



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:38 PM UTC

PDB ID : 9HRQ / pdb\_00009hrq  
Title : Crystal structure of Arabidopsis thaliana Fatty Acid Thioesterase A with an unidentified ligand which closes the N-terminal domain  
Authors : Kot, E.; Ni, X.; Koekemoer, L.; Mulholland, N.P.; Montgomery, M.G.; von Delft, F.  
Deposited on : 2024-12-18  
Resolution : 1.54 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 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

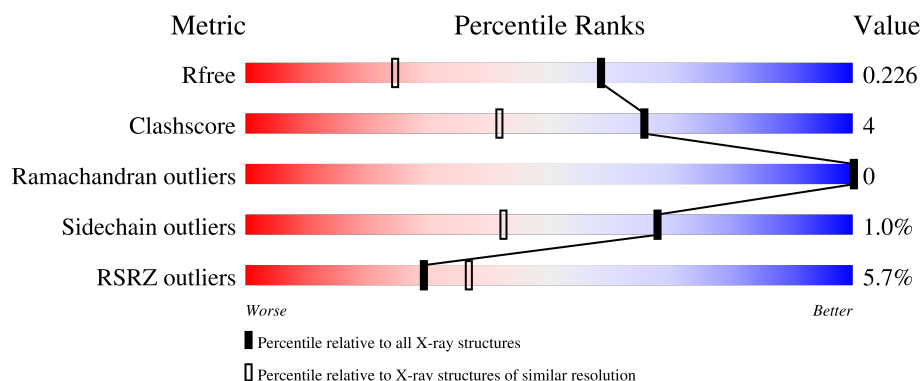
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	295	<div> <div>7%</div> <div>83%</div> <div>5%</div> <div>11%</div> </div>
1	B	295	<div> <div>3%</div> <div>82%</div> <div>8%</div> <div>9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	B	401	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4764 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 Oleoyl-acyl carrier protein thioesterase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	4	0
			2141	1339	378	413	11			
1	B	268	Total	C	N	O	S	0	3	0
			2179	1360	386	422	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	MET	-	initiating methionine	UNP Q42561
A	363	HIS	-	expression tag	UNP Q42561
A	364	HIS	-	expression tag	UNP Q42561
A	365	HIS	-	expression tag	UNP Q42561
A	366	HIS	-	expression tag	UNP Q42561
A	367	HIS	-	expression tag	UNP Q42561
A	368	HIS	-	expression tag	UNP Q42561
B	74	MET	-	initiating methionine	UNP Q42561
B	363	HIS	-	expression tag	UNP Q42561
B	364	HIS	-	expression tag	UNP Q42561
B	365	HIS	-	expression tag	UNP Q42561
B	366	HIS	-	expression tag	UNP Q42561
B	367	HIS	-	expression tag	UNP Q42561
B	368	HIS	-	expression tag	UNP Q42561

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			18	18		

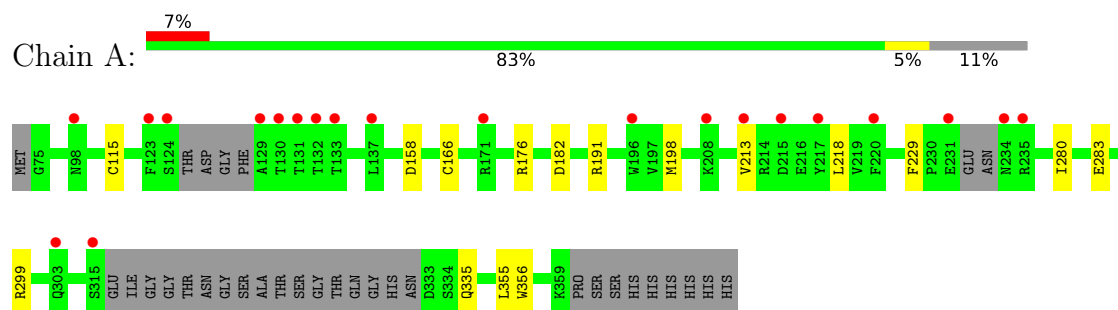
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	183	Total	O	0	0
			183	183		
4	B	238	Total	O	0	0
			238	238		

