



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:28 AM UTC

PDB ID : 5NN3 / pdb_00005nn3
Title : Crystal structure of human lysosomal acid-alpha-glucosidase, GAA
Authors : Roig-Zamboni, V.; Cobucci-Ponzano, B.; Iacono, R.; Ferrara, M.C.; Germany, S.; Parenti, G.; Bourne, Y.; Moracci, M.
Deposited on : 2017-04-08
Resolution : 1.90 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

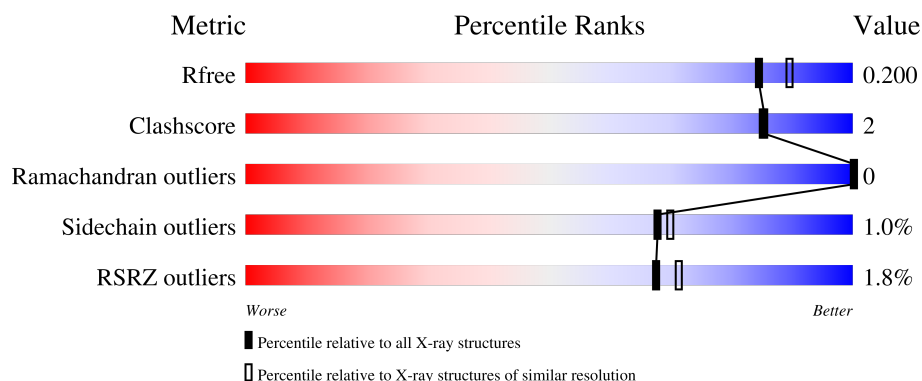
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	872	2% 92% 5%
2	B	3	33% 67%
2	F	3	67% 33%
3	C	3	67% 33%
4	D	2	50% 50%

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Mol	Chain	Length	Quality of chain
5	E	4	 25% 75%

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
10	EDO	A	1031	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7663 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.

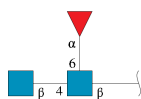
- Molecule 1 is a protein called Lysosomal alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	845	6723	4315	1125	1251	32	0	13	0

There are 3 discrepancies between the modelled and reference sequences:

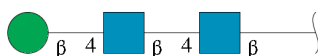
Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ARG	HIS	variant	UNP P10253
A	223	HIS	ARG	variant	UNP P10253
A	780	ILE	VAL	variant	UNP P10253

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	F	3	38	22	2	14	0	0	0

- Molecule 3 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
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



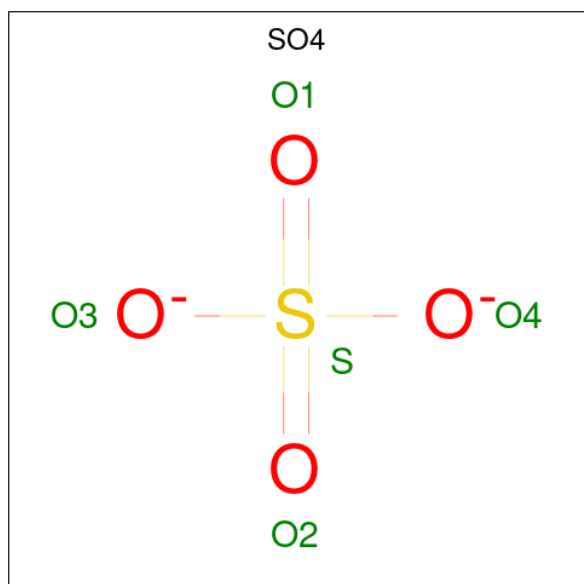
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 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
5	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

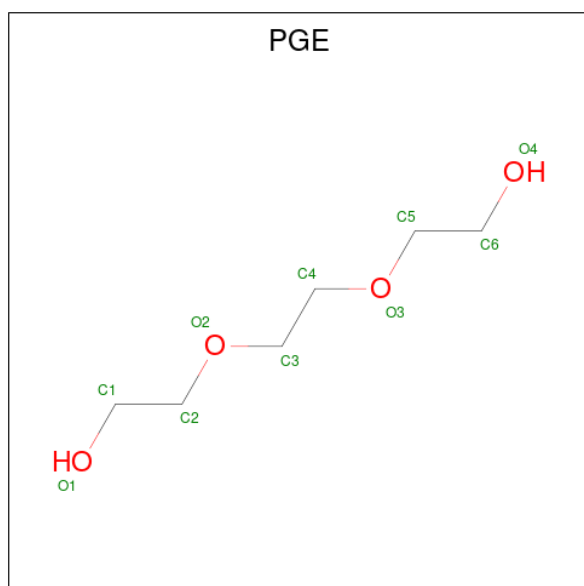


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	Cl	0	0
			8	8		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0

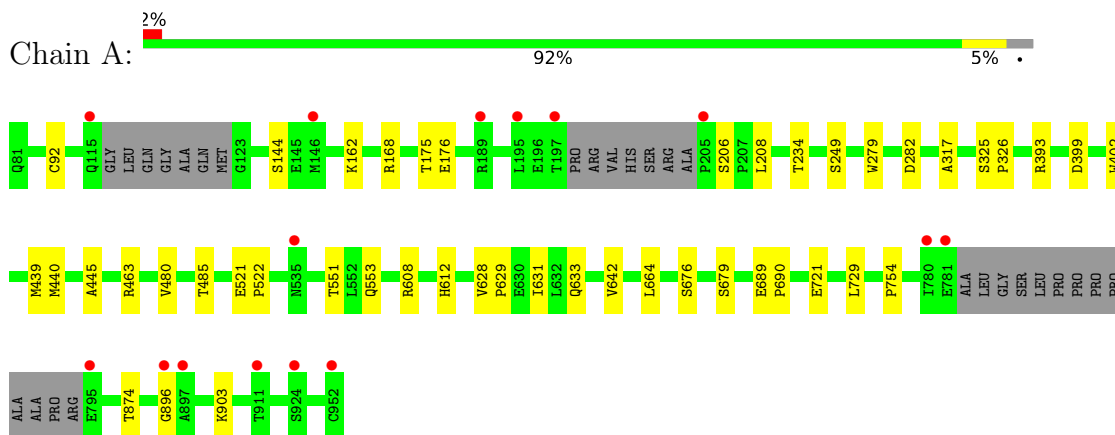
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	668	Total O 668 668	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

