wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 04:18 am GMT

PDB ID	:	5NSL
Title	:	Structure of D80A-fructofuranosidase from Xanthophyllomyces dendrorhous complexed with fructose and hydroxytyrosol
Authors	:	Ramirez-Escudero, M.; Sanz-Aparicio, J.
Deposited on	:	2017-04-26
Resolution	:	1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

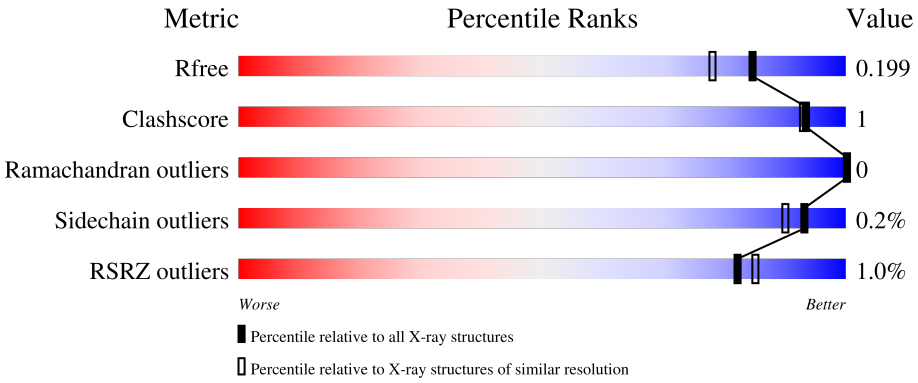
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	665	% 91% · 6%
1	B	665	% 92% · 6%
2	C	9	33% 67%
2	D	9	56% 44%
2	G	9	67% 33%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 50%
3	H	2	50% 50%
4	F	7	43% 57%

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
2	MAN	C	7	-	-	-	X
2	MAN	D	6	-	-	-	X
4	MAN	F	6	-	-	-	X
5	NAG	A	1215	-	-	-	X
5	NAG	A	1512	-	-	-	X
5	NAG	B	1215	-	-	-	X
7	975	A	2025	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 12353 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.

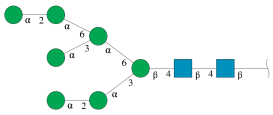
- Molecule 1 is a protein called Beta-fructofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	3	0
			4812	3063	786	956	7			
1	B	624	Total	C	N	O	S	0	1	0
			4800	3057	784	952	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	ILE	conflict	UNP J7HDY4
A	80	ALA	ASP	engineered mutation	UNP J7HDY4
A	663	ALA	SER	conflict	UNP J7HDY4
A	665	TYR	ARG	conflict	UNP J7HDY4
B	2	VAL	ILE	conflict	UNP J7HDY4
B	80	ALA	ASP	engineered mutation	UNP J7HDY4
B	663	ALA	SER	conflict	UNP J7HDY4
B	665	TYR	ARG	conflict	UNP J7HDY4

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	D	9	Total	C	N	O	0	0	0
			105	58	2	45			

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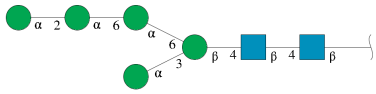
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	9	Total 105	C 58	N 2	O 45	0	0	0

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

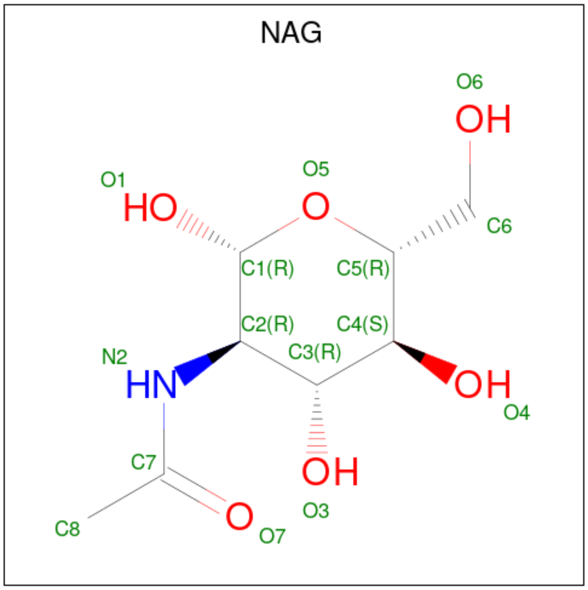
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total 28	C 16	N 2	O 10	0	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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
4	F	7	Total 83	C 46	N 2	O 35	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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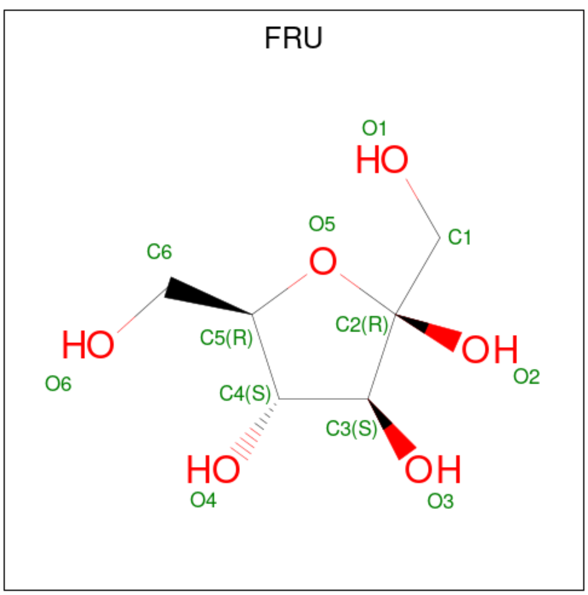
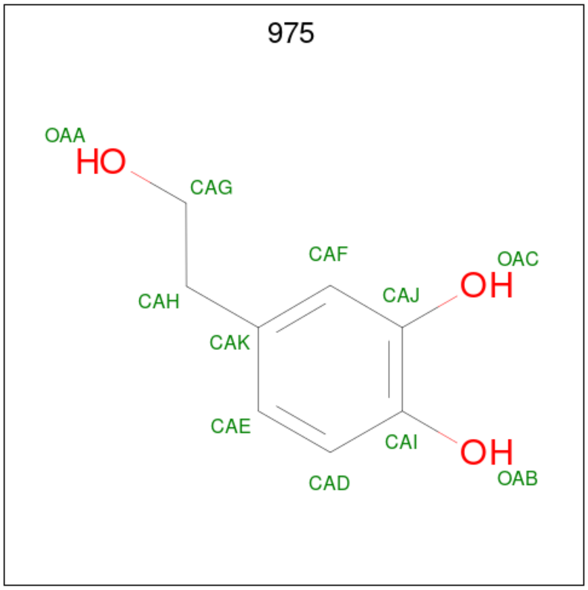
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total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

- Molecule 6 is beta-D-fructofuranose (three-letter code: FRU) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 12 6 6	0	0
6	B	1	Total C O 12 6 6	0	0

- Molecule 7 is 4-(2-hydroxyethyl)benzene-1,2-diol (three-letter code: 975) (formula: $C_8H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	3	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	3	0
7	A	1	Total C O 11 8 3	3	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	A	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0

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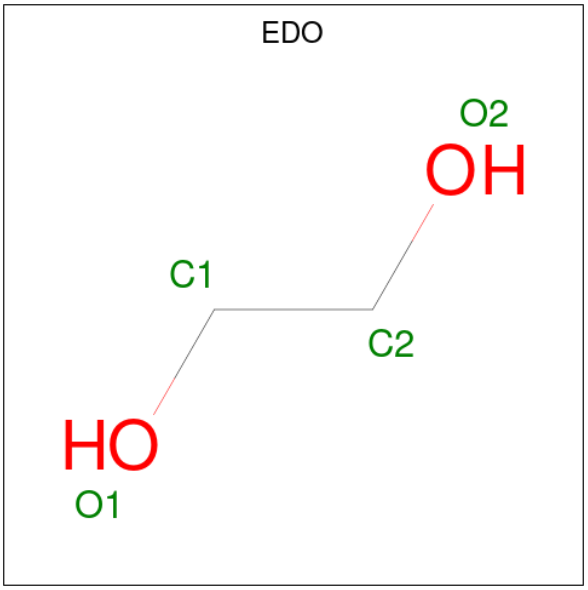
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	0	0
7	B	1	Total C O 11 8 3	1	0
7	B	1	Total C O 11 8 3	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 8 4 4	0	1
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 8 4 4	0	1
8	B	1	Total C O 8 4 4	0	1

- Molecule 9 is water.

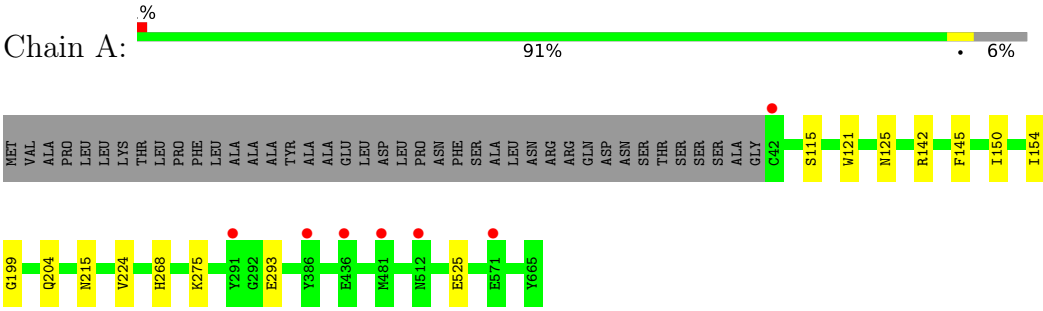
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	647	Total O 647 647	0	0
9	B	657	Total O 657 657	0	0

3 Residue-property plots (i)

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

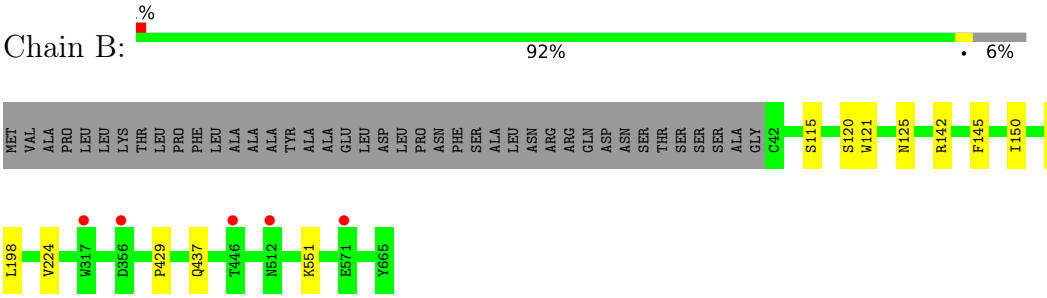
• Molecule 1: Beta-fructofuranosidase

Chain A:



• Molecule 1: Beta-fructofuranosidase

Chain B:

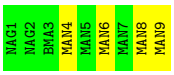


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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

Chain D:



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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

Chain G:

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

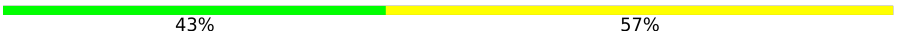
Chain E:

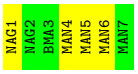
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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 F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.86Å 206.12Å 145.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.88 – 1.70 72.76 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (118.88-1.70) 100.0 (72.76-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.177 , 0.189 0.187 , 0.199	Depositor DCC
R_{free} test set	12454 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12353	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, NAG, EDO, BMA, MAN, 975

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	0.34	0/4946	0.60	0/6762
1	B	0.34	0/4934	0.61	0/6746
All	All	0.34	0/9880	0.61	0/13508

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	4812	0	4506	13	0
1	B	4800	0	4500	12	0
2	C	105	0	88	0	0
2	D	105	0	88	0	1
2	G	105	0	88	0	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
4	F	83	0	70	0	0
5	A	196	0	182	6	0
5	B	154	0	143	1	0
6	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	12	0	0
7	A	242	0	0	2	0
7	B	187	0	0	1	0
8	A	96	0	144	7	0
8	B	84	0	126	4	0
9	A	647	0	0	0	1
9	B	657	0	0	0	0
All	All	12353	0	10009	29	2

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 1.

