



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:54 PM UTC

PDB ID : 5NQ9 / pdb_00005nq9
Title : Crystal structure of laccases from Pycnoporus sanguineus, izoform II, monoclinic
Authors : Orlikowska, M.; de J.Rostro-Alanis, M.; Bujacz, A.; Hernandez-Luna, C.; Rubio, R.; Parra, R.; Bujacz, G.
Deposited on : 2017-04-19
Resolution : 2.72 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 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)
Xtriage (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

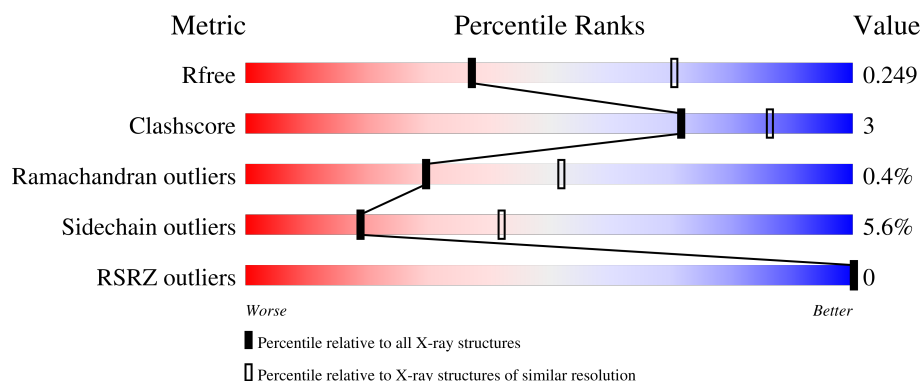
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

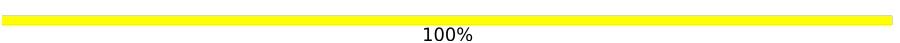
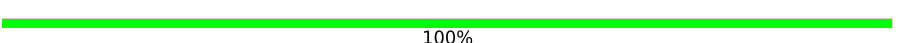
The reported resolution of this entry is 2.72 Å.

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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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 $\leq 5\%$. 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	518	 82% 13% . .
1	C	518	 83% 13% .
2	B	5	 40% 60%
3	D	2	 100%
3	F	2	 100%

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Mol	Chain	Length	Quality of chain
4	E	3	 100%
4	G	3	 67% 33%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7992 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 Laccase, izoform II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3803	2422	642	729	10			
1	C	497	Total	C	N	O	S	0	0	0
			3803	2422	642	729	10			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-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
2	B	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.

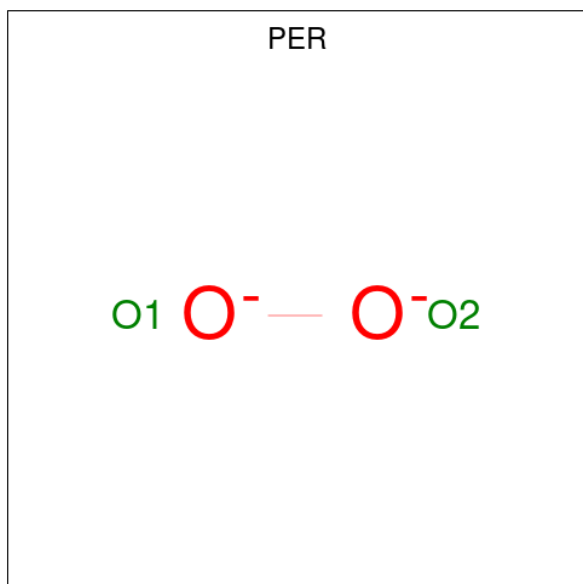


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	Cu	0	0
			6	6		
5	C	6	Total	Cu	0	0
			6	6		

- Molecule 6 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



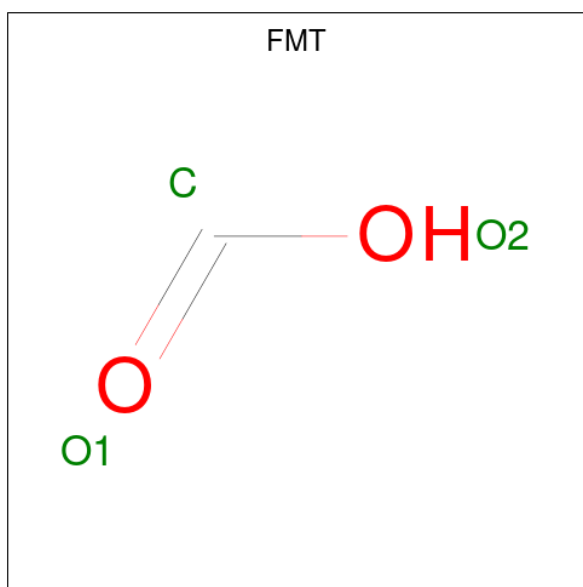
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



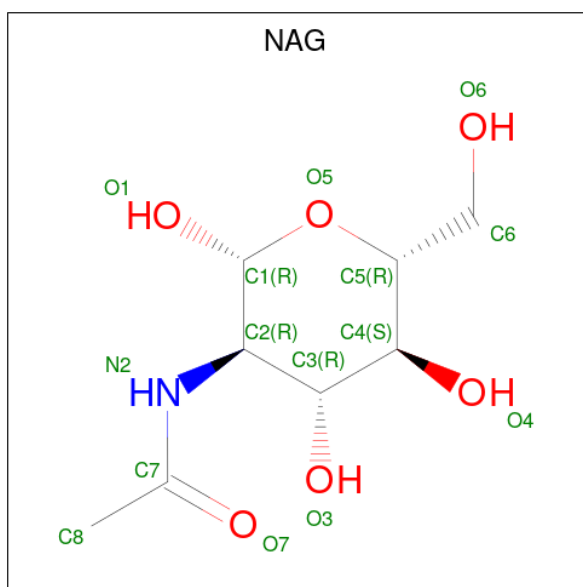
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	C	1	Total	C	O	0	0
			3	1	2		
8	C	1	Total	C	O	0	0
			3	1	2		
8	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			14	8	1	5		

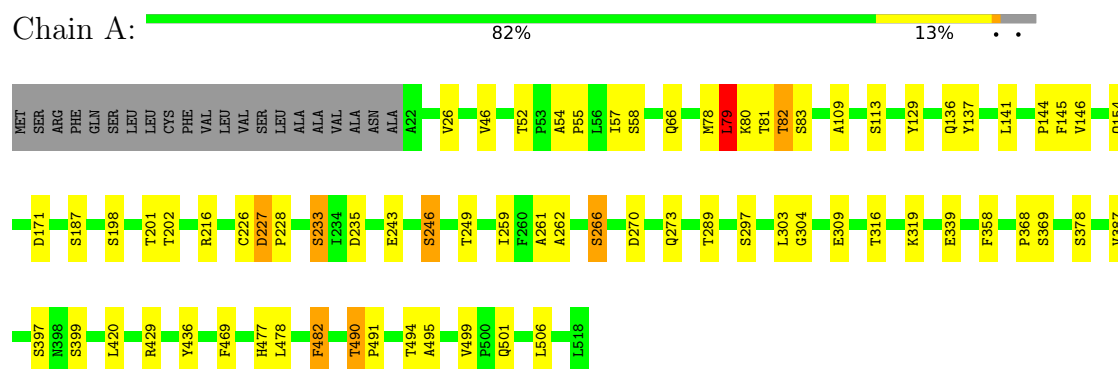
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	38	Total	O	0	0
			38	38		
10	C	41	Total	O	0	0
			41	41		

