WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2023 – 01:42 pm BST

PDB ID	:	4CVU
Title	:	Structure of Fungal beta-mannosidase from Glycoside Hydrolase Family 2 of Trichoderma harzianum
Authors	:	Muniz, J.R.C.; Aparicio, R.; Santos, J.C.; Nascimento, A.S.; Golubev, A.M.; Polikarpov, I.
Deposited on	:	2014-03-31
Resolution	:	1.90 Å(reported)

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

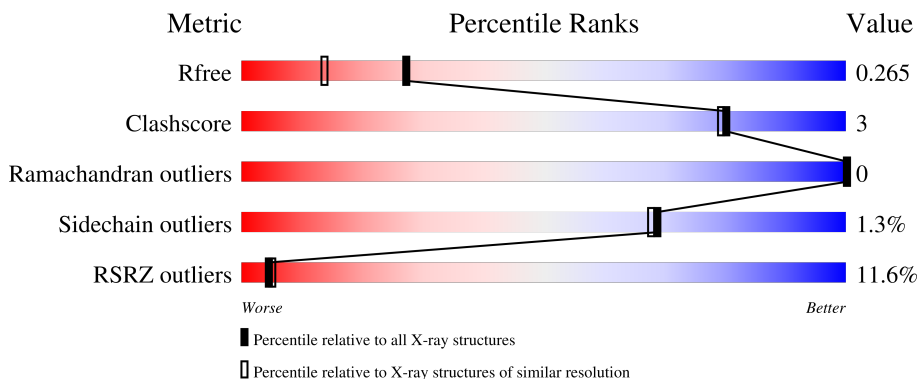|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 1.90 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	Percentile Ranks	Value
Rfree		0.265
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		11.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	942	11% / 90% / 6% ·
2	B	3	33% / 33% / 33%
3	C	8	12% / 62% / 25%
4	D	6	100%
5	E	11	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	C	4	-	-	-	X

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 8456 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 BETA-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	913	Total 7241	C 4645	N 1208	O 1371	S 17	0	6	0

- 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.
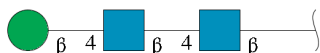
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
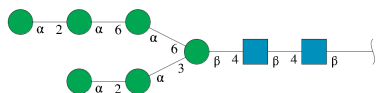
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total 94	C 52	N 2	O 40	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(2-6)]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	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyr anose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2 -acetamido-2-deoxy-beta-D-glucopyranose.
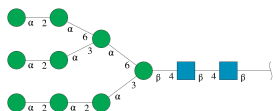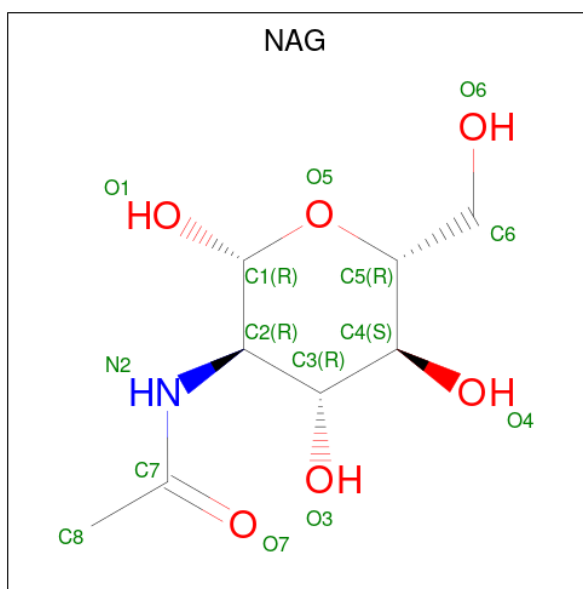

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

- Molecule 7 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total 17	Cd 17	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total 6	Na 6	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
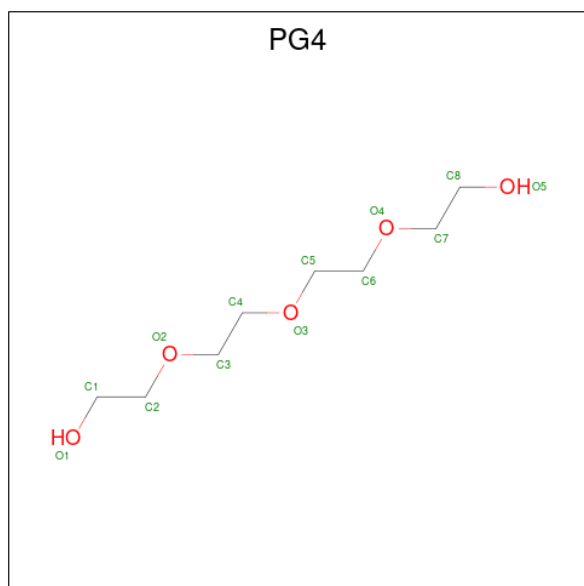
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 12	C 8	O 4	0	0

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
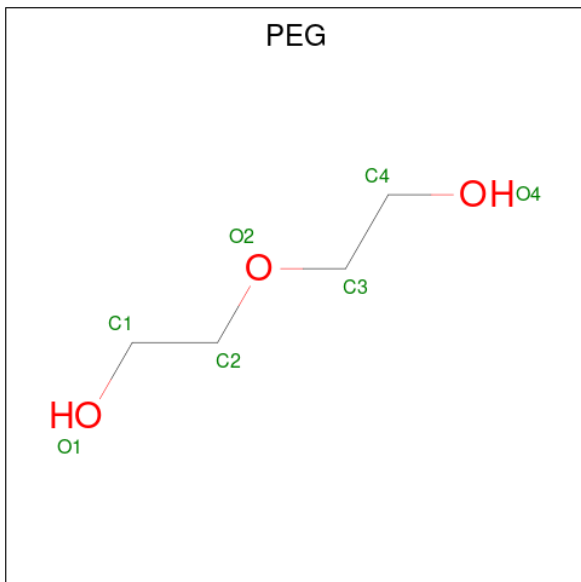
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 7	C 4	O 3	0	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total 1	Ca 1	0	0

