



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 1, 2024 – 12:52 am BST

PDB ID : 4B3J  
Title : Crystal structure of Mycobacterium tuberculosis fatty acid beta- oxidation complex with CoenzymeA bound at the hydratase and thiolase active sites  
Authors : Venkatesan, R.; Wierenga, R.K.  
Deposited on : 2012-07-24  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
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) : 2.36.2

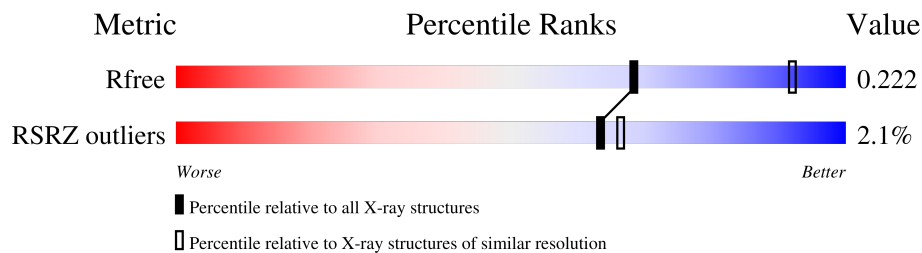
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 18116 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 FATTY ACID BETA-OXIDATION COMPLEX ALPHA-CHAIN FADB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	729	5463	3461	936	1043	23	0	8	0
1	B	726	5440	3447	933	1038	22	0	12	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP O53872
A	-14	GLY	-	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	-	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression tag	UNP O53872
A	0	SER	-	expression tag	UNP O53872
B	-15	MET	-	expression tag	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872

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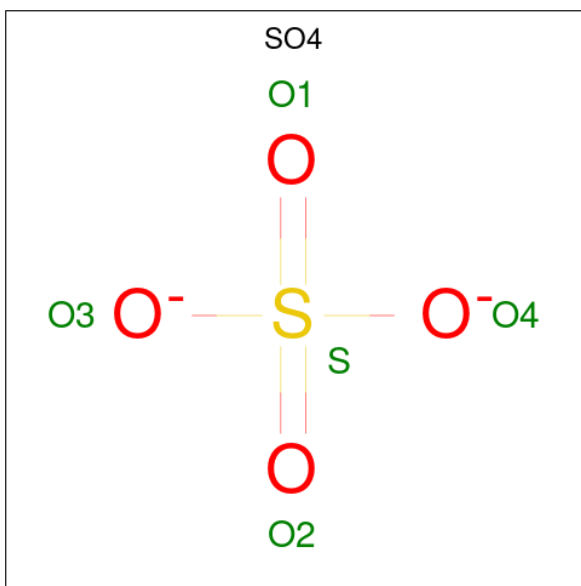
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP O53872
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called FATTY ACID BETA-OXIDATION COMPLEX BETA-CHAIN FADA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	402	2997	1876	529	577	15	0	6	0
2	D	400	2961	1848	524	573	16	0	4	0

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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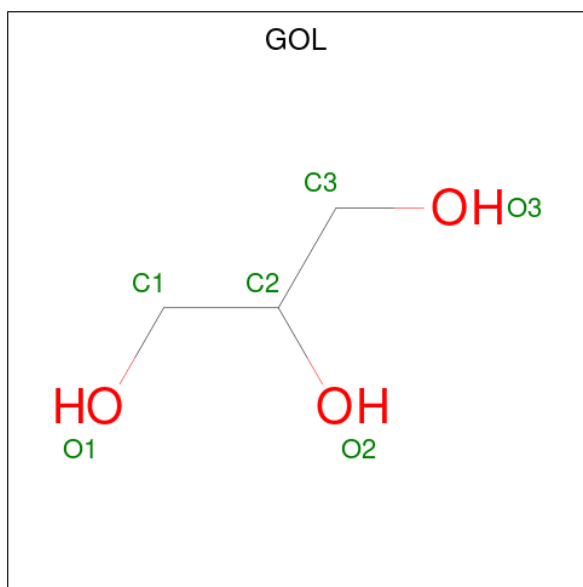
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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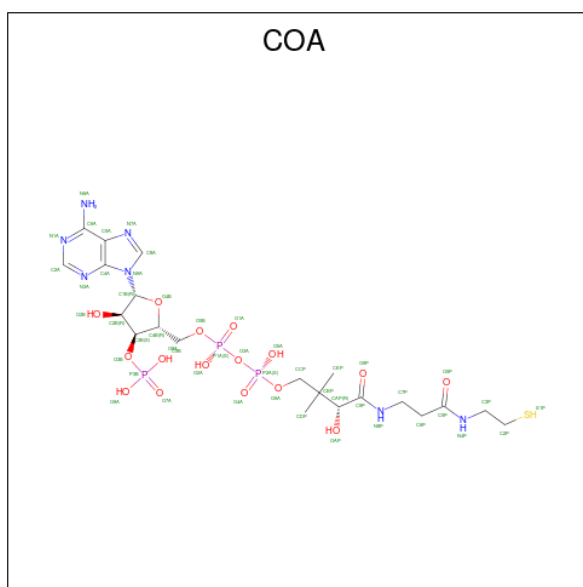
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



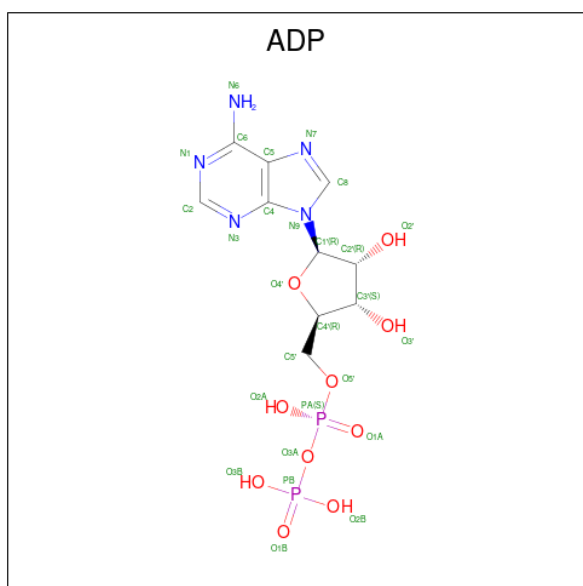
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	251	Total	O	0	0
			251	251		
7	B	284	Total	O	0	0
			284	284		
7	C	177	Total	O	0	0
			177	177		
7	D	125	Total	O	0	0
			125	125		

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### 3 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	248.30Å 135.25Å 118.58Å 90.00° 110.64° 90.00°	Depositor
Resolution (Å)	48.30 – 2.50 48.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.30-2.50) 99.7 (48.30-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.181 , 0.221 0.182 , 0.222	Depositor DCC
$R_{free}$ test set	6303 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

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

MolProbity failed to run properly - this section is therefore empty.

