



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 06:34 PM EDT

PDB ID : 4NHD  
Title : Crystal structure of beta-ketoacyl-ACP synthase III (FabH) from *Vibrio Cholerae* in complex with Coenzyme A  
Authors : Hou, J.; Zheng, H.; Langner, K.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2013-11-04  
Resolution : 1.78 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 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	:	2.27
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)	:	2.27

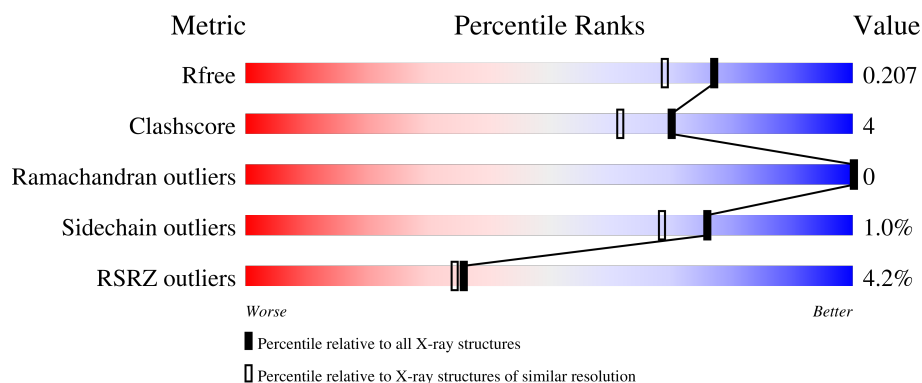
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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))
$R_{free}$	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	319	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>5% ..</div> </div> </div>
1	B	319	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div>5% .</div> </div> </div>
1	C	319	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5% .</div> </div> </div>
1	D	319	<div> <div>9%</div> <div> <div></div> <div>95%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11110 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.

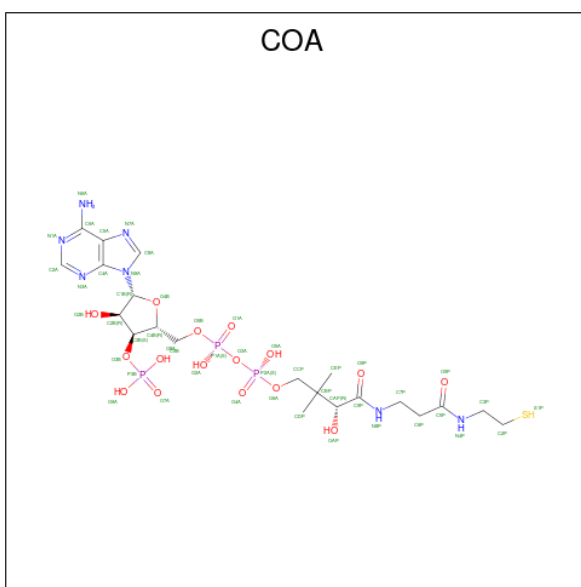
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	4	0
			2394	1502	418	457	17			
1	B	317	Total	C	N	O	S	0	2	0
			2382	1495	416	456	15			
1	C	317	Total	C	N	O	S	0	6	0
			2414	1514	421	462	17			
1	D	318	Total	C	N	O	S	0	0	0
			2361	1481	410	455	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KQH5
A	-1	ASN	-	expression tag	UNP Q9KQH5
A	0	ALA	-	expression tag	UNP Q9KQH5
B	-2	SER	-	expression tag	UNP Q9KQH5
B	-1	ASN	-	expression tag	UNP Q9KQH5
B	0	ALA	-	expression tag	UNP Q9KQH5
C	-2	SER	-	expression tag	UNP Q9KQH5
C	-1	ASN	-	expression tag	UNP Q9KQH5
C	0	ALA	-	expression tag	UNP Q9KQH5
D	-2	SER	-	expression tag	UNP Q9KQH5
D	-1	ASN	-	expression tag	UNP Q9KQH5
D	0	ALA	-	expression tag	UNP Q9KQH5

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	D	1	Total	C	N	O	P	S	0	0
			47	21	7	15	3	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Na	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	340	Total	O	0	0
			340	340		
5	B	335	Total	O	0	0
			335	335		
5	C	348	Total	O	0	0
			348	348		
5	D	239	Total	O	0	0
			239	239		

### 3 Residue-property plots

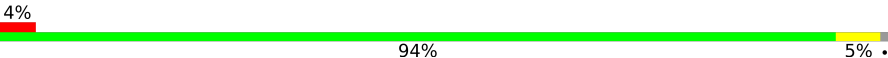
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

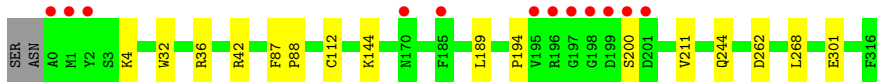
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 1

Chain A: 



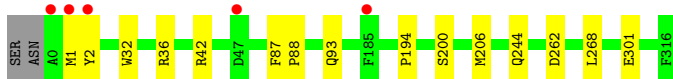
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 1

Chain B: 



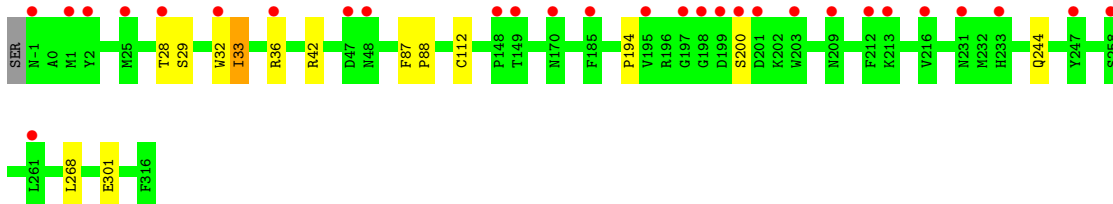
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 1

Chain C: 



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3 protein 1

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.45Å 100.25Å 132.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.78 34.12 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-1.78) 97.9 (34.12-1.78)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.170 , 0.196 0.181 , 0.207	Depositor DCC
$R_{free}$ test set	6294 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11110	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 10.53% 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: CA, SCY, COA, NA

