



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:56 AM UTC

PDB ID : 7EQU / pdb\_00007equ  
Title : Crystal structure of the C-lobe of lactoferrin produced by limited proteolysis using pepsin at 2.74Å resolution  
Authors : Maurya, A.; Singh, J.; Sharma, A.; Sharma, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2021-05-04  
Resolution : 2.74 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](mailto: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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

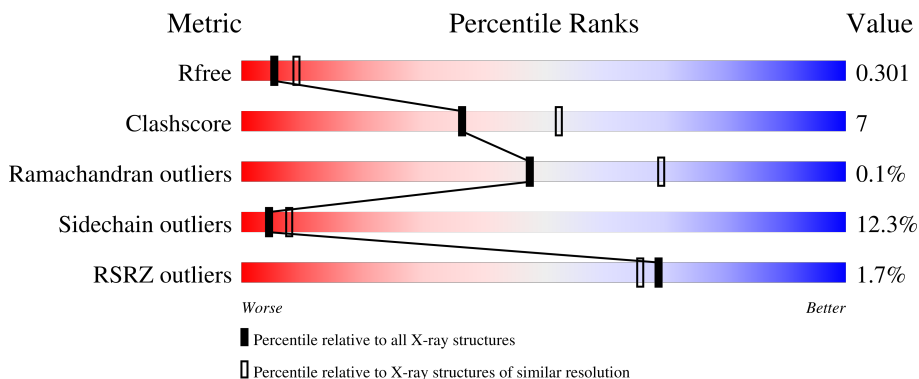
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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.




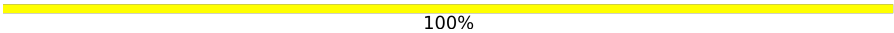

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	
2	C	3	
2	D	3	
2	E	3	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	2	 50% 50%
3	G	2	 100%
4	H	3	 100%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5549 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.

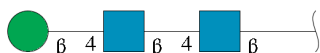
- Molecule 1 is a protein called Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	348	2658	1656	464	517	21	0	0	0
1	B	348	2658	1656	464	517	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	conflict	UNP P24627
A	608	GLU	LYS	conflict	UNP P24627
B	565	LYS	ASN	conflict	UNP P24627
B	608	GLU	LYS	conflict	UNP P24627

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



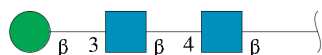
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0
2	E	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			27	16	2	9			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

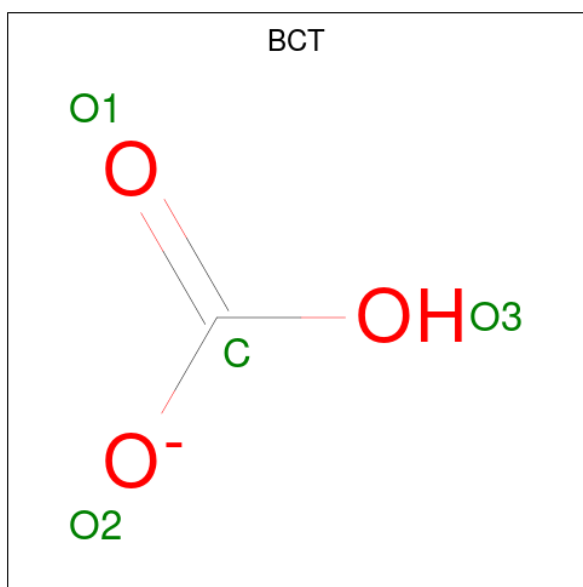


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		
5	B	1	Total	Fe	0	0
			1	1		

- Molecule 6 is BICARBONATE ION (CCD ID: BCT) (formula: CHO<sub>3</sub>).



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

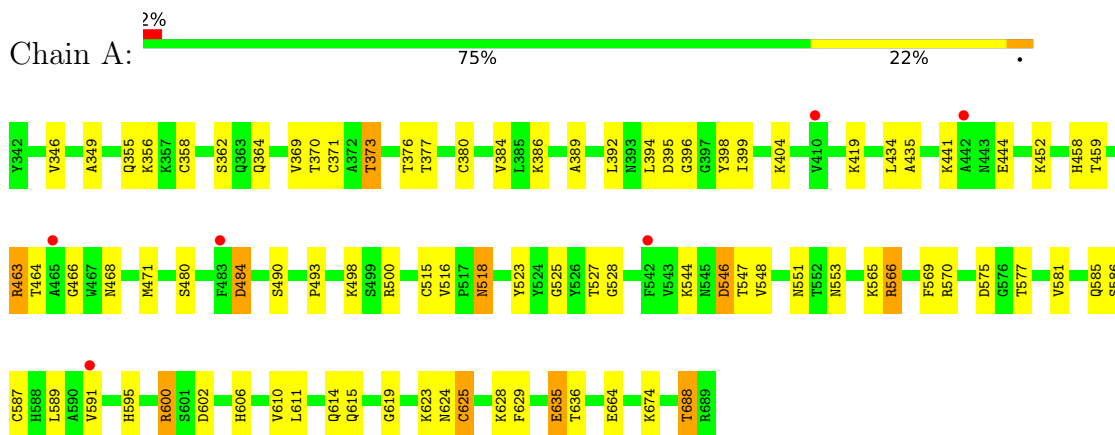
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	B	5	Total O 5 5	0	0

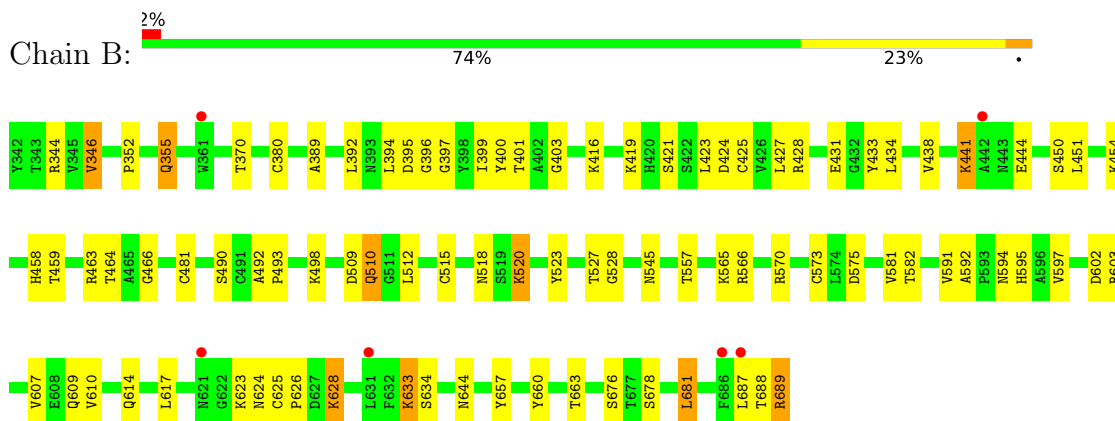
### 3 Residue-property plots i

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 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: Lactotransferrin



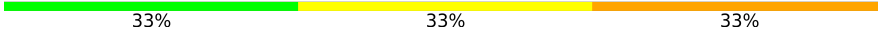
- Molecule 1: Lactotransferrin



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



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

Chain D:  33% 33% 33%

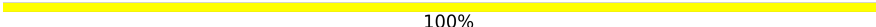
MAG1  
MAG2  
BMA3

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

Chain E:  33% 67%


MAG1  
MAG2  
BMA3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

MAG1  
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%

MAG1  
MAG2

- Molecule 4: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.76Å 81.55Å 111.36Å 90.00° 129.95° 90.00°	Depositor
Resolution (Å)	76.85 – 2.74 76.85 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.0 (76.85-2.74) 97.0 (76.85-2.74)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.239 , 0.298 0.243 , 0.301	Depositor DCC
$R_{free}$ test set	1361 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.7	Xtrriage
Anisotropy	0.211	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 89.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, BCT, NAG, FE

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	1.06	0/2708	1.47	3/3670 (0.1%)
1	B	1.06	1/2708 (0.0%)	1.51	0/3670
All	All	1.06	1/5416 (0.0%)	1.49	3/7340 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	HIS	CE1-NE2	5.13	1.37	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	441	LYS	CA-C-N	5.52	128.44	120.38
1	A	441	LYS	C-N-CA	5.52	128.44	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	SER	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	625	CYS	Peptide

## 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	2658	0	2580	40	0
1	B	2658	0	2581	35	0
2	C	39	0	34	0	0
2	D	39	0	34	1	0
2	E	39	0	34	1	0
3	F	28	0	25	1	0
3	G	27	0	25	0	0
4	H	39	0	34	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	1	0
7	A	7	0	0	0	0
7	B	5	0	0	0	0
All	All	5549	0	5347	78	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 7.