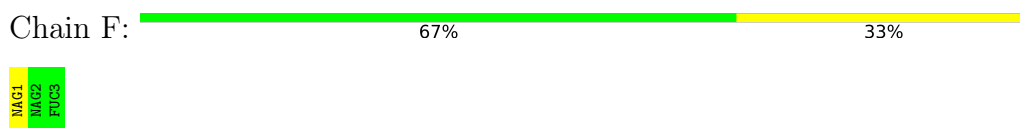
- Molecule 1: Lysosomal alpha-glucosidase



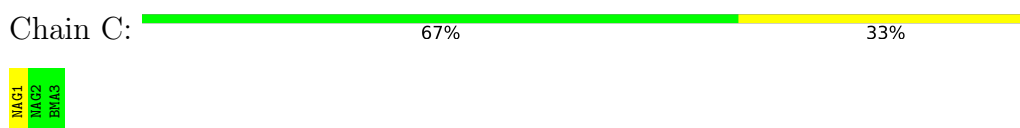
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain D:  50% 50%

MAG1
MAG2

- Molecule 5: 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

Chain E:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.66Å 102.40Å 128.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 1.90 48.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.88-1.90) 100.0 (48.88-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.162 , 0.189 0.173 , 0.200	Depositor DCC
R_{free} test set	5095 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, BMA, FUC, EDO, NAG, SO4, CSO, PEG, CL, MAN

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	0.64	0/6953	0.76	0/9496

There are no bond length outliers.

There are no bond angle outliers.

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	6723	0	6512	28	0
2	B	38	0	34	0	0
2	F	38	0	34	0	0
3	C	39	0	34	0	0
4	D	28	0	25	0	0
5	E	50	0	43	0	0
6	A	10	0	0	0	0
7	A	8	0	0	0	0
8	A	10	0	14	1	0
9	A	7	0	10	1	0
10	A	44	0	66	8	0
11	A	668	0	0	6	0
All	All	7663	0	6772	30	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 2.

All (30) 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:208:LEU:CD2	10:A:1031:EDO:H12	2.22	0.69
1:A:175:THR:C	10:A:1028:EDO:H12	2.21	0.66
1:A:168[A]:ARG:NH1	11:A:1107:HOH:O	2.32	0.62
1:A:551:THR:OG1	1:A:553[A]:GLN:OE1	2.18	0.62
1:A:393[B]:ARG:NH2	11:A:1108:HOH:O	2.34	0.61
1:A:608:ARG:NH1	11:A:1109:HOH:O	2.35	0.59
1:A:162:LYS:H	10:A:1032:EDO:H12	1.67	0.58
1:A:208:LEU:HD21	10:A:1031:EDO:H12	1.86	0.58
1:A:176:GLU:N	10:A:1028:EDO:H12	2.21	0.54
1:A:664:LEU:HD13	1:A:754:PRO:HG3	1.89	0.54
1:A:445:ALA:HB1	1:A:485:THR:HB	1.92	0.52
1:A:874:THR:OG1	1:A:896:GLY:HA3	2.09	0.51
1:A:234:THR:HA	1:A:249:SER:O	2.10	0.51
1:A:463:ARG:HH12	10:A:1029:EDO:H12	1.77	0.50
1:A:206:SER:O	10:A:1031:EDO:H22	2.12	0.49
1:A:325:SER:N	1:A:326:PRO:HA	2.28	0.49
10:A:1031:EDO:H21	11:A:1628:HOH:O	2.13	0.48
1:A:282:ASP:OD1	8:A:1026:PGE:H6	2.17	0.45
1:A:633[B]:GLN:NE2	11:A:1114:HOH:O	2.39	0.44
1:A:689:GLU:HB3	1:A:690:PRO:HD3	1.99	0.44
1:A:521:GLU:N	1:A:522:PRO:HA	2.32	0.44
1:A:628:VAL:HB	1:A:629:PRO:HD3	1.99	0.44
1:A:676:SER:HG	1:A:679:SER:HG	1.66	0.43
1:A:402:TRP:HA	1:A:439:MET:O	2.19	0.42
1:A:721[B]:GLU:OE1	11:A:1104:HOH:O	2.22	0.42
1:A:279:TRP:CE3	1:A:317:ALA:HB2	2.55	0.42
1:A:92:CYS:O	1:A:92:CYS:SG	2.78	0.42
1:A:612:HIS:O	1:A:642:VAL:HA	2.20	0.41
1:A:874:THR:CB	1:A:896:GLY:HA3	2.52	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	849/872 (97%)	833 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	735/741 (99%)	727 (99%)	8 (1%)	65	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144[A]	SER
1	A	144[B]	SER
1	A	399	ASP
1	A	440	MET
1	A	480	VAL
1	A	631	ILE
1	A	729	LEU
1	A	903	LYS

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

Mol	Chain	Res	Type
1	A	115	GLN
1	A	188	ASN
1	A	715	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSO	A	938	1	3,6,7	0.63	0	1,6,8	0.80	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
1	CSO	A	938	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 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	0.38	0	17,19,21	0.79	0
2	NAG	B	2	2	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
2	FUC	B	3	2	10,10,11	0.74	0	14,14,16	2.21	3 (21%)
3	NAG	C	1	3,1	14,14,15	0.57	0	17,19,21	1.15	1 (5%)
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	0.86	0
3	BMA	C	3	3	11,11,12	0.44	0	15,15,17	0.73	0
4	NAG	D	1	4,1	14,14,15	0.56	0	17,19,21	0.79	0
4	NAG	D	2	4	14,14,15	0.63	0	17,19,21	1.06	1 (5%)
5	NAG	E	1	5,1	14,14,15	0.66	0	17,19,21	1.15	1 (5%)
5	NAG	E	2	5	14,14,15	0.49	0	17,19,21	0.84	0
5	BMA	E	3	5	11,11,12	0.44	0	15,15,17	0.85	1 (6%)
5	MAN	E	4	5	11,11,12	0.55	0	15,15,17	0.82	1 (6%)
2	NAG	F	1	2,1	14,14,15	0.65	0	17,19,21	1.11	1 (5%)
2	NAG	F	2	2	14,14,15	0.50	0	17,19,21	0.69	0
2	FUC	F	3	2	10,10,11	0.61	0	14,14,16	0.94	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	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	-	0/2/19/22	0/1/1/1
4	NAG	D	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	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	2/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUC	O5-C1-C2	-6.63	94.98	110.79
2	B	3	FUC	C1-C2-C3	3.41	114.61	109.64
2	B	2	NAG	C1-O5-C5	2.86	116.01	112.19
2	F	1	NAG	C1-C2-N2	2.79	114.83	110.43
5	E	3	BMA	O5-C5-C6	2.65	112.83	107.66
3	C	1	NAG	O5-C1-C2	-2.40	107.57	111.29
2	B	3	FUC	O5-C5-C4	-2.40	105.23	109.55
4	D	2	NAG	C1-C2-N2	-2.40	106.66	110.43
5	E	4	MAN	C1-O5-C5	2.38	115.38	112.19
5	E	1	NAG	O3-C3-C4	2.23	115.64	110.38

There are no chirality outliers.

