



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 03:49 AM UTC

PDB ID : 4PK3 / pdb_00004pk3
Title : tubulin acetyltransferase complex with bisubstrate analog
Authors : Szyk, A.; Roll-Mecak, A.
Deposited on : 2014-05-13
Resolution : 1.35 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
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

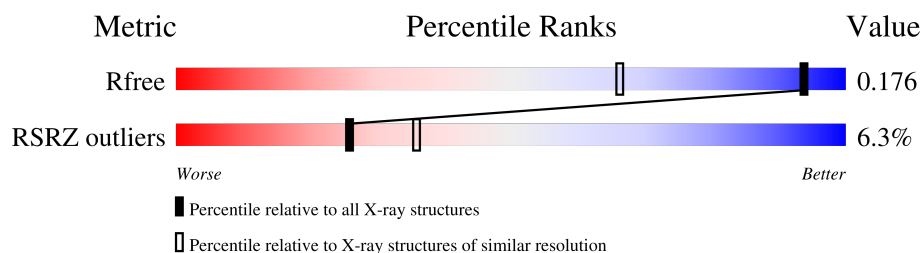
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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}	180053	2194 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3552 atoms, of which 1609 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 Alpha-tubulin N-acetyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	188	3107	999	1550	272	281	5	0	8	0

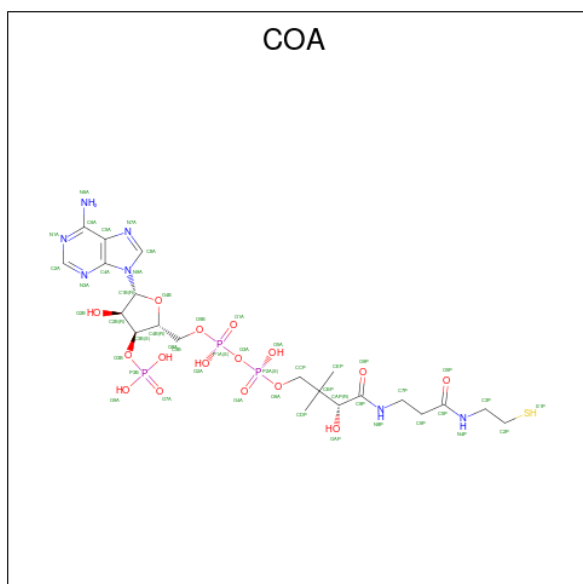
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	PHE	-	expression tag	UNP Q5SQI0
A	0	THR	-	expression tag	UNP Q5SQI0

- Molecule 2 is a protein called ACETYL-SER-ASP-(N-ACETYL-LYS)-THR-NH2 PEPTIDE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O				
2	B	6	64	21	27	6	10		0	0	1

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	S	0	1
			85	21	32	7	20	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	291	Total	O	0	0
			291	291		
4	B	5	Total	O	0	0
			5	5		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.16Å 52.28Å 50.14Å 90.00° 107.13° 90.00°	Depositor
Resolution (Å)	29.38 – 1.35 29.38 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.38-1.35) 96.4 (29.38-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 1.35Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.147 , 0.173 0.151 , 0.176	Depositor DCC
R_{free} test set	2015 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3552	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

1 non-standard protein/DNA/RNA residue is 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	ALY	B	4	2,3	10,11,12	1.22	1 (10%)	7,12,14	2.39	3 (42%)

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	ALY	B	4	2,3	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	ALY	OH-CH	3.73	1.31	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	ALY	CE-NZ-CH	3.97	128.42	122.56
2	B	4	ALY	CH3-CH-NZ	3.83	122.66	116.12
2	B	4	ALY	OH-CH-CH3	-2.72	117.21	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	$\# Z > 2$
3	COA	B	7[A]	-	47,50,50	0.92	2 (4%)	69,75,75	1.57	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	B	7[B]	-	47,50,50	0.83	1 (2%)	69,75,75	1.81	15 (21%)