All (78) 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:395:ASP:HA	1:B:595:HIS:CD2	2.31	0.66
1:A:404:LYS:HD2	1:A:688:THR:HG21	1.80	0.64
1:A:546:ASP:N	1:A:546:ASP:OD1	2.31	0.64
1:A:518:ASN:C	1:A:518:ASN:OD1	2.43	0.62
1:A:553:ASN:OD1	1:A:566:ARG:CZ	2.48	0.61
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.35	0.61
1:A:624:ASN:HB3	1:A:628:LYS:HB2	1.81	0.61
1:A:459:THR:HA	1:A:525:GLY:O	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:LEU:HD11	1:B:394:LEU:HD21	1.84	0.59
1:A:566:ARG:HG2	1:A:581:VAL:HG21	1.83	0.59
1:A:484:ASP:O	1:A:500:ARG:HD2	2.04	0.57
4:H:2:NAG:O4	4:H:3:BMA:H2	2.04	0.57
1:A:575:ASP:HB3	1:A:577:THR:HG22	1.85	0.57
1:B:395:ASP:OD1	1:B:464:THR:N	2.36	0.56
1:B:346:VAL:HB	1:B:389:ALA:HA	1.87	0.55
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.41	0.54
1:B:510:GLN:HB2	1:B:512:LEU:HG	1.91	0.53
1:B:566:ARG:HG2	1:B:581:VAL:HG21	1.90	0.53
4:H:2:NAG:O4	4:H:3:BMA:C2	2.57	0.53
1:A:395:ASP:OD1	1:A:463:ARG:HA	2.09	0.52
1:B:523:TYR:C	1:B:528:GLY:HA3	2.33	0.52
1:A:611:LEU:O	1:A:614:GLN:N	2.41	0.52
4:H:1:NAG:O3	4:H:2:NAG:O5	2.21	0.51
1:A:575:ASP:OD2	1:A:577:THR:HB	2.10	0.51
1:A:349:ALA:O	1:A:373:THR:HA	2.11	0.50
1:A:364:GLN:HE22	3:F:2:NAG:H2	1.76	0.50
1:A:493:PRO:HA	1:A:515:CYS:SG	2.52	0.50
1:A:569:PHE:O	1:A:570:ARG:NH1	2.44	0.50
1:B:518:ASN:OD1	1:B:520:LYS:HB2	2.11	0.50
1:A:553:ASN:OD1	1:A:566:ARG:NE	2.44	0.50
1:A:362:SER:HA	1:A:369:VAL:O	2.11	0.50
1:A:458:HIS:CE1	1:A:471:MET:HE2	2.47	0.50
1:B:594:ASN:O	1:B:660:TYR:OH	2.21	0.50
1:B:459:THR:OG1	1:B:466:GLY:HA3	2.13	0.49
1:A:370:THR:HG21	1:B:481:CYS:SG	2.52	0.49
1:A:435:ALA:O	1:A:589:LEU:N	2.41	0.48
1:B:396:GLY:O	1:B:399:ILE:HB	2.13	0.48
1:A:358:CYS:C	1:A:371:CYS:SG	2.97	0.47
1:B:396:GLY:HA2	1:B:399:ILE:HD12	1.96	0.47
1:B:352:PRO:HA	1:B:355:GLN:HB2	1.97	0.47
1:A:606:HIS:O	1:A:610:VAL:HG23	2.16	0.46
1:A:364:GLN:HG3	1:A:629:PHE:HB2	1.98	0.46
1:A:346:VAL:HB	1:A:389:ALA:HA	1.98	0.45
1:A:547:THR:O	1:A:551:ASN:ND2	2.39	0.45
2:E:2:NAG:H62	2:E:3:BMA:O2	2.16	0.45
1:A:615:GLN:O	1:A:619:GLY:N	2.43	0.45
1:A:434:LEU:O	1:A:544:LYS:HA	2.15	0.45
1:A:523:TYR:HA	1:A:528:GLY:CA	2.47	0.45
1:B:434:LEU:HB2	1:B:545:ASN:OD1	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:THR:HA	1:B:681:LEU:HD21	1.98	0.45
1:B:633:LYS:HD3	1:B:633:LYS:HA	1.56	0.45
1:B:392:LEU:CD1	1:B:394:LEU:HD21	2.46	0.44
1:A:516:VAL:HG23	1:A:516:VAL:O	2.18	0.44
1:A:585:GLN:NE2	2:D:1:NAG:H81	2.33	0.44
1:B:492:ALA:O	1:B:493:PRO:C	2.59	0.44
1:B:433:TYR:CE2	1:B:592:ALA:CB	3.01	0.43
1:B:603:ARG:O	1:B:607:VAL:HG23	2.18	0.43
1:A:396:GLY:HA2	1:A:399:ILE:HD12	2.01	0.43
1:A:458:HIS:HB3	1:A:466:GLY:O	2.19	0.43
1:A:610:VAL:O	1:A:614:GLN:HG2	2.18	0.43
1:B:610:VAL:O	1:B:614:GLN:HG2	2.19	0.42
1:B:392:LEU:O	1:B:597:VAL:HA	2.19	0.42
1:A:392:LEU:HD11	1:A:394:LEU:HD21	2.01	0.42
1:B:678:SER:HB3	1:B:681:LEU:HB2	2.00	0.42
1:B:451:LEU:O	1:B:454:LYS:HB2	2.20	0.41
1:A:523:TYR:C	1:A:528:GLY:HA3	2.46	0.41
1:B:463:ARG:HE	6:B:702:BCT:C	2.33	0.41
1:B:403:GLY:HA3	1:B:657:TYR:CG	2.55	0.41
1:B:441:LYS:HB2	1:B:570:ARG:HG2	2.02	0.41
1:B:395:ASP:OD1	1:B:463:ARG:HA	2.21	0.41
1:B:688:THR:O	1:B:689:ARG:C	2.64	0.41
1:B:397:GLY:O	1:B:400:TYR:HB3	2.21	0.41
1:B:624:ASN:HB3	1:B:628:LYS:HB2	2.03	0.41
1:B:424:ASP:O	1:B:428:ARG:N	2.54	0.40
1:B:424:ASP:OD1	1:B:425:CYS:N	2.55	0.40
1:A:384:VAL:O	1:A:600:ARG:HD2	2.21	0.40
1:A:464:THR:HA	1:A:468:ASN:HB2	2.03	0.40
1:B:625:CYS:HA	1:B:626:PRO:HA	1.93	0.40

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	346/348 (99%)	319 (92%)	26 (8%)	1 (0%)	36	54
1	B	346/348 (99%)	316 (91%)	30 (9%)	0	100	100
All	All	692/696 (99%)	635 (92%)	56 (8%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	GLU

