



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4ZPL / pdb_00004zpl
Title : Crystal Structure of Protocadherin Beta 1 EC1-3
Authors : Goodman, K.M.; Bahna, F.; Shapiro, L.
Deposited on : 2015-05-08
Resolution : 3.30 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:

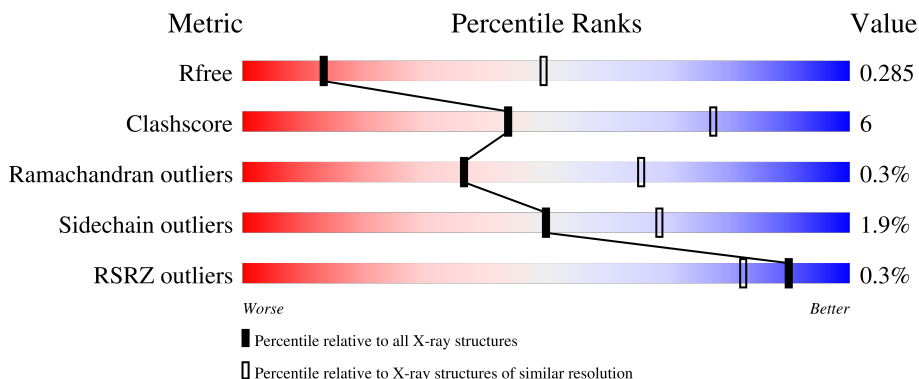
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.



2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2572 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 Protein Pcdhb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2415	1521	420	470	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	Ca 6	0	0

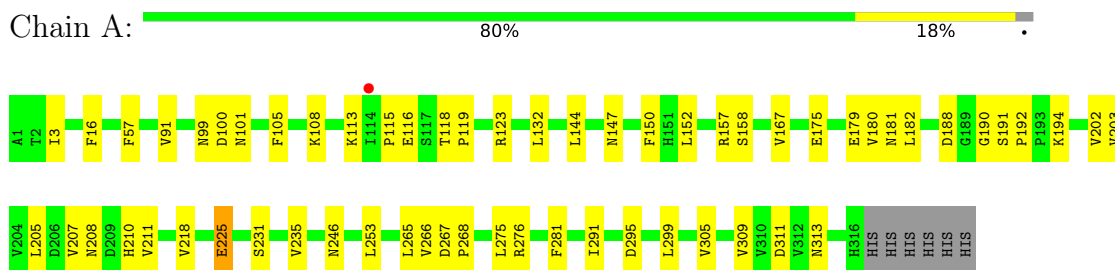
- Molecule 4 is water.

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

3 Residue-property plots

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: Protein Pcdhb1



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.99Å 106.52Å 149.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 3.30 41.70 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.70-3.30) 89.8 (41.70-3.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.231 , 0.278 0.237 , 0.285	Depositor DCC
R_{free} test set	498 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ^{2</}		

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: NAG, FUC, CA, BMA

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	0.27	0/2460	0.75	0/3353

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD23	1:A:276:ARG:HB3	1.78	0.64
1:A:123:ARG:HG2	1:A:167:VAL:HG22	1.83	0.60
1:A:180:VAL:HG13	1:A:202:VAL:HB	1.88	0.56
1:A:99:ASN:HD22	1:A:190:GLY:HA3	1.71	0.56
1:A:188:ASP:OD1	1:A:194:LYS:N	2.39	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	Res	Type
1	A	181	ASN
1	A	218	VAL
1	A	225	GLU
1	A	235	VAL
1	A	305	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	226	ASN
1	A	292	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 ⓘ

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	C	3	2	11,11,12	0.68	0	15,15,17	0.70	0
2	FUC	C	4	2	10,10,11	0.76	0	14,14,16	1.06	1 (7%)
2	NAG	D	1	2,1	14,14,15	0.29	0	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	0.64	0
2	BMA	D	3	2	11,11,12	0.68	0	15		

