



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 09:22 pm BST

PDB ID : 1IXE  
Title : Crystal structure of citrate synthase from *Thermus thermophilus* HB8  
Authors : Murakami, M.; Kanamori, E.; Kawaguchi, S.; Kuramitsu, S.; Kouyama, T.;  
RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2002-06-20  
Resolution : 2.30 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
buster-report	:	1.1.7 (2018)
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

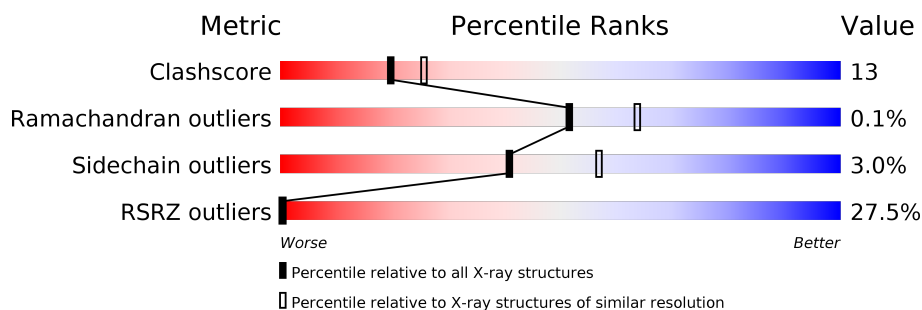
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\leq 5\%$ . 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	377	<div> <div>26%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	B	377	<div> <div>22%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
1	C	377	<div> <div>34%</div> <div>69%</div> <div>26%</div> <div>..</div> </div>
1	D	377	<div> <div>25%</div> <div>69%</div> <div>26%</div> <div>..</div> </div>

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	SO4	C	390	-	-	-	X
3	COA	D	404	-	-	-	X
4	CIT	D	408	-	-	X	-
5	GOL	C	413	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12452 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 citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2920	1870	508	532	10			
1	B	370	Total	C	N	O	S	0	0	0
			2922	1871	507	534	10			
1	C	366	Total	C	N	O	S	0	0	0
			2887	1851	499	527	10			
1	D	366	Total	C	N	O	S	0	0	0
			2888	1851	501	526	10			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



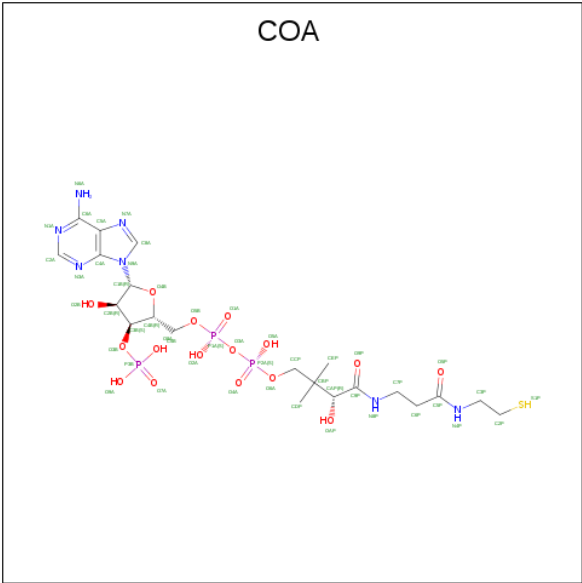
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 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).



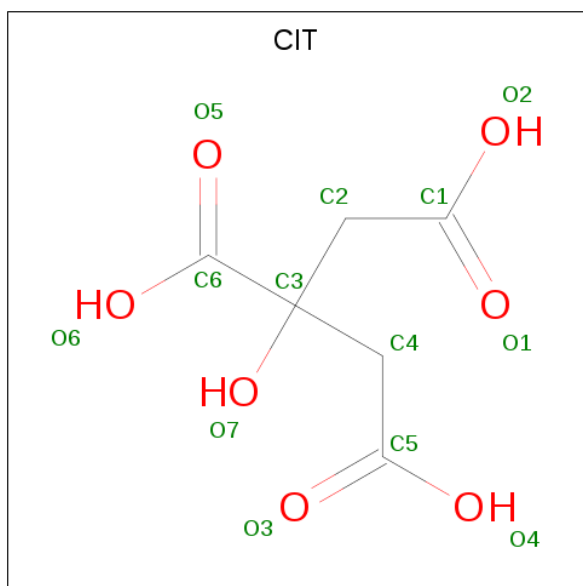
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



