



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2021 – 10:01 PM EDT

PDB ID : 4QCD
Title : Neutron crystal structure of phycocyanobilin:ferredoxin oxidoreductase in complex with biliverdin IXalpha at room temperature.
Authors : Unno, M.; Ishikawa-Suto, K.; Ishihara, M.; Hagiwara, Y.; Sugishima, M.; Wada, K.; Fukuyama, K.
Deposited on : 2014-05-10
Resolution : 1.93 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 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 : 2.19
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) : 2.19

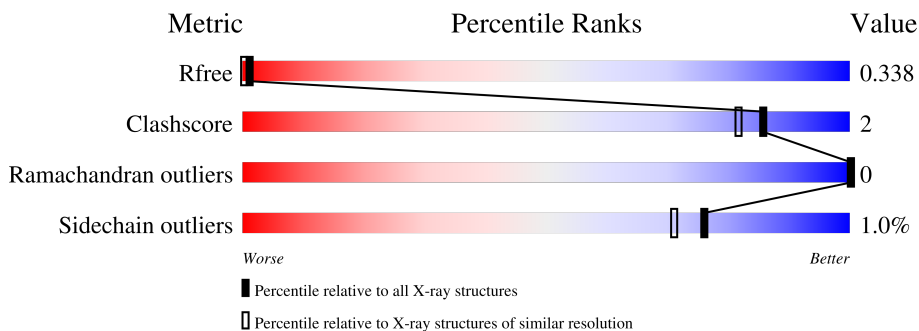
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

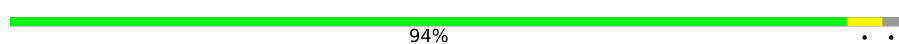
The reported resolution of this entry is 1.93 Å.

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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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	248	 94%

2 Entry composition [i](#)

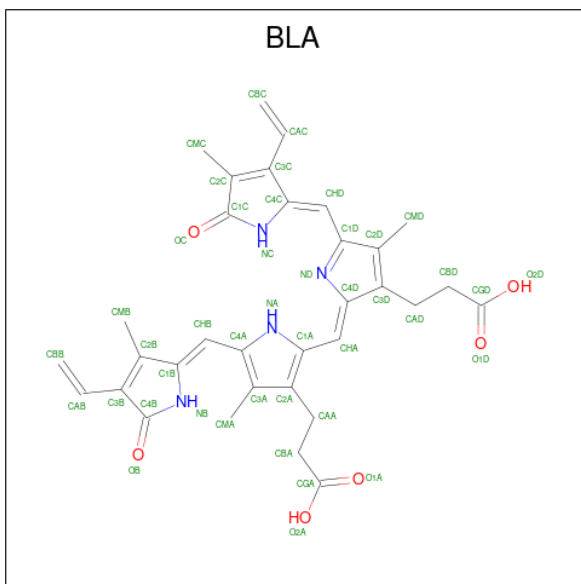
There are 4 unique types of molecules in this entry. The entry contains 5070 atoms, of which 2058 are hydrogens and 760 are deuteriums.

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 Phycocyanobilin:ferredoxin oxidoreductase.

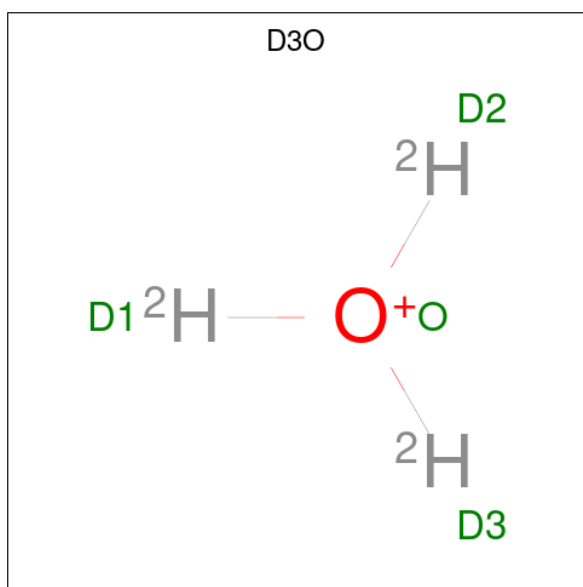
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	242	4458	1298	406	2029	336	374	15	84	225	0