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total 1	Cl 1	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	741	Total 741	O 741	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 res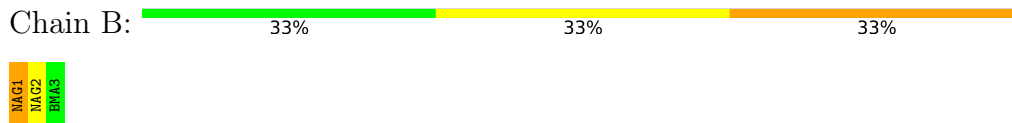idues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BETA-MANNOSIDASE
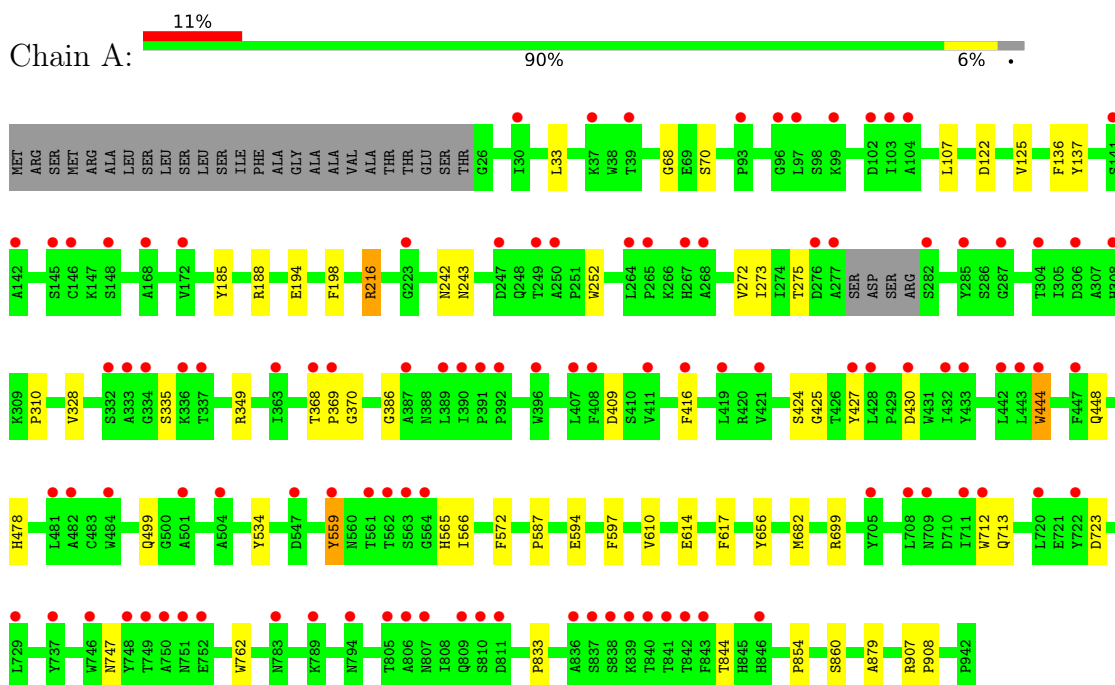
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose

• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran ose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1 -4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos e
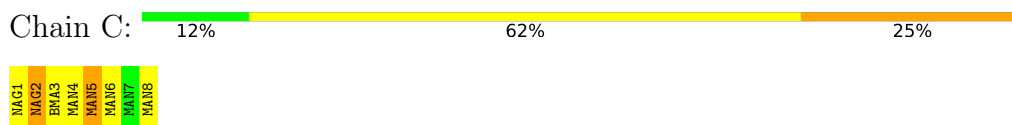
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyran ose-(2-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetam ido-2-deoxy-beta-D-glucopyranose

Chain D:

100%

NAG1 NAG2 BMA3 MAN4 MAN5 MAN6

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]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 MAN4 MAN5 MAN6 MAN7 MAN8 MAN9 MAN10 MAN11

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.46Å 166.46Å 121.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.70 – 1.90	Depositor
	48.30 – 1.90	EDS
% Data completeness	98.8 (117.70-1.90)	Depositor
(in resolution range)	98.8 (48.30-1.90)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.234 , 0.263	Depositor
	0.239 , 0.265	DCC
R_{free} test set	6636 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8456	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NA, NAG, MAN, CL, BMA, CA, PG4, PEG, CD

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	0.67	0/7479	0.72	4/10243 (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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	723	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	409	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	723	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	188	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	SER	Peptide

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	7241	0	6832	39	0
2	B	39	0	34	1	0
3	C	94	0	79	1	0
4	D	72	0	61	0	0
5	E	127	0	105	0	0
6	A	98	0	90	0	0
7	A	17	0	0	0	1
8	A	6	0	0	0	0
9	A	12	0	15	0	0
10	A	7	0	10	0	0
11	A	1	0	0	0	0
12	A	1	0	0	1	0
13	A	741	0	0	7	1
All	All	8456	0	7226	40	1

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 (40) 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)
3:C:2:NAG:H81	3:C:5:MAN:O6	1.81	0.80
1:A:194:GLU:HG3	1:A:425:GLY:HA2	1.67	0.75
1:A:597:PHE:HB2	1:A:682:MET:CE	2.26	0.66
1:A:565:HIS:NE2	12:A:1033:CL:CL	2.58	0.65
1:A:597:PHE:HB2	1:A:682:MET:HE1	1.80	0.64
1:A:844:THR:O	13:A:1101:HOH:O	2.16	0.62
1:A:879:ALA:O	1:A:908:PRO:HA	2.03	0.58
1:A:656:TYR:CE1	1:A:854:PRO:HG2	2.41	0.55
1:A:444:TRP:CD1	1:A:444:TRP:C	2.80	0.54
1:A:860:SER:OG	13:A:1102:HOH:O	2.18	0.53
1:A:272:VAL:HG12	1:A:328:VAL:HG22	1.91	0.52
1:A:617:PHE:CD1	2:B:1:NAG:H82	2.45	0.51
1:A:107:LEU:O	1:A:136:PHE:HA	2.11	0.51
1:A:243:ASN:HD21	1:A:534:TYR:H	1.57	0.51
1:A:610[A]:VAL:CG1	1:A:614:GLU:HB2	2.42	0.50
1:A:572:PHE:CD1	1:A:587:PRO:HD3	2.46	0.49
1:A:597:PHE:HB2	1:A:682:MET:HE2	1.96	0.48
1:A:194:GLU:HG3	1:A:425:GLY:CA	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:GLU:CD	13:A:1179:HOH:O	2.53	0.47
1:A:335:SER:CB	13:A:1333:HOH:O	2.63	0.47
1:A:185:TYR:HB2	1:A:198:PHE:HB3	1.98	0.46
1:A:747:ASN:ND2	13:A:1111:HOH:O	2.39	0.46
1:A:242:ASN:O	1:A:243:ASN:HB2	2.16	0.45
1:A:430:ASP:OD1	1:A:478:HIS:CE1	2.69	0.45
1:A:427:TYR:CE2	1:A:448:GLN:HG2	2.51	0.45
1:A:713:GLN:OE1	1:A:713:GLN:N	2.46	0.45
1:A:762:TRP:CE3	1:A:833:PRO:HB3	2.53	0.44
1:A:125[A]:VAL:HG12	1:A:137:TYR:HB3	1.99	0.44
1:A:860:SER:CB	13:A:1102:HOH:O	2.65	0.43
1:A:273:ILE:HG22	1:A:275[B]:THR:HG23	2.01	0.42
1:A:368:THR:HA	1:A:369:PRO:HD3	1.87	0.42
1:A:33:LEU:HG	1:A:216:ARG:HA	2.01	0.42
1:A:252:TRP:CD1	1:A:310:PRO:HG2	2.55	0.42
1:A:559:TYR:CD1	1:A:559:TYR:N	2.86	0.42
1:A:370:GLY:HA3	1:A:566:ILE:O	2.20	0.41
1:A:444:TRP:C	1:A:444:TRP:HD1	2.22	0.41
1:A:386:GLY:HA2	1:A:416:PHE:CD2	2.55	0.41
1:A:610[A]:VAL:HG13	1:A:614:GLU:HB2	2.02	0.41
1:A:68:GLY:HA3	13:A:1718:HOH:O	2.20	0.41
1:A:243:ASN:HD21	1:A:534:TYR:N	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1011:CD:CD	13:A:1192:HOH:O[3_545]	2.16	0.04

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	915/942 (97%)	891 (97%)	24 (3%)	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	777/811 (96%)	766 (99%)	11 (1%)	67	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	122	ASP
1	A	216	ARG
1	A	349[A]	ARG
1	A	349[B]	ARG
1	A	444	TRP
1	A	499	GLN
1	A	559	TYR
1	A	699	ARG
1	A	712	TRP
1	A	907	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	243	ASN

