



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 13, 2025 – 06:10 PM JST

PDB ID : 8XXF  
Title : TtCS, oxaloacetate, acetyl-CoA complex  
Authors : Yang, L.; Fang, Y.J.  
Deposited on : 2024-01-18  
Resolution : 2.33 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

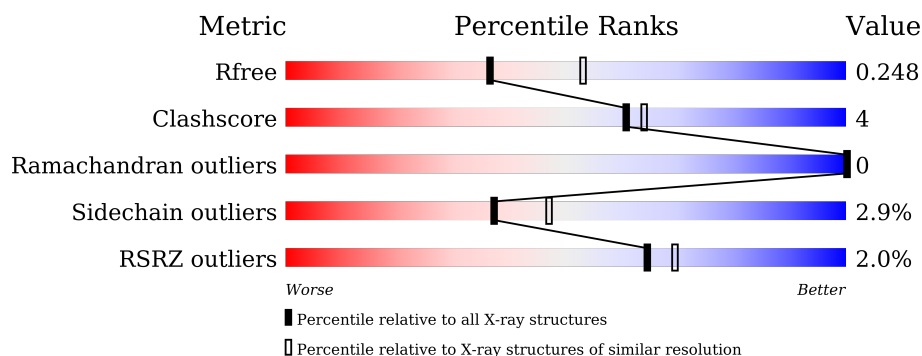
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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))
$R_{free}$	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	449	<div> <div>7%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	B	449	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	C	449	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	D	449	<div> <div></div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	E	449	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	F	449	<div> <div></div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22326 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	435	Total	C	N	O	S	0	0	0
			3502	2254	599	628	21			
1	B	449	Total	C	N	O	S	0	0	0
			3592	2309	616	646	21			
1	C	442	Total	C	N	O	S	0	0	0
			3537	2274	605	637	21			
1	D	440	Total	C	N	O	S	0	1	0
			3545	2280	610	634	21			
1	E	441	Total	C	N	O	S	0	0	0
			3531	2271	604	635	21			
1	F	441	Total	C	N	O	S	0	0	0
			3541	2277	608	635	21			

There are 42 discrepancies between the modelled and reference sequences:

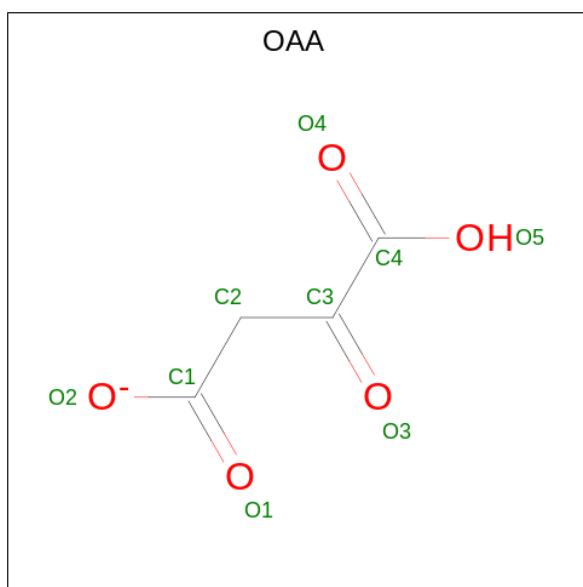
Chain	Residue	Modelled	Actual	Comment	Reference
A	443	LYS	-	expression tag	UNP A0A0S3QTD0
A	444	LEU	-	expression tag	UNP A0A0S3QTD0
A	445	ALA	-	expression tag	UNP A0A0S3QTD0
A	446	ALA	-	expression tag	UNP A0A0S3QTD0
A	447	ALA	-	expression tag	UNP A0A0S3QTD0
A	448	LEU	-	expression tag	UNP A0A0S3QTD0
A	449	GLU	-	expression tag	UNP A0A0S3QTD0
B	443	LYS	-	expression tag	UNP A0A0S3QTD0
B	444	LEU	-	expression tag	UNP A0A0S3QTD0
B	445	ALA	-	expression tag	UNP A0A0S3QTD0
B	446	ALA	-	expression tag	UNP A0A0S3QTD0
B	447	ALA	-	expression tag	UNP A0A0S3QTD0
B	448	LEU	-	expression tag	UNP A0A0S3QTD0
B	449	GLU	-	expression tag	UNP A0A0S3QTD0
C	443	LYS	-	expression tag	UNP A0A0S3QTD0
C	444	LEU	-	expression tag	UNP A0A0S3QTD0
C	445	ALA	-	expression tag	UNP A0A0S3QTD0

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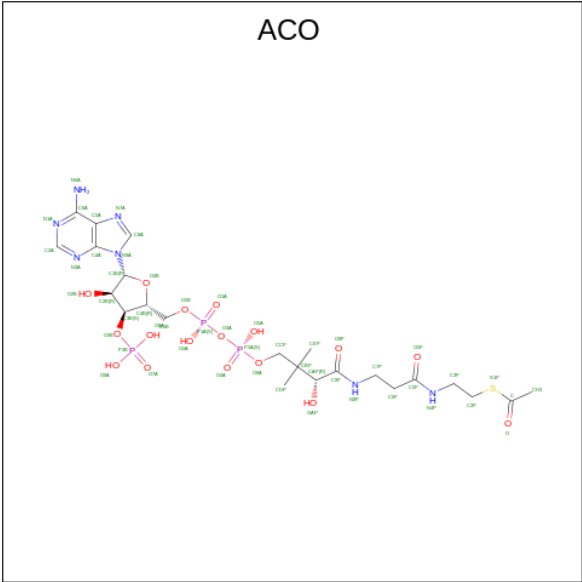
Chain	Residue	Modelled	Actual	Comment	Reference
C	446	ALA	-	expression tag	UNP A0A0S3QTD0
C	447	ALA	-	expression tag	UNP A0A0S3QTD0
C	448	LEU	-	expression tag	UNP A0A0S3QTD0
C	449	GLU	-	expression tag	UNP A0A0S3QTD0
D	443	LYS	-	expression tag	UNP A0A0S3QTD0
D	444	LEU	-	expression tag	UNP A0A0S3QTD0
D	445	ALA	-	expression tag	UNP A0A0S3QTD0
D	446	ALA	-	expression tag	UNP A0A0S3QTD0
D	447	ALA	-	expression tag	UNP A0A0S3QTD0
D	448	LEU	-	expression tag	UNP A0A0S3QTD0
D	449	GLU	-	expression tag	UNP A0A0S3QTD0
E	443	LYS	-	expression tag	UNP A0A0S3QTD0
E	444	LEU	-	expression tag	UNP A0A0S3QTD0
E	445	ALA	-	expression tag	UNP A0A0S3QTD0
E	446	ALA	-	expression tag	UNP A0A0S3QTD0
E	447	ALA	-	expression tag	UNP A0A0S3QTD0
E	448	LEU	-	expression tag	UNP A0A0S3QTD0
E	449	GLU	-	expression tag	UNP A0A0S3QTD0
F	443	LYS	-	expression tag	UNP A0A0S3QTD0
F	444	LEU	-	expression tag	UNP A0A0S3QTD0
F	445	ALA	-	expression tag	UNP A0A0S3QTD0
F	446	ALA	-	expression tag	UNP A0A0S3QTD0
F	447	ALA	-	expression tag	UNP A0A0S3QTD0
F	448	LEU	-	expression tag	UNP A0A0S3QTD0
F	449	GLU	-	expression tag	UNP A0A0S3QTD0

- Molecule 2 is OXALOACETATE ION (three-letter code: OAA) (formula:  $C_4H_3O_5$ ) (labeled as "Ligand of Interest" by depositor).



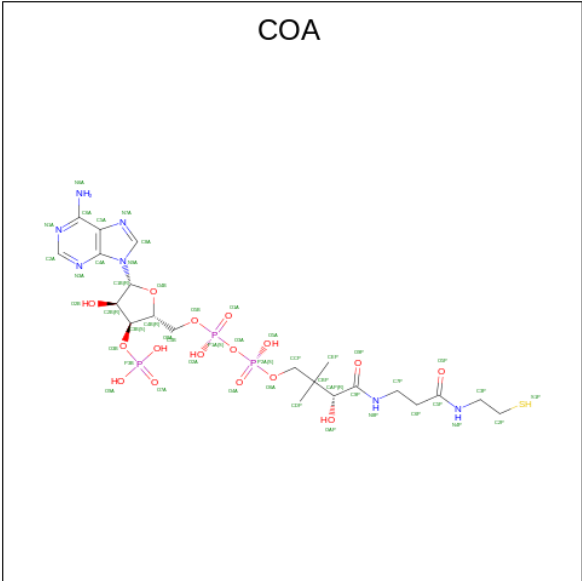
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		
2	E	1	Total	C	O	0	0
			9	4	5		
2	F	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 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) (labeled as "Ligand of Interest" by depositor).