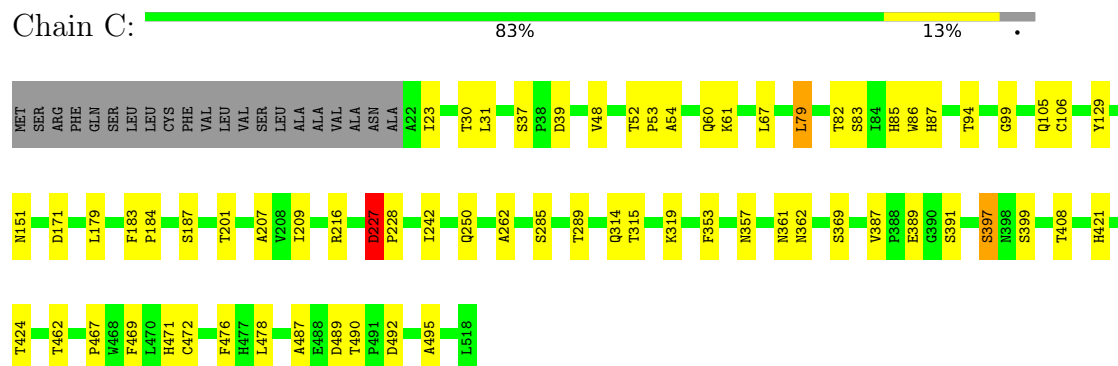
3 Residue-property plots

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.

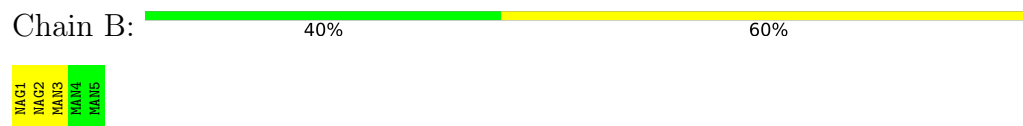
- Molecule 1: Laccase, isoform II



- Molecule 1: Laccase, isoform II



- Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain D:  100%

NAG1
NAG2

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

Chain F:  100%

NAG1
NAG2

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

Chain E:  100%

NAG1
NAG2
BMA3

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

Chain G:  67%  33%

NAG1
NAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.46Å 61.96Å 103.31Å 90.00° 109.82° 90.00°	Depositor
Resolution (Å)	48.65 – 2.72 48.65 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.65-2.72) 99.8 (48.65-2.72)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.170 , 0.246 0.176 , 0.249	Depositor DCC
R_{free} test set	1462 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7992	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: FMT, PER, NAG, MAN, CU, BMA, PEG

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	1.07	6/3924 (0.2%)	1.11	6/5394 (0.1%)
1	C	1.06	1/3924 (0.0%)	1.09	5/5394 (0.1%)
All	All	1.07	7/7848 (0.1%)	1.10	11/10788 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	THR	C-O	-5.95	1.16	1.24
1	A	506	LEU	N-CA	5.64	1.53	1.46
1	A	420	LEU	N-CA	5.54	1.52	1.46
1	A	266	SER	CA-C	-5.25	1.46	1.52
1	C	207	ALA	N-CA	-5.13	1.39	1.46
1	A	233	SER	N-CA	5.06	1.51	1.46
1	A	144	PRO	N-CA	-5.04	1.41	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	GLU	CA-C-N	-7.09	112.46	119.76
1	A	339	GLU	C-N-CA	-7.09	112.46	119.76
1	C	227	ASP	CA-C-N	-6.64	113.45	120.03
1	C	227	ASP	C-N-CA	-6.64	113.45	120.03
1	C	250	GLN	CA-C-N	-6.56	113.01	119.76
1	C	250	GLN	C-N-CA	-6.56	113.01	119.76
1	A	309	GLU	N-CA-C	6.36	117.91	109.83
1	A	273	GLN	CA-C-N	-5.86	114.23	120.03
1	A	273	GLN	C-N-CA	-5.86	114.23	120.03
1	A	235	ASP	N-CA-C	5.20	118.02	110.42
1	C	495	ALA	N-CA-C	-5.10	105.80	111.36

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	3803	0	3601	27	0
1	C	3803	0	3601	24	0
2	B	61	0	52	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	39	0	34	0	0
4	G	39	0	34	0	0
5	A	6	0	0	0	0
5	C	6	0	0	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	28	0	40	0	0
7	C	21	0	30	0	0
8	A	21	0	7	0	0
8	C	12	0	4	0	0
9	C	14	0	13	0	0
10	A	38	0	0	0	0
10	C	41	0	0	0	0
All	All	7992	0	7466	51	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 3.

All (51) 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:82:THR:HG22	1:A:136:GLN:OE1	1.76	0.84
1:C:389:GLU:OE2	1:C:389:GLU:N	2.19	0.72
1:A:198:SER:HG	1:A:201:THR:HG1	1.36	0.71
1:A:243:GLU:HB3	1:A:266:SER:HB2	1.81	0.63
1:A:227:ASP:HB3	1:A:228:PRO:CD	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:HB2	1:C:187:SER:HB3	1.83	0.60
1:A:81:THR:HG22	1:A:109:ALA:HA	1.83	0.60
1:A:243:GLU:OE2	1:A:246:SER:HA	2.02	0.59
1:C:227:ASP:HB3	1:C:228:PRO:CD	2.33	0.58
1:A:54:ALA:HB1	1:A:129:TYR:OH	2.06	0.56
1:C:489:ASP:CG	1:C:492:ASP:HB2	2.33	0.54
1:C:83:SER:OG	1:C:99:GLY:O	2.26	0.53
1:A:358:PHE:HB3	1:A:482:PHE:CD1	2.44	0.53
1:C:471:HIS:ND1	1:C:472:CYS:O	2.31	0.53
1:A:216:ARG:HG2	1:A:270:ASP:HA	1.92	0.52
1:C:52:THR:HA	1:C:53:PRO:C	2.35	0.51
1:C:85:HIS:CE1	1:C:421:HIS:CE1	3.00	0.49
1:A:26:VAL:HG22	1:A:66:GLN:HB2	1.95	0.48
1:C:171:ASP:OD2	1:C:228:PRO:HD2	2.14	0.48
1:C:361:ASN:O	1:C:362:ASN:HB2	2.14	0.48
1:A:78:MET:O	1:A:79:LEU:HB2	2.14	0.47
1:A:171:ASP:HB2	1:A:187:SER:HB3	1.97	0.47
1:A:54:ALA:HB1	1:A:55:PRO:HD2	1.96	0.46
1:A:477:HIS:O	1:A:478:LEU:C	2.56	0.46
1:C:227:ASP:HB3	1:C:228:PRO:HD3	1.98	0.46
1:C:82:THR:OG1	1:C:83:SER:N	2.48	0.45
1:C:353:PHE:HA	1:C:357:ASN:O	2.16	0.45
1:A:171:ASP:OD2	1:A:226:CYS:HB2	2.17	0.44
1:A:494:THR:HG23	1:A:495:ALA:N	2.32	0.44
1:C:54:ALA:HB1	1:C:129:TYR:OH	2.18	0.44
1:C:67:LEU:HD13	1:C:86:TRP:CZ3	2.53	0.44
1:A:368:PRO:HB3	1:A:387:VAL:HG23	2.00	0.44
1:C:87:HIS:CE1	1:C:262:ALA:HB1	2.53	0.43
1:A:259:ILE:HG23	1:A:259:ILE:O	2.19	0.43
1:A:46:VAL:HG11	1:A:141:LEU:HB2	2.00	0.43
1:A:58:SER:HA	1:A:146:VAL:O	2.20	0.42
1:C:184:PRO:HG2	1:C:476:PHE:CZ	2.55	0.42
1:C:60:GLN:O	1:C:61:LYS:C	2.63	0.42
1:C:467:PRO:HA	1:C:487:ALA:HA	2.02	0.41
1:C:105:GLN:HG3	1:C:106:CYS:O	2.20	0.41
1:A:490:THR:N	1:A:491:PRO:CD	2.83	0.41
1:C:39:ASP:O	1:C:201:THR:OG1	2.34	0.41
1:A:261:ALA:O	1:A:262:ALA:HB3	2.20	0.41
1:A:154:GLN:NE2	1:A:249:THR:O	2.54	0.41
1:A:57:ILE:O	1:A:145:PHE:HA	2.20	0.41
1:A:429:ARG:HD2	1:A:436:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:CD2	1:C:48:VAL:HG22	2.51	0.41
1:A:303:LEU:HD23	1:A:304:GLY:N	2.36	0.41
1:C:183:PHE:O	1:C:184:PRO:C	2.63	0.41
1:A:82:THR:CG2	1:A:136:GLN:OE1	2.60	0.40
1:C:397:SER:O	1:C:399:SER:OG	2.35	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	495/518 (96%)	462 (93%)	31 (6%)	2 (0%)	30	52
1	C	495/518 (96%)	458 (92%)	35 (7%)	2 (0%)	30	52
All	All	990/1036 (96%)	920 (93%)	66 (7%)	4 (0%)	30	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	C	227	ASP
1	A	79	LEU
1	C	79	LEU