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	0.51	0/2427	0.70	2/3285 (0.1%)
1	B	0.50	0/2412	0.69	1/3266 (0.0%)
1	C	0.52	0/2450	0.71	1/3314 (0.0%)
1	D	0.47	0/2391	0.67	1/3240 (0.0%)
All	All	0.50	0/9680	0.70	5/13105 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	262	ASP	CB-CG-OD2	5.49	123.25	118.30
1	D	33	ILE	CA-CB-CG1	5.27	121.01	111.00
1	A	187	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	42	ARG	NE-CZ-NH2	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2394	0	2387	21	0
1	B	2382	0	2373	14	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2414	0	2414	9	0
1	D	2361	0	2339	9	0
2	A	96	0	64	13	0
2	B	48	0	32	4	0
2	C	96	0	64	11	0
2	D	47	0	30	5	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	D	2	0	0	0	0
5	A	340	0	0	2	0
5	B	335	0	0	3	0
5	C	348	0	0	1	0
5	D	239	0	0	0	0
All	All	11110	0	9703	70	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 (70) 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:189[B]:LEU:HD11	2:B:401:COA:S1P	1.55	1.42
2:A:401[B]:COA:H131	2:A:401[B]:COA:O9P	1.35	1.15
2:A:401[B]:COA:O9P	2:A:401[B]:COA:CDP	1.99	1.10
1:A:248[A]:ARG:HG2	1:A:248[A]:ARG:HH21	1.02	1.09
1:B:189[B]:LEU:CD1	2:B:401:COA:S1P	2.41	1.09
2:C:401[B]:COA:CEP	2:C:401[B]:COA:O9P	2.09	0.93
1:A:248[A]:ARG:HH21	1:A:248[A]:ARG:CG	1.87	0.86
1:A:248[A]:ARG:HG2	1:A:248[A]:ARG:NH2	1.82	0.84
2:A:401[B]:COA:O9P	2:A:401[B]:COA:H62	1.80	0.80
2:C:401[B]:COA:O9P	2:C:401[B]:COA:H141	1.86	0.75
1:B:112:SCY:HE1	2:B:401:COA:S1P	2.27	0.74
1:D:112:SCY:HE3	2:D:401:COA:S1P	2.28	0.73
2:A:401[A]:COA:O9P	2:A:401[A]:COA:H131	1.92	0.69
1:B:112:SCY:CE	2:B:401:COA:S1P	2.82	0.67
2:A:401[A]:COA:O9P	2:A:401[A]:COA:CDP	2.42	0.65
1:A:112:SCY:HE3	2:A:401[A]:COA:S1P	2.37	0.64
2:A:401[B]:COA:O9P	2:A:401[B]:COA:H132	1.98	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401[B]:COA:O9P	2:A:401[B]:COA:C6P	2.52	0.57
1:B:4:LYS:HE3	5:B:626:HOH:O	2.05	0.56
1:A:36:ARG:O	1:A:248[B]:ARG:NH1	2.40	0.55
1:A:194:PRO:HB3	1:A:200:SER:HA	1.90	0.53
1:A:48:ASN:ND2	5:A:799:HOH:O	2.42	0.52
1:A:112:SCY:HE1	2:A:401[B]:COA:S1P	2.49	0.52
1:C:93:GLN:NE2	5:C:784:HOH:O	2.44	0.51
1:D:194:PRO:HB3	1:D:200:SER:HA	1.93	0.51
1:A:87:PHE:HA	1:A:88:PRO:C	2.32	0.50
1:C:194:PRO:HB3	1:C:200:SER:HA	1.92	0.50
1:B:194:PRO:HB3	1:B:200:SER:HA	1.93	0.50
1:B:144:LYS:NZ	5:B:767:HOH:O	2.29	0.50
2:C:401[A]:COA:O9P	2:C:401[A]:COA:H62	2.11	0.49
1:C:87:PHE:HA	1:C:88:PRO:C	2.34	0.47
2:D:401:COA:O9P	2:D:401:COA:H122	2.14	0.47
1:A:220:SER:HB3	5:A:644:HOH:O	2.14	0.47
1:C:1:MET:HG3	1:C:2:TYR:CD2	2.50	0.46
1:B:87:PHE:HA	1:B:88:PRO:C	2.36	0.46
1:B:244:GLN:HB3	1:B:268:LEU:HB3	1.98	0.46
1:A:189[B]:LEU:HD22	2:A:401[B]:COA:S1P	2.56	0.46
1:C:206[B]:MET:HE1	2:C:401[B]:COA:N4P	2.30	0.46
1:D:87:PHE:HA	1:D:88:PRO:C	2.36	0.45
1:A:112:SCY:CE	2:A:401[B]:COA:S1P	3.05	0.45
1:B:4:LYS:CE	5:B:626:HOH:O	2.63	0.44
2:C:401[A]:COA:O9P	2:C:401[A]:COA:H131	2.16	0.44
1:A:189[B]:LEU:HG	1:A:211:VAL:HG21	1.99	0.44
1:D:244:GLN:HB3	1:D:268:LEU:HB3	1.99	0.44
1:A:189[B]:LEU:CD2	1:A:211:VAL:HG21	2.48	0.43
1:B:32:TRP:CE2	1:B:36:ARG:HG3	2.53	0.43
1:A:248[A]:ARG:CG	1:A:248[A]:ARG:NH2	2.58	0.43
1:C:244:GLN:HB3	1:C:268:LEU:HB3	2.00	0.43
1:B:189[A]:LEU:HD21	1:B:211:VAL:HG21	2.00	0.43
2:C:401[A]:COA:O9P	2:C:401[A]:COA:CDP	2.66	0.43
1:A:244:GLN:HB3	1:A:268:LEU:HB3	2.01	0.43
1:A:189[B]:LEU:HD21	1:A:211:VAL:HG21	2.00	0.42
1:B:189[A]:LEU:CD2	1:B:211:VAL:HG21	2.49	0.42
2:D:401:COA:N8P	2:D:401:COA:H143	2.33	0.42
1:A:245:ALA:HB1	2:A:401[A]:COA:H21	2.01	0.42
1:A:32:TRP:CE2	1:A:36:ARG:HG3	2.55	0.42
2:C:401[A]:COA:H32	2:C:401[A]:COA:H61	1.65	0.41
1:D:112:SCY:CE	2:D:401:COA:S1P	3.04	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:THR:OG1	1:D:33:ILE:HD11	2.20	0.41
1:D:32:TRP:CE2	1:D:36:ARG:HG3	2.56	0.41
2:C:401[B]:COA:H143	2:C:401[B]:COA:H62	2.03	0.41
2:C:401[B]:COA:O1A	2:C:401[B]:COA:O6A	2.39	0.41
1:B:189[A]:LEU:HG	1:B:211:VAL:HG21	2.02	0.41
1:C:32:TRP:CE2	1:C:36:ARG:HG3	2.56	0.41
1:D:29:SER:O	1:D:33:ILE:HG12	2.21	0.41
1:A:189[B]:LEU:HD11	1:A:211:VAL:HG11	2.03	0.40
1:A:211:VAL:HG11	2:A:401[A]:COA:N4P	2.37	0.40
1:C:206[B]:MET:CE	2:C:401[B]:COA:C3P	2.99	0.40
1:C:206[B]:MET:CE	2:C:401[B]:COA:N4P	2.85	0.40
1:D:112:SCY:CD	2:D:401:COA:S1P	3.10	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	318/319 (100%)	309 (97%)	9 (3%)	0	100	100
1	B	316/319 (99%)	305 (96%)	11 (4%)	0	100	100
1	C	320/319 (100%)	310 (97%)	10 (3%)	0	100	100
1	D	315/319 (99%)	306 (97%)	9 (3%)	0	100	100
All	All	1269/1276 (100%)	1230 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	251/252 (100%)	246 (98%)	5 (2%)	55	40
1	B	249/252 (99%)	247 (99%)	2 (1%)	81	76
1	C	255/252 (101%)	253 (99%)	2 (1%)	81	76
1	D	246/252 (98%)	244 (99%)	2 (1%)	81	76
All	All	1001/1008 (99%)	990 (99%)	11 (1%)	76	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	228	LYS
1	A	248[A]	ARG
1	A	248[B]	ARG
1	A	301	GLU
1	B	42	ARG
1	B	301	GLU
1	C	42	ARG
1	C	301	GLU
1	D	42	ARG
1	D	301	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	SCY	D	112	1	7,8,9	0.83	0	3,9,11	0.35	0
1	SCY	C	112	1	7,8,9	0.79	0	3,9,11	0.68	0
1	SCY	B	112	1	7,8,9	0.64	0	3,9,11	0.53	0
1	SCY	A	112	1	7,8,9	0.68	0	3,9,11	0.38	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
1	SCY	D	112	1	-	0/5/7/9	-
1	SCY	C	112	1	-	0/5/7/9	-
1	SCY	B	112	1	-	0/5/7/9	-
1	SCY	A	112	1	-	0/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	112	SCY	3	0
1	B	112	SCY	2	0
1	A	112	SCY	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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	B	401	-	41,50,50	0.95	4 (9%)	52,75,75	2.77	12 (23%)
2	COA	A	401[A]	-	41,50,50	0.90	2 (4%)	52,75,75	3.47	11 (21%)
2	COA	D	401	-	41,49,50	0.82	1 (2%)	51,73,75	2.99	8 (15%)
2	COA	C	401[A]	-	41,50,50	0.93	3 (7%)	52,75,75	3.00	12 (23%)
2	COA	A	401[B]	-	41,50,50	0.87	2 (4%)	52,75,75	3.51	11 (21%)
2	COA	C	401[B]	-	41,50,50	0.79	1 (2%)	52,75,75	3.12	9 (17%)

