wwPDB X-ray Structure Validation Summary Report (i)

Jan 13, 2024 – 02:51 pm GMT

PDB ID	:	6Q7I
Title	:	GH3 exo-beta-xylosidase (XlnD)
Authors	:	Davies, G.J.; Rowland, R.J.; Wu, L.; Moroz, O.; Blagova, E.
Deposited on	:	2018-12-13
Resolution	:	1.48 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 (1)) were used in the production of this report:

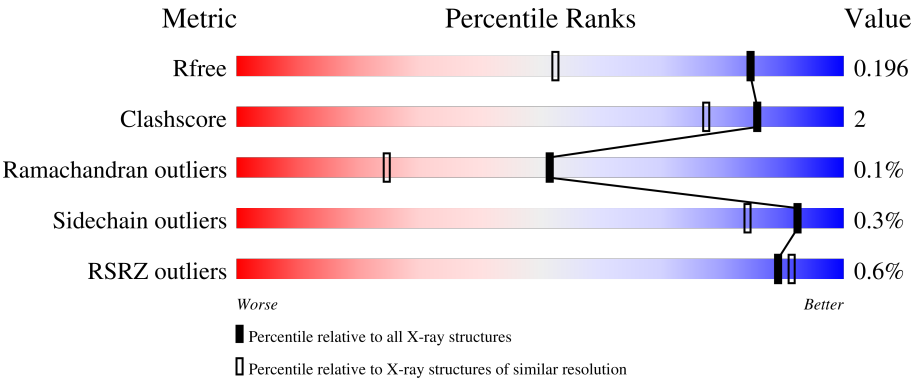
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	785	% 94%
1	B	785	% 94%
2	C	9	100%
3	D	2	100%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
4	E	10	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
6	EDO	B	925	-	-	X	-

2 Entry composition (i)

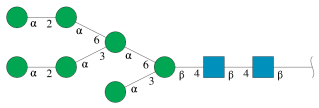
There are 10 unique types of molecules in this entry. The entry contains 14338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Exo-1,4-beta-xylosidase xlnD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	769	Total	C	N	O	S	0	8	0
			5945	3752	982	1195	16			
1	A	770	Total	C	N	O	S	0	11	0
			5987	3775	993	1203	16			

- Molecule 2 is an oligosaccharide called 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)-[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.



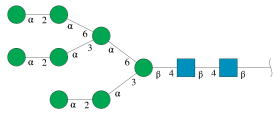
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			

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

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

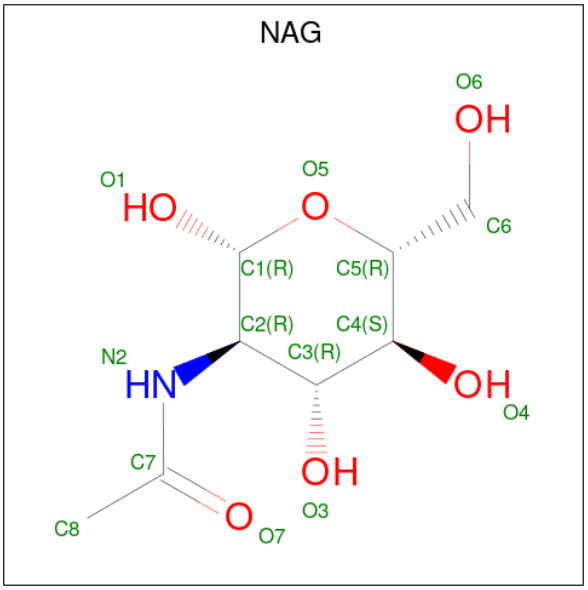
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-3)-[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
4	E	10	Total C N O 116 64 2 50	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	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

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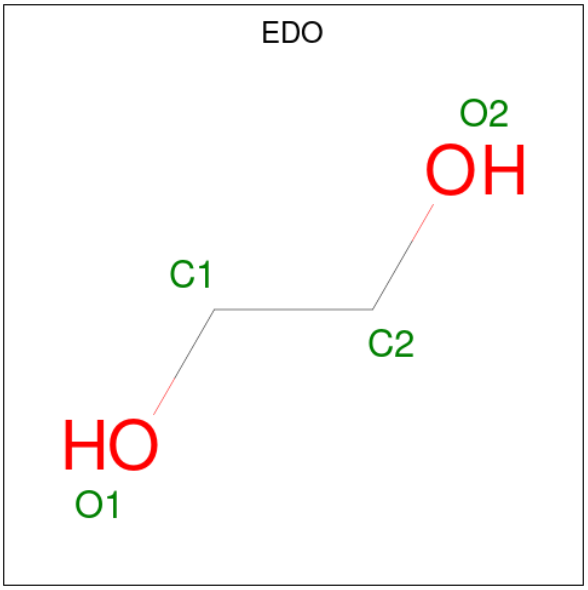
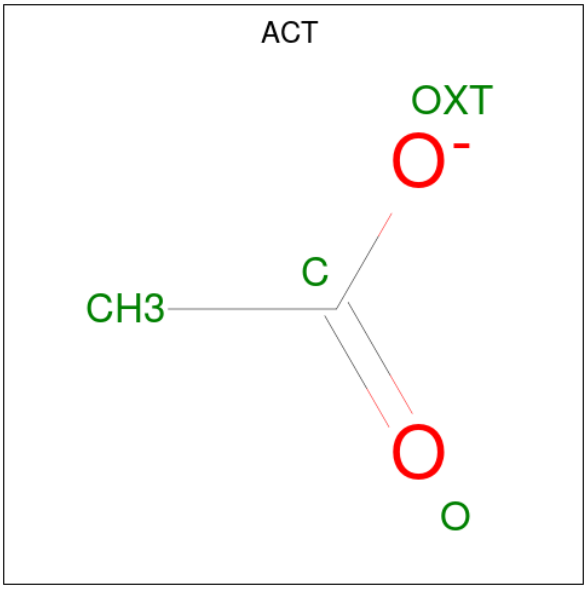
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



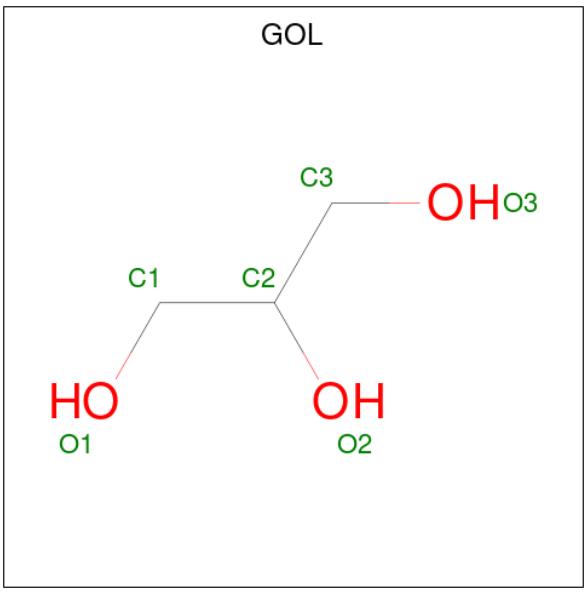
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	3	Total K 3 3	0	0
9	A	1	Total K 1 1	0	0

- Molecule 10 is water.