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	D	H	N	O		
2	A	1	76	33	4	29	4	6	0	0

- Molecule 3 is trideuteriooxidanium (three-letter code: D3O) (formula: D_3O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	D	O	0	0
			4	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	185	Total	D	O	0	0
			532	347	185		

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. 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: Phycocyanobilin:ferredoxin oxidoreductase

Chain A:  94%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.11Å 97.28Å 43.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.19 – 1.93 21.19 – 1.93	Depositor EDS
% Data completeness (in resolution range)	79.4 (21.19-1.93) 79.4 (21.19-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.93Å)	Xtrriage
Refinement program	CNS, PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.167 , 0.227 0.330 , 0.338	Depositor DCC
R_{free} test set	1839 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	5.7	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.84 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	5070	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BLA, D3O

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	0.72	0/3832	0.82	12/5192 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166[A]	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	166[B]	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	A	71[A]	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	71[B]	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	179[A]	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	179[B]	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	183[A]	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	A	183[B]	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	A	14[A]	MET	CG-SD-CE	-5.36	91.62	100.20
1	A	14[B]	MET	CG-SD-CE	-5.36	91.62	100.20
1	A	183[A]	PHE	CB-CG-CD1	5.12	124.38	120.80
1	A	183[B]	PHE	CB-CG-CD1	5.12	124.38	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2429	2029	393	4	0
2	A	47	29	32	4	0
3	A	4	0	0	0	0
4	A	532	0	0	2	0
All	All	3012	2058	425	9	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 2.

All (9) 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)
2:A:301:BLA:HMB1	2:A:301:BLA:HBB1	1.61	0.71
2:A:301:BLA:HBC1	2:A:301:BLA:HMC1	1.76	0.56
1:A:228[A]:LYS:NZ	4:A:569:HOH:O	2.48	0.42

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	465/248 (188%)	457 (98%)	8 (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	405/216 (188%)	401 (99%)	4 (1%)	76 71

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33[A]	GLN
1	A	33[B]	GLN
1	A	41[A]	GLN
1	A	41[B]	GLN

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](#)

Of 2 ligands modelled in this entry, 1 is modelled with single atom - 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	BLA	A	301	-	36,46,46	2.80	9 (25%)	47,67,67	1.89	9 (19%)

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	BLA	A	301	-	-	2/22/74/74	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	BLA	C4C-NC	8.20	1.51	1.37
2	A	301	BLA	C1B-NB	7.55	1.50	1.37
2	A	301	BLA	C1C-NC	6.50	1.51	1.38
2	A	301	BLA	C4B-NB	5.54	1.49	1.38
2	A	301	BLA	C4D-ND	4.62	1.48	1.38
2	A	301	BLA	CHD-C1D	2.92	1.47	1.40
2	A	301	BLA	CHA-C4D	-2.76	1.32	1.35
2	A	301	BLA	C4D-C3D	2.69	1.50	1.45
2	A	301	BLA	C1D-ND	2.45	1.42	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	BLA	C3D-C4D-ND	-5.62	101.88	110.05
2	A	301	BLA	CMB-C2B-C1B	-4.38	118.69	124.17
2	A	301	BLA	C4D-C3D-C2D	4.30	111.54	106.78
2	A	301	BLA	C4C-NC-C1C	-3.79	105.84	110.67
2	A	301	BLA	C3B-C2B-C1B	3.76	112.57	108.03
2	A	301	BLA	C1B-NB-C4B	-3.23	106.56	110.67
2	A	301	BLA	OC-C1C-NC	-2.85	118.45	125.08
2	A	301	BLA	CHA-C4D-ND	2.64	132.49	128.83
2	A	301	BLA	CAD-C3D-C4D	-2.59	120.42	125.01