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	COA	B	7[A]	-	-	1/48/64/64	0/3/3/3
3	COA	B	7[B]	-	-	1/48/64/64	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	7[A]	COA	P3B-O7A	2.35	1.57	1.50
3	B	7[A]	COA	C4A-N9A	-2.05	1.33	1.37
3	B	7[B]	COA	C4A-N9A	-2.05	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	7[B]	COA	P3B-O3B-C3B	-6.01	107.39	123.43
3	B	7[A]	COA	C5A-C4A-N3A	-4.44	120.60	126.72
3	B	7[B]	COA	C5A-C4A-N3A	-4.44	120.60	126.72
3	B	7[A]	COA	N3A-C2A-N1A	-4.43	121.88	128.58
3	B	7[B]	COA	N3A-C2A-N1A	-4.43	121.88	128.58
3	B	7[A]	COA	N9A-C8A-N7A	-3.73	108.64	113.94
3	B	7[B]	COA	N9A-C8A-N7A	-3.73	108.64	113.94
3	B	7[B]	COA	O3B-C3B-C4B	-3.68	97.07	110.03
3	B	7[B]	COA	O9A-P3B-O3B	3.24	118.47	105.85
3	B	7[A]	COA	C4A-C5A-N7A	-2.77	107.42	110.58
3	B	7[B]	COA	C4A-C5A-N7A	-2.77	107.42	110.58
3	B	7[A]	COA	C4A-N9A-C8A	2.75	108.63	105.74
3	B	7[B]	COA	C4A-N9A-C8A	2.75	108.63	105.74
3	B	7[A]	COA	C2P-C3P-N4P	-2.75	106.06	112.31
3	B	7[B]	COA	C2P-C3P-N4P	-2.75	106.06	112.31
3	B	7[A]	COA	N3A-C4A-N9A	2.74	131.83	127.17
3	B	7[B]	COA	N3A-C4A-N9A	2.74	131.83	127.17
3	B	7[A]	COA	C5A-N7A-C8A	2.70	107.69	103.45
3	B	7[B]	COA	C5A-N7A-C8A	2.70	107.69	103.45
3	B	7[A]	COA	C2A-N3A-C4A	2.59	118.16	111.83
3	B	7[B]	COA	C2A-N3A-C4A	2.59	118.16	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	7[A]	COA	O8A-P3B-O3B	2.54	115.76	105.85
3	B	7[B]	COA	O8A-P3B-O7A	-2.44	101.32	110.83
3	B	7[A]	COA	C2B-C1B-N9A	-2.26	107.68	113.30
3	B	7[B]	COA	C2B-C1B-N9A	-2.26	107.68	113.30
3	B	7[A]	COA	C7P-C6P-C5P	2.01	115.74	112.39
3	B	7[B]	COA	C7P-C6P-C5P	2.01	115.74	112.39

There are no chirality outliers.