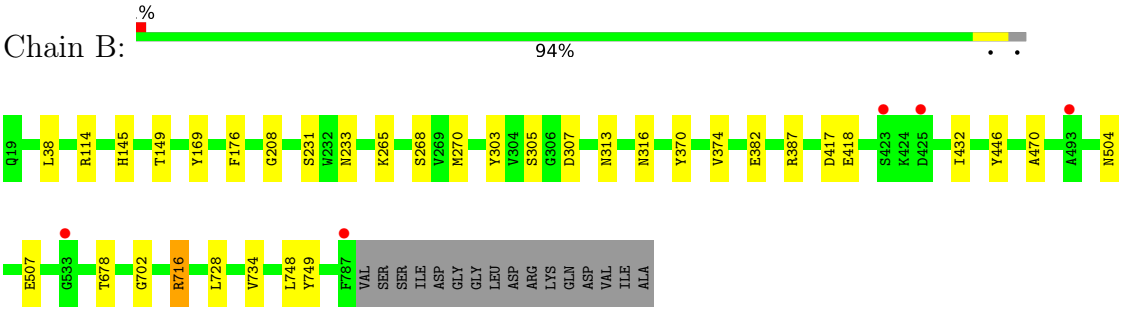
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	873	Total O 873 873	0	0
10	A	948	Total O 948 948	0	0

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.

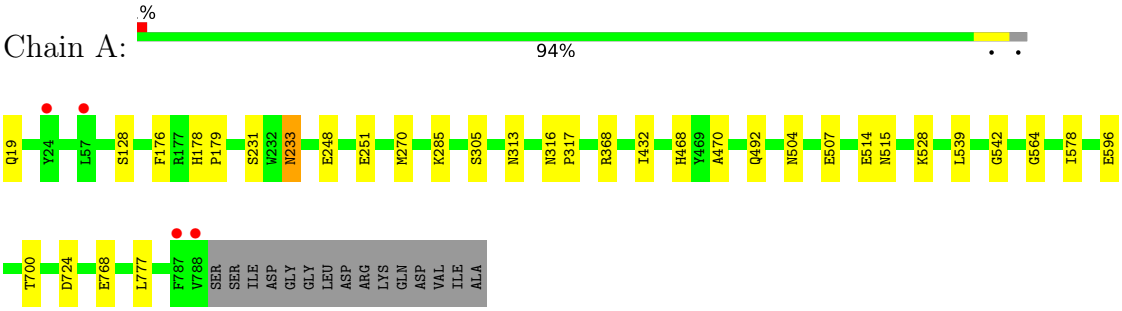
• Molecule 1: Exo-1,4-beta-xylosidase xlnD

Chain B:



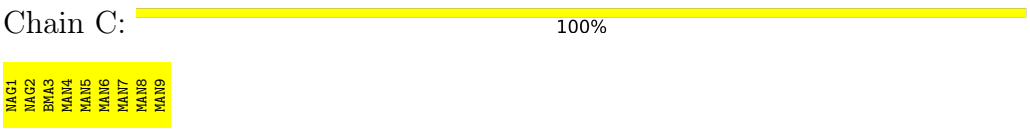
• Molecule 1: Exo-1,4-beta-xylosidase xlnD

Chain A:



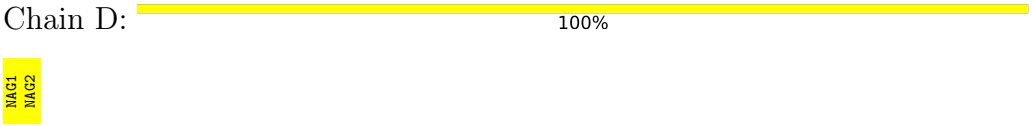
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



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

Chain F:

• Molecule 4: 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)-[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 E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.47Å 90.58Å 244.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.24 – 1.48 33.22 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.24-1.48) 100.0 (33.22-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.159 , 0.193 0.162 , 0.196	Depositor DCC
R_{free} test set	13022 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14338	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.20% 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: GOL, PCA, ACT, EDO, NAG, MAN, BMA, K

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	0.79	1/6127 (0.0%)	0.88	1/8373 (0.0%)
1	B	0.78	0/6086	0.90	5/8320 (0.1%)
All	All	0.79	1/12213 (0.0%)	0.89	6/16693 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	596	GLU	CD-OE2	5.79	1.32	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	114	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	387	ARG	CG-CD-NE	-6.27	98.63	111.80
1	B	716	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	169	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	B	169	TYR	CB-CG-CD1	5.25	124.15	121.00

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	5987	0	5631	21	0
1	B	5945	0	5589	19	0
2	C	105	0	88	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	116	0	97	0	0
5	A	112	0	104	0	0
5	B	126	0	117	0	0
6	A	28	0	41	8	0
6	B	16	0	24	10	0
7	B	4	0	3	1	0
8	A	6	0	8	0	0
8	B	12	0	16	3	0
9	A	1	0	0	0	0
9	B	3	0	0	0	0
10	A	948	0	0	13	0
10	B	873	0	0	7	0
All	All	14338	0	11768	54	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.

The worst 5 of 54 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)
6:A:921:EDO:H11	10:A:1522:HOH:O	1.79	0.83
1:B:208:GLY:HA2	6:B:925:EDO:H21	1.62	0.79
6:A:923:EDO:H22	10:A:1782:HOH:O	1.80	0.79
6:B:924:EDO:HO1	6:B:925:EDO:HO1	1.20	0.78
6:B:924:EDO:O1	6:B:925:EDO:O1	1.92	0.76

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	780/785 (99%)	753 (96%)	26 (3%)	1 (0%)	51 25
1	B	775/785 (99%)	750 (97%)	24 (3%)	1 (0%)	51 25
All	All	1555/1570 (99%)	1503 (97%)	50 (3%)	2 (0%)	51 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	SER
1	B	231	SER

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	641/647 (99%)	639 (100%)	2 (0%)	92 84
1	B	636/647 (98%)	634 (100%)	2 (0%)	92 84
All	All	1277/1294 (99%)	1273 (100%)	4 (0%)	92 84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	176	PHE
1	B	233	ASN
1	A	176	PHE
1	A	233	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	A	19	1	7,8,9	0.61	0	9,10,12	1.01	1 (11%)
1	PCA	B	19	1	7,8,9	0.52	0	9,10,12	0.77	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	PCA	A	19	1	-	0/0/11/13	0/1/1/1
1	PCA	B	19	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	PCA	O-C-CA	-2.10	119.29	124.78

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 (i)

