



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 19, 2024 – 01:46 AM EDT

PDB ID : 4AQD
Title : Crystal structure of fully glycosylated human butyrylcholinesterase
Authors : Brazzolotto, X.; Wandhammer, M.; Ronco, C.; Trovaslet, M.; Jean, L.; Lockridge, O.; Renard, P.Y.; Nachon, F.
Deposited on : 2012-04-16
Resolution : 2.50 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

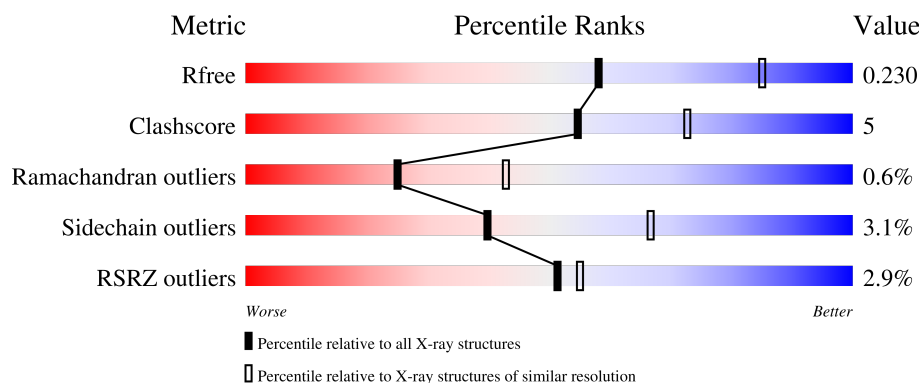
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	531	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	531	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
3	D	3	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	3	 67% 33%
3	H	3	 67% 33%
3	I	3	 100%
3	J	3	 67% 33%
3	K	3	 67% 33%
4	G	3	 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
11	GLY	B	1642	-	X	-	-
12	PEG	B	1530	-	-	-	X
3	NAG	F	2	-	-	-	X
3	NAG	H	1	X	-	-	-
3	NAG	J	1	X	-	-	-
4	MAN	G	3	X	-	-	-
5	BAL	B	550	-	-	X	-
6	NAG	A	651	X	-	-	-
6	NAG	B	621	X	-	-	-
6	NAG	B	671	X	-	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 9253 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 BUTYRYLCHOLINESTERASE.

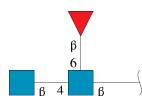
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	12	3	0
			4222	2723	714	770	15			
1	B	526	Total	C	N	O	S	35	0	0
			4191	2704	705	767	15			

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



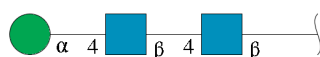
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

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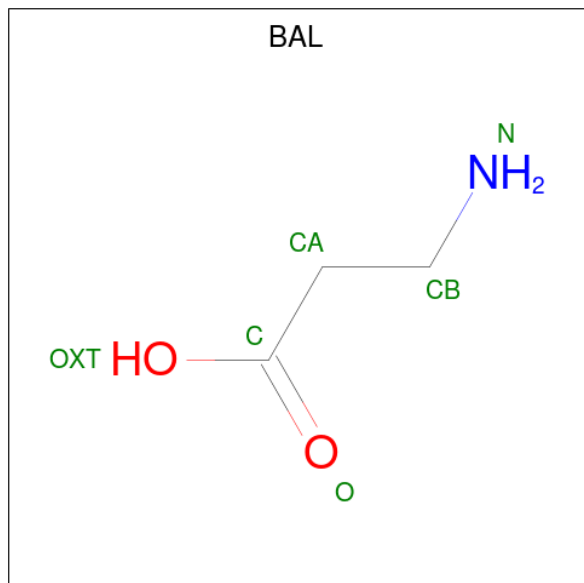
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	J	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



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

- Molecule 5 is BETA-ALANINE (three-letter code: BAL) (formula: C₃H₇NO₂).



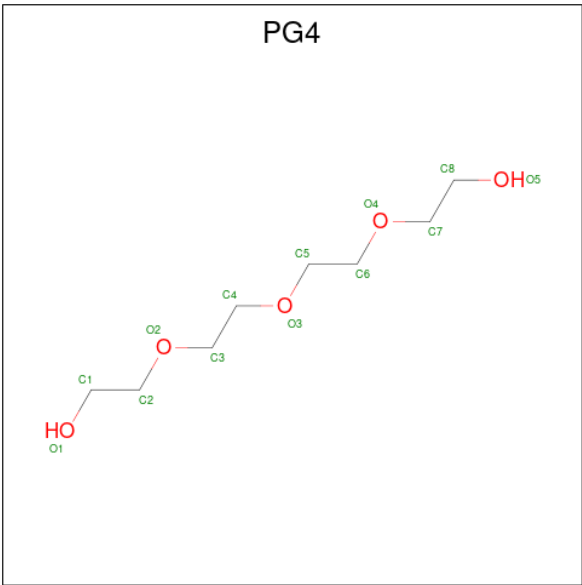
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			6	3	1	2		
5	B	1	Total	C	N	O	0	0
			6	3	1	2		

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



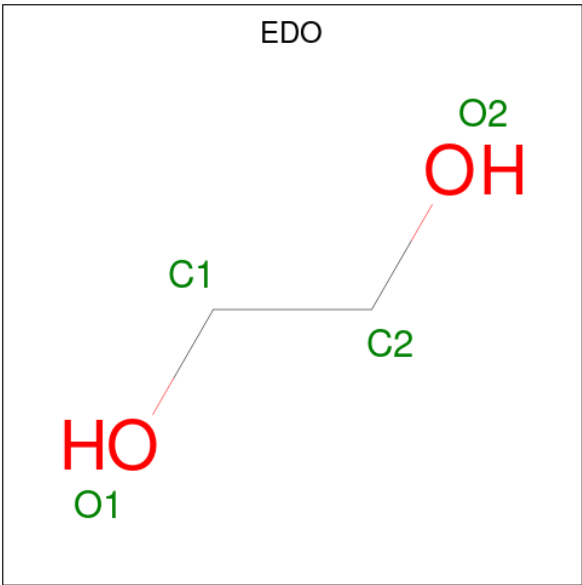
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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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 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	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

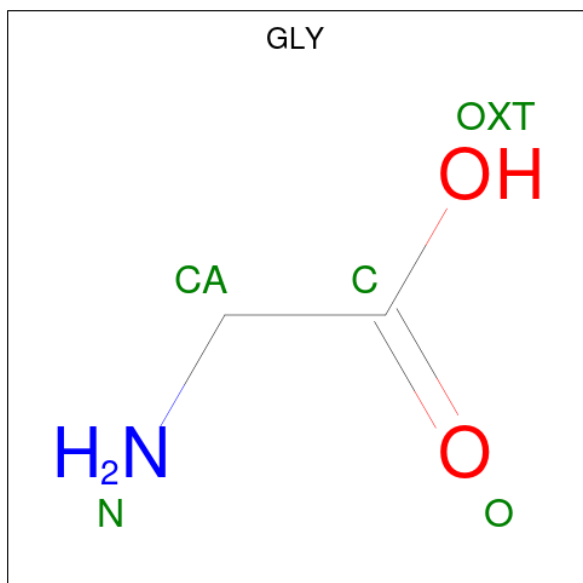
- Molecule 9 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	5	Total X 5 5	0	0
9	B	5	Total X 5 5	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

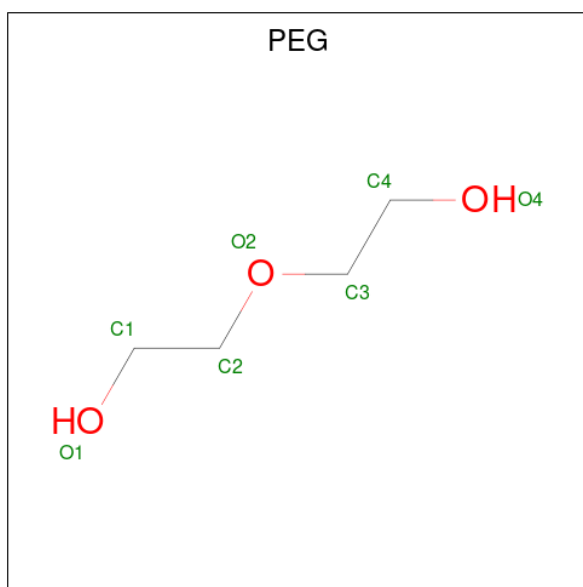
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	3	Total	Cl	0	0
			3	3		
10	B	4	Total	Cl	0	0
			4	4		

- Molecule 11 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			5	2	1	2		
11	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

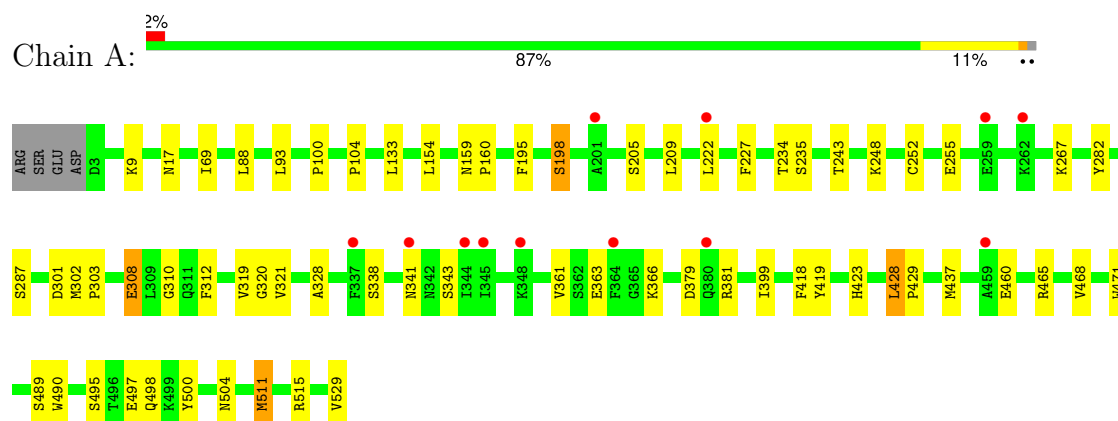
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	160	Total	O	0	0
			160	160		
13	B	118	Total	O	0	0
			118	118		