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

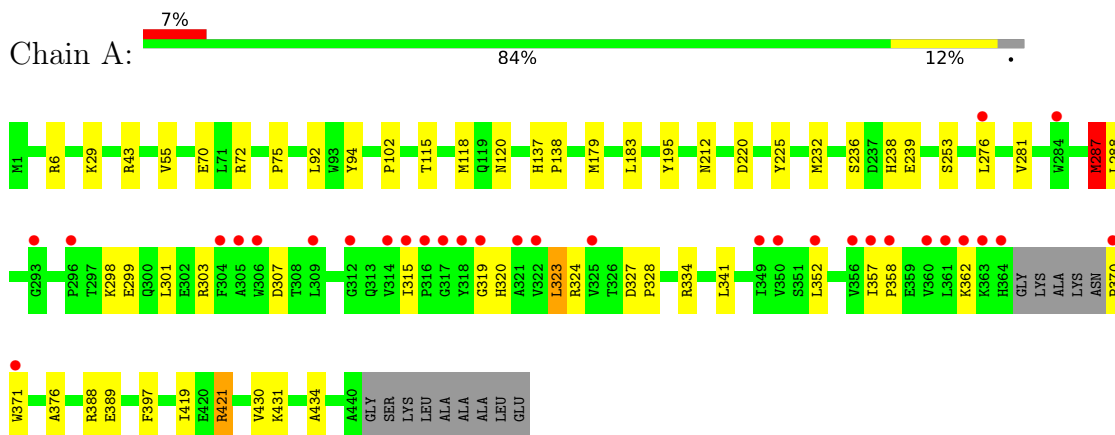
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total 117	O 117	0	0
5	B	152	Total 152	O 152	0	0
5	C	136	Total 136	O 136	0	0
5	D	164	Total 164	O 164	0	0
5	E	147	Total 147	O 147	0	0
5	F	167	Total 167	O 167	0	0

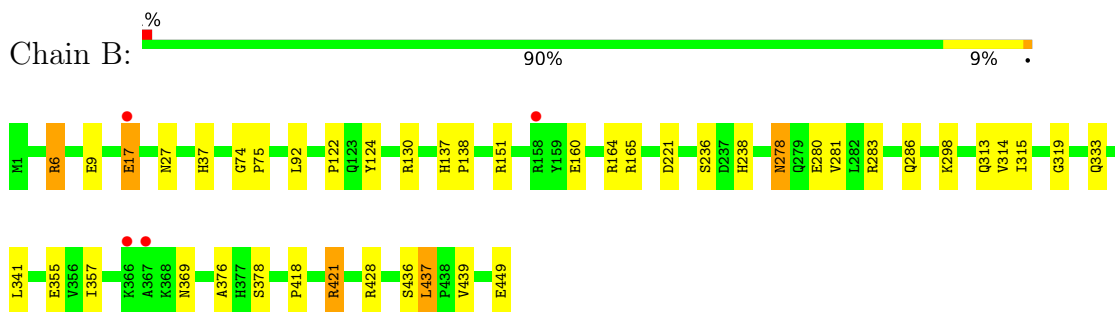
### 3 Residue-property plots

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.

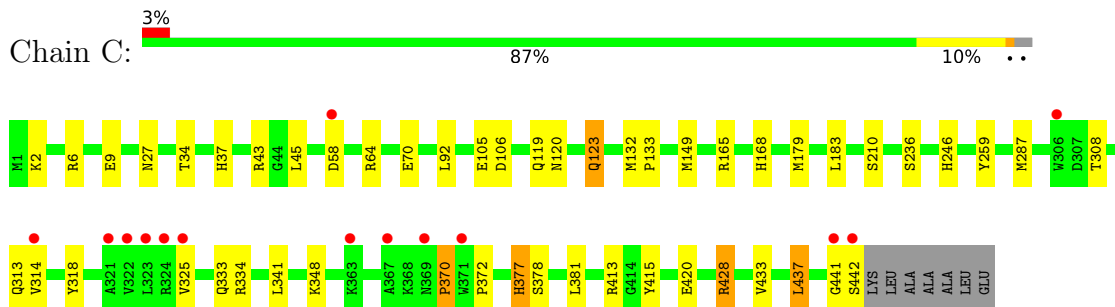
- Molecule 1: Citrate synthase




- Molecule 1: Citrate synthase

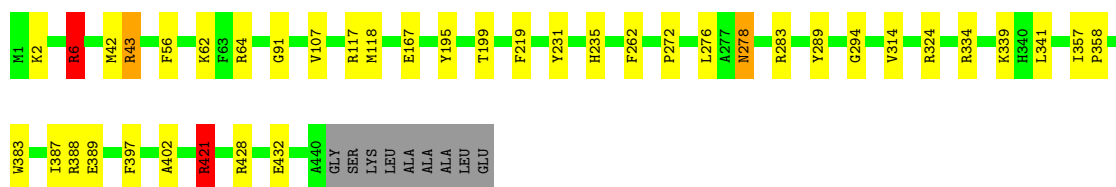


- Molecule 1: Citrate synthase




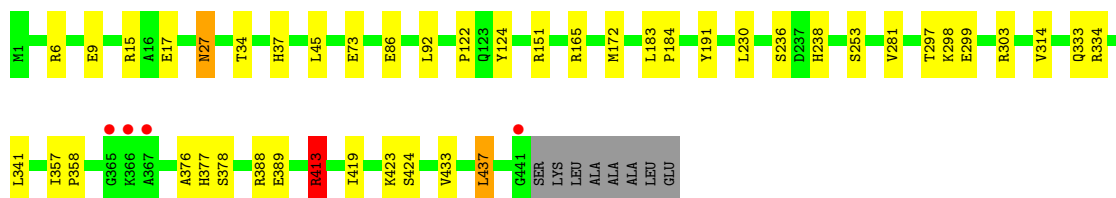
- Molecule 1: Citrate synthase

Chain D:  89% 8% .




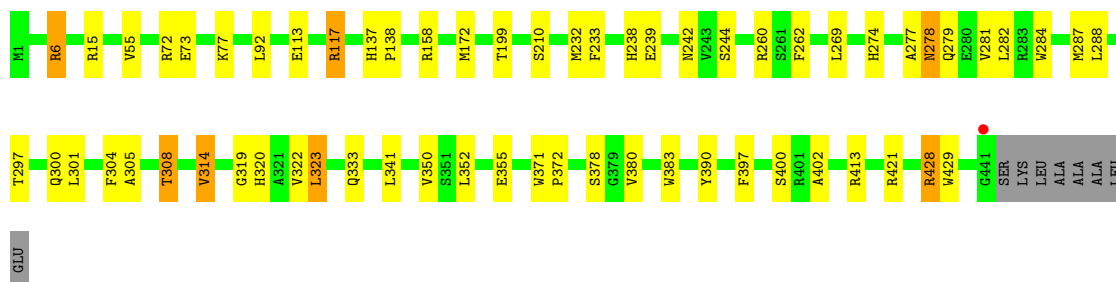
• Molecule 1: Citrate synthase

Chain E:  88% 9% .



