Full wwPDB X-ray Structure Validation Report

Aug 9, 2020 – 09:25 PM BST

PDB ID	:	154L
Title	:	THE REFINED STRUCTURES OF GOOSE LYSOZYME AND ITS COMPLEX WITH A BOUND TRISACCHARIDE SHOW THAT THE "GOOSE-TYPE LYSOZYMES LACK A CATALYTIC ASPARTATE
Authors	:	Weaver, L.H.; Gruetter, M.G.; Matthews, B.W.
Deposited on	:	1994-05-05
Resolution	:	1.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

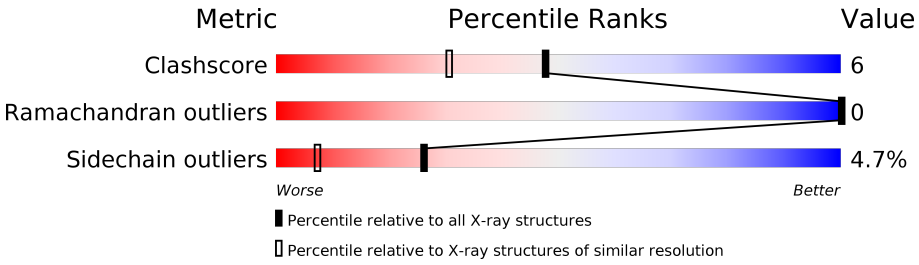
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	185	82% 14%
2	B	3	100%

2 Entry composition

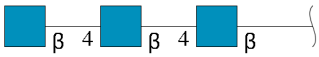
There are 3 unique types of molecules in this entry. The entry contains 1639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GOOSE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1432	891	264	270	7			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			43	24	3	16			

- Molecule 3 is water.

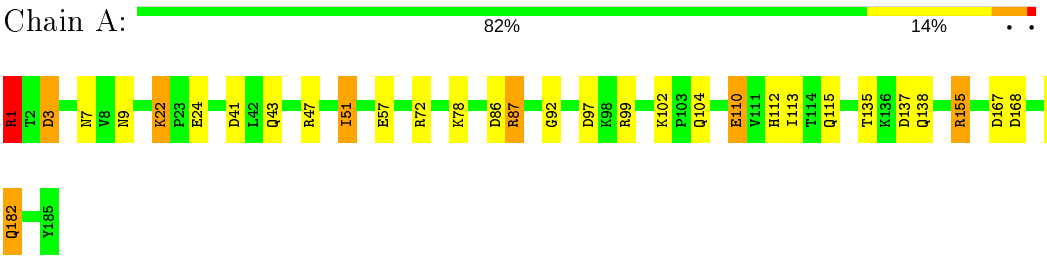
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total	O	0	0
			164	164		

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.

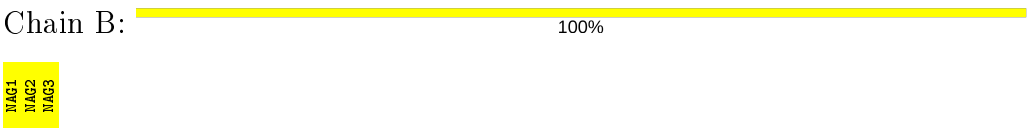
- Molecule 1: GOOSE LYSOZYME

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.30Å 65.40Å 44.70Å 90.00° 117.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.60 19.14 – 1.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-1.60) 72.1 (19.14-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	90275.00 (at 1.57Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.159 , (Not available) 0.304 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.6	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	1639	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.02% 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: NAG

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	1.10	3/1458 (0.2%)	1.45	23/1960 (1.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	GLU	CD-OE1	7.76	1.34	1.25
1	A	24	GLU	CD-OE2	6.50	1.32	1.25
1	A	110	GLU	CD-OE2	5.02	1.31	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ASP	CB-CG-OD2	-10.85	108.53	118.30
1	A	97	ASP	CB-CG-OD2	-9.65	109.61	118.30
1	A	86	ASP	CB-CG-OD1	9.30	126.67	118.30
1	A	99	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	41	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	A	97	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	3	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	3	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	176	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	41	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	155	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	87	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	176	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	47	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	168	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	87	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	155	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	A	182	GLN	N-CA-CB	-5.65	100.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	167	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	172	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	137	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	72	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	1	ARG	CA-CB-CG	-5.05	102.28	113.40

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	1432	0	1425	18	0
2	B	43	0	39	0	0
3	A	164	0	0	4	0
All	All	1639	0	1464	18	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.

