wwPDB X-ray Structure Validation Summary Report (i)

Mar 20, 2026 – 06:19 AM UTC

PDB ID	:	6G4G / pdb_00006g4g
Title	:	Full length ectodomain of ectonucleotide phosphodiesterase/pyrophosphatase -3 (NPP3) including the SMB domains but with a partially disordered active site structure
Authors	:	Dohler, C.; Zebisch, M.; Strater, N.
Deposited on	:	2018-03-27
Resolution	:	2.80 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:

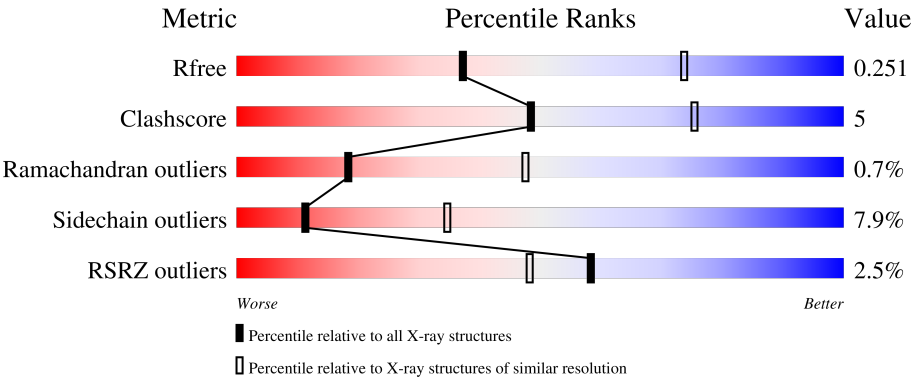
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	840	2% 71% 19% • 9%
1	B	840	2% 72% 17% • 10%
1	C	840	3% 67% 19% • 12%
1	D	840	2% 70% 20% • 7%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	H	2	100%
2	I	2	100%
2	J	2	100%
2	K	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24786 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6131	3903	1040	1140	48			
1	B	759	Total	C	N	O	S	0	0	0
			6087	3871	1035	1134	47			
1	C	742	Total	C	N	O	S	0	0	0
			5982	3818	1016	1102	46			
1	D	781	Total	C	N	O	S	0	0	0
			6274	3991	1064	1171	48			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	-	expression tag	UNP P97675
A	46	GLU	-	expression tag	UNP P97675
A	47	THR	-	expression tag	UNP P97675
A	48	GLY	-	expression tag	UNP P97675
A	201	VAL	MET	variant	UNP P97675
A	596	ASN	SER	variant	UNP P97675
A	597	ARG	GLY	variant	UNP P97675
A	876	GLY	-	expression tag	UNP P97675
A	877	THR	-	expression tag	UNP P97675
A	878	LYS	-	expression tag	UNP P97675
A	879	HIS	-	expression tag	UNP P97675
A	880	HIS	-	expression tag	UNP P97675
A	881	HIS	-	expression tag	UNP P97675
A	882	HIS	-	expression tag	UNP P97675
A	883	HIS	-	expression tag	UNP P97675
A	884	HIS	-	expression tag	UNP P97675
B	45	ALA	-	expression tag	UNP P97675
B	46	GLU	-	expression tag	UNP P97675
B	47	THR	-	expression tag	UNP P97675
B	48	GLY	-	expression tag	UNP P97675