The worst 5 of 29 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:215:ASN:HD21	5:A:1215:NAG:C1	0.94	1.58
1:A:204:GLN:OE1	8:A:2032:EDO:H12	1.81	0.80
1:B:120:SER:O	8:B:2044:EDO:H12	1.93	0.69
8:A:2053:EDO:H12	1:B:125:ASN:H	1.68	0.58
1:A:125:ASN:O	8:B:2053:EDO:H12	2.04	0.58

All (2) 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)
9:A:4094:HOH:O	9:A:4094:HOH:O[2_555]	1.93	0.27
2:D:9:MAN:O4	2:D:9:MAN:O4[2_555]	2.14	0.06

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	625/665 (94%)	600 (96%)	25 (4%)	0	100	100
1	B	623/665 (94%)	597 (96%)	26 (4%)	0	100	100
All	All	1248/1330 (94%)	1197 (96%)	51 (4%)	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	500/529 (94%)	499 (100%)	1 (0%)	93	90
1	B	498/529 (94%)	497 (100%)	1 (0%)	93	90
All	All	998/1058 (94%)	996 (100%)	2 (0%)	93	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ARG
1	B	142	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	215	ASN
1	B	437	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

38 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2,1	14,14,15	0.28	0	17,19,21	1.11	2 (11%)
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.94	0
2	BMA	C	3	2	11,11,12	0.25	0	15,15,17	0.69	0
2	MAN	C	4	2	11,11,12	0.29	0	15,15,17	0.87	1 (6%)
2	MAN	C	5	2	11,11,12	0.42	0	15,15,17	0.86	0
2	MAN	C	6	2	11,11,12	0.36	0	15,15,17	1.09	2 (13%)
2	MAN	C	7	2	11,11,12	0.33	0	15,15,17	0.86	1 (6%)
2	MAN	C	8	2	11,11,12	0.36	0	15,15,17	0.96	1 (6%)
2	MAN	C	9	2	11,11,12	0.50	0	15,15,17	1.87	6 (40%)
2	NAG	D	1	2,1	14,14,15	0.47	0	17,19,21	0.75	0
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.82	0
2	BMA	D	3	2	11,11,12	0.29	0	15,15,17	0.71	0
2	MAN	D	4	2	11,11,12	0.25	0	15,15,17	1.38	2 (13%)
2	MAN	D	5	2	11,11,12	0.30	0	15,15,17	0.55	0
2	MAN	D	6	2	11,11,12	0.26	0	15,15,17	0.79	1 (6%)
2	MAN	D	7	2	11,11,12	0.25	0	15,15,17	0.77	0
2	MAN	D	8	2	11,11,12	0.25	0	15,15,17	0.67	1 (6%)
2	MAN	D	9	2	11,11,12	0.28	0	15,15,17	0.73	0
3	NAG	E	1	1,3	14,14,15	0.25	0	17,19,21	0.77	0
3	NAG	E	2	3	14,14,15	0.39	0	17,19,21	1.47	2 (11%)
4	NAG	F	1	4,1	14,14,15	0.36	0	17,19,21	1.08	2 (11%)
4	NAG	F	2	4	14,14,15	0.37	0	17,19,21	0.80	0
4	BMA	F	3	4	11,11,12	0.33	0	15,15,17	0.73	0
4	MAN	F	4	4	11,11,12	0.43	0	15,15,17	1.07	1 (6%)
4	MAN	F	5	4	11,11,12	0.43	0	15,15,17	1.63	3 (20%)
4	MAN	F	6	4	11,11,12	0.36	0	15,15,17	1.24	2 (13%)
4	MAN	F	7	4	11,11,12	0.36	0	15,15,17	0.71	0
2	NAG	G	1	2,1	14,14,15	0.41	0	17,19,21	0.72	0
2	NAG	G	2	2	14,14,15	0.28	0	17,19,21	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	G	3	2	11,11,12	0.28	0	15,15,17	0.62	0
2	MAN	G	4	2	11,11,12	0.24	0	15,15,17	1.14	1 (6%)
2	MAN	G	5	2	11,11,12	0.32	0	15,15,17	0.70	1 (6%)
2	MAN	G	6	2	11,11,12	0.33	0	15,15,17	0.82	1 (6%)
2	MAN	G	7	2	11,11,12	0.27	0	15,15,17	0.76	0
2	MAN	G	8	2	11,11,12	0.28	0	15,15,17	0.70	0
2	MAN	G	9	2	11,11,12	0.32	0	15,15,17	0.83	0
3	NAG	H	1	1,3	14,14,15	0.30	0	17,19,21	0.80	0
3	NAG	H	2	3	14,14,15	0.36	0	17,19,21	1.88	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
2	NAG	C	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	MAN	D	7	2	-	0/2/19/22	0/1/1/1
2	MAN	D	8	2	-	0/2/19/22	0/1/1/1
2	MAN	D	9	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1
4	MAN	F	6	4	-	0/2/19/22	0/1/1/1
4	MAN	F	7	4	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	2/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	0/2/19/22	0/1/1/1
2	MAN	G	8	2	-	0/2/19/22	0/1/1/1
2	MAN	G	9	2	-	0/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	NAG	C1-O5-C5	5.78	120.02	112.19
4	F	5	MAN	C1-O5-C5	4.09	117.74	112.19
2	D	4	MAN	C1-O5-C5	3.71	117.22	112.19
4	F	6	MAN	C1-O5-C5	3.63	117.11	112.19
4	F	4	MAN	O5-C5-C6	3.46	112.62	107.20

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

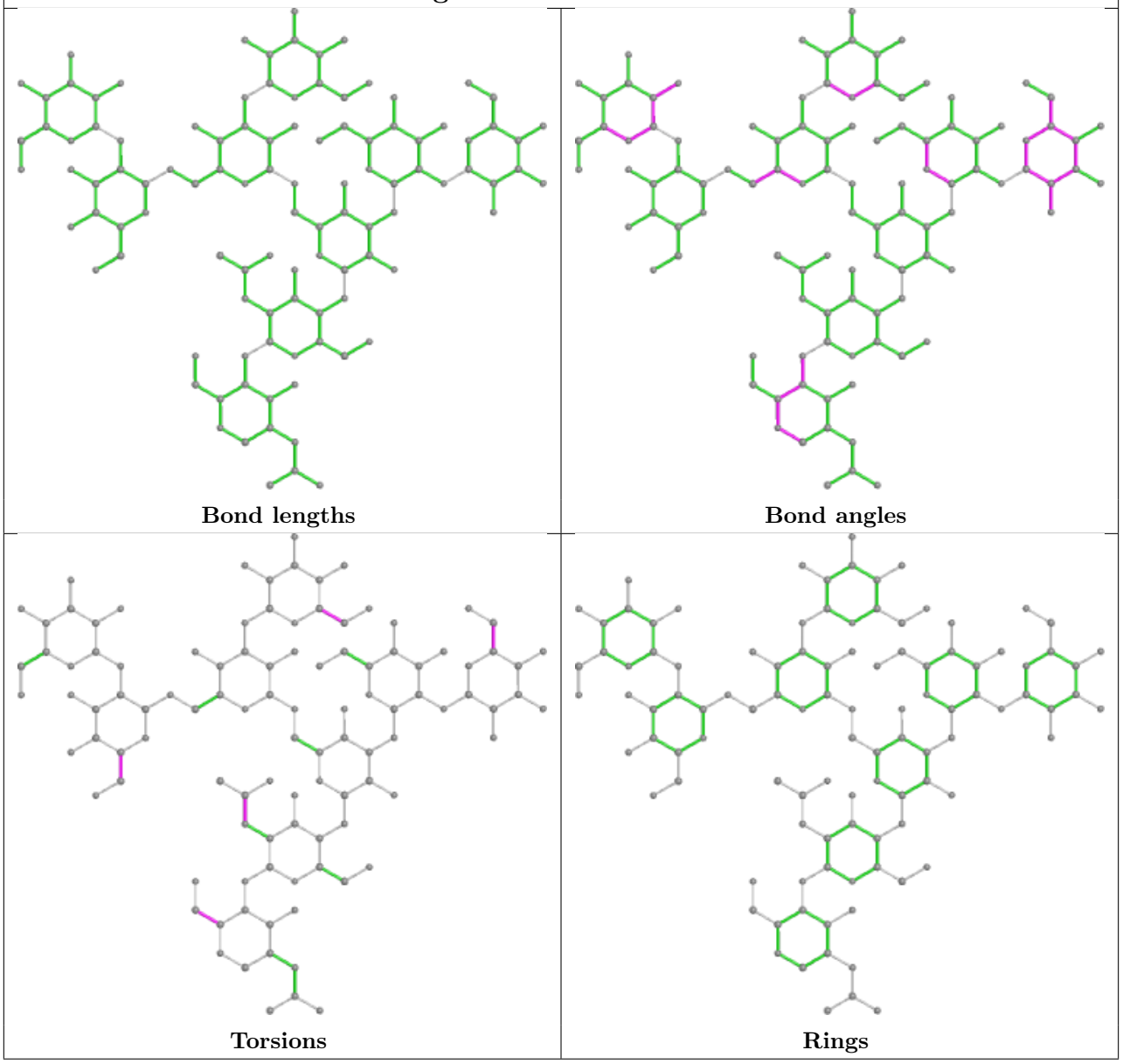
There are no ring outliers.