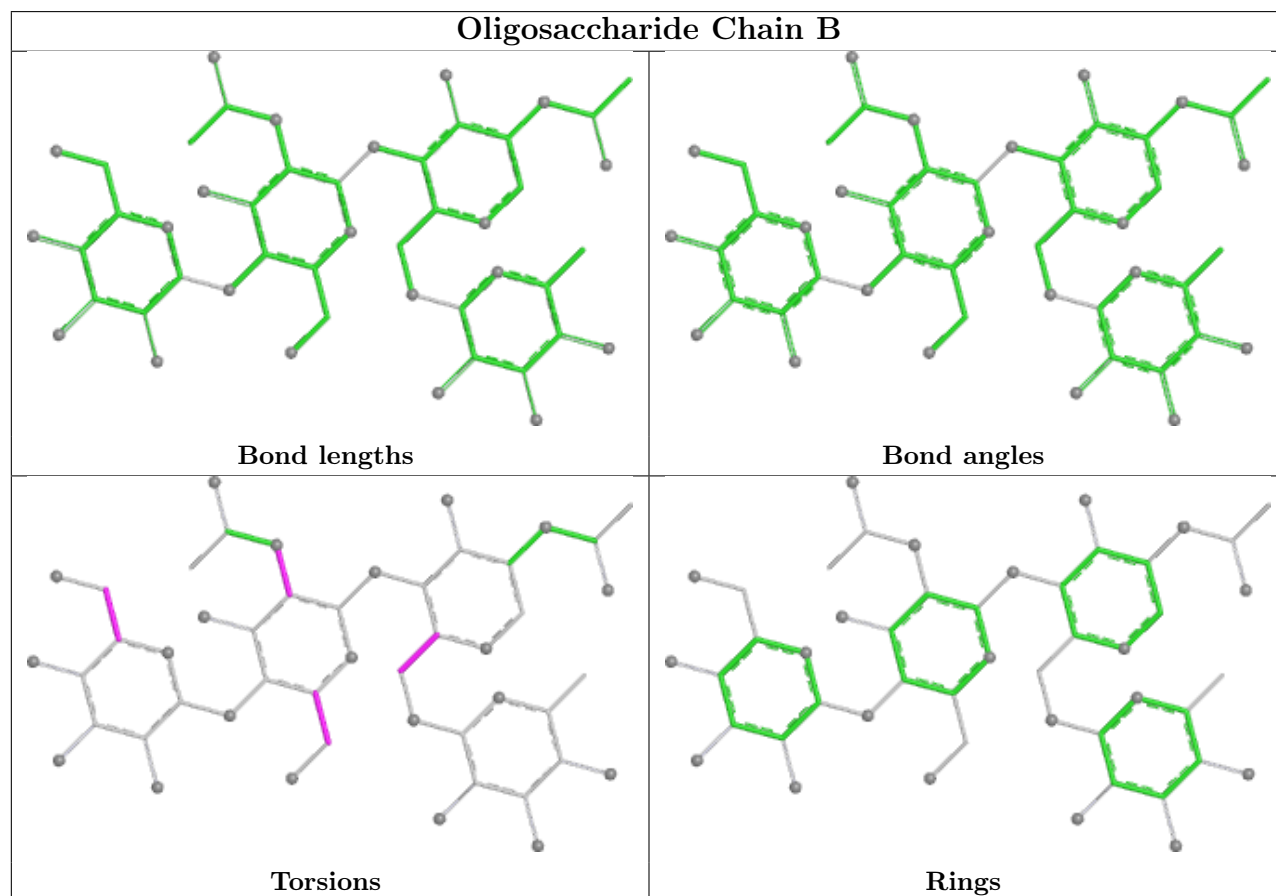
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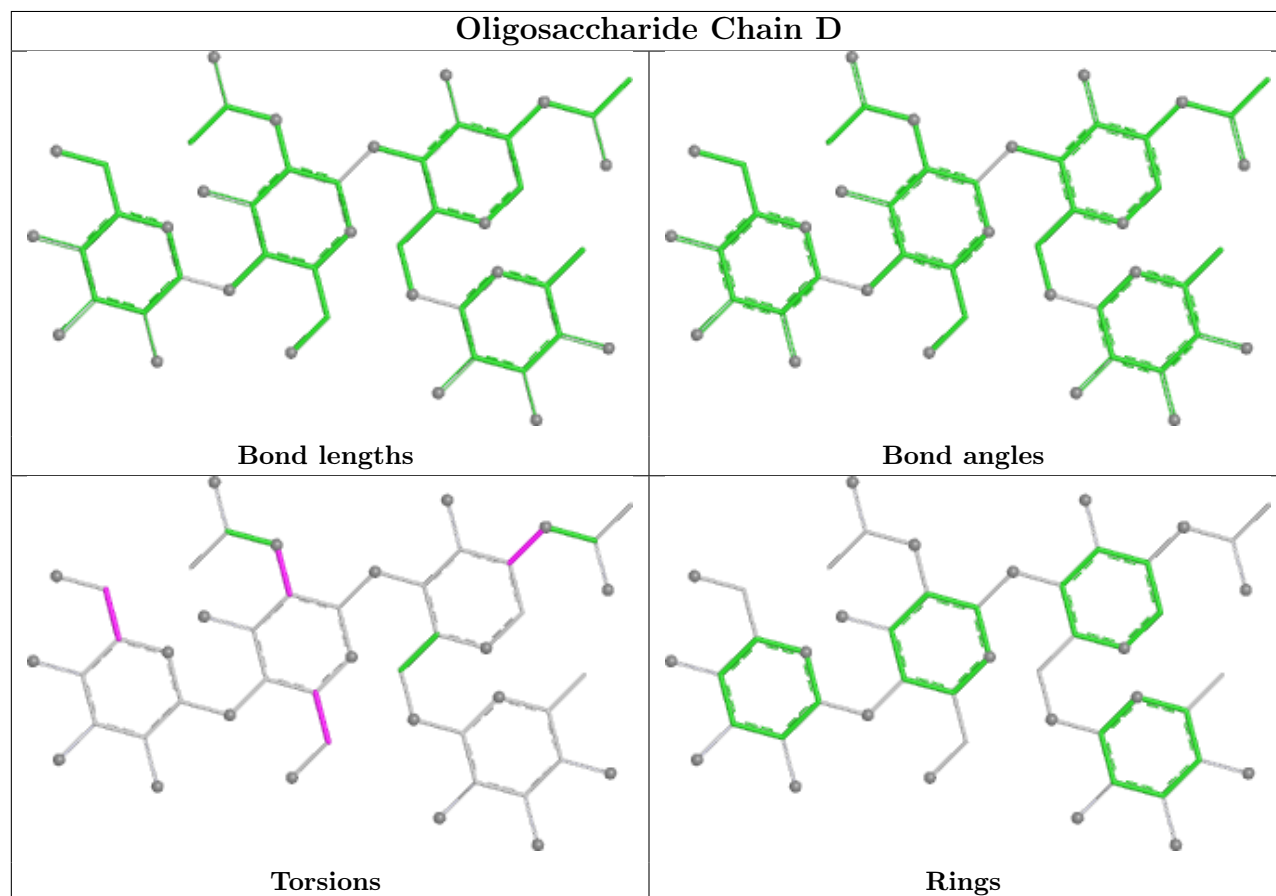