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	417/434 (96%)	395 (95%)	22 (5%)	20	44
1	C	417/434 (96%)	392 (94%)	25 (6%)	17	39
All	All	834/868 (96%)	787 (94%)	47 (6%)	19	42

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	80	LYS
1	A	82	THR
1	A	83	SER
1	A	113	SER
1	A	137	TYR
1	A	202	THR
1	A	233	SER
1	A	246	SER
1	A	289	THR
1	A	297	SER
1	A	316	THR
1	A	319	LYS
1	A	369	SER
1	A	378	SER
1	A	397	SER
1	A	399	SER
1	A	469	PHE
1	A	482	PHE
1	A	490	THR
1	A	499	VAL
1	A	501	GLN
1	C	23	ILE
1	C	30	THR
1	C	37	SER
1	C	79	LEU
1	C	94	THR
1	C	151	ASN
1	C	179	LEU
1	C	209	ILE
1	C	216	ARG
1	C	242	ILE
1	C	285	SER
1	C	289	THR
1	C	314	GLN

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Mol	Chain	Res	Type
1	C	315	THR
1	C	319	LYS
1	C	369	SER
1	C	387	VAL
1	C	391	SER
1	C	397	SER
1	C	408	THR
1	C	424	THR
1	C	462	THR
1	C	469	PHE
1	C	478	LEU
1	C	490	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	348	ASN
1	A	381	GLN
1	C	68	ASN
1	C	105	GLN
1	C	154	GLN
1	C	288	ASN
1	C	363	HIS

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 ⓘ

15 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	2,1	14,14,15	0.31	0	17,19,21	1.88	3 (17%)
2	NAG	B	2	2	14,14,15	0.39	0	17,19,21	1.21	2 (11%)
2	MAN	B	3	2	11,11,12	0.29	0	15,15,17	1.30	2 (13%)
2	MAN	B	4	2	11,11,12	0.26	0	15,15,17	0.79	0
2	MAN	B	5	2	11,11,12	0.29	0	15,15,17	0.53	0
3	NAG	D	1	3,1	14,14,15	0.32	0	17,19,21	1.08	2 (11%)
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.37	0	17,19,21	0.71	1 (5%)
4	NAG	E	2	4	14,14,15	0.40	0	17,19,21	0.96	1 (5%)
4	BMA	E	3	4	11,11,12	0.35	0	15,15,17	0.84	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.29	0	17,19,21	0.75	0
3	NAG	F	2	3	14,14,15	0.35	0	17,19,21	0.67	0
4	NAG	G	1	4,1	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.77	0
4	BMA	G	3	4	11,11,12	0.23	0	15,15,17	1.03	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
2	NAG	B	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1
2	MAN	B	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	6.16	120.45	112.19
2	B	3	MAN	C1-O5-C5	3.26	116.55	112.19
2	B	3	MAN	C1-C2-C3	3.04	114.07	109.64
2	B	2	NAG	C1-C2-N2	-2.79	106.04	110.43
2	B	1	NAG	O5-C1-C2	2.70	115.47	111.29
3	D	1	NAG	C1-O5-C5	2.64	115.72	112.19
4	G	3	BMA	C1-O5-C5	2.52	115.57	112.19
4	E	3	BMA	C1-C2-C3	2.50	113.28	109.64
4	E	1	NAG	C1-C2-N2	-2.46	106.56	110.43
3	D	2	NAG	O5-C1-C2	-2.42	107.55	111.29
2	B	1	NAG	C3-C4-C5	2.42	114.61	110.23
4	E	2	NAG	C4-C3-C2	2.34	114.44	111.02
2	B	2	NAG	C4-C3-C2	2.29	114.38	111.02
3	D	1	NAG	C1-C2-N2	2.09	113.73	110.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