1 monomer is involved in 1 short contact:

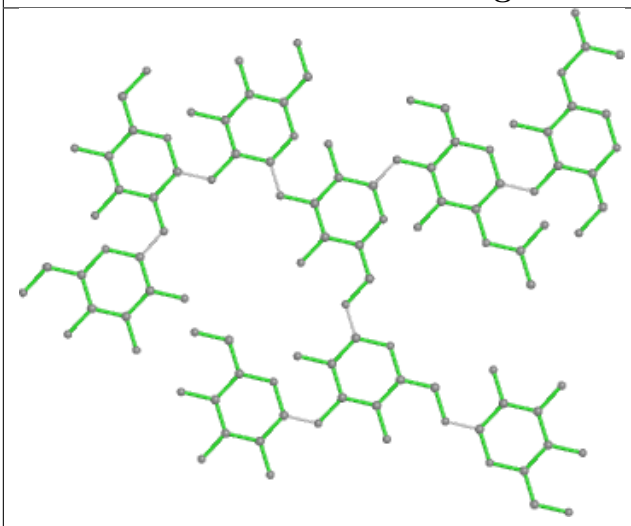
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	9	MAN	0	1

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

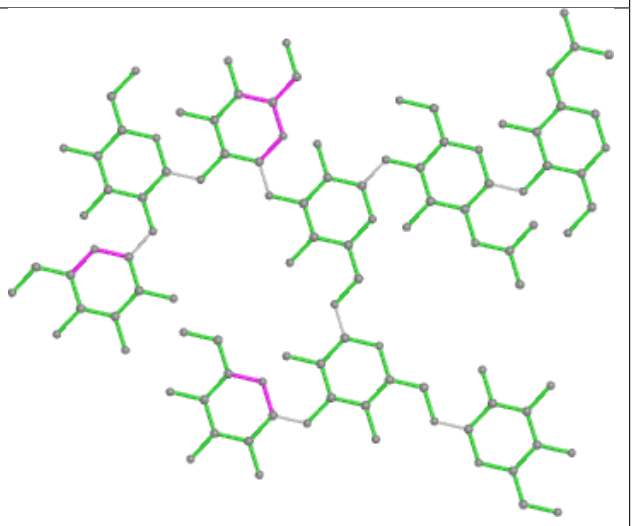
Oligosaccharide Chain C



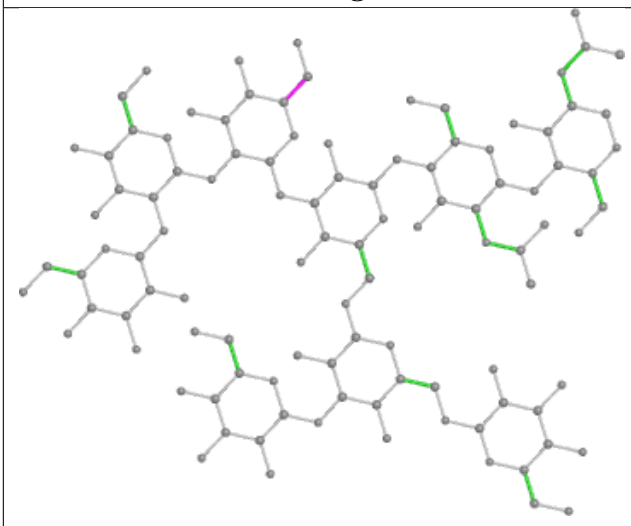
Oligosaccharide Chain D



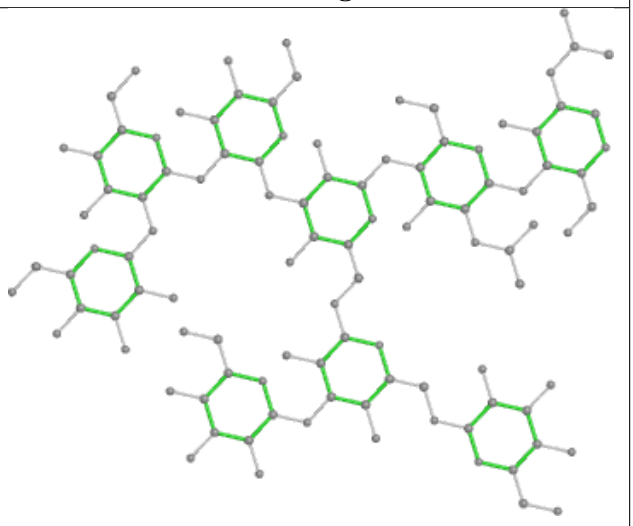
Bond lengths



Bond angles

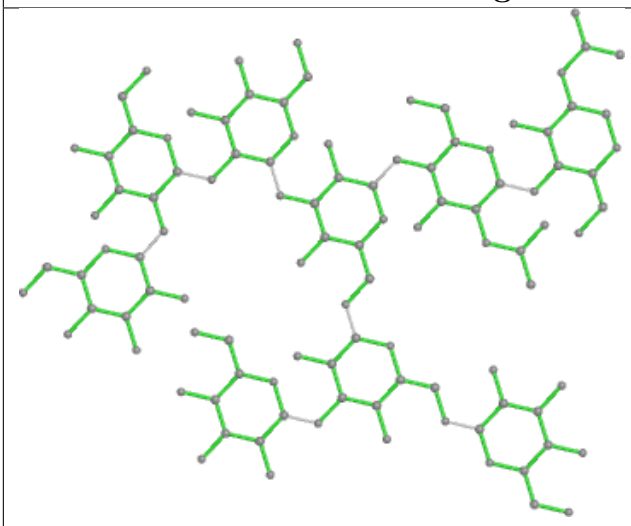


Torsions

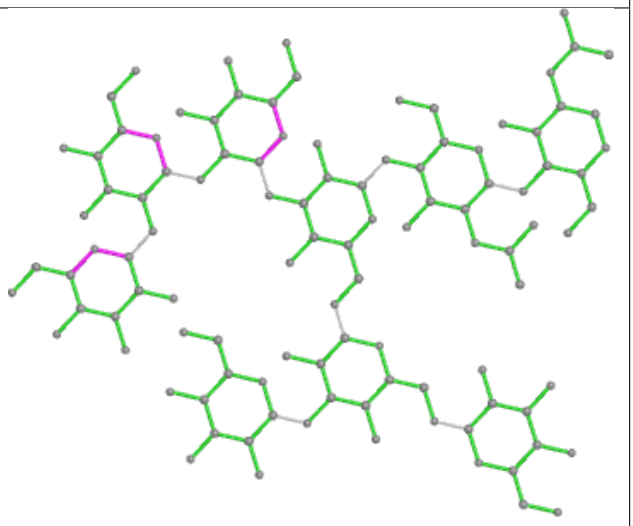


Rings

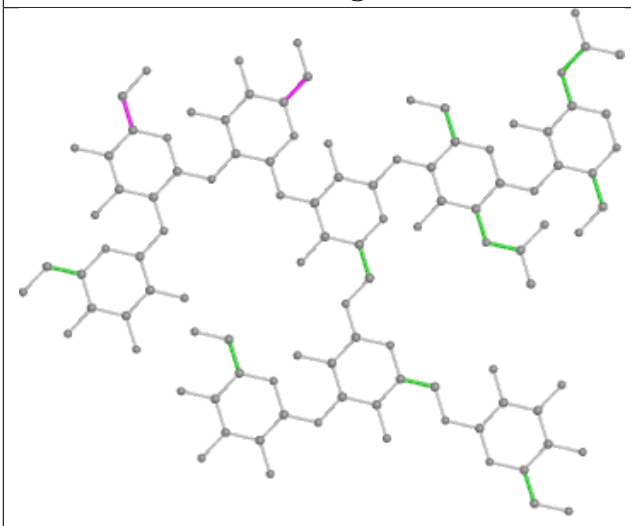
Oligosaccharide Chain G



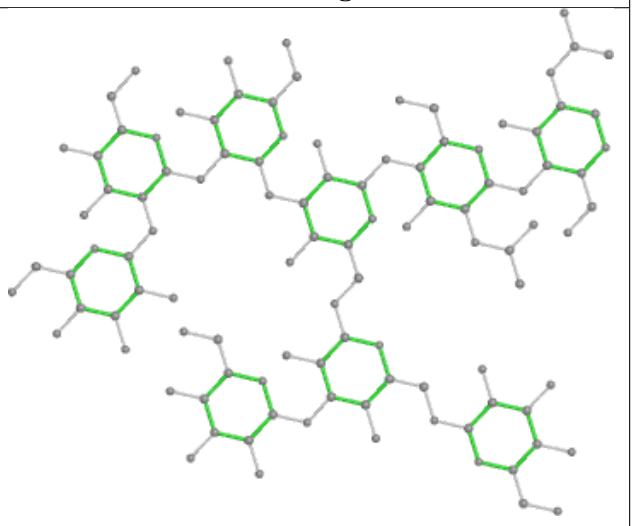
Bond lengths



Bond angles

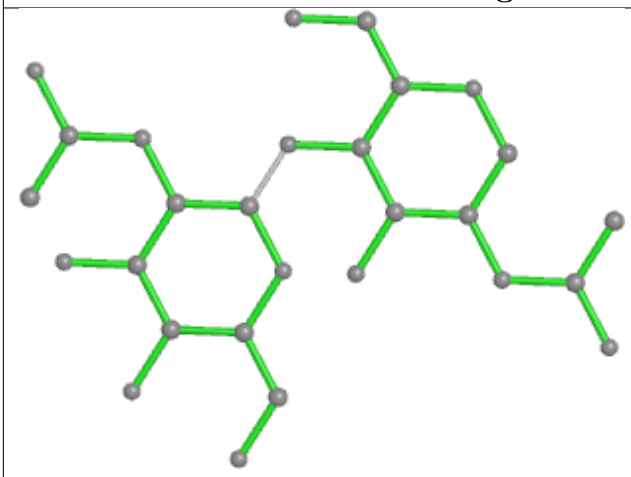


Torsions

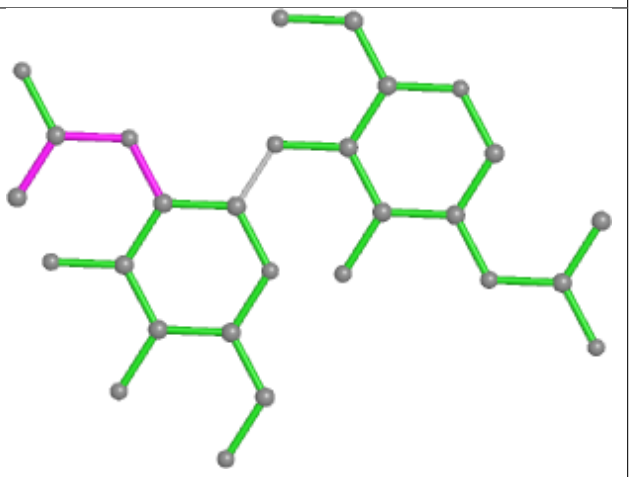


Rings

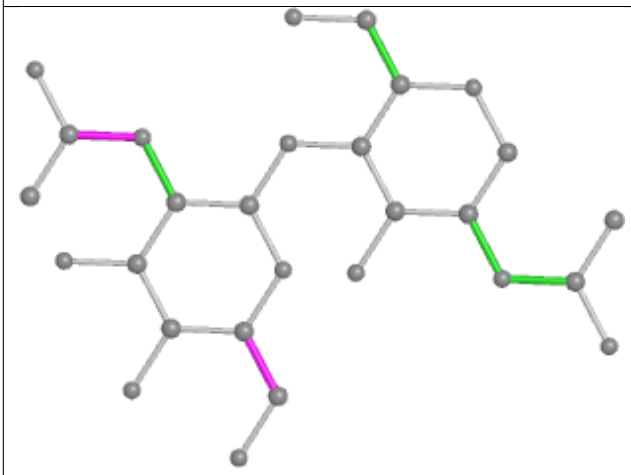
Oligosaccharide Chain E



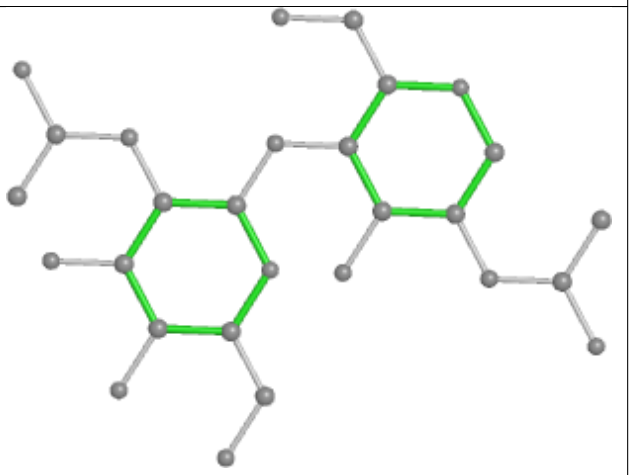
Bond lengths



Bond angles

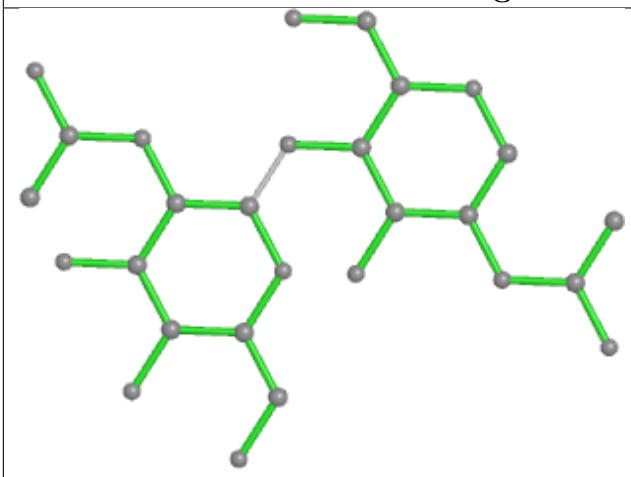


Torsions

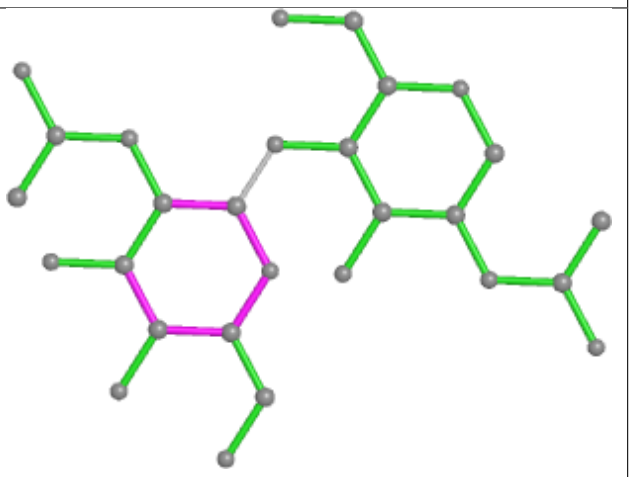


Rings

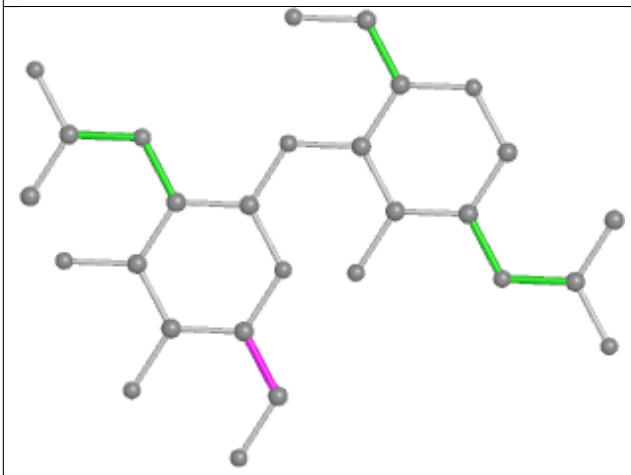
Oligosaccharide Chain H



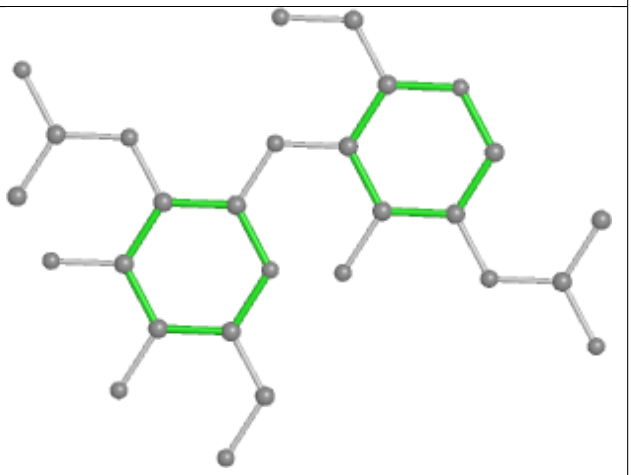
Bond lengths



Bond angles

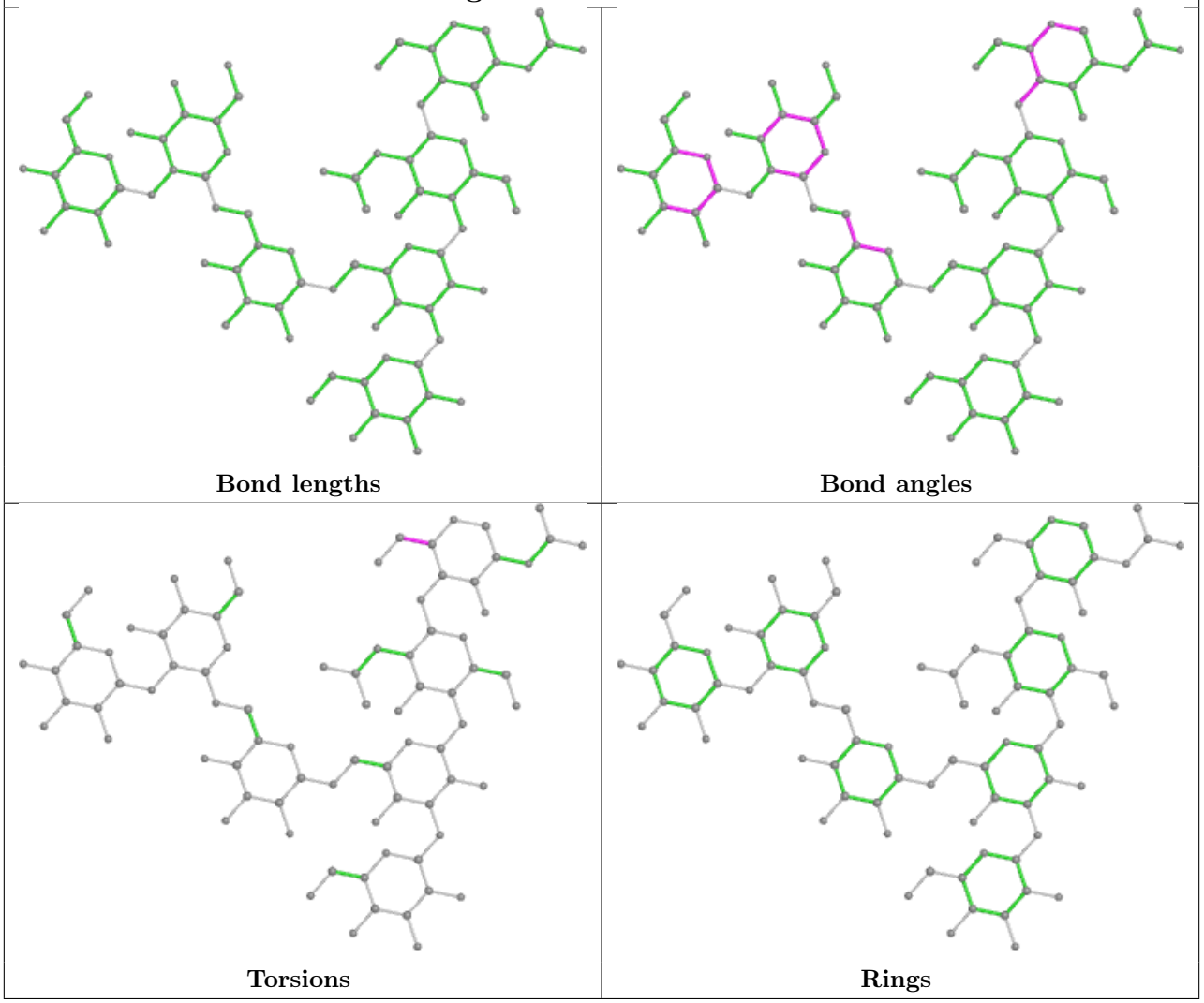


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

111 ligands 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	$\#\|Z\| > 2$
8	EDO	B	2061[B]	-	3,3,3	0.44	0	2,2,2	0.30	0
5	NAG	A	1539	1	14,14,15	0.39	0	17,19,21	1.36	2 (11%)
8	EDO	A	2034	-	3,3,3	0.53	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	975	A	2016	-	11,11,11	1.40	1 (9%)	14,14,14	0.63	0
5	NAG	A	1357	1	14,14,15	0.27	0	17,19,21	1.01	2 (11%)
7	975	B	2011	-	11,11,11	1.42	1 (9%)	14,14,14	0.78	1 (7%)
5	NAG	A	1512	1	14,14,15	0.34	0	17,19,21	2.08	4 (23%)
8	EDO	B	2042	-	3,3,3	0.51	0	2,2,2	0.19	0
7	975	B	2003	-	11,11,11	1.46	1 (9%)	14,14,14	0.68	0
7	975	B	2009	-	11,11,11	1.39	1 (9%)	14,14,14	1.00	1 (7%)
8	EDO	B	2043	-	3,3,3	0.51	0	2,2,2	0.16	0
7	975	A	2005	-	11,11,11	1.48	1 (9%)	14,14,14	0.61	0
8	EDO	B	2036	-	3,3,3	0.50	0	2,2,2	0.19	0
7	975	A	2021	-	11,11,11	2.98	1 (9%)	14,14,14	0.76	0
7	975	B	2002	-	11,11,11	1.41	1 (9%)	14,14,14	0.60	0
8	EDO	B	2035	-	3,3,3	0.54	0	2,2,2	0.24	0
8	EDO	A	2039	-	3,3,3	0.46	0	2,2,2	0.37	0
7	975	B	2017	-	11,11,11	1.47	1 (9%)	14,14,14	0.84	0
7	975	A	2013	-	11,11,11	1.50	1 (9%)	14,14,14	0.67	0
7	975	A	2008	-	11,11,11	1.56	1 (9%)	14,14,14	0.80	0
5	NAG	B	1357	1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
7	975	A	2007	-	11,11,11	1.43	1 (9%)	14,14,14	1.60	2 (14%)
7	975	A	2022	-	11,11,11	3.97	1 (9%)	14,14,14	6.16	3 (21%)
7	975	A	2018	-	11,11,11	1.64	1 (9%)	14,14,14	0.84	0
8	EDO	B	2047	-	3,3,3	0.56	0	2,2,2	0.15	0
7	975	A	2024	-	11,11,11	1.37	1 (9%)	14,14,14	1.12	1 (7%)
5	NAG	B	1555	1	14,14,15	0.28	0	17,19,21	0.88	0
6	FRU	B	2000	-	11,12,12	0.61	0	10,18,18	0.71	0
8	EDO	A	2048	-	3,3,3	0.51	0	2,2,2	0.22	0
8	EDO	A	2037[B]	-	3,3,3	0.44	0	2,2,2	0.34	0
5	NAG	B	1215	1	14,14,15	0.49	0	17,19,21	1.01	0
8	EDO	B	2034	-	3,3,3	0.46	0	2,2,2	0.11	0
7	975	B	2008	-	11,11,11	1.51	1 (9%)	14,14,14	1.44	2 (14%)
5	NAG	A	1555	1	14,14,15	0.31	0	17,19,21	1.30	3 (17%)
5	NAG	A	1644	1	14,14,15	0.27	0	17,19,21	0.81	0
8	EDO	A	2033	-	3,3,3	0.48	0	2,2,2	0.19	0
8	EDO	A	2056	-	3,3,3	0.53	0	2,2,2	0.17	0
8	EDO	B	2031	-	3,3,3	0.54	0	2,2,2	0.23	0
7	975	B	2004	-	11,11,11	1.44	1 (9%)	14,14,14	0.68	0
8	EDO	A	2037[A]	-	3,3,3	0.46	0	2,2,2	0.25	0
6	FRU	A	2000	-	11,12,12	0.60	0	10,18,18	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	EDO	B	2055	-	3,3,3	0.50	0	2,2,2	0.12	0
8	EDO	A	2055	-	3,3,3	0.52	0	2,2,2	0.10	0
7	975	A	2014	-	11,11,11	1.53	1 (9%)	14,14,14	0.80	0
7	975	A	2004	-	11,11,11	1.47	1 (9%)	14,14,14	0.65	0