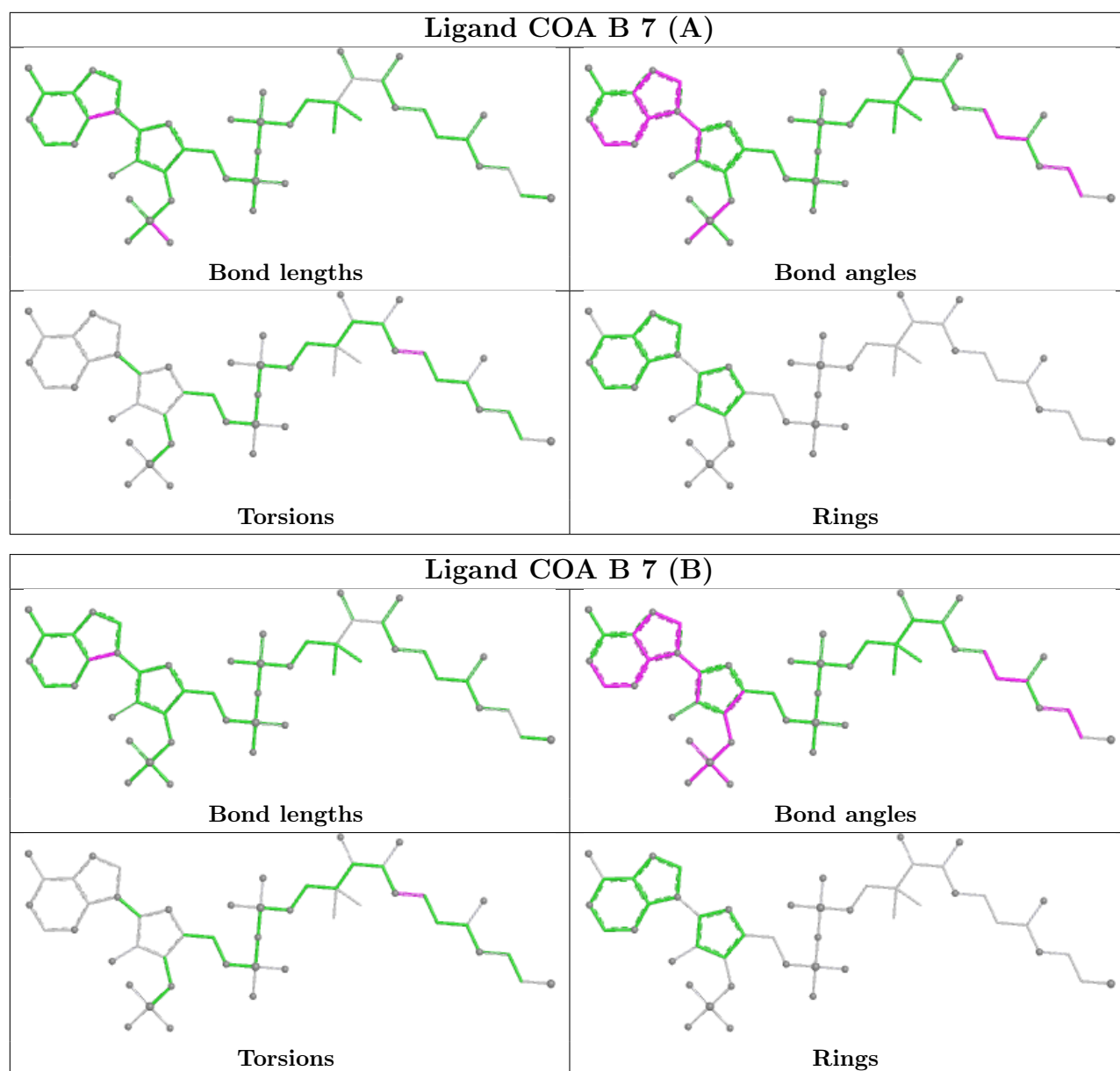
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	7[A]	COA	C6P-C7P-N8P-C9P
3	B	7[B]	COA	C6P-C7P-N8P-C9P

There are no ring outliers.

No monomer is involved in short contacts.

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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, 95th 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 ²)	Q<0.9
1	A	188/198 (94%)	-0.11	11 (5%) 28 39	8, 17, 46, 74	8 (4%)
2	B	3/6 (50%)	1.86	1 (33%) 1 1	14, 14, 19, 57	0
All	All	191/204 (93%)	-0.08	12 (6%) 26 36	8, 17, 47, 74	8 (4%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	THR	7.3
1	A	117	GLU	5.2
1	A	87	PRO	5.1
1	A	26	ALA	4.4
1	A	196	PRO	3.9
1	A	86	ARG	3.6
1	A	187[A]	GLU	3.4
1	A	-1	PHE	3.0
1	A	88	ALA	2.9
1	A	37	VAL	2.8
1	A	0	THR	2.2
1	A	85	ALA	2.1

5.2 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, 95th 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 ²)	Q<0.9
2	ALY	B	4	12/13	0.97	0.06	13,19,28,32	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