### 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	289/289 (100%)	259 (90%)	30 (10%)	7	13
1	B	289/289 (100%)	248 (86%)	41 (14%)	3	5
All	All	578/578 (100%)	507 (88%)	71 (12%)	4	8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	356	LYS
1	A	373	THR
1	A	376	THR
1	A	380	CYS
1	A	386	LYS
1	A	419	LYS
1	A	444	GLU
1	A	452	LYS
1	A	463	ARG
1	A	480	SER
1	A	484	ASP
1	A	498	LYS
1	A	518	ASN
1	A	527	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	546	ASP
1	A	548	VAL
1	A	565	LYS
1	A	566	ARG
1	A	586	SER
1	A	587	CYS
1	A	591	VAL
1	A	600	ARG
1	A	623	LYS
1	A	625	CYS
1	A	635	GLU
1	A	636	THR
1	A	664	GLU
1	A	674	LYS
1	A	688	THR
1	B	344	ARG
1	B	346	VAL
1	B	355	GLN
1	B	370	THR
1	B	380	CYS
1	B	416	LYS
1	B	419	LYS
1	B	421	SER
1	B	423	LEU
1	B	427	LEU
1	B	431	GLU
1	B	438	VAL
1	B	441	LYS
1	B	444	GLU
1	B	450	SER
1	B	490	SER
1	B	498	LYS
1	B	509	ASP
1	B	510	GLN
1	B	515	CYS
1	B	520	LYS
1	B	527	THR
1	B	557	THR
1	B	565	LYS
1	B	573	CYS
1	B	575	ASP
1	B	582	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	591	VAL
1	B	602	ASP
1	B	609	GLN
1	B	617	LEU
1	B	623	LYS
1	B	628	LYS
1	B	633	LYS
1	B	634	SER
1	B	644	ASN
1	B	663	THR
1	B	676	SER
1	B	681	LEU
1	B	687	LEU
1	B	689	ARG

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

Mol	Chain	Res	Type
1	A	355	GLN
1	A	364	GLN
1	A	468	ASN
1	A	585	GLN
1	B	367	GLN
1	B	510	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](#)

16 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	C	1	2,1	14,14,15	0.43	0	17,19,21	2.04	2 (11%)
2	NAG	C	2	2	14,14,15	0.73	0	17,19,21	2.23	4 (23%)
2	BMA	C	3	2	11,11,12	0.59	0	15,15,17	0.70	0
2	NAG	D	1	2,1	14,14,15	0.65	0	17,19,21	2.14	6 (35%)
2	NAG	D	2	2	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
2	BMA	D	3	2	11,11,12	0.62	0	15,15,17	0.81	0
2	NAG	E	1	2,1	14,14,15	1.41	3 (21%)	17,19,21	3.01	7 (41%)
2	NAG	E	2	2	14,14,15	1.44	4 (28%)	17,19,21	2.55	7 (41%)
2	BMA	E	3	2	11,11,12	0.91	0	15,15,17	2.35	4 (26%)
3	NAG	F	1	1,3	14,14,15	0.42	0	17,19,21	1.13	2 (11%)
3	NAG	F	2	3	14,14,15	0.60	0	17,19,21	1.58	2 (11%)
3	NAG	G	1	1,3	14,14,15	0.69	0	17,19,21	2.11	4 (23%)
3	NAG	G	2	3	13,13,15	0.78	0	16,17,21	1.55	3 (18%)
4	NAG	H	1	4,1	14,14,15	0.86	0	17,19,21	1.81	5 (29%)
4	NAG	H	2	4	14,14,15	0.61	0	17,19,21	1.50	2 (11%)
4	BMA	H	3	4	11,11,12	0.59	0	15,15,17	1.25	2 (13%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/5/22/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	C1-C2	3.42	1.57	1.52
2	E	1	NAG	O4-C4	2.98	1.50	1.43
2	E	1	NAG	O5-C1	2.59	1.48	1.43
2	E	2	NAG	O5-C1	2.30	1.47	1.43
2	E	1	NAG	O5-C5	2.30	1.47	1.43
2	E	2	NAG	O5-C5	2.08	1.47	1.43
2	E	2	NAG	O4-C4	2.02	1.48	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	7.16	121.78	112.19
2	C	2	NAG	C1-O5-C5	6.74	121.22	112.19
2	E	1	NAG	C1-O5-C5	6.37	120.73	112.19
3	G	1	NAG	C1-O5-C5	5.95	120.16	112.19
2	E	3	BMA	C1-C2-C3	5.62	117.83	109.64
2	E	2	NAG	C1-O5-C5	5.62	119.72	112.19
2	E	1	NAG	O5-C1-C2	-5.51	102.77	111.29
2	E	1	NAG	C3-C4-C5	-5.09	101.00	110.23
2	E	3	BMA	C1-O5-C5	4.77	118.58	112.19
2	E	2	NAG	O5-C1-C2	-4.71	104.00	111.29
2	D	1	NAG	C1-O5-C5	4.71	118.50	112.19
2	C	2	NAG	O4-C4-C5	4.58	120.61	109.32
2	E	1	NAG	C4-C3-C2	4.54	117.68	111.02
4	H	2	NAG	C1-O5-C5	4.20	117.81	112.19
3	G	2	NAG	C7-N2-C2	4.10	120.68	114.43
2	D	1	NAG	C1-C2-N2	-3.71	104.58	110.43
3	F	2	NAG	C1-O5-C5	3.66	117.09	112.19
2	E	3	BMA	O5-C5-C6	3.64	114.75	107.66
2	E	2	NAG	O5-C5-C6	3.58	114.62	107.66
4	H	1	NAG	C4-C3-C2	3.53	116.19	111.02
3	F	2	NAG	O5-C1-C2	3.46	116.65	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O5-C5-C4	3.31	118.88	110.83
2	E	2	NAG	C1-C2-N2	3.26	115.58	110.43
2	D	2	NAG	C1-C2-N2	3.20	115.48	110.43
2	C	2	NAG	C3-C4-C5	-3.07	104.66	110.23
4	H	2	NAG	C4-C3-C2	-3.03	106.58	111.02
4	H	1	NAG	C6-C5-C4	3.02	120.45	113.02
3	G	1	NAG	C6-C5-C4	-2.97	105.74	113.02
2	E	1	NAG	O4-C4-C5	2.89	116.43	109.32
2	E	1	NAG	O5-C5-C6	2.85	113.21	107.66
2	E	2	NAG	C4-C3-C2	2.80	115.12	111.02
2	E	2	NAG	C6-C5-C4	-2.78	106.19	113.02
4	H	1	NAG	C1-O5-C5	-2.78	108.47	112.19
2	D	1	NAG	O5-C5-C6	-2.77	102.27	107.66
2	E	2	NAG	C3-C4-C5	-2.56	105.59	110.23
2	D	1	NAG	C2-N2-C7	2.52	126.28	122.90
4	H	3	BMA	C1-C2-C3	2.44	113.20	109.64
2	D	1	NAG	C4-C3-C2	2.44	114.59	111.02
3	G	2	NAG	O5-C1-C2	-2.43	107.53	111.29
2	E	1	NAG	C1-C2-N2	-2.40	106.66	110.43
4	H	3	BMA	O2-C2-C3	-2.39	105.19	110.15
4	H	1	NAG	O5-C5-C4	-2.37	105.06	110.83
3	G	1	NAG	O3-C3-C4	-2.37	104.80	110.38
2	E	3	BMA	O2-C2-C3	-2.37	105.25	110.15
3	F	1	NAG	O4-C4-C3	-2.36	104.81	110.38
3	F	1	NAG	C3-C4-C5	2.33	114.46	110.23
2	D	1	NAG	C3-C4-C5	2.32	114.44	110.23
4	H	1	NAG	O5-C5-C6	-2.29	103.20	107.66
2	C	1	NAG	O6-C6-C5	-2.14	104.05	111.33
2	C	2	NAG	C4-C3-C2	-2.11	107.93	111.02
3	G	2	NAG	O5-C5-C6	2.00	111.56	107.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	3	BMA	O5-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C1-C2-N2-C7

Continued on next page...