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

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

39 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	SO4	C	1404	-	4,4,4	0.30	0	6,6,6	0.39	0
4	GOL	C	1411	-	5,5,5	0.41	0	5,5,5	0.43	0
4	GOL	A	1730	-	5,5,5	0.23	0	5,5,5	0.36	0
3	SO4	D	1406	-	4,4,4	0.35	0	6,6,6	0.15	0
3	SO4	B	1725	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	B	1727	-	4,4,4	0.36	0	6,6,6	0.07	0
3	SO4	C	1410	-	4,4,4	0.37	0	6,6,6	0.24	0
5	COA	C	1412	-	41,50,50	0.84	1 (2%)	52,75,75	1.22	4 (7%)
3	SO4	D	1405	-	4,4,4	0.34	0	6,6,6	0.16	0
3	SO4	C	1406	-	4,4,4	0.36	0	6,6,6	0.19	0
5	COA	B	1730	-	41,50,50	0.83	1 (2%)	52,75,75	1.22	5 (9%)
3	SO4	C	1405	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	B	1728	-	4,4,4	0.36	0	6,6,6	0.13	0
4	GOL	A	1729	-	5,5,5	0.34	0	5,5,5	0.15	0
3	SO4	A	1724	-	4,4,4	0.35	0	6,6,6	0.17	0
4	GOL	A	1727	-	5,5,5	0.36	0	5,5,5	0.16	0
6	ADP	C	1413	-	24,29,29	1.08	2 (8%)	29,45,45	1.34	4 (13%)
3	SO4	B	1726	-	4,4,4	0.31	0	6,6,6	0.27	0
3	SO4	A	1722	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	B	1724	-	4,4,4	0.35	0	6,6,6	0.11	0
3	SO4	A	1721	-	4,4,4	0.41	0	6,6,6	0.16	0
3	SO4	C	1409	-	4,4,4	0.39	0	6,6,6	0.22	0
5	COA	D	1409	-	41,50,50	0.83	1 (2%)	52,75,75	1.16	3 (5%)
3	SO4	A	1726	-	4,4,4	0.34	0	6,6,6	0.17	0
3	SO4	B	1721	-	4,4,4	0.30	0	6,6,6	0.24	0
3	SO4	B	1722	-	4,4,4	0.39	0	6,6,6	0.14	0
3	SO4	A	1723	-	4,4,4	0.33	0	6,6,6	0.10	0
4	GOL	A	1728	-	5,5,5	0.38	0	5,5,5	0.21	0
3	SO4	B	1723	-	4,4,4	0.40	0	6,6,6	0.16	0
3	SO4	D	1408	-	4,4,4	0.33	0	6,6,6	0.11	0
5	COA	A	1731	-	41,50,50	0.83	2 (4%)	52,75,75	1.11	5 (9%)
4	GOL	D	1411	-	5,5,5	0.45	0	5,5,5	0.49	0
3	SO4	D	1407	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	C	1407	-	4,4,4	0.36	0	6,6,6	0.09	0
6	ADP	D	1410	-	24,29,29	1.07	3 (12%)	29,45,45	1.46	4 (13%)
3	SO4	A	1725	-	4,4,4	0.35	0	6,6,6	0.10	0
3	SO4	D	1404	-	4,4,4	0.32	0	6,6,6	0.30	0
3	SO4	C	1408	-	4,4,4	0.35	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	1729	-	5,5,5	0.43	0	5,5,5	0.59	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
4	GOL	C	1411	-	-	2/4/4/4	-
5	COA	D	1409	-	-	22/44/64/64	0/3/3/3
4	GOL	A	1730	-	-	2/4/4/4	-
5	COA	A	1731	-	-	13/44/64/64	0/3/3/3
4	GOL	D	1411	-	-	4/4/4/4	-
5	COA	B	1730	-	-	27/44/64/64	0/3/3/3
6	ADP	D	1410	-	-	8/12/32/32	0/3/3/3
4	GOL	A	1729	-	-	0/4/4/4	-
4	GOL	A	1728	-	-	2/4/4/4	-
4	GOL	A	1727	-	-	4/4/4/4	-
6	ADP	C	1413	-	-	0/12/32/32	0/3/3/3
5	COA	C	1412	-	-	23/44/64/64	0/3/3/3
4	GOL	B	1729	-	-	1/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1413	ADP	C5-C4	2.77	1.48	1.40
6	D	1410	ADP	C5-C4	2.76	1.48	1.40
6	C	1413	ADP	O4'-C1'	2.59	1.44	1.41
5	B	1730	COA	C5A-C4A	2.56	1.47	1.40
5	A	1731	COA	C5A-C4A	2.47	1.47	1.40

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1410	ADP	C3'-C2'-C1'	4.11	107.17	100.98
5	B	1730	COA	P2A-O3A-P1A	-3.83	119.68	132.83
6	D	1410	ADP	N3-C2-N1	-3.66	122.95	128.68
5	A	1731	COA	N3A-C2A-N1A	-3.63	123.00	128.68
6	C	1413	ADP	N3-C2-N1	-3.50	123.20	128.68

There are no chirality outliers.