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 ⓘ

28 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	0.65	0	17,19,21	1.16	1 (5%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	0.93	1 (5%)
2	BMA	B	3	2	11,11,12	0.52	0	15,15,17	0.76	0
3	NAG	C	1	3,1	14,14,15	0.80	1 (7%)	17,19,21	0.90	0
3	NAG	C	2	3	14,14,15	0.66	0	17,19,21	1.30	2 (11%)
3	BMA	C	3	3	11,11,12	0.78	0	15,15,17	1.10	2 (13%)
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	2.07	3 (20%)
3	MAN	C	5	3	11,11,12	0.77	0	15,15,17	1.50	2 (13%)
3	MAN	C	6	3	11,11,12	0.68	0	15,15,17	0.87	1 (6%)
3	MAN	C	7	3	11,11,12	0.62	0	15,15,17	0.87	0
3	MAN	C	8	3	11,11,12	0.53	0	15,15,17	1.04	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.52	0	17,19,21	1.00	1 (5%)
4	NAG	D	2	4	14,14,15	0.74	0	17,19,21	1.21	1 (5%)
4	BMA	D	3	4	11,11,12	0.59	0	15,15,17	1.10	1 (6%)
4	MAN	D	4	4	11,11,12	0.63	0	15,15,17	1.27	2 (13%)
4	MAN	D	5	4	11,11,12	0.59	0	15,15,17	1.03	1 (6%)
4	MAN	D	6	4	11,11,12	0.95	0	13,15,17	2.05	2 (15%)
5	NAG	E	1	5,1	14,14,15	0.69	0	17,19,21	1.10	2 (11%)
5	MAN	E	10	5	11,11,12	0.78	1 (9%)	15,15,17	0.87	0
5	MAN	E	11	5	11,11,12	0.65	0	15,15,17	0.72	1 (6%)
5	NAG	E	2	5	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
5	BMA	E	3	5	11,11,12	0.53	0	15,15,17	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	MAN	E	4	5	11,11,12	0.58	0	15,15,17	1.12	2 (13%)
5	MAN	E	5	5	11,11,12	1.02	1 (9%)	15,15,17	1.11	2 (13%)
5	MAN	E	6	5	11,11,12	0.62	0	15,15,17	1.12	1 (6%)
5	MAN	E	7	5	11,11,12	1.40	1 (9%)	15,15,17	3.23	2 (13%)
5	MAN	E	8	5	11,11,12	0.75	0	15,15,17	1.52	4 (26%)
5	MAN	E	9	5	11,11,12	0.71	0	15,15,17	1.34	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	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	1/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	1/2/18/22	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	MAN	E	10	5	-	0/2/19/22	0/1/1/1
5	MAN	E	11	5	-	0/2/19/22	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	2/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1
5	MAN	E	8	5	-	0/2/19/22	0/1/1/1
5	MAN	E	9	5	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	7	MAN	O3-C3	-4.02	1.33	1.43
5	E	10	MAN	O5-C5	-2.19	1.39	1.43
3	C	1	NAG	C1-C2	2.07	1.55	1.52
5	E	5	MAN	O5-C1	-2.02	1.40	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	7	MAN	O3-C3-C2	11.67	132.35	109.99
3	C	4	MAN	C1-O5-C5	5.86	120.14	112.19
4	D	6	MAN	C3-C4-C5	5.27	115.22	109.97
4	D	6	MAN	C1-C2-C3	-4.50	100.55	110.91
3	C	4	MAN	O5-C5-C4	3.48	119.30	110.83
3	C	5	MAN	C1-C2-C3	3.44	113.89	109.67
3	C	2	NAG	C2-N2-C7	3.17	127.42	122.90