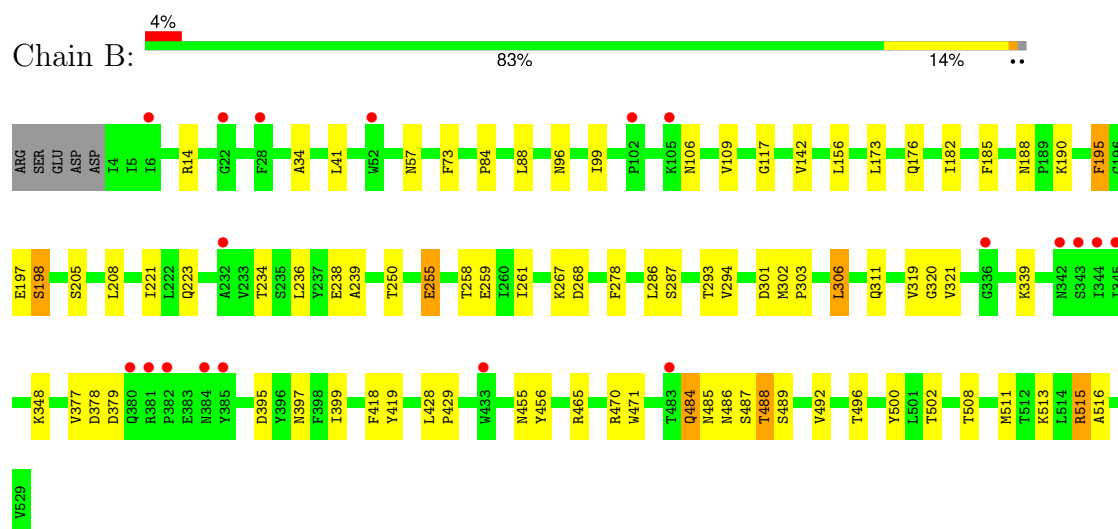
3 Residue-property plots [i](#)

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: BUTYRYLCHOLINESTERASE



• Molecule 1: BUTYRYLCHOLINESTERASE



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



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

Chain E:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 67%

MAG1
MAG2
FUL3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%

MAG1
MAG2
FUL3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

MAG1
MAG2
FUL3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2
FUL3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%

MAG1
MAG2
FUL3

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%

MAG1
MAG2
FOL3

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

Chain G:

100%

MAG1
MAG2
MAN3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.75Å 79.26Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.50 46.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.04-2.50) 99.4 (46.17-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.232 0.164 , 0.230	Depositor DCC
R_{free} test set	1383 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9253	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, EDO, CL, MAN, UNX, FUL, NAG, BAL

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	0.41	0/4351	0.57	0/5906
1	B	0.39	0/4310	0.54	0/5852
All	All	0.40	0/8661	0.56	0/11758

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 [i](#)

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	4222	0	4125	37	0
1	B	4191	0	4084	52	0
2	C	28	0	25	1	0
2	E	28	0	25	0	0
3	D	38	0	34	0	0
3	F	38	0	34	1	0
3	H	38	0	34	0	0
3	I	38	0	34	3	0
3	J	38	0	34	1	0
3	K	38	0	34	1	0
4	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	6	3	0
5	B	6	0	6	5	0
6	A	14	0	12	0	0
6	B	70	0	64	4	0
7	A	26	0	36	1	0
8	A	36	0	54	1	0
8	B	40	0	60	4	0
9	A	5	0	0	0	0
9	B	5	0	0	0	0
10	A	3	0	0	1	0
10	B	4	0	0	0	0
11	A	5	0	2	0	0
11	B	5	0	2	0	0
12	B	14	0	20	2	0
13	A	160	0	0	3	0
13	B	118	0	0	1	0
All	All	9253	0	8759	92	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 5.

The worst 5 of 92 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:198:SER:OG	5:A:550:BAL:C	2.07	1.01
1:B:198:SER:OG	5:B:550:BAL:C	2.08	1.00
1:B:99:ILE:HD11	1:B:185:PHE:HB3	1.66	0.76
1:A:338:SER:HB3	1:A:341:ASN:HB2	1.69	0.74
3:I:1:NAG:H61	3:I:2:NAG:HN2	1.54	0.73

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	528/531 (99%)	506 (96%)	20 (4%)	2 (0%)	34	54
1	B	524/531 (99%)	494 (94%)	26 (5%)	4 (1%)	19	35
All	All	1052/1062 (99%)	1000 (95%)	46 (4%)	6 (1%)	25	43

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	484	GLN
1	B	485	ASN
1	B	488	THR
1	B	489	SER
1	A	255	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/456 (100%)	444 (98%)	11 (2%)	49	74
1	B	451/456 (99%)	434 (96%)	17 (4%)	33	58
All	All	906/912 (99%)	878 (97%)	28 (3%)	40	67

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	255	GLU
1	B	515	ARG
1	B	286	LEU
1	B	471	TRP
1	B	268	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

25 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	0.68	0	17,19,21	1.13	2 (11%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	1.14	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.54	0	17,19,21	1.46	2 (11%)
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	1.37	1 (5%)
3	FUL	D	3	3	10,10,11	0.70	0	14,14,16	0.84	0
2	NAG	E	1	2,1	14,14,15	0.61	0	17,19,21	1.30	3 (17%)
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.15	2 (11%)
3	NAG	F	1	3,1	14,14,15	0.51	0	17,19,21	1.18	1 (5%)
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	1.22	2 (11%)
3	FUL	F	3	3	10,10,11	0.61	0	14,14,16	1.18	1 (7%)
4	NAG	G	1	4,1	14,14,15	0.43	0	17,19,21	1.20	1 (5%)
4	NAG	G	2	4	14,14,15	0.65	0	17,19,21	1.21	1 (5%)
4	MAN	G	3	4	11,11,12	0.60	0	15,15,17	1.04	1 (6%)
3	NAG	H	1	3,1	14,14,15	0.72	0	17,19,21	1.26	1 (5%)
3	NAG	H	2	3	14,14,15	0.56	0	17,19,21	0.74	0
3	FUL	H	3	3	10,10,11	0.67	0	14,14,16	0.68	0
3	NAG	I	1	3,1	14,14,15	0.39	0	17,19,21	1.64	2 (11%)
3	NAG	I	2	3	14,14,15	0.44	0	17,19,21	1.21	1 (5%)
3	FUL	I	3	3	10,10,11	0.61	0	14,14,16	1.30	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	1	3,1	14,14,15	0.50	0	17,19,21	1.36	2 (11%)
3	NAG	J	2	3	14,14,15	0.47	0	17,19,21	0.93	0
3	FUL	J	3	3	10,10,11	0.65	0	14,14,16	0.67	0
3	NAG	K	1	3,1	14,14,15	0.54	0	17,19,21	1.46	3 (17%)
3	NAG	K	2	3	14,14,15	0.59	0	17,19,21	1.36	2 (11%)
3	FUL	K	3	3	10,10,11	0.66	0	14,14,16	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	5/6/23/26	0/1/1/1
3	FUL	D	3	3	-	-	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	FUL	F	3	3	-	-	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	MAN	G	3	4	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	FUL	H	3	3	-	-	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	FUL	I	3	3	-	-	0/1/1/1
3	NAG	J	1	3,1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	FUL	J	3	3	-	-	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	FUL	K	3	3	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-O5-C5	4.66	118.43	112.19
3	D	2	NAG	C1-O5-C5	4.32	117.98	112.19
3	K	1	NAG	C1-O5-C5	4.15	117.75	112.19
3	F	2	NAG	C1-O5-C5	3.93	117.46	112.19
3	F	1	NAG	C1-O5-C5	3.83	117.32	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1	NAG	C1
3	J	1	NAG	C1
4	G	3	MAN	C1

5 of 37 torsion outliers are listed below:

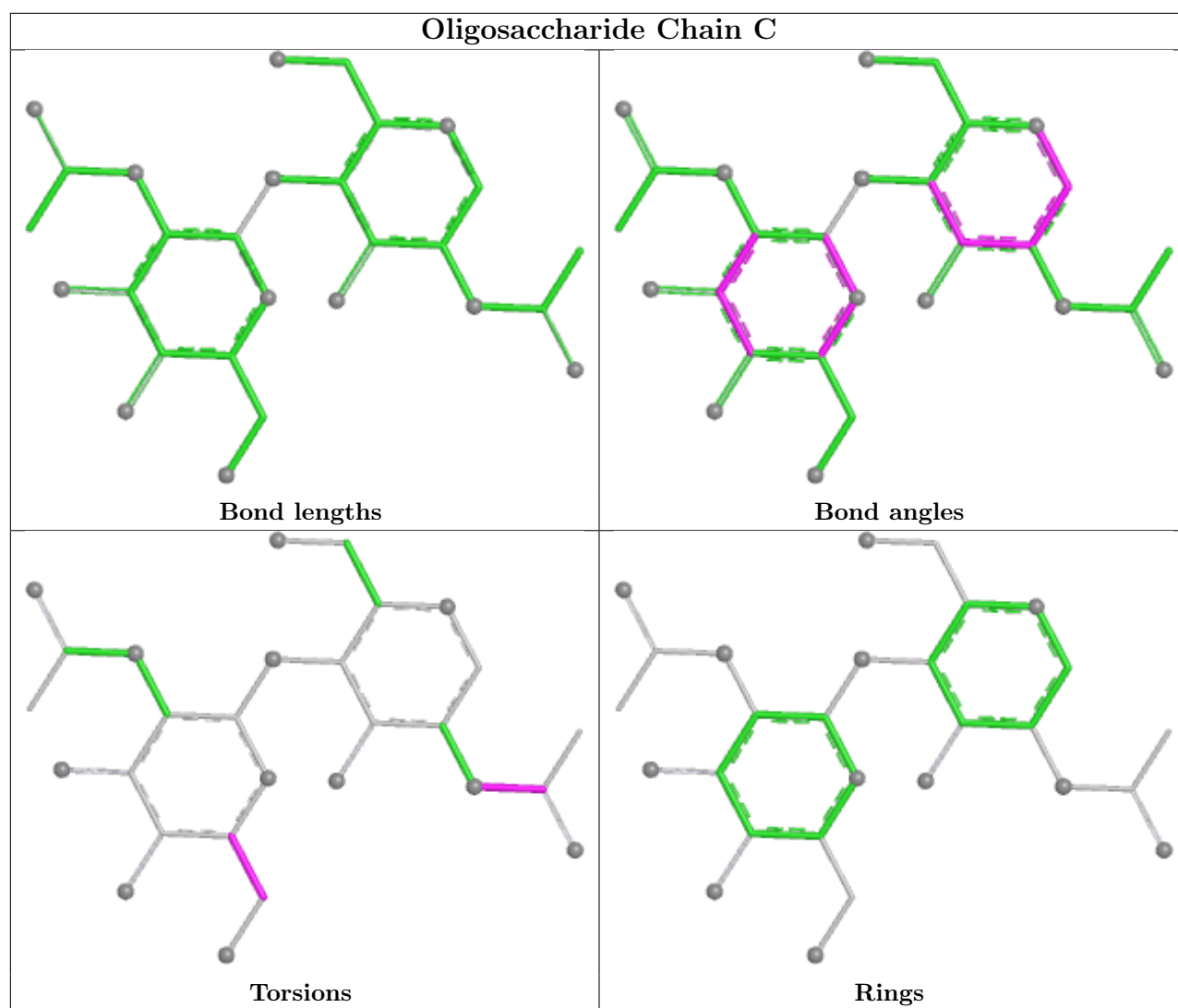
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C3-C2-N2-C7