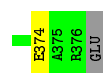
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

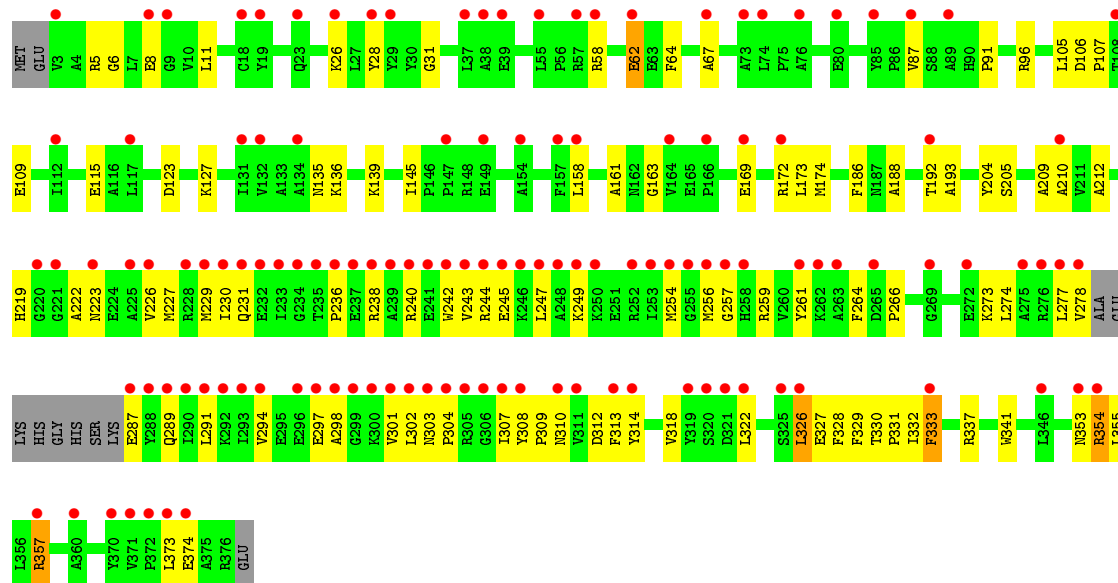
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	138	Total	O	0	0
			138	138		
6	C	120	Total	O	0	0
			120	120		
6	D	134	Total	O	0	0
			134	134		



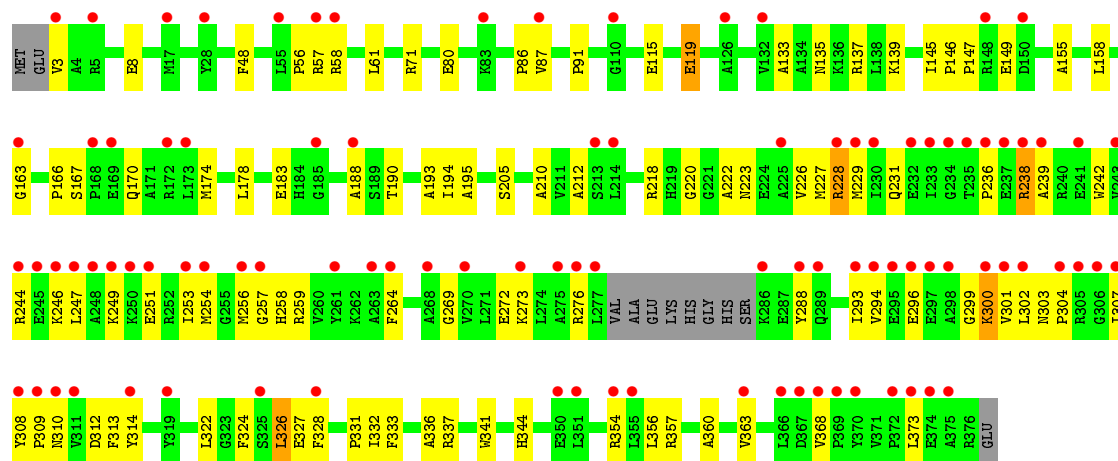




• Molecule 1: citrate synthase



• Molecule 1: citrate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.01Å 110.63Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.79 – 2.30 14.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (14.79-2.30) 90.7 (14.79-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.177 , 0.217 0.173 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: COA, GOL, SO4, CIT