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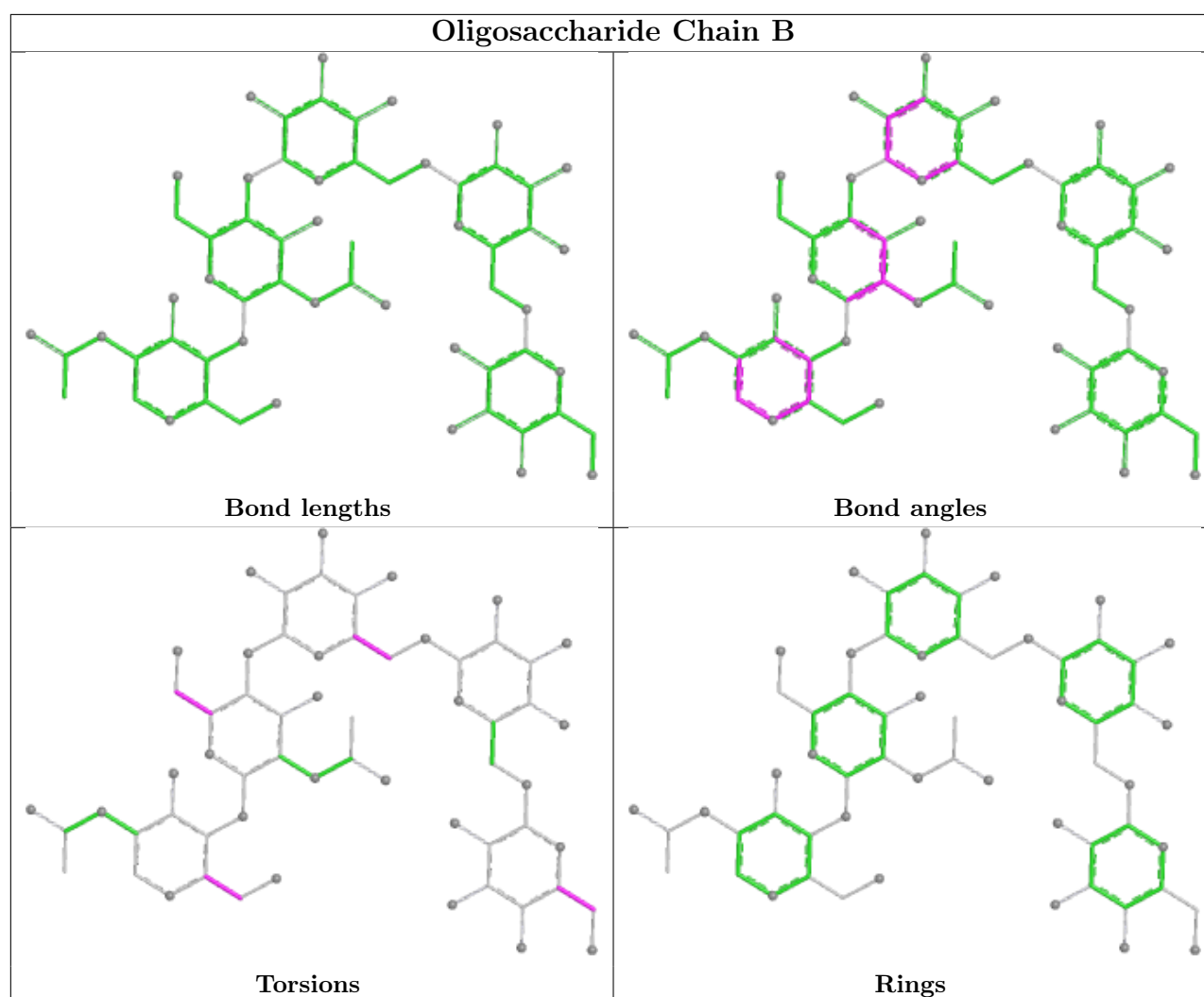
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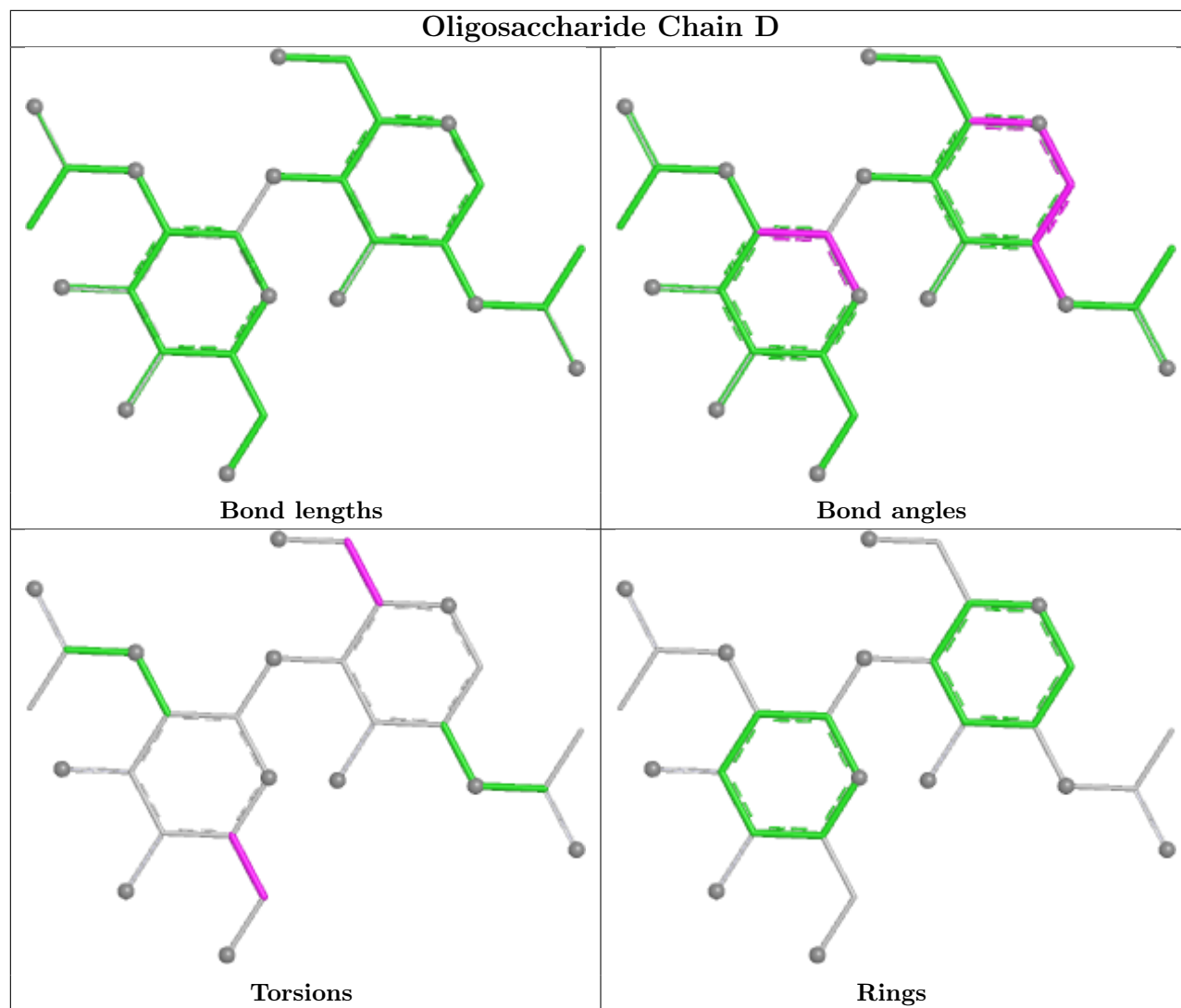
Mol	Chain	Res	Type	Atoms
2	B	3	MAN	O5-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