23 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	0.91	1 (7%)	17,19,21	1.68	3 (17%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
2	BMA	C	3	2	11,11,12	1.56	1 (9%)	15,15,17	1.31	2 (13%)
2	MAN	C	4	2	11,11,12	0.67	0	15,15,17	1.24	2 (13%)
2	MAN	C	5	2	11,11,12	0.88	0	15,15,17	1.52	3 (20%)
2	MAN	C	6	2	11,11,12	0.65	0	15,15,17	1.39	2 (13%)
2	MAN	C	7	2	11,11,12	0.71	0	15,15,17	1.36	1 (6%)
2	MAN	C	8	2	11,11,12	1.09	1 (9%)	15,15,17	0.96	0
2	MAN	C	9	2	11,11,12	0.90	1 (9%)	15,15,17	1.85	4 (26%)
3	NAG	D	1	3,1	14,14,15	0.69	0	17,19,21	1.25	1 (5%)
3	NAG	D	2	3	14,14,15	0.76	0	17,19,21	1.26	3 (17%)
4	NAG	E	1	4,1	14,14,15	1.47	2 (14%)	17,19,21	2.28	4 (23%)
4	MAN	E	10	4	11,11,12	1.01	0	15,15,17	1.48	4 (26%)
4	NAG	E	2	4	14,14,15	0.92	1 (7%)	17,19,21	1.58	4 (23%)
4	BMA	E	3	4	11,11,12	0.65	0	15,15,17	1.71	2 (13%)
4	MAN	E	4	4	11,11,12	0.80	0	15,15,17	1.53	4 (26%)
4	MAN	E	5	4	11,11,12	0.88	1 (9%)	15,15,17	3.07	6 (40%)
4	MAN	E	6	4	11,11,12	1.32	2 (18%)	15,15,17	2.75	5 (33%)
4	MAN	E	7	4	11,11,12	0.48	0	15,15,17	1.00	1 (6%)
4	MAN	E	8	4	11,11,12	0.48	0	15,15,17	1.06	1 (6%)
4	MAN	E	9	4	11,11,12	0.63	0	15,15,17	1.67	4 (26%)
3	NAG	F	1	3,1	14,14,15	0.76	0	17,19,21	1.39	3 (17%)
3	NAG	F	2	3	14,14,15	0.91	0	17,19,21	1.78	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	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	-	0/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	MAN	E	10	4	-	2/2/19/22	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	1/2/19/22	0/1/1/1
4	MAN	E	7	4	-	0/2/19/22	0/1/1/1
4	MAN	E	8	4	-	0/2/19/22	0/1/1/1
4	MAN	E	9	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	BMA	O5-C1	-4.11	1.37	1.43
4	E	1	NAG	C1-C2	3.71	1.57	1.52
4	E	6	MAN	O5-C1	-2.94	1.39	1.43
4	E	1	NAG	C8-C7	2.73	1.56	1.50
4	E	2	NAG	C1-C2	2.30	1.55	1.52

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	5	MAN	O2-C2-C3	-8.48	93.16	110.14
4	E	1	NAG	O5-C1-C2	-7.50	99.45	111.29
4	E	6	MAN	C1-O5-C5	6.33	120.77	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	6	MAN	O5-C5-C6	-6.08	97.68	107.20
2	C	1	NAG	O5-C1-C2	-4.95	103.48	111.29

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

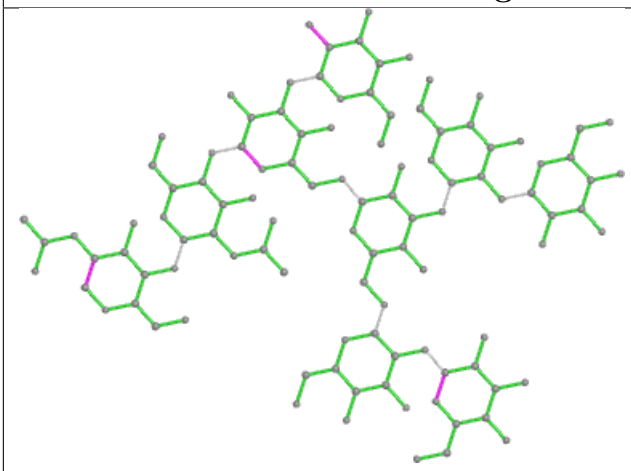
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
4	E	9	MAN	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6

There are no ring outliers.

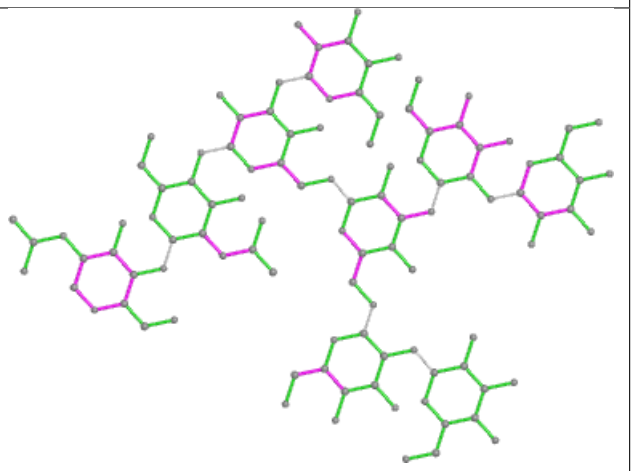
No monomer is involved in short contacts.