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	VAL	MET	variant	UNP P97675
B	596	ASN	SER	variant	UNP P97675
B	597	ARG	GLY	variant	UNP P97675
B	876	GLY	-	expression tag	UNP P97675
B	877	THR	-	expression tag	UNP P97675
B	878	LYS	-	expression tag	UNP P97675
B	879	HIS	-	expression tag	UNP P97675
B	880	HIS	-	expression tag	UNP P97675
B	881	HIS	-	expression tag	UNP P97675
B	882	HIS	-	expression tag	UNP P97675
B	883	HIS	-	expression tag	UNP P97675
B	884	HIS	-	expression tag	UNP P97675
C	45	ALA	-	expression tag	UNP P97675
C	46	GLU	-	expression tag	UNP P97675
C	47	THR	-	expression tag	UNP P97675
C	48	GLY	-	expression tag	UNP P97675
C	201	VAL	MET	variant	UNP P97675
C	596	ASN	SER	variant	UNP P97675
C	597	ARG	GLY	variant	UNP P97675
C	876	GLY	-	expression tag	UNP P97675
C	877	THR	-	expression tag	UNP P97675
C	878	LYS	-	expression tag	UNP P97675
C	879	HIS	-	expression tag	UNP P97675
C	880	HIS	-	expression tag	UNP P97675
C	881	HIS	-	expression tag	UNP P97675
C	882	HIS	-	expression tag	UNP P97675
C	883	HIS	-	expression tag	UNP P97675
C	884	HIS	-	expression tag	UNP P97675
D	45	ALA	-	expression tag	UNP P97675
D	46	GLU	-	expression tag	UNP P97675
D	47	THR	-	expression tag	UNP P97675
D	48	GLY	-	expression tag	UNP P97675
D	201	VAL	MET	variant	UNP P97675
D	596	ASN	SER	variant	UNP P97675
D	597	ARG	GLY	variant	UNP P97675
D	876	GLY	-	expression tag	UNP P97675
D	877	THR	-	expression tag	UNP P97675
D	878	LYS	-	expression tag	UNP P97675
D	879	HIS	-	expression tag	UNP P97675
D	880	HIS	-	expression tag	UNP P97675
D	881	HIS	-	expression tag	UNP P97675
D	882	HIS	-	expression tag	UNP P97675

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Chain	Residue	Modelled	Actual	Comment	Reference
D	883	HIS	-	expression tag	UNP P97675
D	884	HIS	-	expression tag	UNP P97675

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

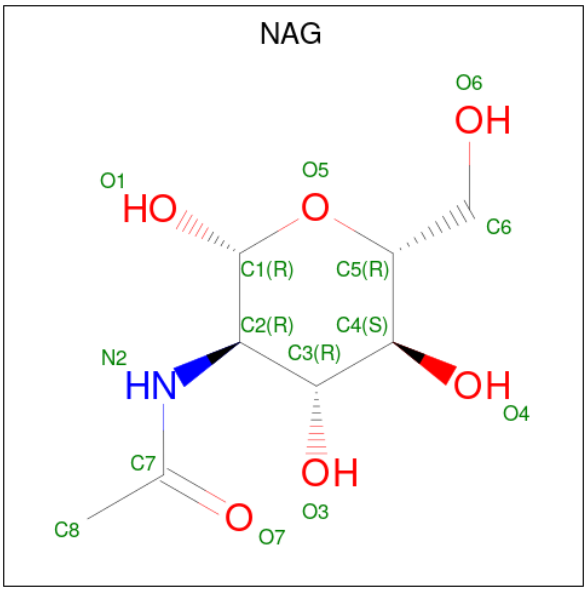


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	2	Total C N O 28 16 2 10	0	0	0
2	F	2	Total C N O 28 16 2 10	0	0	0
2	G	2	Total C N O 28 16 2 10	0	0	0
2	H	2	Total C N O 28 16 2 10	0	0	0
2	I	2	Total C N O 28 16 2 10	0	0	0
2	J	2	Total C N O 28 16 2 10	0	0	0
2	K	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