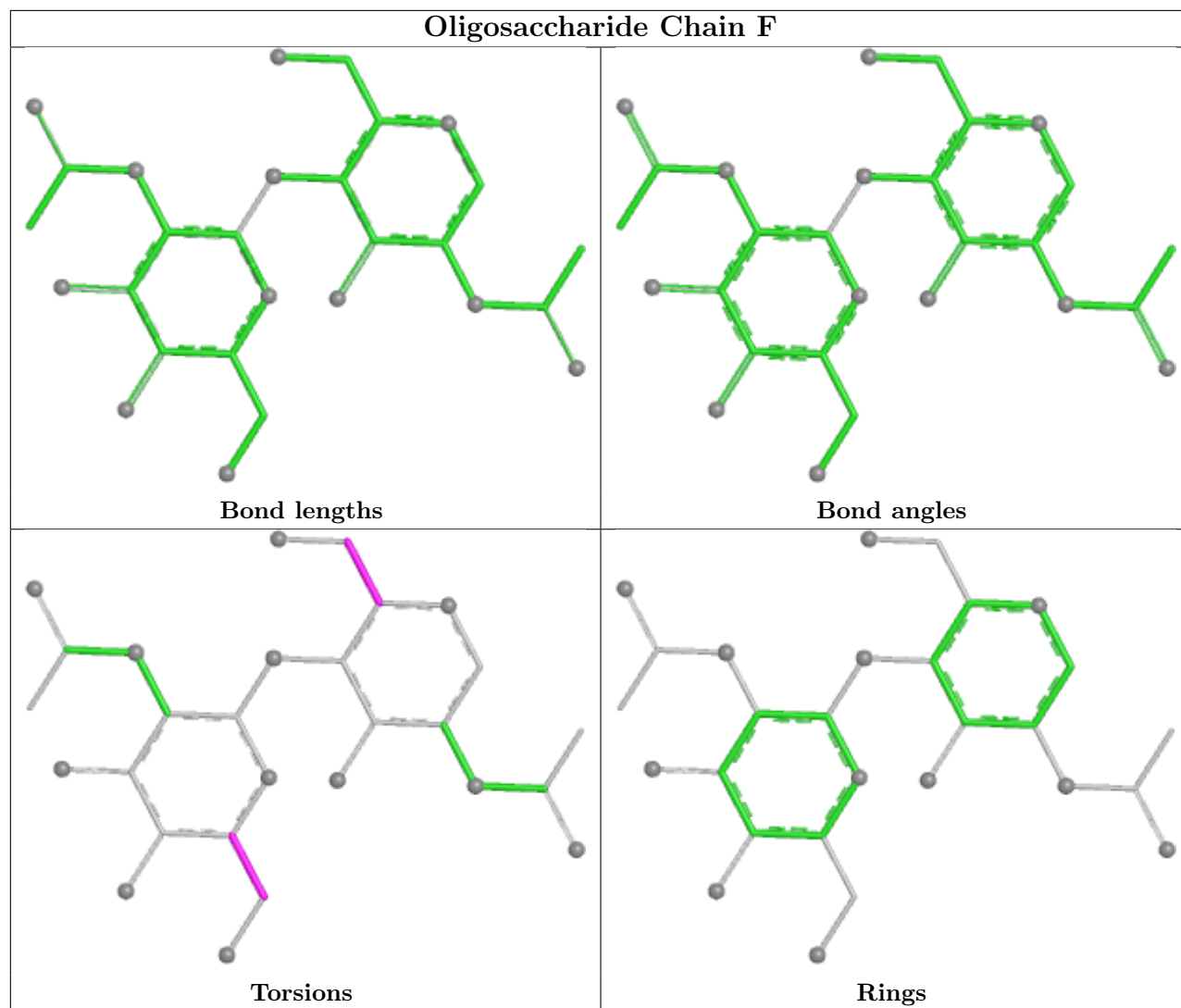
There are no ring outliers.

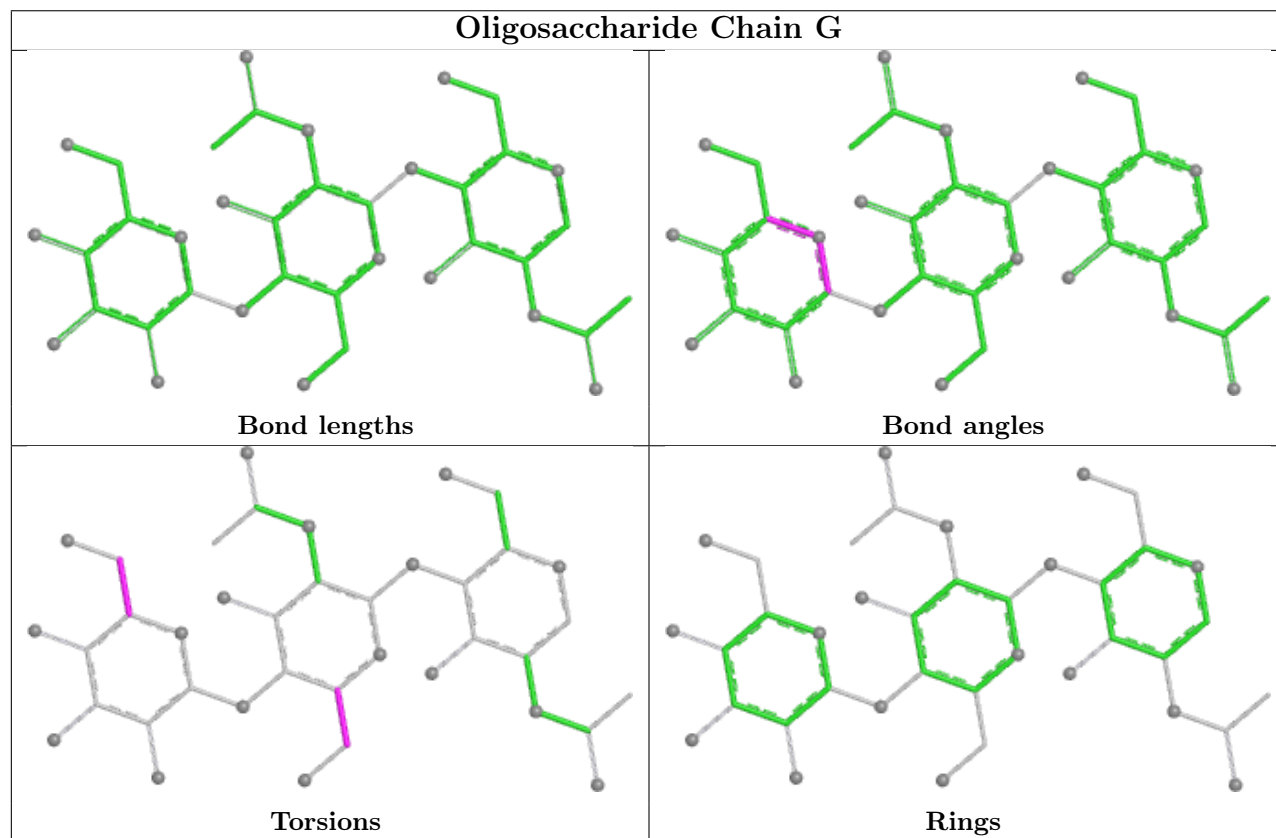
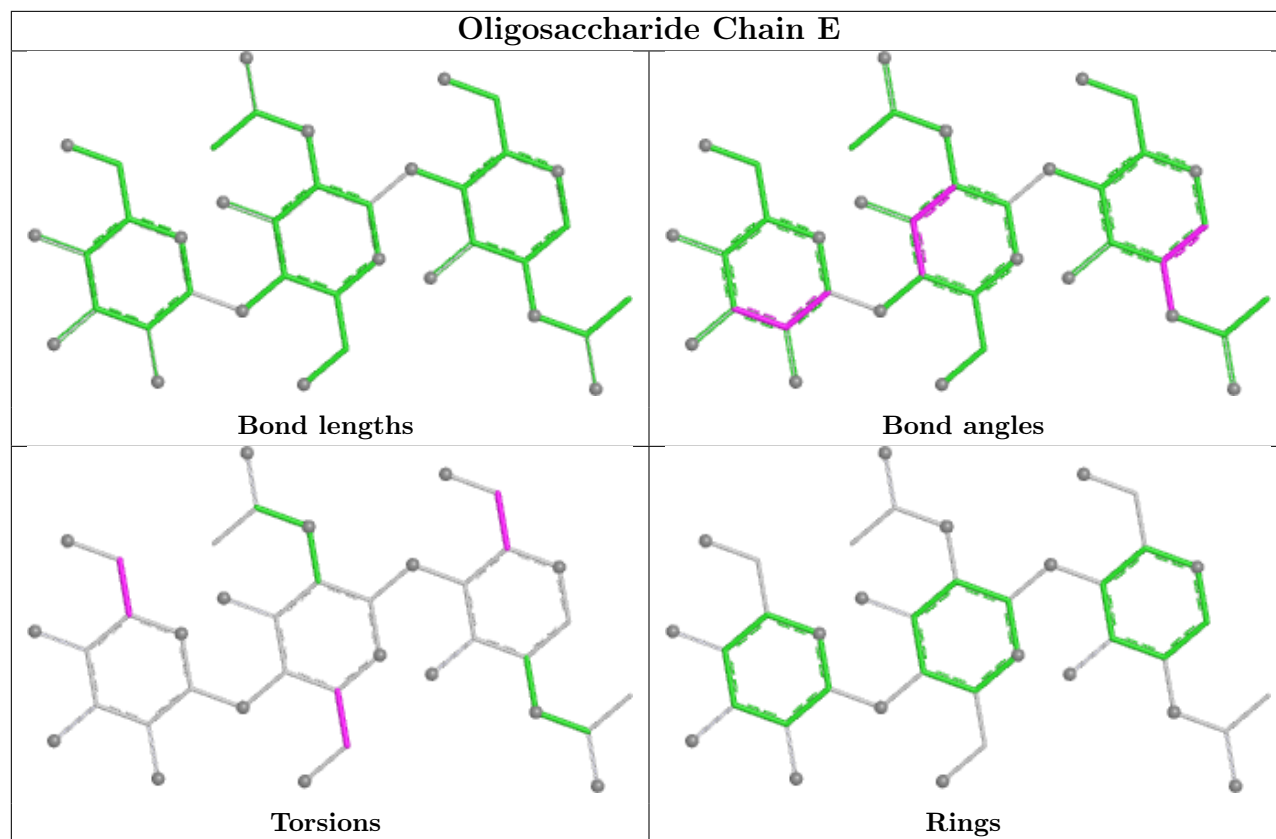
No monomer is involved in short contacts.