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	0.33	0/2986	0.47	0/4036
1	B	0.37	0/2987	0.51	0/4035
1	C	0.34	0/2952	0.48	0/3990
1	D	0.41	0/2953	0.54	0/3990
All	All	0.36	0/11878	0.50	0/16051

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	LYS	Mainchain

### 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	2920	0	2911	81	0
1	B	2922	0	2924	76	0
1	C	2887	0	2884	87	0
1	D	2888	0	2888	89	0
2	A	10	0	0	0	0
2	B	15	0	0	2	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
3	A	48	0	32	2	0
3	B	48	0	32	1	0
3	C	48	0	32	1	0
3	D	48	0	32	11	0
4	A	13	0	5	1	0
4	B	13	0	5	1	0
4	C	13	0	5	0	0
4	D	13	0	5	6	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	125	0	0	1	0
6	B	138	0	0	6	0
6	C	120	0	0	1	0
6	D	134	0	0	3	0
All	All	12452	0	11787	302	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 13.

The worst 5 of 302 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)
3:D:404:COA:H21	4:D:408:CIT:O4	1.53	1.06
3:D:404:COA:H21	4:D:408:CIT:C5	1.94	0.97
1:A:35:GLN:HE21	1:A:35:GLN:H	1.16	0.88
1:A:35:GLN:NE2	1:A:35:GLN:H	1.73	0.87
3:D:404:COA:C2P	4:D:408:CIT:O4	2.26	0.83

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	367/377 (97%)	356 (97%)	10 (3%)	1 (0%)	41	50
1	B	366/377 (97%)	356 (97%)	10 (3%)	0	100	100
1	C	362/377 (96%)	349 (96%)	13 (4%)	0	100	100
1	D	362/377 (96%)	350 (97%)	12 (3%)	0	100	100
All	All	1457/1508 (97%)	1411 (97%)	45 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	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	298/307 (97%)	288 (97%)	10 (3%)	37	51
1	B	300/307 (98%)	290 (97%)	10 (3%)	38	53
1	C	296/307 (96%)	289 (98%)	7 (2%)	49	66
1	D	296/307 (96%)	287 (97%)	9 (3%)	41	57
All	All	1190/1228 (97%)	1154 (97%)	36 (3%)	41	57

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	287	GLU
1	C	62	GLU
1	D	300	LYS
1	B	333	PHE
1	C	135	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	231	GLN
1	C	23	GLN
1	A	170	GLN
1	B	289	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

22 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	CIT	B	406	-	3,12,12	1.81	1 (33%)	3,17,17	7.62	2 (66%)
2	SO4	C	388	-	4,4,4	0.26	0	6,6,6	0.10	0
3	COA	B	402	-	41,50,50	1.83	11 (26%)	52,75,75	1.60	10 (19%)
5	GOL	B	412	-	5,5,5	0.81	0	5,5,5	0.30	0
2	SO4	D	389	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	B	383	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	A	391	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	386	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	B	385	-	4,4,4	0.28	0	6,6,6	0.09	0
5	GOL	A	411	-	5,5,5	0.80	0	5,5,5	0.20	0
2	SO4	A	387	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	C	390	-	4,4,4	0.23	0	6,6,6	0.08	0
5	GOL	D	414	-	5,5,5	0.73	0	5,5,5	0.20	0
4	CIT	A	405	-	3,12,12	2.44	2 (66%)	3,17,17	7.30	3 (100%)
2	SO4	C	381	-	4,4,4	0.19	0	6,6,6	0.12	0
5	GOL	C	413	-	5,5,5	0.88	0	5,5,5	0.59	0
3	COA	D	404	-	41,50,50	2.32	13 (31%)	52,75,75	1.82	14 (26%)
4	CIT	C	407	-	3,12,12	2.22	1 (33%)	3,17,17	7.06	2 (66%)
3	COA	A	401	-	41,50,50	1.89	9 (21%)	52,75,75	1.66	10 (19%)
2	SO4	B	382	-	4,4,4	0.25	0	6,6,6	0.10	0
4	CIT	D	408	-	3,12,12	2.38	1 (33%)	3,17,17	5.19	2 (66%)
3	COA	C	403	-	41,50,50	1.89	10 (24%)	52,75,75	1.68	10 (19%)

