



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:38 am BST

PDB ID : 2IU9
Title : Chlamydia trachomatis LpxD with 100mM UDPGlcNAc (Complex II)
Authors : Buetow, L.; Smith, T.K.; Dawson, A.; Fyffe, S.; Hunter, W.N.
Deposited on : 2006-05-30
Resolution : 3.10 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

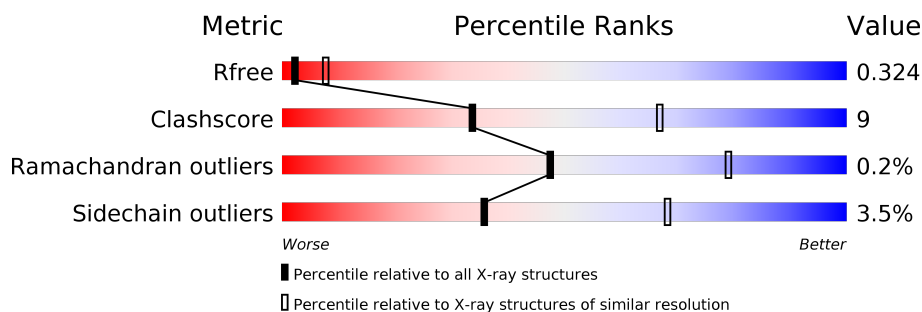
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	
1	C	374	

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
2	BME	A	1347	-	-	X	-

2 Entry composition [i](#)

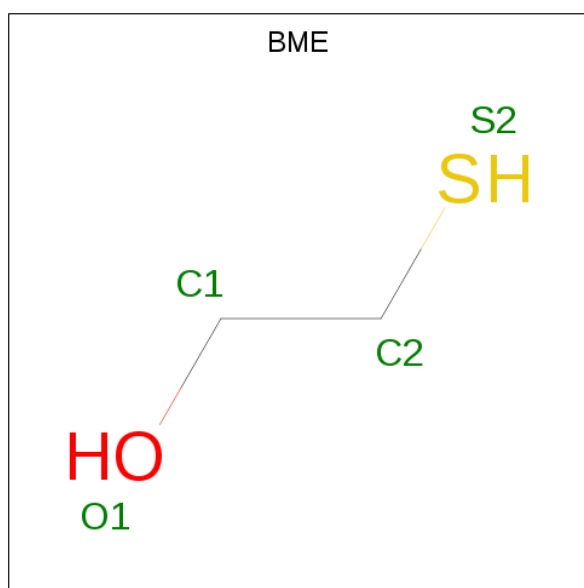
There are 6 unique types of molecules in this entry. The entry contains 8271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	8	0
			2675	1688	480	495	12			
1	B	345	Total	C	N	O	S	0	7	0
			2665	1682	476	497	10			
1	C	346	Total	C	N	O	S	0	5	0
			2666	1684	479	493	10			

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



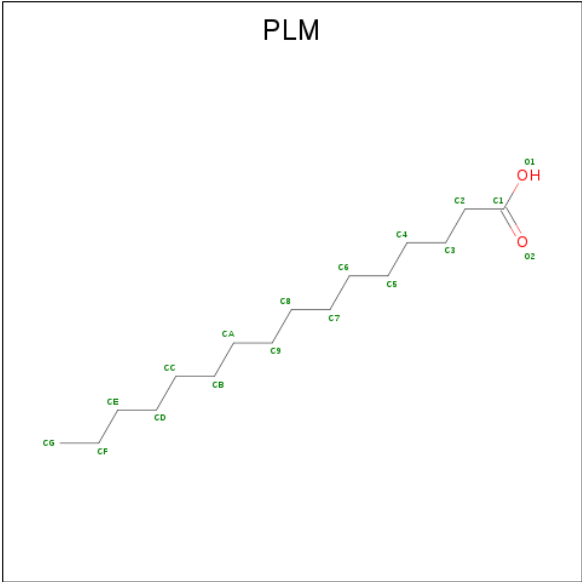
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



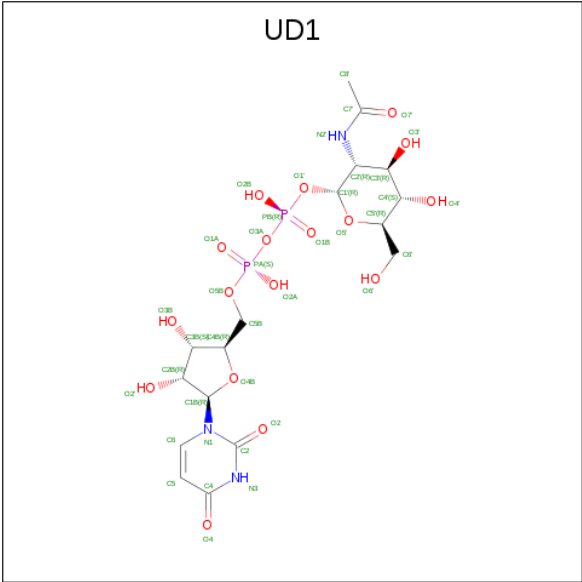
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			18	16	2		
4	B	1	Total	C	O	0	0
			18	16	2		
4	C	1	Total	C	O	0	0
			18	16	2		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
5	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