• Molecule 1: Citrate synthase

Chain F:  84% 12% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.49Å 131.76Å 207.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.15 – 2.33 30.15 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.15-2.33) 99.9 (30.15-2.33)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.187 , 0.245 0.194 , 0.248	Depositor DCC
$R_{free}$ test set	6296 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22326	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, ACO, COA

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	0.41	0/3597	0.89	3/4875 (0.1%)
1	B	0.44	0/3688	0.89	4/4999 (0.1%)
1	C	0.44	0/3633	0.90	7/4926 (0.1%)
1	D	0.44	0/3644	0.89	9/4938 (0.2%)
1	E	0.43	0/3627	0.88	1/4918 (0.0%)
1	F	0.44	0/3637	0.93	8/4929 (0.2%)
All	All	0.44	0/21826	0.89	32/29585 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	D	0	4
1	E	0	5
1	F	0	3
All	All	0	17

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	260	ARG	NE-CZ-NH1	11.45	126.02	120.30
1	B	151	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	A	287	MET	CG-SD-CE	7.89	112.82	100.20
1	D	6	ARG	CG-CD-NE	-7.08	96.94	111.80
1	E	413	ARG	NE-CZ-NH2	-6.68	116.96	120.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ARG	Sidechain
1	A	388	ARG	Sidechain
1	A	421	ARG	Sidechain
1	A	6	ARG	Sidechain
1	A	72	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3502	0	3459	37	0
1	B	3592	0	3552	24	0
1	C	3537	0	3485	31	0
1	D	3545	0	3512	22	0
1	E	3531	0	3480	25	0
1	F	3541	0	3502	40	0
2	A	9	0	2	0	0
2	B	9	0	2	1	0
2	D	9	0	2	0	0
2	E	9	0	2	1	0
2	F	9	0	2	3	0
3	A	51	0	34	15	0
3	F	51	0	34	7	0
4	D	48	0	32	1	0
5	A	117	0	0	2	0
5	B	152	0	0	6	0
5	C	136	0	0	6	0
5	D	164	0	0	2	0
5	E	147	0	0	2	0
5	F	167	0	0	0	0
All	All	22326	0	21100	175	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.

The worst 5 of 175 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:D:167:GLU:HG3	5:D:755:HOH:O	1.55	1.06
1:A:43:ARG:HH11	3:A:502:ACO:CCP	1.70	1.05
3:A:502:ACO:H72	3:A:502:ACO:H21	1.38	1.04
1:C:2:LYS:HB3	5:C:614:HOH:O	1.59	1.01
1:A:43:ARG:HH11	3:A:502:ACO:H121	1.34	0.90

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	431/449 (96%)	419 (97%)	12 (3%)	0	100	100
1	B	447/449 (100%)	439 (98%)	8 (2%)	0	100	100
1	C	440/449 (98%)	425 (97%)	15 (3%)	0	100	100
1	D	439/449 (98%)	429 (98%)	10 (2%)	0	100	100
1	E	439/449 (98%)	429 (98%)	10 (2%)	0	100	100
1	F	439/449 (98%)	428 (98%)	11 (2%)	0	100	100
All	All	2635/2694 (98%)	2569 (98%)	66 (2%)	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	368/376 (98%)	357 (97%)	11 (3%)	36	45
1	B	375/376 (100%)	361 (96%)	14 (4%)	29	37
1	C	370/376 (98%)	358 (97%)	12 (3%)	34	42
1	D	372/376 (99%)	366 (98%)	6 (2%)	58	70
1	E	369/376 (98%)	363 (98%)	6 (2%)	58	70
1	F	371/376 (99%)	356 (96%)	15 (4%)	27	34
All	All	2225/2256 (99%)	2161 (97%)	64 (3%)	37	47

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	322	VAL
1	F	341	LEU
1	B	449	GLU
1	B	439	VAL
1	F	352	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	27	ASN
1	F	300	GLN
1	E	37	HIS
1	E	333	GLN
1	F	408	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OAA	B	501	-	8,8,8	5.64	3 (37%)	9,10,10	1.92	2 (22%)
3	ACO	A	502	-	45,53,53	0.68	1 (2%)	56,79,79	1.30	4 (7%)
2	OAA	A	501	-	8,8,8	5.76	2 (25%)	9,10,10	1.93	4 (44%)
2	OAA	F	501	-	8,8,8	9.88	2 (25%)	9,10,10	3.84	4 (44%)
3	ACO	F	502	-	45,53,53	0.78	2 (4%)	56,79,79	1.19	6 (10%)
2	OAA	D	501	-	8,8,8	4.61	2 (25%)	9,10,10	2.26	4 (44%)
4	COA	D	502	-	41,50,50	0.64	0	52,75,75	1.10	4 (7%)
2	OAA	E	501	-	8,8,8	5.36	2 (25%)	9,10,10	2.55	3 (33%)

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	OAA	B	501	-	-	0/8/8/8	-
3	ACO	A	502	-	-	22/47/67/67	0/3/3/3
2	OAA	A	501	-	-	1/8/8/8	-
2	OAA	F	501	-	-	0/8/8/8	-
3	ACO	F	502	-	-	15/47/67/67	0/3/3/3
2	OAA	D	501	-	-	0/8/8/8	-
4	COA	D	502	-	-	4/44/64/64	0/3/3/3
2	OAA	E	501	-	-	2/8/8/8	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	OAA	C3-C4	-27.59	1.16	1.53

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	OAA	C3-C4	-15.94	1.32	1.53
2	B	501	OAA	C3-C4	-15.53	1.32	1.53
2	E	501	OAA	C3-C4	-14.59	1.33	1.53
2	D	501	OAA	C3-C4	-12.16	1.37	1.53

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	OAA	O3-C3-C4	-8.59	106.99	119.43
2	F	501	OAA	C2-C3-C4	5.93	127.86	117.85
2	E	501	OAA	C2-C3-C4	5.91	127.83	117.85
3	A	502	ACO	C2P-S1P-C	5.80	132.21	101.68
2	B	501	OAA	C2-C3-C4	4.45	125.37	117.85

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	OAA	O2-C1-C2-C3
3	A	502	ACO	C5B-O5B-P1A-O1A
3	A	502	ACO	C5B-O5B-P1A-O2A
3	A	502	ACO	CCP-O6A-P2A-O4A
3	A	502	ACO	CCP-O6A-P2A-O5A

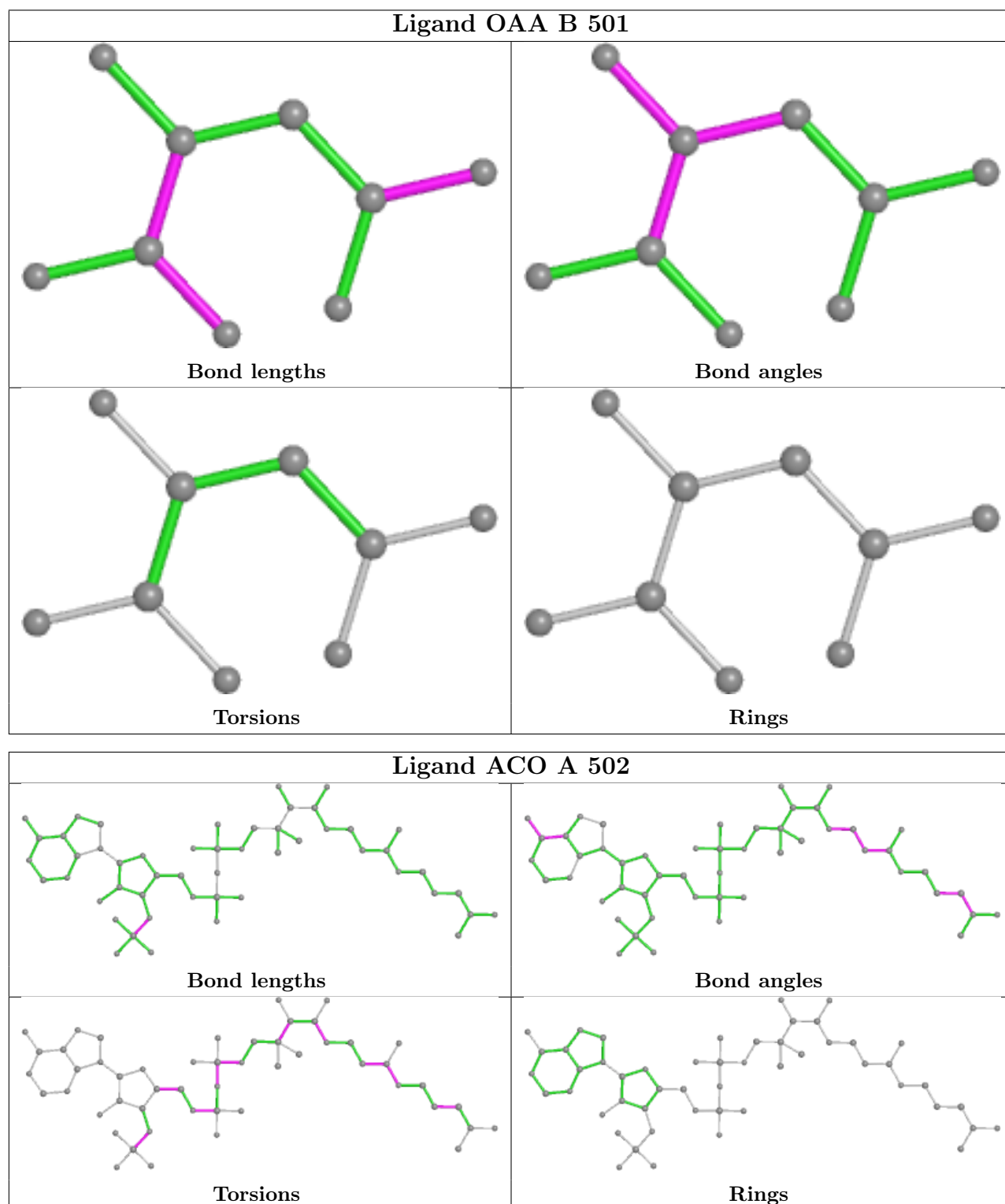
There are no ring outliers.