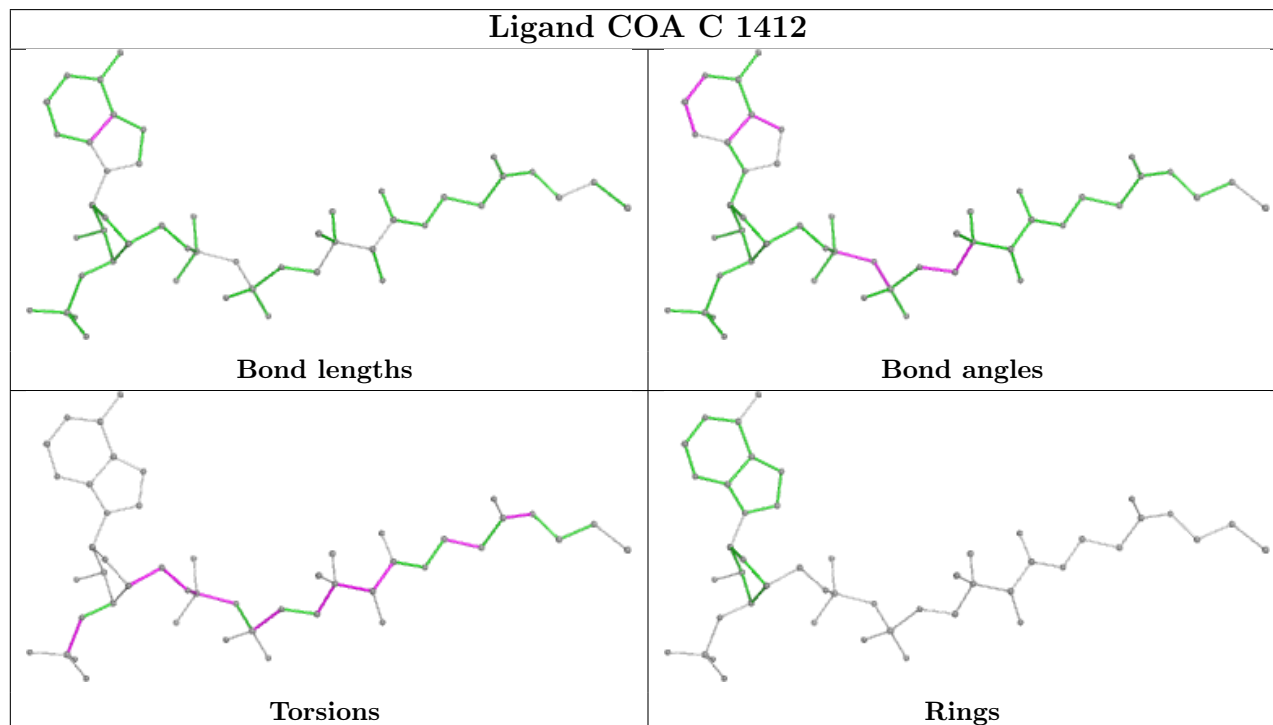
5 of 108 torsion outliers are listed below:

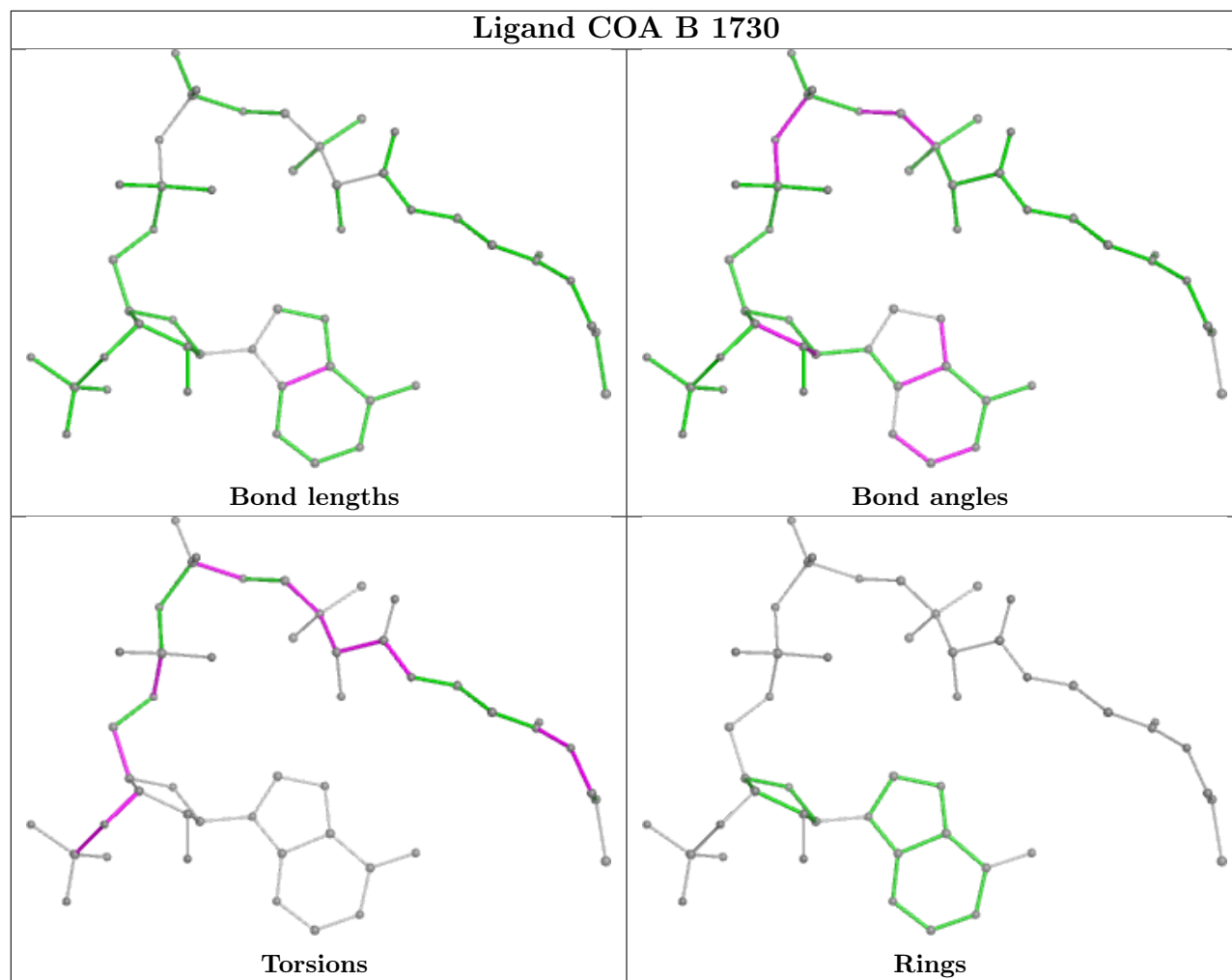
Mol	Chain	Res	Type	Atoms
4	A	1727	GOL	O1-C1-C2-C3
4	A	1727	GOL	C1-C2-C3-O3
4	A	1727	GOL	O2-C2-C3-O3
4	C	1411	GOL	O1-C1-C2-C3
4	D	1411	GOL	C1-C2-C3-O3