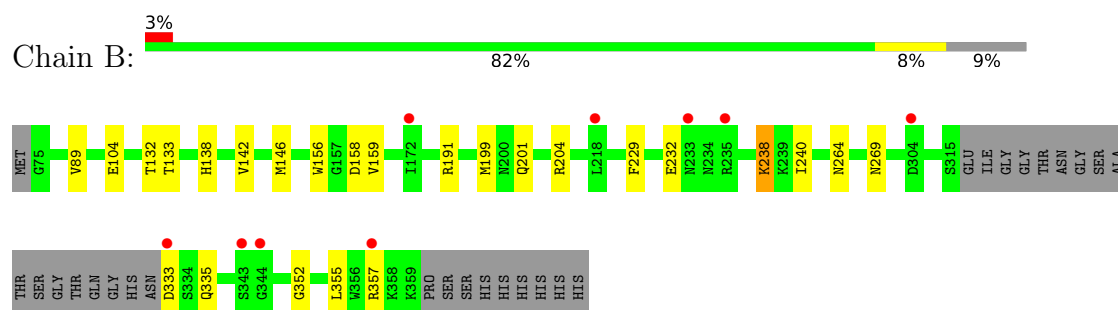
### 3 Residue-property plots [i](#)

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: Oleoyl-acyl carrier protein thioesterase 1, chloroplastic



- Molecule 1: Oleoyl-acyl carrier protein thioesterase 1, chloroplastic



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.79Å 98.58Å 128.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 1.54 49.29 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-1.54) 99.7 (49.29-1.54)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.189 , 0.217 0.199 , 0.226	Depositor DCC
$R_{free}$ test set	4539 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4764	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 4.40% 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: UNL, SO4