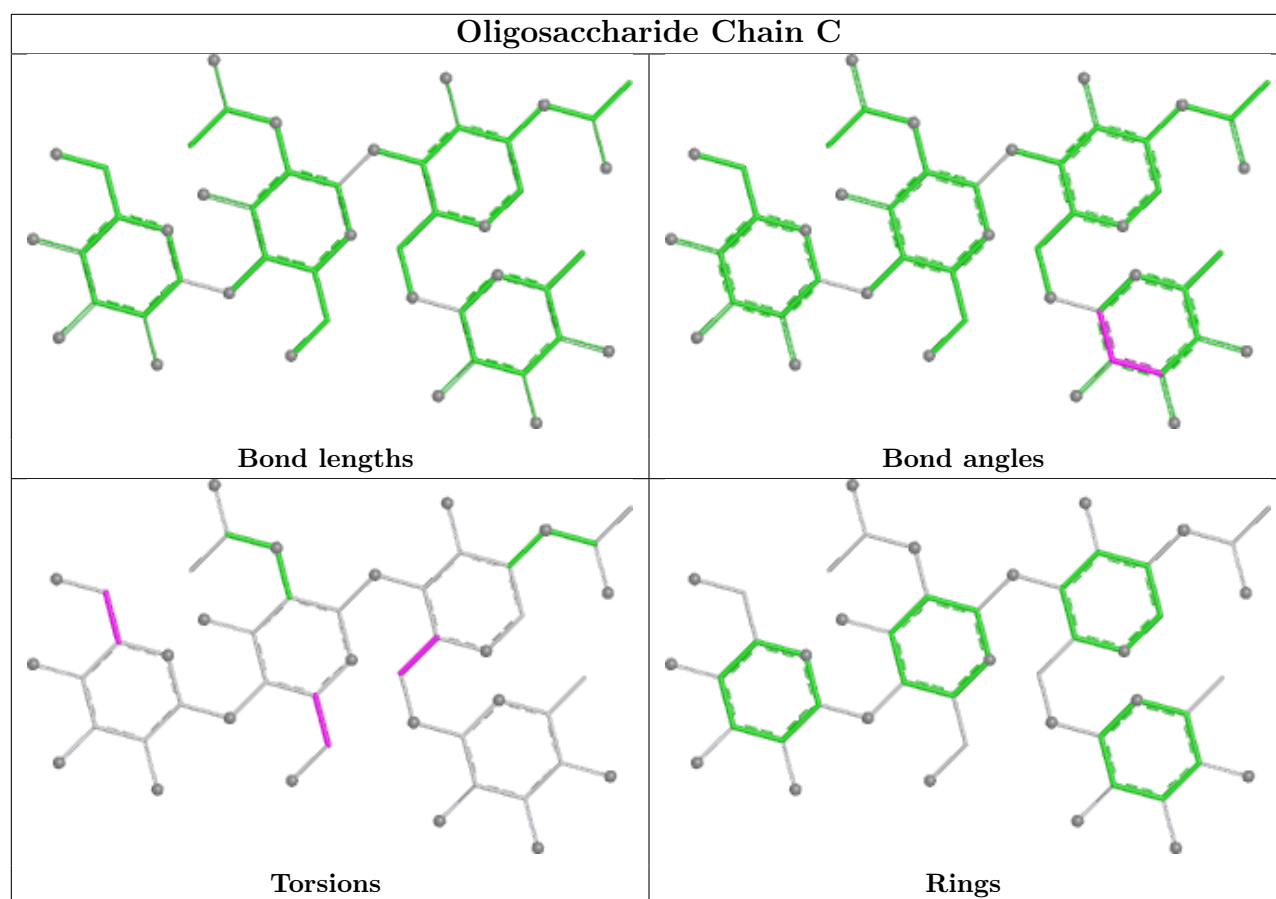
Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	316/322 (98%)	0.25	1 (0%) 90 82	45, 80, 108, 171	0