5	E	8	MAN	O5-C1-C2	3.06	115.49	110.77
5	E	9	MAN	C1-O5-C5	2.92	116.15	112.19
3	C	6	MAN	C1-O5-C5	2.92	116.15	112.19
3	C	8	MAN	C1-O5-C5	2.87	116.08	112.19
4	D	4	MAN	O2-C2-C3	-2.82	104.49	110.14
5	E	6	MAN	C2-C3-C4	-2.66	106.30	110.89
5	E	8	MAN	C3-C4-C5	2.65	114.97	110.24
5	E	8	MAN	C1-C2-C3	-2.63	106.44	109.67
5	E	1	NAG	C1-O5-C5	2.61	115.73	112.19
3	C	3	BMA	O3-C3-C4	-2.59	104.36	110.35
4	D	3	BMA	O4-C4-C3	-2.53	104.49	110.35
3	C	2	NAG	C8-C7-N2	2.53	120.38	116.10
4	D	2	NAG	C3-C4-C5	-2.50	105.78	110.24
2	B	1	NAG	C1-O5-C5	2.48	115.56	112.19
5	E	5	MAN	C1-O5-C5	2.38	115.42	112.19
3	C	5	MAN	O2-C2-C1	-2.32	104.41	109.15
4	D	1	NAG	C1-O5-C5	2.29	115.30	112.19
3	C	4	MAN	O5-C5-C6	-2.26	103.66	107.20
5	E	1	NAG	O5-C1-C2	-2.24	107.75	111.29
5	E	11	MAN	C1-O5-C5	2.24	115.22	112.19
5	E	2	NAG	O7-C7-C8	-2.22	117.94	122.06
4	D	5	MAN	O5-C5-C6	2.21	110.67	107.20
5	E	4	MAN	O4-C4-C5	2.18	114.70	109.30
5	E	8	MAN	O4-C4-C3	-2.13	105.42	110.35
2	B	2	NAG	C1-O5-C5	2.12	115.07	112.19
5	E	5	MAN	C6-C5-C4	-2.07	108.15	113.00
5	E	7	MAN	C1-O5-C5	2.06	114.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	3	BMA	O6-C6-C5	-2.05	104.25	111.29
4	D	4	MAN	C1-C2-C3	-2.04	107.16	109.67
3	C	3	BMA	O4-C4-C3	-2.01	105.70	110.35
5	E	4	MAN	O2-C2-C1	-2.00	105.06	109.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MAN	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
5	E	6	MAN	O5-C5-C6-O6
5	E	6	MAN	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
4	D	6	MAN	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
5	E	9	MAN	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
3	C	2	NAG	1	0
3	C	5	MAN	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.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
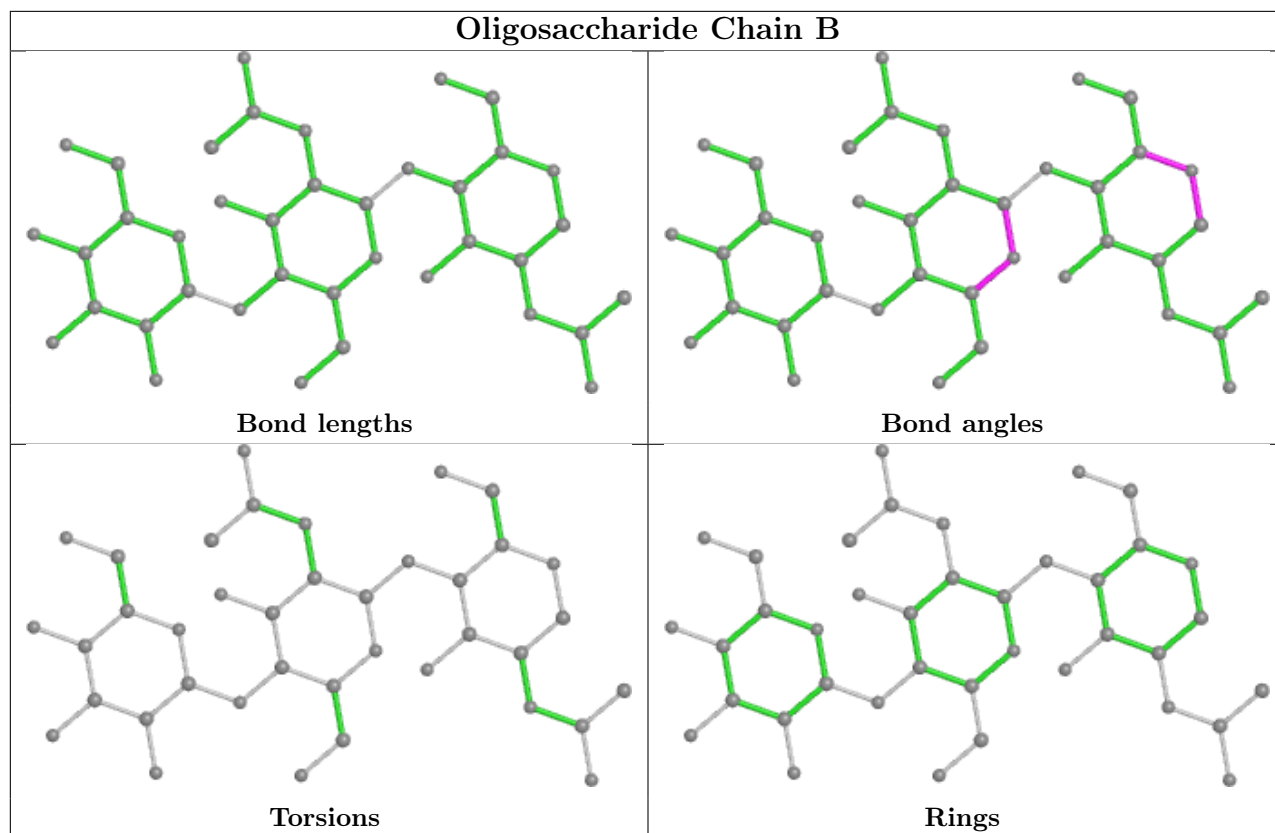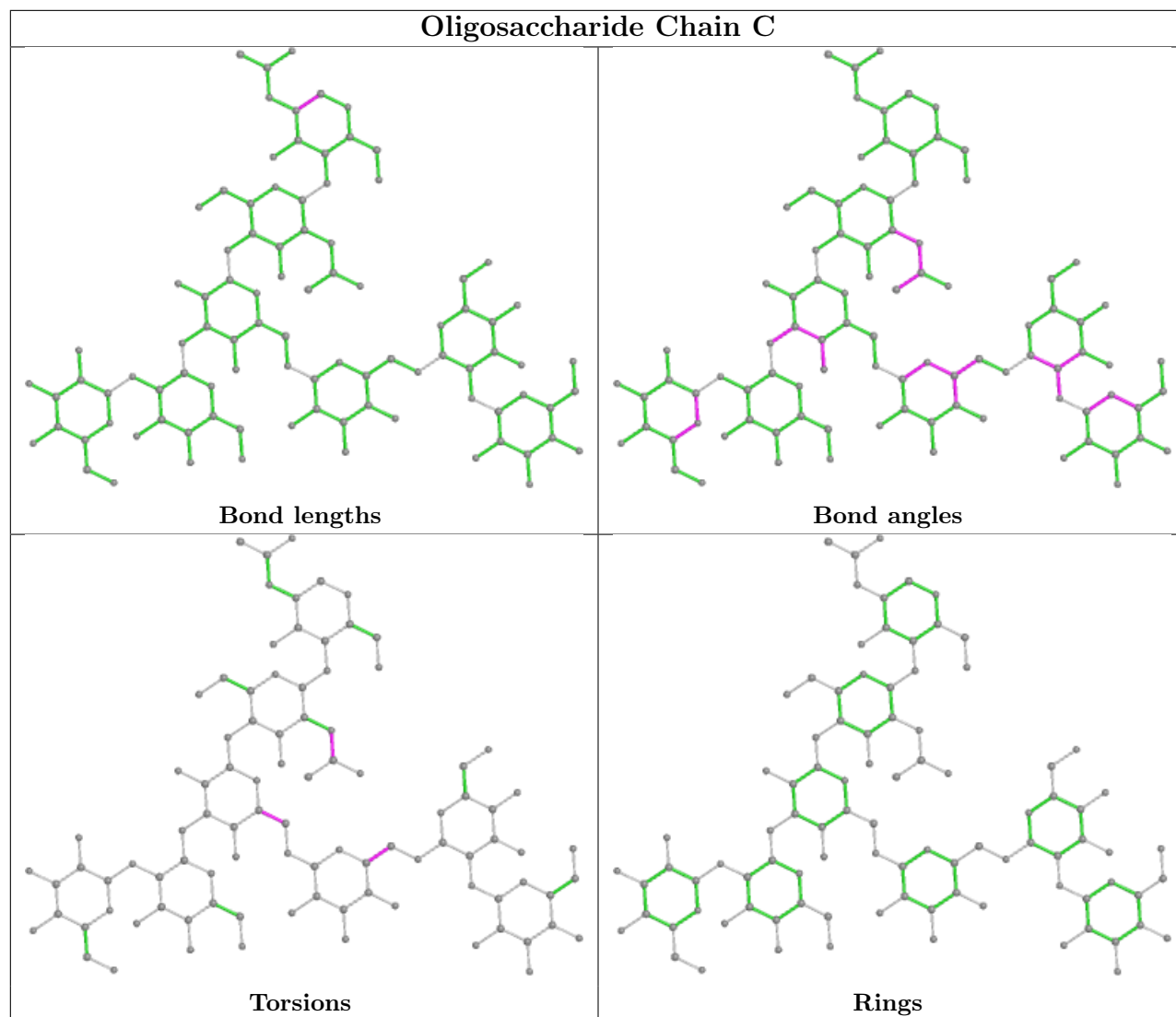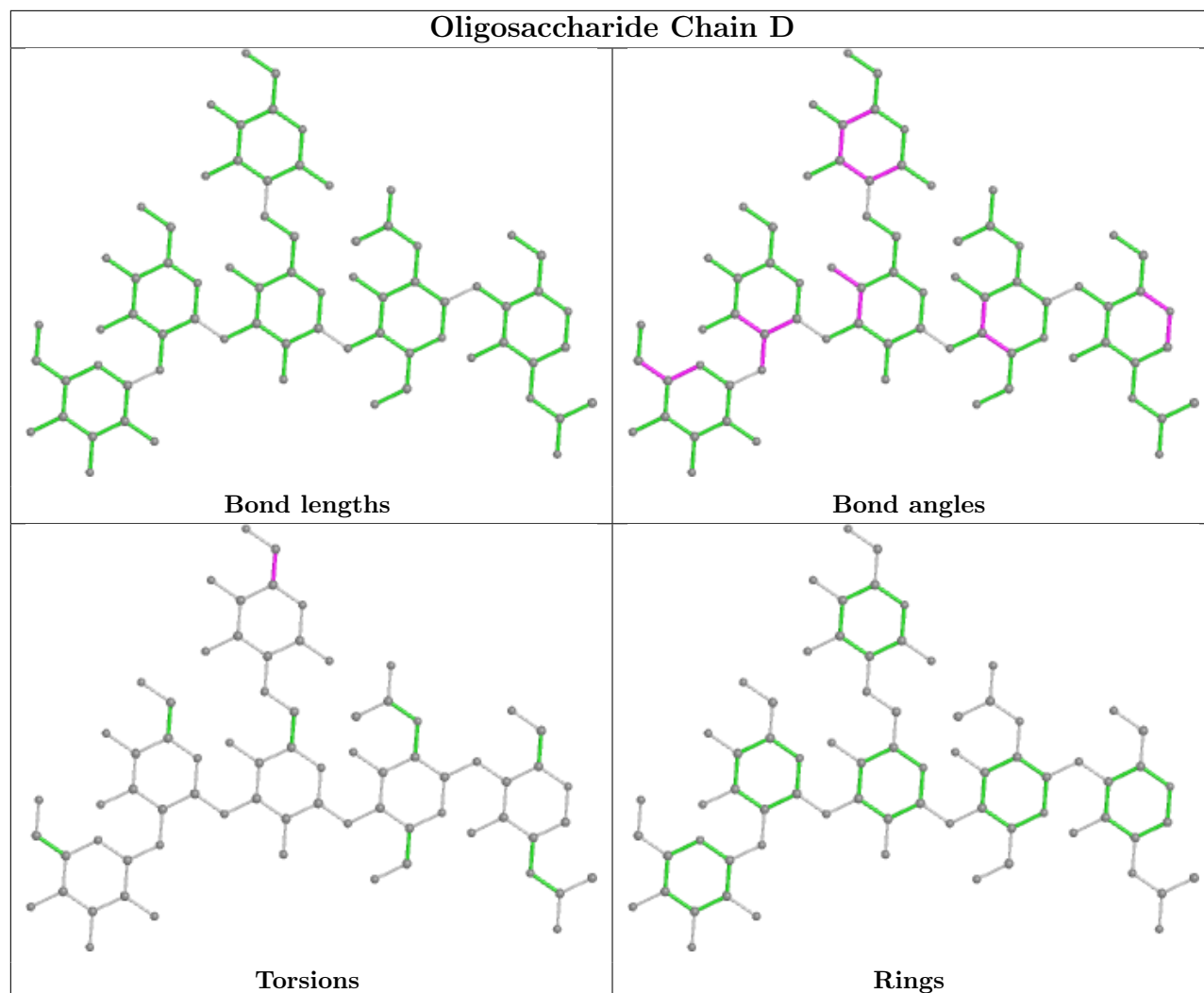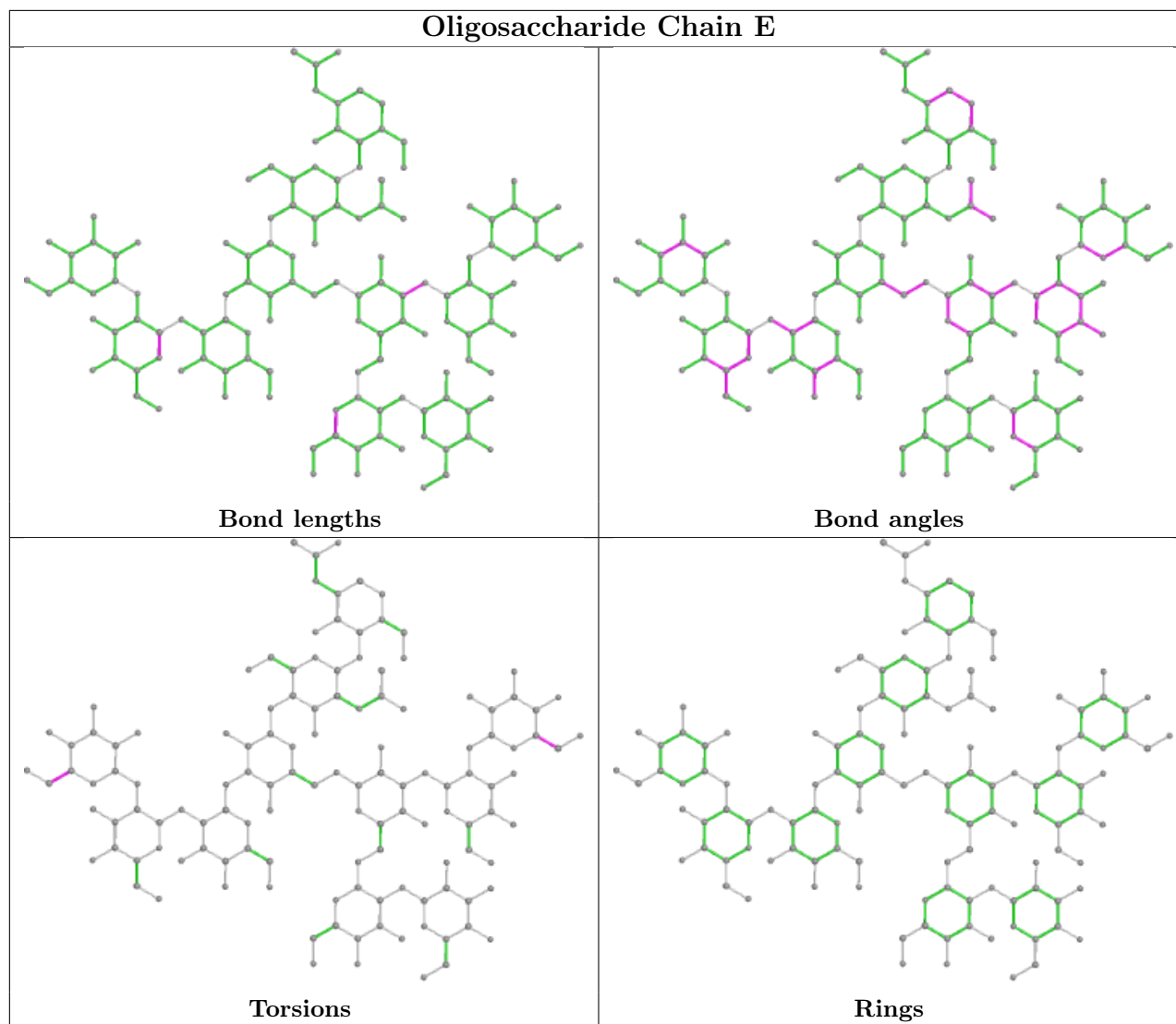
5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 25 are monoatomic - leaving 9 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	$\#|Z| > 2$
9	PG4	A	1030	-	11,11,12	0.54	0	10,10,11	0.44	0
6	NAG	A	1007	1	14,14,15	0.50	0	17,19,21	1.08	0
6	NAG	A	1004	1	14,14,15	0.48	0	17,19,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	NAG	A	1001	1	14,14,15	0.96	1 (7%)	17,19,21	1.22	1 (5%)
10	PEG	A	1031	-	6,6,6	0.53	0	5,5,5	0.28	0
6	NAG	A	1002	-	14,14,15	0.66	0	19,19,21	2.14	7 (36%)
6	NAG	A	1006	1	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
6	NAG	A	1003	1	14,14,15	0.93	1 (7%)	17,19,21	1.36	1 (5%)
6	NAG	A	1005	1	14,14,15	0.44	0	17,19,21	1.44	3 (17%)