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	BLA	ND-C4D-CHA-C1A

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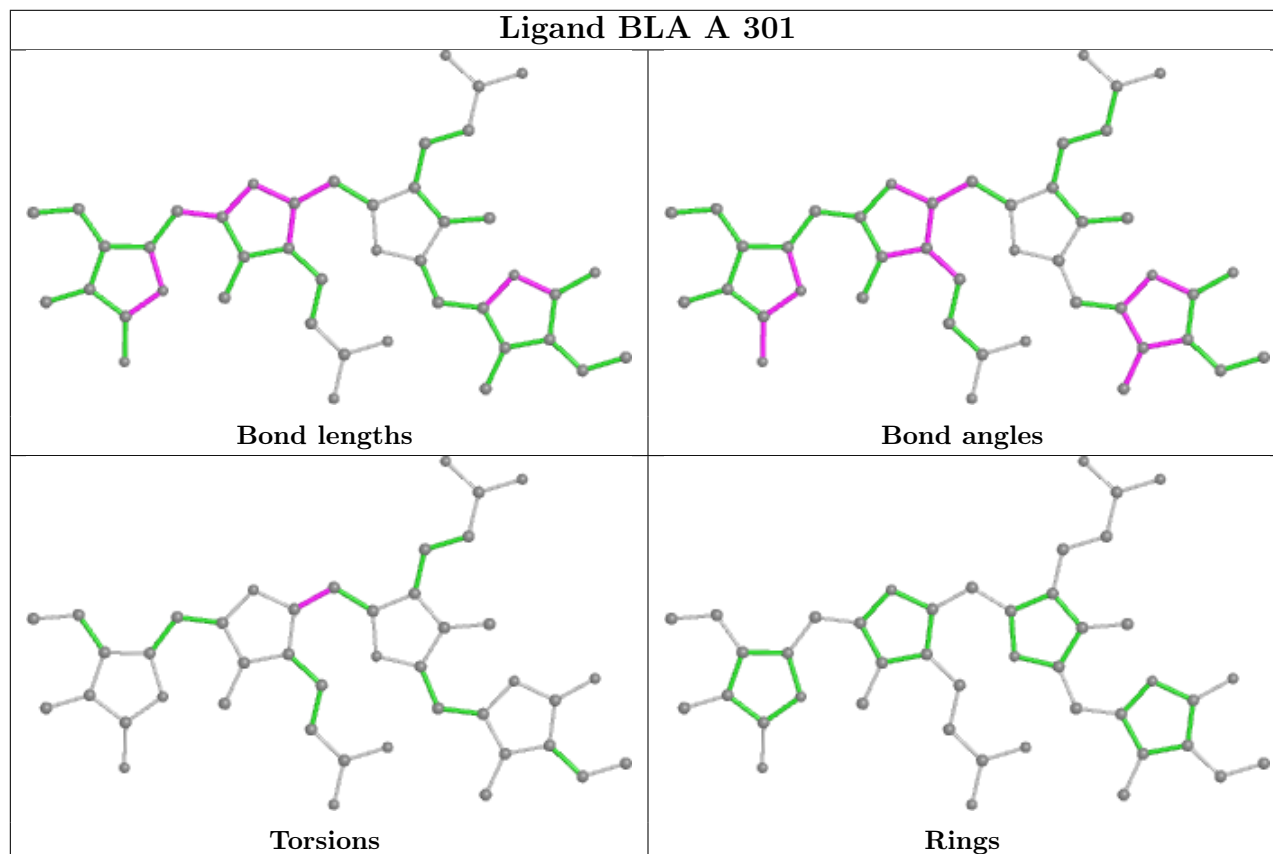
Mol	Chain	Res	Type	Atoms
2	A	301	BLA	C3D-C4D-CHA-C1A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	BLA	4	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.