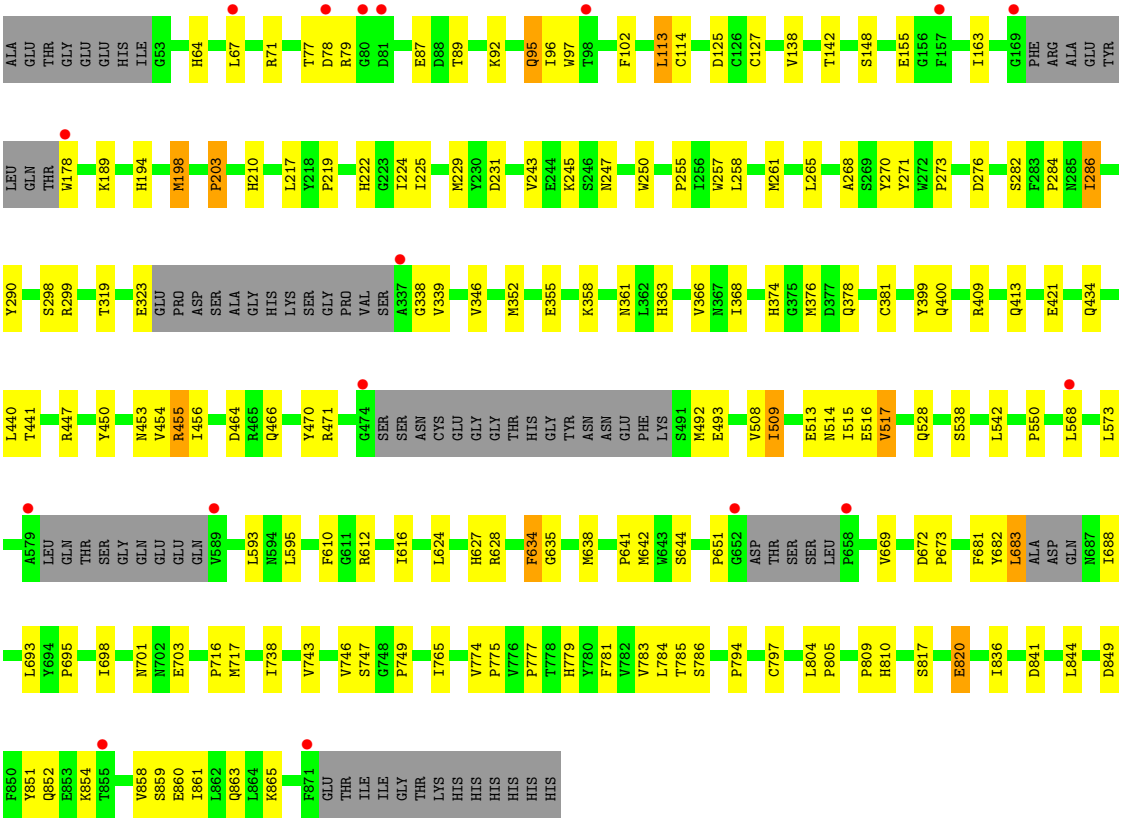
3 Residue-property plots (i)

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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3

Chain A:

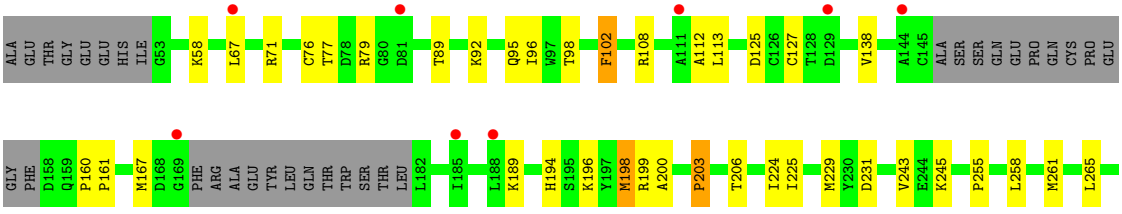


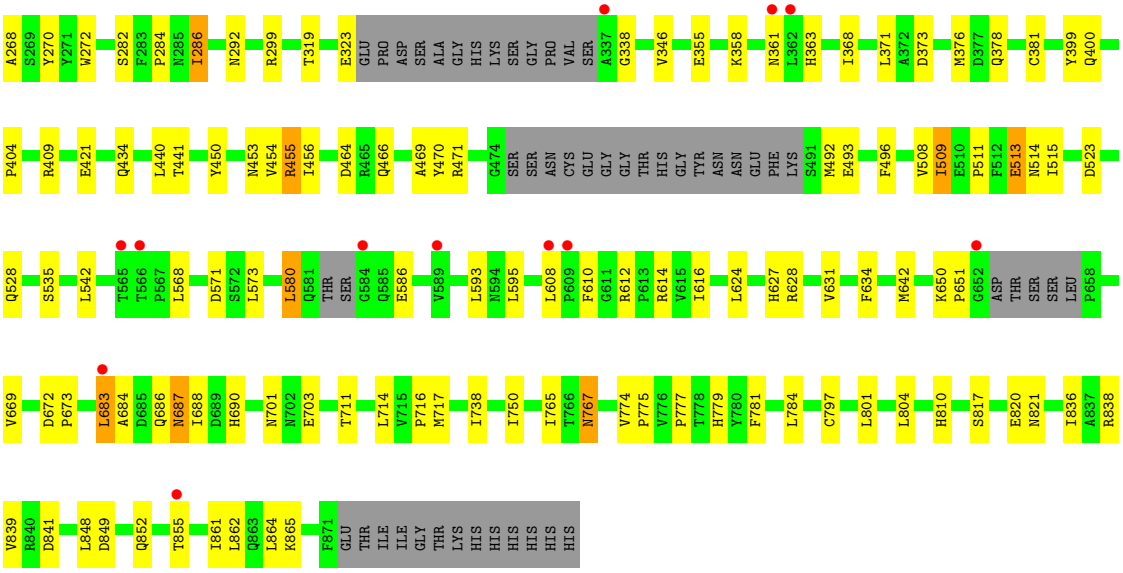


• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3

Chain B:



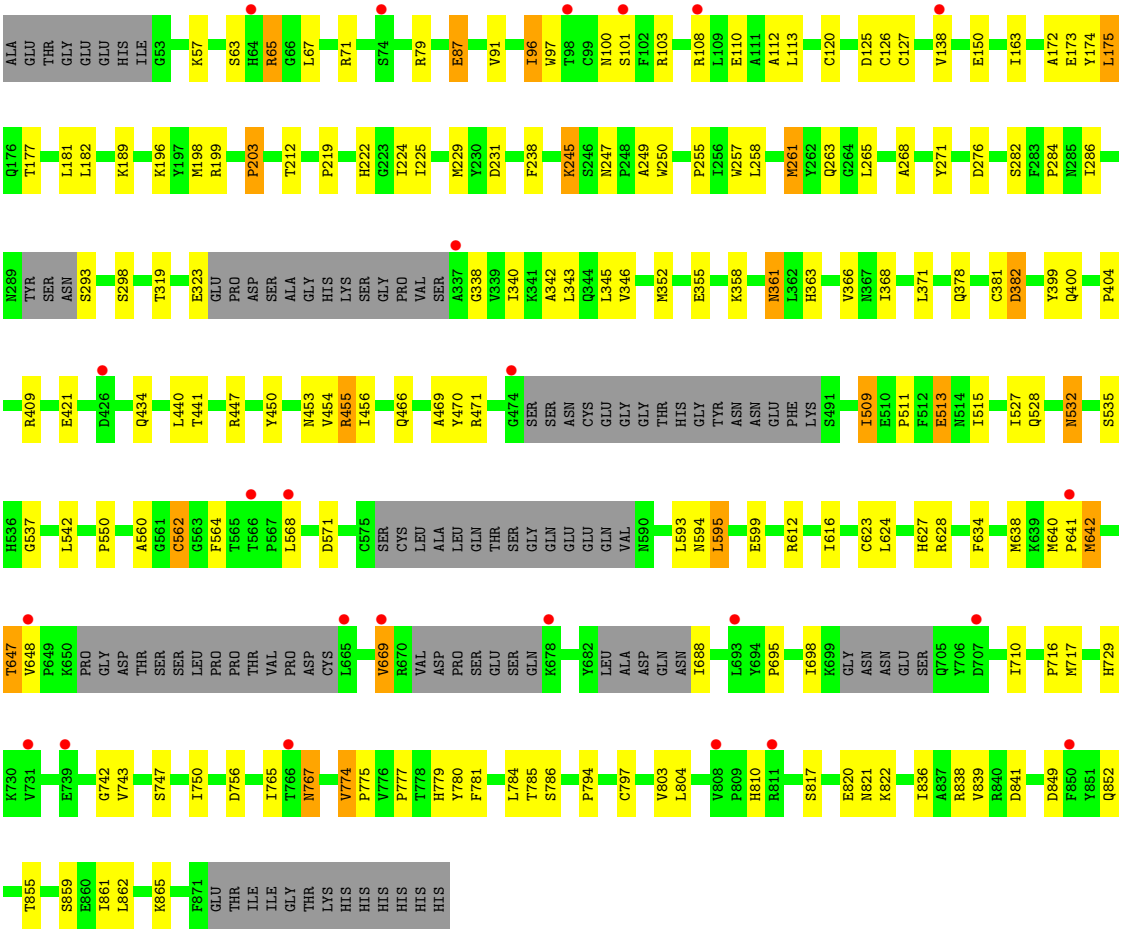




• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3

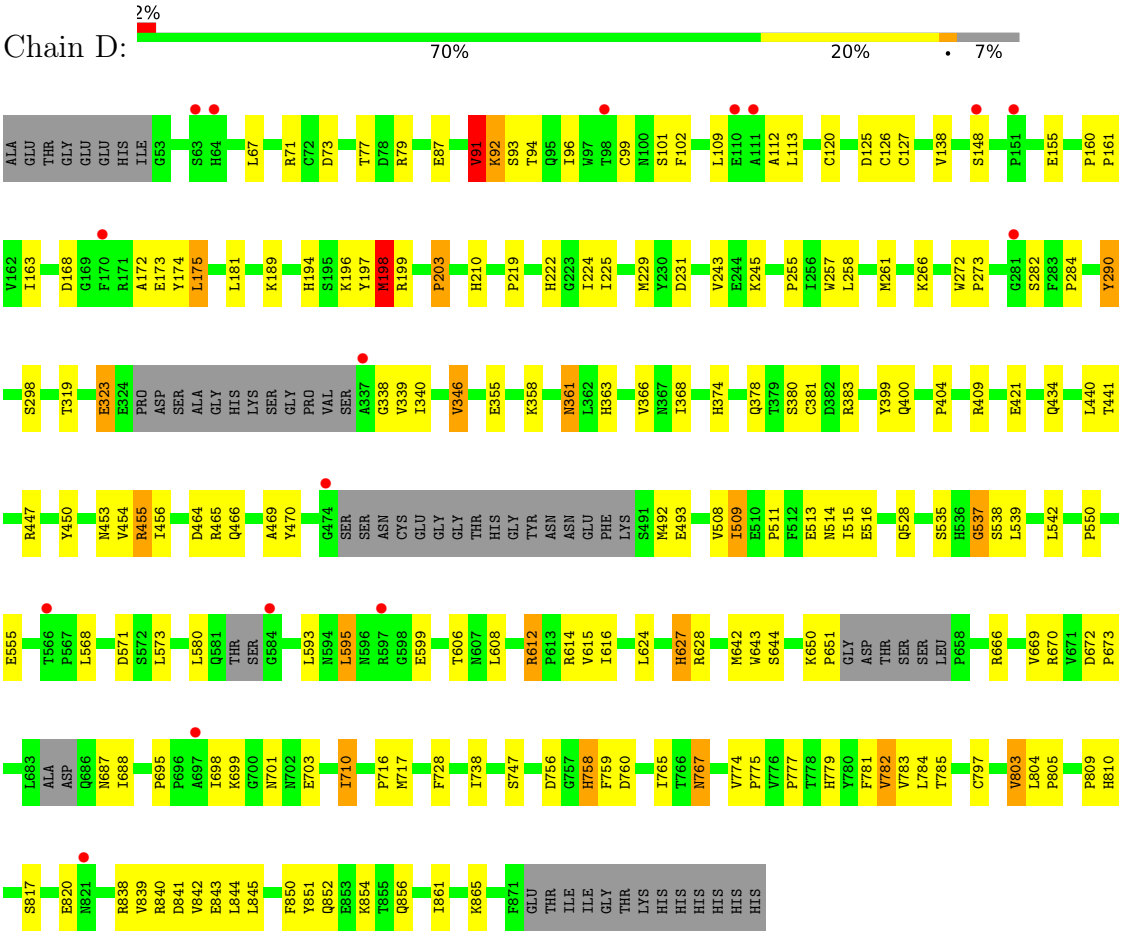
Chain C:





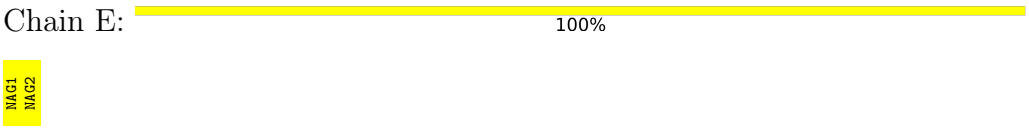
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3

Chain D:



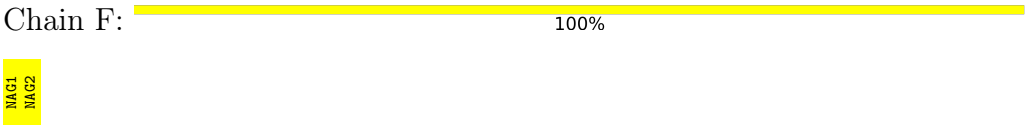
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