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
9	PG4	A	1030	-	-	4/9/9/10	-
6	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
10	PEG	A	1031	-	-	3/4/4/4	-
6	NAG	A	1002	-	-	4/6/22/26	0/1/1/1
6	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1005	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	NAG	O5-C1	-2.16	1.40	1.43
6	A	1003	NAG	O5-C1	-2.03	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1002	NAG	C8-C7-N2	5.15	124.83	116.10
6	A	1003	NAG	C1-O5-C5	4.66	118.51	112.19
6	A	1002	NAG	C2-N2-C7	4.10	128.75	122.90
6	A	1004	NAG	C1-O5-C5	3.51	116.95	112.19
6	A	1001	NAG	C1-O5-C5	3.24	116.58	112.19
6	A	1002	NAG	C3-C2-N2	3.16	115.75	110.86
6	A	1005	NAG	C1-O5-C5	2.81	116.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1002	NAG	C3-C4-C5	2.79	114.39	110.77
6	A	1005	NAG	O5-C5-C6	2.52	111.16	107.20
6	A	1005	NAG	O5-C1-C2	-2.50	107.34	111.29
6	A	1002	NAG	O7-C7-C8	-2.43	117.53	122.06
6	A	1006	NAG	C1-O5-C5	2.42	115.47	112.19
6	A	1002	NAG	O7-C7-N2	-2.35	117.64	121.95
6	A	1002	NAG	O5-C1-C2	-2.02	107.49	109.52