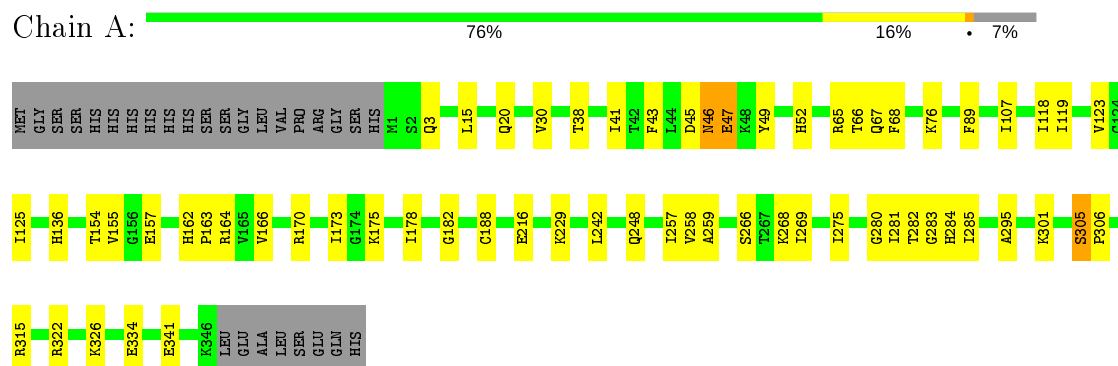
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	32	Total	O	0	0
			32	32		
6	C	20	Total	O	0	0
			20	20		

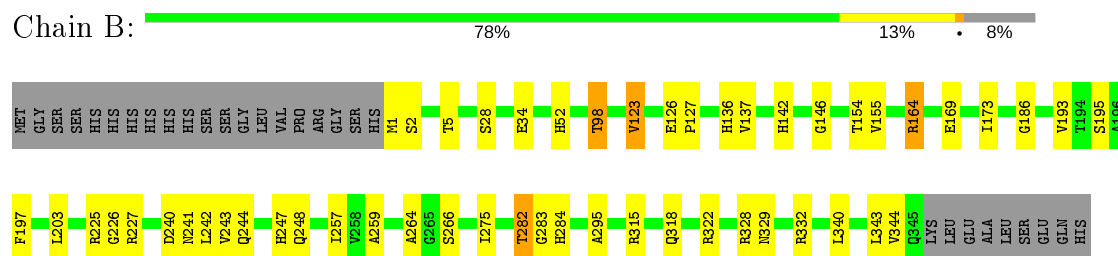
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

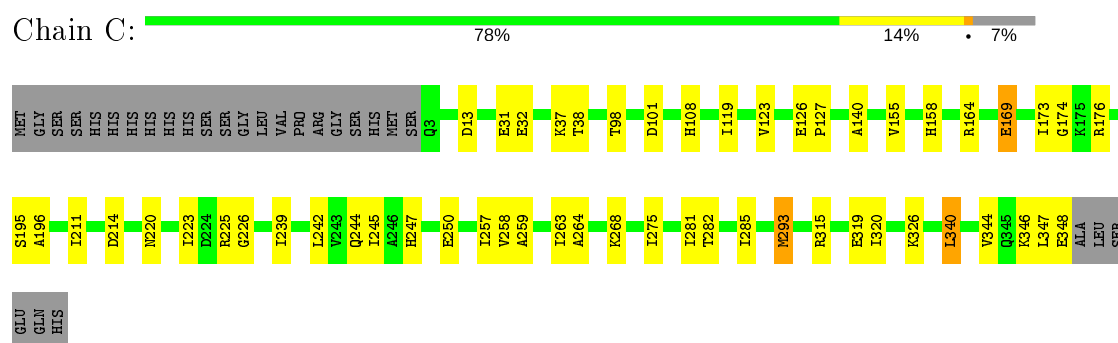
- Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE



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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.87Å 98.87Å 283.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.50 – 3.10 28.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.50-3.10) 99.0 (28.48-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.281 0.279 , 0.324	Depositor DCC
R_{free} test set	1323 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8271	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PLM, UD1, SO4, BME

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	0.35	0/2758	0.50	0/3729
1	B	0.34	0/2744	0.52	0/3712
1	C	0.37	1/2737 (0.0%)	0.51	0/3702
All	All	0.35	1/8239 (0.0%)	0.51	0/11143

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	GLU	C-O	7.46	1.37	1.23

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	2675	0	2695	63	0
1	B	2665	0	2680	48	0
1	C	2666	0	2688	49	0
2	A	4	0	6	5	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	31	3	0
4	B	18	0	31	3	0
4	C	18	0	31	7	0
5	B	39	0	25	1	0
5	C	39	0	25	13	0
6	A	47	0	0	1	0
6	B	32	0	0	1	0
6	C	20	0	0	0	0
All	All	8271	0	8212	139	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 9.