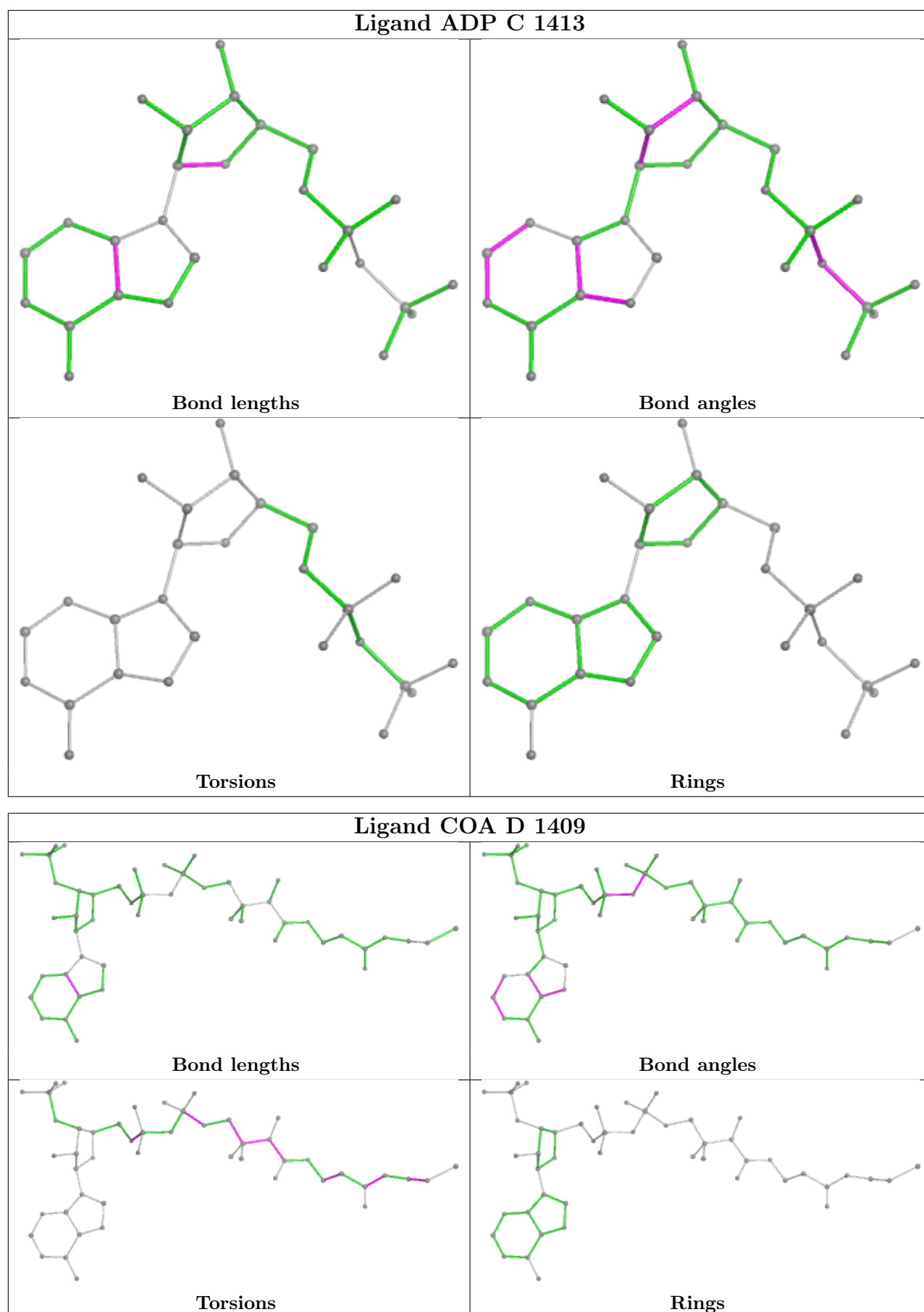
There are no ring outliers.

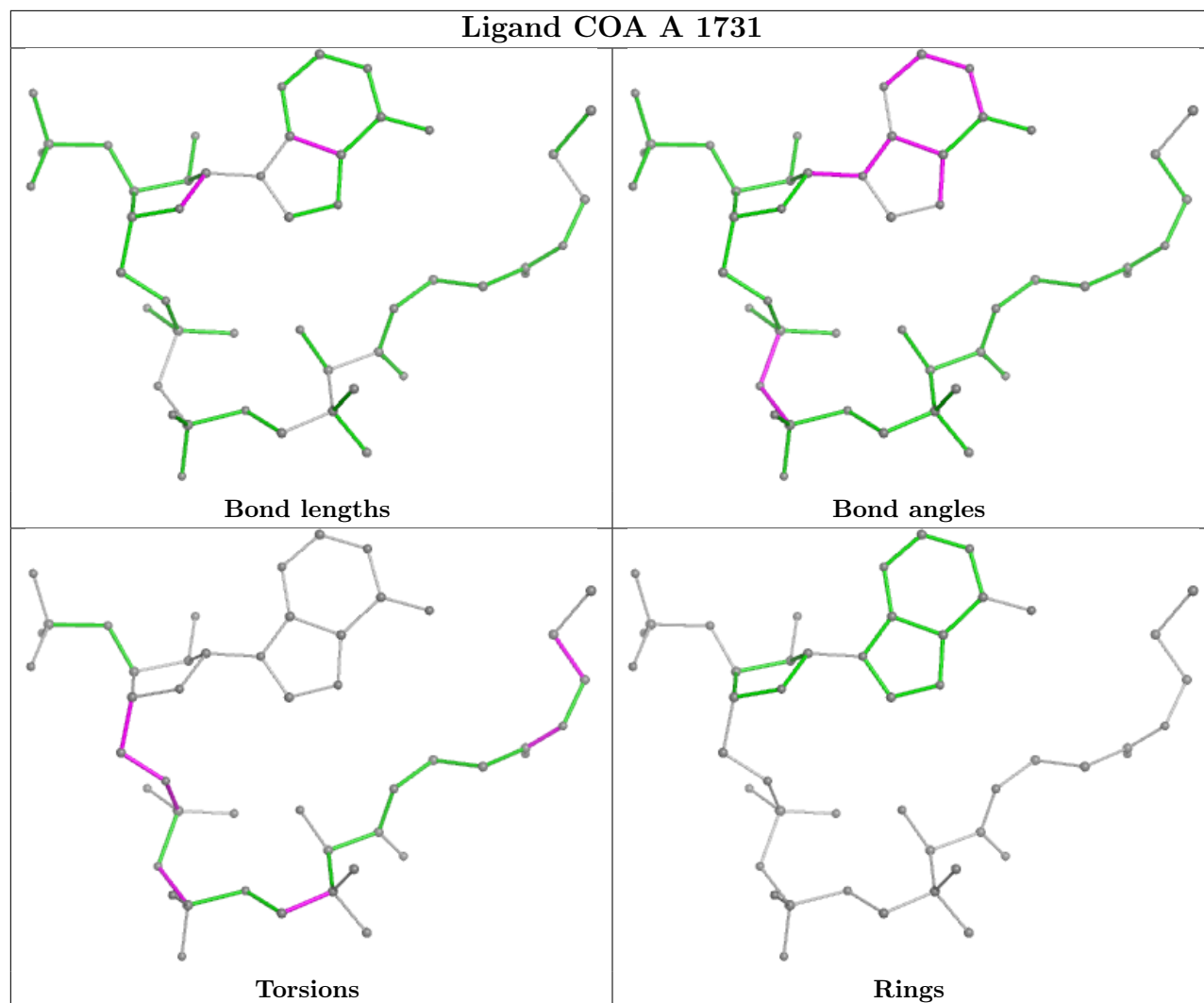
No monomer is involved in short contacts.