*Continued from previous page...*

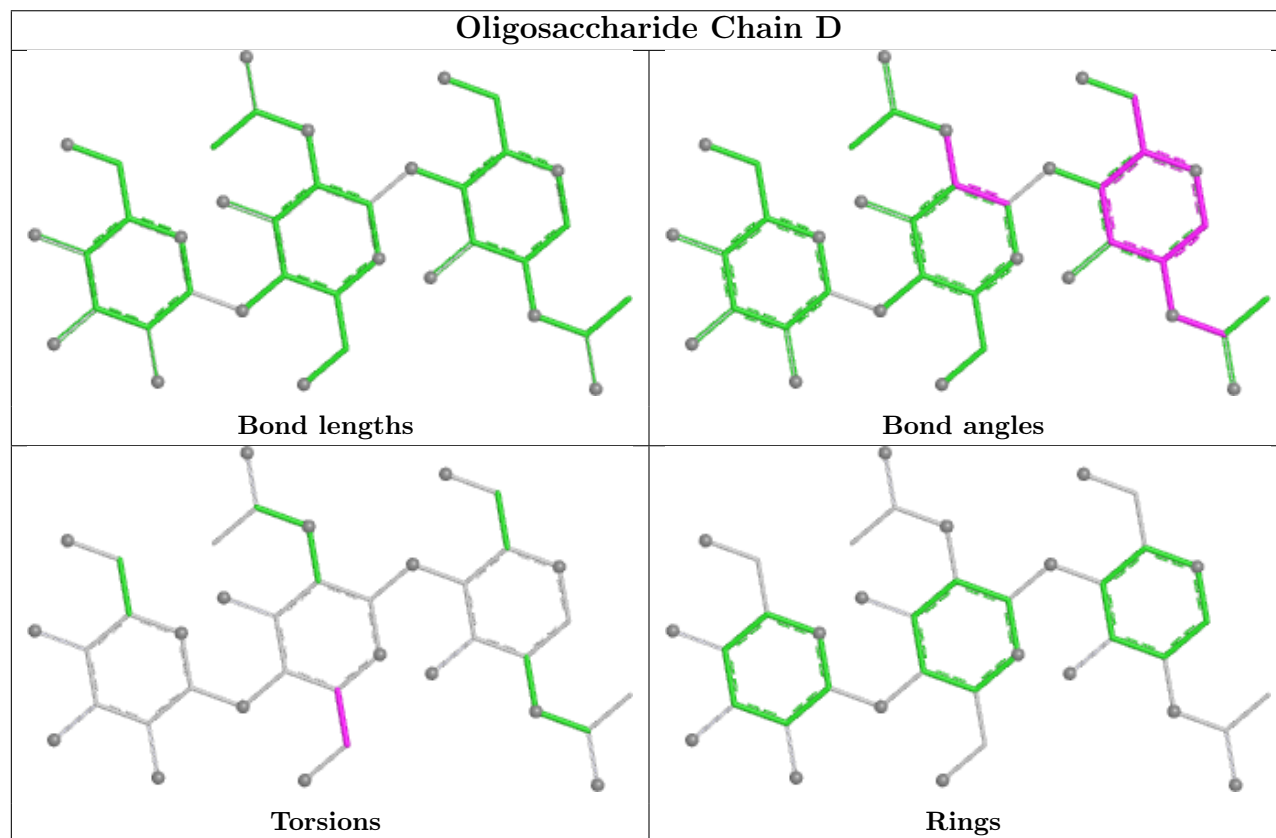
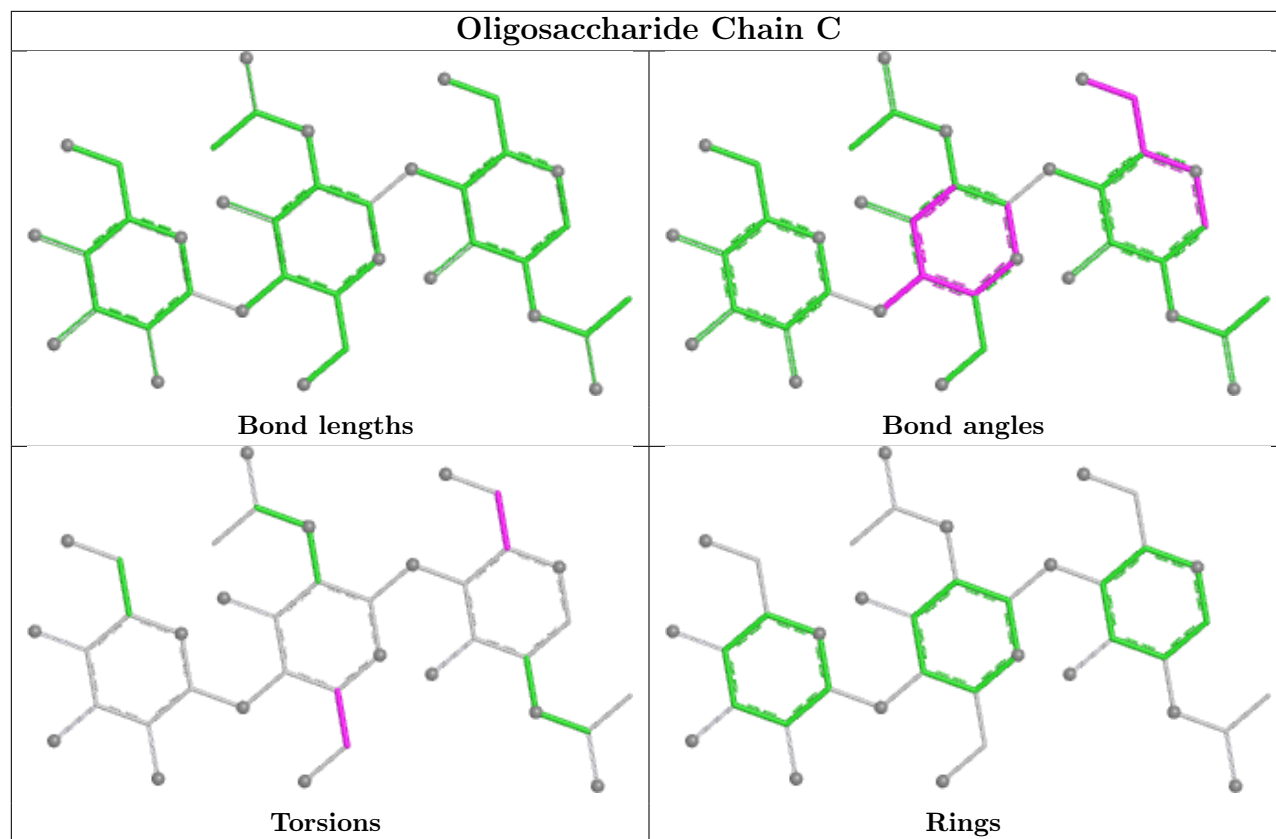
Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C3-C2-N2-C7
4	H	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