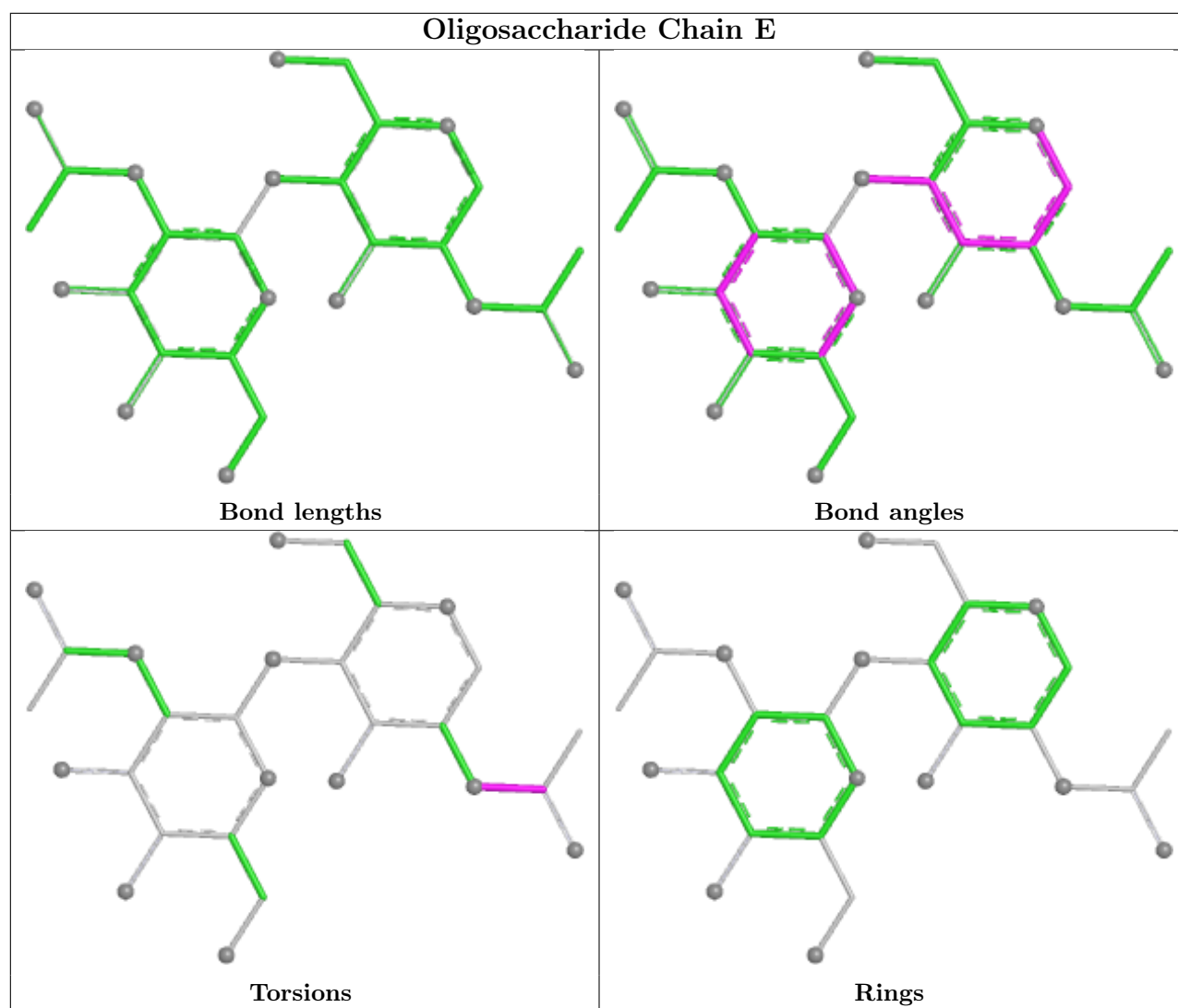
There are no ring outliers.

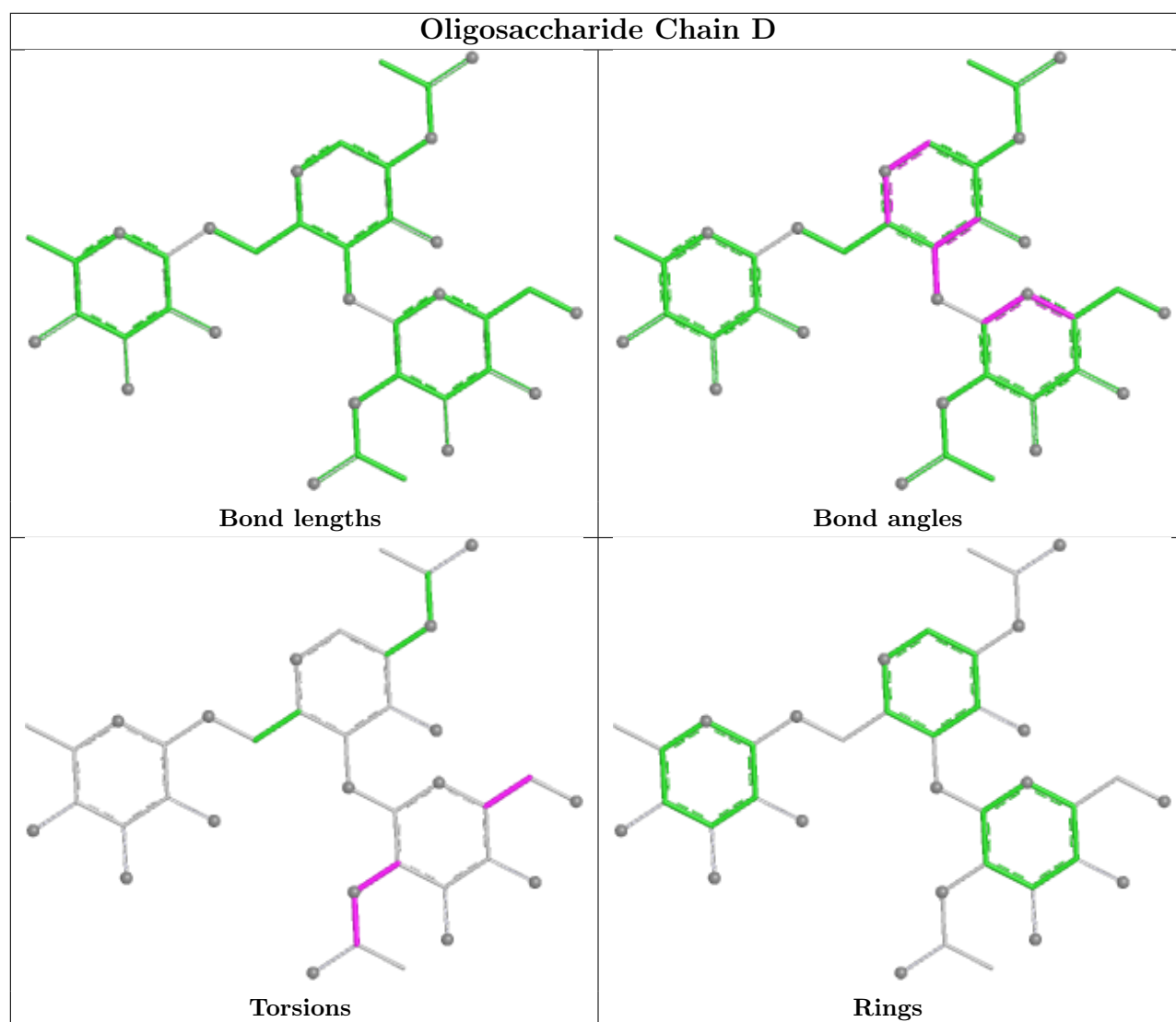
8 monomers are involved in 7 short contacts:

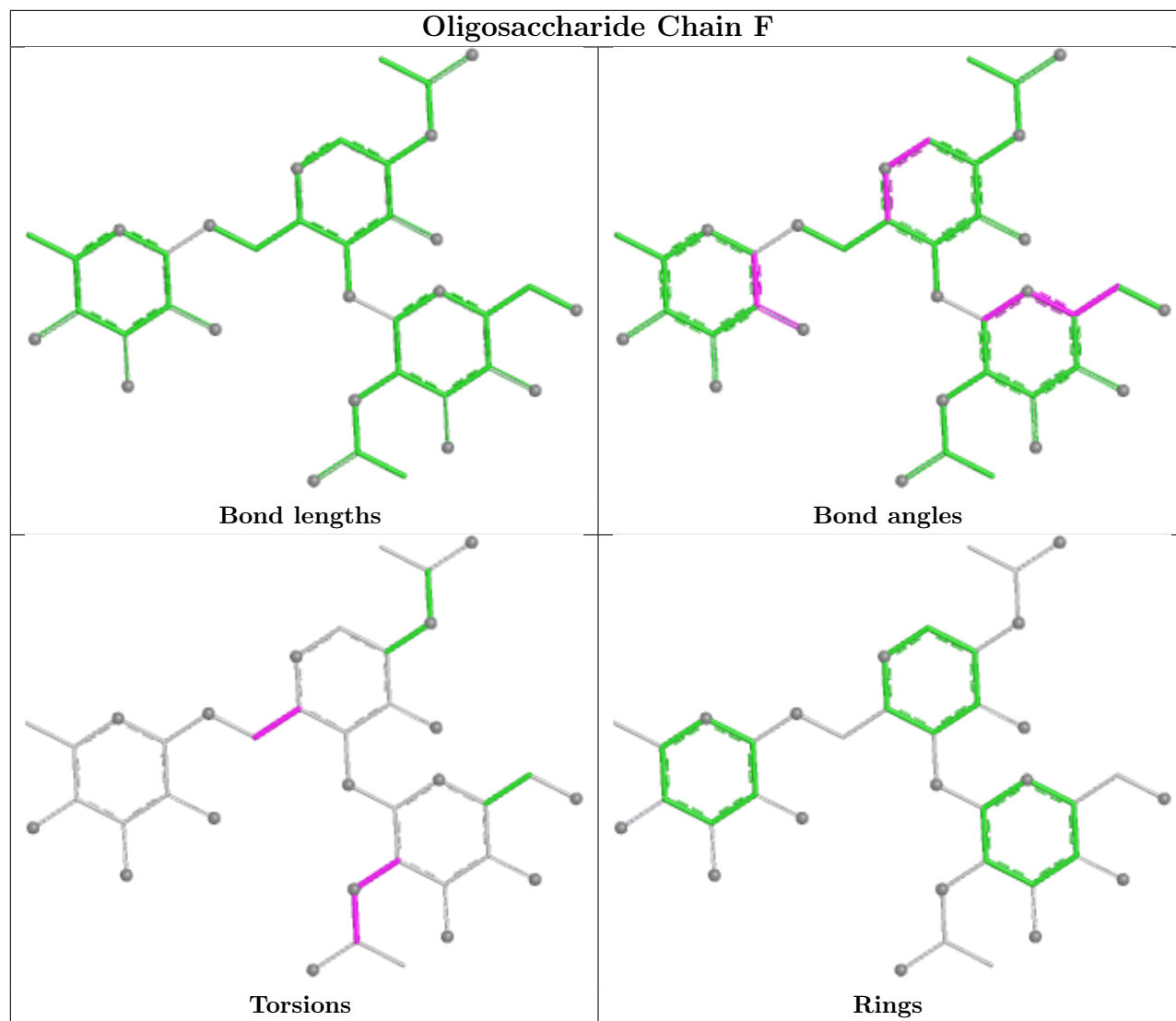
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1	NAG	2	0
3	F	3	FUL	1	0
2	C	1	NAG	1	0
3	I	3	FUL	1	0
3	I	2	NAG	2	0
3	K	3	FUL	1	0
3	J	1	NAG	1	0
3	K	1	NAG	1	0

