



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2022 – 06:37 am GMT

PDB ID : 7QZ8
Title : Transcriptional regulator LmrR with bound daunomycin and with Trp-67 and Trp-96 replaced by the unnatural amino acid 5,6-difluoroTrp
Authors : Thunnissen, A.M.W.H.
Deposited on : 2022-01-30
Resolution : 2.30 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 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 : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

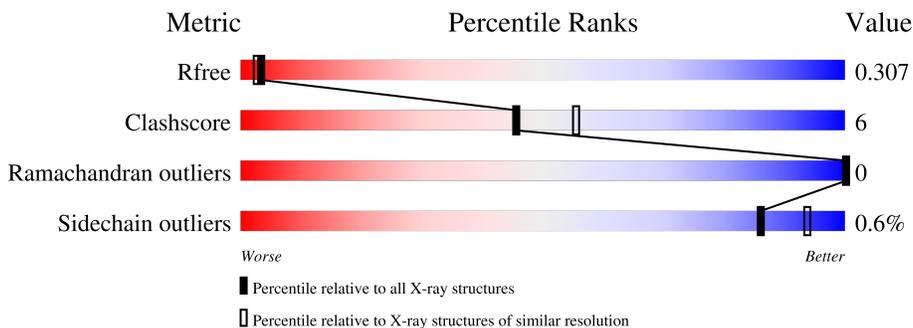
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	122	77% (green), 9% (yellow), 14% (grey)
1	B	122	68% (green), 15% (yellow), 17% (grey)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3391 atoms, of which 1639 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.

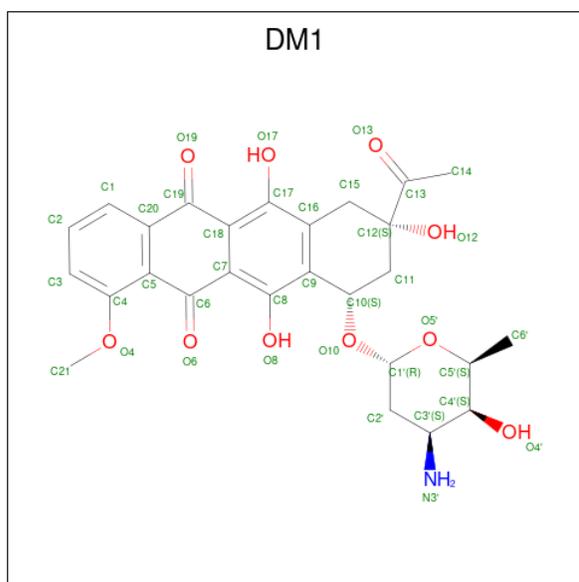
- Molecule 1 is a protein called Transcriptional regulator, PadR-like family.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	F	H	N	O	S			
1	A	105	1686	544	4	822	151	162	3	0	0	0
1	B	101	1628	533	4	789	141	158	3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	HIS	-	expression tag	UNP A2RI36
A	118	HIS	-	expression tag	UNP A2RI36
A	119	HIS	-	expression tag	UNP A2RI36
A	120	HIS	-	expression tag	UNP A2RI36
A	121	HIS	-	expression tag	UNP A2RI36
A	122	HIS	-	expression tag	UNP A2RI36
B	117	HIS	-	expression tag	UNP A2RI36
B	118	HIS	-	expression tag	UNP A2RI36
B	119	HIS	-	expression tag	UNP A2RI36
B	120	HIS	-	expression tag	UNP A2RI36
B	121	HIS	-	expression tag	UNP A2RI36
B	122	HIS	-	expression tag	UNP A2RI36

- Molecule 2 is DAUNOMYCIN (three-letter code: DM1) (formula: C₂₇H₂₉NO₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	66	27	28	1	10	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.15Å 35.74Å 71.15Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	70.51 – 2.30 70.51 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (70.51-2.30) 98.7 (70.51-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.241 , 0.317 0.238 , 0.307	Depositor DCC
R_{free} test set	716 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3391	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.63% 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: DM1, I3D

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	0.38	0/838	0.57	0/1114
1	B	0.30	0/814	0.54	0/1087
All	All	0.34	0/1652	0.55	0/2201

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	864	822	848	6	0
1	B	839	789	825	16	0
2	A	38	28	29	3	0
3	A	10	0	0	0	0
3	B	1	0	0	0	0
All	All	1752	1639	1702	22	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 6.

