Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 09:21 AM EDT

PDB ID	:	7ACI
Title	:	In meso structure of apolipoprotein N-acyltransferase, Lnt, from Escherichia coli in 9.8 monoacylglycerol
Authors	:	Smithers, L.; van Dalsen, L.; Boland, C.; Caffrey, M.
Deposited on	:	2020-09-10
Resolution	:	2.30 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*
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.

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

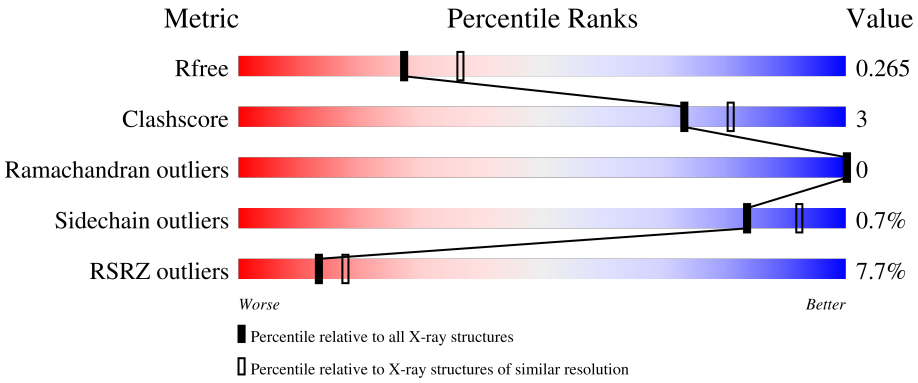
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	532	7%, 86%, 8%, 5%

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	LH9	A	612	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8538 atoms, of which 4308 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.

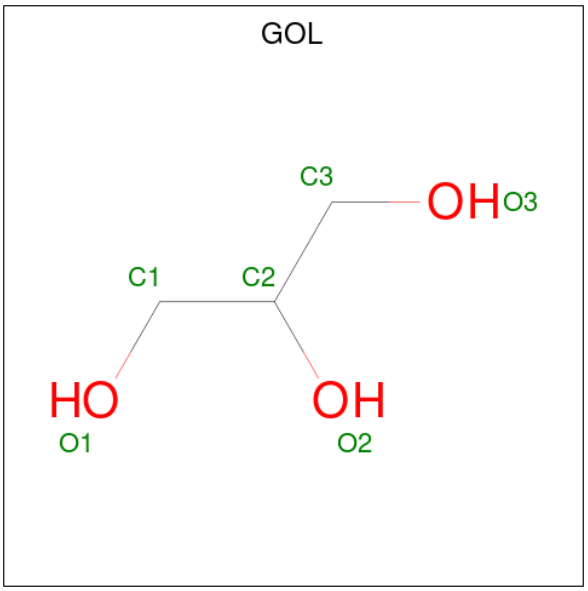
- Molecule 1 is a protein called Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	505	Total	C	H	N	O	S	0	2	0
			8011	2612	4034	660	689	16			

There are 20 discrepancies between the modelled and reference sequences:

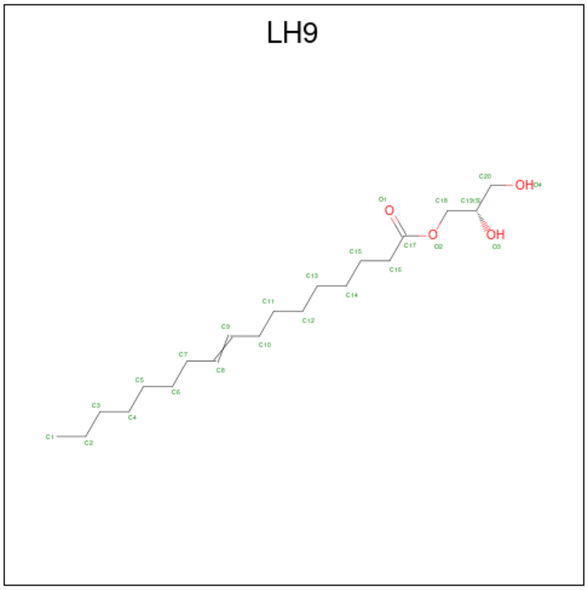
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A037YBN4
A	-18	GLY	-	expression tag	UNP A0A037YBN4
A	-17	SER	-	expression tag	UNP A0A037YBN4
A	-16	SER	-	expression tag	UNP A0A037YBN4
A	-15	HIS	-	expression tag	UNP A0A037YBN4
A	-14	HIS	-	expression tag	UNP A0A037YBN4
A	-13	HIS	-	expression tag	UNP A0A037YBN4
A	-12	HIS	-	expression tag	UNP A0A037YBN4
A	-11	HIS	-	expression tag	UNP A0A037YBN4
A	-10	HIS	-	expression tag	UNP A0A037YBN4
A	-9	SER	-	expression tag	UNP A0A037YBN4
A	-8	SER	-	expression tag	UNP A0A037YBN4
A	-7	GLY	-	expression tag	UNP A0A037YBN4
A	-6	LEU	-	expression tag	UNP A0A037YBN4
A	-5	VAL	-	expression tag	UNP A0A037YBN4
A	-4	PRO	-	expression tag	UNP A0A037YBN4
A	-3	ARG	-	expression tag	UNP A0A037YBN4
A	-2	GLY	-	expression tag	UNP A0A037YBN4
A	-1	SER	-	expression tag	UNP A0A037YBN4
A	0	HIS	-	expression tag	UNP A0A037YBN4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			13	3	7	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is [(2 {S})-2,3-bis(oxidanyl)propyl] heptadec-9-enoate (three-letter code: LH9) (formula: $C_{20}H_{38}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 62 20 38 4	0	0
3	A	1	Total C H O 62 20 38 4	0	0
3	A	1	Total C H O 62 20 38 4	0	0
3	A	1	Total C H O 62 20 38 4	0	0
3	A	1	Total C H O 62 20 38 4	0	0
3	A	1	Total C H O 62 20 38 4	0	0

- Molecule 4 is water.