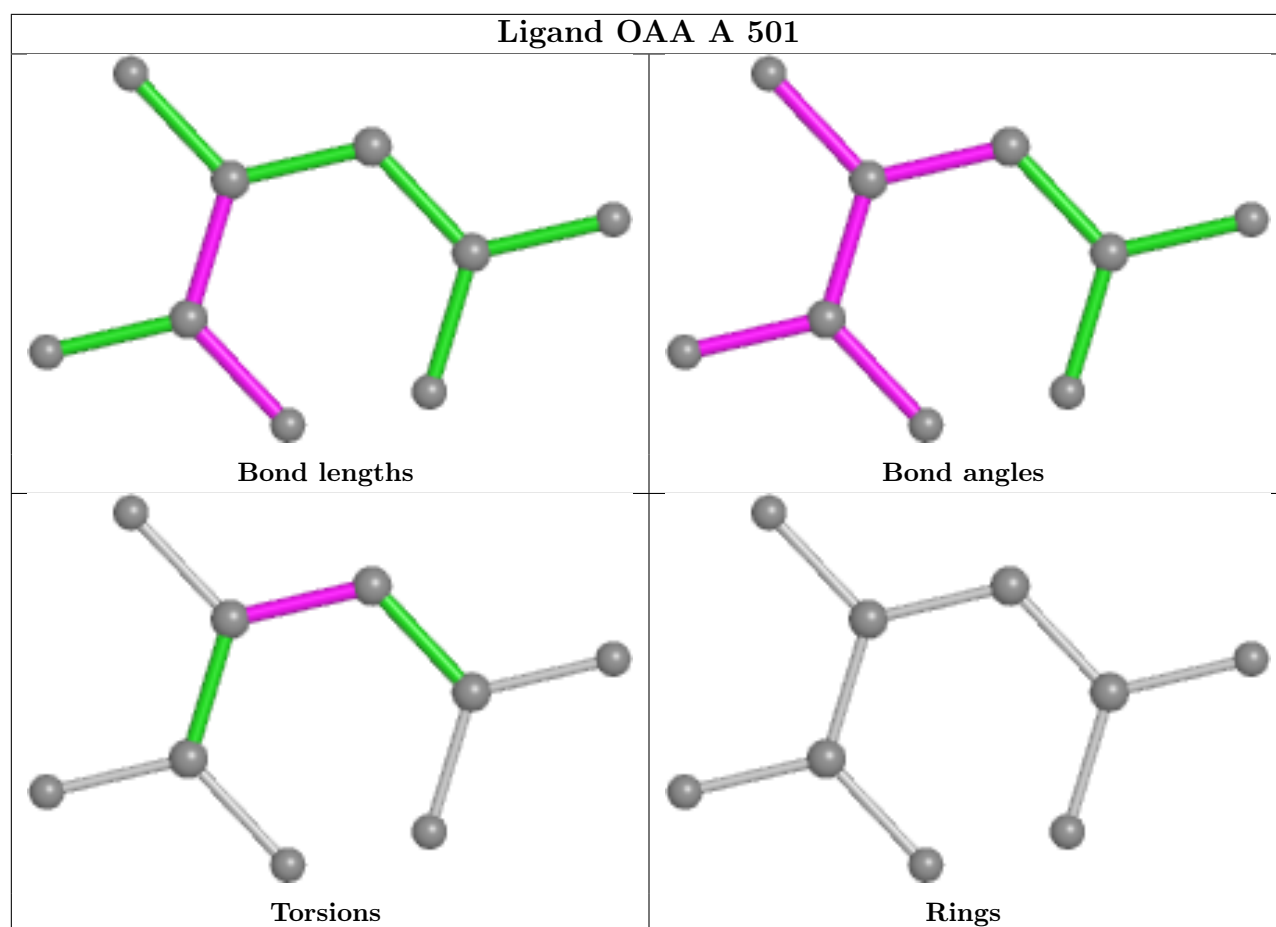
6 monomers are involved in 28 short contacts:

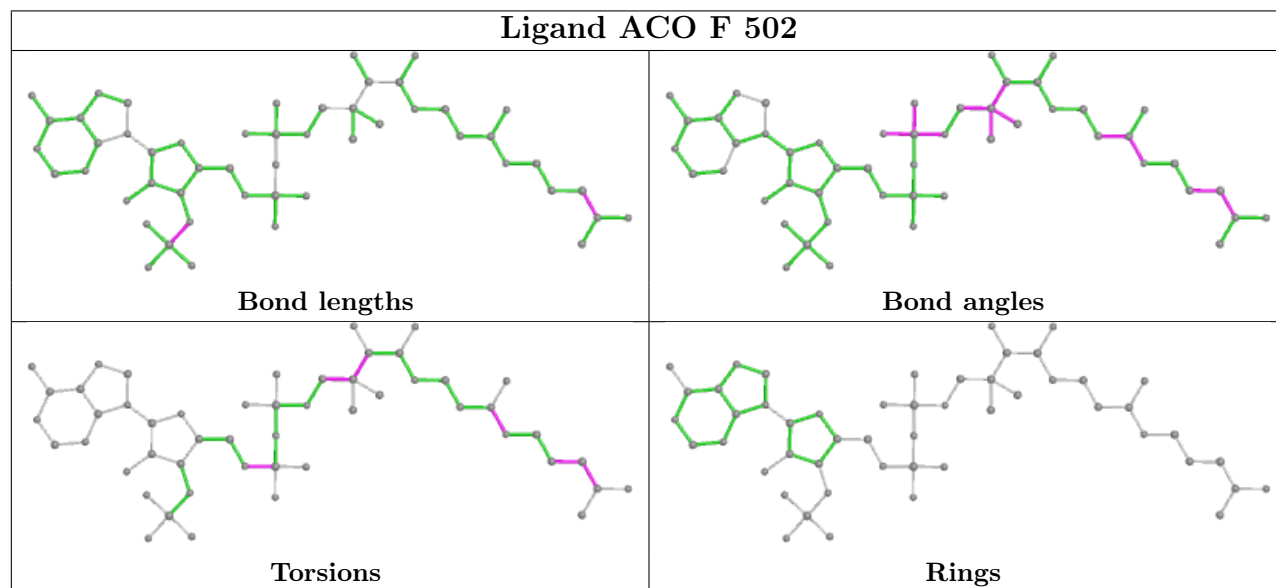
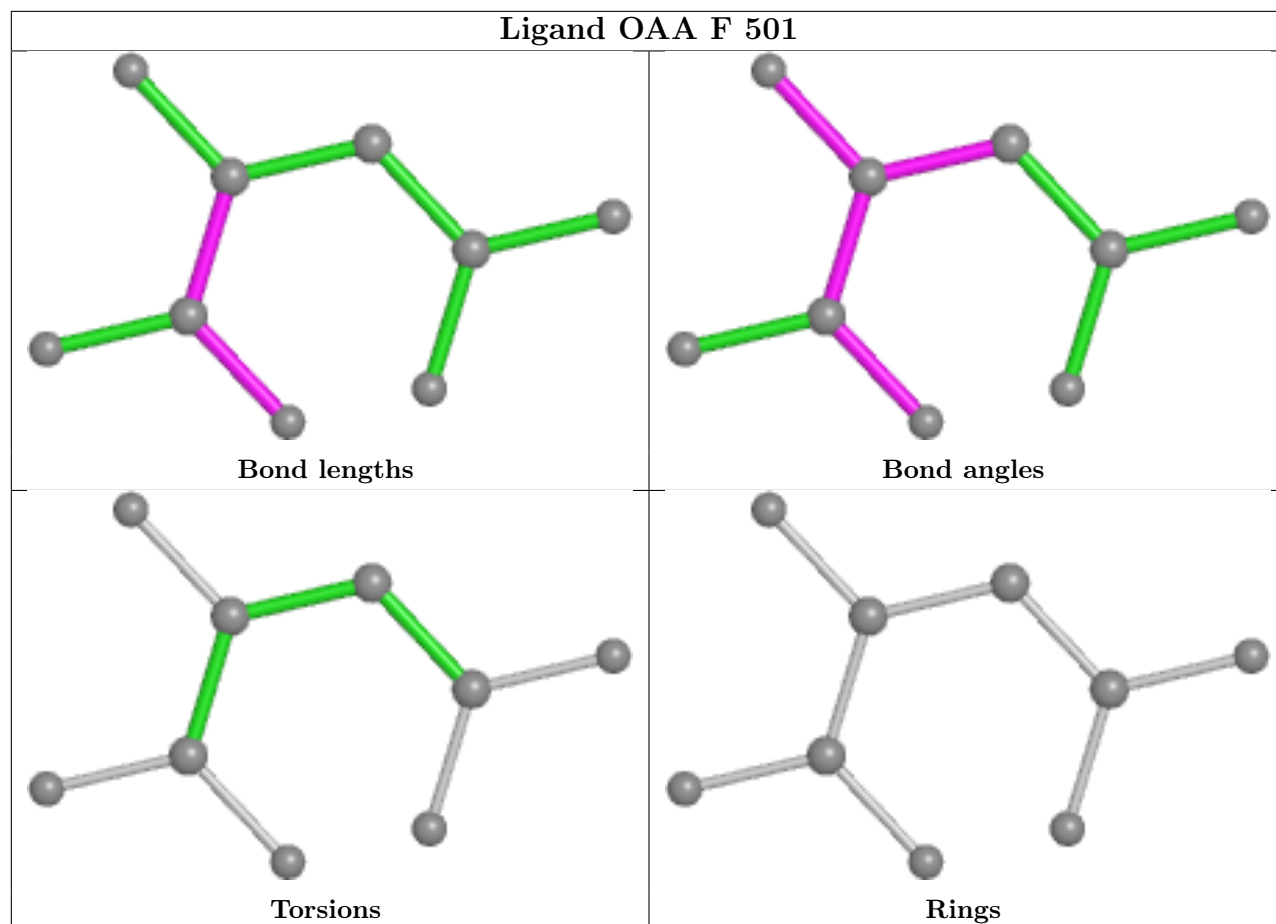
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	OAA	1	0
3	A	502	ACO	15	0
2	F	501	OAA	3	0
3	F	502	ACO	7	0
4	D	502	COA	1	0
2	E	501	OAA	1	0

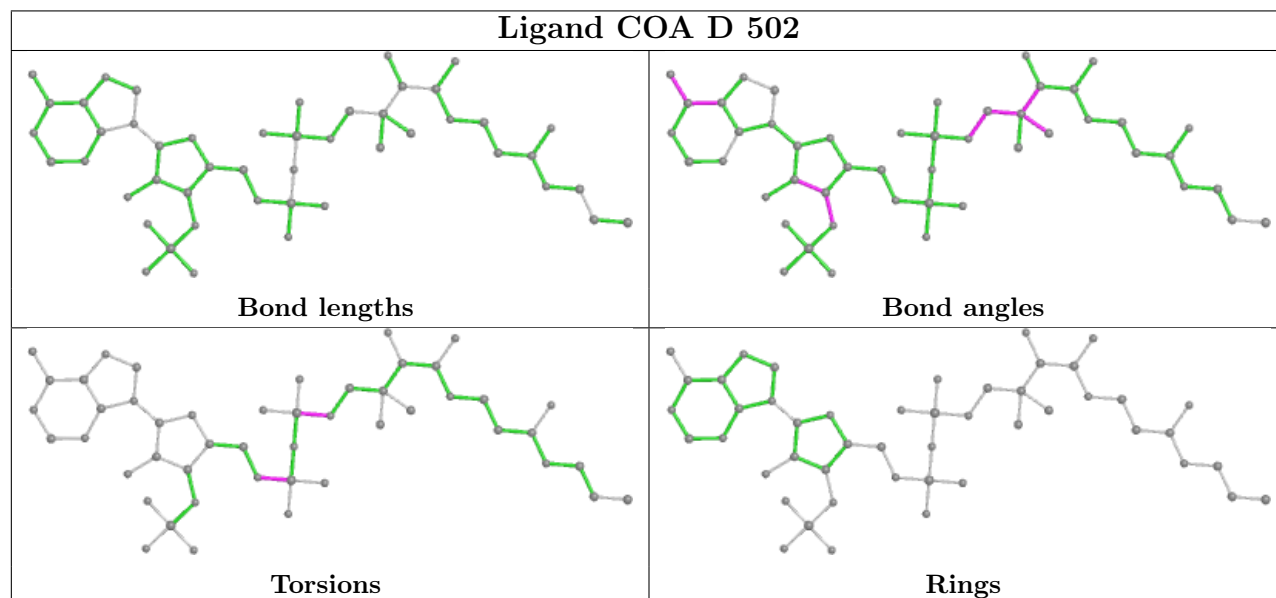
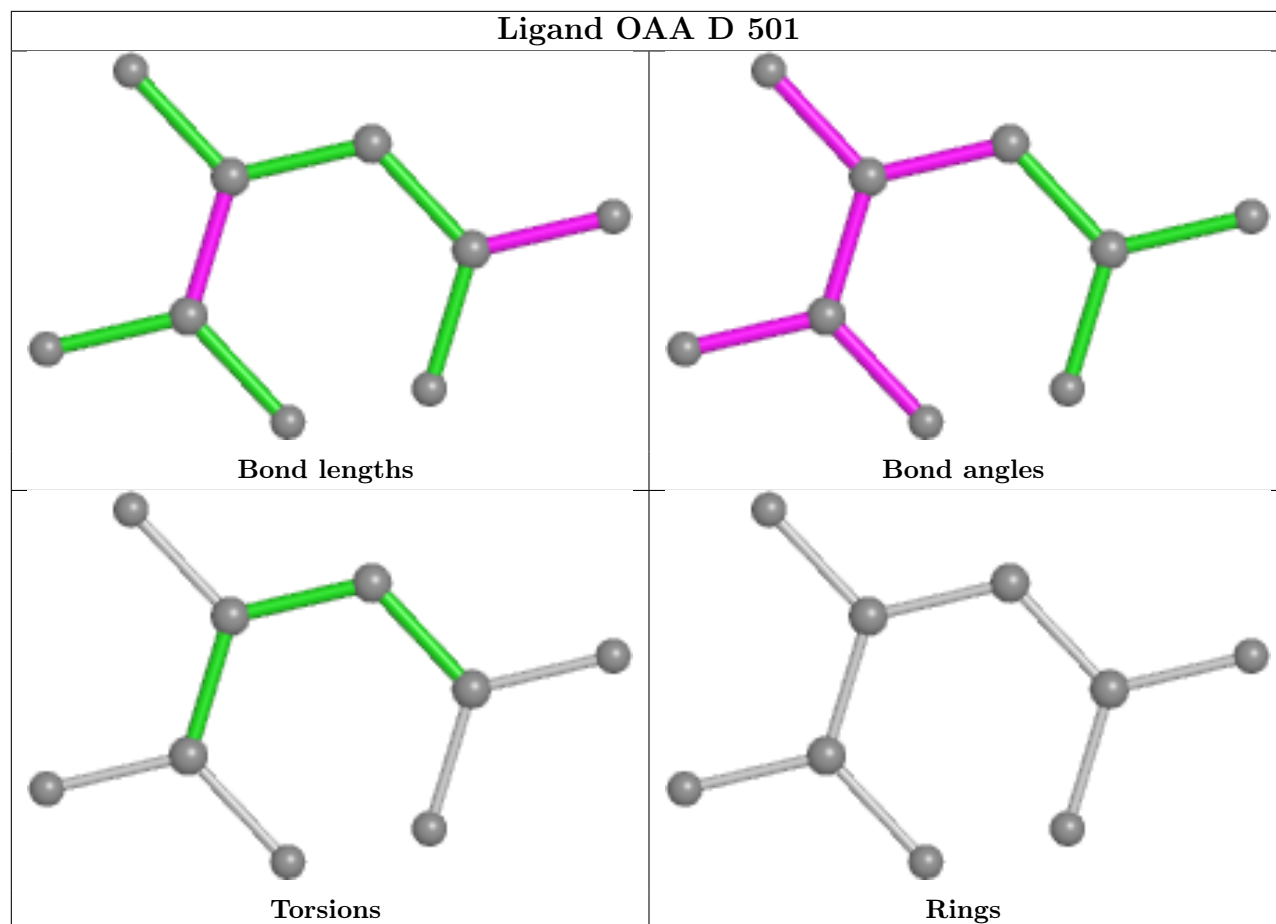
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