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 33 ligands modelled in this entry, 12 are monoatomic - leaving 21 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	$\# Z > 2$
7	PEG	C	613	-	6,6,6	0.52	0	5,5,5	0.19	0
8	FMT	A	621	-	2,2,2	0.69	0	1,1,1	0.72	0
7	PEG	A	619	-	6,6,6	0.65	0	5,5,5	0.45	0
7	PEG	C	612	-	6,6,6	0.68	0	5,5,5	0.64	0
8	FMT	A	624	-	2,2,2	0.74	0	1,1,1	0.70	0
7	PEG	A	618	-	6,6,6	0.58	0	5,5,5	0.49	0
8	FMT	C	616	-	2,2,2	0.69	0	1,1,1	0.71	0
8	FMT	C	615	-	2,2,2	0.73	0	1,1,1	0.66	0
7	PEG	A	616	-	6,6,6	0.65	0	5,5,5	0.63	0
6	PER	C	601	5	1,1,1	0.29	0	-		
8	FMT	A	623	-	2,2,2	0.70	0	1,1,1	0.70	0
8	FMT	C	618	-	2,2,2	0.77	0	1,1,1	0.65	0
8	FMT	A	620	-	2,2,2	0.76	0	1,1,1	0.69	0
9	NAG	C	606	1	14,14,15	0.61	0	17,19,21	1.00	1 (5%)
8	FMT	A	626	-	2,2,2	0.69	0	1,1,1	0.78	0
7	PEG	C	614	-	6,6,6	0.54	0	5,5,5	0.42	0
7	PEG	A	617	-	6,6,6	0.60	0	5,5,5	0.38	0
8	FMT	A	625	-	2,2,2	0.71	0	1,1,1	0.67	0
8	FMT	C	617	-	2,2,2	0.64	0	1,1,1	0.75	0
8	FMT	A	622	-	2,2,2	0.69	0	1,1,1	0.68	0
6	PER	A	605	5	1,1,1	0.12	0	-		

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
7	PEG	C	613	-	-	0/4/4/4	-
7	PEG	A	617	-	-	1/4/4/4	-
7	PEG	C	614	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	C	606	1	-	4/6/23/26	0/1/1/1
7	PEG	A	619	-	-	3/4/4/4	-
7	PEG	A	616	-	-	1/4/4/4	-
7	PEG	C	612	-	-	3/4/4/4	-
7	PEG	A	618	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	606	NAG	C8-C7-N2	2.41	120.11	116.12

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	606	NAG	O5-C5-C6-O6
7	C	612	PEG	C4-C3-O2-C2
9	C	606	NAG	C4-C5-C6-O6
9	C	606	NAG	C8-C7-N2-C2
9	C	606	NAG	O7-C7-N2-C2
7	A	617	PEG	O1-C1-C2-O2
7	A	618	PEG	O2-C3-C4-O4
7	C	612	PEG	O1-C1-C2-O2
7	A	616	PEG	O1-C1-C2-O2
7	A	619	PEG	C4-C3-O2-C2
7	C	614	PEG	C1-C2-O2-C3
7	A	618	PEG	C1-C2-O2-C3
7	A	618	PEG	C4-C3-O2-C2
7	A	619	PEG	O1-C1-C2-O2
7	C	612	PEG	O2-C3-C4-O4
7	A	619	PEG	O2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	497/518 (95%)	-0.47	0 100 100	34, 51, 72, 90	0
1	C	497/518 (95%)	-0.42	0 100 100	38, 55, 75, 103	0
All	All	994/1036 (95%)	-0.45	0 100 100	34, 53, 74, 103	0

There are no RSRZ outliers to report.

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, 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.