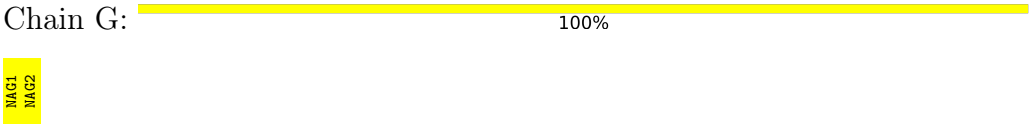
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



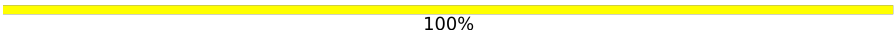
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

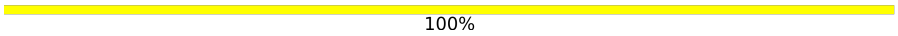
Chain H:





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

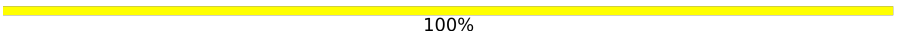
Chain I:





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

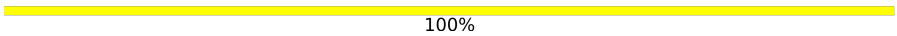
Chain J:





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

Chain K:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.36Å 116.30Å 124.16Å 86.77° 87.76° 88.20°	Depositor
Resolution (Å)	47.22 – 2.80 47.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	65.3 (47.22-2.80) 65.3 (47.22-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.196 , 0.237 0.209 , 0.251	Depositor DCC
R_{free} test set	3360 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 75.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	24786	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NAG, CA

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	0.89	2/6303 (0.0%)	1.34	37/8565 (0.4%)
1	B	0.81	0/6254	1.32	27/8495 (0.3%)
1	C	0.85	1/6148 (0.0%)	1.33	23/8345 (0.3%)
1	D	0.88	1/6449 (0.0%)	1.37	49/8763 (0.6%)
All	All	0.86	4/25154 (0.0%)	1.34	136/34168 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	MET	SD-CE	-8.95	1.57	1.79
1	A	114	CYS	CA-C	6.57	1.61	1.53
1	D	758	HIS	CA-C	-5.72	1.45	1.52
1	C	261	MET	SD-CE	-5.08	1.66	1.79

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	101	SER	CA-C-N	8.41	132.38	120.28
1	D	101	SER	C-N-CA	8.41	132.38	120.28
1	A	516	GLU	CA-C-N	8.14	131.10	120.60
1	A	516	GLU	C-N-CA	8.14	131.10	120.60
1	C	767	ASN	CA-CB-CG	7.62	120.22	112.60

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	6131	0	5886	65	0
1	B	6087	0	5850	55	0
1	C	5982	0	5757	77	0
1	D	6274	0	6017	69	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
4	D	28	0	26	1	0
All	All	24786	0	23789	266	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 266 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:C:247:ASN:HD21	1:C:249:ALA:HB3	1.48	0.78
1:B:750:ILE:HD11	1:B:781:PHE:HB3	1.69	0.72
1:A:198:MET:HE1	1:A:517:VAL:HG21	1.73	0.70
1:A:509:ILE:HD13	1:A:542:LEU:HD11	1.77	0.66
1:A:409:ARG:HH22	1:A:471:ARG:NE	1.94	0.66

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	751/840 (89%)	700 (93%)	47 (6%)	4 (0%)	24	55
1	B	745/840 (89%)	694 (93%)	44 (6%)	7 (1%)	14	41
1	C	724/840 (86%)	674 (93%)	44 (6%)	6 (1%)	16	44
1	D	769/840 (92%)	710 (92%)	54 (7%)	5 (1%)	18	47
All	All	2989/3360 (89%)	2778 (93%)	189 (6%)	22 (1%)	18	47

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	683	LEU
1	B	820	GLU
1	D	148	SER
1	A	820	GLU
1	C	820	GLU

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	686/749 (92%)	634 (92%)	52 (8%)	12	36
1	B	680/749 (91%)	629 (92%)	51 (8%)	12	37
1	C	665/749 (89%)	611 (92%)	54 (8%)	11	33
1	D	701/749 (94%)	642 (92%)	59 (8%)	10	32
All	All	2732/2996 (91%)	2516 (92%)	216 (8%)	11	35