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1005	NAG	O5-C5-C6-O6
6	A	1005	NAG	C4-C5-C6-O6
6	A	1002	NAG	C8-C7-N2-C2
6	A	1002	NAG	O7-C7-N2-C2
6	A	1004	NAG	O5-C5-C6-O6
9	A	1030	PG4	O2-C3-C4-O3
10	A	1031	PEG	O2-C3-C4-O4
6	A	1006	NAG	C4-C5-C6-O6
6	A	1004	NAG	C4-C5-C6-O6
6	A	1006	NAG	O5-C5-C6-O6
10	A	1031	PEG	O1-C1-C2-O2
10	A	1031	PEG	C4-C3-O2-C2
6	A	1002	NAG	C1-C2-N2-C7
6	A	1002	NAG	O5-C5-C6-O6
9	A	1030	PG4	C3-C4-O3-C5
9	A	1030	PG4	C5-C6-O4-C7
9	A	1030	PG4	O4-C7-C8-O5

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	913/942 (96%)	0.74	106 (11%)	4	5	28, 45, 69, 105	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	749	THR	7.7
1	A	839	LYS	6.2
1	A	750	ALA	5.9
1	A	334	GLY	5.7
1	A	838	SER	5.4
1	A	751	ASN	5.2
1	A	389	LEU	4.9
1	A	563	SER	4.9
1	A	419	LEU	4.9
1	A	421	VAL	4.6
1	A	265	PRO	4.5
1	A	267	HIS	4.4
1	A	443	LEU	4.3
1	A	432	ILE	4.2
1	A	268	ALA	4.1
1	A	708	LEU	4.1
1	A	428	LEU	4.0
1	A	308	HIS	4.0
1	A	168	ALA	4.0
1	A	306	ASP	3.9
1	A	805	THR	3.9
1	A	810	SER	3.9
1	A	811	ASP	3.8
1	A	807	ASN	3.8
1	A	840	THR	3.7
1	A	142	ALA	3.6
1	A	333	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	3.5
1	A	103	ILE	3.4
1	A	411	VAL	3.4
1	A	276	ASP	3.3
1	A	564	GLY	3.3
1	A	141	SER	3.3
1	A	748	TYR	3.3
1	A	390	ILE	3.2
1	A	392	PRO	3.2
1	A	396	TRP	3.1
1	A	250	ALA	3.1
1	A	37	LYS	3.1
1	A	148	SER	3.1
1	A	146	CYS	3.0
1	A	722	TYR	3.0
1	A	249	THR	3.0
1	A	337	THR	3.0
1	A	752	GLU	3.0
1	A	336	LYS	3.0
1	A	481	LEU	3.0
1	A	391	PRO	3.0
1	A	737	TYR	2.9
1	A	720	LEU	2.9
1	A	93	PRO	2.8
1	A	794	ASN	2.8
1	A	427	TYR	2.8
1	A	145	SER	2.8
1	A	837	SER	2.7
1	A	363	ILE	2.7
1	A	97	LEU	2.7
1	A	562	THR	2.7
1	A	559	TYR	2.6
1	A	746	TRP	2.6
1	A	501	ALA	2.6
1	A	433	TYR	2.6
1	A	172	VAL	2.6
1	A	729	LEU	2.5
1	A	30	ILE	2.5
1	A	561	THR	2.5
1	A	285	TYR	2.5
1	A	712	TRP	2.5
1	A	287	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	282	SER	2.5
1	A	102	ASP	2.5
1	A	447	PHE	2.5
1	A	223	GLY	2.4
1	A	547	ASP	2.4
1	A	332	SER	2.4
1	A	836	ALA	2.4
1	A	841	THR	2.4
1	A	846	HIS	2.4
1	A	484	TRP	2.4
1	A	368	THR	2.4
1	A	416	PHE	2.4
1	A	705	TYR	2.4
1	A	277	ALA	2.4
1	A	387	ALA	2.4
1	A	482	ALA	2.3
1	A	99	LYS	2.3
1	A	809	GLN	2.3
1	A	783	ASN	2.3
1	A	408	PHE	2.3
1	A	504	ALA	2.2
1	A	806	ALA	2.2
1	A	407	LEU	2.2
1	A	444	TRP	2.2
1	A	789	LYS	2.2
1	A	709	ASN	2.2
1	A	369	PRO	2.2
1	A	104	ALA	2.1
1	A	247	ASP	2.1
1	A	430	ASP	2.1
1	A	842	THR	2.1
1	A	711	ILE	2.1
1	A	442	LEU	2.0
1	A	843	PHE	2.0
1	A	264	LEU	2.0
1	A	39	THR	2.0
1	A	304	THR	2.0

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

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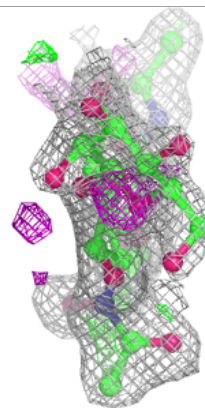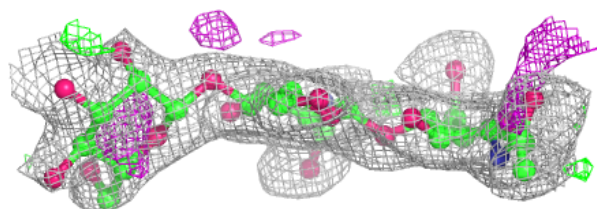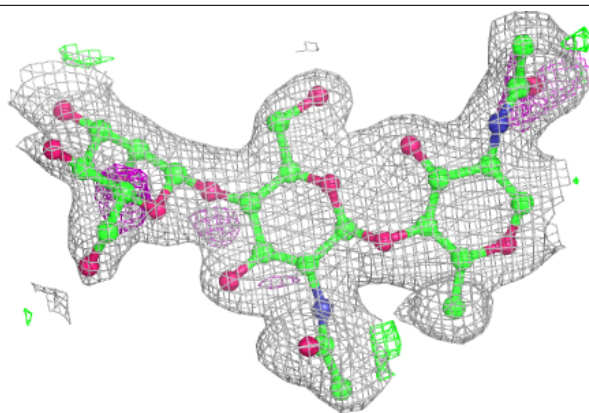
6.3 Carbohydrates ⓘ