8	EDO	B	2061[A]	-	3,3,3	0.46	0	2,2,2	0.25	0
8	EDO	A	2038	-	3,3,3	0.55	0	2,2,2	0.30	0
8	EDO	A	2035	-	3,3,3	0.47	0	2,2,2	0.48	0
7	975	A	2006	-	11,11,11	1.55	1 (9%)	14,14,14	0.99	0
7	975	B	2024	-	11,11,11	1.42	1 (9%)	14,14,14	1.29	2 (14%)
8	EDO	A	2052	-	3,3,3	0.51	0	2,2,2	0.13	0
5	NAG	A	1444	1	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
5	NAG	A	1606	1	14,14,15	0.33	0	17,19,21	1.65	3 (17%)
8	EDO	A	2041	-	3,3,3	0.33	0	2,2,2	0.11	0
8	EDO	A	2051	-	3,3,3	0.50	0	2,2,2	0.15	0
7	975	A	2026	-	11,11,11	1.78	1 (9%)	14,14,14	1.09	0
5	NAG	B	1644	1	14,14,15	0.26	0	17,19,21	0.74	0
8	EDO	B	2057	-	3,3,3	0.51	0	2,2,2	0.18	0
8	EDO	B	2046	-	3,3,3	0.53	0	2,2,2	0.13	0
8	EDO	A	2059	-	3,3,3	0.55	0	2,2,2	0.31	0
8	EDO	A	2049	-	3,3,3	0.49	0	2,2,2	0.13	0
7	975	B	2010	-	11,11,11	1.57	1 (9%)	14,14,14	0.78	0
7	975	A	2019	-	11,11,11	1.81	1 (9%)	14,14,14	2.78	2 (14%)
8	EDO	B	2058[B]	-	3,3,3	0.48	0	2,2,2	0.26	0
7	975	A	2011	-	11,11,11	1.63	1 (9%)	14,14,14	0.80	0
8	EDO	A	2057	-	3,3,3	0.49	0	2,2,2	0.20	0
8	EDO	A	2053	-	3,3,3	0.51	0	2,2,2	0.10	0
5	NAG	B	1471	1	14,14,15	0.32	0	17,19,21	0.70	0
5	NAG	B	1539	1	14,14,15	0.49	0	17,19,21	1.46	2 (11%)
5	NAG	A	1483	1	14,14,15	0.25	0	17,19,21	0.69	0
7	975	A	2020	-	11,11,11	1.63	1 (9%)	14,14,14	0.92	0
5	NAG	B	1242	1	14,14,15	0.23	0	17,19,21	1.17	2 (11%)
8	EDO	B	2056	-	3,3,3	0.45	0	2,2,2	0.29	0
7	975	B	2014	-	11,11,11	1.51	1 (9%)	14,14,14	0.80	0
7	975	B	2007	-	11,11,11	1.52	1 (9%)	14,14,14	0.71	0
7	975	B	2018	-	11,11,11	1.63	1 (9%)	14,14,14	0.88	0
7	975	B	2015	-	11,11,11	1.40	1 (9%)	14,14,14	1.03	1 (7%)
7	975	A	2025	-	11,11,11	1.59	1 (9%)	14,14,14	0.64	0
8	EDO	A	2040	-	3,3,3	0.50	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	1319	1	14,14,15	0.20	0	17,19,21	1.07	1 (5%)
7	975	B	2023	-	11,11,11	2.05	2 (18%)	14,14,14	2.01	3 (21%)
8	EDO	B	2058[A]	-	3,3,3	0.46	0	2,2,2	0.24	0
5	NAG	A	1471	1	14,14,15	0.36	0	17,19,21	1.10	2 (11%)
8	EDO	B	2054	-	3,3,3	0.55	0	2,2,2	0.32	0
8	EDO	A	2042	-	3,3,3	0.54	0	2,2,2	0.24	0
5	NAG	A	1319	1	14,14,15	0.24	0	17,19,21	1.38	1 (5%)
5	NAG	A	1242	1	14,14,15	0.27	0	17,19,21	0.89	1 (5%)
7	975	A	2003	-	11,11,11	1.60	1 (9%)	14,14,14	0.82	0
7	975	A	2009	-	11,11,11	1.44	1 (9%)	14,14,14	1.17	1 (7%)
7	975	B	2012	-	11,11,11	1.42	1 (9%)	14,14,14	0.72	0
7	975	A	2002	-	11,11,11	1.40	1 (9%)	14,14,14	0.61	0
8	EDO	B	2038	-	3,3,3	0.51	0	2,2,2	0.23	0
7	975	A	2017	-	11,11,11	1.51	1 (9%)	14,14,14	0.76	0
8	EDO	A	2032	-	3,3,3	0.40	0	2,2,2	0.50	0
5	NAG	B	1052	1	14,14,15	0.32	0	17,19,21	0.88	0
5	NAG	B	1483	1	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
8	EDO	A	2047	-	3,3,3	0.53	0	2,2,2	0.13	0
5	NAG	B	1444	1	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
8	EDO	B	2037	-	3,3,3	0.53	0	2,2,2	0.18	0
5	NAG	A	1052	1	14,14,15	0.25	0	17,19,21	1.08	2 (11%)
8	EDO	A	2050	-	3,3,3	0.51	0	2,2,2	0.15	0
5	NAG	A	1215	1	14,14,15	1.19	2 (14%)	17,19,21	1.22	1 (5%)
8	EDO	B	2044	-	3,3,3	0.55	0	2,2,2	0.19	0
7	975	B	2001	-	11,11,11	1.46	1 (9%)	14,14,14	0.64	0
8	EDO	A	2045	-	3,3,3	0.56	0	2,2,2	0.20	0
7	975	A	2001	-	11,11,11	1.39	1 (9%)	14,14,14	0.66	0
8	EDO	B	2030	-	3,3,3	0.50	0	2,2,2	0.27	0
5	NAG	A	1236	1	14,14,15	0.25	0	17,19,21	0.65	0
8	EDO	A	2060	-	3,3,3	0.55	0	2,2,2	0.28	0
7	975	B	2016	-	11,11,11	1.43	1 (9%)	14,14,14	0.94	1 (7%)
8	EDO	B	2053	-	3,3,3	0.64	0	2,2,2	0.18	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
8	EDO	B	2061[B]	-	-	1/1/1/1	-
5	NAG	A	1539	1	-	0/6/23/26	0/1/1/1
8	EDO	A	2034	-	-	1/1/1/1	-
7	975	A	2016	-	-	0/3/3/3	0/1/1/1
5	NAG	A	1357	1	-	2/6/23/26	0/1/1/1
7	975	B	2011	-	-	3/3/3/3	0/1/1/1
5	NAG	A	1512	1	-	3/6/23/26	0/1/1/1
8	EDO	B	2042	-	-	0/1/1/1	-
7	975	B	2003	-	-	1/3/3/3	0/1/1/1
7	975	B	2009	-	-	3/3/3/3	0/1/1/1