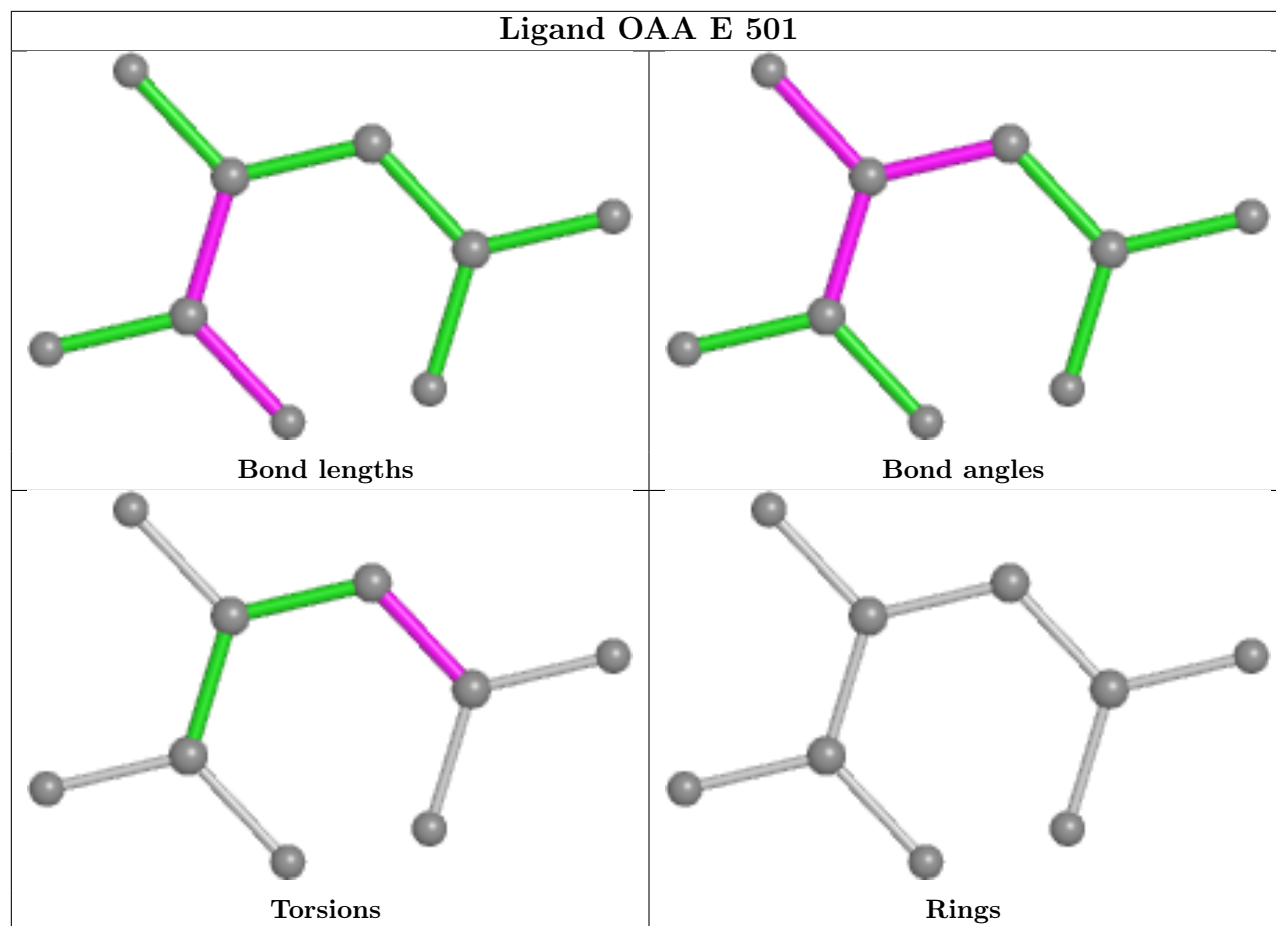
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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	435/449 (96%)	-0.06	31 (7%) 23 29	23, 39, 107, 145	0
1	B	449/449 (100%)	-0.38	4 (0%) 81 84	21, 35, 66, 133	0
1	C	442/449 (98%)	-0.18	14 (3%) 50 57	22, 36, 77, 123	0
1	D	440/449 (97%)	-0.54	0 100 100	20, 31, 55, 77	1 (0%)
1	E	441/449 (98%)	-0.43	4 (0%) 81 84	20, 32, 63, 124	0
1	F	441/449 (98%)	-0.49	1 (0%) 92 93	21, 33, 59, 78	0
All	All	2648/2694 (98%)	-0.35	54 (2%) 64 69	20, 34, 71, 145	1 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	VAL	7.4
1	B	367	ALA	4.2
1	A	315	ILE	4.0
1	A	364	HIS	3.8
1	B	366	LYS	3.7

### 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](#)

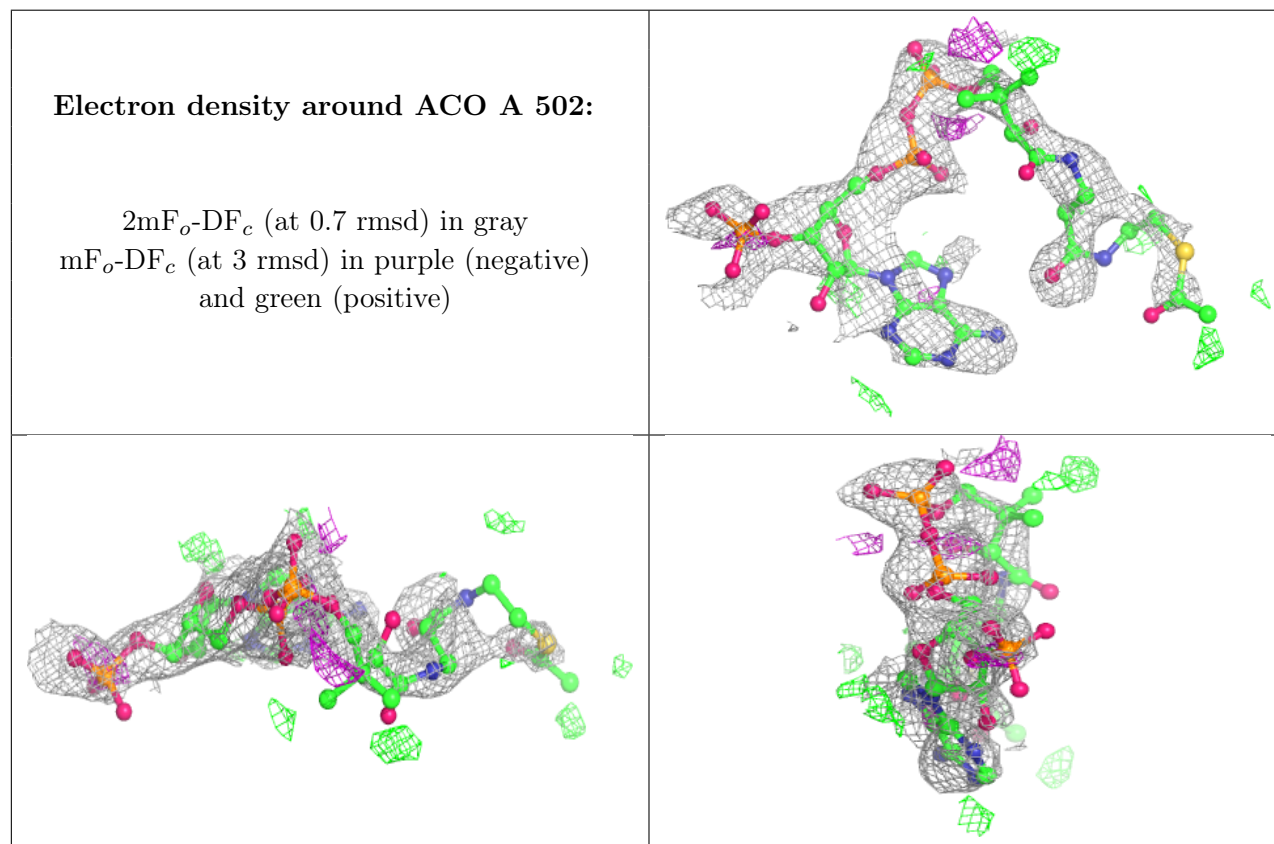
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