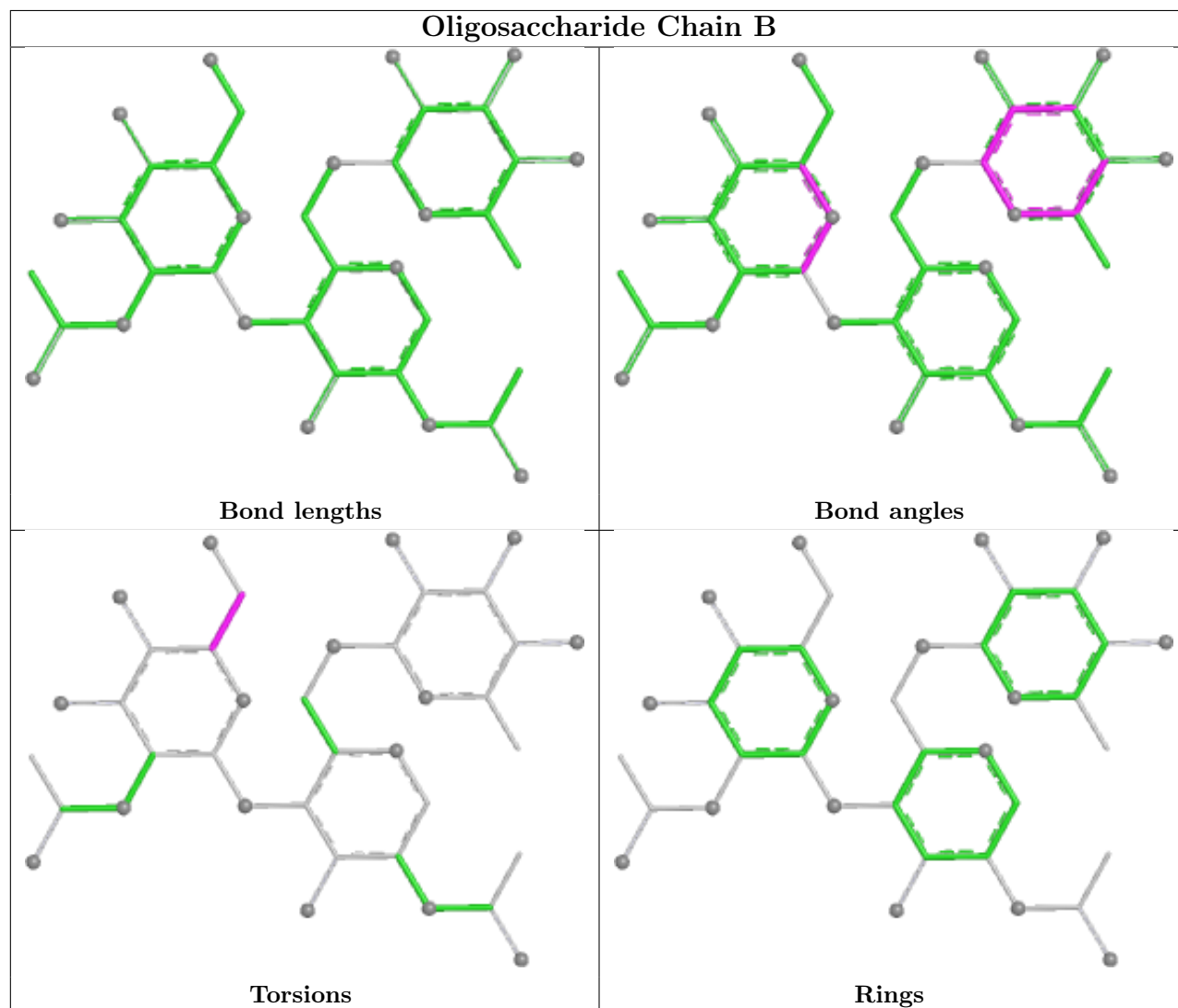
All (12) torsion outliers are listed below:

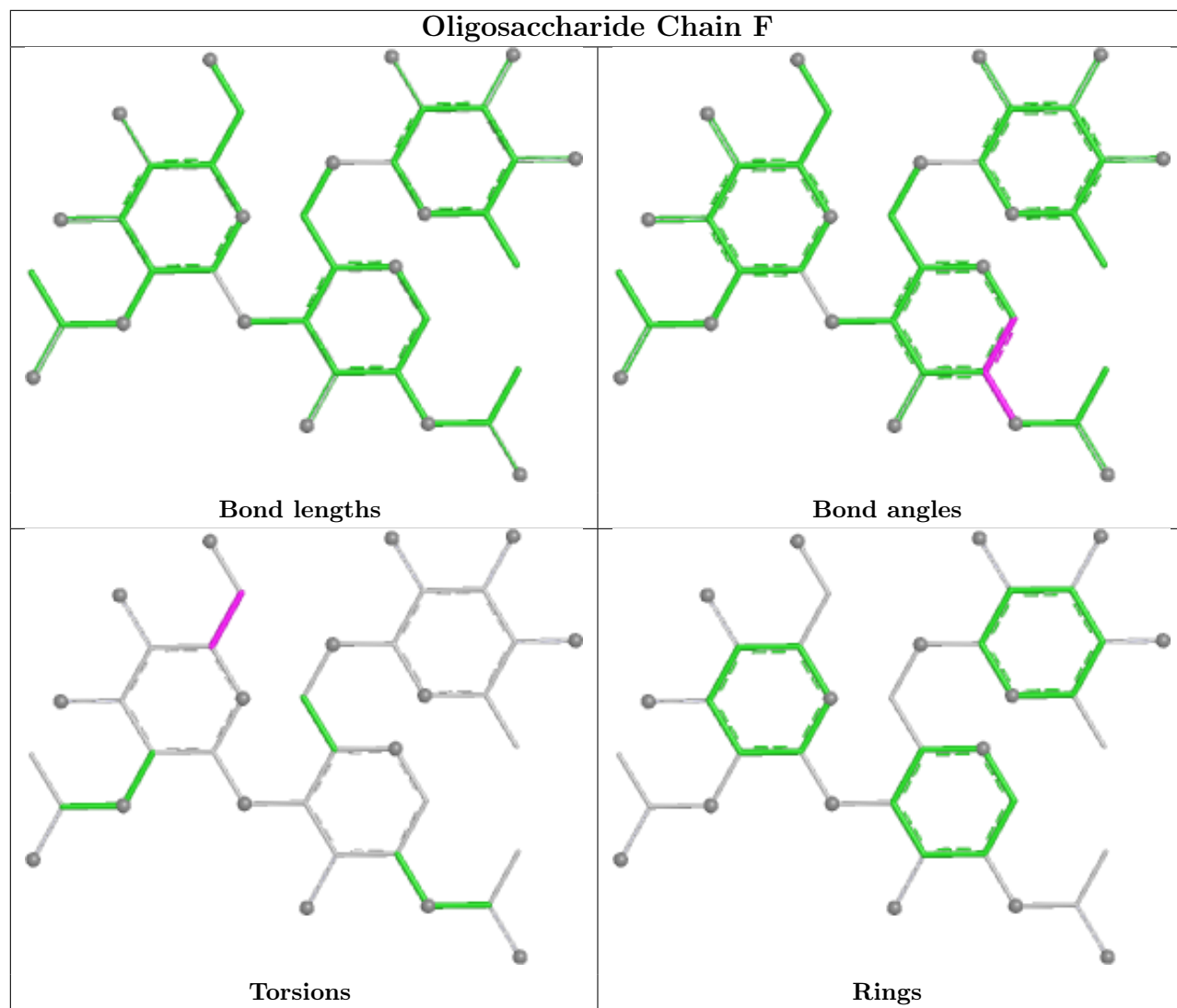
Mol	Chain	Res	Type	Atoms
5	E	4	MAN	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	E	4	MAN	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