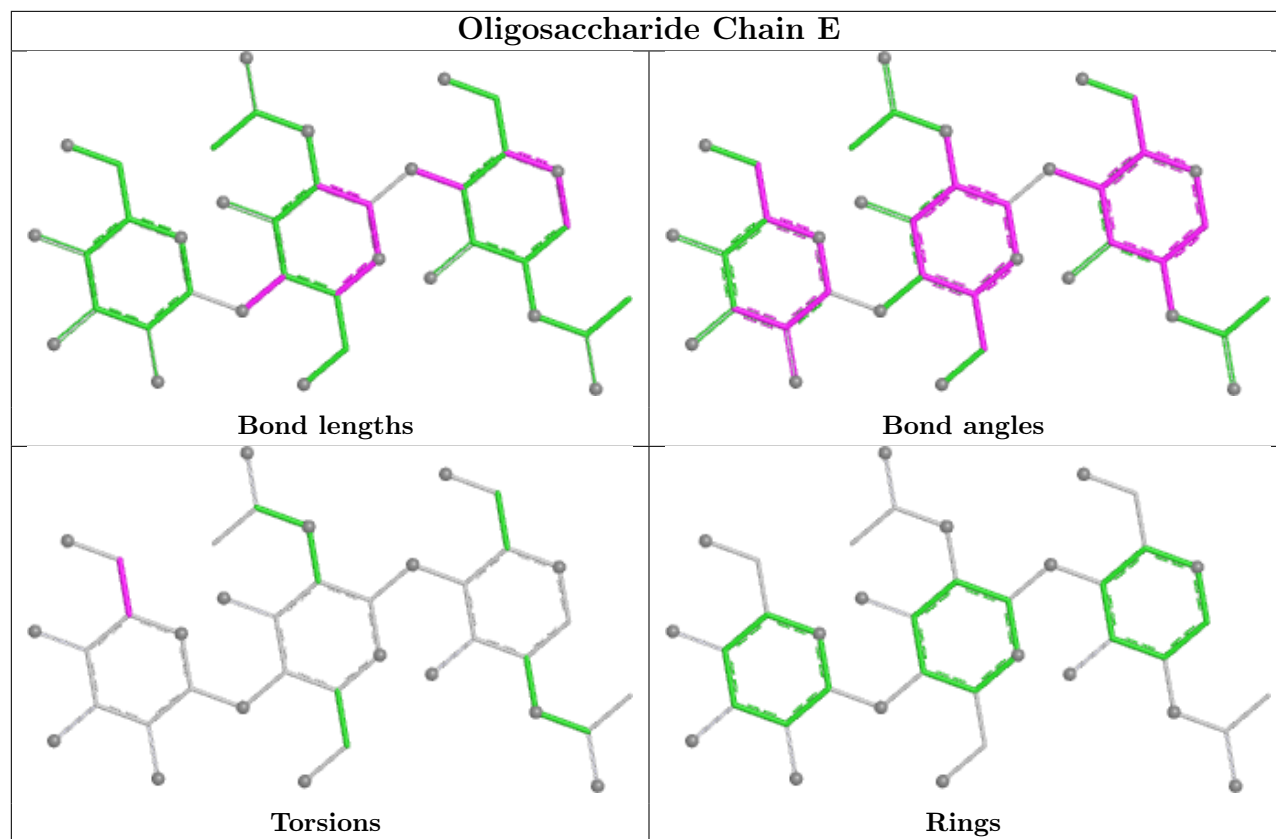
There are no ring outliers.

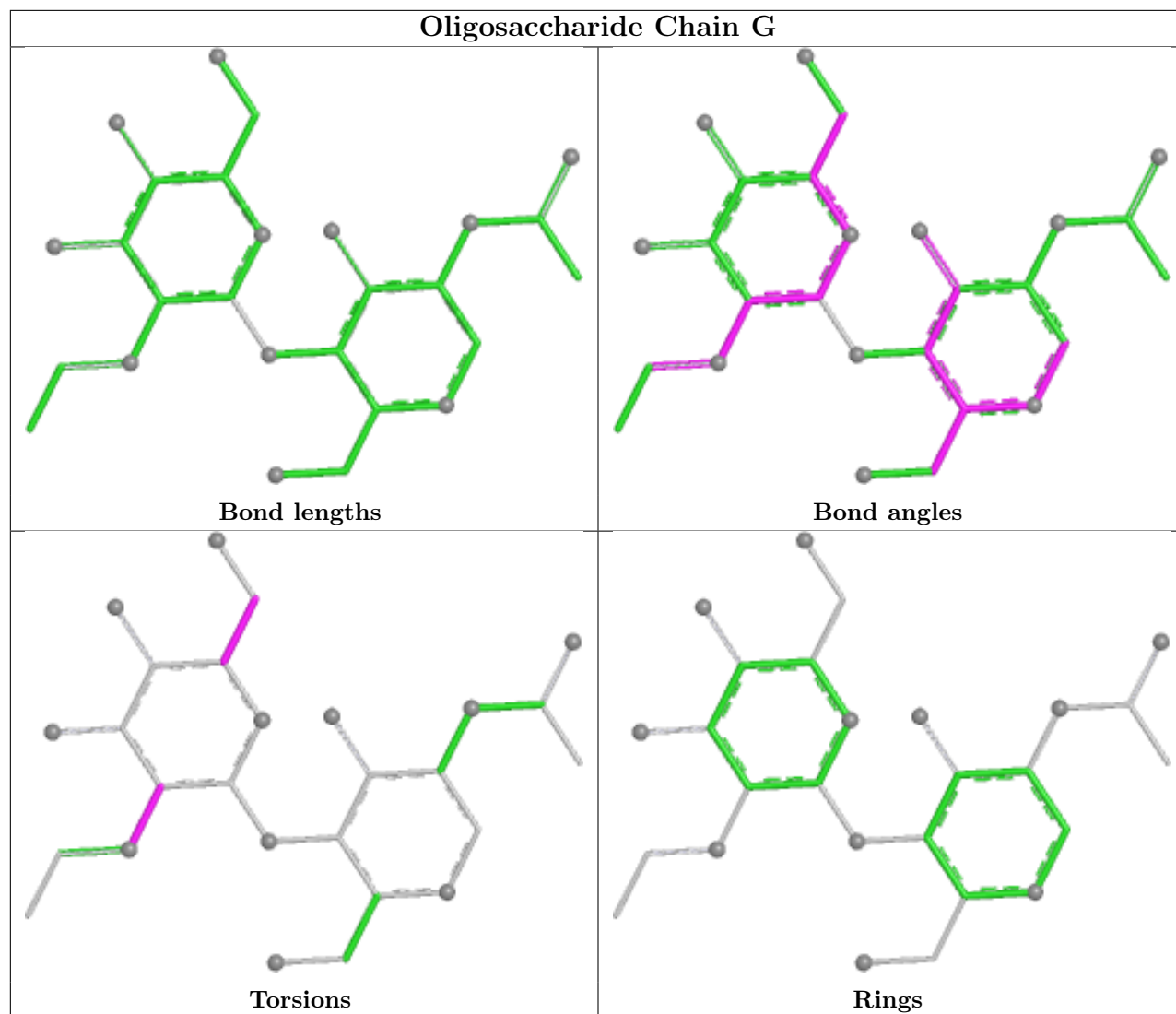
7 monomers are involved in 6 short contacts:

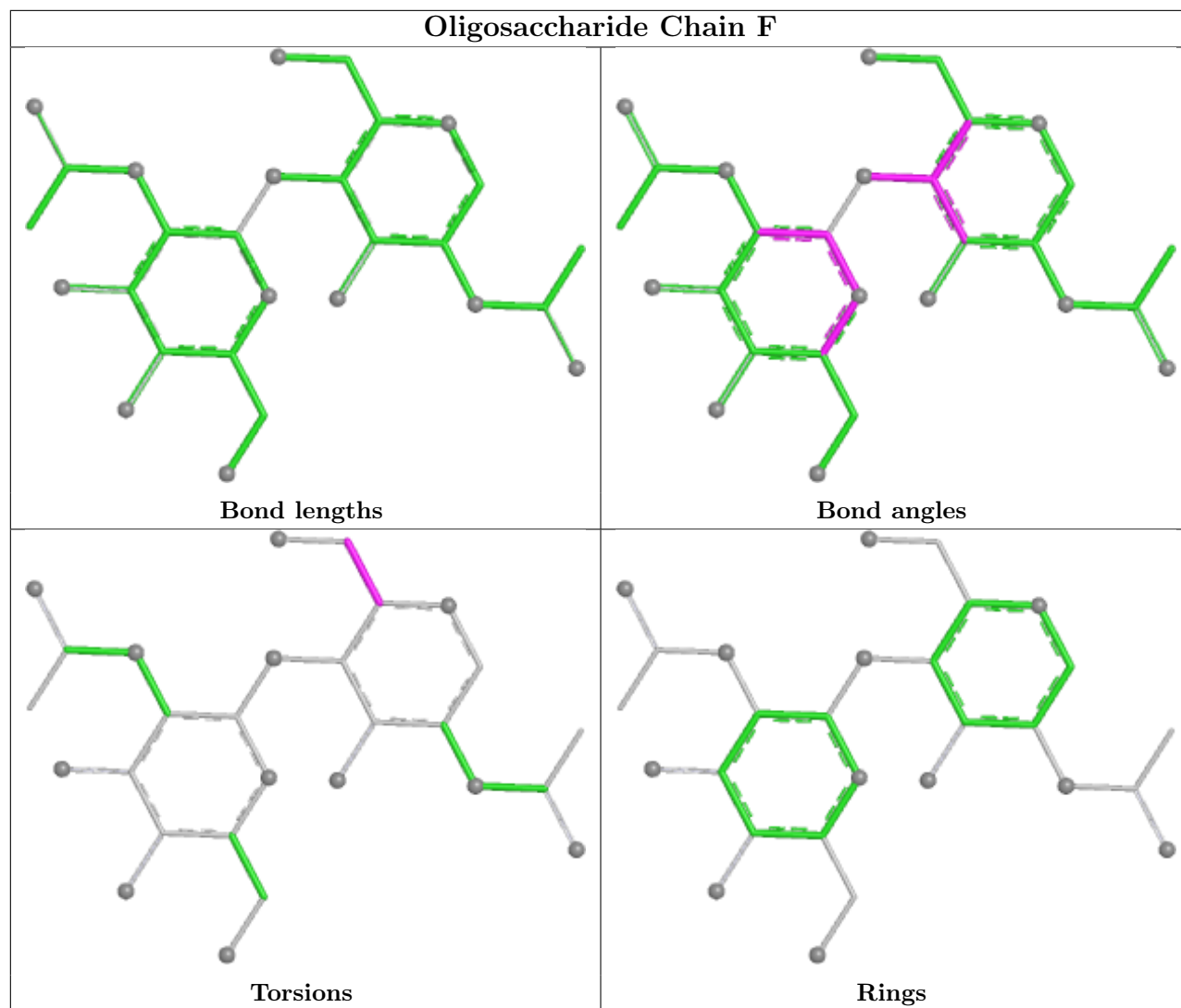
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	3	0
3	F	2	NAG	1	0
2	D	1	NAG	1	0
2	E	2	NAG	1	0
2	E	3	BMA	1	0
4	H	3	BMA	2	0
4	H	1	NAG	1	0

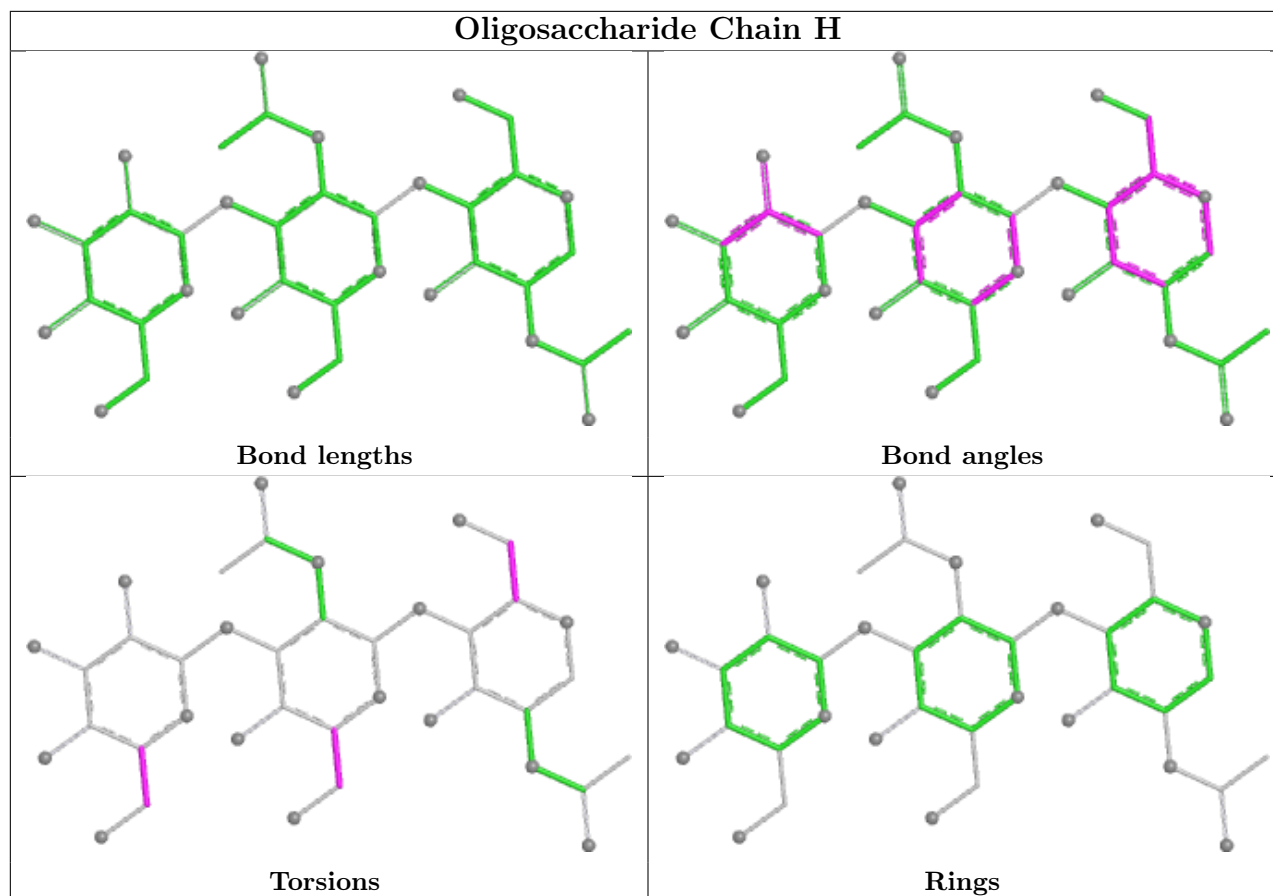
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
6	BCT	A	702	5	3,3,3	0.62	0	2,3,3	1.21	0
6	BCT	B	702	5	3,3,3	1.50	1 (33%)	2,3,3	1.19	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	702	BCT	O1-C	2.47	1.34	1.25