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	0.67	0/2182	1.11	3/2952 (0.1%)
1	B	0.68	0/2225	1.07	4/3013 (0.1%)
All	All	0.67	0/4407	1.09	7/5965 (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	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	158	ASP	CA-CB-CG	8.61	121.20	112.60
1	B	232	GLU	CB-CA-C	7.67	122.76	109.65
1	A	182	ASP	CA-CB-CG	7.14	119.74	112.60
1	B	158	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	133	THR	CA-CB-OG1	-5.30	101.64	109.60
1	A	299	ARG	N-CA-C	-5.21	100.82	108.79
1	B	264	ASN	CA-CB-CG	5.09	117.69	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	204	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	2141	0	2110	8	0
1	B	2179	0	2148	15	0
2	A	5	0	0	0	0
3	B	18	0	0	12	0
4	A	183	0	0	0	0
4	B	238	0	0	5	0
All	All	4764	0	4258	33	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 (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:401:UNL:O11	3:B:401:UNL:O10	1.55	1.23
3:B:401:UNL:O14	3:B:401:UNL:O16	1.53	1.23
3:B:401:UNL:O14	3:B:401:UNL:O13	1.55	1.23
3:B:401:UNL:O18	3:B:401:UNL:O17	1.58	1.22
3:B:401:UNL:O7	3:B:401:UNL:O9	1.60	1.19
3:B:401:UNL:O4	3:B:401:UNL:O5	1.63	1.16
3:B:401:UNL:O16	3:B:401:UNL:O17	1.61	1.15
3:B:401:UNL:O14	3:B:401:UNL:O15	1.71	1.08
3:B:401:UNL:O4	3:B:401:UNL:O3	1.72	1.04
1:A:335:GLN:HG2	1:A:355:LEU:HD13	1.77	0.66
1:A:198:MET:HE1	1:A:213:VAL:HG11	1.81	0.63
1:B:335:GLN:HG2	1:B:355:LEU:HD13	1.84	0.59
1:A:280:ILE:HD13	1:A:356:TRP:CZ2	2.37	0.59
1:A:115[B]:CYS:SG	1:B:156:TRP:HZ2	2.26	0.58
1:B:201:GLN:HB2	4:B:610:HOH:O	2.03	0.57
1:B:333:ASP:OD1	1:B:357:ARG:HD3	2.07	0.54
1:B:269:ASN:CB	4:B:714:HOH:O	2.56	0.54
1:B:240:ILE:HD13	1:B:352:GLY:HA2	1.90	0.53
1:B:269:ASN:HB3	4:B:714:HOH:O	2.08	0.52
1:B:191[C]:ARG:HG3	1:B:229:PHE:CZ	2.45	0.52
1:A:191:ARG:HG3	1:A:229:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LYS:HE3	4:B:709:HOH:O	2.10	0.50
3:B:401:UNL:O16	3:B:401:UNL:O13	2.31	0.48
1:A:166:CYS:SG	1:A:176:ARG:NH1	2.87	0.47
1:B:104:GLU:HG3	4:B:668:HOH:O	2.14	0.47
1:A:335:GLN:HG2	1:A:355:LEU:CD1	2.45	0.47
1:A:115[B]:CYS:HG	1:B:156:TRP:HZ2	1.62	0.46
1:B:142:VAL:HG21	1:B:199:MET:HB2	1.98	0.45
3:B:401:UNL:O4	3:B:401:UNL:O2	2.34	0.44
1:B:138:HIS:HB3	1:B:201:GLN:HG2	1.99	0.44
3:B:401:UNL:O14	3:B:401:UNL:O17	2.35	0.43
1:B:89:VAL:HG22	1:B:159:VAL:HG22	2.00	0.43
1:B:335:GLN:HG2	1:B:355:LEU:CD1	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/295 (88%)	257 (100%)	1 (0%)	0	100	100
1	B	267/295 (90%)	265 (99%)	2 (1%)	0	100	100
All	All	525/590 (89%)	522 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/263 (92%)	239 (99%)	2 (1%)	73	51
1	B	245/263 (93%)	242 (99%)	3 (1%)	63	34
All	All	486/526 (92%)	481 (99%)	5 (1%)	68	42

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	LEU
1	A	283	GLU
1	B	132	THR
1	B	146	MET
1	B	238	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	GLN
1	B	223	GLN
1	B	264	ASN
1	B	282	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is unknown - leaving 1 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	SO4	A	401	-	4,4,4	0.40	0	6,6,6	0.12	0

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.

No monomer is involved in short contacts.

## 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	262/295 (88%)	0.53	21 (8%)	18 23	12, 24, 48, 70	4 (1%)
1	B	268/295 (90%)	0.26	9 (3%)	48 57	11, 23, 39, 59	3 (1%)
All	All	530/590 (89%)	0.40	30 (5%)	29 37	11, 23, 43, 70	7 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	5.0
1	A	124	SER	4.6
1	A	123	PHE	4.4
1	A	132	THR	4.1
1	A	217	TYR	3.7
1	A	231	GLU	3.4
1	A	137	LEU	3.2
1	A	133	THR	3.1
1	A	315	SER	3.0
1	A	131	THR	3.0
1	A	220[A]	PHE	3.0
1	B	344	GLY	2.8
1	A	235	ARG	2.7
1	B	218	LEU	2.5
1	B	172	ILE	2.4
1	B	304	ASP	2.4
1	A	208	LYS	2.4
1	B	343	SER	2.4
1	A	303	GLN	2.3
1	A	130	THR	2.3
1	A	234	ASN	2.3
1	B	233	ASN	2.3
1	A	213	VAL	2.2
1	B	357	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	196	TRP	2.2
1	A	171	ARG	2.2
1	A	98	ASN	2.1
1	B	333	ASP	2.1
1	B	235	ARG	2.1
1	A	215	ASP	2.0