8	EDO	B	2043	-	-	0/1/1/1	-
7	975	A	2005	-	-	3/3/3/3	0/1/1/1
8	EDO	B	2036	-	-	0/1/1/1	-
7	975	A	2021	-	-	0/3/3/3	0/1/1/1
7	975	B	2002	-	-	1/3/3/3	0/1/1/1
8	EDO	B	2035	-	-	1/1/1/1	-
8	EDO	A	2039	-	-	1/1/1/1	-
7	975	B	2017	-	-	0/3/3/3	0/1/1/1
7	975	A	2013	-	-	0/3/3/3	0/1/1/1
7	975	A	2008	-	-	1/3/3/3	0/1/1/1
5	NAG	B	1357	1	-	0/6/23/26	0/1/1/1
7	975	A	2007	-	-	2/3/3/3	0/1/1/1
7	975	A	2022	-	-	1/3/3/3	0/1/1/1
7	975	A	2018	-	-	0/3/3/3	0/1/1/1
8	EDO	B	2047	-	-	1/1/1/1	-
7	975	A	2024	-	-	3/3/3/3	0/1/1/1
5	NAG	B	1555	1	-	0/6/23/26	0/1/1/1
6	FRU	B	2000	-	-	0/5/24/24	0/1/1/1
8	EDO	A	2048	-	-	0/1/1/1	-
8	EDO	A	2037[B]	-	-	1/1/1/1	-
5	NAG	B	1215	1	-	0/6/23/26	0/1/1/1
8	EDO	B	2034	-	-	1/1/1/1	-
7	975	B	2008	-	-	2/3/3/3	0/1/1/1
5	NAG	A	1555	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1644	1	-	0/6/23/26	0/1/1/1
8	EDO	A	2033	-	-	1/1/1/1	-
8	EDO	A	2056	-	-	1/1/1/1	-
8	EDO	B	2031	-	-	1/1/1/1	-
7	975	B	2004	-	-	0/3/3/3	0/1/1/1
8	EDO	A	2037[A]	-	-	0/1/1/1	-
6	FRU	A	2000	-	-	0/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	2055	-	-	0/1/1/1	-
8	EDO	A	2055	-	-	1/1/1/1	-
7	975	A	2014	-	-	0/3/3/3	0/1/1/1
7	975	A	2004	-	-	0/3/3/3	0/1/1/1
8	EDO	B	2061[A]	-	-	1/1/1/1	-
8	EDO	A	2038	-	-	1/1/1/1	-
8	EDO	A	2035	-	-	1/1/1/1	-
7	975	A	2006	-	-	1/3/3/3	0/1/1/1
7	975	B	2024	-	-	2/3/3/3	0/1/1/1
8	EDO	A	2052	-	-	1/1/1/1	-
5	NAG	A	1444	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1606	1	-	3/6/23/26	0/1/1/1
8	EDO	A	2041	-	-	1/1/1/1	-
8	EDO	A	2051	-	-	1/1/1/1	-
7	975	A	2026	-	-	0/3/3/3	0/1/1/1
5	NAG	B	1644	1	-	0/6/23/26	0/1/1/1
8	EDO	B	2057	-	-	1/1/1/1	-
8	EDO	B	2046	-	-	1/1/1/1	-
8	EDO	A	2059	-	-	0/1/1/1	-
8	EDO	A	2049	-	-	1/1/1/1	-
7	975	B	2010	-	-	0/3/3/3	0/1/1/1
7	975	A	2019	-	-	1/3/3/3	0/1/1/1
8	EDO	B	2058[B]	-	-	0/1/1/1	-
7	975	A	2011	-	-	1/3/3/3	0/1/1/1
8	EDO	A	2057	-	-	0/1/1/1	-
8	EDO	A	2053	-	-	1/1/1/1	-
5	NAG	B	1471	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1539	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1483	1	-	0/6/23/26	0/1/1/1
7	975	A	2020	-	-	1/3/3/3	0/1/1/1
5	NAG	B	1242	1	-	2/6/23/26	0/1/1/1
8	EDO	B	2056	-	-	1/1/1/1	-
7	975	B	2014	-	-	0/3/3/3	0/1/1/1
7	975	B	2007	-	-	1/3/3/3	0/1/1/1
7	975	B	2018	-	-	1/3/3/3	0/1/1/1
7	975	B	2015	-	-	2/3/3/3	0/1/1/1
7	975	A	2025	-	-	0/3/3/3	0/1/1/1
8	EDO	A	2040	-	-	0/1/1/1	-
5	NAG	B	1319	1	-	0/6/23/26	0/1/1/1
7	975	B	2023	-	-	2/3/3/3	0/1/1/1
8	EDO	B	2058[A]	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1471	1	-	2/6/23/26	0/1/1/1
8	EDO	B	2054	-	-	1/1/1/1	-
8	EDO	A	2042	-	-	1/1/1/1	-
5	NAG	A	1319	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1242	1	-	0/6/23/26	0/1/1/1
7	975	A	2003	-	-	0/3/3/3	0/1/1/1
7	975	A	2009	-	-	3/3/3/3	0/1/1/1
7	975	B	2012	-	-	0/3/3/3	0/1/1/1
7	975	A	2002	-	-	1/3/3/3	0/1/1/1
8	EDO	B	2038	-	-	1/1/1/1	-
7	975	A	2017	-	-	1/3/3/3	0/1/1/1
8	EDO	A	2032	-	-	0/1/1/1	-
5	NAG	B	1052	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1483	1	-	0/6/23/26	0/1/1/1
8	EDO	A	2047	-	-	1/1/1/1	-
5	NAG	B	1444	1	-	0/6/23/26	0/1/1/1
8	EDO	B	2037	-	-	1/1/1/1	-
5	NAG	A	1052	1	-	2/6/23/26	0/1/1/1
8	EDO	A	2050	-	-	1/1/1/1	-
5	NAG	A	1215	1	-	0/6/23/26	0/1/1/1
8	EDO	B	2044	-	-	0/1/1/1	-
7	975	B	2001	-	-	1/3/3/3	0/1/1/1
8	EDO	A	2045	-	-	1/1/1/1	-
7	975	A	2001	-	-	2/3/3/3	0/1/1/1
8	EDO	B	2030	-	-	1/1/1/1	-
5	NAG	A	1236	1	-	0/6/23/26	0/1/1/1
8	EDO	A	2060	-	-	1/1/1/1	-
7	975	B	2016	-	-	2/3/3/3	0/1/1/1
8	EDO	B	2053	-	-	0/1/1/1	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2022	975	CAH-CAK	-13.05	1.13	1.51
7	A	2021	975	CAH-CAK	-9.73	1.23	1.51
7	A	2026	975	CAH-CAK	-5.87	1.34	1.51
7	A	2019	975	CAH-CAK	-5.79	1.34	1.51
7	A	2018	975	CAH-CAK	-5.25	1.36	1.51