The worst 5 of 139 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:164[A]:ARG:HD2	1:C:164[A]:ARG:CG	1.71	1.19
5:C:1351:UD1:H6	5:C:1351:UD1:O1A	1.50	1.10
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:HG2	1.89	1.02
1:A:164[A]:ARG:NE	1:C:164[A]:ARG:HE	1.61	0.97
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:HG2	0.97	0.96

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	352/374 (94%)	333 (95%)	17 (5%)	2 (1%)	25	59
1	B	350/374 (94%)	325 (93%)	25 (7%)	0	100	100
1	C	349/374 (93%)	332 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1051/1122 (94%)	990 (94%)	59 (6%)	2 (0%)	47 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	47	GLU

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	293/309 (95%)	284 (97%)	9 (3%)	40 70
1	B	291/309 (94%)	278 (96%)	13 (4%)	27 60
1	C	290/309 (94%)	281 (97%)	9 (3%)	40 70
All	All	874/927 (94%)	843 (96%)	31 (4%)	36 68

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	242	LEU
1	B	322	ARG
1	C	319	GLU
1	B	282	THR
1	B	328	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	52	HIS
1	B	162	HIS
1	B	290	HIS
1	A	253	GLN
1	B	253	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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$
5	UD1	C	1351	-	34,41,41	1.47	4 (11%)	45,62,62	1.35	3 (6%)
3	SO4	A	1349	-	4,4,4	0.11	0	6,6,6	0.11	0
4	PLM	C	1352	-	14,17,17	0.29	0	13,17,17	0.48	0
4	PLM	B	1348	-	14,17,17	0.27	0	13,17,17	0.52	0
3	SO4	C	1350	-	4,4,4	0.12	0	6,6,6	0.13	0
3	SO4	B	1346	-	4,4,4	0.15	0	6,6,6	0.12	0
2	BME	A	1347	1	3,3,3	0.32	0	1,2,2	0.86	0
3	SO4	B	1351	-	4,4,4	0.16	0	6,6,6	0.05	0
5	UD1	B	1347	-	34,41,41	1.36	3 (8%)	45,62,62	1.39	4 (8%)
3	SO4	A	1348	-	4,4,4	0.16	0	6,6,6	0.08	0
4	PLM	A	1350	-	14,17,17	0.31	0	13,17,17	0.49	0
3	SO4	C	1349	-	4,4,4	0.15	0	6,6,6	0.06	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
5	UD1	C	1351	-	-	9/24/63/63	0/3/3/3
4	PLM	C	1352	-	-	10/13/15/15	-
4	PLM	B	1348	-	-	12/13/15/15	-
5	UD1	B	1347	-	-	12/24/63/63	0/3/3/3
2	BME	A	1347	1	-	0/1/1/1	-
4	PLM	A	1350	-	-	11/13/15/15	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1351	UD1	C4-N3	4.64	1.41	1.33
5	C	1351	UD1	C6-N1	4.48	1.41	1.35
5	B	1347	UD1	C4-N3	4.27	1.40	1.33
5	B	1347	UD1	C6-N1	4.08	1.40	1.35
5	C	1351	UD1	O5'-C1'	2.64	1.48	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1351	UD1	O5'-C1'-O1'	4.88	117.74	111.36
5	B	1347	UD1	PB-O3A-PA	-4.30	118.07	132.83
5	C	1351	UD1	PB-O3A-PA	-3.50	120.81	132.83
5	B	1347	UD1	O4B-C1B-C2B	-3.47	101.86	106.93
5	B	1347	UD1	O5'-C5'-C4'	3.37	115.81	109.69

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1351	UD1	O5'-C1'-O1'-PB
5	C	1351	UD1	C2B-C1B-N1-C6
5	C	1351	UD1	O4B-C1B-N1-C6
5	C	1351	UD1	O4B-C4B-C5B-O5B
5	C	1351	UD1	C5B-O5B-PA-O1A

There are no ring outliers.