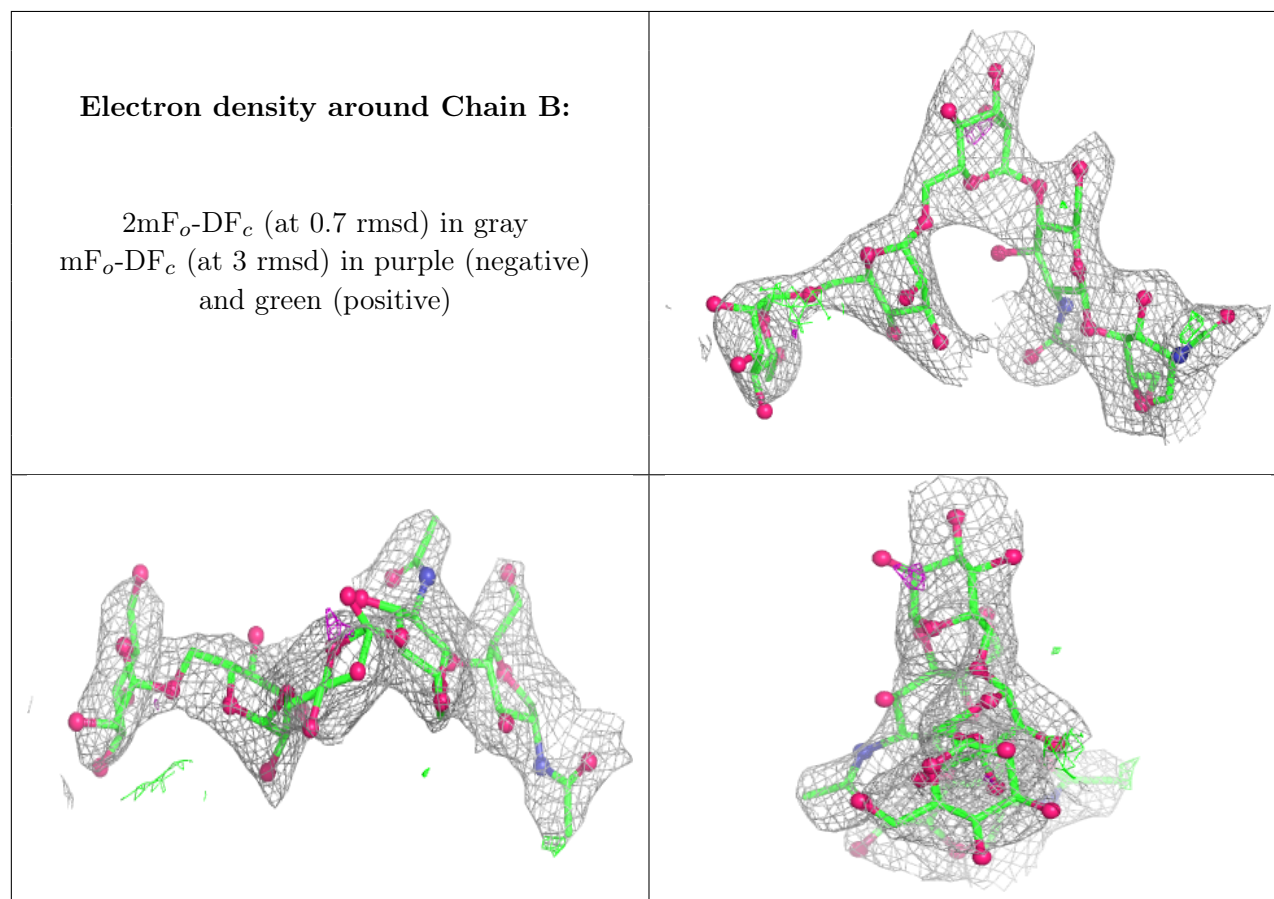
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	1	14/15	-	-	81,88,92,93	0
2	NAG	B	2	14/15	-	-	81,100,107,111	0
2	MAN	B	3	11/12	-	-	82,95,103,104	0
2	MAN	B	4	11/12	-	-	84,96,101,103	0
2	MAN	B	5	11/12	-	-	90,95,101,102	0
4	BMA	G	3	11/12	0.63	0.11	81,92,99,103	0
4	BMA	E	3	11/12	0.75	0.10	73,79,84,91	0
3	NAG	D	2	14/15	0.79	0.10	73,90,99,101	0
3	NAG	F	2	14/15	0.83	0.12	80,92,111,119	0
3	NAG	D	1	14/15	0.88	0.10	64,71,79,88	0
3	NAG	F	1	14/15	0.91	0.08	58,63,69,74	0

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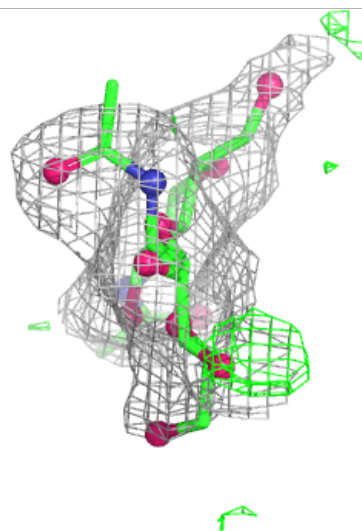
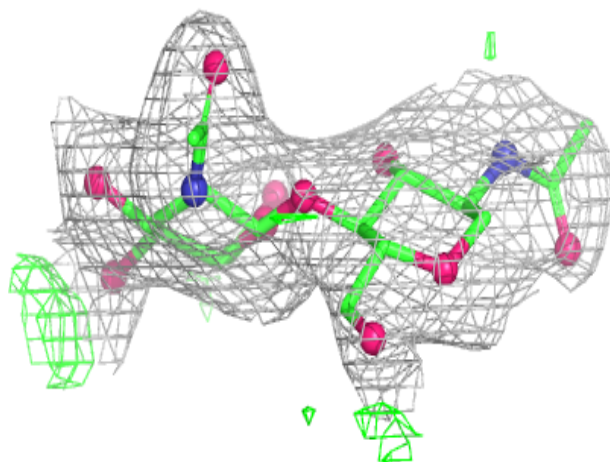
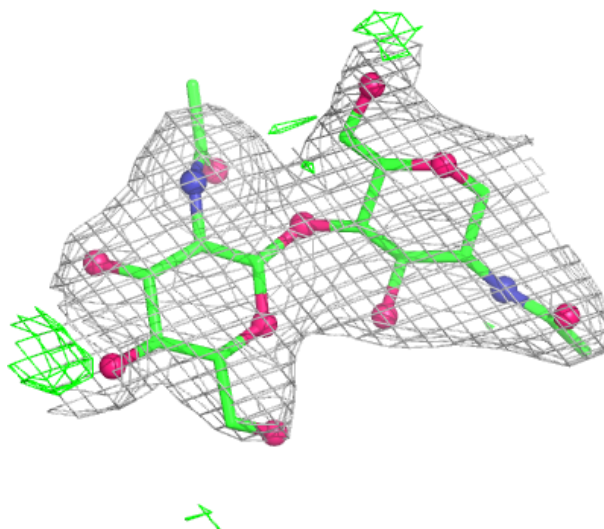
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	E	2	14/15	0.92	0.09	46,63,70,72	0
4	NAG	G	2	14/15	0.94	0.07	46,52,61,66	0
4	NAG	G	1	14/15	0.94	0.08	41,48,49,49	0
4	NAG	E	1	14/15	0.95	0.06	44,50,55,58	0

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.



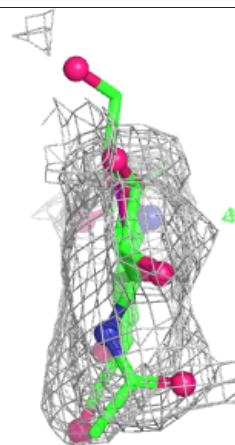
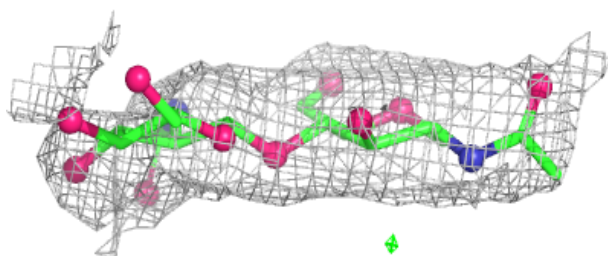
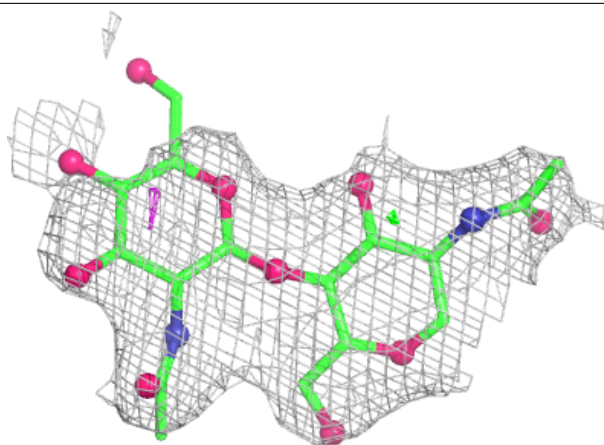
Electron density around Chain D:

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

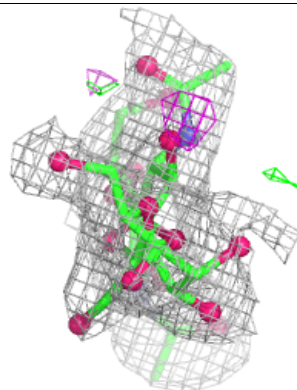
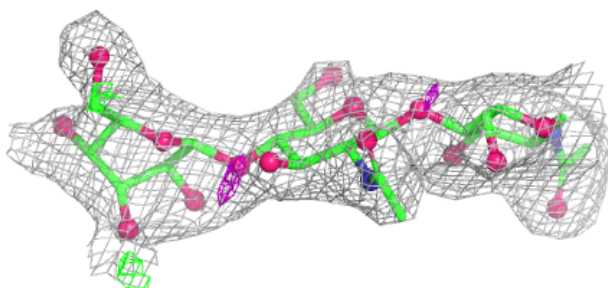
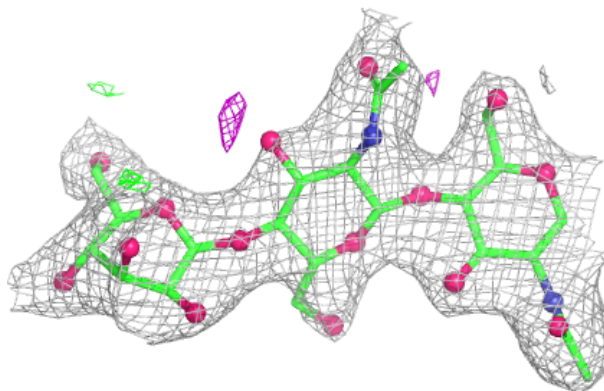


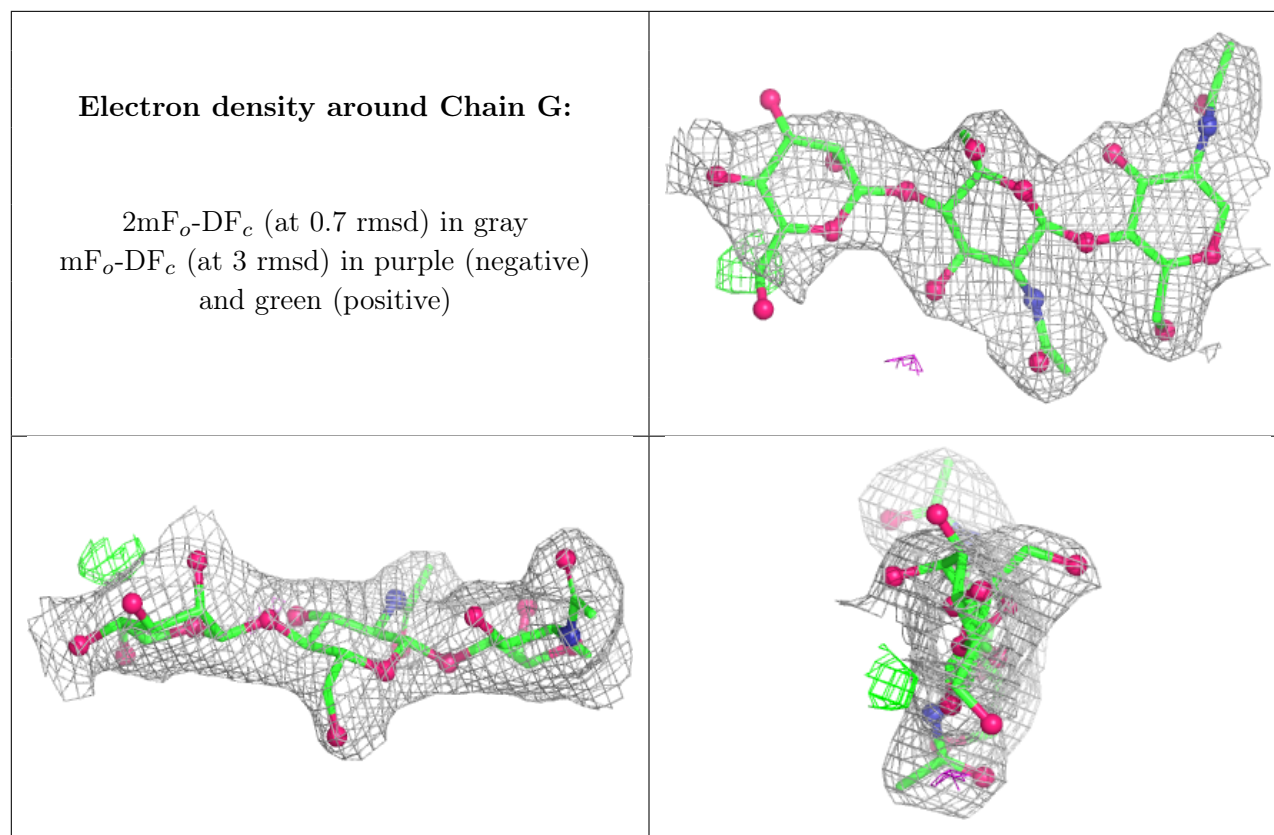
Electron density around Chain F:

$2mF_o-DF_c$ (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)





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
9	NAG	C	606	14/15	0.69	0.14	74,84,100,102	0
8	FMT	A	624	3/3	0.74	0.21	74,74,82,82	0
8	FMT	A	623	3/3	0.76	0.10	61,61,66,66	0
7	PEG	A	617	7/7	0.79	0.14	63,72,74,75	0
8	FMT	A	626	3/3	0.80	0.14	68,68,71,73	0
5	CU	C	619	1/1	0.80	0.11	116,116,116,116	0
7	PEG	C	614	7/7	0.81	0.13	63,71,76,79	0
8	FMT	C	618	3/3	0.83	0.10	67,67,71,72	0
5	CU	A	627	1/1	0.84	0.09	109,109,109,109	0
8	FMT	C	616	3/3	0.85	0.12	72,72,74,76	0
8	FMT	C	617	3/3	0.85	0.11	71,71,73,74	0
7	PEG	C	613	7/7	0.85	0.18	76,77,81,81	0
8	FMT	C	615	3/3	0.85	0.11	71,71,73,76	0
7	PEG	A	616	7/7	0.87	0.12	58,62,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FMT	A	625	3/3	0.88	0.11	64,64,71,75	0
7	PEG	C	612	7/7	0.89	0.13	61,66,67,69	0
5	CU	C	620	1/1	0.90	0.08	113,113,113,113	0
5	CU	A	628	1/1	0.92	0.09	111,111,111,111	0
7	PEG	A	618	7/7	0.92	0.09	54,57,59,59	0
7	PEG	A	619	7/7	0.92	0.10	61,63,65,66	0
8	FMT	A	620	3/3	0.93	0.08	59,59,65,66	0
6	PER	A	605	2/2	0.93	0.21	69,69,69,76	0
8	FMT	A	621	3/3	0.94	0.11	57,57,60,63	0
8	FMT	A	622	3/3	0.96	0.07	52,52,54,58	0
6	PER	C	601	2/2	0.97	0.08	62,62,62,71	0
5	CU	C	604	1/1	0.99	0.02	52,52,52,52	0
5	CU	A	601	1/1	0.99	0.02	52,52,52,52	0
5	CU	A	603	1/1	0.99	0.03	46,46,46,46	0
5	CU	C	602	1/1	0.99	0.02	46,46,46,46	0
5	CU	C	605	1/1	1.00	0.02	47,47,47,47	0
5	CU	A	602	1/1	1.00	0.02	56,56,56,56	0
5	CU	C	603	1/1	1.00	0.01	58,58,58,58	0
5	CU	A	604	1/1	1.00	0.02	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.