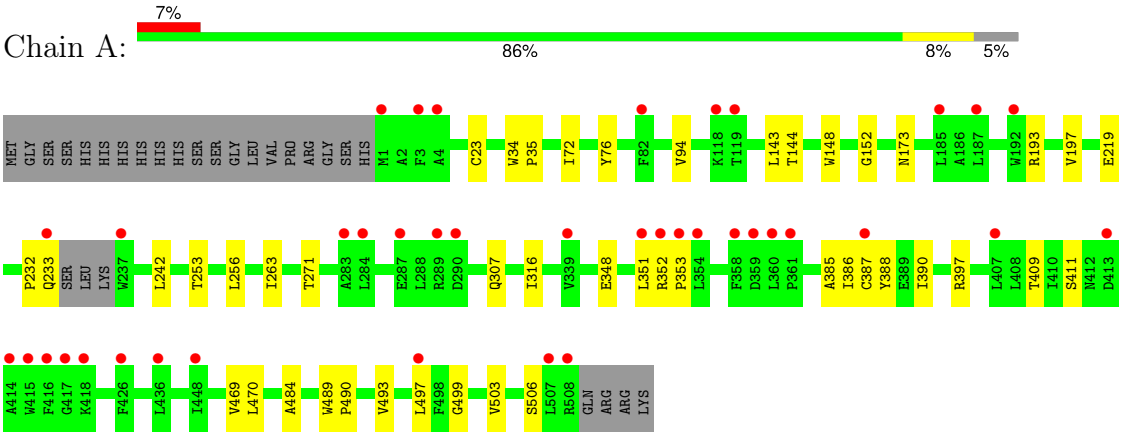
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	73	Total O 73 73	0	0

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: Apolipoprotein N-acyltransferase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	48.77Å 76.17Å 156.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 2.30 46.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.57-2.30) 99.4 (46.57-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.214 , 0.258 0.219 , 0.265	Depositor DCC
R_{free} test set	1423 reflections (5.36%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8538	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LH9, GOL

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	0.28	0/4089	0.46	0/5586

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3977	4034	4036	27	0
2	A	36	46	48	0	0
3	A	144	228	0	3	0
4	A	73	0	0	0	0
All	All	4230	4308	4084	27	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 3.

All (27) 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:A:397:ARG:NH1	1:A:484:ALA:O	2.32	0.63
1:A:143:LEU:O	1:A:144:THR:OG1	2.18	0.57
1:A:348:GLU:HA	1:A:351:LEU:HD11	1.86	0.56
1:A:307:GLN:N	1:A:307:GLN:OE1	2.39	0.55
1:A:72:ILE:HG22	1:A:72:ILE:O	2.09	0.52
1:A:470:LEU:C	1:A:470:LEU:HD23	2.29	0.52
1:A:253:THR:HG23	1:A:263:ILE:HD13	1.92	0.51
1:A:387:CYS:SG	1:A:388:TYR:N	2.86	0.49
1:A:256:LEU:HD11	1:A:469:VAL:HG11	1.95	0.47
1:A:34:TRP:N	1:A:35:PRO:CD	2.78	0.47
1:A:242:LEU:HD12	1:A:271:THR:OG1	2.14	0.46
1:A:387:CYS:SG	3:A:608:LH9:O4	2.74	0.45
1:A:23:CYS:HB2	3:A:609:LH9:C9	2.47	0.45
1:A:197:VAL:HG11	3:A:612:LH9:O3	2.18	0.44
1:A:72:ILE:O	1:A:72:ILE:CG2	2.66	0.43
1:A:72:ILE:HD11	1:A:148:TRP:CD1	2.53	0.43
1:A:316:ILE:HG13	1:A:386:ILE:HD11	2.00	0.43
1:A:352:ARG:N	1:A:353:PRO:CD	2.82	0.43
1:A:219:GLU:OE1	1:A:219:GLU:N	2.41	0.43
1:A:385:ALA:O	1:A:409:THR:HA	2.18	0.43
1:A:493:VAL:O	1:A:497:LEU:HD13	2.18	0.43
1:A:76:TYR:HB2	1:A:94:VAL:HG21	2.01	0.42
1:A:489:TRP:N	1:A:490:PRO:CD	2.82	0.42
1:A:152:GLY:N	1:A:173:ASN:OD1	2.48	0.42
1:A:499:GLY:O	1:A:503:VAL:HG12	2.20	0.42
1:A:232:PRO:O	1:A:233:GLN:C	2.57	0.41
1:A:390:ILE:HD13	1:A:409:THR:OG1	2.19	0.41

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	503/532 (94%)	487 (97%)	16 (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	420/444 (95%)	417 (99%)	3 (1%)	84 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	A	411	SER
1	A	506	SER

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	LH9	A	607	-	23,23,23	0.97	0	24,24,24	0.83	0
3	LH9	A	609	-	23,23,23	0.92	0	24,24,24	0.72	0
2	GOL	A	605	-	5,5,5	0.90	0	5,5,5	1.12	0
3	LH9	A	608	-	23,23,23	1.02	0	24,24,24	0.87	0
2	GOL	A	602	-	5,5,5	0.88	0	5,5,5	1.08	0
2	GOL	A	604	-	5,5,5	0.89	0	5,5,5	1.08	0
3	LH9	A	610	-	23,23,23	0.83	0	24,24,24	0.76	0
3	LH9	A	611	-	23,23,23	1.01	0	24,24,24	0.85	0
2	GOL	A	601	-	5,5,5	0.86	0	5,5,5	1.08	0
3	LH9	A	612	-	23,23,23	1.40	2 (8%)	24,24,24	0.95	1 (4%)
2	GOL	A	606	-	5,5,5	0.86	0	5,5,5	0.98	0
2	GOL	A	603	-	5,5,5	0.94	0	5,5,5	1.08	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
3	LH9	A	607	-	-	8/23/23/23	-
3	LH9	A	609	-	-	14/23/23/23	-
2	GOL	A	605	-	-	1/4/4/4	-
3	LH9	A	608	-	-	12/23/23/23	-
2	GOL	A	602	-	-	0/4/4/4	-
2	GOL	A	604	-	-	0/4/4/4	-
3	LH9	A	610	-	-	12/23/23/23	-
3	LH9	A	611	-	-	14/23/23/23	-
2	GOL	A	601	-	-	2/4/4/4	-
3	LH9	A	612	-	-	6/23/23/23	-
2	GOL	A	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	603	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	LH9	C18-C19	2.40	1.59	1.51
3	A	612	LH9	O2-C17	2.17	1.39	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	612	LH9	C11-C10-C9	2.01	123.87	112.60

