279	LEU	3.5
1	B	241	PHE	3.4
1	B	209	SER	3.3
1	B	399	ILE	3.3
1	B	237	LEU	3.3
1	A	243	LYS	3.2
1	B	273	ALA	3.1
1	B	274	GLN	3.1
1	B	217	VAL	3.1
1	B	229	ALA	2.9
1	B	234	PHE	2.7
1	B	271	ALA	2.7
1	A	209	SER	2.7
1	B	235	THR	2.7
1	A	242	VAL	2.6
1	B	240	VAL	2.6

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	B	227	HIS	2.6
1	B	268	ALA	2.6
1	A	6	ALA	2.6
1	B	212	THR	2.5
1	B	270	ALA	2.4
1	B	218	ALA	2.3
1	B	230	GLY	2.3
1	A	7	ALA	2.2
1	B	174	TYR	2.2
1	B	211	ARG	2.2
1	A	212	THR	2.2
1	A	244	GLU	2.1
1	B	186	LEU	2.1
1	B	185	ALA	2.1
1	B	250	ALA	2.1
1	B	8	LYS	2.0
1	B	357	ILE	2.0
1	B	13	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	CY4	A	95	11/12	0.96	0.09	43,47,55,55	0
1	CY4	B	95	11/12	0.97	0.11	49,57,63,63	0

## 6.3 Carbohydrates [i](#)

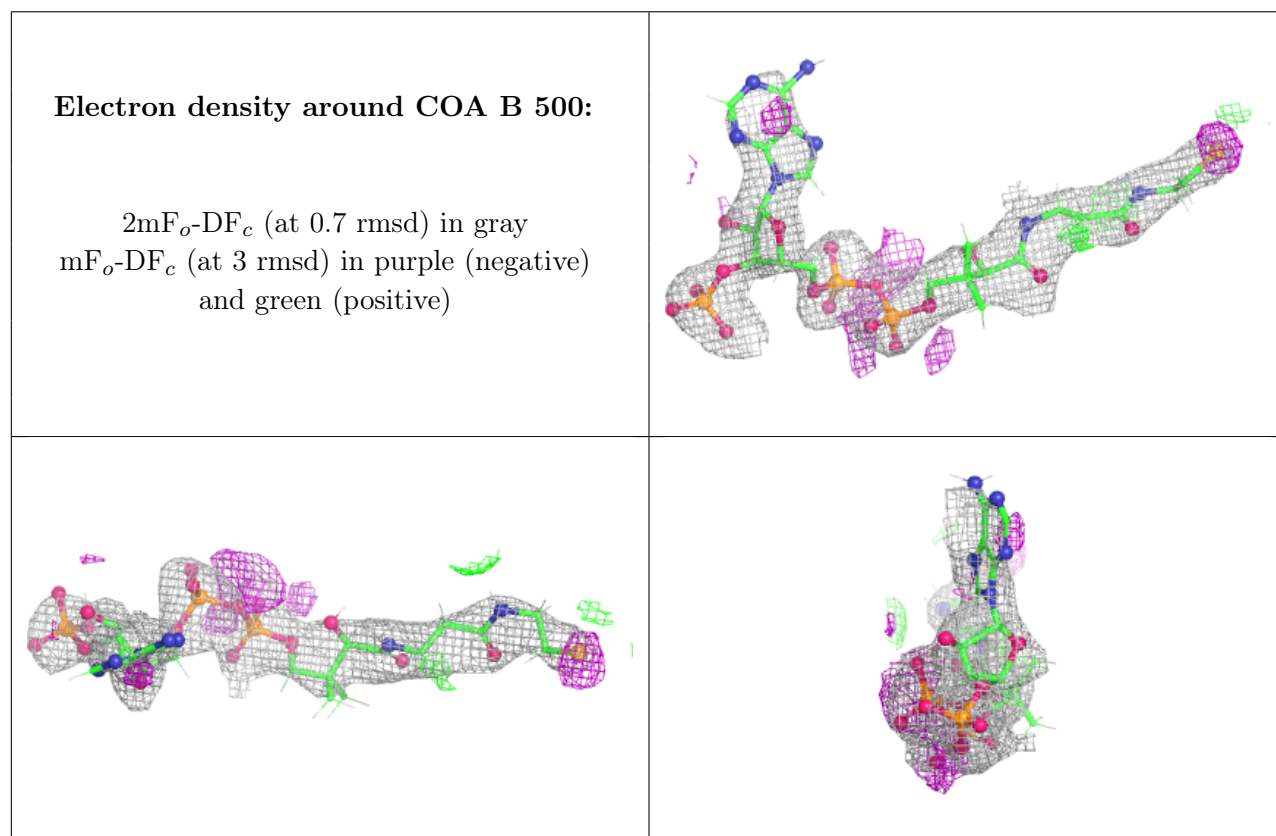
There are no oligosaccharides in this entry.