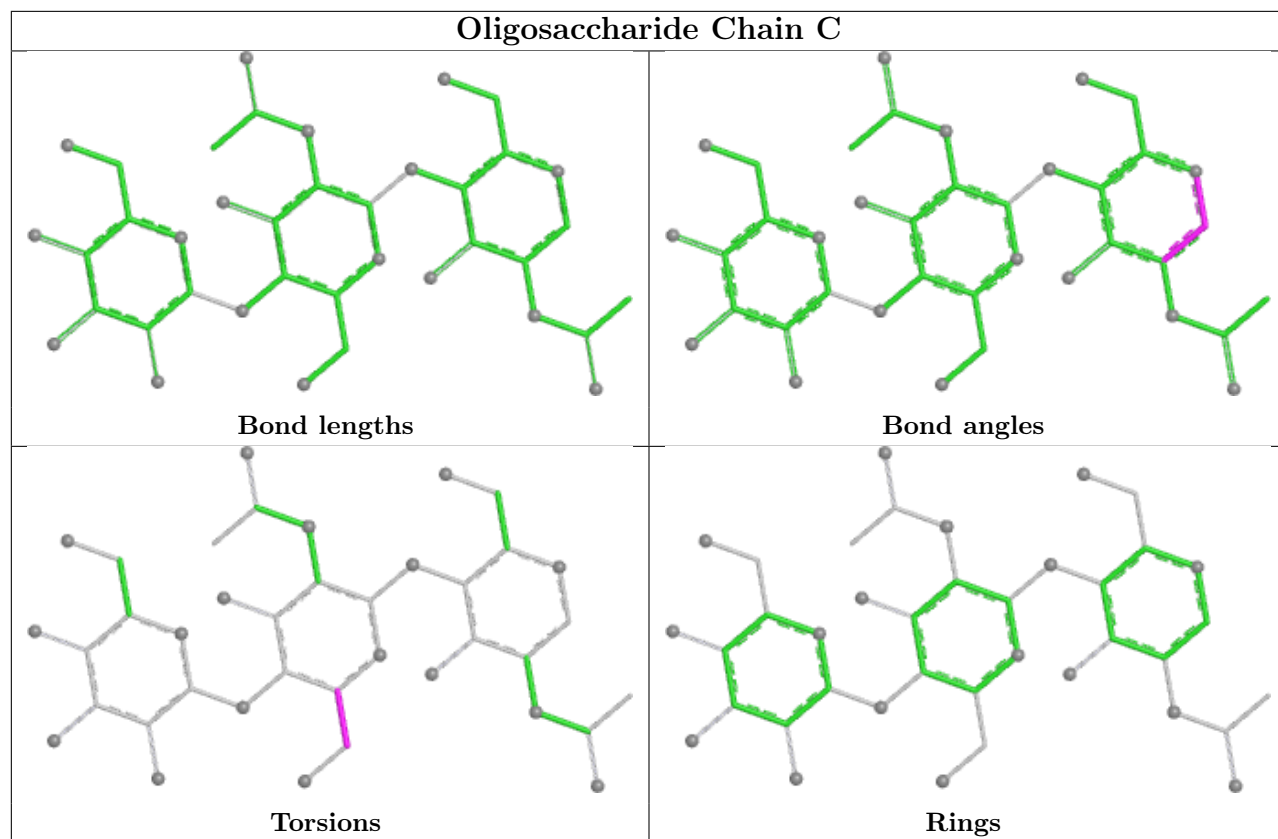
There are no ring outliers.