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
4	CIT	B	406	-	-	1/6/16/16	-
5	GOL	C	413	-	-	0/4/4/4	-
3	COA	D	404	-	-	17/44/64/64	0/3/3/3
4	CIT	C	407	-	-	0/6/16/16	-
5	GOL	D	414	-	-	2/4/4/4	-
3	COA	A	401	-	-	5/44/64/64	0/3/3/3
4	CIT	A	405	-	-	3/6/16/16	-
5	GOL	A	411	-	-	0/4/4/4	-
3	COA	B	402	-	-	9/44/64/64	0/3/3/3
4	CIT	D	408	-	-	2/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	412	-	-	0/4/4/4	-
3	COA	C	403	-	-	2/44/64/64	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	404	COA	O4B-C1B	6.65	1.50	1.41
3	A	401	COA	P3B-O3B	5.71	1.70	1.59
3	C	403	COA	P3B-O3B	5.52	1.69	1.59
3	D	404	COA	O9P-C9P	5.34	1.34	1.23
3	B	402	COA	P3B-O3B	5.00	1.68	1.59

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	CIT	C3-C4-C5	11.59	133.54	114.98
4	B	406	CIT	C3-C4-C5	11.12	132.80	114.98
4	C	407	CIT	C3-C4-C5	10.57	131.91	114.98
4	B	406	CIT	C3-C2-C1	6.98	126.16	114.98
4	D	408	CIT	C3-C4-C5	6.23	124.97	114.98

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	414	GOL	O1-C1-C2-C3
4	A	405	CIT	C2-C3-C4-C5
4	A	405	CIT	O7-C3-C4-C5
4	A	405	CIT	C6-C3-C4-C5
3	D	404	COA	C4B-C3B-O3B-P3B

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	406	CIT	1	0
3	B	402	COA	1	0
2	B	383	SO4	1	0
4	A	405	CIT	1	0
3	D	404	COA	11	0
3	A	401	COA	2	0