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
3	MAN	C	4	11/12	0.64	0.44	63,65,67,68	0
4	MAN	D	6	11/12	0.72	0.23	65,66,68,70	0
3	NAG	C	2	14/15	0.80	0.19	44,48,53,54	0
5	MAN	E	7	11/12	0.80	0.20	47,51,53,53	0
2	BMA	B	3	11/12	0.82	0.34	54,57,59,62	0
5	MAN	E	6	11/12	0.83	0.21	52,57,61,65	0
3	MAN	C	8	11/12	0.84	0.18	57,61,64,69	0
3	NAG	C	1	14/15	0.85	0.18	40,43,47,49	0
3	MAN	C	6	11/12	0.85	0.28	52,60,62,64	0
4	NAG	D	2	14/15	0.86	0.15	44,48,50,58	0
3	MAN	C	5	11/12	0.86	0.26	51,60,62,64	0
3	BMA	C	3	11/12	0.87	0.27	50,55,57,59	0
4	BMA	D	3	11/12	0.88	0.20	48,51,55,58	0
3	MAN	C	7	11/12	0.88	0.27	57,60,64,64	0
5	MAN	E	8	11/12	0.88	0.15	48,55,62,63	0
4	MAN	D	4	11/12	0.89	0.15	43,46,47,48	0
4	MAN	D	5	11/12	0.89	0.17	43,47,53,56	0
4	NAG	D	1	14/15	0.89	0.16	44,46,47,47	0
5	MAN	E	9	11/12	0.89	0.18	51,53,54,56	0
5	MAN	E	4	11/12	0.90	0.11	43,44,47,48	0
5	MAN	E	11	11/12	0.90	0.11	49,51,52,52	0
5	NAG	E	1	14/15	0.91	0.13	42,45,51,51	0
5	NAG	E	2	14/15	0.91	0.12	41,44,47,48	0
5	MAN	E	5	11/12	0.92	0.17	45,48,53,57	0
2	NAG	B	1	14/15	0.92	0.12	35,38,42,45	0
2	NAG	B	2	14/15	0.92	0.18	46,50,51,52	0
5	MAN	E	10	11/12	0.93	0.12	46,50,52,53	0
5	BMA	E	3	11/12	0.95	0.12	43,45,50,50	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 B:

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 C:

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

Electron density around Chain D:

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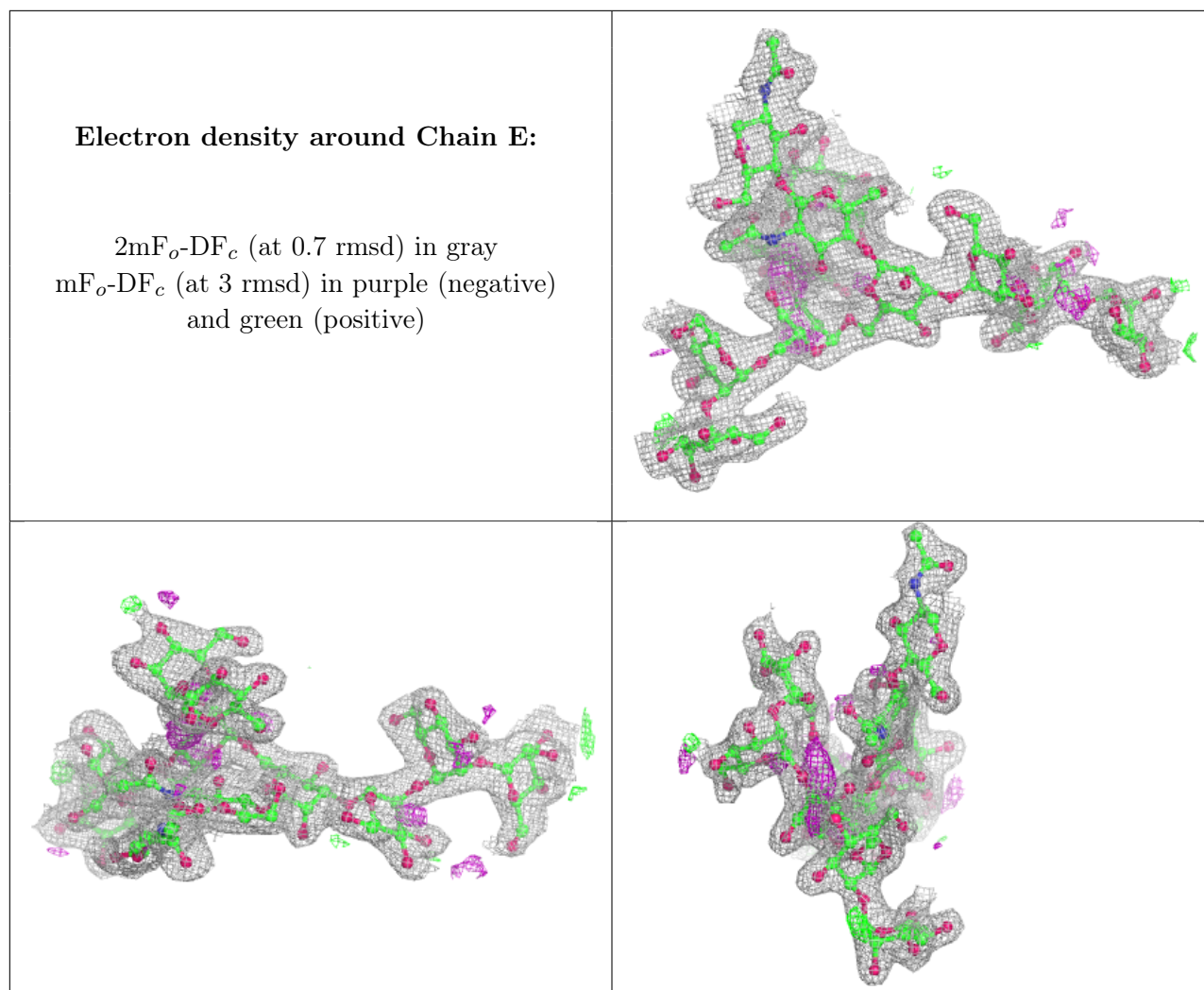and green (positive)