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	B	401	-	-	4/44/64/64	0/3/3/3
2	COA	A	401[A]	-	-	6/44/64/64	0/3/3/3
2	COA	D	401	-	-	3/44/60/64	0/3/3/3
2	COA	C	401[A]	-	-	7/44/64/64	0/3/3/3
2	COA	A	401[B]	-	-	12/44/64/64	0/3/3/3
2	COA	C	401[B]	-	-	24/44/64/64	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	COA	OAP-CAP	2.66	1.47	1.42
2	B	401	COA	O4B-C1B	2.55	1.44	1.41
2	D	401	COA	C5A-C4A	2.44	1.47	1.40
2	A	401[A]	COA	C5A-C4A	2.43	1.47	1.40
2	C	401[A]	COA	C5A-C4A	2.41	1.47	1.40
2	A	401[B]	COA	C5A-C4A	2.40	1.47	1.40
2	A	401[A]	COA	O4B-C1B	2.38	1.44	1.41
2	B	401	COA	P3B-O3B	2.36	1.63	1.59
2	C	401[B]	COA	C5A-C4A	2.33	1.47	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	COA	O4B-C1B	2.27	1.44	1.41
2	C	401[A]	COA	O4B-C1B	2.21	1.44	1.41
2	B	401	COA	C5A-C4A	2.16	1.46	1.40
2	C	401[A]	COA	C2A-N3A	2.13	1.35	1.32

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	COA	CDP-CBP-CAP	-15.88	81.28	108.82
2	A	401[A]	COA	CDP-CBP-CAP	-14.80	83.16	108.82
2	C	401[A]	COA	CDP-CBP-CAP	-14.38	83.89	108.82
2	A	401[B]	COA	CEP-CBP-CAP	-13.42	85.55	108.82
2	C	401[B]	COA	CDP-CBP-CAP	-13.34	85.70	108.82
2	D	401	COA	CEP-CBP-CCP	12.48	128.59	108.23
2	A	401[A]	COA	CEP-CBP-CAP	-11.63	88.66	108.82
2	C	401[B]	COA	CEP-CBP-CAP	-11.43	89.00	108.82
2	D	401	COA	CEP-CBP-CAP	-10.62	90.40	108.82
2	A	401[A]	COA	CEP-CBP-CDP	9.91	129.36	109.17
2	B	401	COA	CEP-CBP-CDP	9.86	129.26	109.17
2	B	401	COA	CEP-CBP-CAP	-9.82	91.80	108.82
2	A	401[B]	COA	CEP-CBP-CDP	9.38	128.29	109.17
2	D	401	COA	CDP-CBP-CAP	-8.91	93.38	108.82
2	C	401[A]	COA	CDP-CBP-CCP	8.87	122.70	108.23
2	B	401	COA	CDP-CBP-CAP	-8.15	94.69	108.82
2	A	401[A]	COA	CDP-CBP-CCP	7.91	121.13	108.23
2	C	401[B]	COA	CDP-CBP-CCP	7.58	120.59	108.23
2	C	401[B]	COA	CEP-CBP-CCP	7.35	120.22	108.23
2	A	401[B]	COA	CDP-CBP-CCP	5.96	117.96	108.23
2	D	401	COA	CDP-CBP-CCP	5.66	117.46	108.23
2	C	401[A]	COA	CEP-CBP-CCP	5.36	116.97	108.23
2	B	401	COA	CDP-CBP-CCP	5.32	116.90	108.23
2	C	401[A]	COA	CEP-CBP-CDP	5.25	119.86	109.17
2	C	401[A]	COA	CEP-CBP-CAP	-4.84	100.43	108.82
2	B	401	COA	O6A-CCP-CBP	4.70	118.10	110.55
2	C	401[B]	COA	CEP-CBP-CDP	4.51	118.36	109.17
2	A	401[A]	COA	O6A-CCP-CBP	4.47	117.74	110.55
2	B	401	COA	N3A-C2A-N1A	-4.13	122.22	128.68
2	A	401[B]	COA	N3A-C2A-N1A	-3.90	122.58	128.68
2	A	401[A]	COA	N3A-C2A-N1A	-3.88	122.61	128.68
2	C	401[B]	COA	N3A-C2A-N1A	-3.87	122.63	128.68
2	C	401[A]	COA	N3A-C2A-N1A	-3.82	122.70	128.68
2	D	401	COA	N3A-C2A-N1A	-3.67	122.94	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401[A]	COA	C7P-N8P-C9P	3.58	128.98	122.59
2	A	401[A]	COA	C6P-C7P-N8P	3.18	118.32	111.90
2	B	401	COA	OAP-CAP-CBP	3.07	117.47	110.25
2	C	401[A]	COA	C4A-C5A-N7A	-3.06	106.21	109.40
2	A	401[B]	COA	CEP-CBP-CCP	2.97	113.08	108.23
2	C	401[B]	COA	C4A-C5A-N7A	-2.96	106.31	109.40
2	D	401	COA	C4A-C5A-N7A	-2.84	106.44	109.40
2	C	401[B]	COA	C3B-C2B-C1B	2.78	106.05	99.89
2	C	401[A]	COA	C6P-C7P-N8P	2.74	117.44	111.90
2	D	401	COA	P2A-O3A-P1A	-2.70	123.55	132.83
2	B	401	COA	C4A-C5A-N7A	-2.60	106.69	109.40
2	B	401	COA	CEP-CBP-CCP	2.58	112.44	108.23
2	C	401[A]	COA	CAP-C9P-N8P	-2.51	111.59	116.58
2	A	401[B]	COA	P2A-O3A-P1A	-2.50	124.25	132.83
2	A	401[A]	COA	C6P-C5P-N4P	2.49	120.61	116.42
2	A	401[A]	COA	P2A-O3A-P1A	-2.47	124.35	132.83
2	C	401[A]	COA	O9A-P3B-O8A	2.45	117.00	107.64
2	A	401[B]	COA	O6A-CCP-CBP	2.41	114.43	110.55
2	C	401[A]	COA	O4B-C1B-C2B	-2.33	103.51	106.93
2	B	401	COA	C1B-N9A-C4A	-2.32	122.56	126.64
2	C	401[B]	COA	P2A-O3A-P1A	-2.30	124.95	132.83
2	A	401[A]	COA	O4B-C1B-C2B	-2.27	103.61	106.93
2	B	401	COA	C7P-C6P-C5P	-2.25	108.61	112.36
2	A	401[B]	COA	C7P-C6P-C5P	-2.23	108.64	112.36
2	D	401	COA	CEP-CBP-CDP	2.10	113.45	109.17
2	B	401	COA	O9A-P3B-O8A	2.10	115.64	107.64
2	A	401[A]	COA	C2A-N1A-C6A	2.08	122.31	118.75
2	A	401[B]	COA	C2A-N1A-C6A	2.08	122.31	118.75
2	A	401[B]	COA	O4B-C1B-C2B	-2.05	103.93	106.93