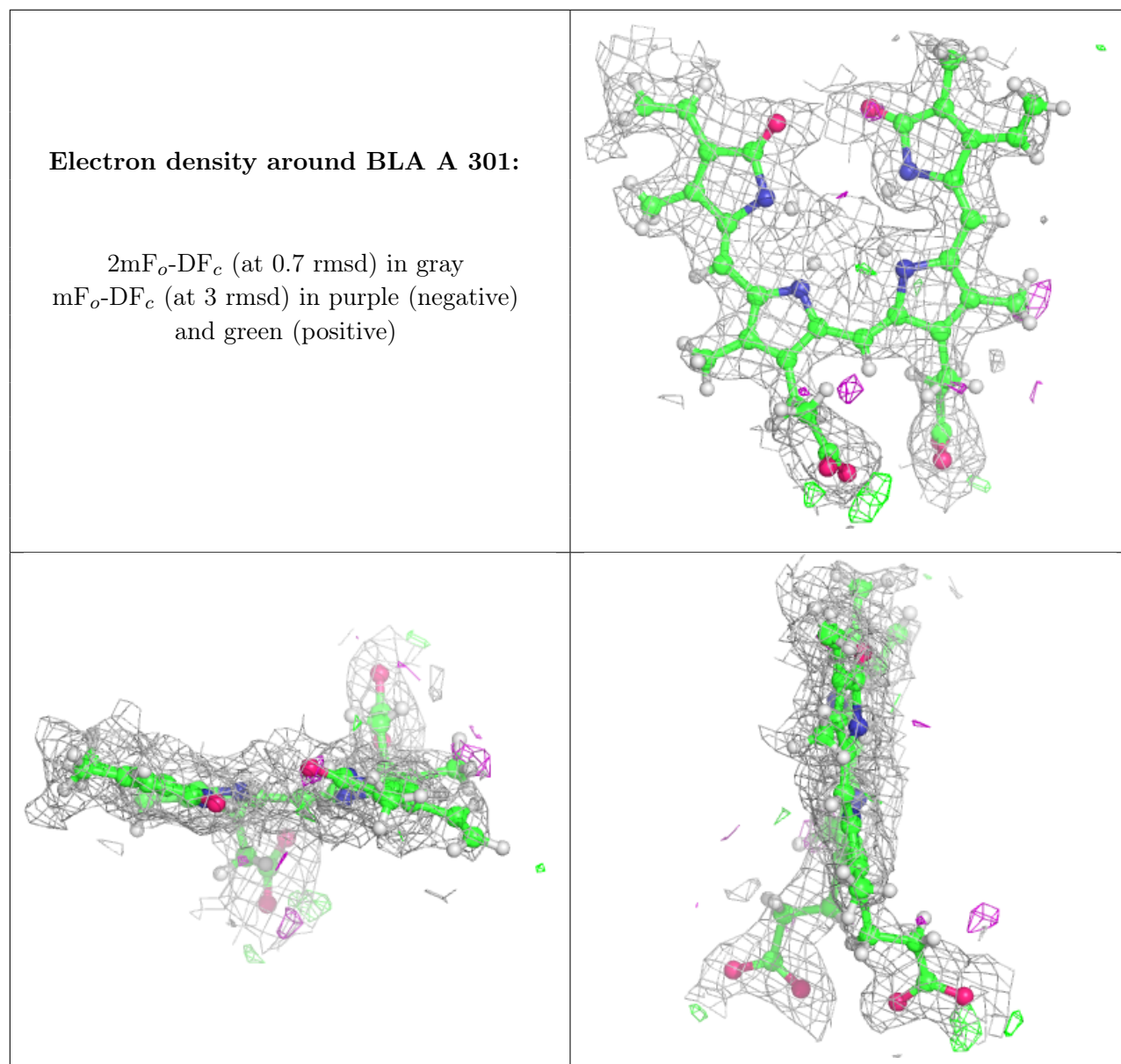
6.3 Carbohydrates

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.



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

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