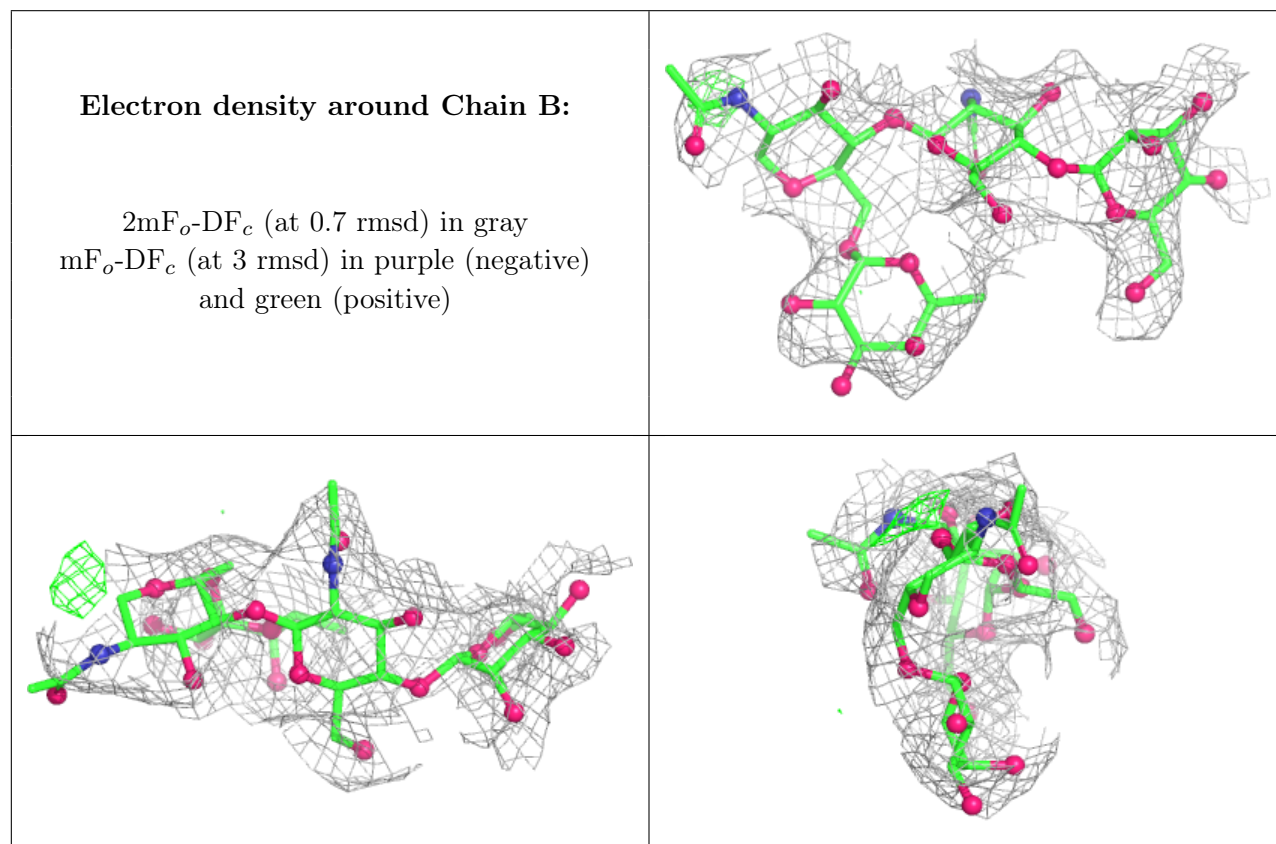
All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	ILE	3.2