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	702	BCT	1	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	348/348 (100%)	0.32	6 (1%) 69 66	57, 97, 142, 183	0
1	B	348/348 (100%)	0.25	6 (1%) 69 66	57, 106, 149, 215	0
All	All	696/696 (100%)	0.29	12 (1%) 69 66	57, 102, 147, 215	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	442	ALA	5.1
1	B	687	LEU	4.6
1	A	442	ALA	3.3
1	A	542	PHE	2.9
1	A	591	VAL	2.8
1	B	686	PHE	2.7
1	A	410	VAL	2.6
1	A	465	ALA	2.4
1	B	631	LEU	2.2
1	B	621	ASN	2.2
1	B	361	TRP	2.1
1	A	483	PHE	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

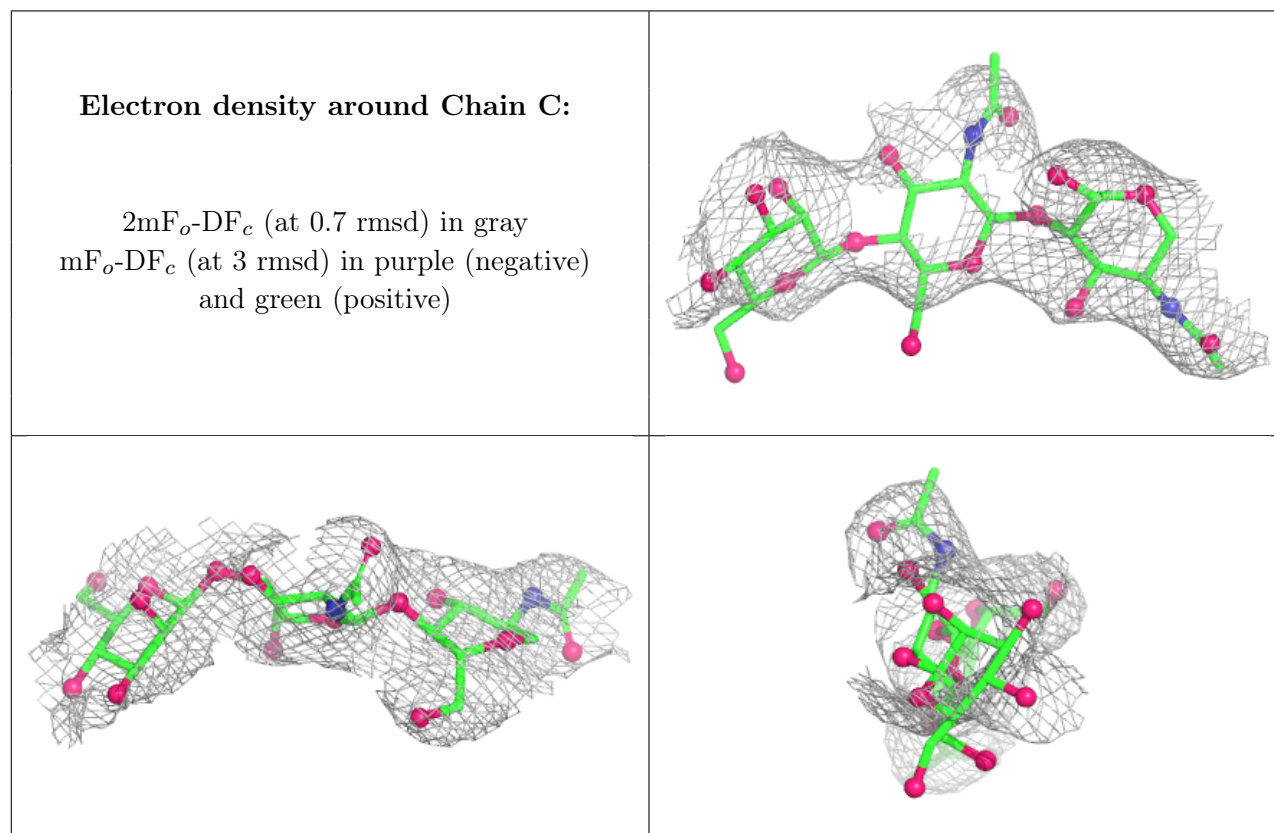
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [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, 95<sup>th</sup> 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.

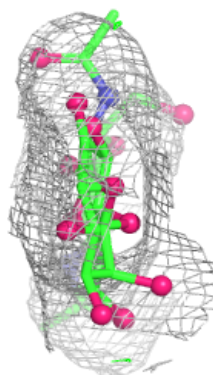
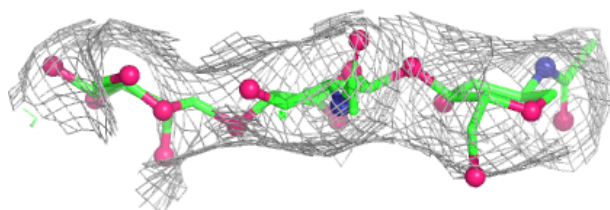
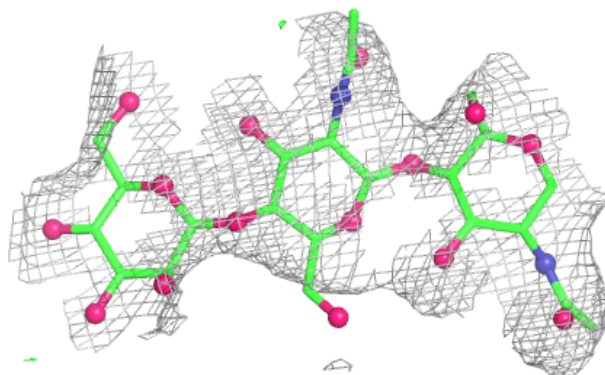
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	H	3	11/12	0.44	0.11	143,158,164,166	0
2	BMA	E	3	11/12	0.60	0.09	156,172,178,193	0
2	BMA	D	3	11/12	0.60	0.11	145,164,175,175	0
4	NAG	H	1	14/15	0.67	0.14	140,149,181,203	0
3	NAG	F	2	14/15	0.67	0.13	154,166,184,187	0
3	NAG	F	1	14/15	0.69	0.15	104,137,154,155	0
2	BMA	C	3	11/12	0.69	0.08	143,165,177,177	0
3	NAG	G	2	13/15	0.73	0.12	164,194,219,229	0
2	NAG	E	2	14/15	0.75	0.10	111,126,138,156	0
4	NAG	H	2	14/15	0.76	0.09	139,157,165,181	0
2	NAG	E	1	14/15	0.77	0.11	100,109,124,129	0
3	NAG	G	1	14/15	0.80	0.11	163,176,208,219	0
2	NAG	C	2	14/15	0.81	0.09	123,157,165,171	0
2	NAG	D	2	14/15	0.91	0.09	110,129,146,166	0
2	NAG	C	1	14/15	0.91	0.08	94,106,111,114	0
2	NAG	D	1	14/15	0.92	0.08	96,123,130,131	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.