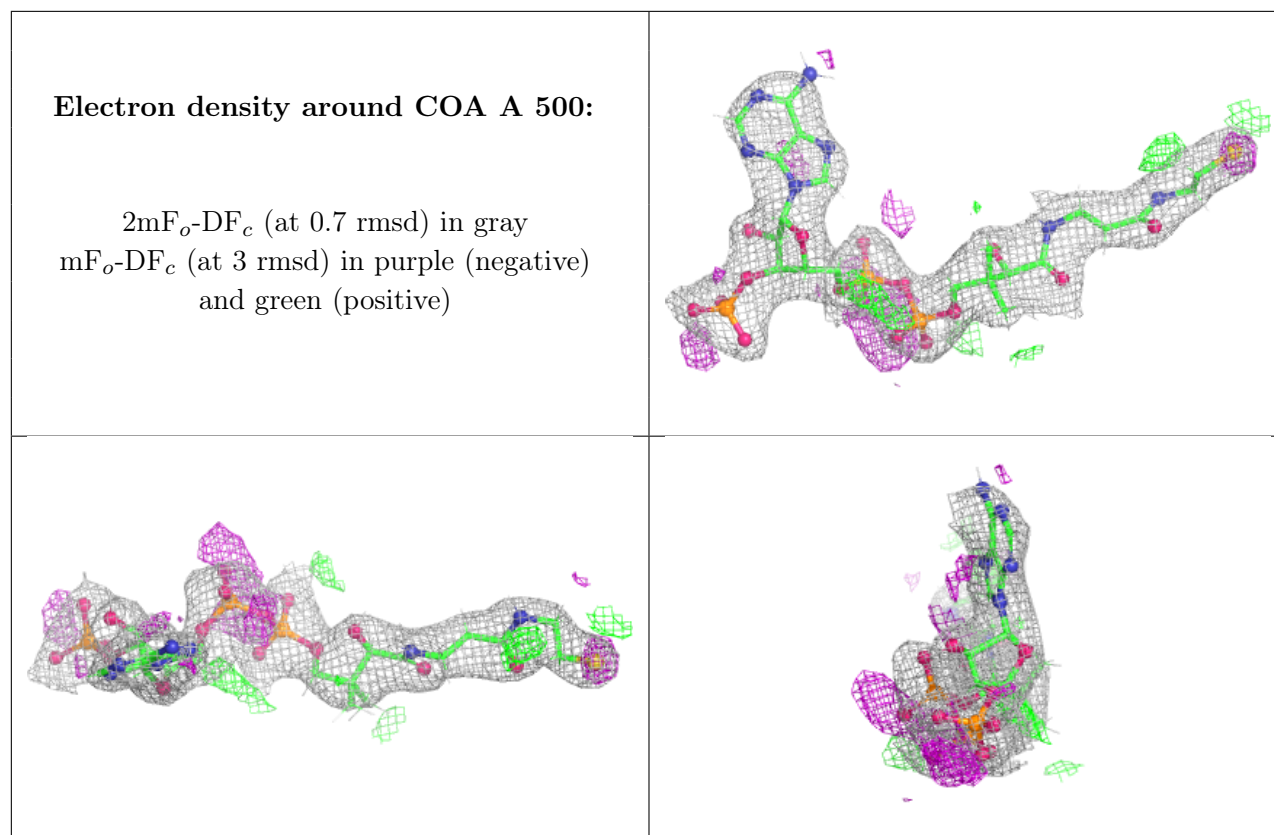
## 6.4 Ligands [i](#)

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	COA	B	500	48/48	0.84	0.12	73,122,168,176	0
2	COA	A	500	48/48	0.89	0.11	54,83,126,132	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.