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

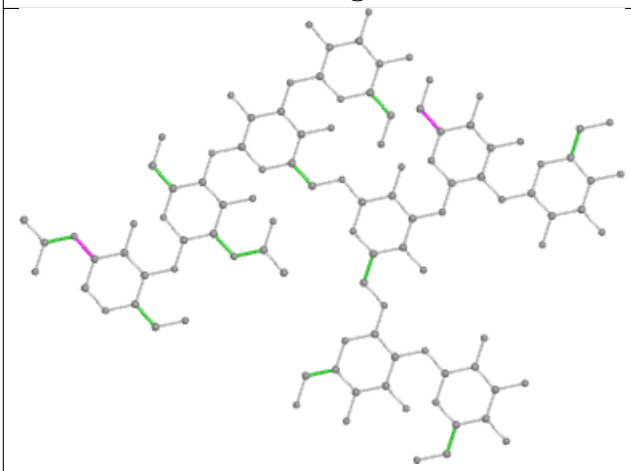
Oligosaccharide Chain C



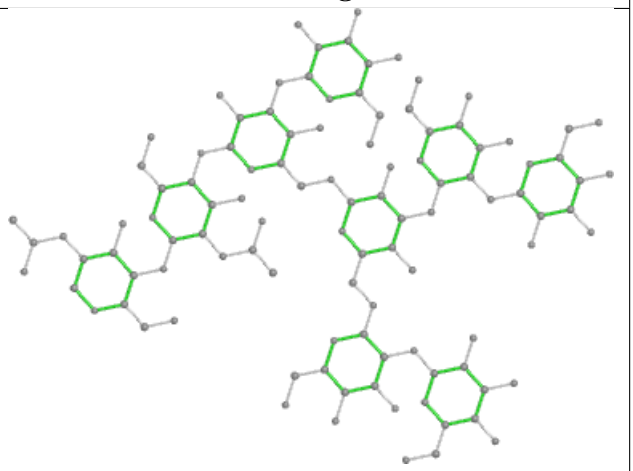
Bond lengths



Bond angles

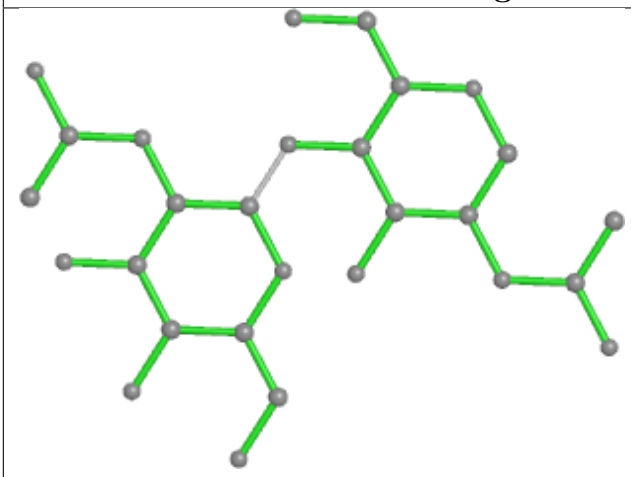


Torsions

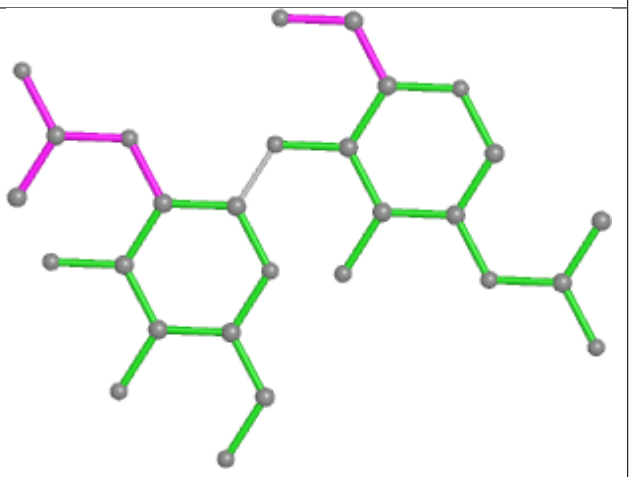


Rings

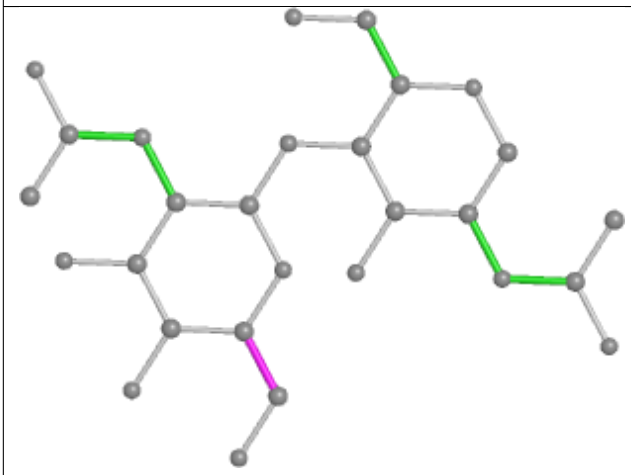
Oligosaccharide Chain D



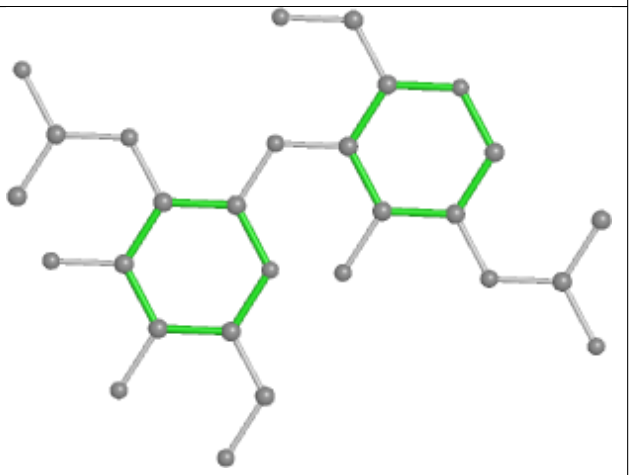
Bond lengths



Bond angles

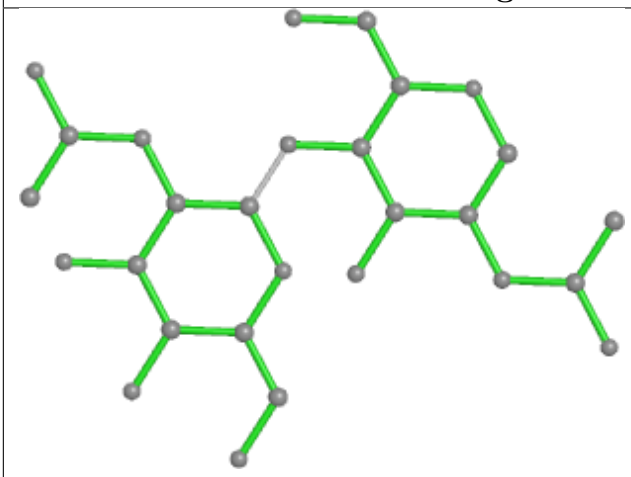


Torsions

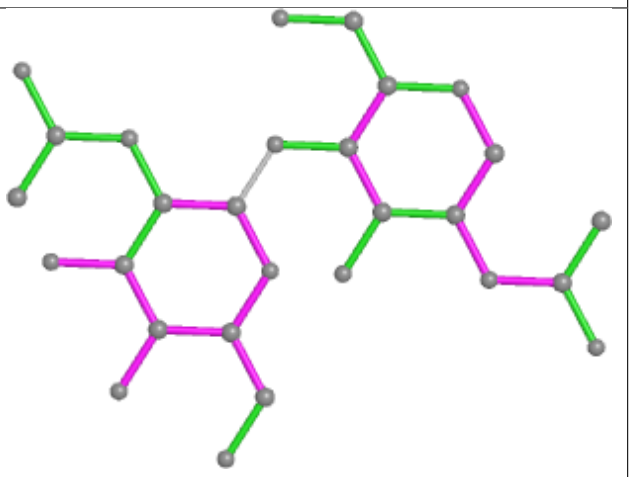


Rings

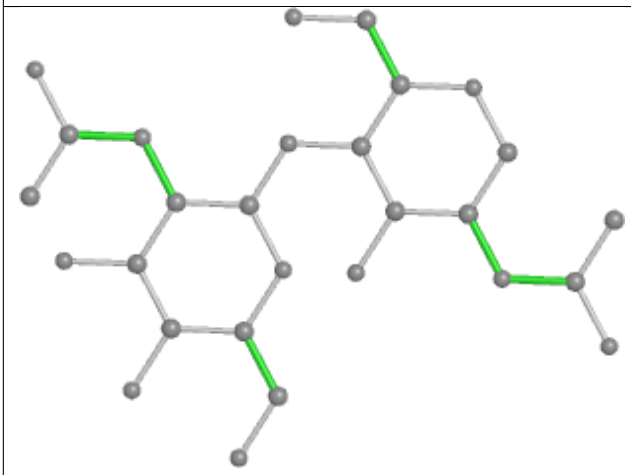
Oligosaccharide Chain F



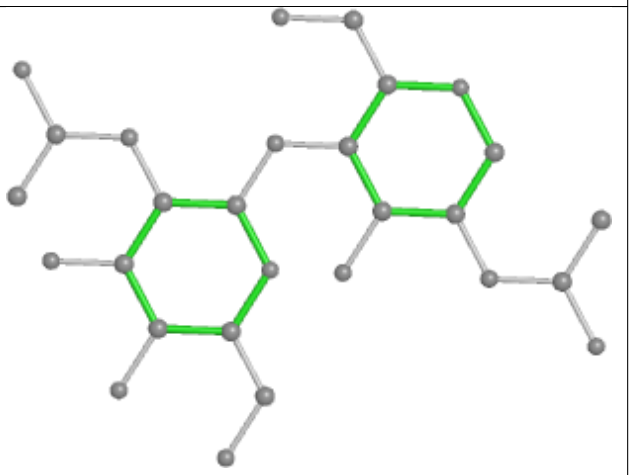
Bond lengths



Bond angles

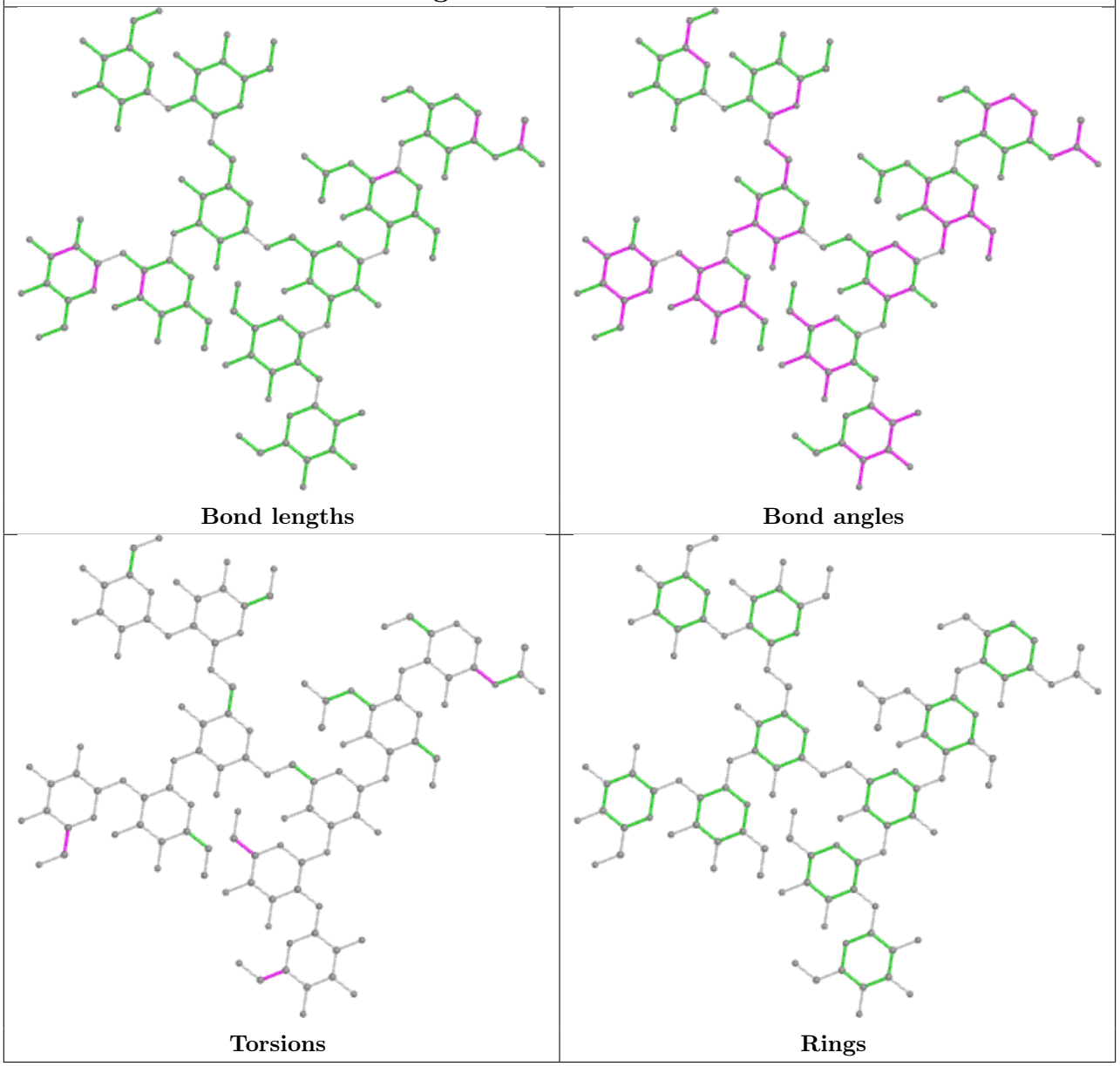


Torsions



Rings

Oligosaccharide Chain E



5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	A	923	-	3,3,3	0.52	0	2,2,2	0.13	0
6	EDO	A	926	6	3,3,3	0.26	0	2,2,2	0.47	0
5	NAG	A	901	1	14,14,15	0.88	0	17,19,21	1.52	4 (23%)
6	EDO	B	925	-	3,3,3	0.47	0	2,2,2	1.21	0
5	NAG	A	917	1	14,14,15	0.72	0	17,19,21	1.54	4 (23%)
7	ACT	B	922	-	3,3,3	0.77	0	3,3,3	1.33	0
5	NAG	B	901	1	14,14,15	1.19	2 (14%)	17,19,21	2.18	3 (17%)
8	GOL	B	926	-	5,5,5	0.18	0	5,5,5	1.10	0
5	NAG	A	920	1	14,14,15	0.97	1 (7%)	17,19,21	1.84	6 (35%)
8	GOL	B	927	-	5,5,5	0.11	0	5,5,5	0.36	0
5	NAG	B	917	1	14,14,15	0.61	0	17,19,21	2.29	8 (47%)
5	NAG	A	919	1	14,14,15	0.51	0	17,19,21	0.81	0
6	EDO	B	921	-	3,3,3	0.32	0	2,2,2	0.36	0
8	GOL	A	928	-	5,5,5	0.08	0	5,5,5	0.49	0
6	EDO	B	924	-	3,3,3	0.33	0	2,2,2	0.19	0
6	EDO	A	925	-	3,3,3	0.32	0	2,2,2	0.38	0
5	NAG	B	918	1	14,14,15	0.52	0	17,19,21	1.24	3 (17%)
5	NAG	B	913	1	14,14,15	0.68	0	17,19,21	0.86	0
5	NAG	B	914	1	14,14,15	0.94	1 (7%)	17,19,21	1.66	4 (23%)
5	NAG	B	920	1	14,14,15	1.34	2 (14%)	17,19,21	1.85	2 (11%)
6	EDO	A	924	-	3,3,3	0.57	0	2,2,2	0.62	0
5	NAG	B	912	1	14,14,15	0.75	0	17,19,21	0.95	0
5	NAG	B	919	1	14,14,15	0.77	1 (7%)	17,19,21	1.10	2 (11%)
5	NAG	A	914	1	14,14,15	1.14	1 (7%)	17,19,21	2.14	4 (23%)