7 monomers are involved in 33 short contacts:

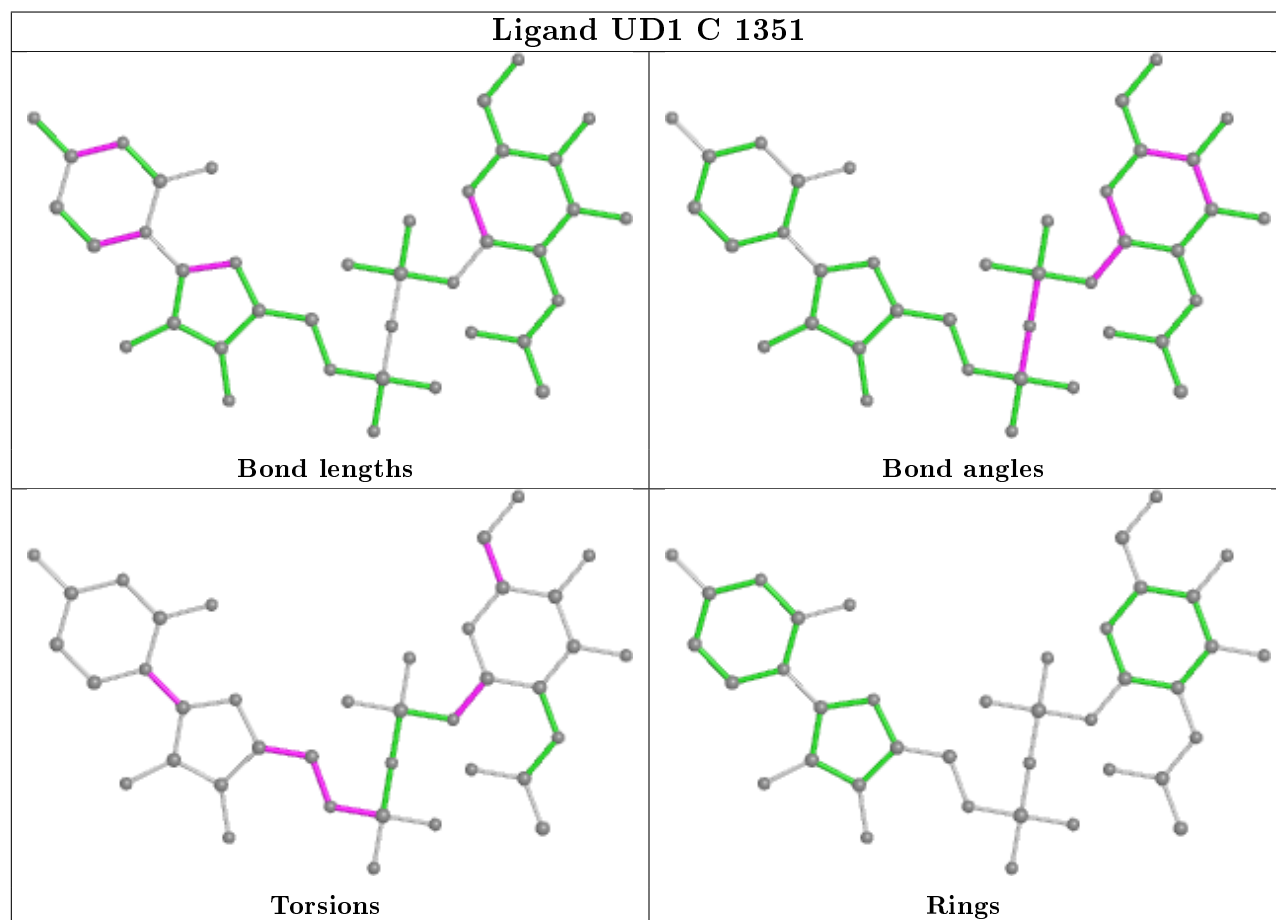
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1351	UD1	13	0
4	C	1352	PLM	7	0