The worst 5 of 22 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:B:4:ILE:HD12	1:B:8:MET:CE	2.20	0.72
1:A:87:GLU:OE2	1:A:90:ARG:NH2	2.26	0.68
1:B:4:ILE:HD12	1:B:8:MET:HE1	1.77	0.66
1:B:46:ASN:ND2	1:B:49:THR:OG1	2.29	0.65
1:B:4:ILE:HG23	1:B:8:MET:HE2	1.89	0.53

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	99/122 (81%)	99 (100%)	0	0	100	100
1	B	96/122 (79%)	96 (100%)	0	0	100	100
All	All	195/244 (80%)	195 (100%)	0	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	90/105 (86%)	90 (100%)	0	100	100
1	B	89/105 (85%)	88 (99%)	1 (1%)	73	86
All	All	179/210 (85%)	178 (99%)	1 (1%)	86	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	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](#)

4 non-standard protein/DNA/RNA residues 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
1	I3D	A	67	1	15,17,18	1.09	1 (6%)	16,24,26	1.49	2 (12%)
1	I3D	B	67	1	15,17,18	1.06	1 (6%)	16,24,26	1.66	2 (12%)
1	I3D	A	96	1	15,17,18	1.03	1 (6%)	16,24,26	1.46	2 (12%)
1	I3D	B	96	1	15,17,18	1.01	1 (6%)	16,24,26	1.35	1 (6%)

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
1	I3D	A	67	1	-	0/4/6/8	0/2/2/2
1	I3D	B	67	1	-	0/4/6/8	0/2/2/2
1	I3D	A	96	1	-	1/4/6/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	I3D	B	96	1	-	0/4/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	I3D	CE3-CZ3	2.92	1.39	1.35
1	B	67	I3D	CE3-CZ3	2.68	1.39	1.35
1	B	96	I3D	CE3-CZ3	2.53	1.39	1.35
1	A	96	I3D	CE3-CZ3	2.15	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	I3D	CG-CB-CA	-4.82	107.07	114.53
1	B	96	I3D	CG-CB-CA	-4.55	107.50	114.53
1	A	67	I3D	CG-CB-CA	-4.10	108.18	114.53
1	A	96	I3D	CG-CB-CA	-3.48	109.14	114.53
1	A	67	I3D	CB-CG-CD1	-2.99	124.27	127.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	96	I3D	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	DM1	A	201	-	40,42,42	2.38	8 (20%)	54,66,66	1.21	5 (9%)

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	DM1	A	201	-	-	3/12/58/58	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	DM1	O4-C4	-7.77	1.24	1.37
2	A	201	DM1	C17-C16	7.25	1.51	1.40
2	A	201	DM1	C8-C9	5.24	1.49	1.40
2	A	201	DM1	O13-C13	4.90	1.31	1.21
2	A	201	DM1	C20-C19	-4.17	1.39	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	DM1	C21-O4-C4	4.31	124.04	117.53
2	A	201	DM1	C20-C5-C4	2.62	120.94	118.11
2	A	201	DM1	O5'-C5'-C6'	2.61	112.33	106.70
2	A	201	DM1	O4-C4-C5	2.55	119.40	115.85
2	A	201	DM1	C8-C7-C6	-2.15	116.84	120.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

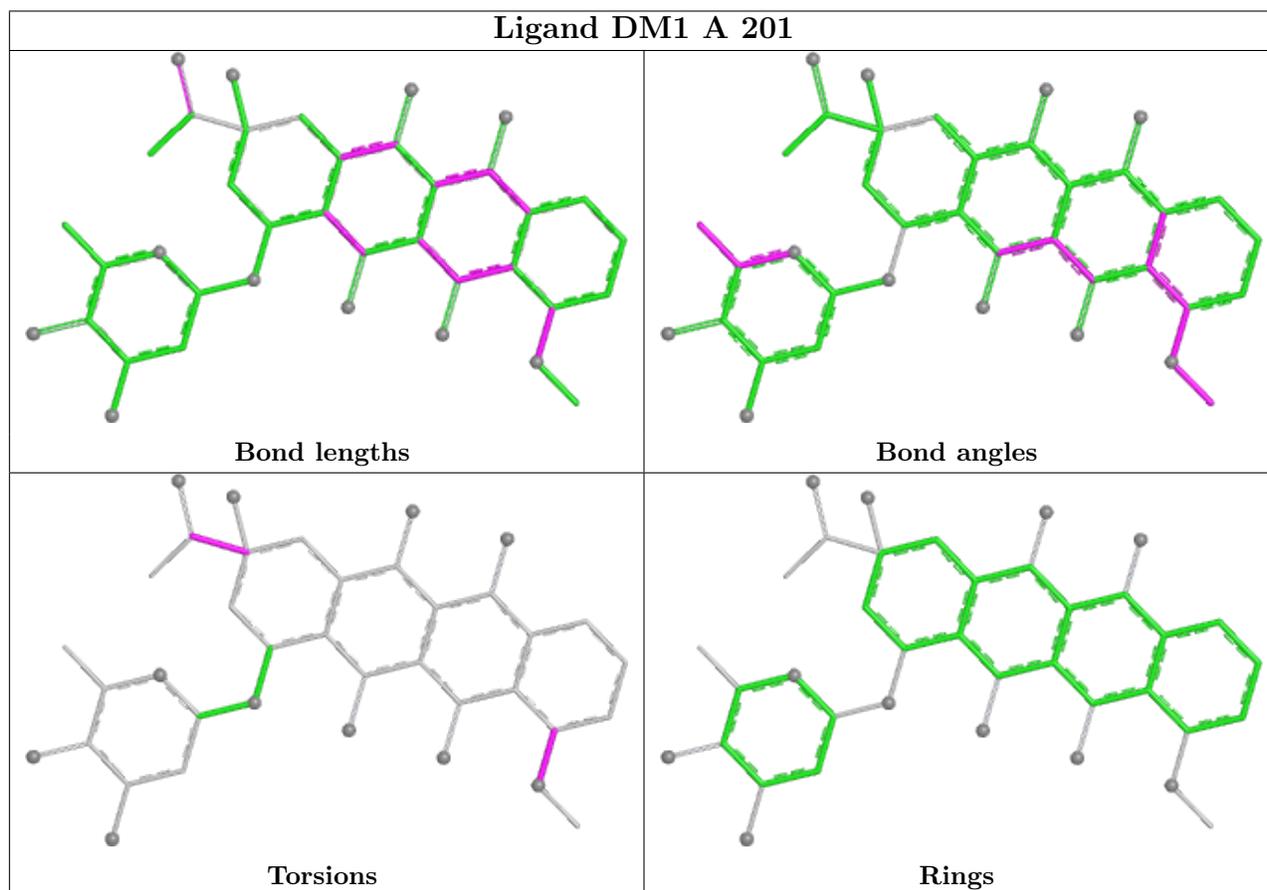
Mol	Chain	Res	Type	Atoms
2	A	201	DM1	C3-C4-O4-C21
2	A	201	DM1	C5-C4-O4-C21
2	A	201	DM1	O12-C12-C13-O13