5	NAG	A	918	1	14,14,15	1.01	0	17,19,21	1.61	3 (17%)
6	EDO	A	921	-	3,3,3	0.15	0	2,2,2	0.21	0
5	NAG	B	911	1	14,14,15	0.60	0	17,19,21	0.97	0
5	NAG	A	915	1	14,14,15	0.51	0	17,19,21	1.22	1 (5%)
5	NAG	A	916	1	14,14,15	0.87	1 (7%)	17,19,21	1.08	1 (5%)
6	EDO	B	923	-	3,3,3	0.66	0	2,2,2	0.63	0
6	EDO	A	922	-	3,3,3	0.11	0	2,2,2	0.70	0
6	EDO	A	927	6	3,3,3	0.27	0	2,2,2	0.58	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
6	EDO	A	923	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	926	6	-	1/1/1/1	-
5	NAG	A	901	1	-	0/6/23/26	0/1/1/1
6	EDO	B	925	-	-	0/1/1/1	-
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
5	NAG	B	901	1	-	1/6/23/26	0/1/1/1
8	GOL	B	926	-	-	3/4/4/4	-
5	NAG	A	920	1	-	0/6/23/26	0/1/1/1
8	GOL	B	927	-	-	0/4/4/4	-
5	NAG	B	917	1	-	2/6/23/26	0/1/1/1
5	NAG	A	919	1	-	0/6/23/26	0/1/1/1
6	EDO	B	921	-	-	1/1/1/1	-
8	GOL	A	928	-	-	0/4/4/4	-
6	EDO	B	924	-	-	0/1/1/1	-
6	EDO	A	925	-	-	1/1/1/1	-
5	NAG	B	918	1	-	0/6/23/26	0/1/1/1
5	NAG	B	913	1	-	0/6/23/26	0/1/1/1
5	NAG	B	914	1	-	0/6/23/26	0/1/1/1
5	NAG	B	920	1	-	0/6/23/26	0/1/1/1
6	EDO	A	924	-	-	0/1/1/1	-
5	NAG	B	912	1	-	0/6/23/26	0/1/1/1
5	NAG	B	919	1	-	0/6/23/26	0/1/1/1
5	NAG	A	914	1	-	0/6/23/26	0/1/1/1
5	NAG	A	918	1	-	0/6/23/26	0/1/1/1
6	EDO	A	921	-	-	0/1/1/1	-
5	NAG	B	911	1	-	0/6/23/26	0/1/1/1
5	NAG	A	915	1	-	0/6/23/26	0/1/1/1
5	NAG	A	916	1	-	0/6/23/26	0/1/1/1
6	EDO	B	923	-	-	1/1/1/1	-
6	EDO	A	922	-	-	1/1/1/1	-
6	EDO	A	927	6	-	0/1/1/1	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	920	NAG	C1-C2	3.55	1.57	1.52
5	B	901	NAG	C8-C7	2.86	1.56	1.50
5	B	920	NAG	O5-C1	2.51	1.47	1.43
5	A	914	NAG	O7-C7	2.49	1.28	1.23
5	B	914	NAG	O5-C5	2.41	1.48	1.43

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	901	NAG	C2-N2-C7	6.88	132.71	122.90
5	A	914	NAG	C8-C7-N2	-6.30	105.44	116.10
5	B	917	NAG	C1-O5-C5	4.88	118.81	112.19
5	B	920	NAG	C1-O5-C5	4.85	118.77	112.19
5	A	920	NAG	C1-O5-C5	4.55	118.36	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	926	GOL	C1-C2-C3-O3
5	B	917	NAG	C4-C5-C6-O6