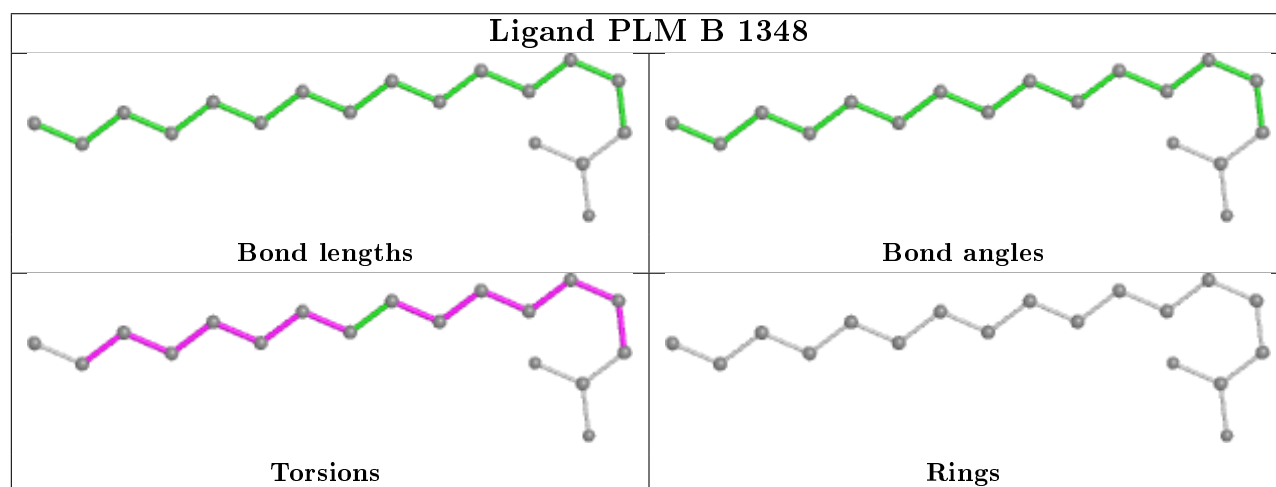
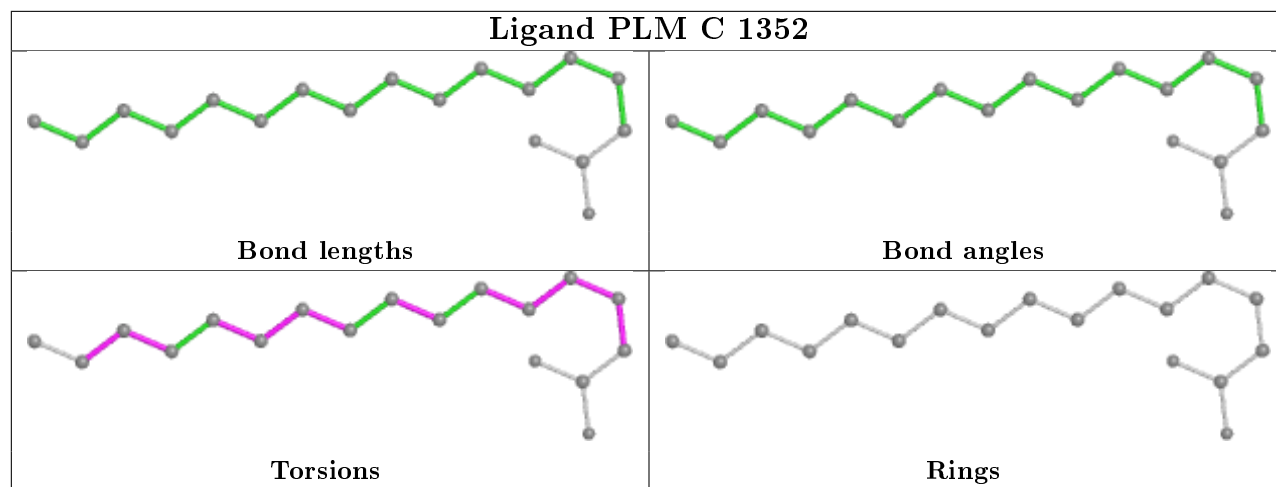
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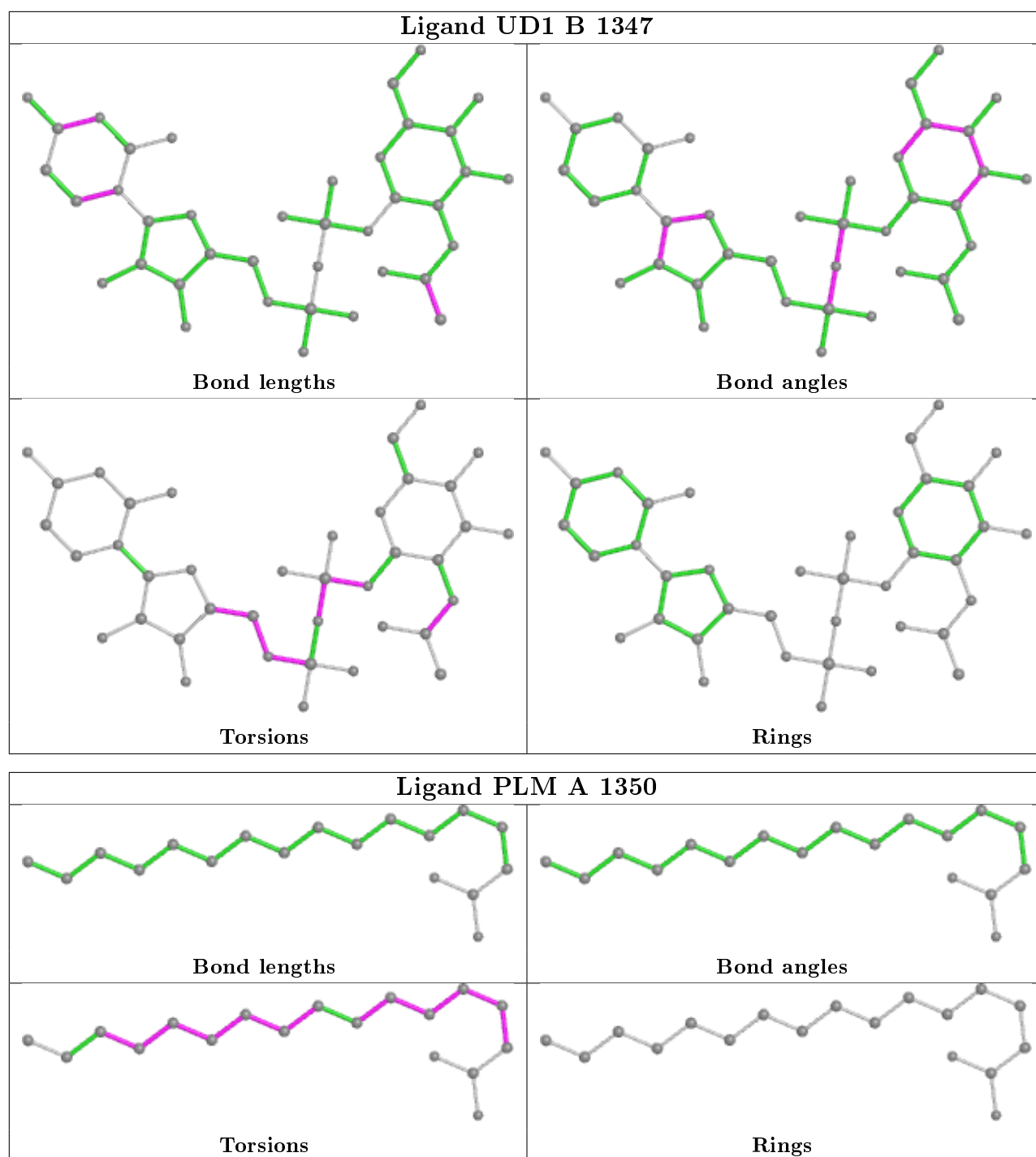
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1348	PLM	3	0
2	A	1347	BME	5	0
5	B	1347	UD1	1	0
3	A	1348	SO4	1	0
4	A	1350	PLM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