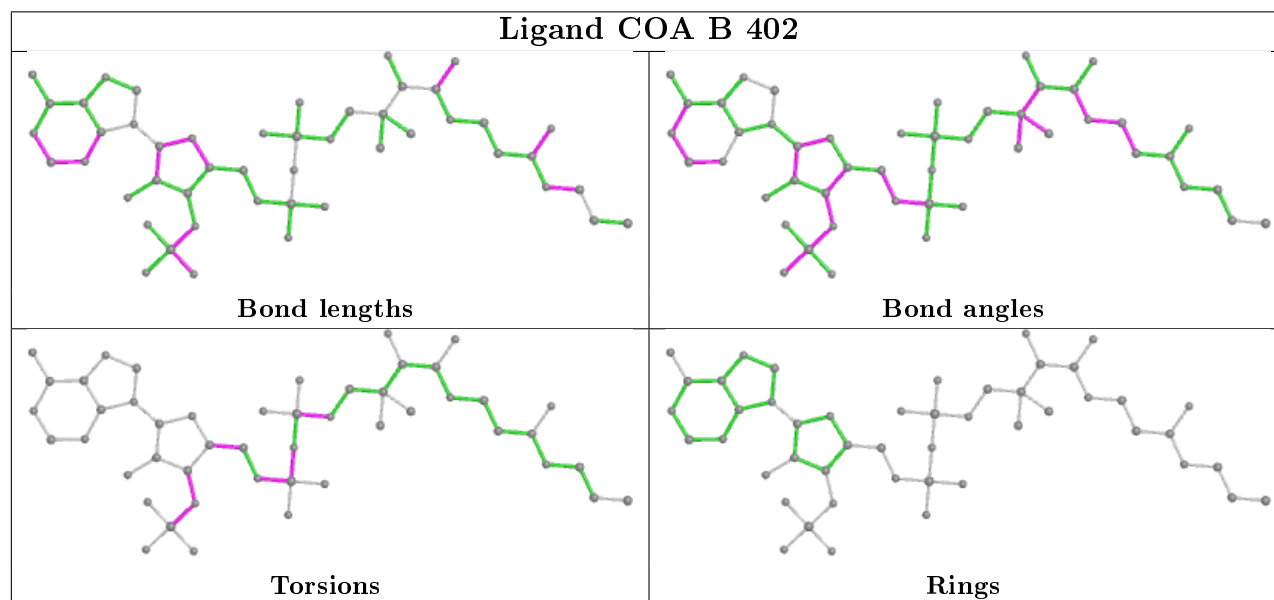
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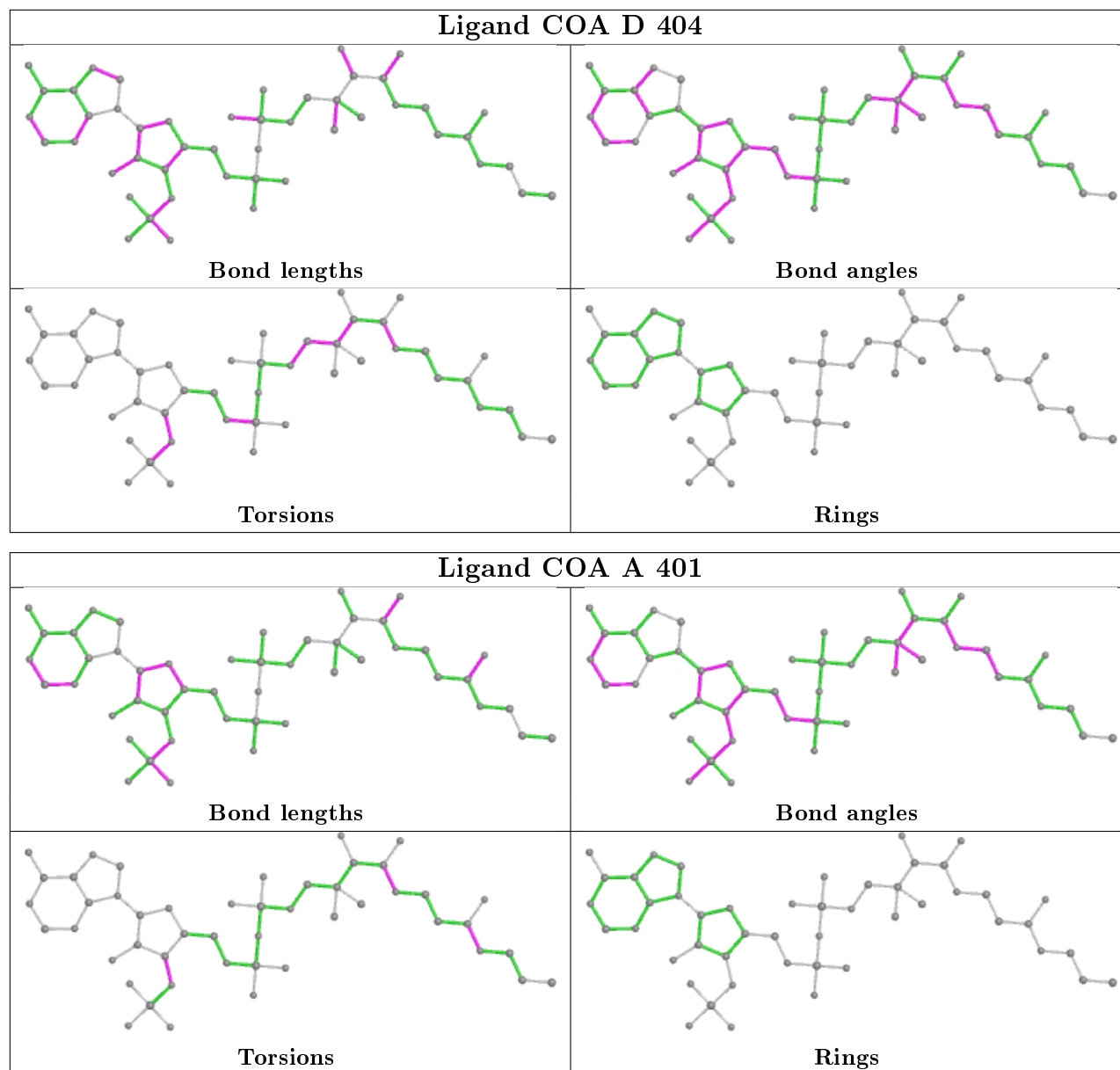