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.

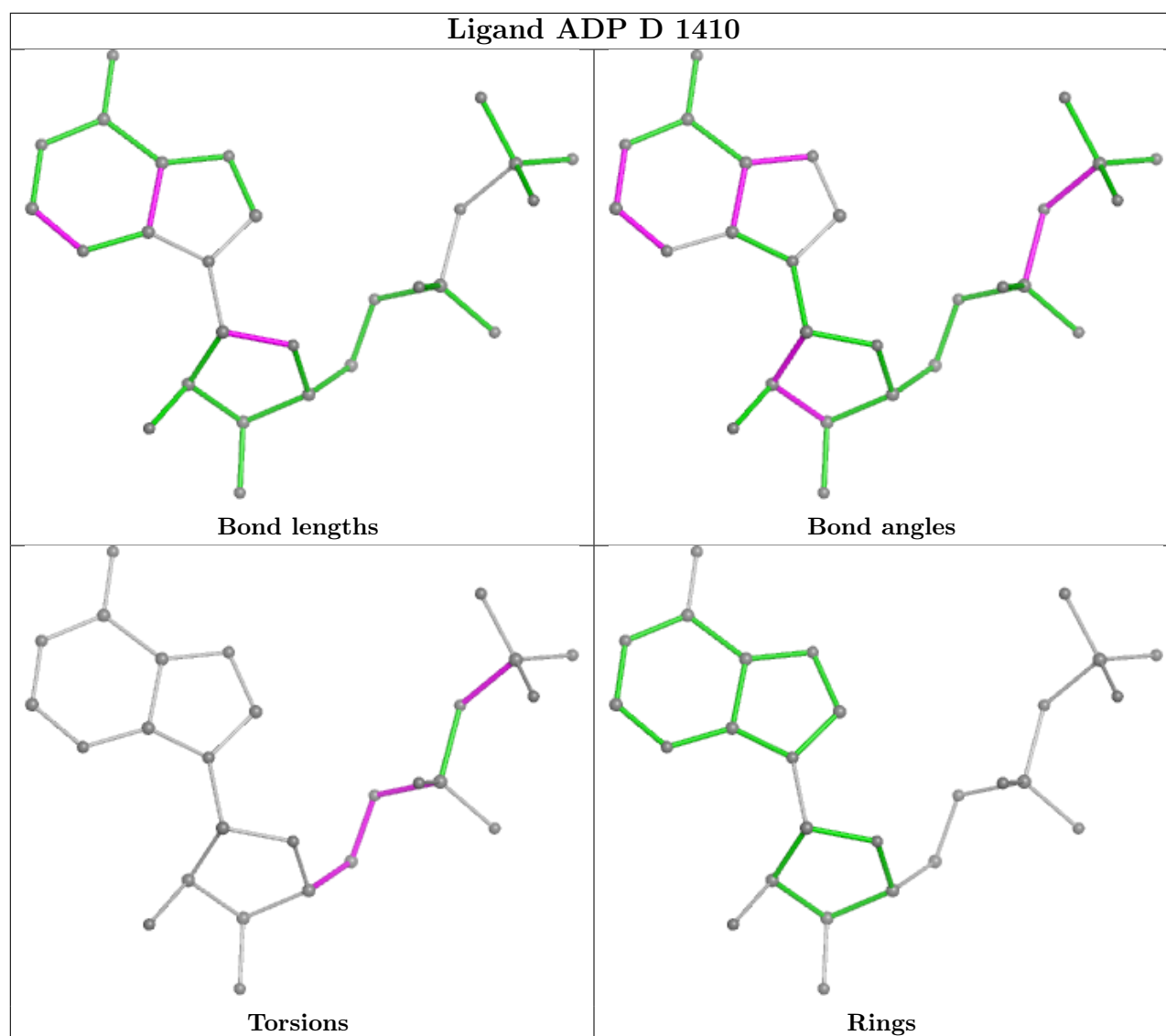












#### 4.7 Other polymers [i](#)

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, 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	729/736 (99%)	-0.18	15 (2%) 63 66	19, 39, 62, 99	0
1	B	726/736 (98%)	-0.22	16 (2%) 62 65	19, 34, 64, 99	0
2	C	402/403 (99%)	-0.14	7 (1%) 70 72	19, 29, 57, 96	0
2	D	400/403 (99%)	-0.09	10 (2%) 57 61	20, 31, 65, 98	0
All	All	2257/2278 (99%)	-0.17	48 (2%) 63 66	19, 35, 63, 99	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	230	ALA	5.5
2	D	231	LEU	4.8
1	A	-6	HIS	4.0
2	C	229	ALA	4.0
2	D	1	MET	3.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates [i](#)