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	DM1	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

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.

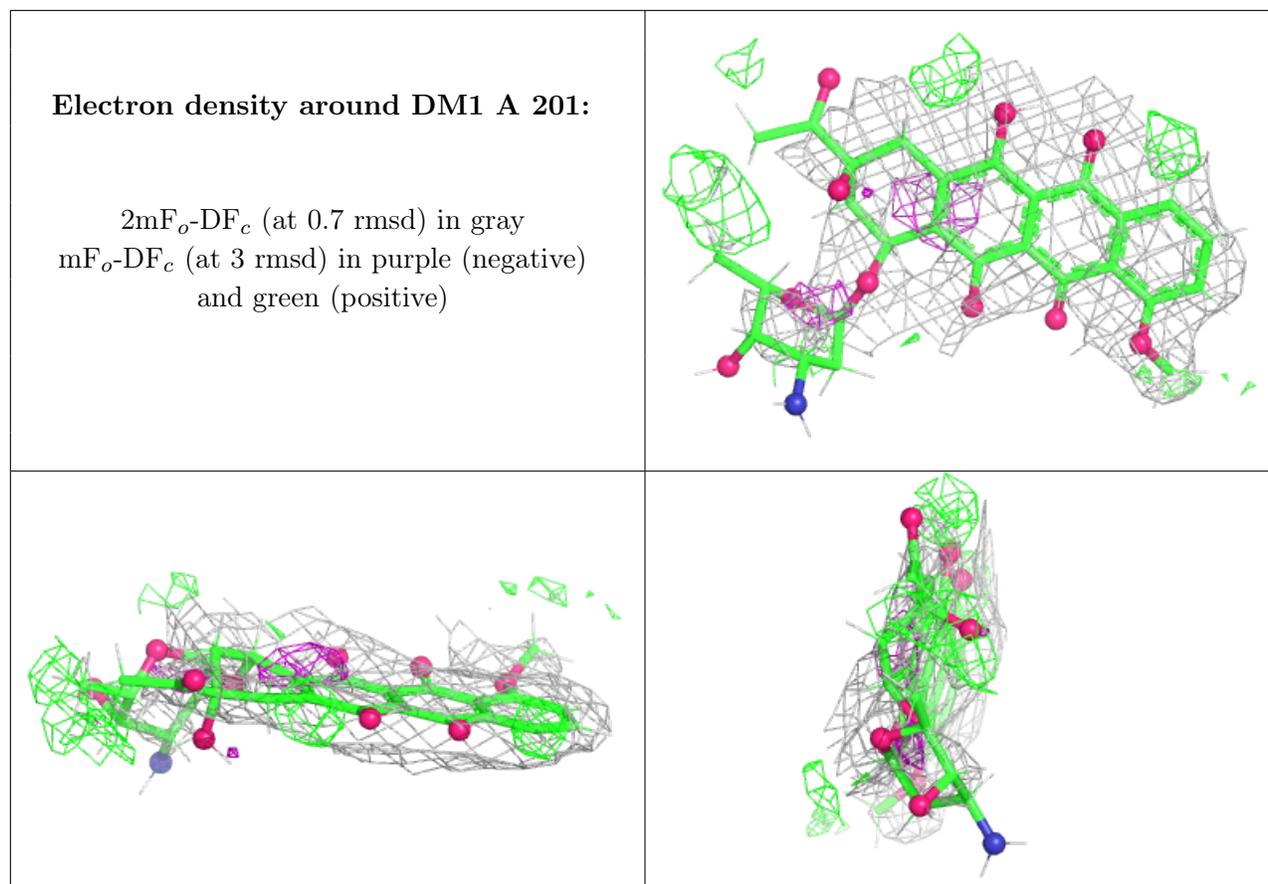
6.3 Carbohydrates

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.



6.5 Other polymers [\(i\)](#)

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