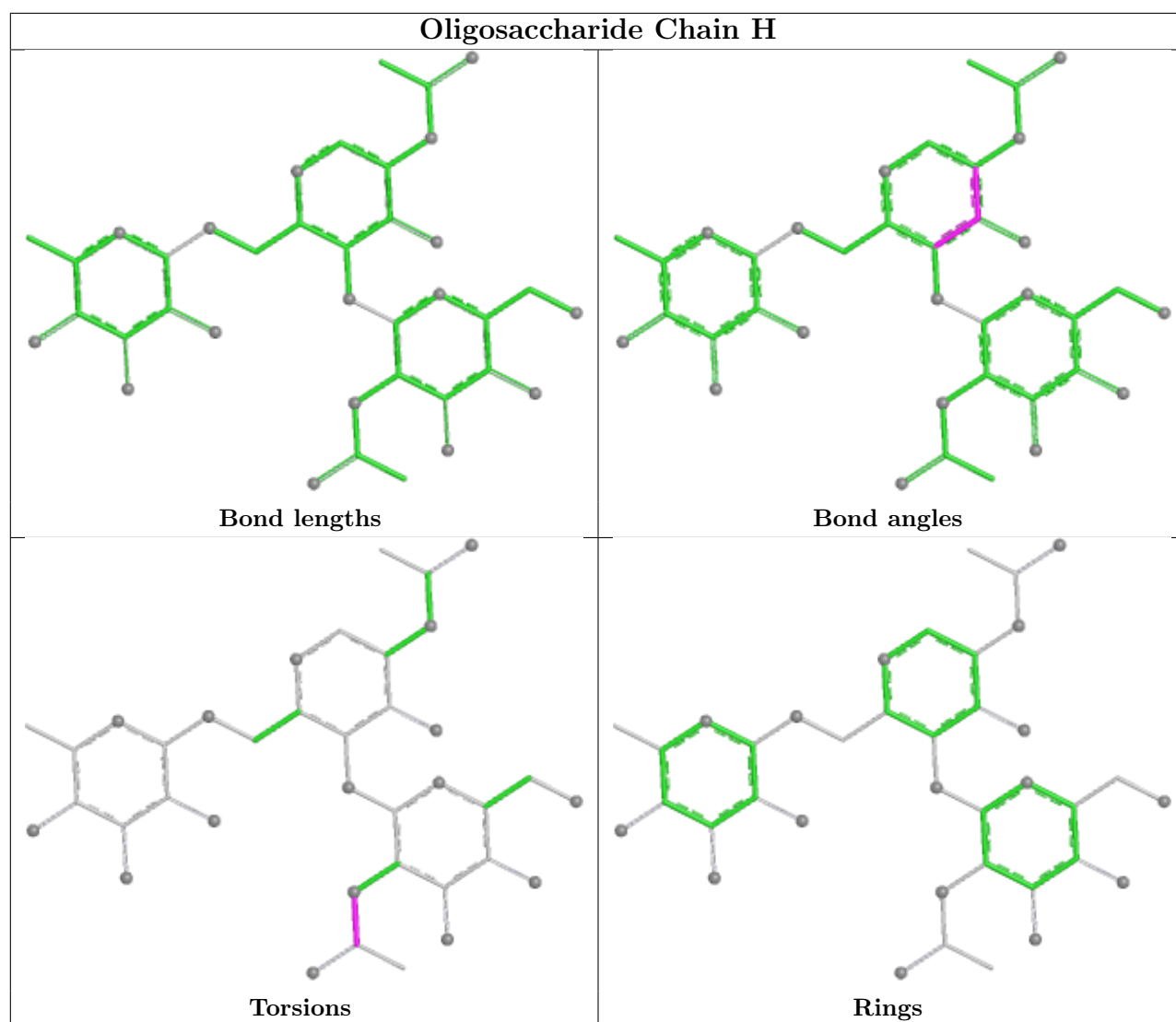
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