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	608	LH9	O2-C18-C19-C20
3	A	608	LH9	C7-C8-C9-C10
3	A	609	LH9	C18-C19-C20-O4
3	A	611	LH9	O1-C17-O2-C18
3	A	611	LH9	C16-C17-O2-C18
3	A	612	LH9	C7-C8-C9-C10
3	A	611	LH9	C3-C4-C5-C6
3	A	609	LH9	O2-C18-C19-O3
3	A	607	LH9	C7-C8-C9-C10
3	A	610	LH9	C7-C8-C9-C10
3	A	611	LH9	C7-C8-C9-C10
3	A	607	LH9	C16-C17-O2-C18
3	A	607	LH9	O1-C17-O2-C18
3	A	608	LH9	C16-C17-O2-C18
3	A	608	LH9	C14-C15-C16-C17
3	A	611	LH9	C14-C15-C16-C17
3	A	609	LH9	C7-C8-C9-C10
3	A	608	LH9	O1-C17-O2-C18
2	A	606	GOL	C1-C2-C3-O3
3	A	611	LH9	C2-C3-C4-C5
3	A	609	LH9	O3-C19-C20-O4
3	A	611	LH9	O3-C19-C20-O4
3	A	610	LH9	C3-C4-C5-C6
3	A	609	LH9	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	611	LH9	C13-C14-C15-C16
3	A	608	LH9	C3-C4-C5-C6
3	A	608	LH9	C10-C11-C12-C13
3	A	607	LH9	C10-C11-C12-C13
3	A	609	LH9	C4-C5-C6-C7
3	A	609	LH9	O2-C18-C19-C20
3	A	612	LH9	C4-C5-C6-C7
3	A	610	LH9	C11-C10-C9-C8
3	A	612	LH9	C9-C10-C11-C12
3	A	610	LH9	C4-C5-C6-C7
3	A	607	LH9	C5-C6-C7-C8
3	A	609	LH9	C9-C10-C11-C12
3	A	611	LH9	C12-C13-C14-C15
2	A	601	GOL	O1-C1-C2-O2
2	A	603	GOL	O2-C2-C3-O3
2	A	605	GOL	O1-C1-C2-O2
2	A	606	GOL	O2-C2-C3-O3
3	A	610	LH9	C11-C12-C13-C14
3	A	609	LH9	C2-C3-C4-C5
3	A	610	LH9	C14-C15-C16-C17
3	A	609	LH9	C14-C15-C16-C17
3	A	611	LH9	C11-C12-C13-C14
3	A	608	LH9	C11-C12-C13-C14
3	A	607	LH9	C4-C5-C6-C7
3	A	609	LH9	C16-C17-O2-C18
2	A	601	GOL	O1-C1-C2-C3
3	A	610	LH9	C1-C2-C3-C4
3	A	608	LH9	C4-C5-C6-C7
3	A	608	LH9	C9-C10-C11-C12
3	A	612	LH9	C3-C4-C5-C6
3	A	609	LH9	O1-C17-O2-C18
3	A	607	LH9	C6-C7-C8-C9
3	A	612	LH9	C13-C14-C15-C16
3	A	608	LH9	O2-C18-C19-O3
3	A	610	LH9	C16-C17-O2-C18
3	A	608	LH9	C6-C7-C8-C9
3	A	609	LH9	C6-C7-C8-C9
3	A	611	LH9	C18-C19-C20-O4
3	A	610	LH9	C9-C10-C11-C12
3	A	609	LH9	C3-C4-C5-C6
3	A	610	LH9	O1-C17-O2-C18
3	A	611	LH9	O2-C18-C19-C20

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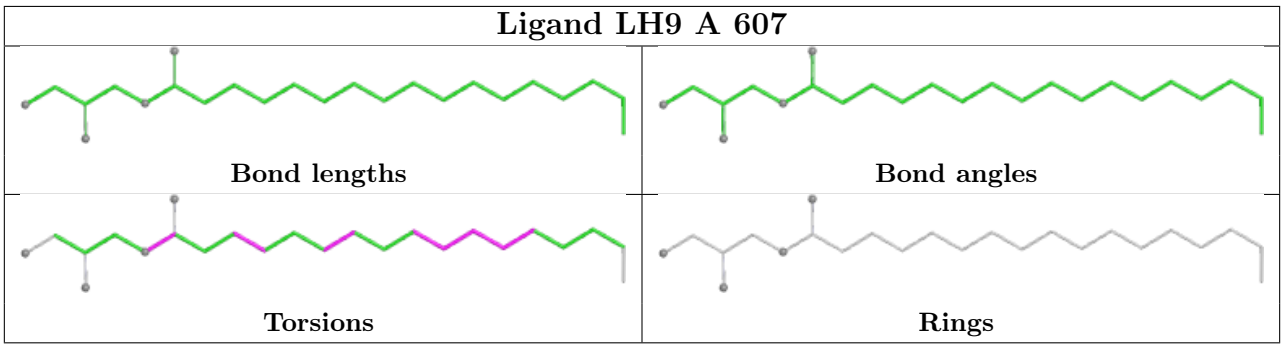
Mol	Chain	Res	Type	Atoms
3	A	611	LH9	O2-C18-C19-O3
3	A	612	LH9	C10-C11-C12-C13
3	A	607	LH9	C13-C14-C15-C16
3	A	611	LH9	C1-C2-C3-C4
3	A	610	LH9	O2-C18-C19-O3
3	A	610	LH9	C10-C11-C12-C13

There are no ring outliers.