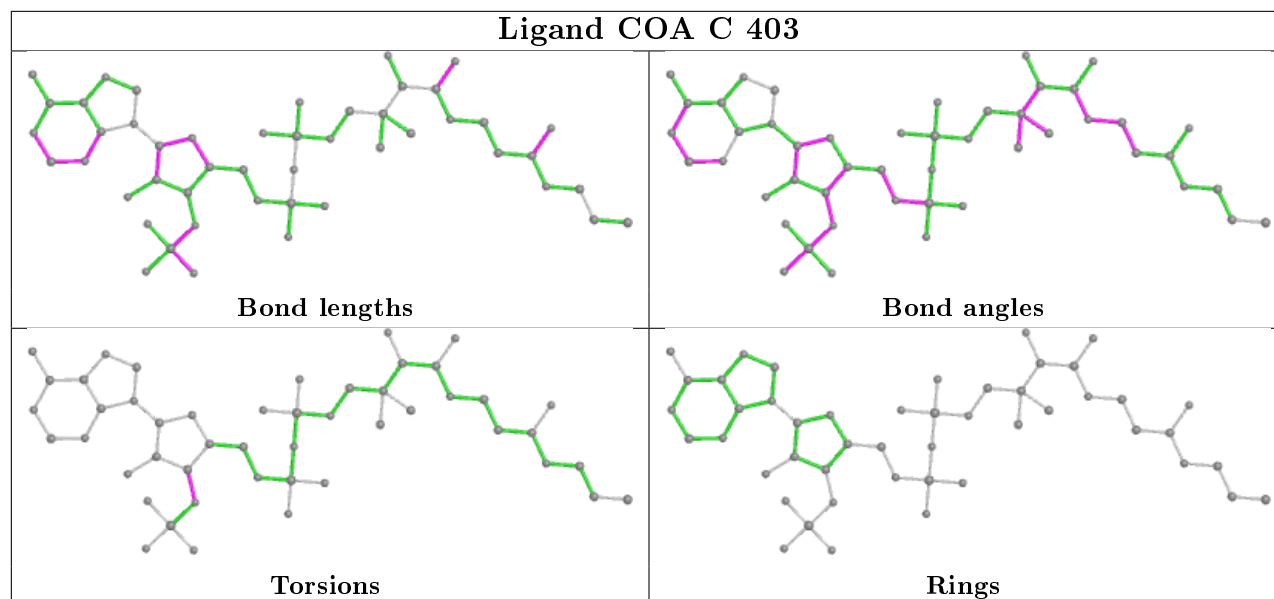
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	382	SO4	1	0
4	D	408	CIT	6	0
3	C	403	COA	1	0

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	371/377 (98%)	1.62	97 (26%) 0 0	8, 21, 39, 57	21 (5%)
1	B	370/377 (98%)	1.49	84 (22%) 0 1	10, 21, 39, 55	24 (6%)
1	C	366/377 (97%)	1.86	128 (34%) 0 0	10, 25, 65, 79	30 (8%)
1	D	366/377 (97%)	1.66	96 (26%) 0 0	10, 23, 52, 64	28 (7%)
All	All	1473/1508 (97%)	1.66	405 (27%) 0 0	8, 22, 51, 79	103 (6%)

The worst 5 of 405 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	PHE	15.8
1	C	288	TYR	9.4
1	C	278	VAL	8.7
1	C	247	LEU	8.5
1	C	302	LEU	8.2