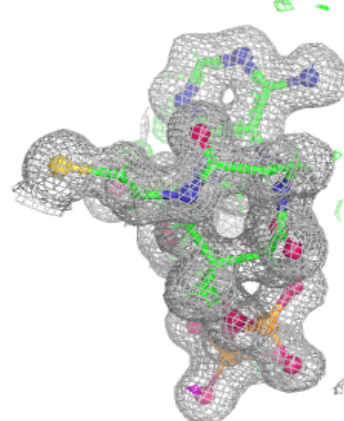
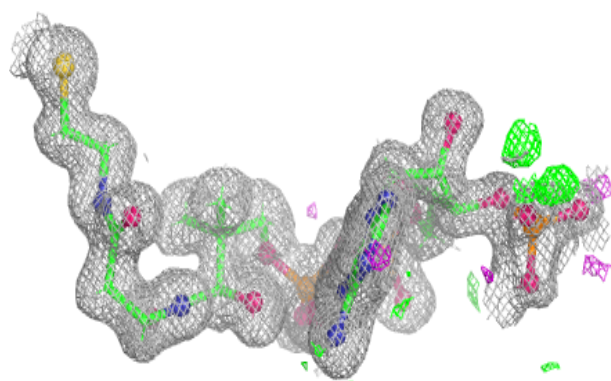
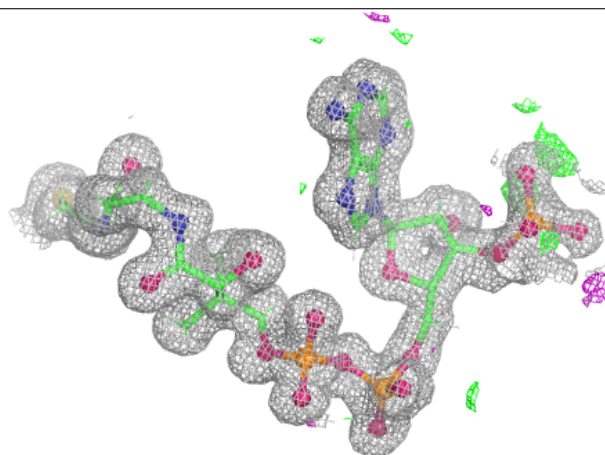
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	COA	B	7[A]	48/48	0.99	0.04	9,13,16,18	7
3	COA	B	7[B]	48/48	0.99	0.04	9,13,16,18	7

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.

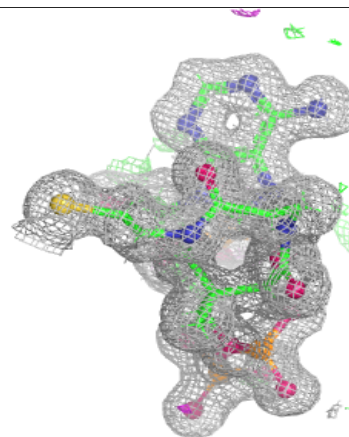
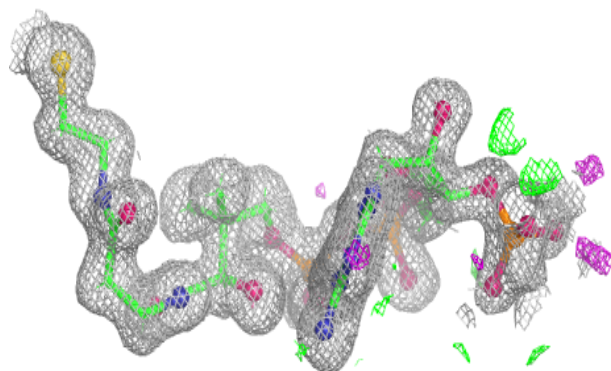
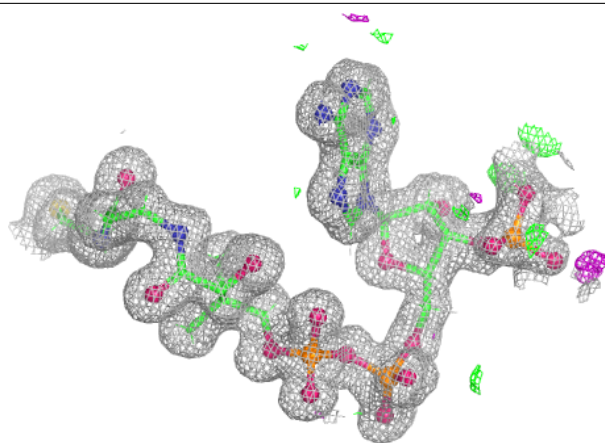
Electron density around COA B 7 (A):

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 COA B 7 (B):

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



5.5 Other polymers [i](#)

There are no such residues in this entry.