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	2022	975	CAH-CAK-CAF	-19.75	88.14	120.54
7	A	2019	975	CAH-CAK-CAF	-9.18	105.48	120.54
7	A	2022	975	CAH-CAK-CAE	9.05	144.11	121.23
7	A	2022	975	CAG-CAH-CAK	-7.38	79.45	112.15
5	A	1512	NAG	C1-O5-C5	6.44	120.92	112.19

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2002	975	OAA-CAG-CAH-CAK
7	A	2005	975	OAA-CAG-CAH-CAK
7	A	2008	975	OAA-CAG-CAH-CAK
7	A	2009	975	OAA-CAG-CAH-CAK
7	A	2019	975	OAA-CAG-CAH-CAK

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	2047	EDO	2	0
8	A	2056	EDO	1	0
5	A	1606	NAG	2	0
8	A	2053	EDO	3	0
7	A	2025	975	2	0
7	B	2023	975	1	0
8	A	2032	EDO	3	0
5	B	1444	NAG	1	0
5	A	1215	NAG	4	0
8	B	2044	EDO	1	0
8	B	2053	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

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, 95^{th} 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	624/665 (93%)	0.07	7 (1%)	80	83	12, 20, 30, 40	2 (0%)
1	B	624/665 (93%)	0.00	5 (0%)	86	88	14, 22, 34, 41	2 (0%)
All	All	1248/1330 (93%)	0.04	12 (0%)	82	85	12, 21, 32, 41	4 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	THR	3.6
1	B	317	TRP	3.1
1	B	571	GLU	2.7
1	A	386	TYR	2.7
1	A	42	CYS	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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
4	MAN	F	6	11/12	0.42	0.42	65,66,67,67	0
2	MAN	C	7	11/12	0.51	0.48	63,66,67,67	0
2	MAN	C	6	11/12	0.62	0.36	57,57,57,58	0
2	MAN	C	5	11/12	0.65	0.33	58,60,61,61	0
2	MAN	D	9	11/12	0.66	0.26	32,35,36,37	0

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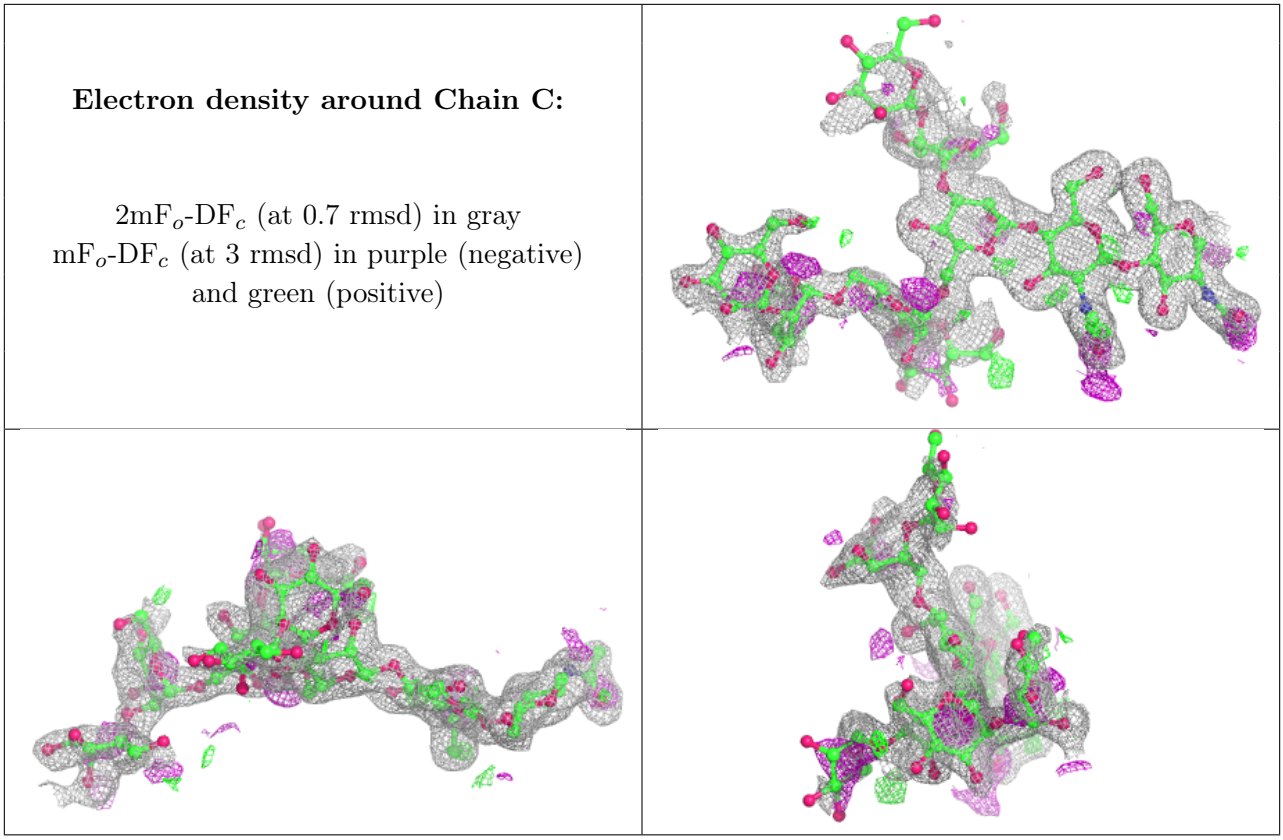
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	2	14/15	0.67	0.31	55,59,61,68	0
4	MAN	F	4	11/12	0.70	0.33	52,55,58,60	0
2	MAN	D	5	11/12	0.72	0.18	45,47,49,56	0
2	MAN	G	9	11/12	0.73	0.28	34,36,38,38	0
2	MAN	D	6	11/12	0.74	0.43	63,68,70,73	0
4	MAN	F	5	11/12	0.78	0.39	63,65,65,65	0
3	NAG	H	2	14/15	0.78	0.27	55,59,60,60	0
2	MAN	C	8	11/12	0.79	0.26	53,58,58,64	0
2	MAN	C	4	11/12	0.79	0.28	50,54,57,59	0
2	MAN	G	6	11/12	0.79	0.33	58,61,63,63	0
2	MAN	C	9	11/12	0.81	0.53	71,76,78,78	0
2	MAN	G	4	11/12	0.83	0.13	32,35,36,39	0
4	MAN	F	7	11/12	0.84	0.29	50,52,54,54	0
2	MAN	D	4	11/12	0.85	0.14	31,34,36,39	0
2	MAN	G	5	11/12	0.85	0.17	44,45,47,52	0
3	NAG	E	1	14/15	0.86	0.12	36,38,43,49	0
2	NAG	C	2	14/15	0.89	0.12	23,24,26,29	0
2	BMA	C	3	11/12	0.91	0.11	34,39,45,46	0
3	NAG	H	1	14/15	0.91	0.08	37,39,43,49	0
2	MAN	G	7	11/12	0.91	0.11	19,21,26,30	0
4	BMA	F	3	11/12	0.91	0.11	36,41,45,48	0
4	NAG	F	2	14/15	0.94	0.09	25,27,28,32	0
2	NAG	C	1	14/15	0.94	0.11	19,21,23,23	0
2	MAN	D	7	11/12	0.94	0.11	17,20,24,28	0
2	NAG	D	2	14/15	0.95	0.10	15,16,17,18	0
2	BMA	D	3	11/12	0.95	0.10	20,20,22,26	0
4	NAG	F	1	14/15	0.95	0.08	22,23,26,26	0
2	NAG	D	1	14/15	0.96	0.10	14,14,14,15	0
2	NAG	G	1	14/15	0.96	0.08	16,16,17,17	0
2	NAG	G	2	14/15	0.96	0.08	17,18,18,20	0
2	BMA	G	3	11/12	0.96	0.09	21,22,23,27	0
2	MAN	D	8	11/12	0.97	0.10	15,15,15,16	0
2	MAN	G	8	11/12	0.97	0.09	17,17,17,18	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.