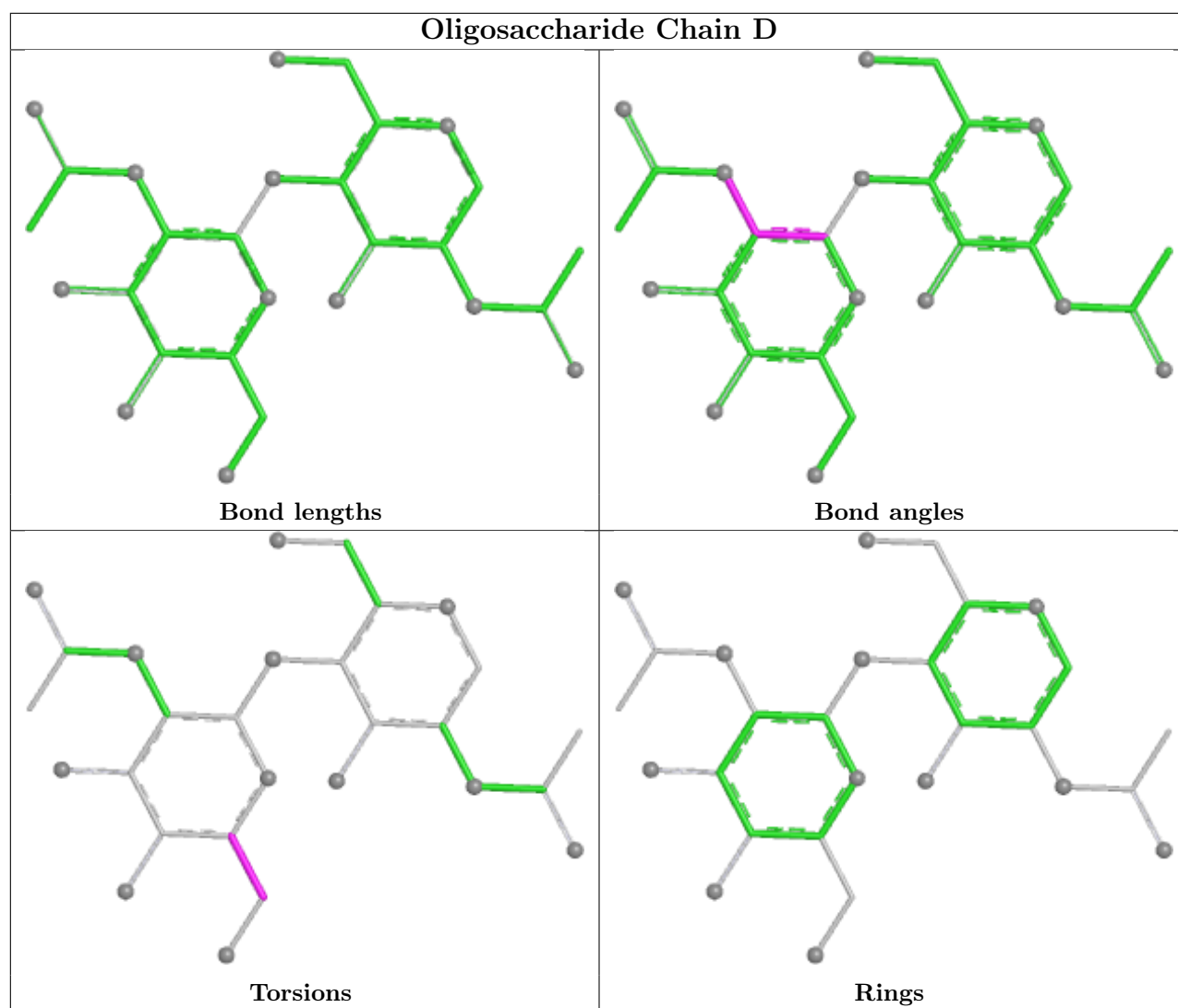
No monomer is involved in short contacts.

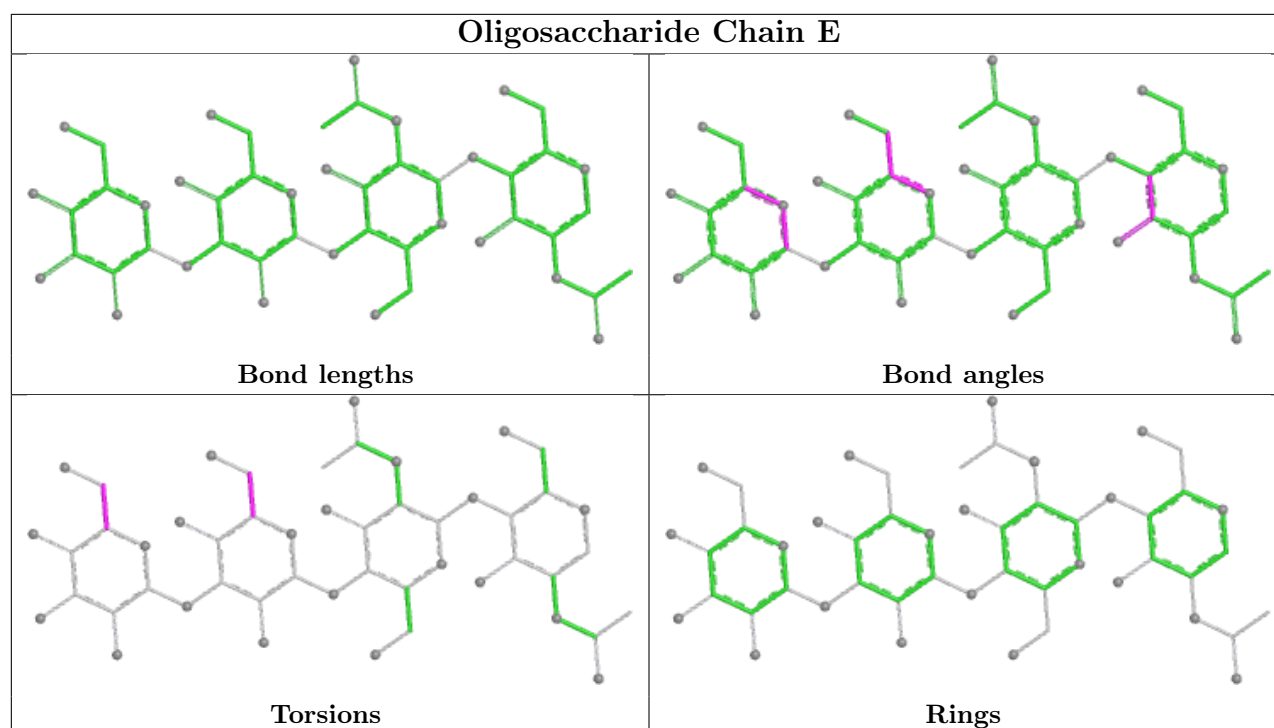
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	PEG	A	1027	-	6,6,6	0.52	0	5,5,5	0.31	0
8	PGE	A	1026	-	9,9,9	0.49	0	8,8,8	0.56	0
6	SO4	A	1017	-	4,4,4	0.64	0	6,6,6	0.41	0
6	SO4	A	1016	-	4,4,4	0.39	0	6,6,6	0.48	0
10	EDO	A	1034	-	3,3,3	0.48	0	2,2,2	0.56	0
10	EDO	A	1031	-	3,3,3	0.65	0	2,2,2	0.18	0
10	EDO	A	1036	-	3,3,3	0.54	0	2,2,2	0.33	0
10	EDO	A	1038	-	3,3,3	0.44	0	2,2,2	0.40	0
10	EDO	A	1032	-	3,3,3	0.40	0	2,2,2	0.45	0
10	EDO	A	1035	-	3,3,3	0.40	0	2,2,2	0.38	0
10	EDO	A	1033	-	3,3,3	0.43	0	2,2,2	1.00	0
10	EDO	A	1028	-	3,3,3	0.59	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	A	1030	-	3,3,3	0.60	0	2,2,2	0.27	0
10	EDO	A	1037	-	3,3,3	0.49	0	2,2,2	0.15	0
10	EDO	A	1029	-	3,3,3	0.42	0	2,2,2	0.63	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
9	PEG	A	1027	-	-	2/4/4/4	-
8	PGE	A	1026	-	-	7/7/7/7	-
10	EDO	A	1034	-	-	0/1/1/1	-
10	EDO	A	1031	-	-	1/1/1/1	-
10	EDO	A	1036	-	-	1/1/1/1	-
10	EDO	A	1038	-	-	0/1/1/1	-
10	EDO	A	1032	-	-	1/1/1/1	-
10	EDO	A	1035	-	-	0/1/1/1	-
10	EDO	A	1033	-	-	1/1/1/1	-
10	EDO	A	1028	-	-	0/1/1/1	-
10	EDO	A	1030	-	-	1/1/1/1	-
10	EDO	A	1037	-	-	0/1/1/1	-
10	EDO	A	1029	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1026	PGE	O1-C1-C2-O2
8	A	1026	PGE	O3-C5-C6-O4
8	A	1026	PGE	O2-C3-C4-O3
10	A	1030	EDO	O1-C1-C2-O2
8	A	1026	PGE	C4-C3-O2-C2
10	A	1031	EDO	O1-C1-C2-O2
8	A	1026	PGE	C1-C2-O2-C3
8	A	1026	PGE	C6-C5-O3-C4
9	A	1027	PEG	O2-C3-C4-O4
8	A	1026	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
10	A	1029	EDO	O1-C1-C2-O2
9	A	1027	PEG	C1-C2-O2-C3
10	A	1032	EDO	O1-C1-C2-O2
10	A	1036	EDO	O1-C1-C2-O2
10	A	1033	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1027	PEG	1	0
8	A	1026	PGE	1	0
10	A	1031	EDO	4	0
10	A	1032	EDO	1	0
10	A	1028	EDO	2	0
10	A	1029	EDO	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, 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	844/872 (96%)	-0.16	15 (1%) 67 71	17, 29, 47, 82	13 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	PRO	5.2
1	A	897	ALA	4.4
1	A	780	ILE	4.3
1	A	197	THR	4.2
1	A	146	MET	3.6
1	A	795	GLU	3.3
1	A	115	GLN	2.7
1	A	781	GLU	2.6
1	A	535	ASN	2.5
1	A	952	CYS	2.5
1	A	911	THR	2.4
1	A	195	LEU	2.4
1	A	924	SER	2.2
1	A	189	ARG	2.1
1	A	896	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	938	7/8	0.97	0.06	35,36,42,43	0