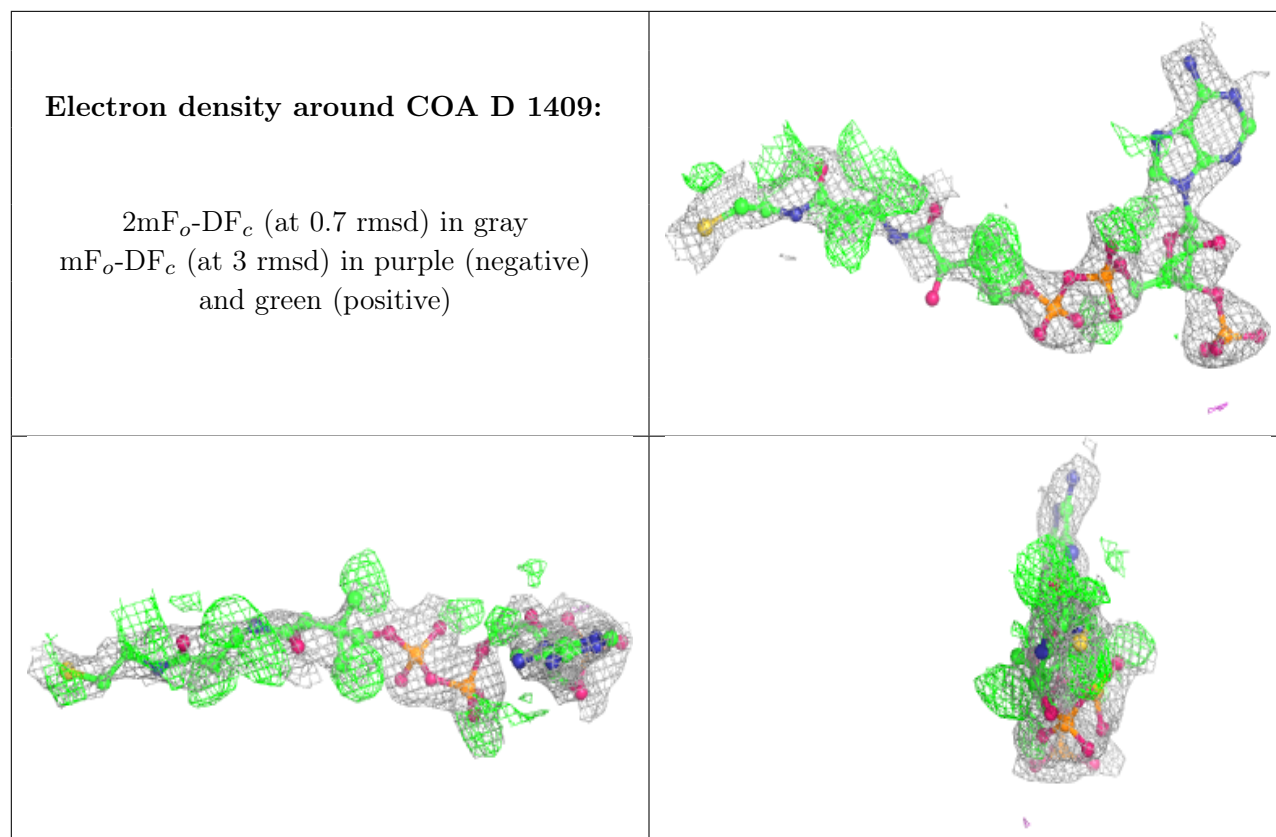
There are no monosaccharides in this entry.

### 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, 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.

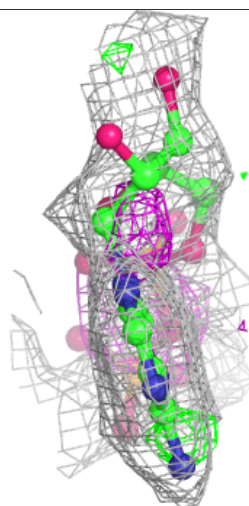
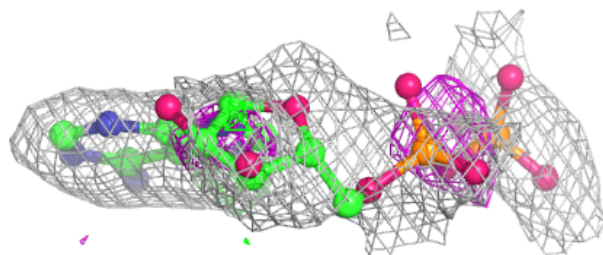
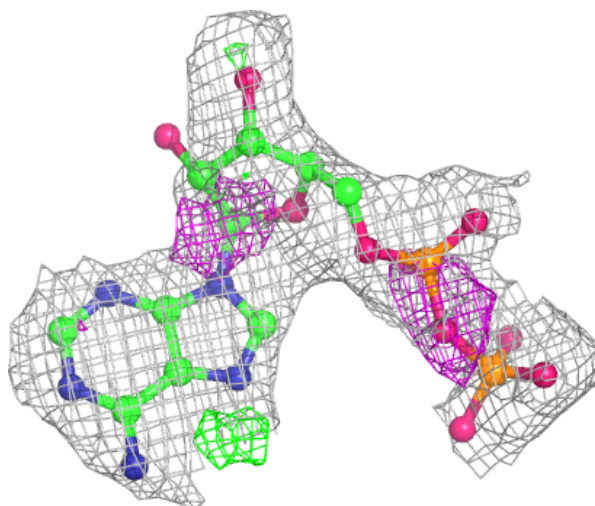
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	COA	D	1409	48/48	0.69	0.36	40,44,46,49	48
6	ADP	D	1410	27/27	0.73	0.30	60,92,132,135	0
3	SO4	B	1726	5/5	0.77	0.32	65,65,66,67	5
6	ADP	C	1413	27/27	0.81	0.24	48,80,133,138	0
5	COA	B	1730	48/48	0.83	0.30	41,50,57,57	48
4	GOL	D	1411	6/6	0.84	0.33	37,37,39,40	0
3	SO4	A	1724	5/5	0.84	0.23	65,65,68,68	5
5	COA	C	1412	48/48	0.84	0.25	32,38,46,51	48
3	SO4	B	1727	5/5	0.86	0.30	63,64,66,67	5
5	COA	A	1731	48/48	0.87	0.24	37,45,53,62	48
4	GOL	A	1728	6/6	0.87	0.22	50,55,55,56	0
3	SO4	B	1725	5/5	0.87	0.20	51,51,52,53	5
4	GOL	C	1411	6/6	0.90	0.28	50,53,54,55	0
3	SO4	D	1408	5/5	0.90	0.12	80,81,84,84	5
4	GOL	A	1727	6/6	0.90	0.24	48,52,53,55	0
3	SO4	C	1410	5/5	0.90	0.18	65,67,70,73	0
3	SO4	A	1726	5/5	0.91	0.36	62,62,64,64	5
3	SO4	B	1728	5/5	0.91	0.18	40,40,42,42	5
3	SO4	B	1724	5/5	0.91	0.27	65,66,67,68	5
4	GOL	B	1729	6/6	0.91	0.20	41,46,47,48	0
3	SO4	C	1408	5/5	0.92	0.34	51,54,55,55	5
3	SO4	C	1406	5/5	0.92	0.20	73,73,75,77	0
3	SO4	C	1409	5/5	0.93	0.32	39,40,41,41	5
4	GOL	A	1730	6/6	0.94	0.17	23,23,24,24	6
3	SO4	A	1725	5/5	0.95	0.12	73,74,78,79	0
3	SO4	D	1404	5/5	0.95	0.10	59,61,65,65	0
3	SO4	A	1723	5/5	0.95	0.20	76,76,78,78	0
3	SO4	B	1722	5/5	0.96	0.12	54,57,59,59	0
4	GOL	A	1729	6/6	0.96	0.21	49,51,54,56	0
3	SO4	D	1406	5/5	0.97	0.27	63,65,66,66	0
3	SO4	B	1723	5/5	0.97	0.10	62,63,66,66	0
3	SO4	C	1407	5/5	0.97	0.25	72,72,74,74	0
3	SO4	A	1722	5/5	0.97	0.12	48,49,50,51	0
3	SO4	D	1405	5/5	0.97	0.27	63,66,67,69	0
3	SO4	C	1404	5/5	0.98	0.11	46,47,50,50	0
3	SO4	C	1405	5/5	0.98	0.25	57,58,59,60	0
3	SO4	B	1721	5/5	0.98	0.10	39,40,40,41	0
3	SO4	A	1721	5/5	0.98	0.13	44,46,47,47	0
3	SO4	D	1407	5/5	0.99	0.24	62,63,64,64	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.