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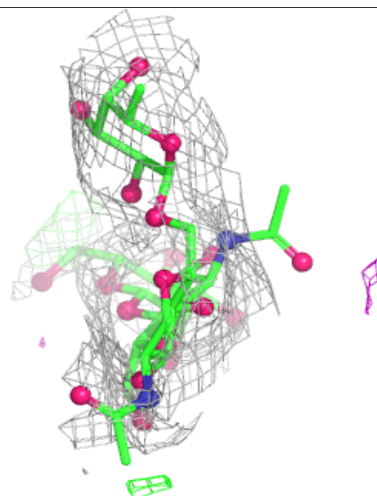
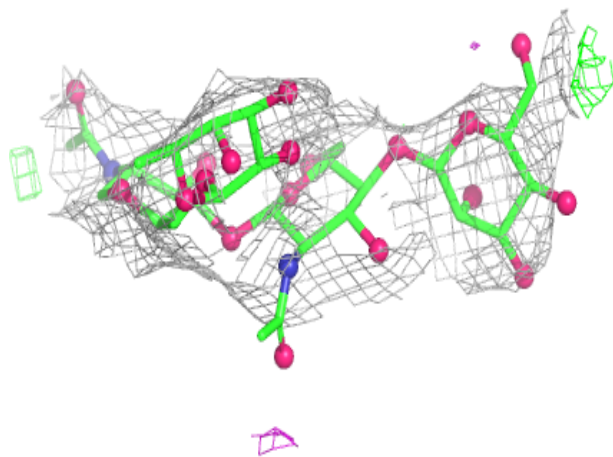
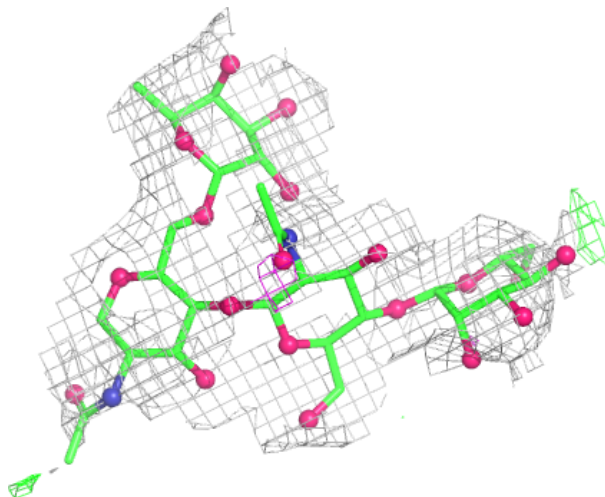
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	1	14/15	0.83	0.11	104,126,132,140	0