6.3 Carbohydrates

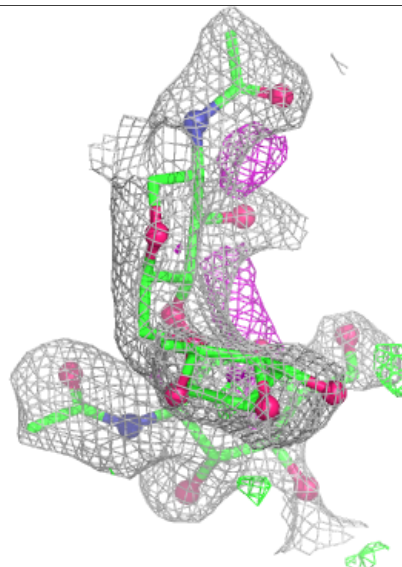
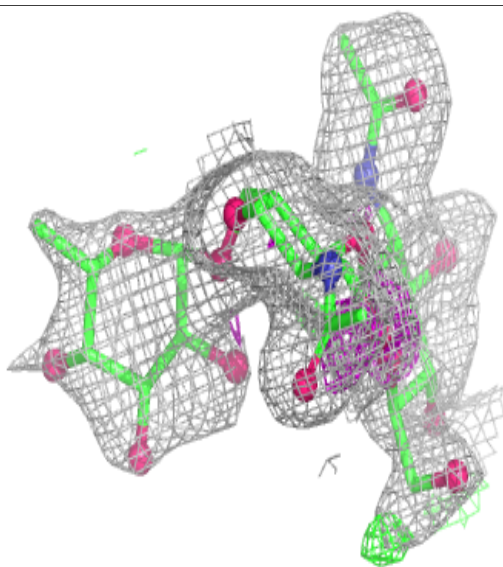
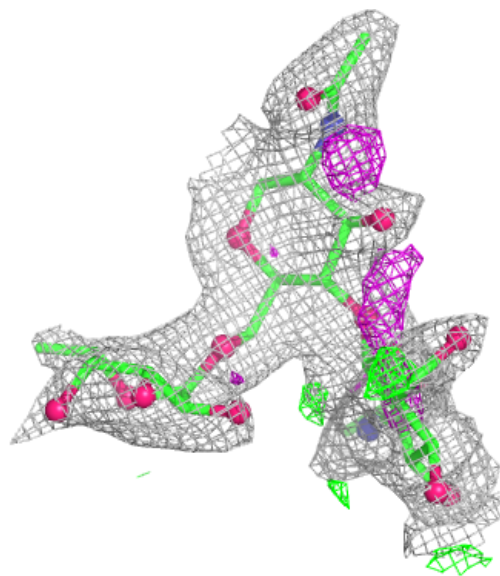
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	BMA	C	3	11/12	0.38	0.15	89,97,101,102	0
5	MAN	E	4	11/12	0.45	0.16	76,89,97,98	0
2	NAG	F	2	14/15	0.56	0.16	78,91,99,99	0
4	NAG	D	2	14/15	0.61	0.16	73,81,89,95	0
2	FUC	F	3	10/11	0.67	0.17	69,77,83,84	0
2	NAG	B	2	14/15	0.67	0.16	52,67,78,80	0
2	FUC	B	3	10/11	0.73	0.14	72,80,84,85	0
5	BMA	E	3	11/12	0.76	0.12	61,75,84,85	0
3	NAG	C	2	14/15	0.76	0.14	63,68,80,90	0
2	NAG	F	1	14/15	0.86	0.12	47,58,69,78	0
3	NAG	C	1	14/15	0.91	0.09	31,38,43,53	0
2	NAG	B	1	14/15	0.91	0.09	35,44,57,58	0
4	NAG	D	1	14/15	0.92	0.09	31,40,58,64	0
5	NAG	E	2	14/15	0.93	0.08	32,38,45,52	0
5	NAG	E	1	14/15	0.97	0.06	26,31,35,38	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.