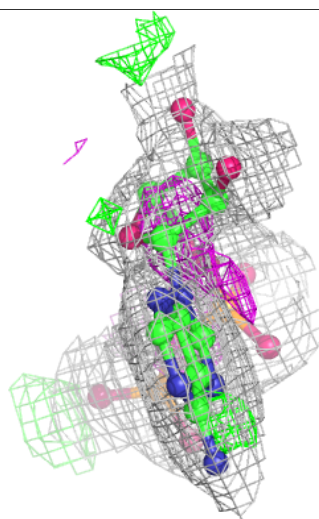
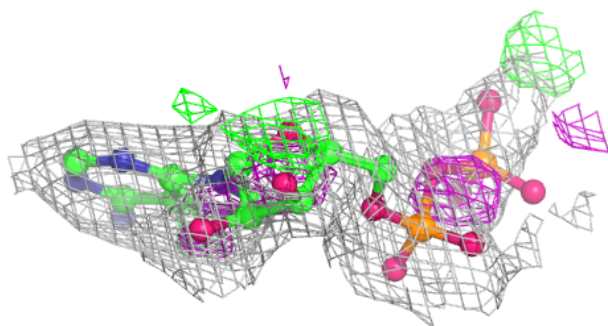
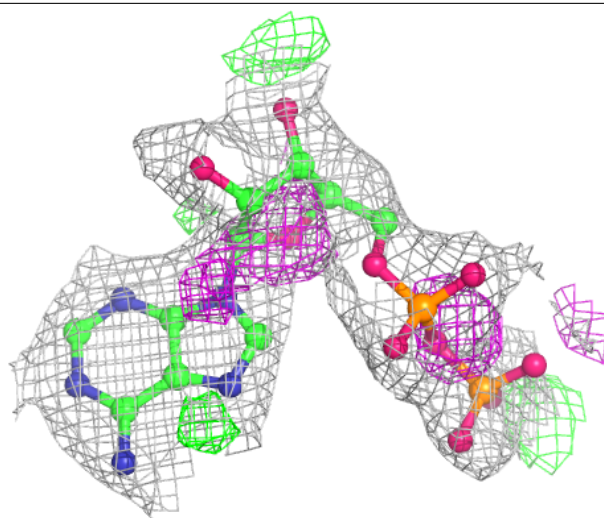
**Electron density around ADP D 1410:**

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



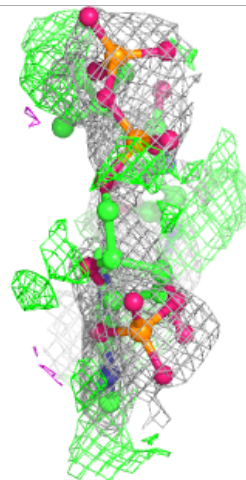
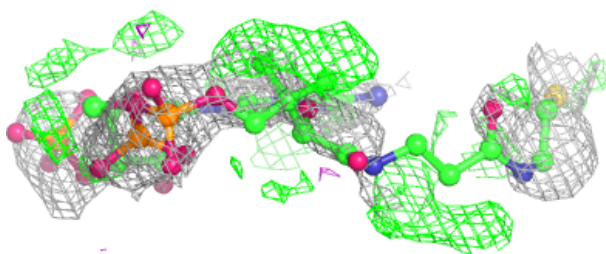
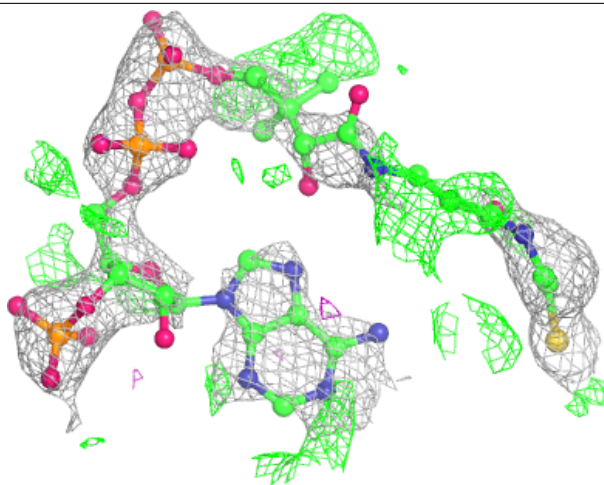
**Electron density around ADP C 1413:**