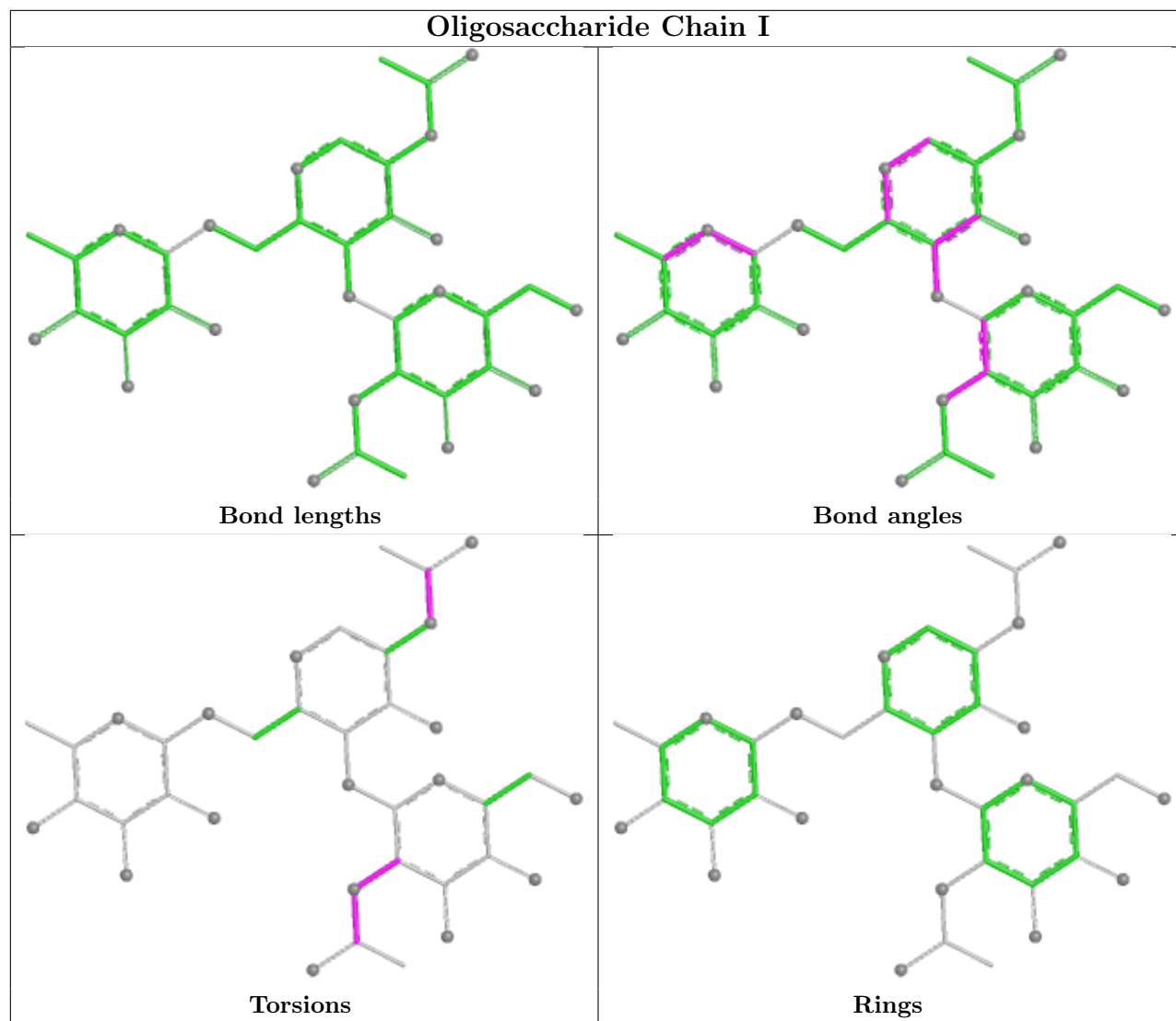


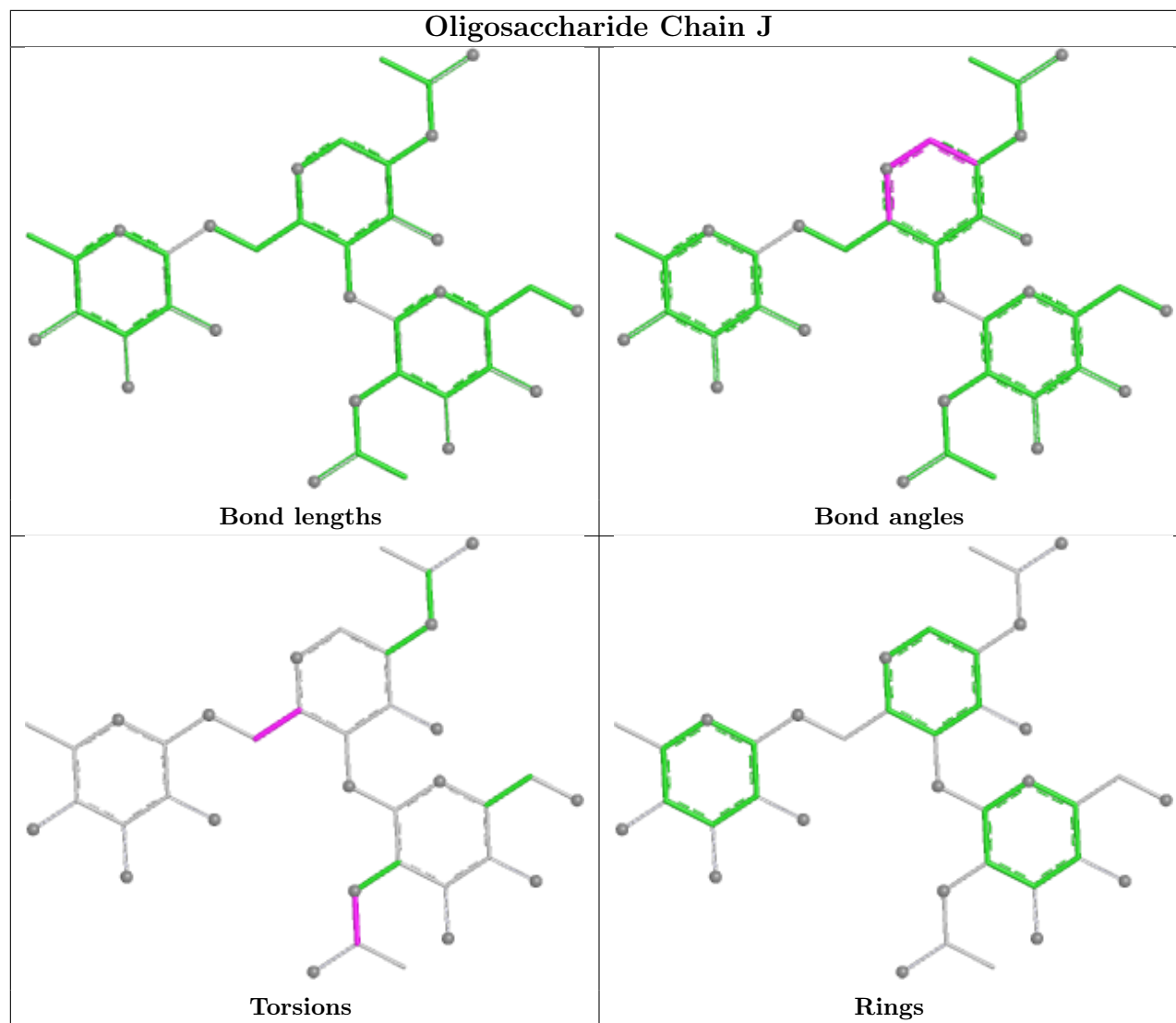


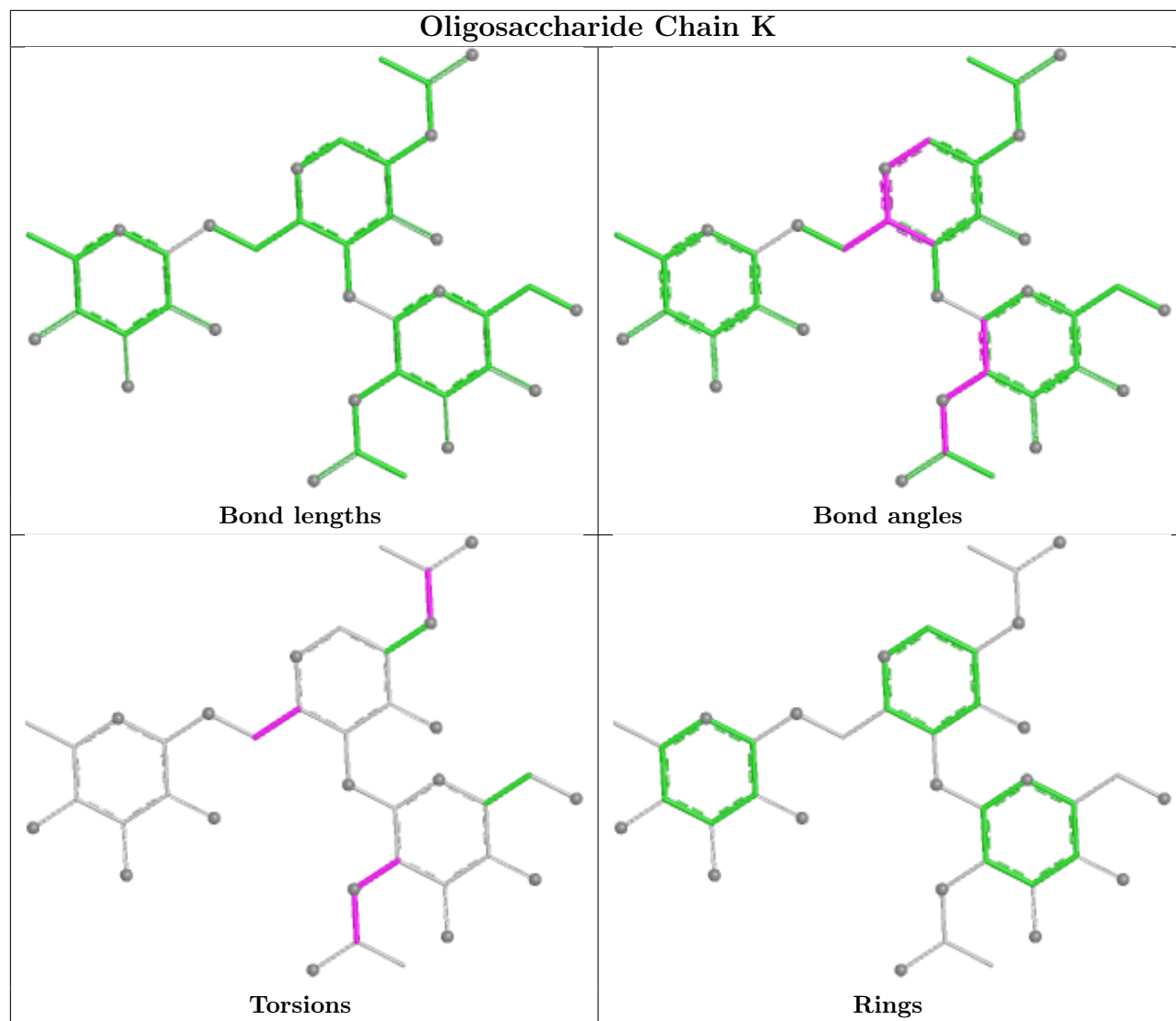


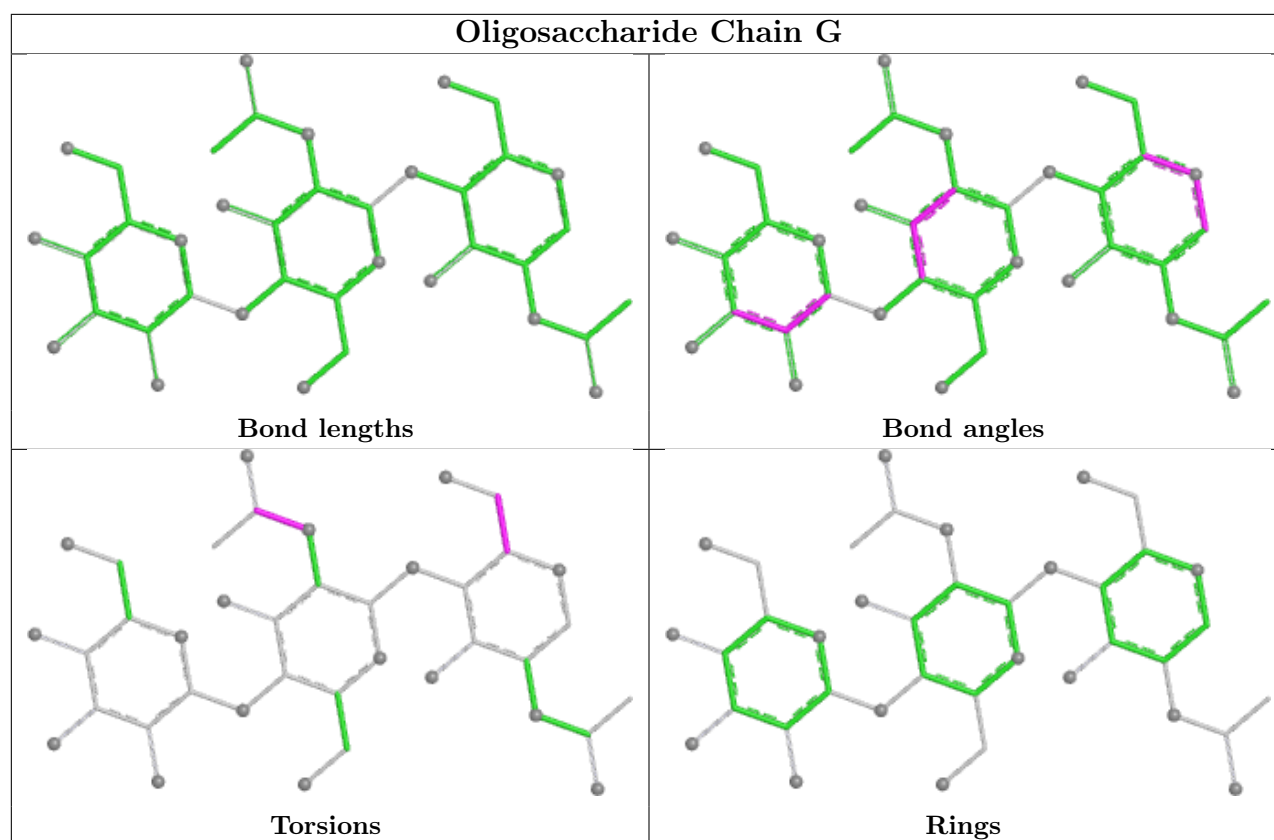












5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 10 are unknown and 7 are monoatomic - leaving 33 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	$\# Z > 2$
8	EDO	A	1535	-	3,3,3	0.47	0	2,2,2	0.24	0
8	EDO	B	1533	-	3,3,3	0.46	0	2,2,2	0.30	0
12	PEG	B	1531	-	6,6,6	0.71	0	5,5,5	1.31	0
6	NAG	B	651	1	14,14,15	0.55	0	17,19,21	1.23	1 (5%)
8	EDO	B	1540	-	3,3,3	0.46	0	2,2,2	0.36	0
8	EDO	B	1541	-	3,3,3	0.40	0	2,2,2	0.49	0
12	PEG	B	1530	-	6,6,6	0.61	0	5,5,5	1.49	1 (20%)
7	PG4	A	1530	-	12,12,12	0.66	0	11,11,11	1.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	B	1536	-	3,3,3	0.43	0	2,2,2	0.44	0
8	EDO	A	1539	-	3,3,3	0.47	0	2,2,2	0.21	0
8	EDO	A	1536	-	3,3,3	0.43	0	2,2,2	0.47	0
8	EDO	B	1538	-	3,3,3	0.44	0	2,2,2	0.32	0
8	EDO	A	1540	-	3,3,3	0.55	0	2,2,2	0.11	0
8	EDO	B	1534	-	3,3,3	0.43	0	2,2,2	0.61	0
8	EDO	B	1532	-	3,3,3	0.48	0	2,2,2	0.34	0
8	EDO	A	1532	-	3,3,3	0.47	0	2,2,2	0.42	0
6	NAG	B	621	1	14,14,15	0.60	0	17,19,21	1.64	3 (17%)
5	BAL	A	550	-	5,5,5	0.73	0	5,5,5	2.05	3 (60%)
6	NAG	B	601	1	14,14,15	0.66	0	17,19,21	1.43	3 (17%)
11	GLY	A	1643	-	4,4,4	1.04	0	3,4,4	1.63	1 (33%)
6	NAG	B	671	1	14,14,15	0.59	0	17,19,21	0.85	0
8	EDO	A	1533	-	3,3,3	0.49	0	2,2,2	0.26	0
7	PG4	A	1531	-	12,12,12	0.68	0	11,11,11	1.48	0
8	EDO	A	1534	-	3,3,3	0.50	0	2,2,2	0.32	0
11	GLY	B	1642	-	4,4,4	1.08	1 (25%)	3,4,4	1.59	1 (33%)
8	EDO	B	1537	-	3,3,3	0.42	0	2,2,2	0.58	0
8	EDO	B	1539	-	3,3,3	0.42	0	2,2,2	0.35	0
6	NAG	B	611	1	14,14,15	0.46	0	17,19,21	0.81	1 (5%)
6	NAG	A	651	1	14,14,15	0.57	0	17,19,21	0.63	0
5	BAL	B	550	-	5,5,5	1.00	0	5,5,5	1.90	2 (40%)
8	EDO	A	1538	-	3,3,3	0.45	0	2,2,2	0.31	0
8	EDO	B	1535	-	3,3,3	0.49	0	2,2,2	0.24	0
8	EDO	A	1537	-	3,3,3	0.49	0	2,2,2	0.33	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	A	1535	-	-	0/1/1/1	-
8	EDO	B	1533	-	-	0/1/1/1	-
12	PEG	B	1531	-	-	1/4/4/4	-
6	NAG	B	651	1	-	2/6/23/26	0/1/1/1
8	EDO	B	1540	-	-	0/1/1/1	-
8	EDO	B	1541	-	-	1/1/1/1	-
12	PEG	B	1530	-	-	3/4/4/4	-
7	PG4	A	1530	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	1536	-	-	0/1/1/1	-
8	EDO	A	1539	-	-	0/1/1/1	-
8	EDO	A	1536	-	-	1/1/1/1	-
8	EDO	B	1538	-	-	0/1/1/1	-
8	EDO	A	1540	-	-	0/1/1/1	-
8	EDO	B	1534	-	-	0/1/1/1	-
8	EDO	B	1532	-	-	0/1/1/1	-
8	EDO	A	1532	-	-	1/1/1/1	-
6	NAG	B	621	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	B	601	1	-	2/6/23/26	0/1/1/1
5	BAL	A	550	-	-	1/3/3/3	-
11	GLY	A	1643	-	-	2/2/2/2	-
6	NAG	B	671	1	1/1/5/7	1/6/23/26	0/1/1/1
8	EDO	A	1533	-	-	0/1/1/1	-
7	PG4	A	1531	-	-	5/10/10/10	-
8	EDO	A	1534	-	-	0/1/1/1	-
11	GLY	B	1642	-	-	2/2/2/2	-
8	EDO	B	1537	-	-	1/1/1/1	-
8	EDO	B	1539	-	-	1/1/1/1	-
6	NAG	B	611	1	-	2/6/23/26	0/1/1/1
6	NAG	A	651	1	1/1/5/7	4/6/23/26	0/1/1/1