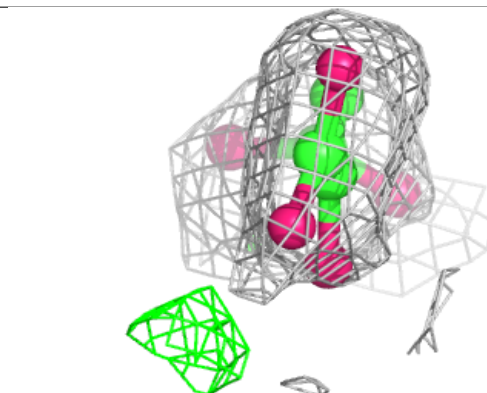
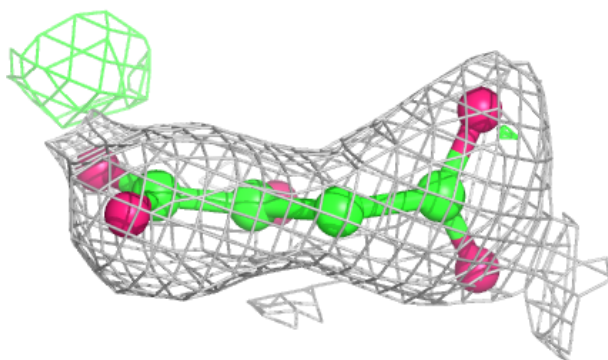
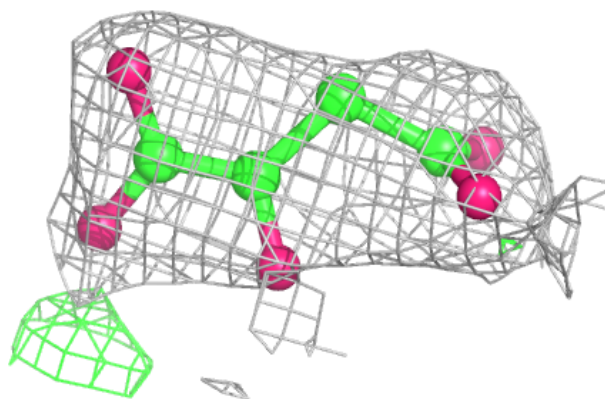
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACO	A	502	51/51	0.67	0.17	63,96,119,142	0
2	OAA	E	501	9/9	0.82	0.12	53,62,67,68	0
2	OAA	B	501	9/9	0.84	0.12	56,68,79,82	0
2	OAA	F	501	9/9	0.91	0.10	30,38,49,67	0
2	OAA	A	501	9/9	0.91	0.10	44,56,72,81	0
2	OAA	D	501	9/9	0.93	0.11	27,37,63,65	0
4	COA	D	502	48/48	0.93	0.08	32,45,64,80	0
3	ACO	F	502	51/51	0.97	0.07	24,30,59,90	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.

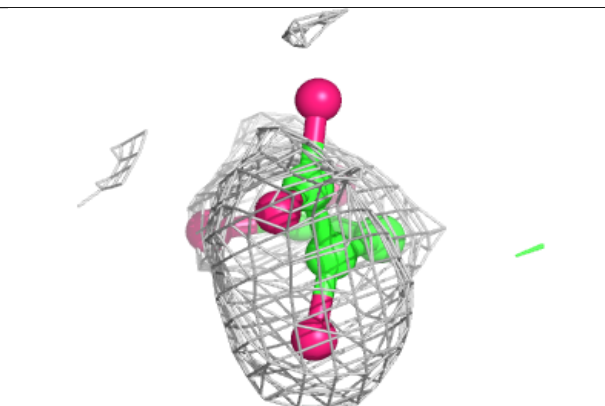
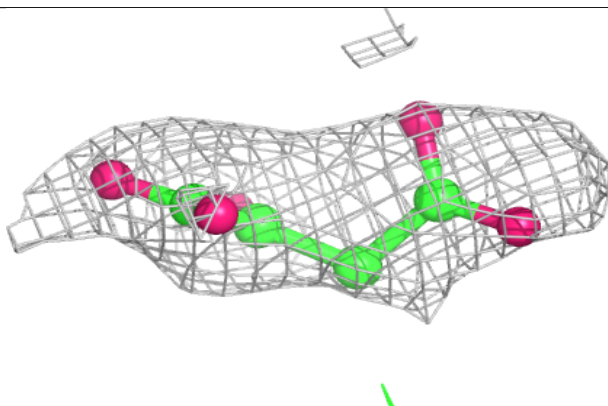
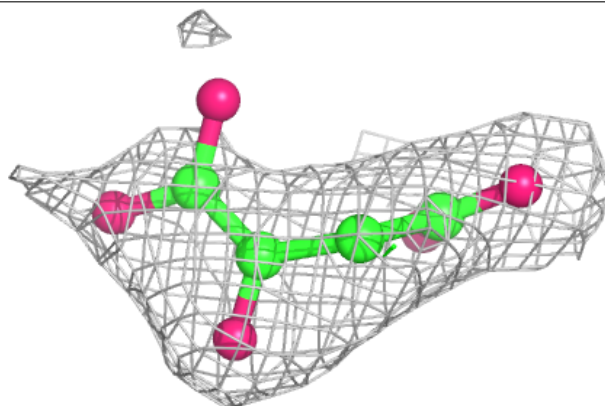


**Electron density around OAA E 501:**

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

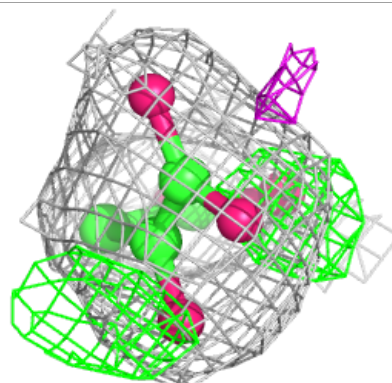
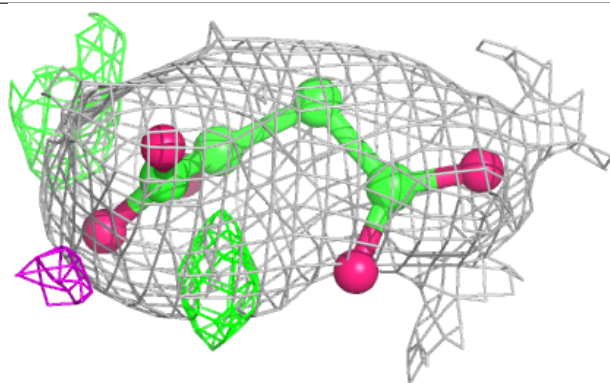
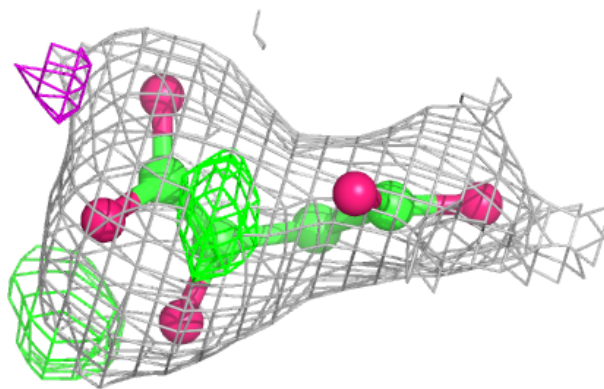
**Electron density around OAA B 501:**