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	175	LEU
1	C	624	LEU
1	D	624	LEU
1	C	282	SER
1	C	382	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	622	HIS
1	D	687	ASN
1	B	528	GLN
1	B	514	ASN
1	D	701	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)

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

5.5 Carbohydrates (i)

14 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	E	1	1,2	14,14,15	0.37	0	17,19,21	1.49	2 (11%)
2	NAG	E	2	2	14,14,15	0.35	0	17,19,21	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	1	1,2	14,14,15	0.34	0	17,19,21	1.76	3 (17%)
2	NAG	F	2	2	14,14,15	0.39	0	17,19,21	1.15	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.35	0	17,19,21	1.49	2 (11%)
2	NAG	G	2	2	14,14,15	0.33	0	17,19,21	1.05	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.36	0	17,19,21	1.45	2 (11%)
2	NAG	H	2	2	14,14,15	0.33	0	17,19,21	1.01	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.29	0	17,19,21	1.38	3 (17%)
2	NAG	I	2	2	14,14,15	0.34	0	17,19,21	0.83	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.38	0	17,19,21	1.51	2 (11%)
2	NAG	J	2	2	14,14,15	0.34	0	17,19,21	1.05	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.26	0	17,19,21	1.26	2 (11%)
2	NAG	K	2	2	14,14,15	0.35	0	17,19,21	1.20	1 (5%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	NAG	C1-O5-C5	5.85	120.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	NAG	O5-C1-C2	-5.33	103.05	111.29
2	J	1	NAG	O5-C1-C2	-5.29	103.11	111.29
2	E	1	NAG	O5-C1-C2	-4.99	103.57	111.29
2	H	1	NAG	O5-C1-C2	-4.83	103.81	111.29

There are no chirality outliers.

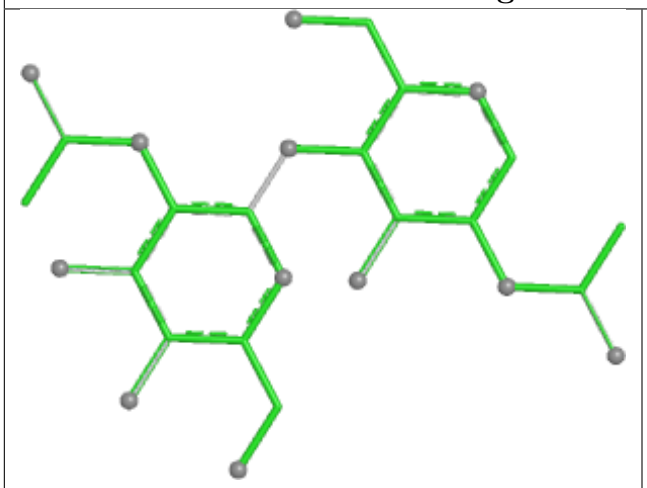
There are no torsion outliers.

There are no ring outliers.

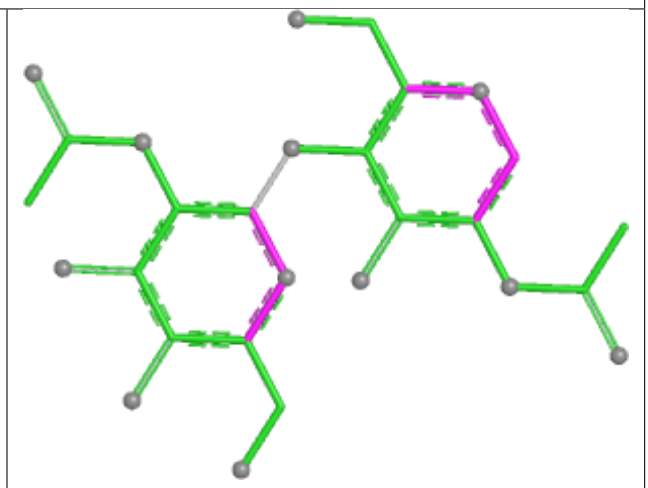
No monomer is involved in short contacts.