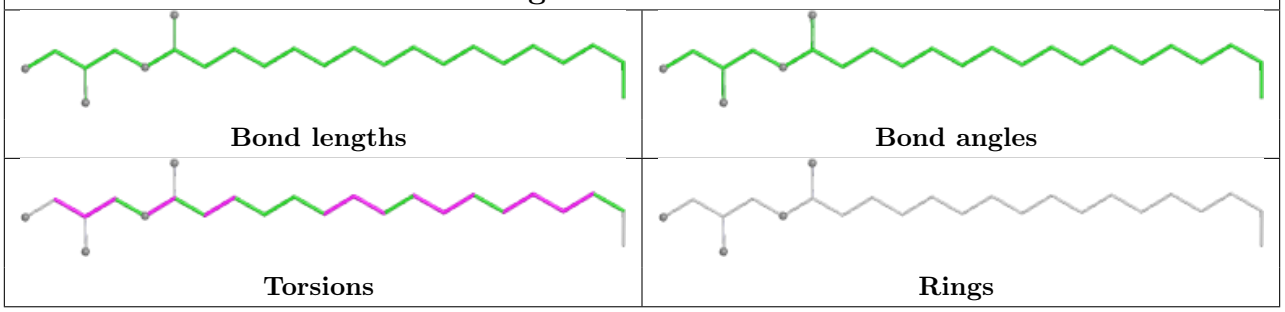
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	609	LH9	1	0
3	A	608	LH9	1	0
3	A	612	LH9	1	0

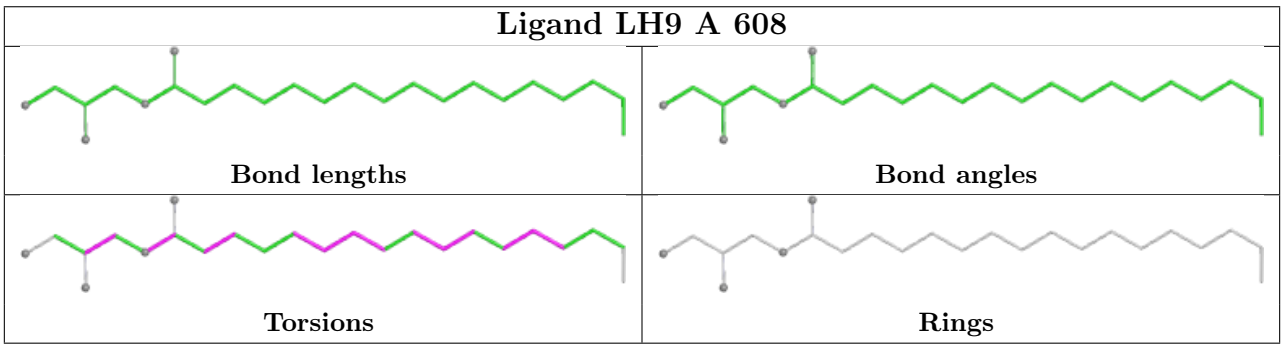
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