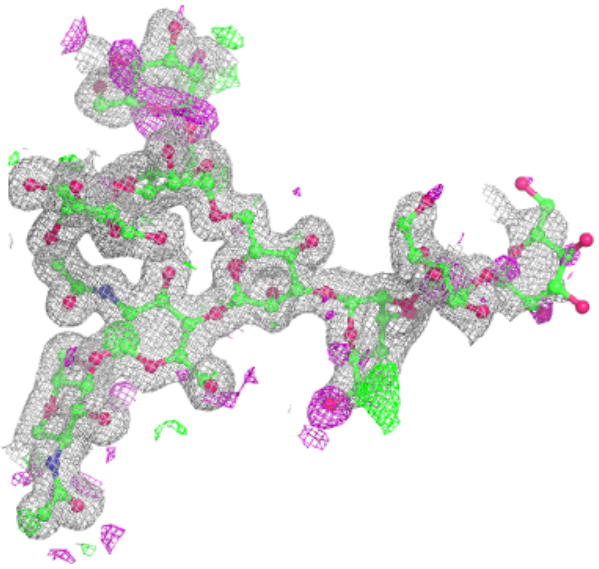
Electron density around Chain C:

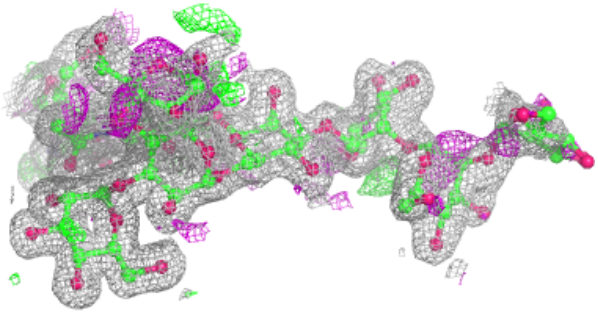
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

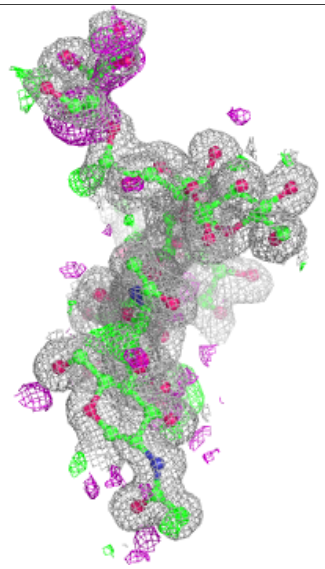


Electron density around Chain D:

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

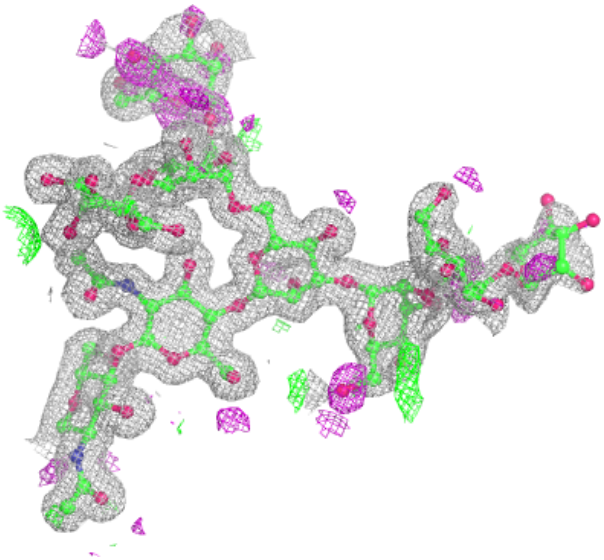


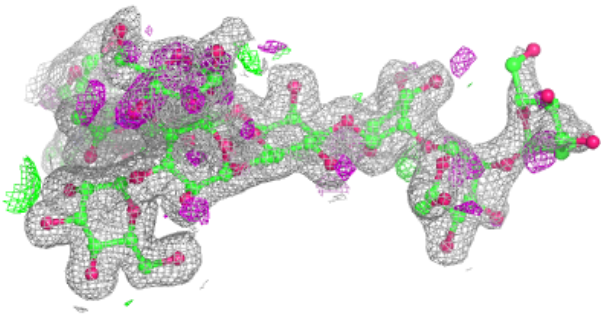


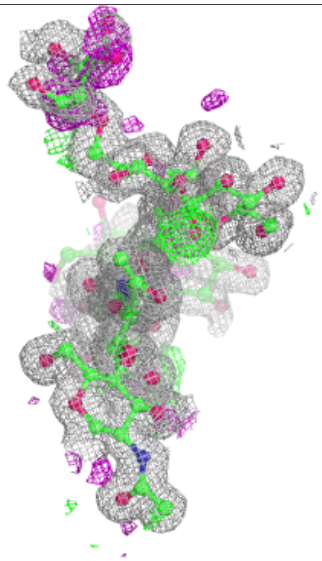


Electron density around Chain G:

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

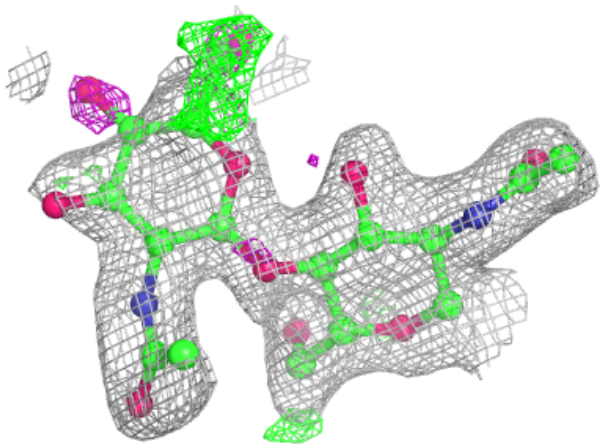


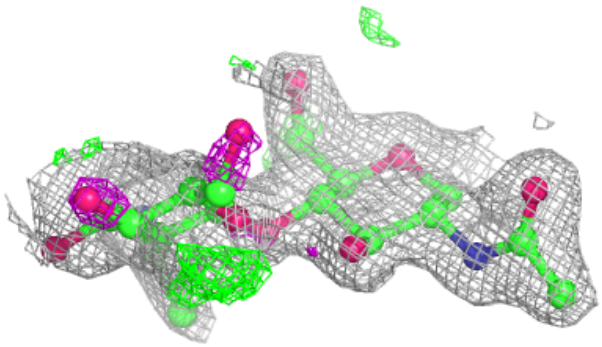


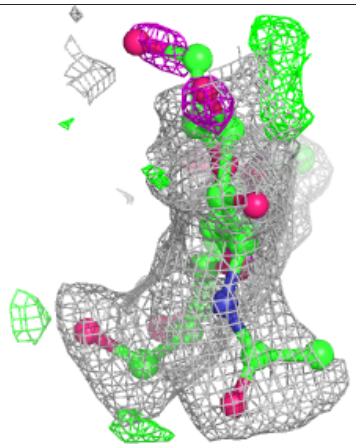


Electron density around Chain E:

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

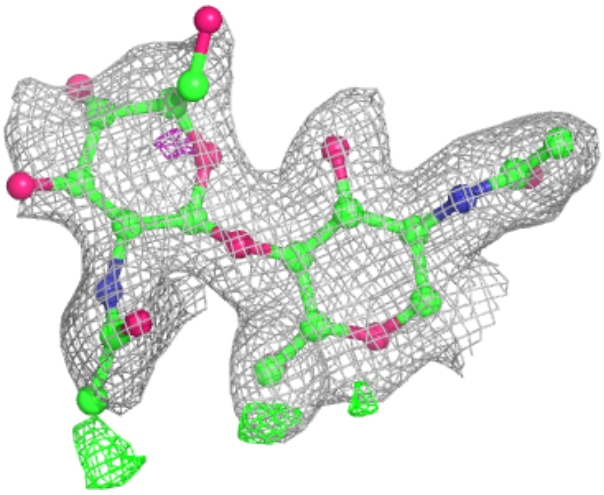


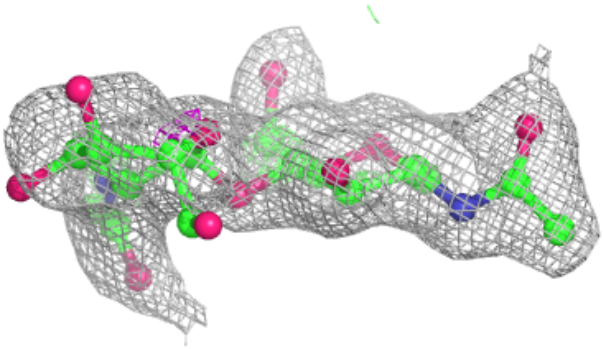


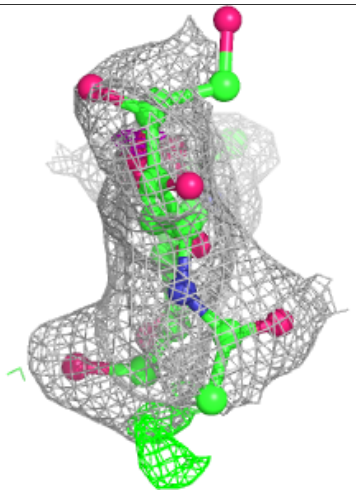


Electron density around Chain H:

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

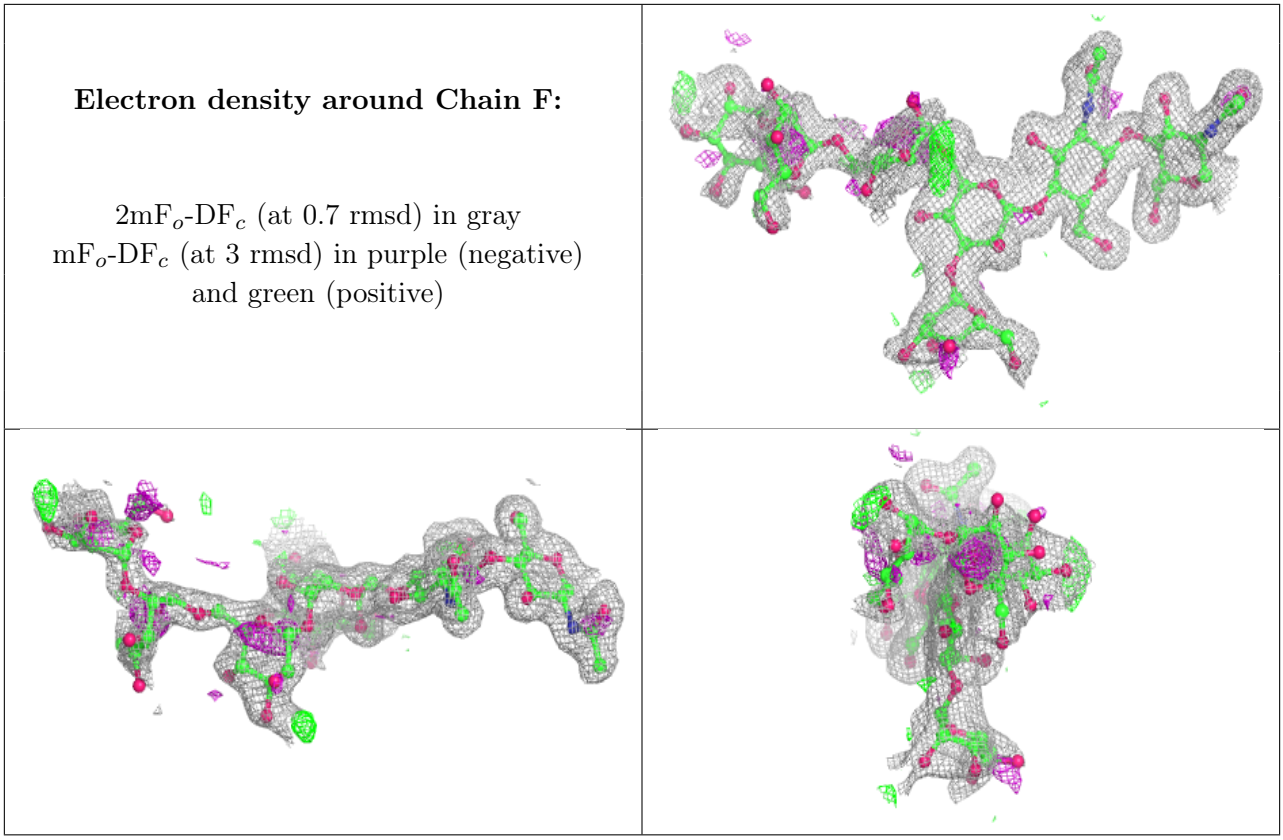






Electron density around Chain F:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	NAG	A	1512	14/15	0.41	0.52	60,65,69,69	0
7	975	B	2014	11/11	0.47	0.32	46,46,47,47	0
7	975	B	2010	11/11	0.48	0.29	63,66,67,68	0
7	975	B	2004	11/11	0.49	0.24	41,41,42,42	0
7	975	A	2005	11/11	0.50	0.27	56,59,59,60	0
7	975	A	2014	11/11	0.53	0.32	40,41,42,43	0
8	EDO	B	2046	4/4	0.53	0.26	45,45,45,45	0
7	975	B	2008	11/11	0.55	0.30	48,48,49,49	0
8	EDO	A	2042	4/4	0.55	0.23	40,40,40,40	0
8	EDO	A	2050	4/4	0.55	0.23	32,32,32,32	0
7	975	A	2025	11/11	0.55	0.42	62,62,63,63	0
8	EDO	A	2053	4/4	0.56	0.32	36,36,36,37	0
7	975	A	2009	11/11	0.59	0.32	44,48,48,48	0
8	EDO	A	2032	4/4	0.59	0.30	34,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	A	2049	4/4	0.60	0.27	40,41,41,41	0
8	EDO	B	2053	4/4	0.60	0.27	41,41,41,41	0
7	975	B	2009	11/11	0.61	0.28	66,66,67,67	0
7	975	A	2002	11/11	0.62	0.29	34,36,36,36	0
7	975	A	2004	11/11	0.62	0.23	38,39,39,39	0
8	EDO	B	2037	4/4	0.63	0.29	43,43,43,43	0
7	975	B	2024	11/11	0.63	0.33	76,76,76,77	0
8	EDO	B	2047	4/4	0.63	0.19	44,44,44,45	0
7	975	B	2015	11/11	0.63	0.24	44,45,45,45	0
7	975	B	2002	11/11	0.64	0.29	39,42,42,42	0
8	EDO	A	2045	4/4	0.65	0.28	37,37,37,37	4
7	975	A	2006	11/11	0.65	0.20	50,51,51,51	0
8	EDO	B	2057	4/4	0.65	0.35	26,26,27,27	0
8	EDO	A	2059	4/4	0.66	0.27	43,43,44,44	0
8	EDO	A	2055	4/4	0.66	0.28	24,25,25,25	0
8	EDO	A	2057	4/4	0.66	0.20	46,46,46,46	0
8	EDO	B	2061[A]	4/4	0.66	0.21	22,22,22,22	4
8	EDO	B	2061[B]	4/4	0.66	0.21	21,21,21,22	4
7	975	B	2003	11/11	0.67	0.25	43,46,47,47	0
5	NAG	A	1606	14/15	0.67	0.30	38,40,41,41	0
7	975	B	2023	11/11	0.68	0.39	54,54,57,76	3
7	975	B	2001	11/11	0.69	0.30	38,39,39,39	0
7	975	A	2008	11/11	0.69	0.32	45,45,45,46	0
8	EDO	A	2039	4/4	0.69	0.15	40,41,41,41	0
7	975	A	2016	11/11	0.69	0.23	40,41,43,43	0
7	975	A	2022	11/11	0.69	0.23	69,69,90,93	3
7	975	A	2007	11/11	0.69	0.22	38,40,41,41	0
8	EDO	B	2058[A]	4/4	0.70	0.30	30,30,30,30	4
8	EDO	B	2058[B]	4/4	0.70	0.30	29,29,29,29	4
7	975	B	2011	11/11	0.70	0.18	52,53,53,53	0
7	975	A	2024	11/11	0.70	0.23	66,66,67,67	0
5	NAG	A	1555	14/15	0.71	0.22	34,36,37,37	0
5	NAG	A	1539	14/15	0.71	0.30	39,42,45,45	0
8	EDO	A	2051	4/4	0.71	0.24	45,46,46,46	0
8	EDO	A	2048	4/4	0.71	0.29	44,44,44,44	0
5	NAG	A	1215	14/15	0.72	0.46	50,55,58,58	0
7	975	A	2017	11/11	0.72	0.30	43,46,47,47	0
7	975	A	2020	11/11	0.72	0.26	57,58,59,59	3
8	EDO	A	2035	4/4	0.72	0.20	36,36,36,36	0
5	NAG	B	1215	14/15	0.72	0.48	52,57,58,59	0
7	975	B	2017	11/11	0.72	0.27	45,47,48,48	0
8	EDO	B	2043	4/4	0.73	0.19	48,48,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	A	2041	4/4	0.74	0.29	24,24,24,25	4
8	EDO	A	2052	4/4	0.74	0.17	50,50,50,50	0
7	975	A	2026	11/11	0.74	0.32	54,54,55,55	11
8	EDO	A	2034	4/4	0.74	0.16	38,38,39,39	0
7	975	B	2018	11/11	0.75	0.24	65,65,66,66	0
8	EDO	A	2038	4/4	0.76	0.23	49,49,49,50	0
5	NAG	A	1242	14/15	0.76	0.31	44,47,48,48	0
7	975	A	2003	11/11	0.76	0.31	43,46,47,47	0
7	975	B	2016	11/11	0.76	0.28	40,42,44,45	0
5	NAG	B	1539	14/15	0.76	0.36	39,43,44,44	0
7	975	A	2021	11/11	0.76	0.28	44,44,76,86	3
8	EDO	B	2036	4/4	0.77	0.18	36,36,36,36	0
5	NAG	B	1052	14/15	0.77	0.29	45,48,51,51	0
5	NAG	B	1242	14/15	0.77	0.32	53,57,58,58	0
8	EDO	B	2044	4/4	0.77	0.26	23,23,23,23	4
5	NAG	B	1319	14/15	0.78	0.31	53,56,57,58	0
8	EDO	A	2056	4/4	0.78	0.24	42,42,43,43	0
8	EDO	B	2030	4/4	0.78	0.27	55,55,55,56	0
5	NAG	A	1319	14/15	0.79	0.28	48,52,53,53	0
7	975	A	2019	11/11	0.79	0.24	43,44,90,92	3
7	975	A	2011	11/11	0.79	0.20	49,49,49,50	0
8	EDO	B	2034	4/4	0.79	0.17	39,39,39,39	0
8	EDO	B	2055	4/4	0.80	0.22	35,36,36,36	0
7	975	A	2001	11/11	0.80	0.27	37,38,38,38	0
7	975	B	2007	11/11	0.80	0.20	43,45,45,45	0
8	EDO	A	2040	4/4	0.80	0.18	33,33,34,34	0
8	EDO	A	2037[A]	4/4	0.80	0.20	35,35,35,35	4
8	EDO	A	2037[B]	4/4	0.80	0.20	32,32,32,32	4
8	EDO	B	2042	4/4	0.81	0.24	37,37,37,38	0
5	NAG	A	1052	14/15	0.81	0.26	43,46,48,48	0
5	NAG	B	1483	14/15	0.81	0.24	45,47,49,49	0
8	EDO	B	2038	4/4	0.82	0.28	50,50,50,50	0
7	975	A	2013	11/11	0.82	0.18	36,37,39,39	0
8	EDO	B	2056	4/4	0.82	0.37	26,26,27,27	0
5	NAG	A	1471	14/15	0.82	0.15	30,31,32,33	0
7	975	A	2018	11/11	0.83	0.24	58,58,59,59	0
8	EDO	A	2047	4/4	0.84	0.25	49,49,49,49	0
8	EDO	B	2035	4/4	0.84	0.19	45,45,45,45	0
8	EDO	A	2060	4/4	0.85	0.30	37,37,37,37	0
8	EDO	B	2031	4/4	0.85	0.11	36,36,36,36	0
5	NAG	A	1236	14/15	0.86	0.14	26,27,28,29	0
8	EDO	B	2054	4/4	0.86	0.23	37,37,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	975	B	2012	11/11	0.86	0.18	37,38,38,38	0
5	NAG	A	1483	14/15	0.87	0.21	39,41,43,43	0
5	NAG	B	1471	14/15	0.88	0.13	31,32,35,35	0
5	NAG	B	1644	14/15	0.89	0.11	24,25,27,28	0
8	EDO	A	2033	4/4	0.89	0.15	45,45,45,45	0
5	NAG	B	1555	14/15	0.89	0.18	31,33,33,34	0
5	NAG	A	1357	14/15	0.91	0.10	30,30,31,31	0
5	NAG	B	1357	14/15	0.92	0.12	34,35,35,36	0
5	NAG	A	1644	14/15	0.92	0.09	23,24,25,26	0
5	NAG	A	1444	14/15	0.94	0.09	26,26,26,27	0
6	FRU	B	2000	12/12	0.94	0.08	18,19,20,21	0
6	FRU	A	2000	12/12	0.95	0.09	16,16,17,18	0
5	NAG	B	1444	14/15	0.95	0.08	27,27,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.