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

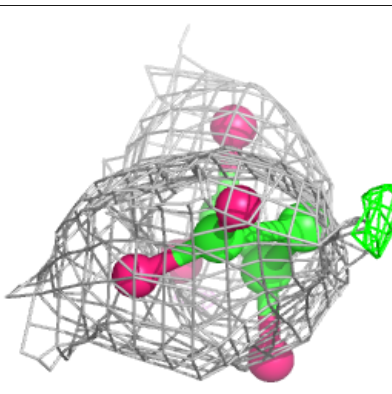
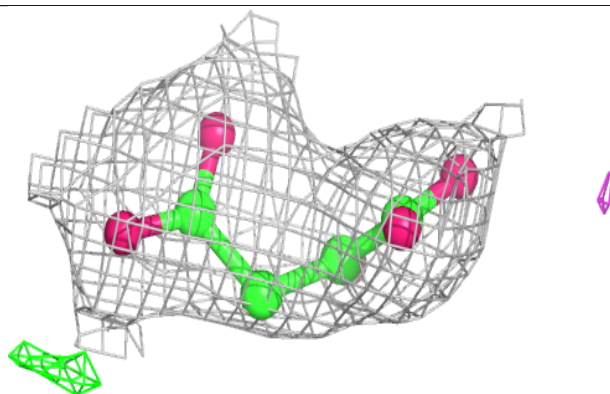
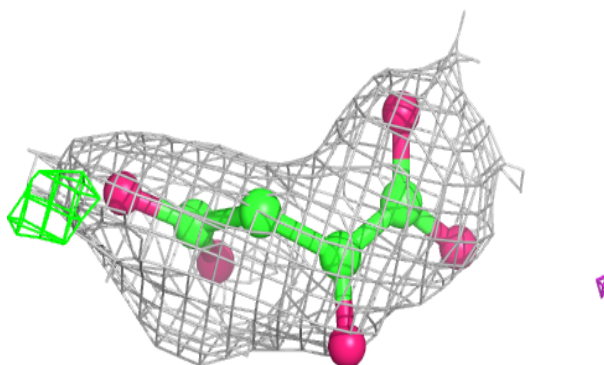


**Electron density around OAA F 501:**

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

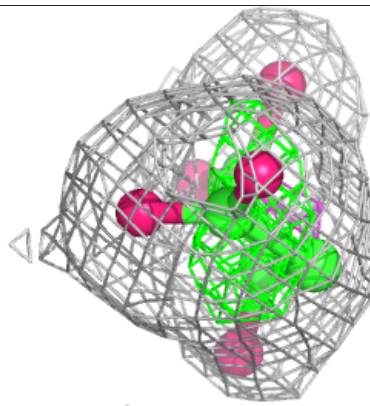
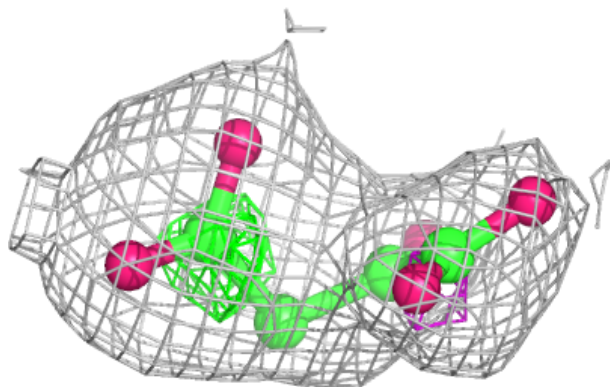
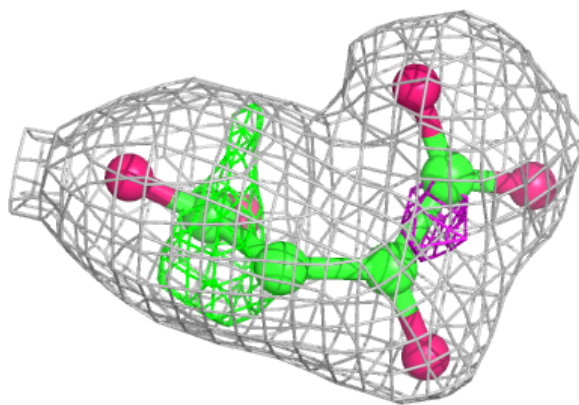
**Electron density around OAA A 501:**

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



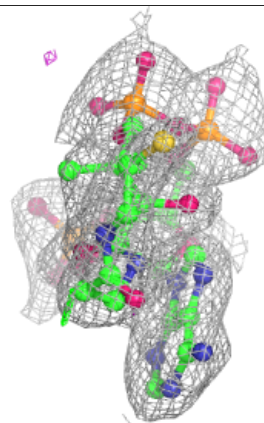
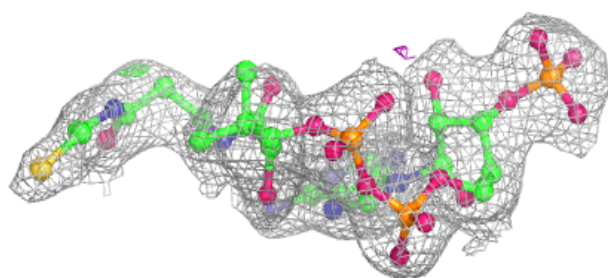
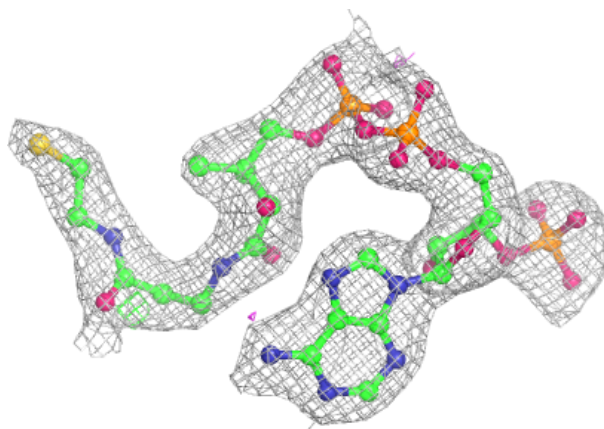
**Electron density around OAA D 501:**

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

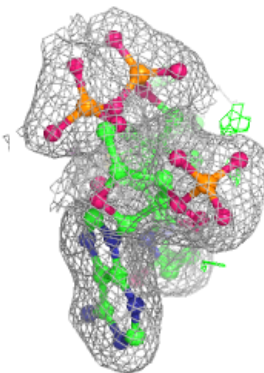
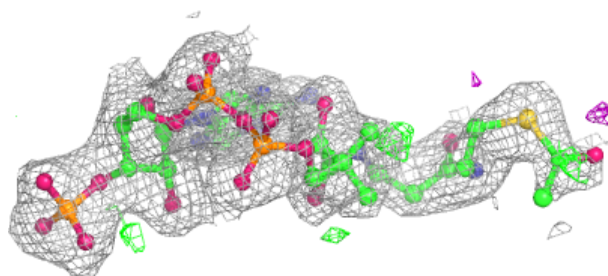
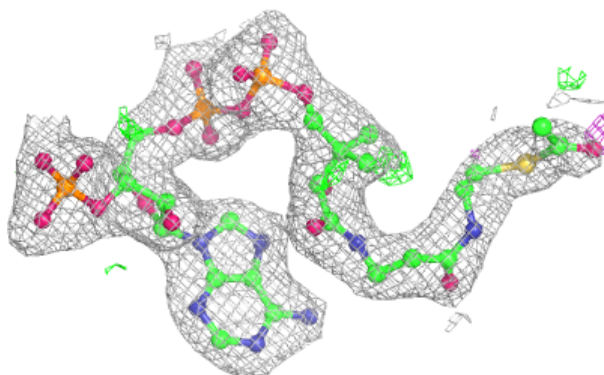


**Electron density around COA D 502:**

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

**Electron density around ACO F 502:**

$2mF_o-DF_c$  (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.