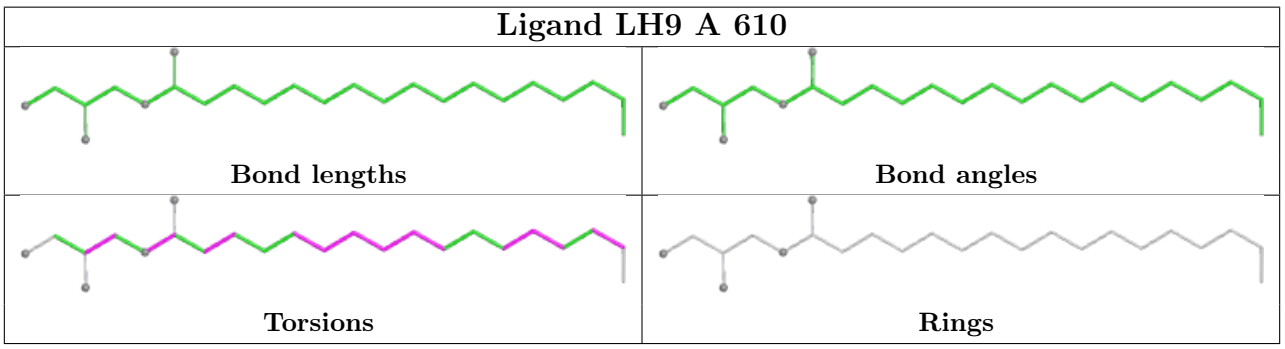
Ligand LH9 A 609



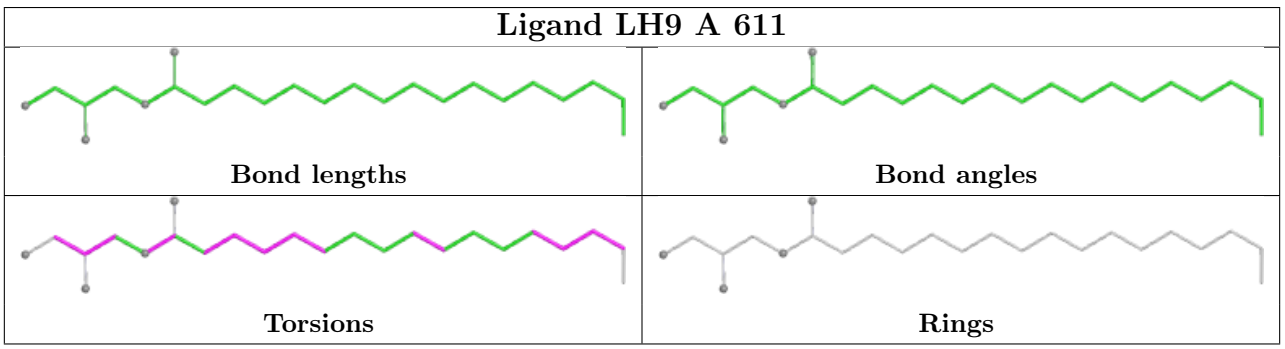
Ligand LH9 A 608



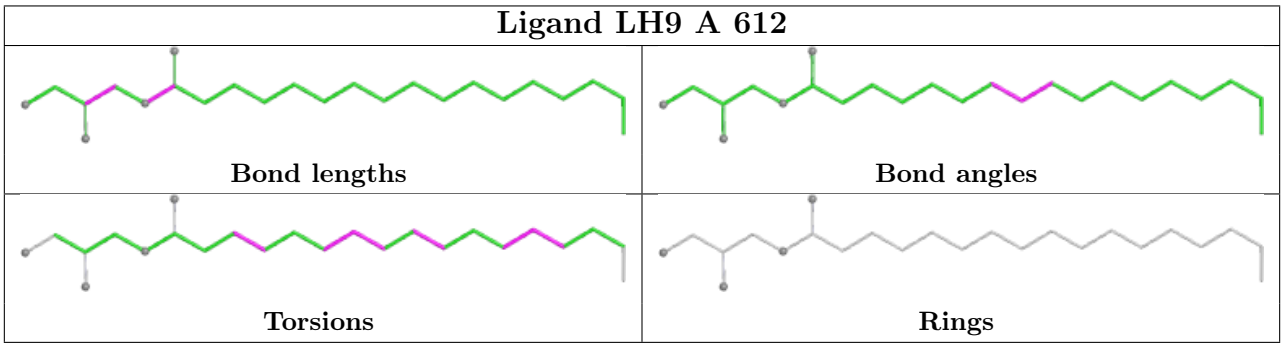
Ligand LH9 A 610



Ligand LH9 A 611



Ligand LH9 A 612



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^{th} 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^2)	Q<0.9
1	A	505/532 (94%)	0.45	39 (7%)	13	17	29, 41, 64, 87	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	LEU	6.6
1	A	358	PHE	5.1
1	A	508	ARG	4.7
1	A	352	ARG	4.5
1	A	415	TRP	4.4
1	A	353	PRO	4.3
1	A	351	LEU	4.0
1	A	418	LYS	4.0
1	A	192	TRP	3.8
1	A	426	PHE	3.7
1	A	119	THR	3.6
1	A	416	PHE	3.6
1	A	359	ASP	3.6
1	A	290	ASP	3.4
1	A	187	LEU	3.4
1	A	507	LEU	3.3
1	A	361	PRO	3.2
1	A	354	LEU	3.1
1	A	417	GLY	3.0
1	A	4	ALA	3.0
1	A	185	LEU	2.9
1	A	118	LYS	2.9
1	A	237	TRP	2.9
1	A	82	PHE	2.7
1	A	436	LEU	2.6
1	A	289	ARG	2.5
1	A	387	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	407	LEU	2.4
1	A	233	GLN	2.4
1	A	284	LEU	2.4
1	A	448	ILE	2.3
1	A	339	VAL	2.3
1	A	283	ALA	2.3
1	A	1	MET	2.2
1	A	287	GLU	2.2
1	A	414	ALA	2.1
1	A	497	LEU	2.1
1	A	413	ASP	2.0
1	A	3	PHE	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 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^{th} 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^2)	Q<0.9
3	LH9	A	612	24/24	0.54	0.41	62,81,96,98	0
2	GOL	A	601	6/6	0.60	0.24	88,106,107,107	0
3	LH9	A	611	24/24	0.65	0.38	79,96,102,102	0
2	GOL	A	604	6/6	0.67	0.29	69,70,84,84	0
3	LH9	A	607	24/24	0.67	0.34	66,81,93,93	0
3	LH9	A	608	24/24	0.71	0.30	67,81,91,93	0
3	LH9	A	610	24/24	0.71	0.25	66,79,94,95	0
3	LH9	A	609	24/24	0.72	0.24	66,81,86,87	0
2	GOL	A	605	6/6	0.73	0.26	67,80,85,85	0
2	GOL	A	603	6/6	0.76	0.27	74,76,91,91	0
2	GOL	A	606	6/6	0.76	0.20	76,91,91,92	0

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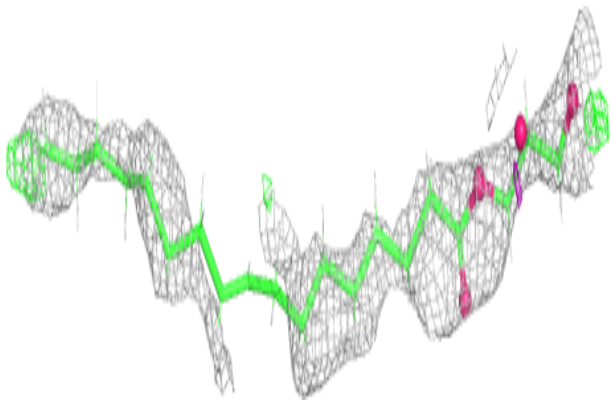
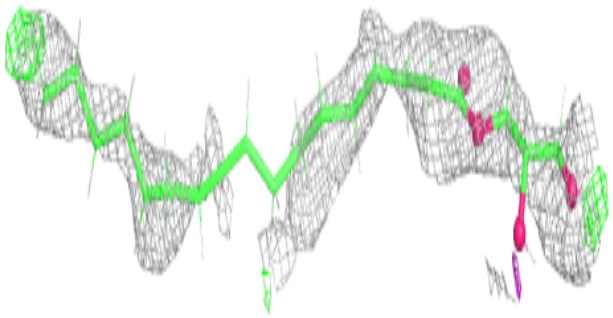
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	602	6/6	0.89	0.16	65,78,82,82	0