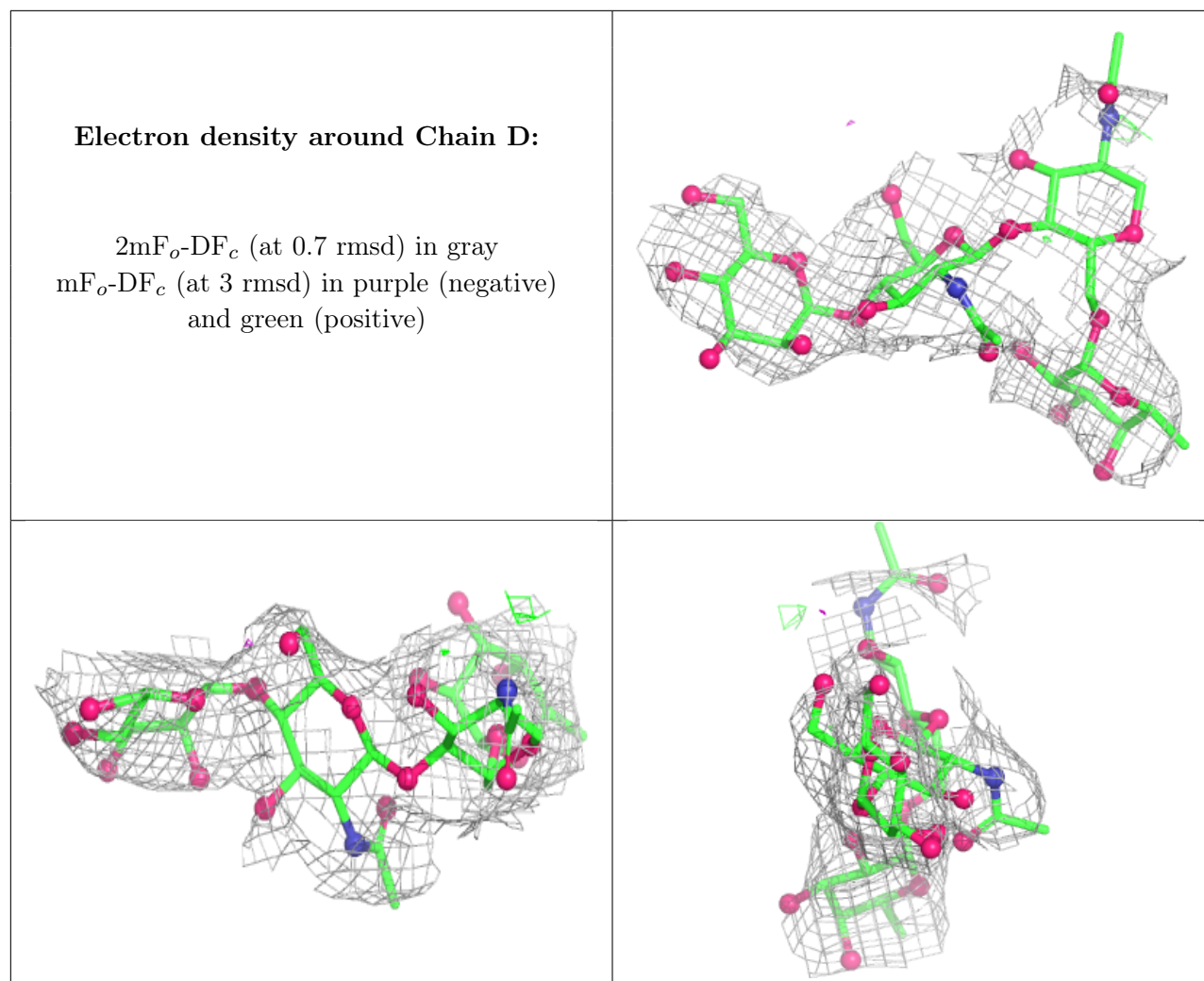
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

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





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, 95th 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
3	CA	A	417	1/1	0.95	0.09	72,72,72,72	0
3	CA	A	414	1/1	0.96	0.09	58,58,58,58	0
3	CA	A						

6.5 Other polymers [i](#)

There are no such residues in this entry.