8	B	926	GOL	O1-C1-C2-O2
8	B	926	GOL	O2-C2-C3-O3
5	B	917	NAG	O5-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	923	EDO	3	0
6	B	925	EDO	5	0
7	B	922	ACT	1	0
8	B	926	GOL	2	0
8	B	927	GOL	1	0
6	B	921	EDO	2	0
6	B	924	EDO	3	0
6	A	924	EDO	3	0
6	A	921	EDO	2	0
6	B	923	EDO	2	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	769/785 (97%)	-0.38	4 (0%)	91	93	14, 19, 31, 45	19 (2%)
1	B	768/785 (97%)	-0.28	5 (0%)	87	90	14, 21, 36, 48	14 (1%)
All	All	1537/1570 (97%)	-0.33	9 (0%)	89	91	14, 20, 33, 48	33 (2%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	788	VAL	4.8
1	A	787	PHE	3.2
1	A	57	LEU	3.1
1	B	425	ASP	2.7
1	A	24	TYR	2.2

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

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
1	PCA	A	19	8/9	0.95	0.07	17,19,20,20	0
1	PCA	B	19	8/9	0.98	0.04	17,18,20,20	0

6.3 Carbohydrates

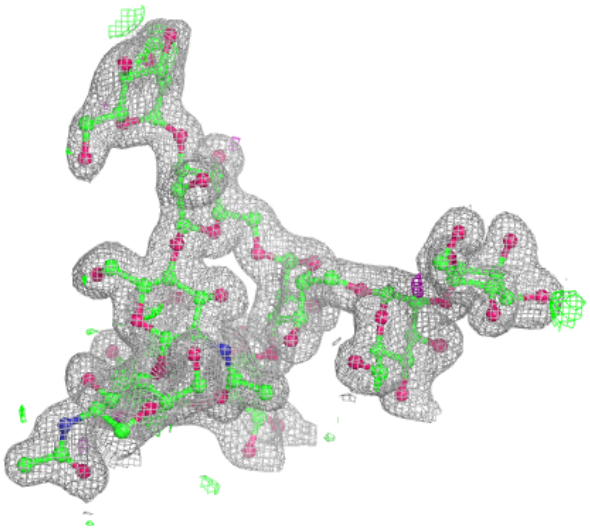
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

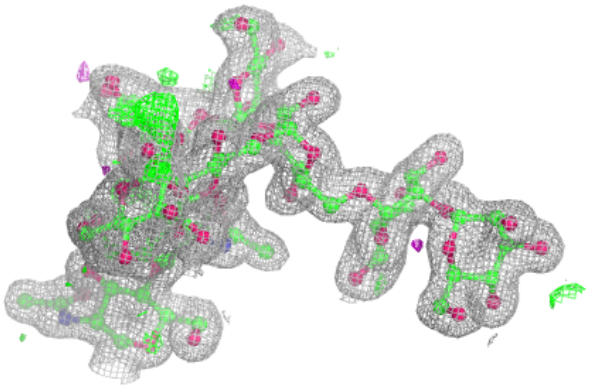
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	E	10	11/12	0.62	0.19	58,63,68,70	0
3	NAG	F	2	14/15	0.78	0.24	47,63,73,74	0
3	NAG	D	2	14/15	0.84	0.28	40,45,55,66	0
4	MAN	E	6	11/12	0.85	0.20	42,47,51,64	0
2	MAN	C	6	11/12	0.85	0.18	39,47,51,55	0
4	MAN	E	5	11/12	0.86	0.22	34,41,46,50	0
2	MAN	C	9	11/12	0.89	0.11	29,39,45,49	0
2	MAN	C	5	11/12	0.89	0.15	34,40,42,46	0
4	MAN	E	9	11/12	0.90	0.12	37,45,56,57	0
3	NAG	F	1	14/15	0.91	0.10	25,29,41,45	0
3	NAG	D	1	14/15	0.91	0.12	25,27,37,41	0
2	MAN	C	7	11/12	0.93	0.08	27,31,40,42	0
4	MAN	E	8	11/12	0.94	0.07	19,23,28,31	0
2	MAN	C	8	11/12	0.94	0.11	21,25,30,33	0
4	BMA	E	3	11/12	0.94	0.09	22,25,30,30	0
4	NAG	E	1	14/15	0.95	0.07	17,22,29,29	0
2	MAN	C	4	11/12	0.95	0.10	26,28,29,31	0
4	MAN	E	7	11/12	0.95	0.10	26,29,33,35	0
4	NAG	E	2	14/15	0.96	0.07	22,23,29,31	0
2	BMA	C	3	11/12	0.96	0.09	23,26,30,31	0
4	MAN	E	4	11/12	0.96	0.09	24,26,28,32	0
2	NAG	C	2	14/15	0.97	0.06	22,23,26,32	0
2	NAG	C	1	14/15	0.97	0.04	18,21,26,29	0