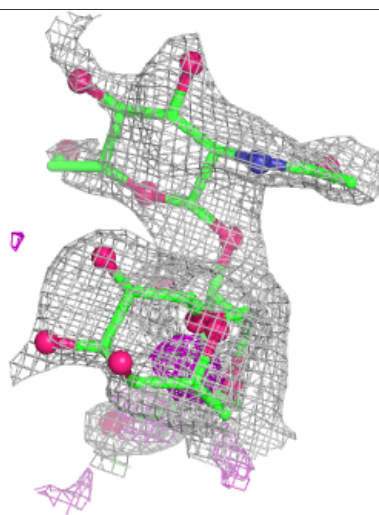
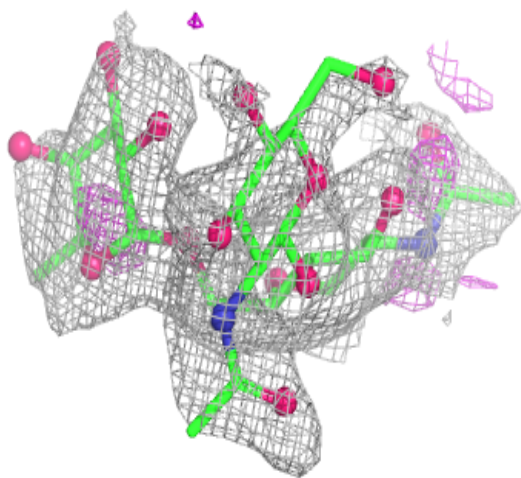
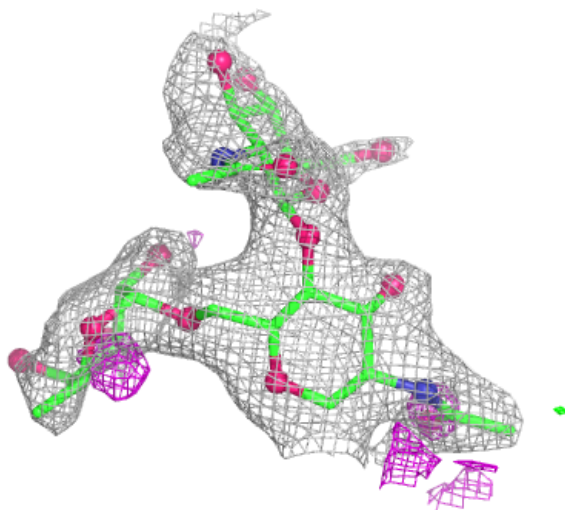
Electron density around Chain B:

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



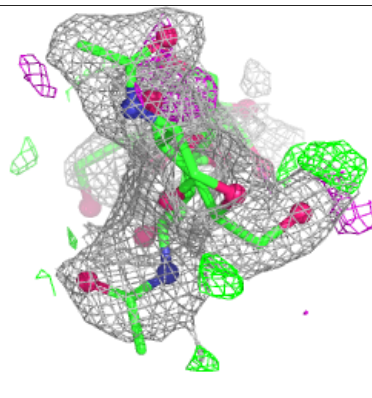
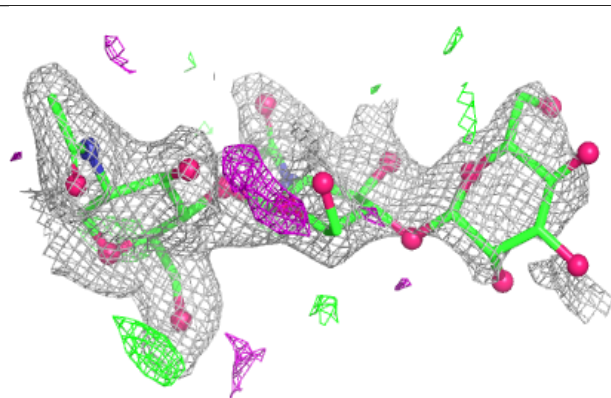
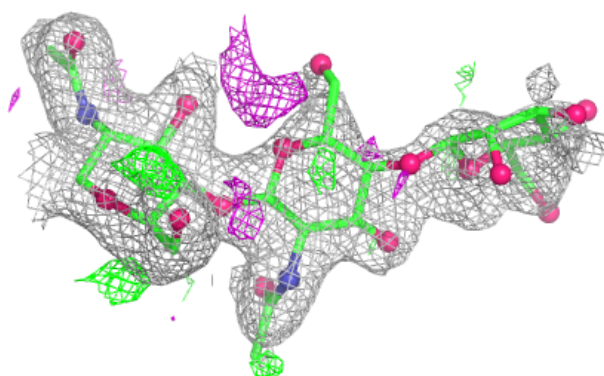
Electron density around Chain F:

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



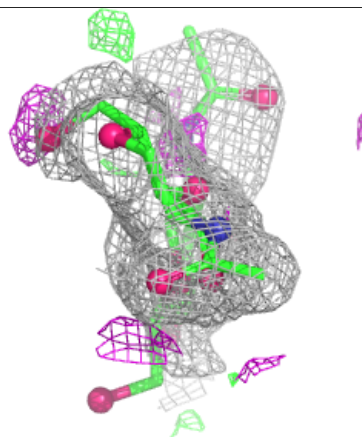
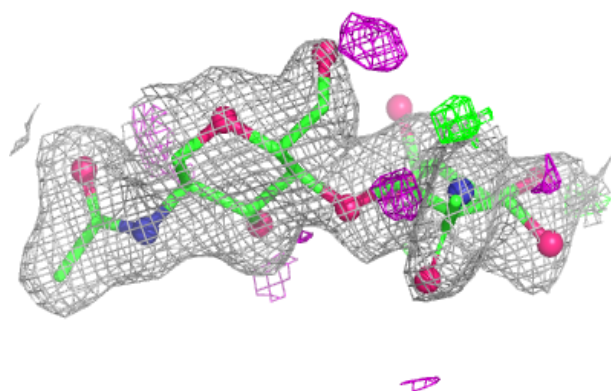
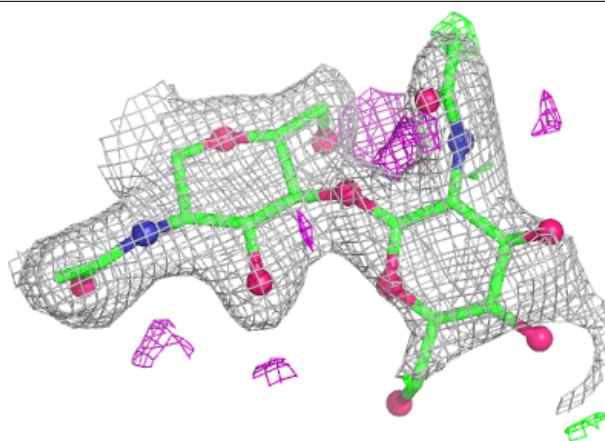
Electron density around Chain C:

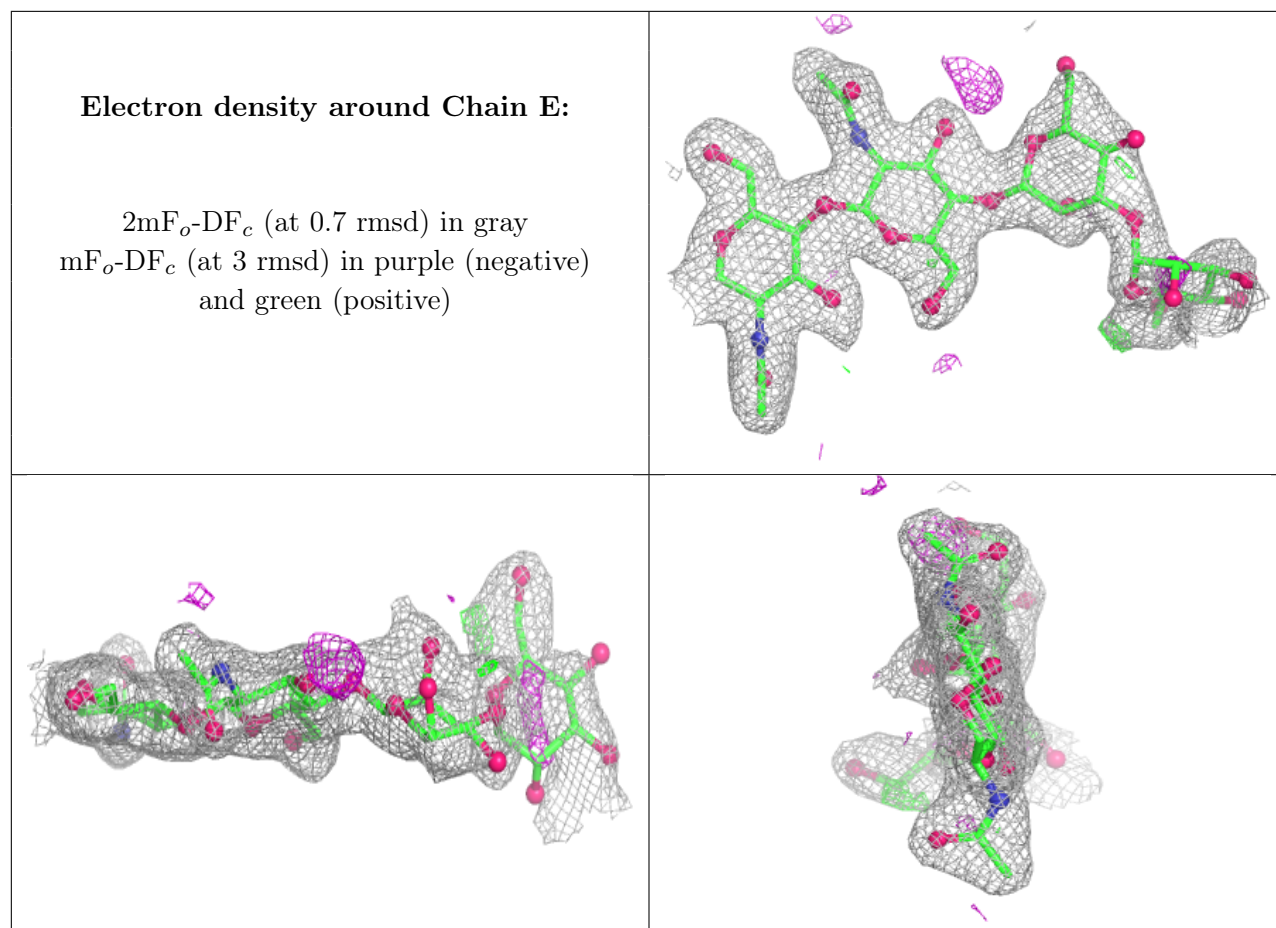
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





6.4 Ligands ⓘ

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
10	EDO	A	1034	4/4	0.74	0.18	42,48,48,51	0
9	PEG	A	1027	7/7	0.79	0.20	65,67,69,71	0
10	EDO	A	1033	4/4	0.81	0.18	34,36,41,41	0
10	EDO	A	1032	4/4	0.81	0.15	38,42,45,46	0
10	EDO	A	1038	4/4	0.81	0.15	48,49,51,53	0
10	EDO	A	1028	4/4	0.82	0.27	39,40,42,48	0
10	EDO	A	1030	4/4	0.82	0.15	44,45,46,49	0
8	PGE	A	1026	10/10	0.83	0.16	42,45,50,52	0
10	EDO	A	1037	4/4	0.85	0.19	45,45,47,47	0
10	EDO	A	1035	4/4	0.85	0.14	41,41,42,45	0
10	EDO	A	1029	4/4	0.86	0.14	45,45,46,49	0
10	EDO	A	1036	4/4	0.86	0.17	47,49,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CL	A	1024	1/1	0.87	0.13	67,67,67,67	0
10	EDO	A	1031	4/4	0.89	0.17	37,40,44,44	0
6	SO4	A	1017	5/5	0.89	0.16	31,31,42,42	5
7	CL	A	1019	1/1	0.93	0.09	57,57,57,57	0
7	CL	A	1022	1/1	0.94	0.12	49,49,49,49	0
7	CL	A	1025	1/1	0.95	0.08	53,53,53,53	0
6	SO4	A	1016	5/5	0.95	0.09	37,38,39,41	5
7	CL	A	1021	1/1	0.96	0.17	46,46,46,46	0
7	CL	A	1023	1/1	0.97	0.14	44,44,44,44	0
7	CL	A	1020	1/1	0.98	0.07	31,31,31,31	0
7	CL	A	1018	1/1	0.99	0.06	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.