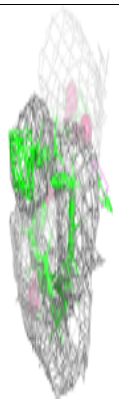
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LH9 A 612:

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

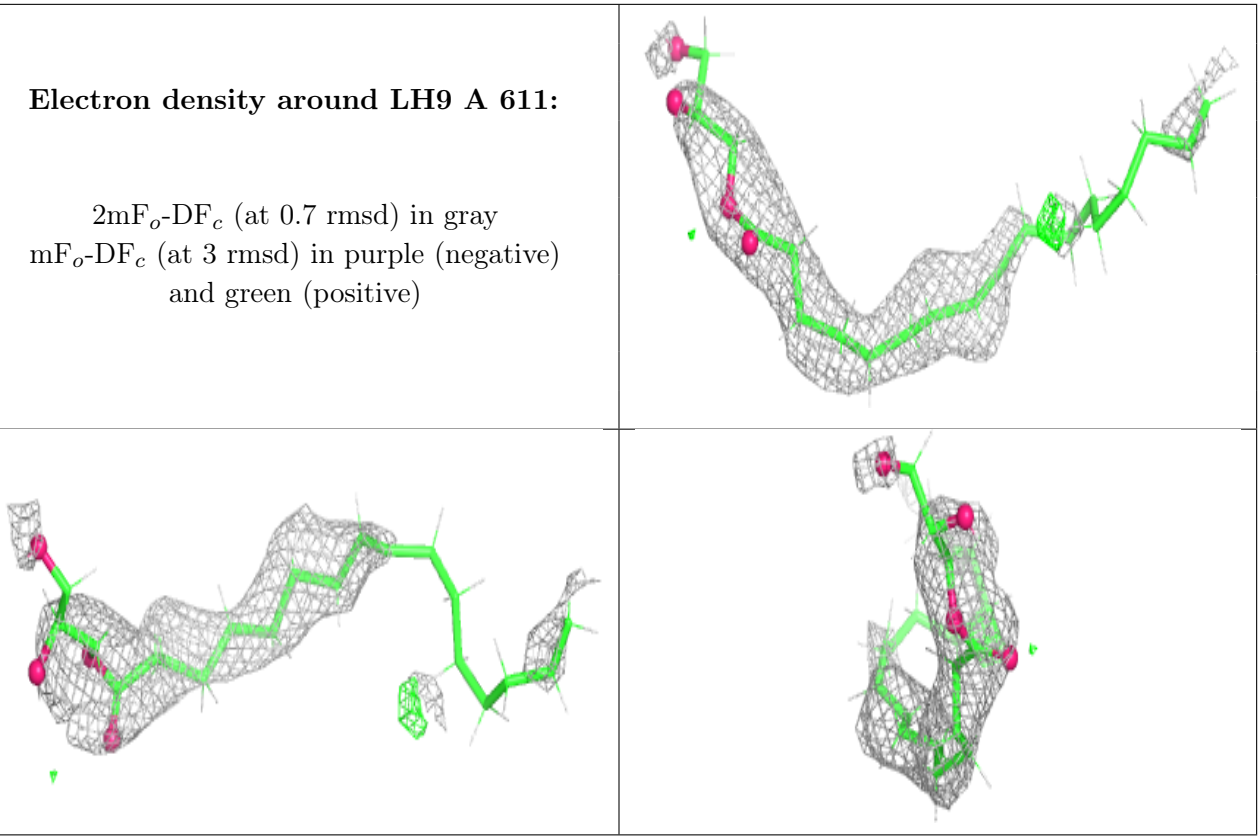






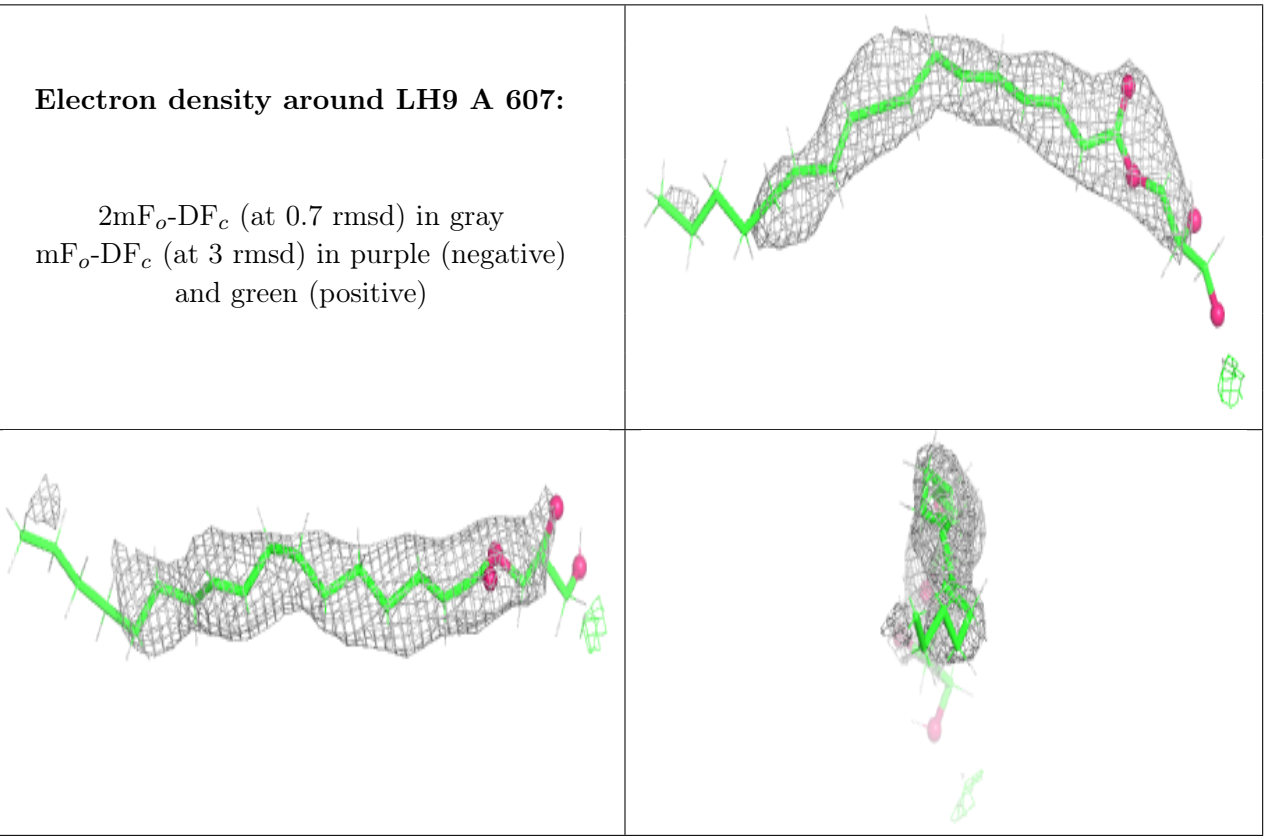
Electron density around LH9 A 611:

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



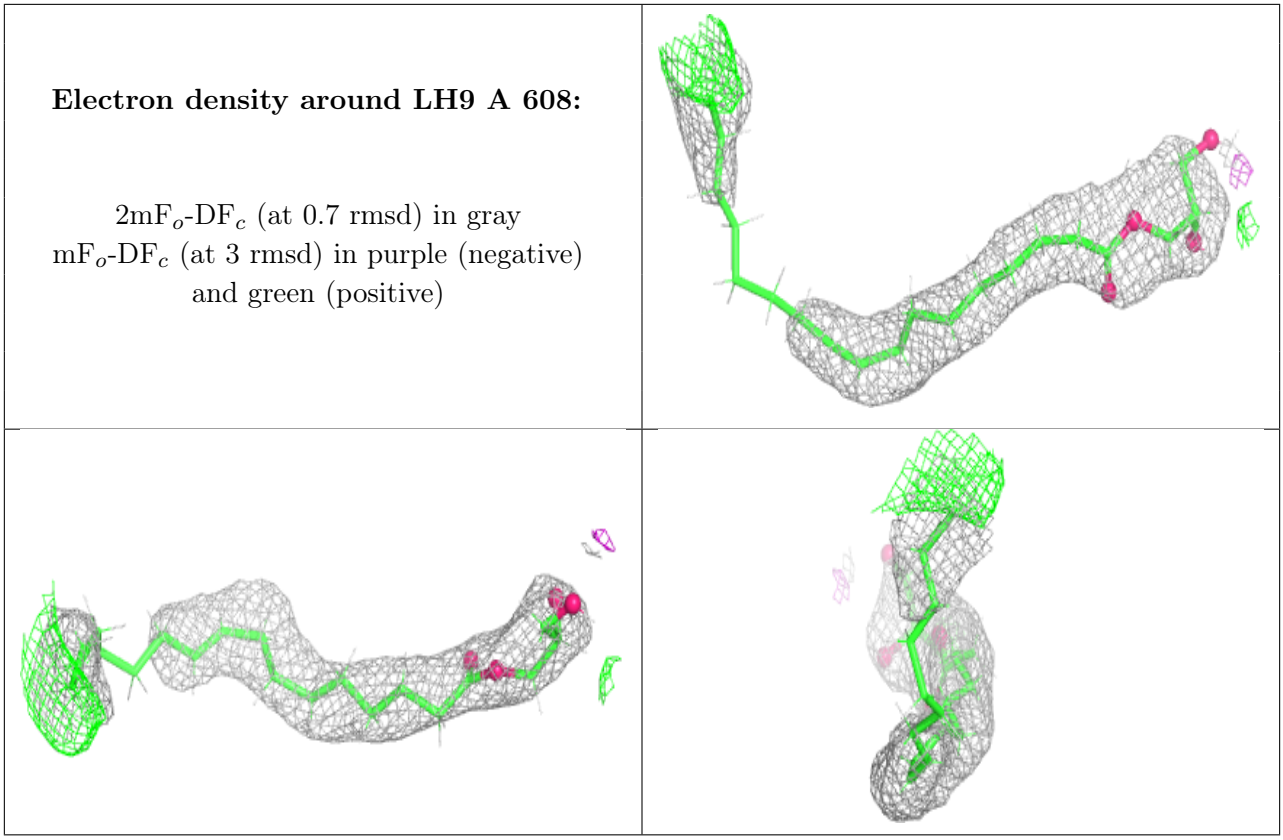
Electron density around LH9 A 607:

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



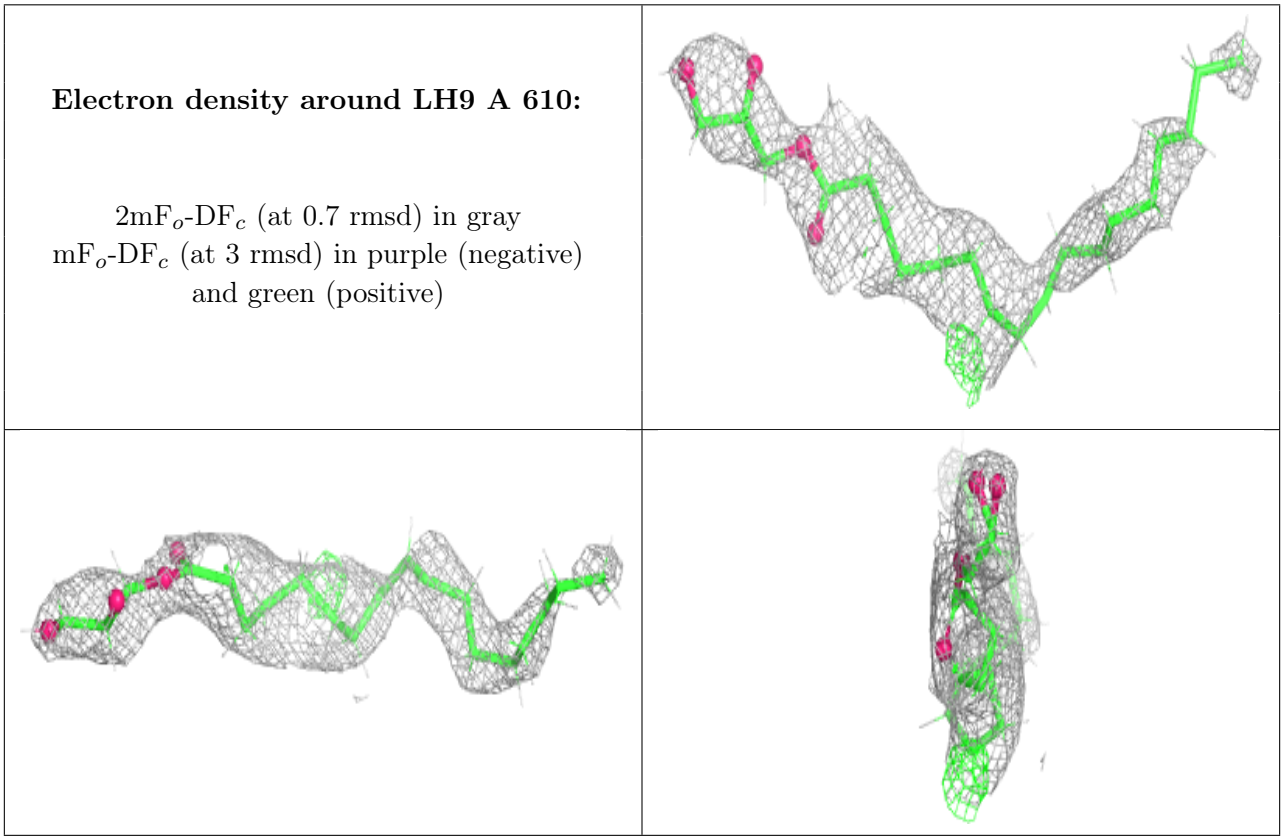
Electron density around LH9 A 608:

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



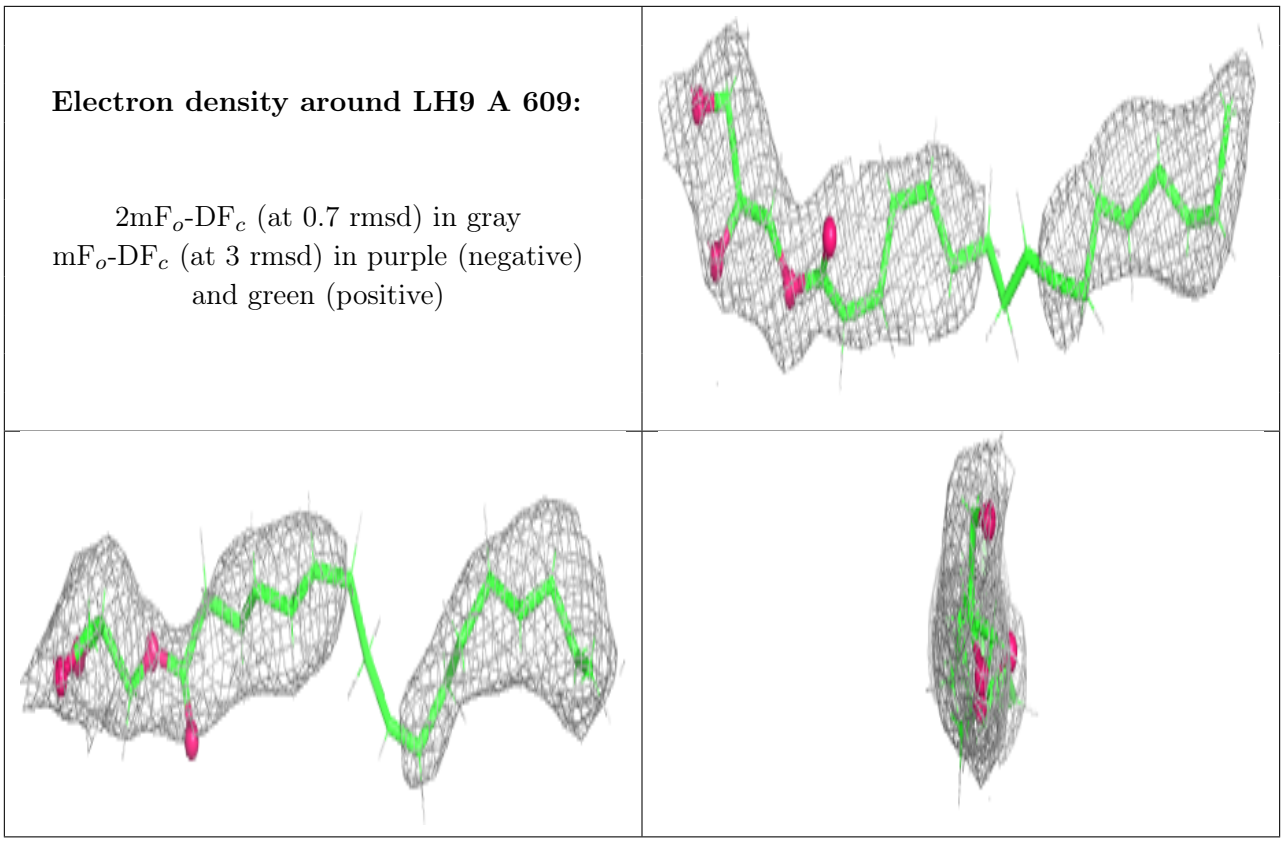
Electron density around LH9 A 610:

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



Electron density around LH9 A 609:

$2mF_o$-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.