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	COA	CEP-CBP-CCP-O6A
2	A	401[A]	COA	S1P-C2P-C3P-N4P
2	A	401[B]	COA	CCP-O6A-P2A-O3A
2	A	401[B]	COA	CEP-CBP-CCP-O6A
2	A	401[B]	COA	CAP-CBP-CCP-O6A
2	A	401[B]	COA	C5P-C6P-C7P-N8P
2	B	401	COA	C3B-O3B-P3B-O8A
2	C	401[A]	COA	C3B-O3B-P3B-O9A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	C	401[A]	COA	CDP-CBP-CCP-O6A
2	C	401[A]	COA	S1P-C2P-C3P-N4P
2	C	401[B]	COA	CCP-O6A-P2A-O3A
2	C	401[B]	COA	CBP-CCP-O6A-P2A
2	C	401[B]	COA	CAP-CBP-CCP-O6A
2	C	401[B]	COA	OAP-CAP-CBP-CCP
2	C	401[B]	COA	C9P-CAP-CBP-CCP
2	C	401[B]	COA	OAP-CAP-CBP-CDP
2	C	401[B]	COA	C9P-CAP-CBP-CDP
2	C	401[B]	COA	OAP-CAP-CBP-CEP
2	C	401[B]	COA	C9P-CAP-CBP-CEP
2	C	401[B]	COA	C5P-C6P-C7P-N8P
2	C	401[A]	COA	C6P-C7P-N8P-C9P
2	A	401[B]	COA	C6P-C7P-N8P-C9P
2	A	401[A]	COA	C6P-C5P-N4P-C3P
2	C	401[A]	COA	C6P-C5P-N4P-C3P
2	A	401[A]	COA	O5P-C5P-N4P-C3P
2	C	401[A]	COA	O5P-C5P-N4P-C3P
2	C	401[B]	COA	C6P-C7P-N8P-C9P
2	C	401[B]	COA	C2B-C3B-O3B-P3B
2	C	401[B]	COA	C4B-C3B-O3B-P3B
2	A	401[A]	COA	CDP-CBP-CCP-O6A
2	C	401[B]	COA	CDP-CBP-CCP-O6A
2	D	401	COA	CEP-CBP-CCP-O6A
2	B	401	COA	CEP-CBP-CCP-O6A
2	C	401[B]	COA	P1A-O3A-P2A-O6A
2	C	401[B]	COA	C3B-O3B-P3B-O7A
2	B	401	COA	CDP-CBP-CCP-O6A
2	C	401[A]	COA	C5P-C6P-C7P-N8P
2	A	401[B]	COA	C3B-O3B-P3B-O8A
2	C	401[B]	COA	P2A-O3A-P1A-O1A
2	A	401[B]	COA	CCP-O6A-P2A-O4A
2	A	401[B]	COA	CCP-O6A-P2A-O5A
2	C	401[B]	COA	C5B-O5B-P1A-O2A
2	C	401[B]	COA	CCP-O6A-P2A-O5A
2	D	401	COA	O9P-C9P-CAP-OAP
2	D	401	COA	CDP-CBP-CCP-O6A
2	B	401	COA	P1A-O3A-P2A-O4A
2	A	401[B]	COA	O9P-C9P-CAP-CBP
2	C	401[B]	COA	CEP-CBP-CCP-O6A
2	A	401[B]	COA	N8P-C9P-CAP-CBP
2	A	401[A]	COA	P1A-O3A-P2A-O4A