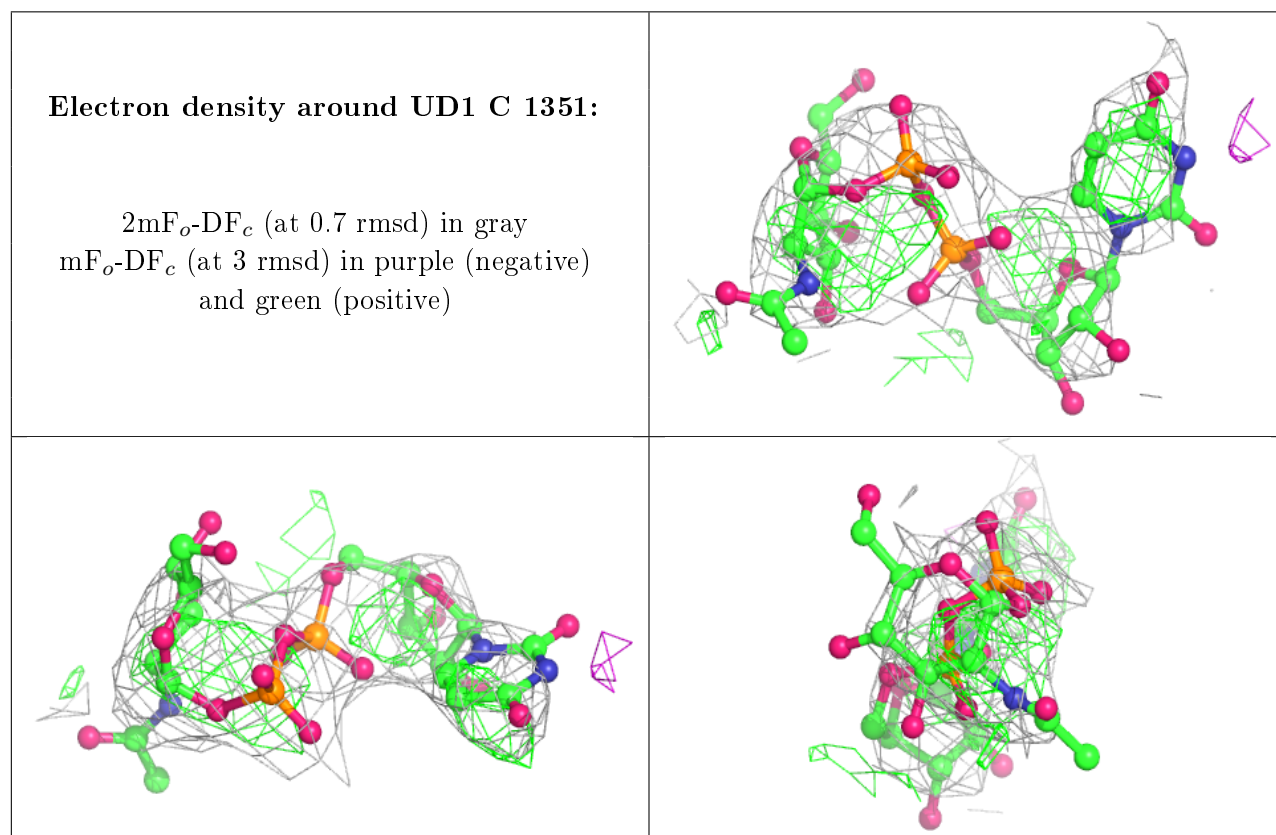
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