5	BAL	B	550	-	-	1/3/3/3	-
8	EDO	A	1538	-	-	0/1/1/1	-
8	EDO	B	1535	-	-	1/1/1/1	-
8	EDO	A	1537	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1642	GLY	OXT-C	-2.01	1.24	1.30

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	651	NAG	C1-O5-C5	4.38	118.06	112.19
6	B	621	NAG	C2-N2-C7	3.60	127.72	122.90
6	B	621	NAG	C1-O5-C5	3.39	116.73	112.19
6	B	621	NAG	C1-C2-N2	3.23	115.53	110.43
5	B	550	BAL	O-C-CA	-3.15	113.10	123.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	651	NAG	C1
6	B	621	NAG	C1
6	B	671	NAG	C1

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	550	BAL	C-CA-CB-N
6	A	651	NAG	C8-C7-N2-C2
6	A	651	NAG	O7-C7-N2-C2
6	B	601	NAG	C8-C7-N2-C2
6	B	601	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1531	PEG	2	0
8	A	1536	EDO	1	0
8	B	1538	EDO	1	0
8	B	1534	EDO	2	0
6	B	621	NAG	4	0
5	A	550	BAL	3	0
7	A	1531	PG4	1	0
8	B	1539	EDO	1	0
5	B	550	BAL	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	527/531 (99%)	-0.11	12 (2%) 60 63	26, 44, 72, 117	4 (0%)
1	B	526/531 (99%)	0.01	19 (3%) 42 46	27, 52, 88, 119	12 (2%)
All	All	1053/1062 (99%)	-0.05	31 (2%) 51 55	26, 48, 81, 119	16 (1%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	GLN	4.3
1	B	344	ILE	4.1
1	B	380	GLN	3.5
1	B	52	TRP	3.3
1	B	384	ASN	3.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUL	K	3	10/11	0.70	0.37	124,127,131,132	0
3	NAG	K	2	14/15	0.75	0.39	88,106,120,121	0
3	NAG	F	2	14/15	0.75	0.64	145,148,151,153	0
4	MAN	G	3	11/12	0.75	0.30	118,125,131,137	0
3	NAG	F	1	14/15	0.76	0.27	97,111,128,137	0

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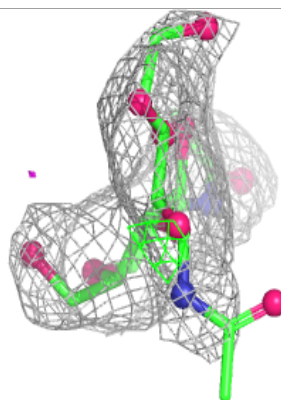
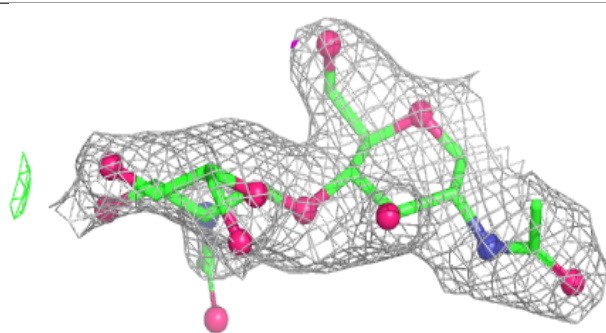
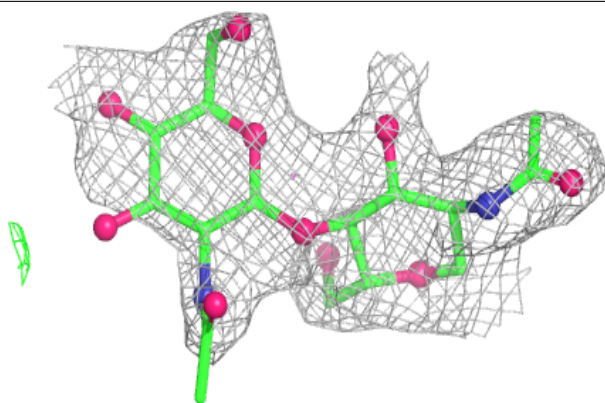
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	2	14/15	0.78	0.38	93,108,123,124	0
3	NAG	H	2	14/15	0.78	0.37	104,116,121,121	0
3	FUL	I	3	10/11	0.78	0.30	96,106,109,112	0
2	NAG	C	2	14/15	0.79	0.39	91,100,108,111	0
3	NAG	H	1	14/15	0.80	0.26	92,101,109,114	0
3	NAG	J	2	14/15	0.83	0.40	110,115,126,126	0
3	FUL	F	3	10/11	0.83	0.43	125,130,131,132	0
3	NAG	D	2	14/15	0.84	0.26	90,105,113,116	0
3	FUL	J	3	10/11	0.85	0.40	119,124,127,127	0
3	NAG	K	1	14/15	0.86	0.18	67,78,101,111	0
3	FUL	H	3	10/11	0.88	0.22	90,100,106,108	0
3	FUL	D	3	10/11	0.88	0.21	96,98,100,101	0
3	NAG	I	1	14/15	0.90	0.27	71,91,107,111	0
3	NAG	I	2	14/15	0.91	0.35	90,105,112,113	0
2	NAG	E	1	14/15	0.91	0.17	42,64,70,92	0
3	NAG	D	1	14/15	0.92	0.14	67,78,96,103	0
2	NAG	C	1	14/15	0.92	0.24	51,65,83,91	0
3	NAG	J	1	14/15	0.93	0.19	72,89,102,108	0
4	NAG	G	2	14/15	0.94	0.13	66,81,91,108	0
4	NAG	G	1	14/15	0.95	0.12	43,57,71,71	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.

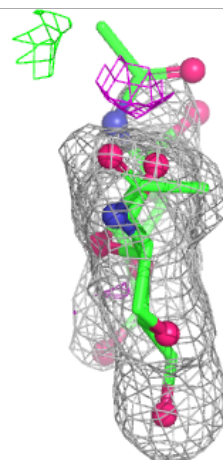
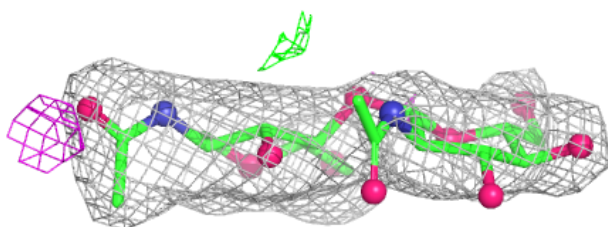
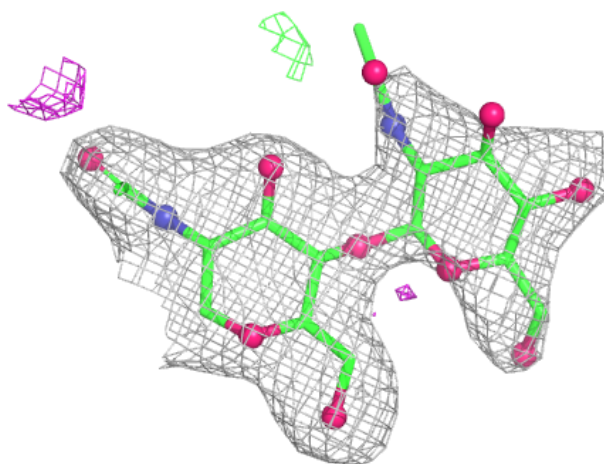
Electron density around Chain C:

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



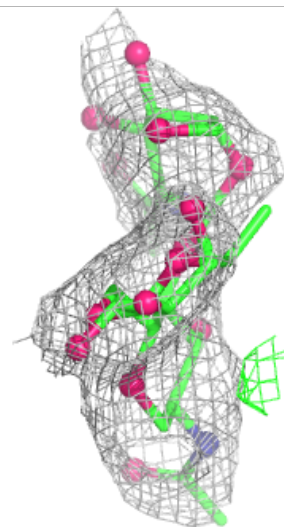
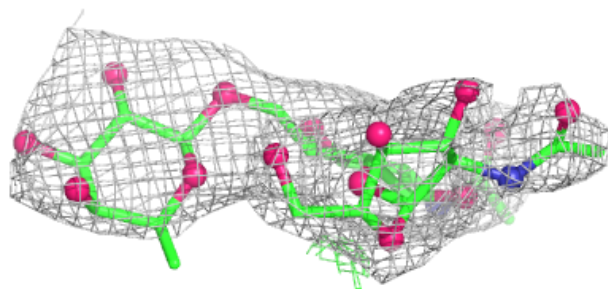
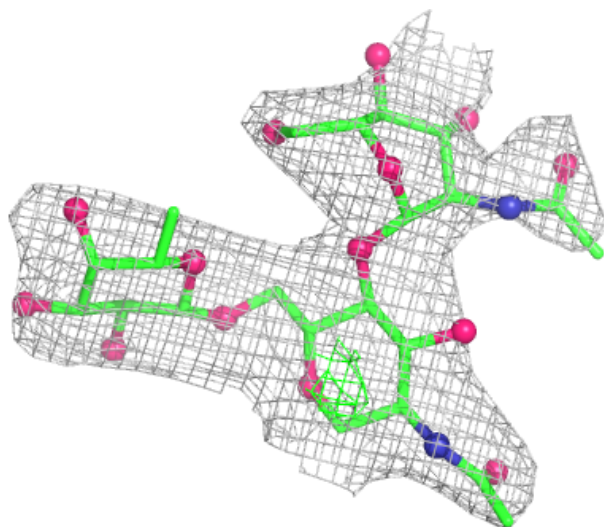
Electron density around Chain E:

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



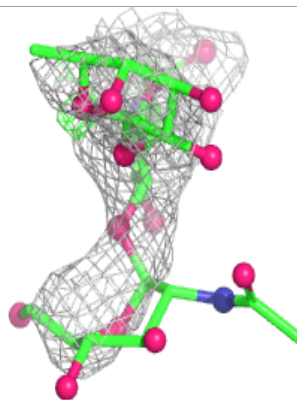
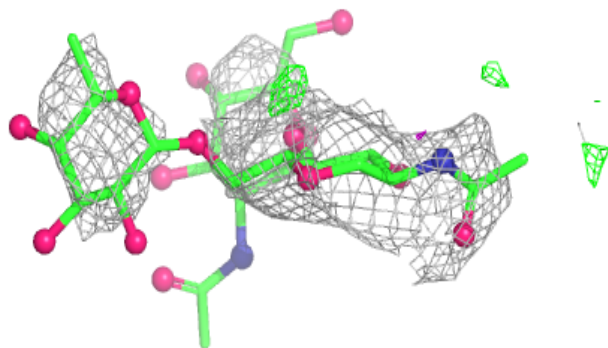
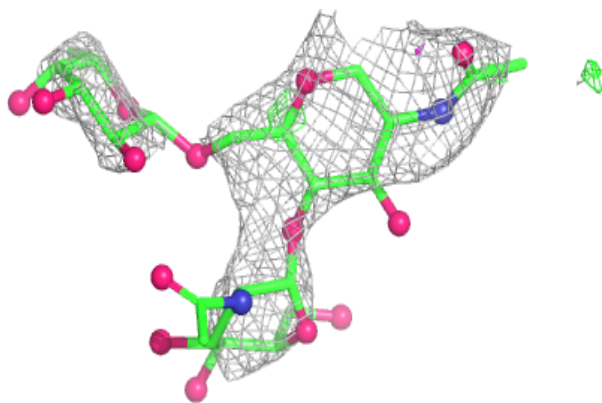
Electron density around Chain D:

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



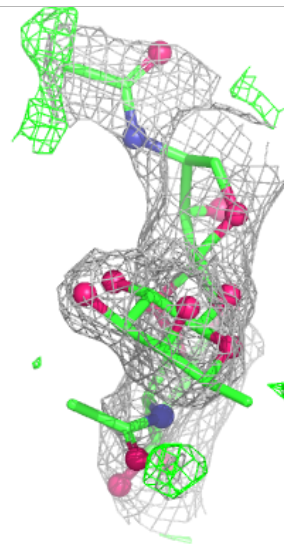
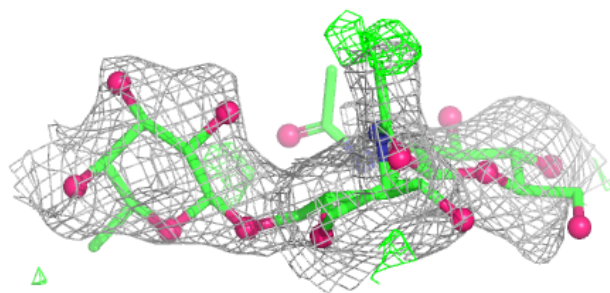
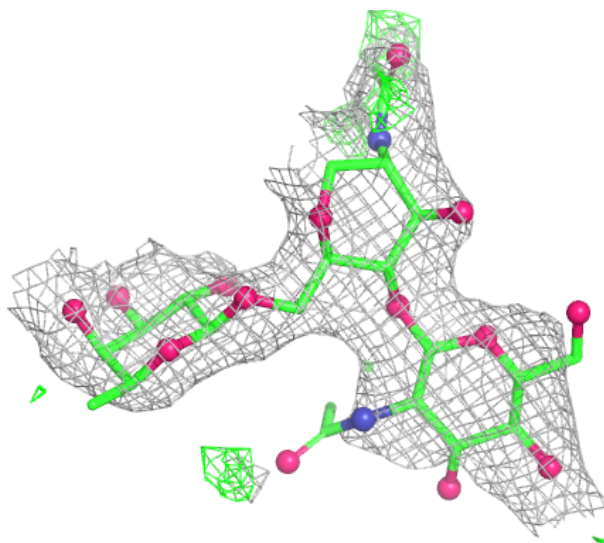
Electron density around Chain F:

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



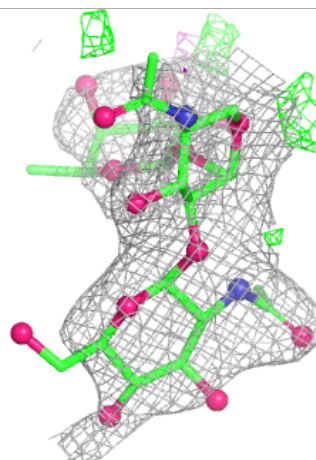
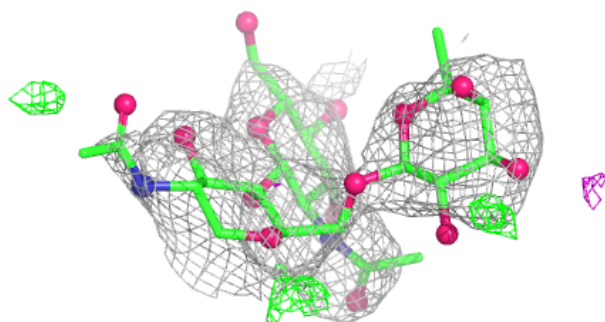
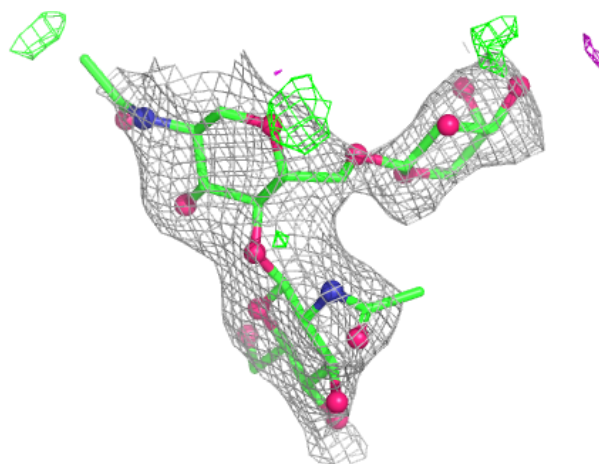
Electron density around Chain H:

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



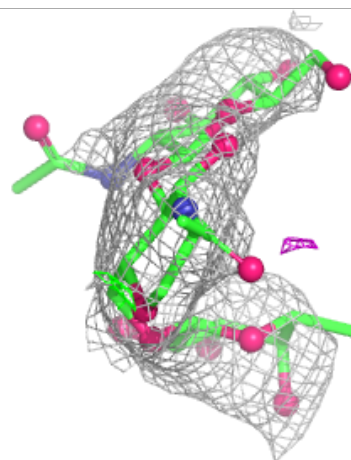
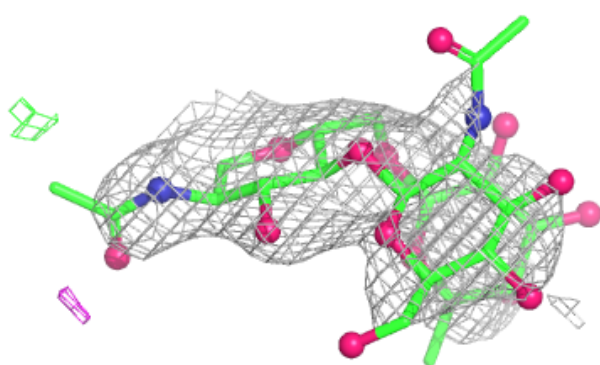
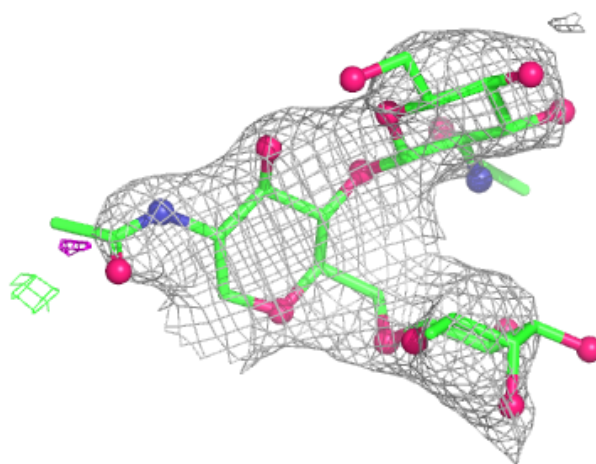
Electron density around Chain I:

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



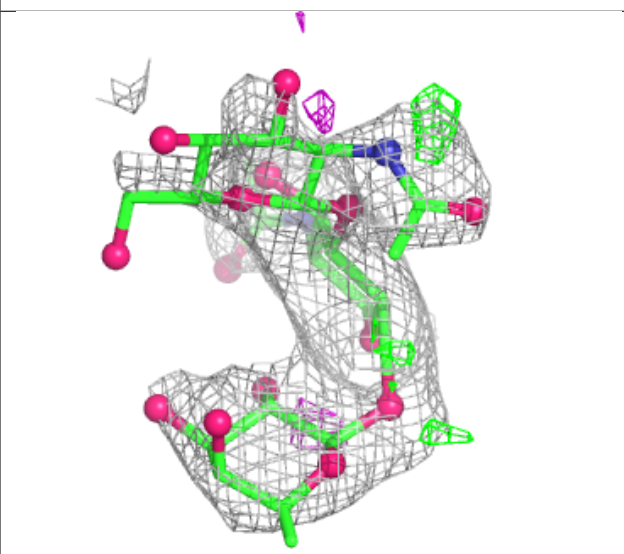
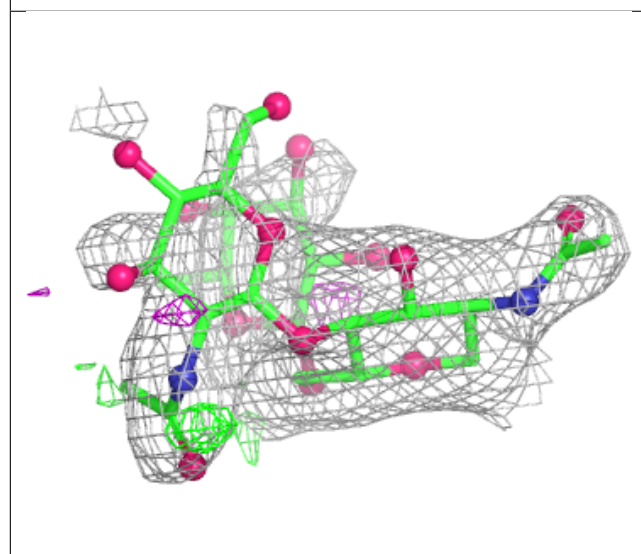
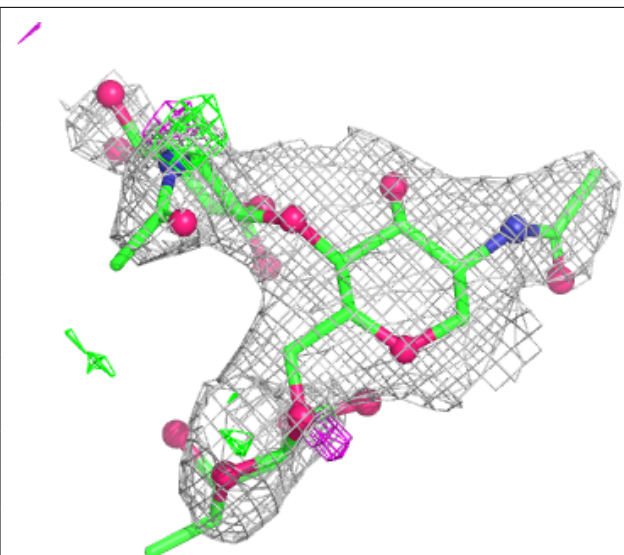
Electron density around Chain J:

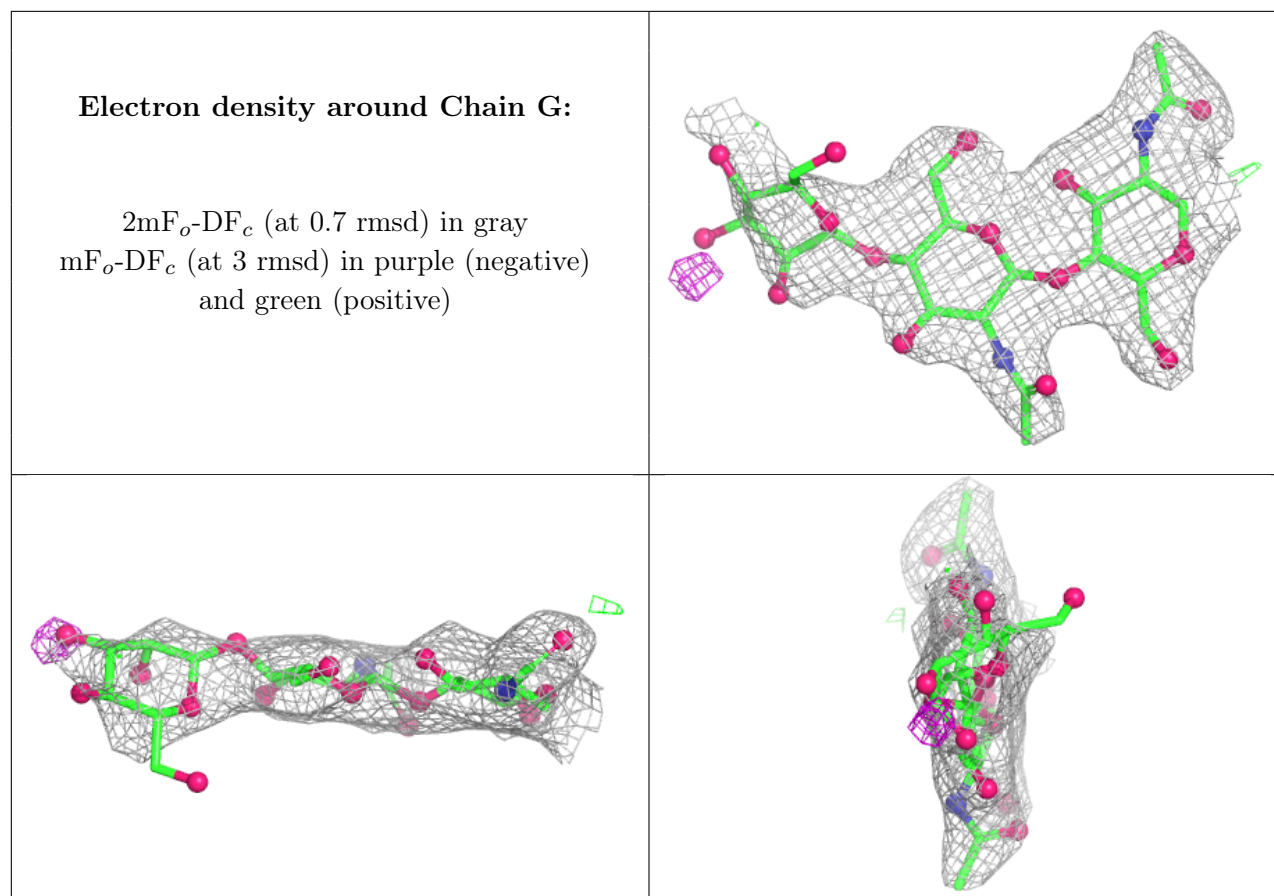
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	UNX	A	1548	1/1	0.39	0.20	71,71,71,71	0
10	CL	A	1547	1/1	0.62	0.21	99,99,99,99	0
6	NAG	B	601	14/15	0.67	0.31	94,104,119,120	0
8	EDO	A	1535	4/4	0.73	0.20	84,85,88,88	0
6	NAG	B	671	14/15	0.75	0.20	92,103,111,112	0
10	CL	B	1549	1/1	0.76	0.19	95,95,95,95	0
6	NAG	B	611	14/15	0.77	0.20	102,109,114,116	0
12	PEG	B	1530	7/7	0.80	0.40	66,86,98,100	0
8	EDO	A	1533	4/4	0.82	0.25	68,74,75,78	0
9	UNX	A	1543	1/1	0.82	1.25	83,83,83,83	0
9	UNX	B	1548	1/1	0.83	0.07	68,68,68,68	0
7	PG4	A	1530	13/13	0.83	0.30	76,82,84,84	0
10	CL	A	1545	1/1	0.84	0.10	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	CL	B	1546	1/1	0.85	0.50	102,102,102,102	0
8	EDO	A	1540	4/4	0.86	0.20	64,65,72,73	0
8	EDO	B	1534	4/4	0.87	0.27	55,65,69,73	0
8	EDO	A	1536	4/4	0.87	0.30	74,76,77,82	0
5	BAL	B	550	6/6	0.87	0.31	49,55,68,79	0
12	PEG	B	1531	7/7	0.88	0.31	70,73,88,89	0
6	NAG	B	621	14/15	0.89	0.28	75,88,96,97	0
11	GLY	B	1642	5/5	0.89	0.16	57,60,68,70	0
8	EDO	A	1534	4/4	0.89	0.11	66,71,75,76	0
8	EDO	B	1537	4/4	0.89	0.16	69,73,76,77	0
10	CL	B	1547	1/1	0.90	0.11	96,96,96,96	0
7	PG4	A	1531	13/13	0.90	0.28	59,80,87,92	0
10	CL	B	1550	1/1	0.90	0.14	82,82,82,82	0
8	EDO	B	1541	4/4	0.90	0.24	74,75,76,78	0
8	EDO	A	1532	4/4	0.90	0.30	64,66,68,76	0
8	EDO	B	1536	4/4	0.90	0.48	64,65,73,74	0
6	NAG	A	651	14/15	0.91	0.26	58,78,87,91	0
6	NAG	B	651	14/15	0.92	0.25	56,71,80,87	0
8	EDO	B	1532	4/4	0.92	0.19	62,64,69,79	0
8	EDO	B	1540	4/4	0.92	0.27	67,74,81,81	0
10	CL	A	1546	1/1	0.92	0.15	73,73,73,73	0
8	EDO	A	1537	4/4	0.92	0.30	51,52,58,64	0
8	EDO	B	1535	4/4	0.92	0.18	68,75,76,77	0
8	EDO	B	1538	4/4	0.93	0.19	64,65,67,69	0
5	BAL	A	550	6/6	0.94	0.27	50,56,70,84	0
8	EDO	B	1533	4/4	0.95	0.12	65,73,74,76	0
8	EDO	A	1539	4/4	0.95	0.47	77,82,84,85	0
8	EDO	B	1539	4/4	0.95	0.43	57,59,61,61	0
11	GLY	A	1643	5/5	0.96	0.12	42,48,53,58	0
9	UNX	A	1544	1/1	0.97	0.57	53,53,53,53	0
8	EDO	A	1538	4/4	0.97	0.22	61,65,67,68	0
9	UNX	B	1543	1/1	0.97	0.57	43,43,43,43	0
9	UNX	B	1545	1/1	0.97	0.62	53,53,53,53	0
9	UNX	A	1542	1/1	0.98	0.44	54,54,54,54	0
9	UNX	B	1544	1/1	0.98	0.57	67,67,67,67	0
9	UNX	B	1542	1/1	0.98	0.64	59,59,59,59	0
9	UNX	A	1541	1/1	0.99	0.53	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.