*Continued on next page...*

*Continued from previous page...*

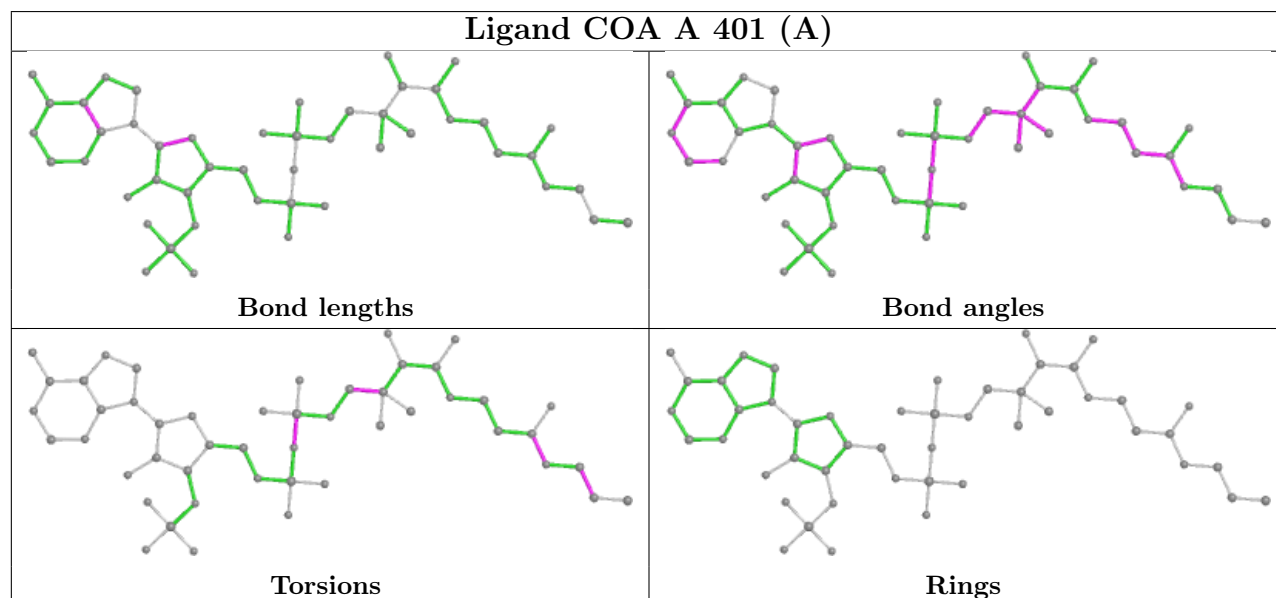
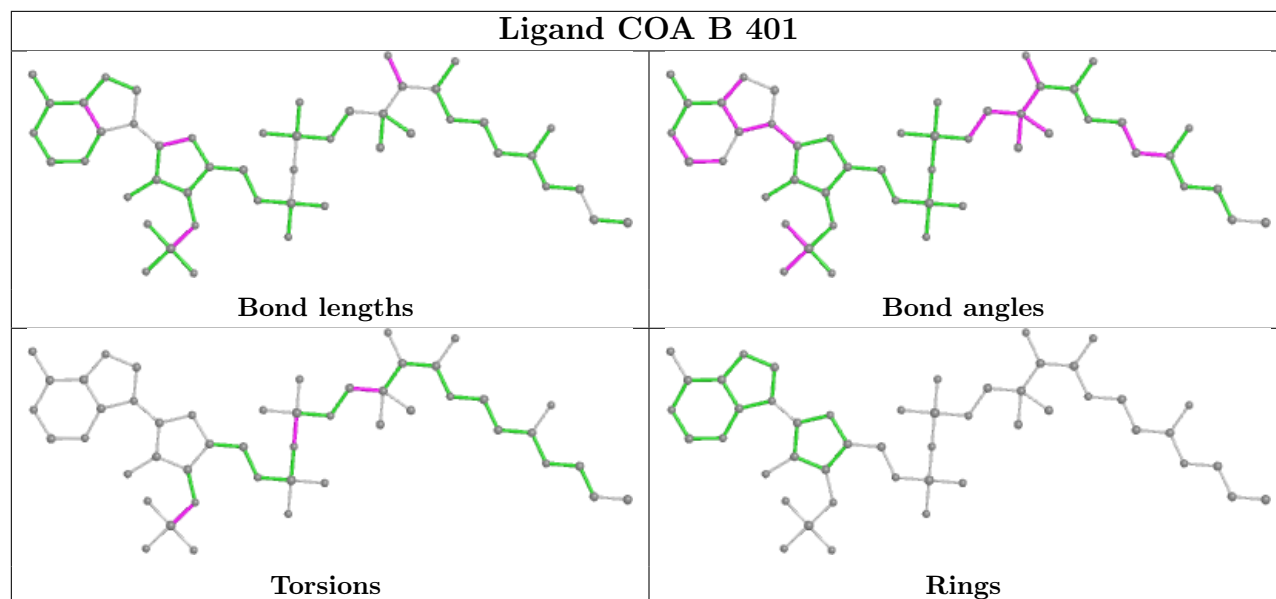
Mol	Chain	Res	Type	Atoms
2	A	401[B]	COA	C5B-O5B-P1A-O3A
2	C	401[B]	COA	C3B-O3B-P3B-O8A
2	C	401[B]	COA	C5B-O5B-P1A-O3A
2	C	401[B]	COA	P1A-O3A-P2A-O5A
2	A	401[B]	COA	C5B-O5B-P1A-O1A
2	C	401[B]	COA	C5B-O5B-P1A-O1A

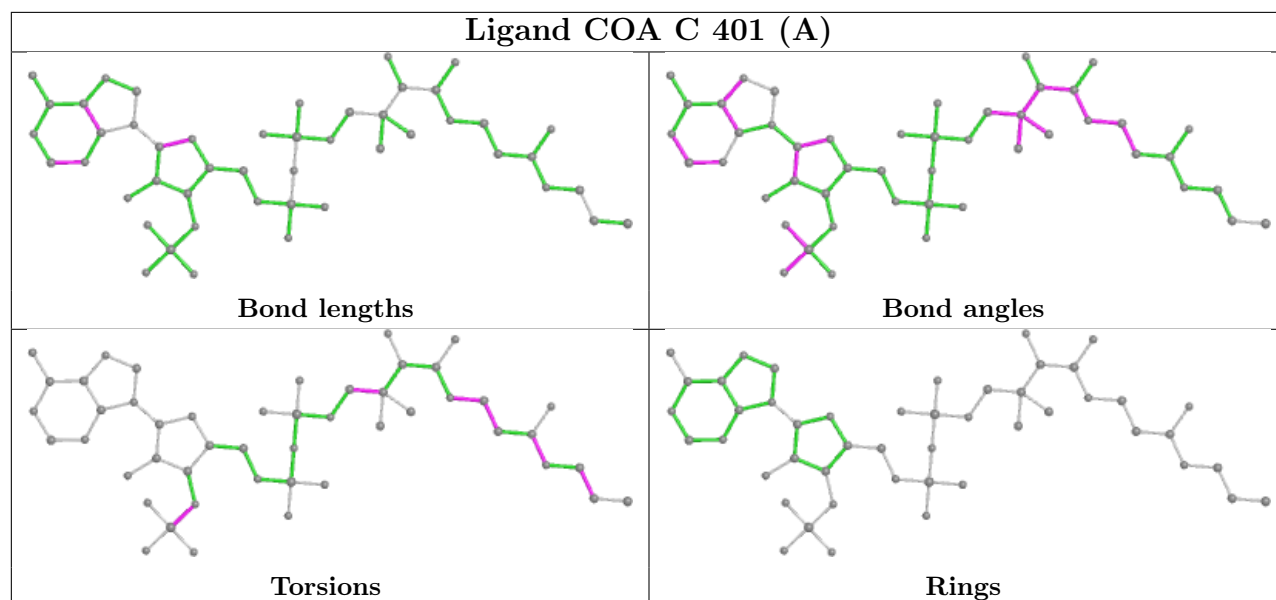
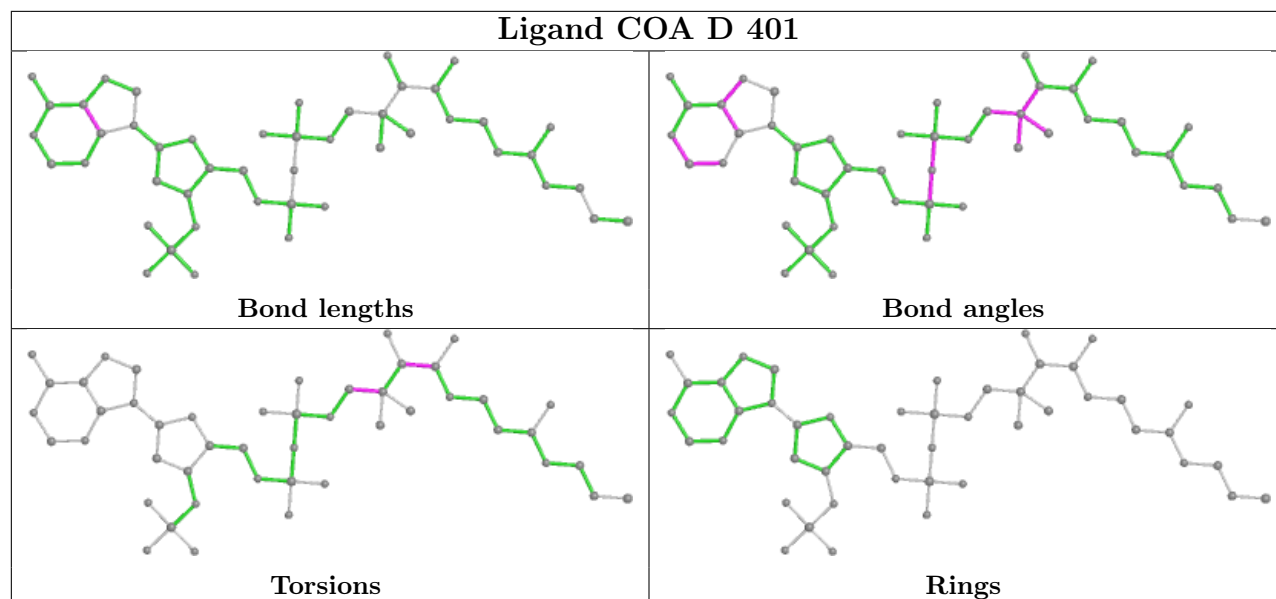
There are no ring outliers.