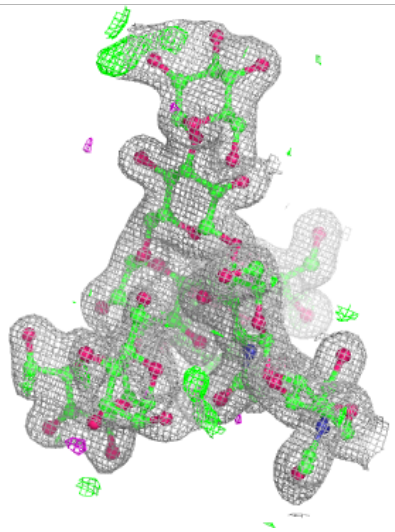
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

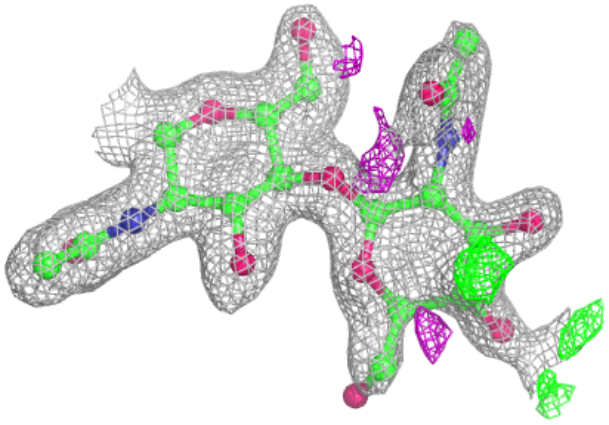


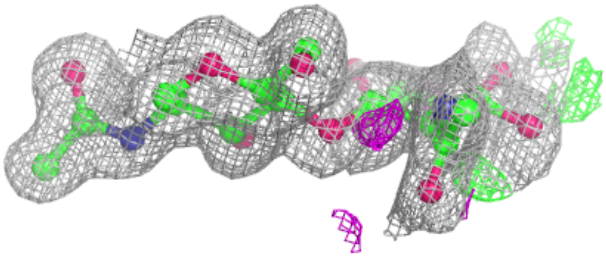


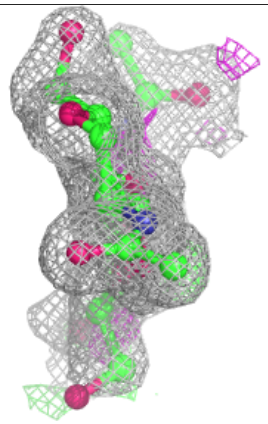


Electron density around Chain D:

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

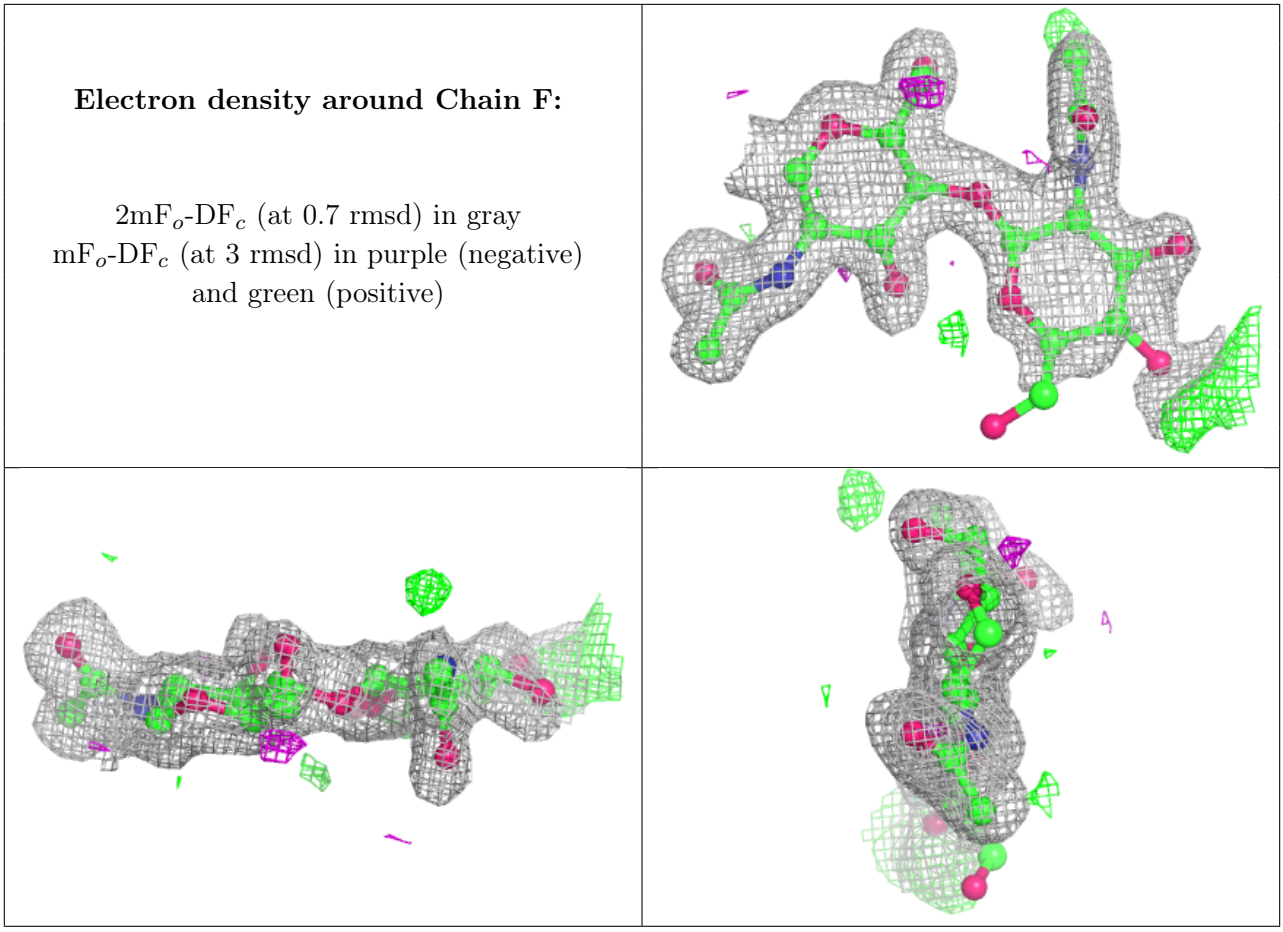






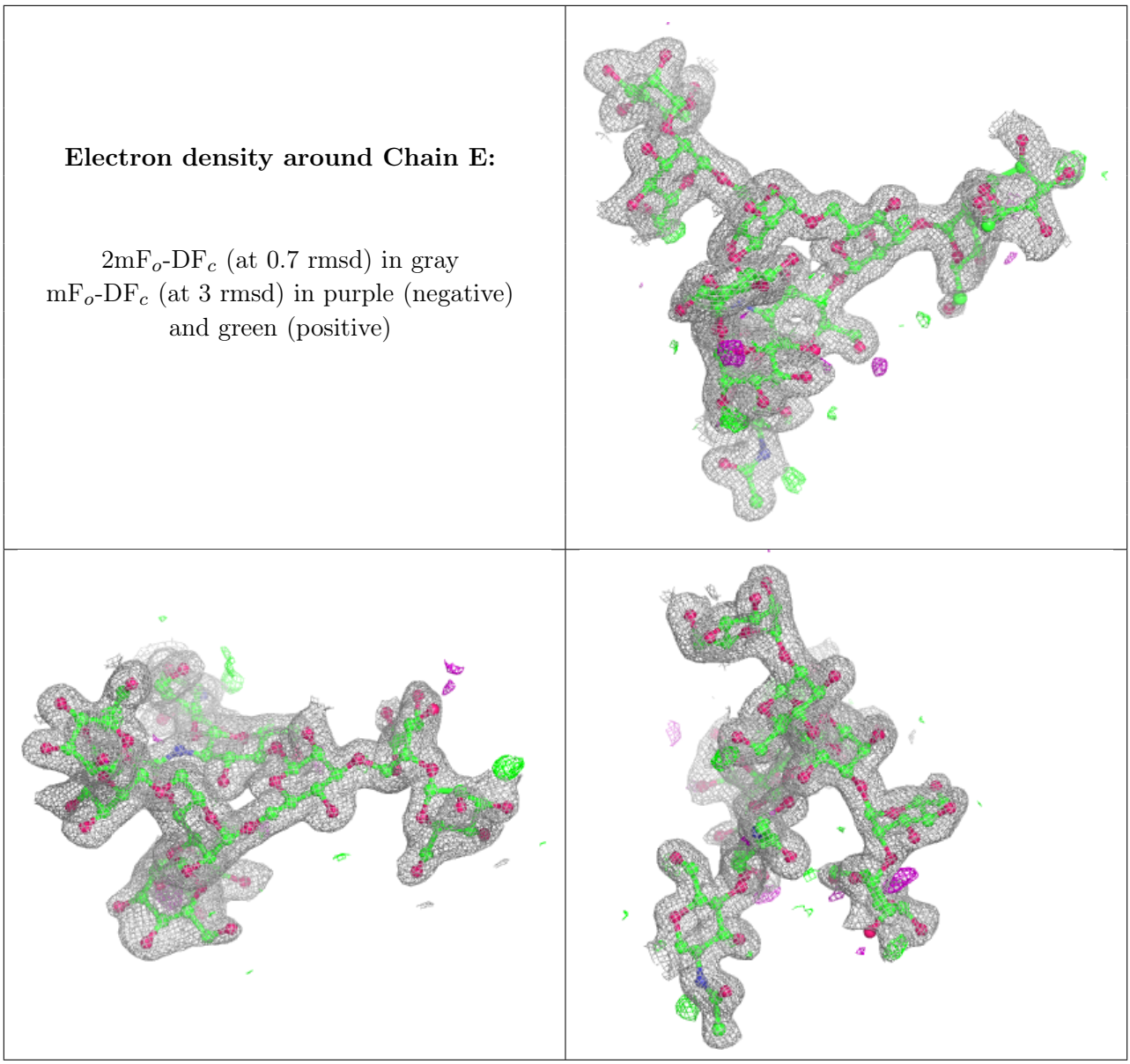
Electron density around Chain F:

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



Electron density around Chain E:

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



6.4 Ligands

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
6	EDO	B	921	4/4	0.75	0.14	45,57,58,59	0
5	NAG	B	920	14/15	0.76	0.24	26,41,44,49	0
6	EDO	A	925	4/4	0.82	0.15	34,47,49,56	0
6	EDO	B	923	4/4	0.84	0.13	33,37,39,41	0
8	GOL	B	927	6/6	0.84	0.13	32,42,50,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	926	4/4	0.85	0.14	37,39,39,42	4
5	NAG	B	917	14/15	0.86	0.13	32,39,48,53	0
6	EDO	A	927	4/4	0.86	0.12	21,23,26,26	4
5	NAG	B	919	14/15	0.86	0.14	36,39,48,50	0
6	EDO	A	924	4/4	0.87	0.15	36,37,41,45	0
6	EDO	B	925	4/4	0.88	0.21	30,31,34,38	0
5	NAG	B	914	14/15	0.88	0.11	22,28,30,40	0
5	NAG	B	918	14/15	0.89	0.14	34,41,52,53	0
6	EDO	A	922	4/4	0.90	0.16	32,36,37,52	0
5	NAG	A	919	14/15	0.90	0.13	40,48,52,52	0
5	NAG	A	916	14/15	0.90	0.11	30,34,42,43	0
6	EDO	B	924	4/4	0.91	0.24	30,38,39,41	0
5	NAG	A	918	14/15	0.91	0.09	21,28,31,37	0
5	NAG	B	901	14/15	0.92	0.10	21,24,38,40	0
5	NAG	A	920	14/15	0.92	0.10	27,31,38,39	0
8	GOL	B	926	6/6	0.92	0.10	20,22,23,29	0
5	NAG	A	915	14/15	0.92	0.13	29,36,45,47	0
5	NAG	B	913	14/15	0.93	0.12	29,39,48,52	0
6	EDO	A	923	4/4	0.93	0.10	26,28,31,32	0
7	ACT	B	922	4/4	0.94	0.11	16,20,22,29	0
5	NAG	A	914	14/15	0.94	0.07	20,26,34,37	0
5	NAG	B	911	14/15	0.94	0.10	25,30,34,36	0
8	GOL	A	928	6/6	0.94	0.07	19,22,24,24	0
5	NAG	B	912	14/15	0.96	0.09	20,22,27,27	0
5	NAG	A	901	14/15	0.96	0.06	20,22,25,28	0
9	K	B	929	1/1	0.96	0.06	39,39,39,39	0
6	EDO	A	921	4/4	0.97	0.05	27,30,30,31	0
5	NAG	A	917	14/15	0.97	0.07	22,26,28,30	0
9	K	B	930	1/1	0.97	0.13	37,37,37,37	0
9	K	B	928	1/1	0.99	0.03	32,32,32,32	0
9	K	A	929	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.