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

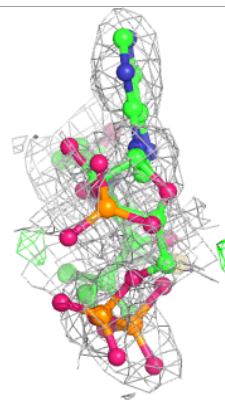
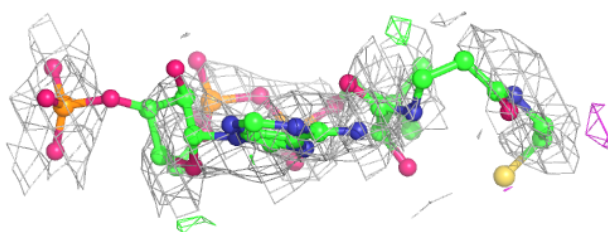
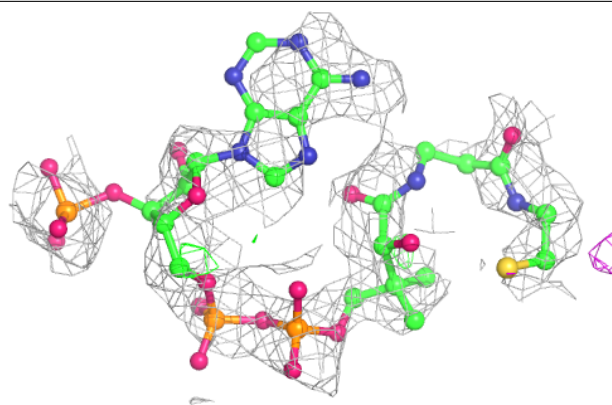
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
3	COA	D	404	48/48	0.47	0.43	82,86,89,90	0
5	GOL	B	412	6/6	0.59	0.37	35,39,40,42	0
3	COA	C	403	48/48	0.60	0.35	63,73,81,82	0
5	GOL	C	413	6/6	0.62	0.57	43,47,50,51	0
3	COA	A	401	48/48	0.65	0.32	42,52,62,65	0
4	CIT	D	408	13/13	0.69	0.30	32,39,47,49	0
5	GOL	D	414	6/6	0.70	0.27	59,61,62,62	0
4	CIT	C	407	13/13	0.71	0.30	36,43,51,53	0
4	CIT	B	406	13/13	0.77	0.33	22,31,42,43	0
4	CIT	A	405	13/13	0.78	0.28	22,28,42,45	0
3	COA	B	402	48/48	0.79	0.22	18,25,43,45	0
2	SO4	C	390	5/5	0.79	0.52	80,82,83,83	0
5	GOL	A	411	6/6	0.80	0.40	22,30,31,36	0
2	SO4	B	383	5/5	0.83	0.50	59,62,63,64	0
2	SO4	D	386	5/5	0.83	0.22	42,43,44,45	0
2	SO4	D	389	5/5	0.85	0.39	70,70,72,73	0
2	SO4	A	387	5/5	0.89	0.31	42,43,43,46	0
2	SO4	B	382	5/5	0.90	0.23	52,55,56,58	0
2	SO4	C	388	5/5	0.91	0.14	49,50,51,53	0
2	SO4	B	385	5/5	0.92	0.25	43,43,44,45	0
2	SO4	C	381	5/5	0.95	0.14	25,26,27,29	0
2	SO4	A	391	5/5	0.96	0.14	15,16,17,19	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.

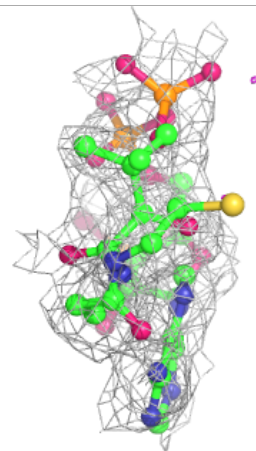
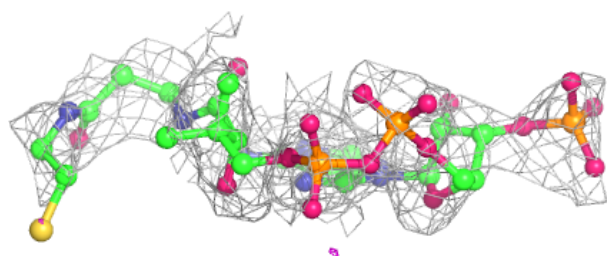
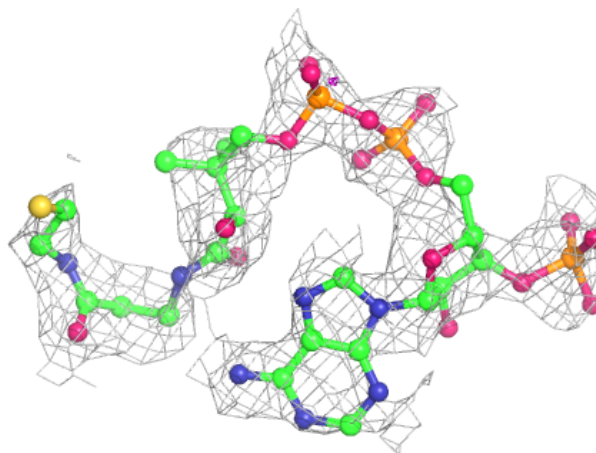
**Electron density around COA D 404:**