All (18) 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:51:ILE:CD1	1:A:113:ILE:HD12	2.02	0.88
1:A:51:ILE:HD13	1:A:113:ILE:HD12	1.64	0.78
1:A:135:THR:H	1:A:138:GLN:HE21	1.33	0.78
1:A:22:LYS:HE3	3:A:454:HOH:O	1.85	0.77
1:A:1:ARG:HH21	1:A:3:ASP:HB3	1.58	0.68
1:A:51:ILE:HD11	1:A:113:ILE:HD12	1.79	0.64
1:A:51:ILE:HD11	1:A:110:GLU:HA	1.81	0.63
1:A:43:GLN:HG2	3:A:318:HOH:O	2.05	0.56
1:A:1:ARG:NH1	1:A:1:ARG:HB2	2.20	0.56
1:A:104:GLN:H	1:A:115:GLN:HE22	1.56	0.54
1:A:7:ASN:OD1	1:A:9:ASN:HB2	2.10	0.52
1:A:155:ARG:NE	3:A:433:HOH:O	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:HD3	3:A:432:HOH:O	2.12	0.48
1:A:104:GLN:H	1:A:115:GLN:NE2	2.11	0.47
1:A:135:THR:H	1:A:138:GLN:NE2	2.09	0.45
1:A:1:ARG:HB2	1:A:1:ARG:HH11	1.82	0.43
1:A:92:GLY:HA3	1:A:112:HIS:CE1	2.54	0.42
1:A:51:ILE:HD13	1:A:113:ILE:CD1	2.43	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	183/185 (99%)	179 (98%)	4 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	149/149 (100%)	142 (95%)	7 (5%)	26 7

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	22	LYS
1	A	51	ILE
1	A	78	LYS
1	A	87	ARG
1	A	102	LYS
1	A	182	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	82	ASN
1	A	104	GLN
1	A	115	GLN
1	A	128	GLN
1	A	138	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

3 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	B	1	2	15,15,15	1.09	0	21,21,21	2.79	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	2	2	14,14,15	0.98	0	17,19,21	1.81	2 (11%)
2	NAG	B	3	2	14,14,15	0.68	0	17,19,21	1.65	4 (23%)

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	NAG	B	1	2	-	4/6/26/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	B	3	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O7-C7-C8	-10.09	103.31	122.06
2	B	2	NAG	O6-C6-C5	-5.27	93.21	111.29
2	B	3	NAG	C1-O5-C5	4.75	118.63	112.19
2	B	1	NAG	C1-C2-C3	4.57	116.78	110.54
2	B	1	NAG	C3-C2-N2	4.06	118.28	110.62
2	B	2	NAG	C2-N2-C7	-3.14	118.42	122.90
2	B	3	NAG	O5-C5-C6	-2.80	102.82	107.20
2	B	1	NAG	O7-C7-N2	2.55	126.64	121.95
2	B	1	NAG	O5-C1-C2	2.45	111.98	109.52
2	B	3	NAG	O4-C4-C3	-2.41	104.78	110.35
2	B	3	NAG	C2-N2-C7	-2.17	119.81	122.90
2	B	1	NAG	O1-C1-O5	-2.16	103.89	110.38

There are no chirality outliers.

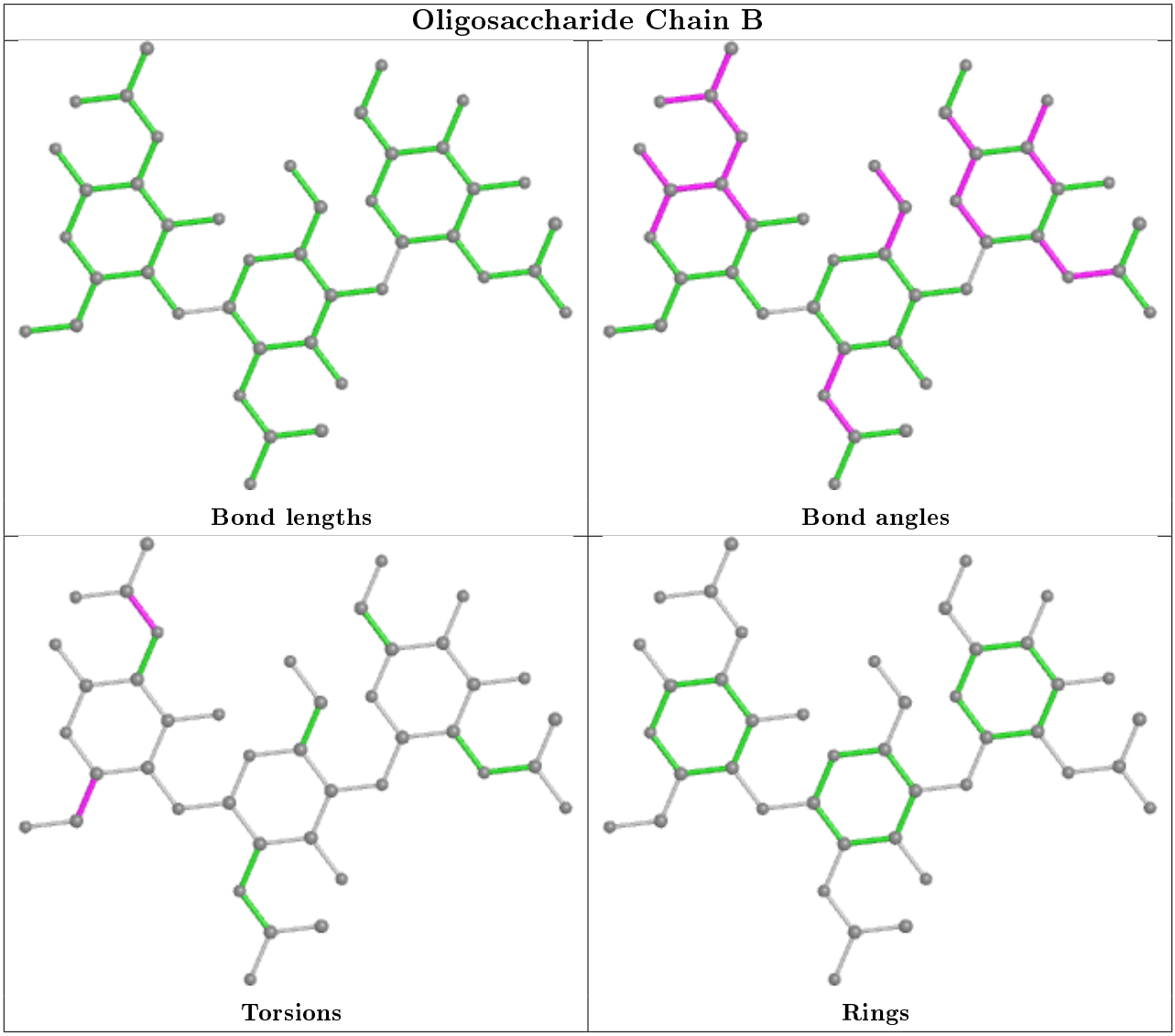
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-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