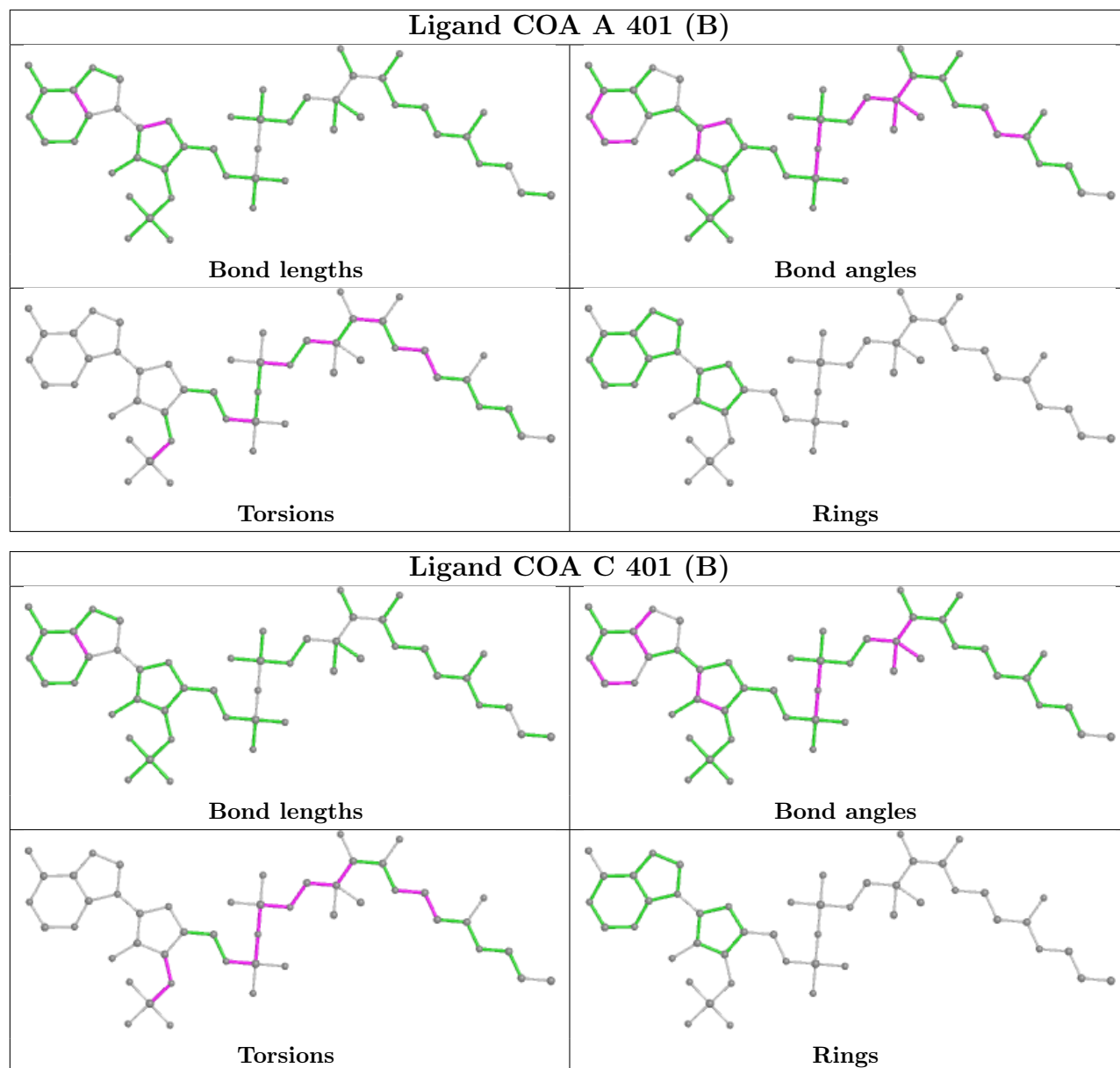
6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	COA	4	0
2	A	401[A]	COA	5	0
2	D	401	COA	5	0
2	C	401[A]	COA	4	0
2	A	401[B]	COA	8	0
2	C	401[B]	COA	7	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	316/319 (99%)	0.10	7 (2%) 62 61	11, 20, 39, 64	0
1	B	316/319 (99%)	-0.01	12 (3%) 40 39	12, 20, 41, 74	0
1	C	316/319 (99%)	-0.05	5 (1%) 72 72	10, 19, 37, 58	0
1	D	317/319 (99%)	0.42	29 (9%) 9 8	14, 28, 58, 78	0
All	All	1265/1276 (99%)	0.11	53 (4%) 36 34	10, 21, 47, 78	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.2
1	B	197	GLY	5.5
1	A	2	TYR	5.2
1	D	199	ASP	4.7
1	B	198	GLY	4.7
1	C	0	ALA	4.6
1	D	197	GLY	4.4
1	B	185	PHE	4.3
1	D	195	VAL	4.1
1	D	200	SER	4.1
1	B	0	ALA	4.1
1	C	1	MET	4.1
1	D	2	TYR	4.0
1	D	201	ASP	3.8
1	D	203	TRP	3.5
1	D	198	GLY	3.5
1	B	170	ASN	3.4
1	D	32	TRP	3.4
1	B	1	MET	3.4
1	D	149	THR	3.2
1	C	185	PHE	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	47	ASP	3.1
1	D	209	ASN	3.1
1	D	170	ASN	3.1
1	B	2	TYR	2.9
1	D	247	TYR	2.9
1	D	1	MET	2.8
1	D	213	LYS	2.8
1	A	199	ASP	2.8
1	B	199	ASP	2.8
1	D	148	PRO	2.8
1	D	258	SER	2.6
1	A	195	VAL	2.5
1	D	212	PHE	2.4
1	B	196	ARG	2.4
1	D	-1	ASN	2.4
1	B	200	SER	2.4
1	B	195	VAL	2.4
1	D	233	HIS	2.3
1	A	247	TYR	2.3
1	A	47	ASP	2.3
1	D	261	LEU	2.3
1	A	172	PRO	2.2
1	D	25	MET	2.2
1	D	36	ARG	2.2
1	D	216	VAL	2.2
1	B	201	ASP	2.2
1	C	2	TYR	2.1
1	D	185	PHE	2.1
1	D	28	THR	2.0
1	C	47	ASP	2.0
1	D	48	ASN	2.0
1	D	231	ASN	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	SCY	A	112	9/10	0.89	0.14	15,16,29,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SCY	D	112	9/10	0.89	0.17	20,21,26,28	4
1	SCY	B	112	9/10	0.93	0.13	15,17,28,30	0
1	SCY	C	112	9/10	0.96	0.12	13,14,16,17	4