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



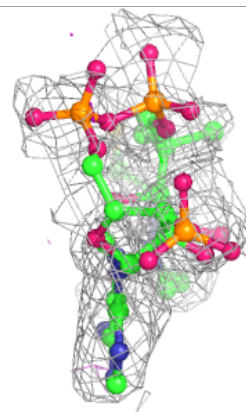
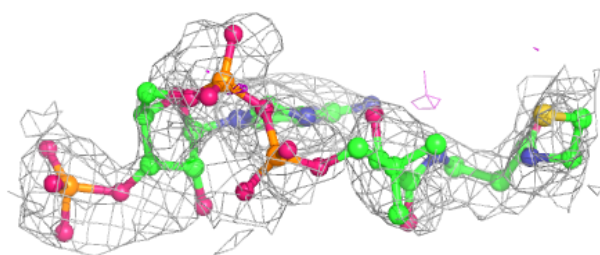
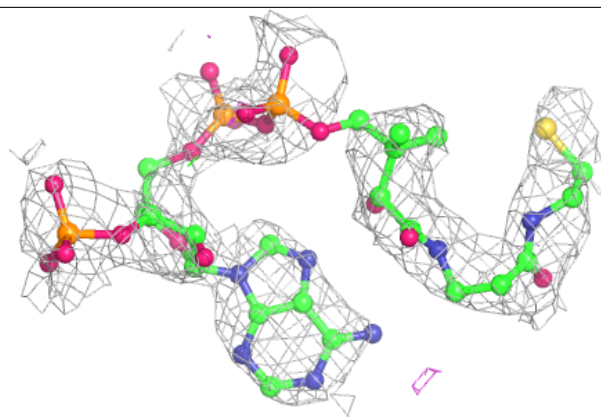
**Electron density around COA C 403:**

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

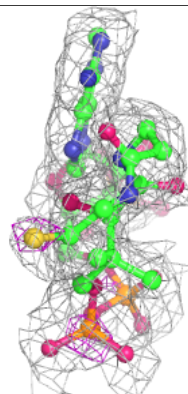
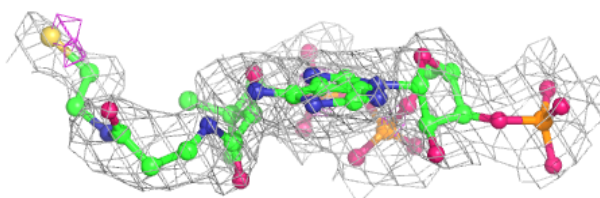
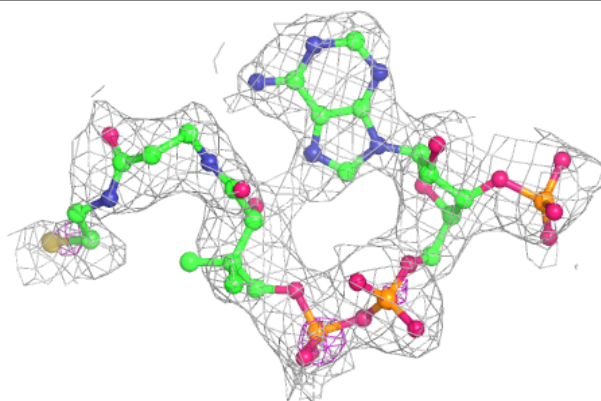


**Electron density around COA A 401:**

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

**Electron density around COA B 402:**

$2mF_o-DF_c$  (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.