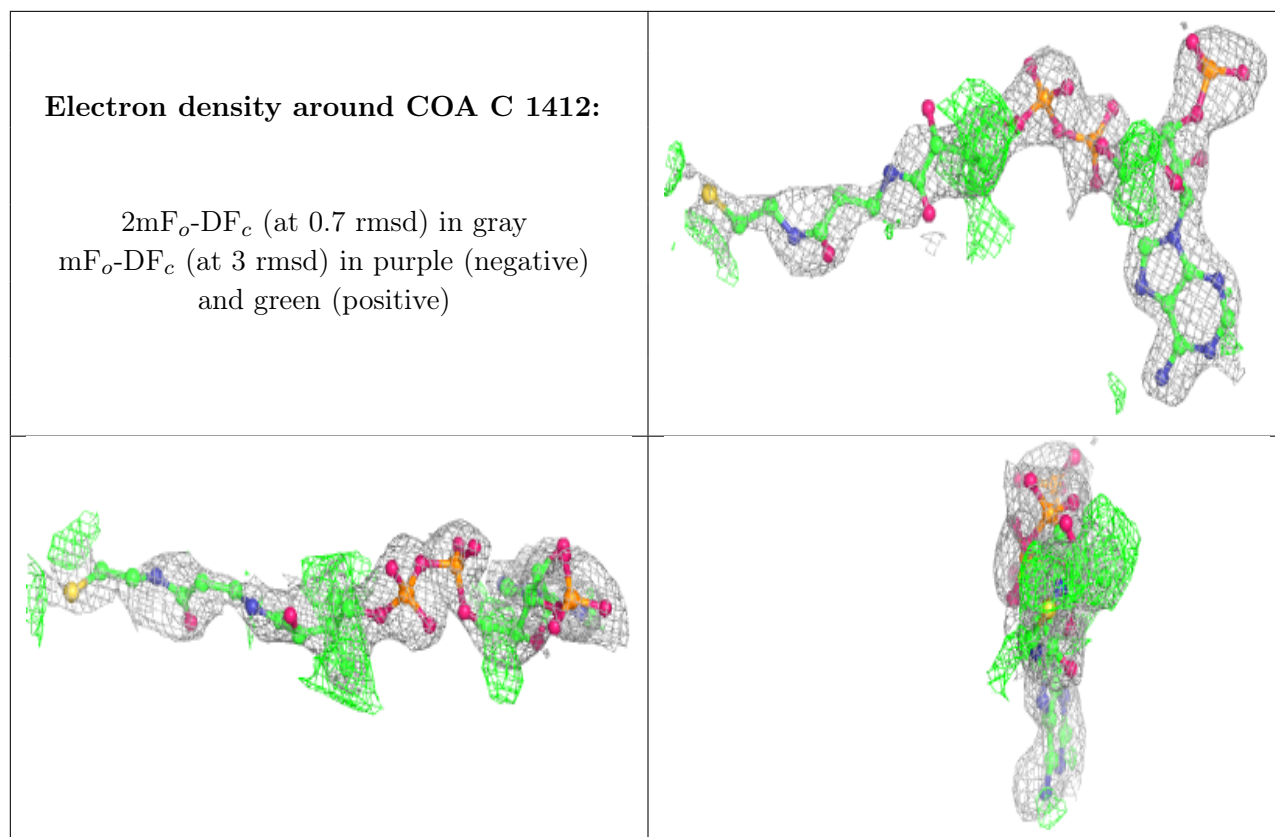
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



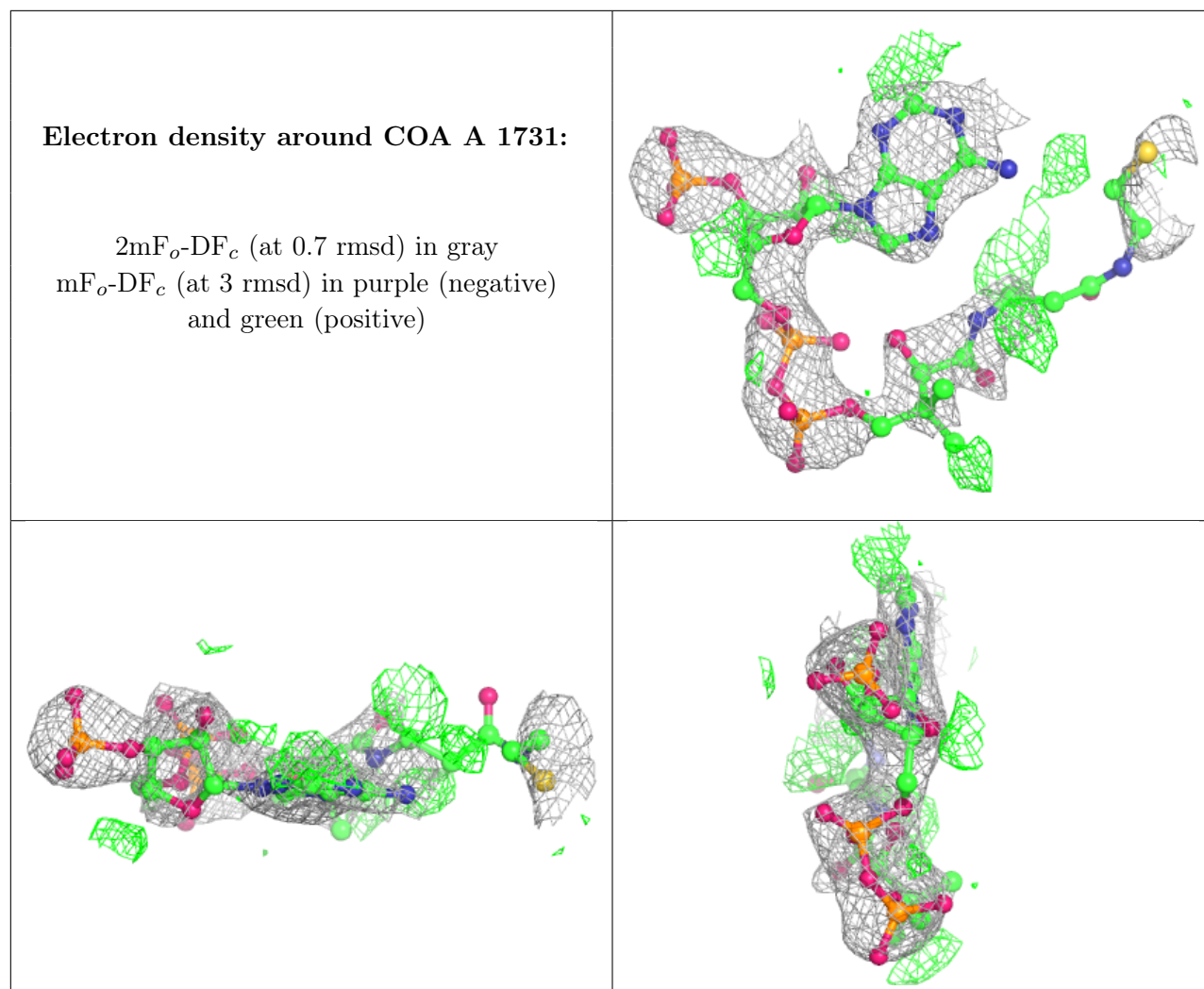
**Electron density around COA B 1730:**

$2mF_o-DF_c$  (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.