### 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.

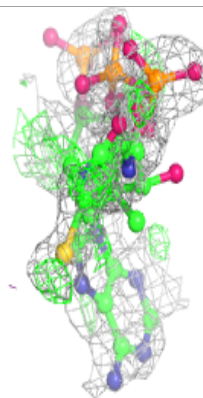
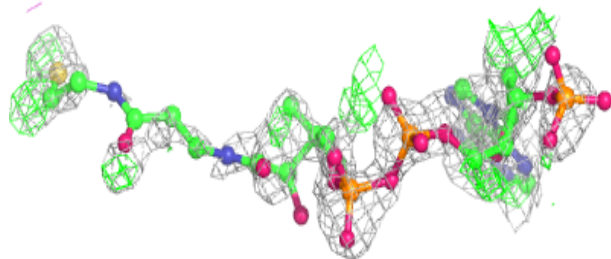
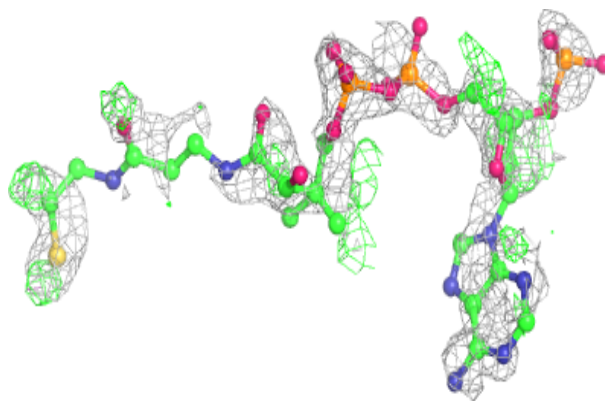
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	COA	D	401	47/48	0.57	0.29	45,58,64,67	47
2	COA	A	401[B]	48/48	0.85	0.20	32,54,68,70	48
2	COA	A	401[A]	48/48	0.85	0.20	28,33,57,58	48
4	NA	A	403	1/1	0.86	0.09	33,33,33,33	0
3	CA	C	403	1/1	0.88	0.12	37,37,37,37	0
2	COA	C	401[B]	48/48	0.90	0.21	39,76,97,98	48
2	COA	C	401[A]	48/48	0.90	0.21	16,19,31,33	48
4	NA	D	404	1/1	0.92	0.05	40,40,40,40	0
2	COA	B	401	48/48	0.94	0.12	19,27,49,51	0
3	CA	B	402	1/1	0.95	0.15	35,35,35,35	0
3	CA	B	403	1/1	0.96	0.26	46,46,46,46	0
3	CA	D	402	1/1	0.96	0.11	42,42,42,42	0
3	CA	A	402	1/1	0.98	0.12	35,35,35,35	0
3	CA	D	403	1/1	0.98	0.09	27,27,27,27	0
4	NA	D	405	1/1	0.98	0.07	21,21,21,21	0
3	CA	C	402	1/1	0.99	0.09	25,25,25,25	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.

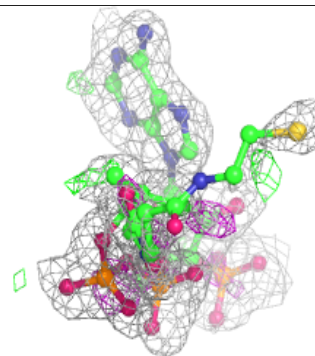
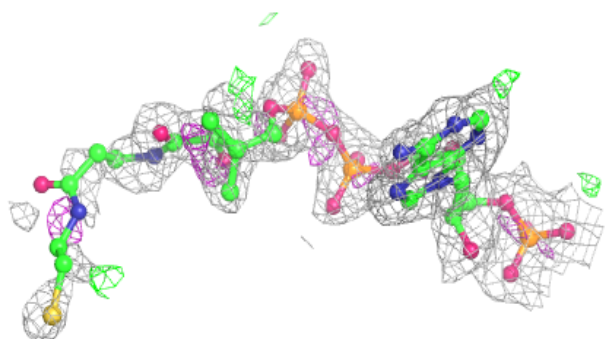
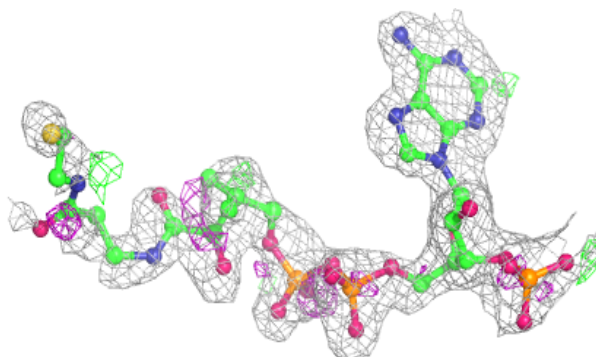