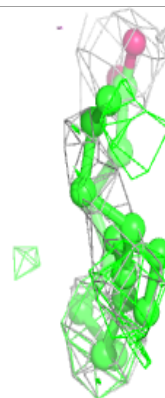
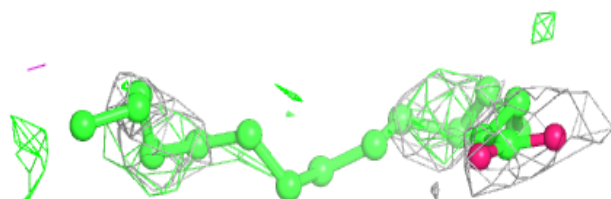
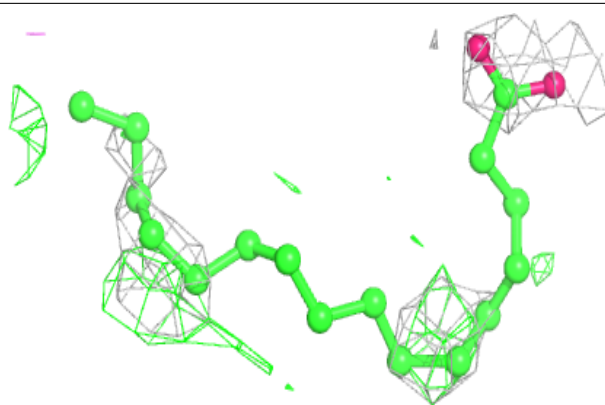
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

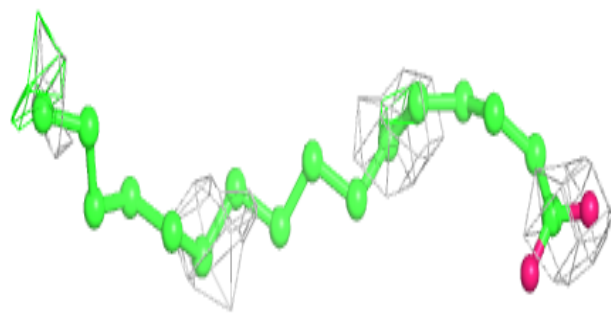
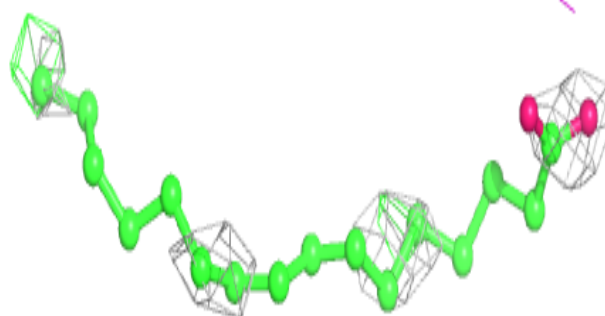


Electron density around PLM C 1352:

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

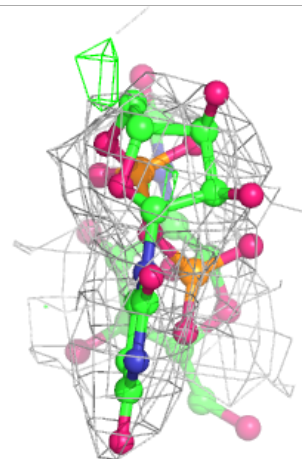
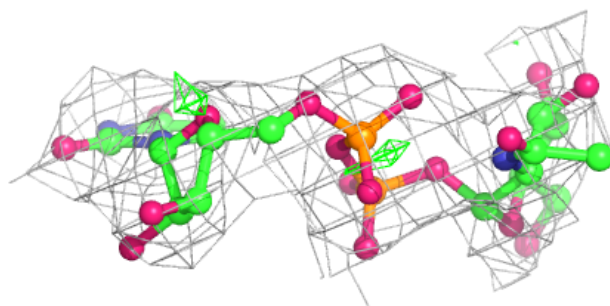
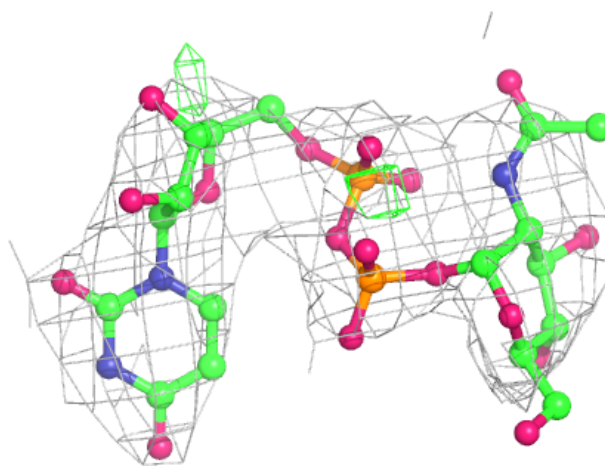
**Electron density around PLM B 1348:**

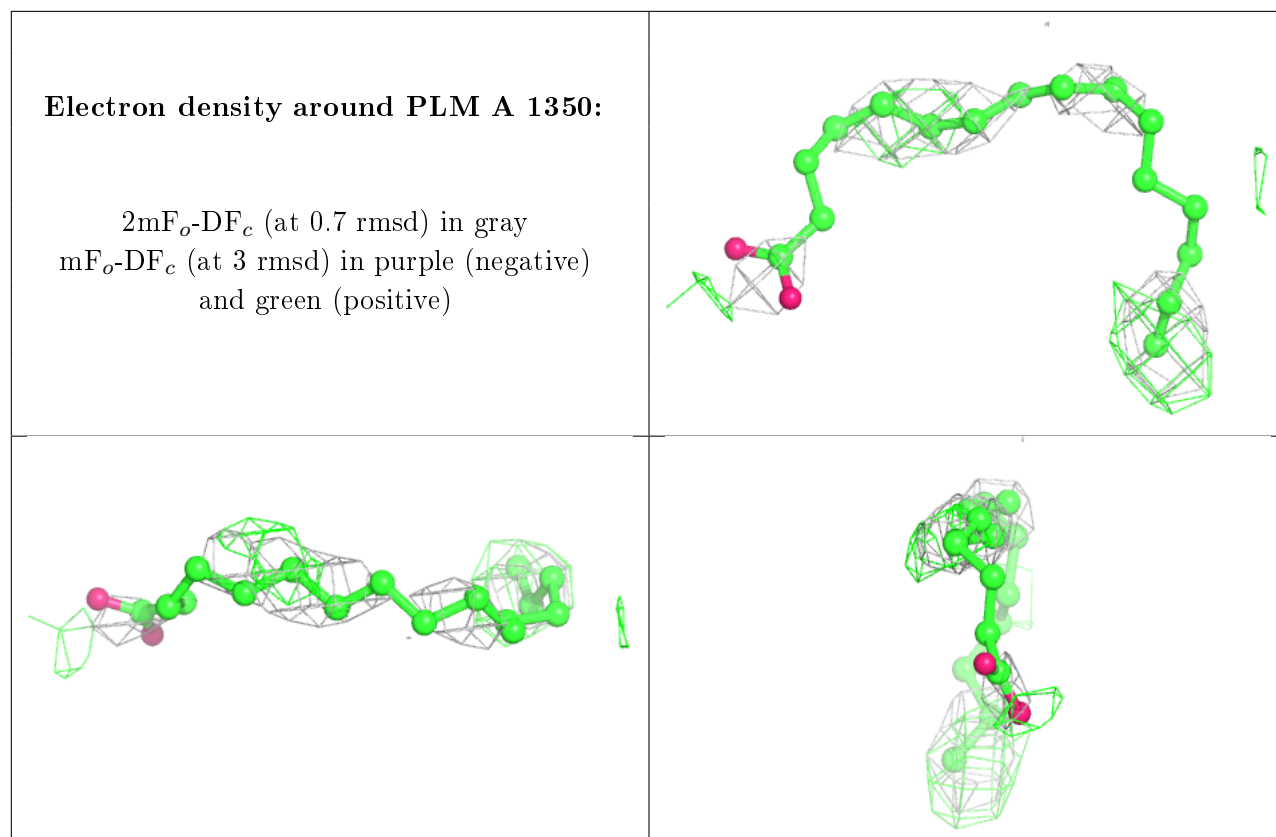
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UD1 B 1347:

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.