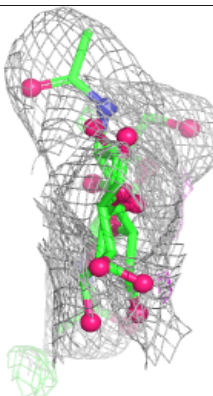
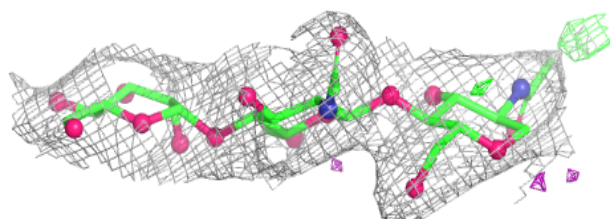
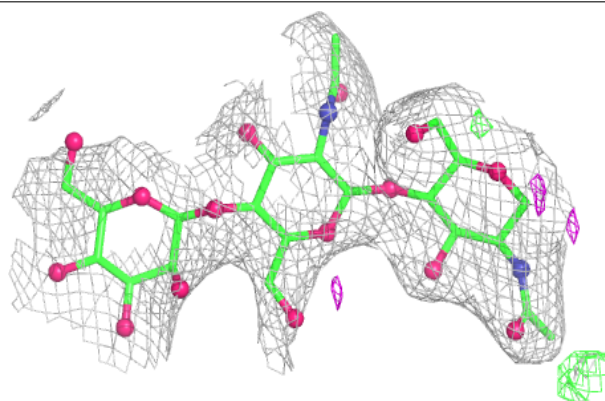


**Electron density around Chain D:**

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

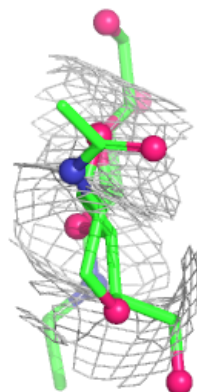
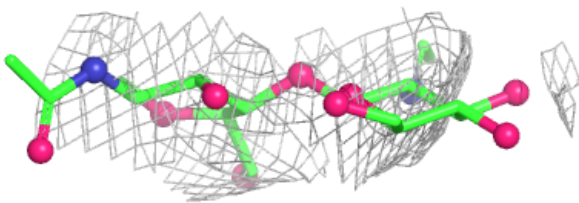
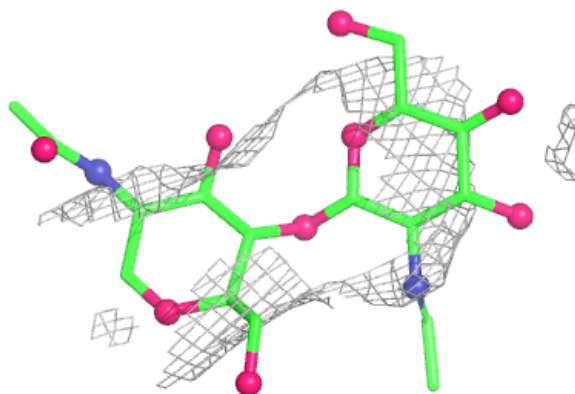
**Electron density around Chain E:**

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

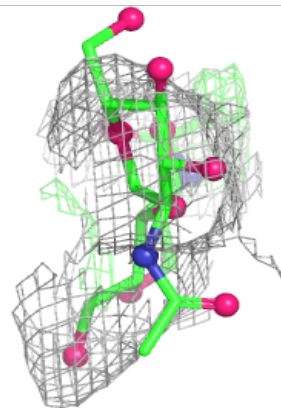
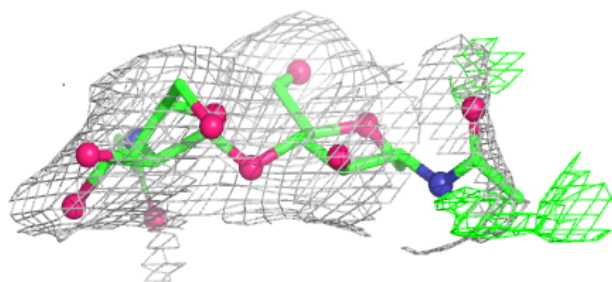
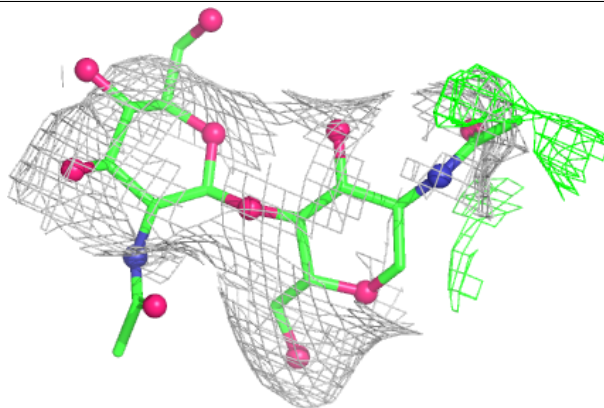


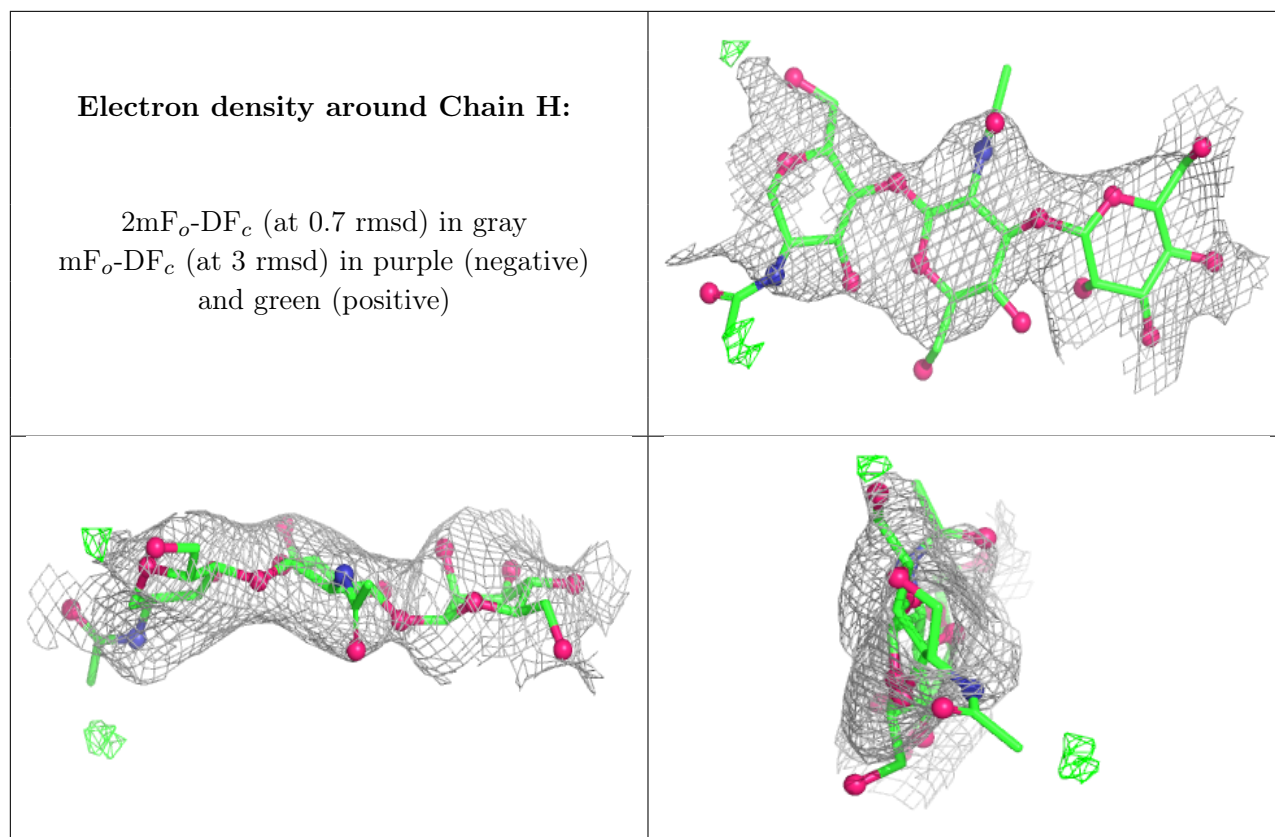
**Electron density around Chain G:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
6	BCT	B	702	4/4	0.91	0.08	46,55,57,61	0
6	BCT	A	702	4/4	0.95	0.06	58,64,79,83	0
5	FE	B	701	1/1	0.97	0.09	86,86,86,86	0
5	FE	A	701	1/1	0.99	0.05	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.