**Electron density around COA D 401:**

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

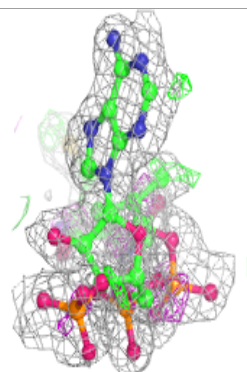
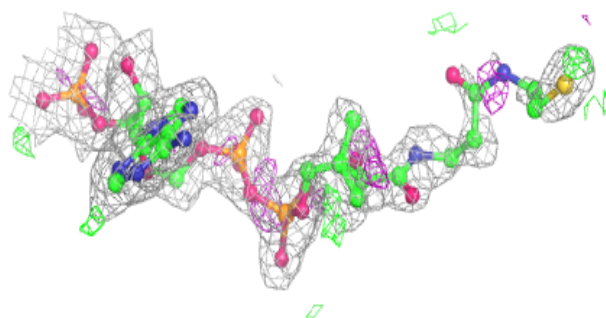
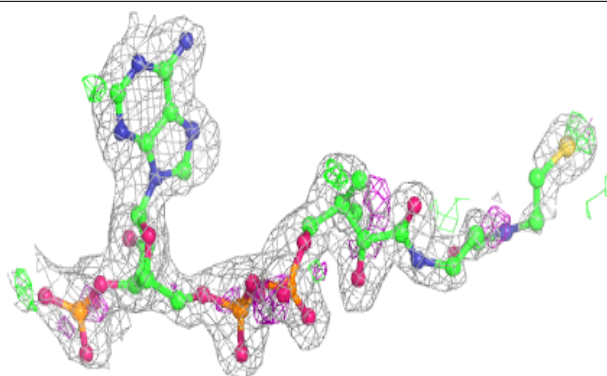
**Electron density around COA A 401 (B):**

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

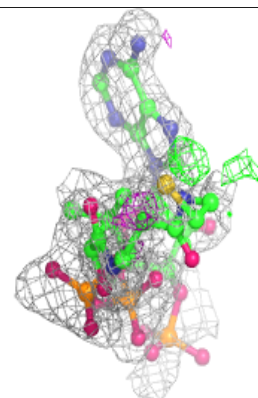
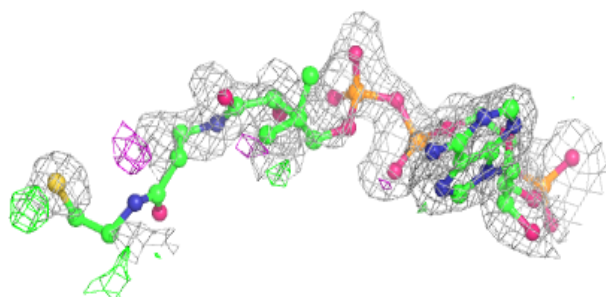
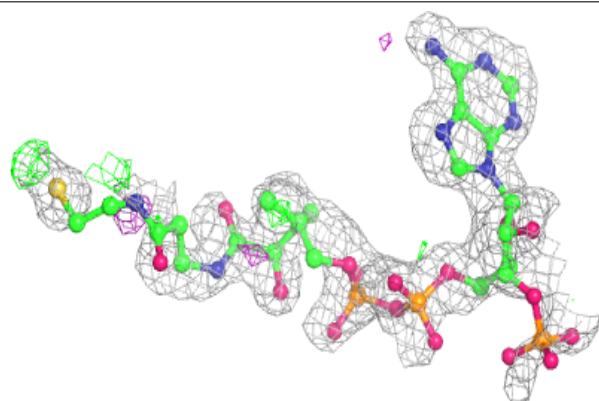


**Electron density around COA A 401 (A):**

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

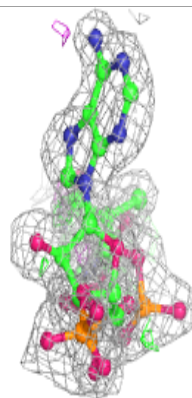
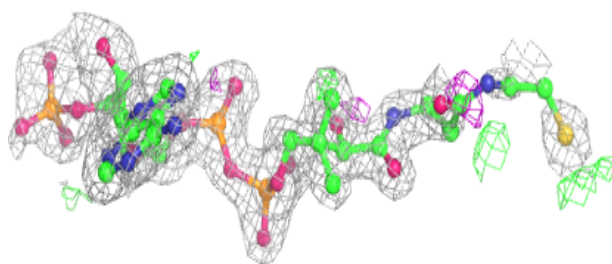
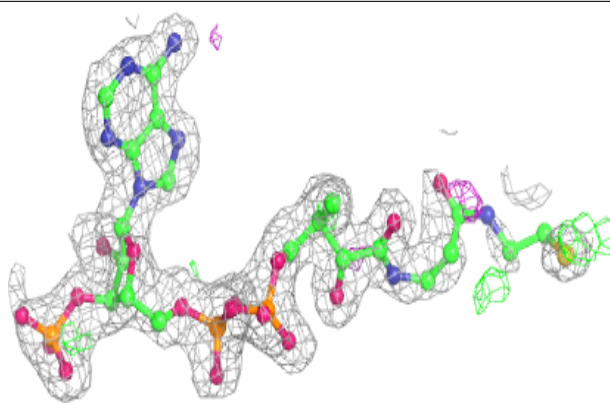
**Electron density around COA C 401 (B):**

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

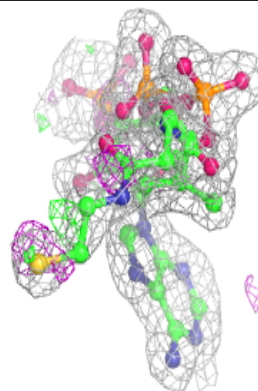
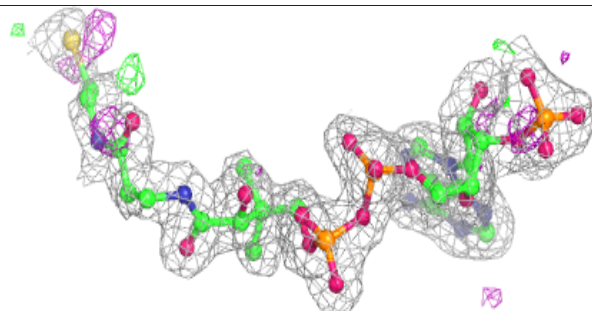
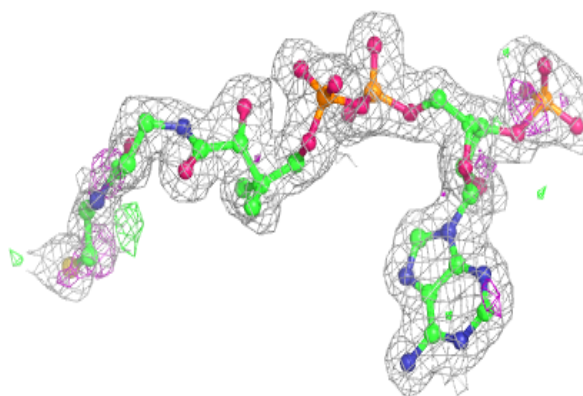


**Electron density around COA C 401 (A):**

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

**Electron density around COA B 401:**

$2mF_o-DF_c$  (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.