There are no ligands in this entry.

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

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.

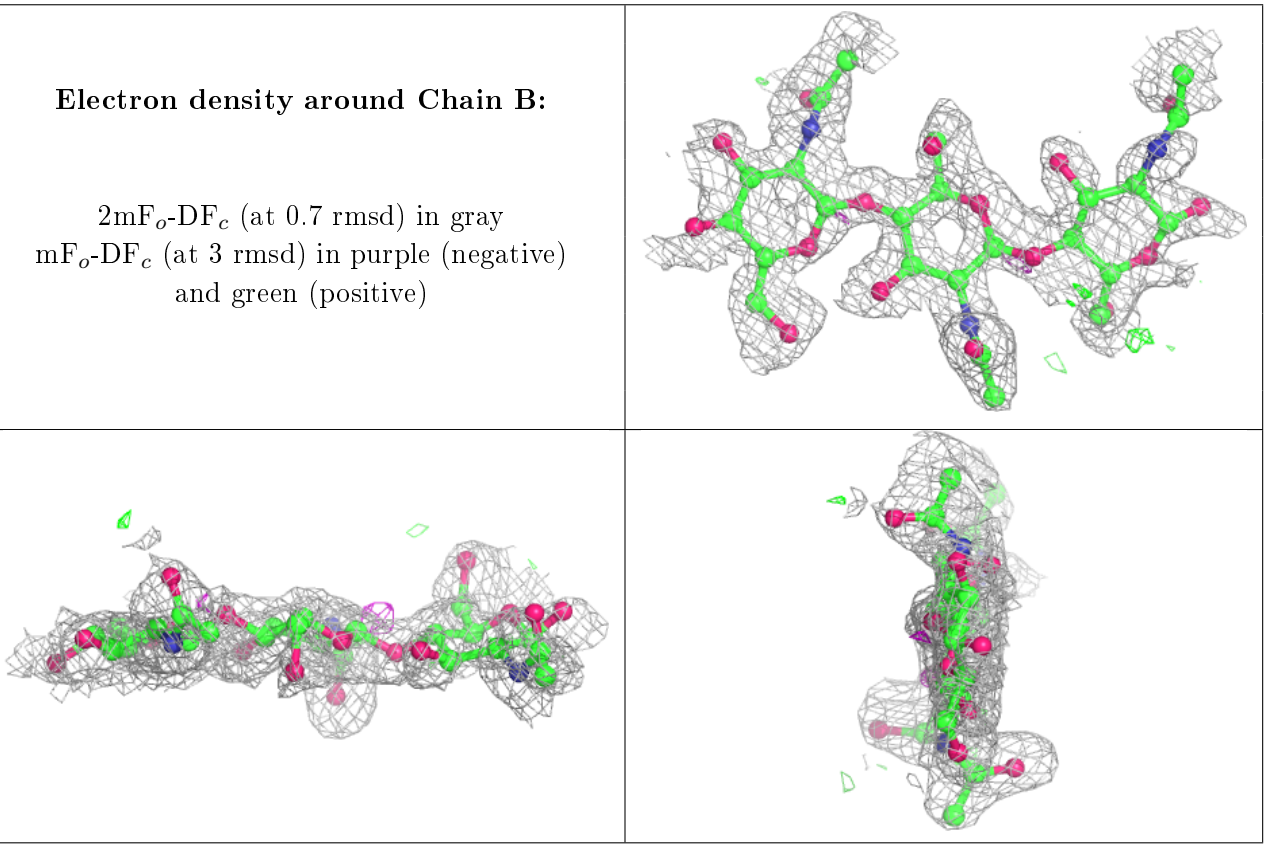
6.3 Carbohydrates

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

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 B:

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



6.4 Ligands

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

6.5 Other polymers (i)

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