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)
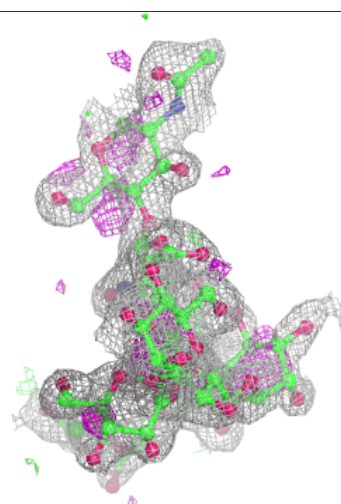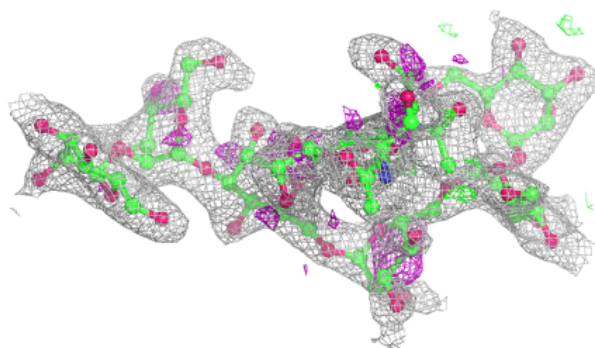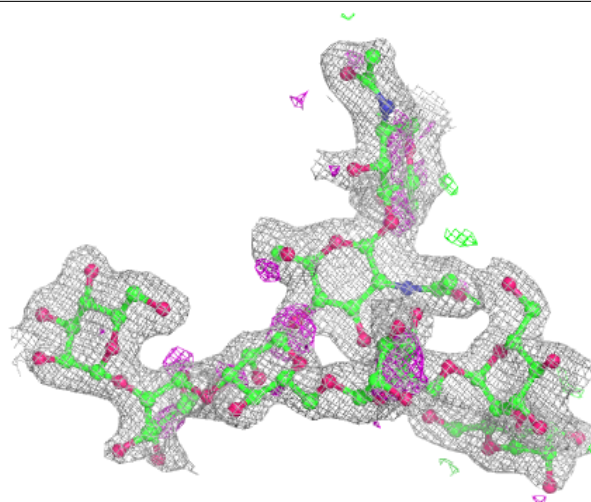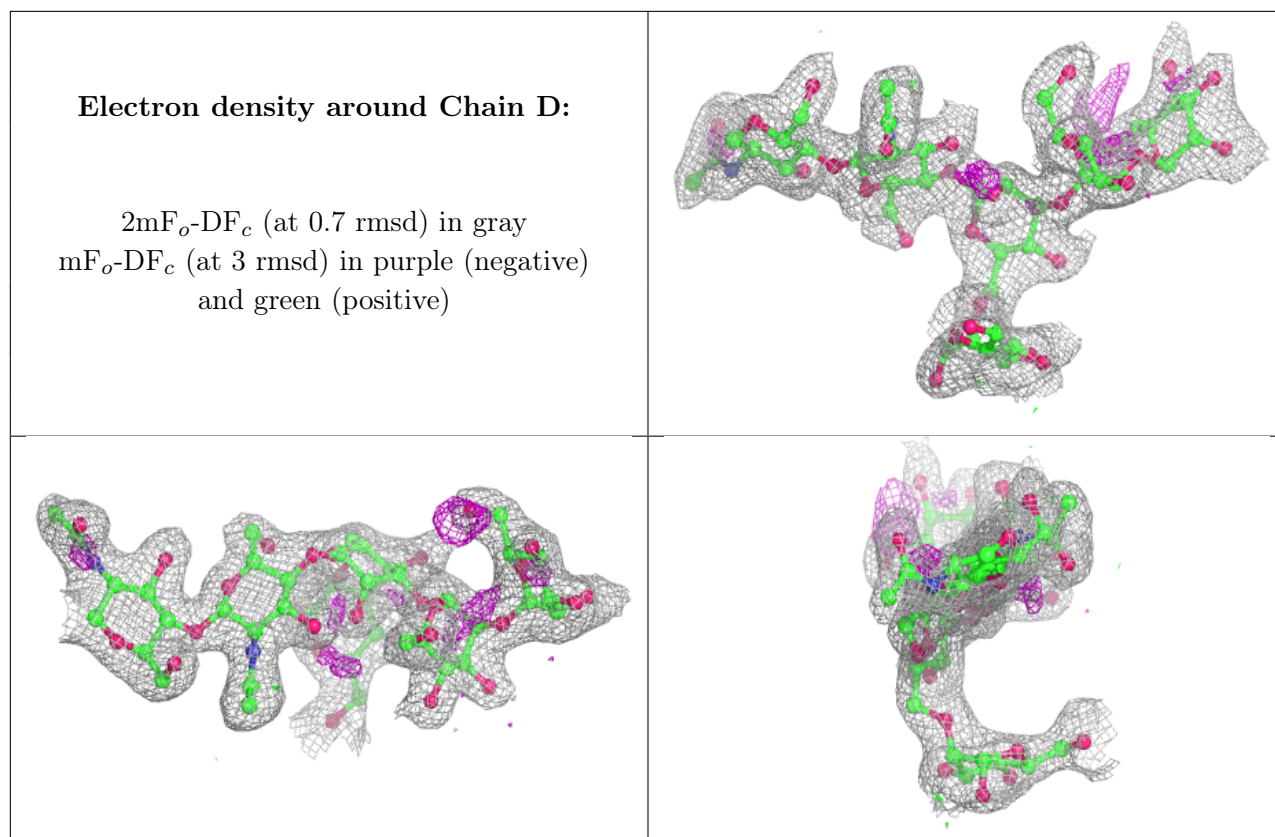
6.4 Ligands (i)

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(Å^2)	Q<0.9
8	NA	A	1025	1/1	0.68	0.29	54,54,54,54	0
7	CD	A	1021	1/1	0.71	0.21	125,125,125,125	1
10	PEG	A	1031	7/7	0.78	0.19	58,60,62,64	0
9	PG4	A	1030	12/13	0.79	0.17	57,61,66,66	0
6	NAG	A	1005	14/15	0.79	0.31	56,60,63,68	0
6	NAG	A	1002	14/15	0.84	0.29	67,73,78,80	0
6	NAG	A	1006	14/15	0.84	0.31	54,59,68,70	0
6	NAG	A	1004	14/15	0.88	0.14	54,59,64,67	0
8	NA	A	1028	1/1	0.88	0.17	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
6	NAG	A	1003	14/15	0.89	0.14	39,44,48,48	0
6	NAG	A	1007	14/15	0.90	0.18	40,43,46,47	0
6	NAG	A	1001	14/15	0.90	0.20	46,51,55,57	0
12	CL	A	1033	1/1	0.90	0.14	49,49,49,49	0
7	CD	A	1023	1/1	0.91	0.39	44,44,44,44	0
7	CD	A	1012	1/1	0.91	0.06	72,72,72,72	0
7	CD	A	1024	1/1	0.92	0.62	44,44,44,44	0
7	CD	A	1019	1/1	0.93	0.05	80,80,80,80	0
8	NA	A	1027	1/1	0.93	0.28	30,30,30,30	0
7	CD	A	1014	1/1	0.94	0.08	76,76,76,76	0
8	NA	A	1029	1/1	0.95	0.19	33,33,33,33	0
11	CA	A	1032	1/1	0.95	0.09	54,54,54,54	0
8	NA	A	1026	1/1	0.95	0.29	48,48,48,48	0
7	CD	A	1022	1/1	0.96	0.17	87,87,87,87	1
7	CD	A	1020	1/1	0.96	0.10	77,77,77,77	0
7	CD	A	1013	1/1	0.96	0.08	52,52,52,52	0
8	NA	A	1034	1/1	0.97	0.33	37,37,37,37	0
7	CD	A	1011	1/1	0.98	0.07	50,50,50,50	0
7	CD	A	1015	1/1	0.98	0.09	51,51,51,51	0
7	CD	A	1016	1/1	0.98	0.05	59,59,59,59	0
7	CD	A	1017	1/1	0.98	0.08	81,81,81,81	0
7	CD	A	1018	1/1	0.98	0.07	74,74,74,74	0
7	CD	A	1009	1/1	0.98	0.08	43,43,43,43	0
7	CD	A	1010	1/1	0.98	0.10	58,58,58,58	0
7	CD	A	1008	1/1	0.99	0.10	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.