## 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](#)

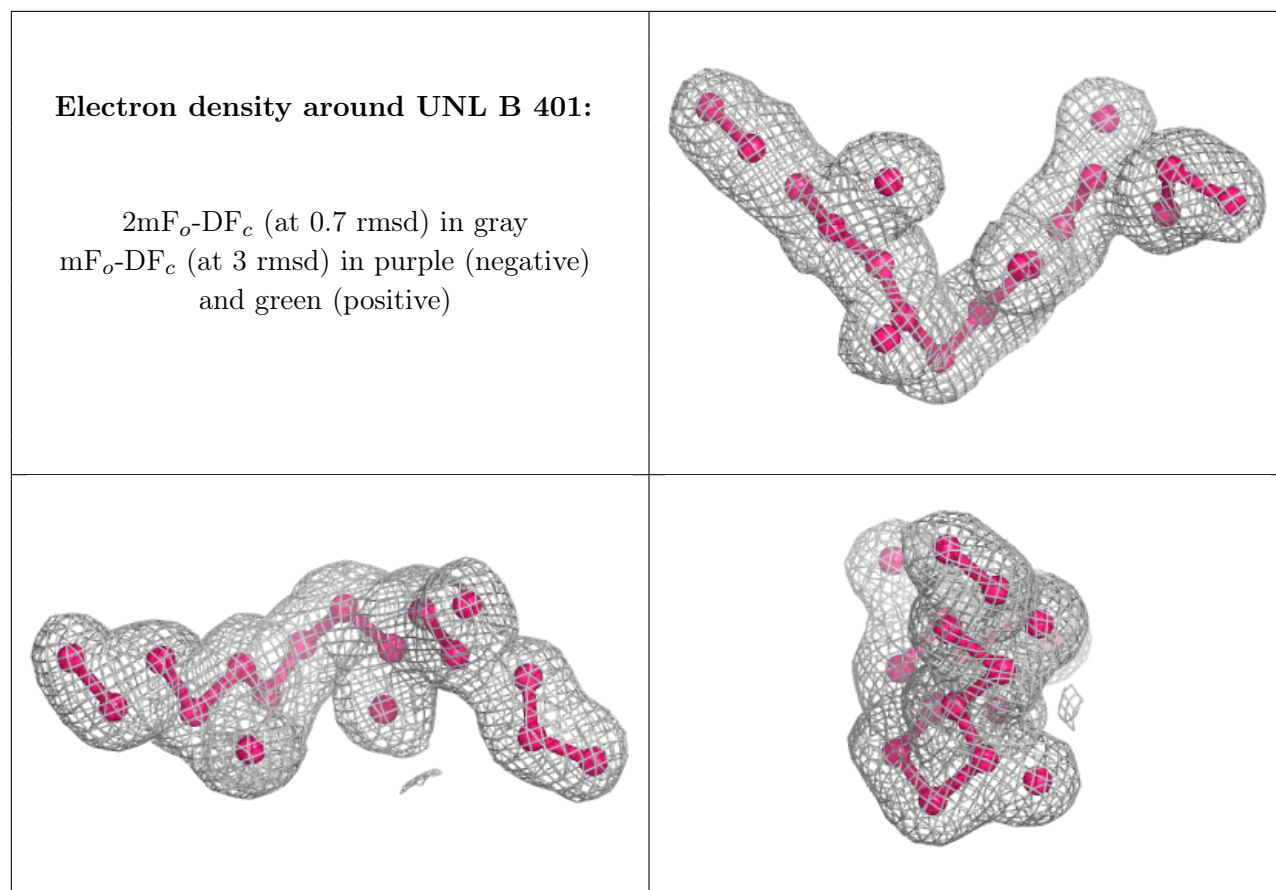
There are no oligosaccharides in this entry.

## 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	SO4	A	401	5/5	0.96	0.07	39,39,44,51	0
3	UNL	B	401	18/-	0.97	0.06	19,29,33,34	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.