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

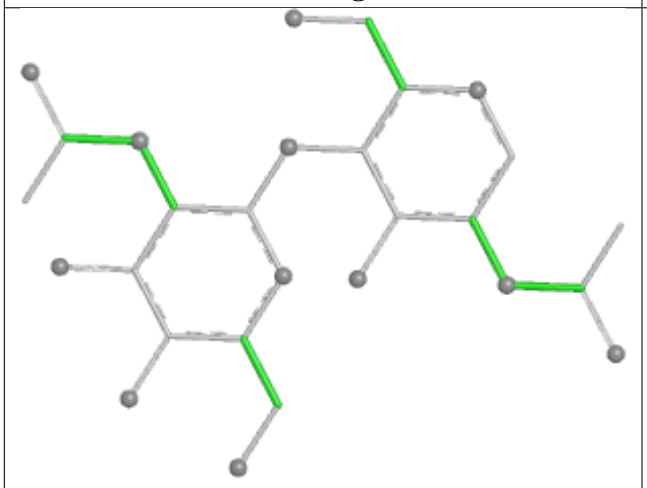
Oligosaccharide Chain E



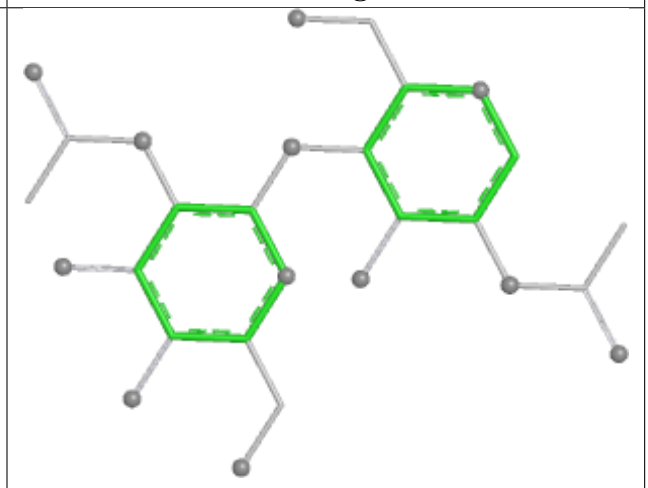
Bond lengths



Bond angles

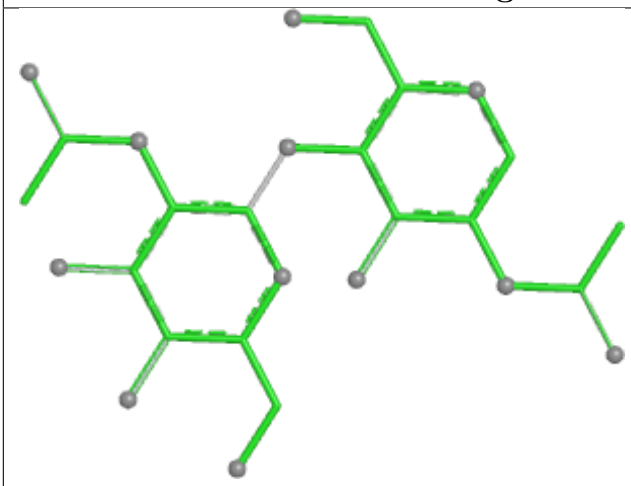


Torsions

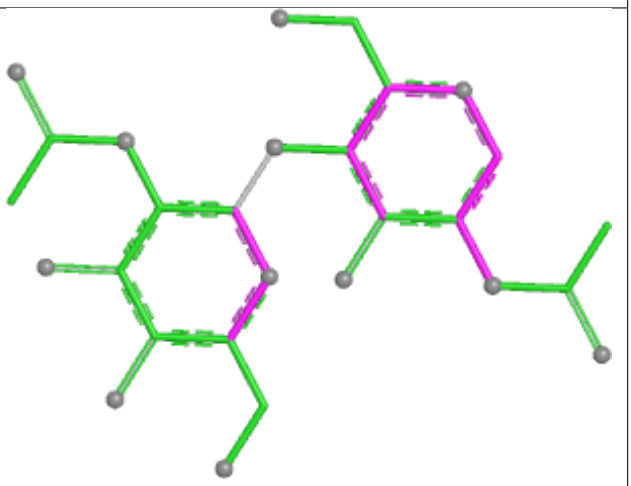


Rings

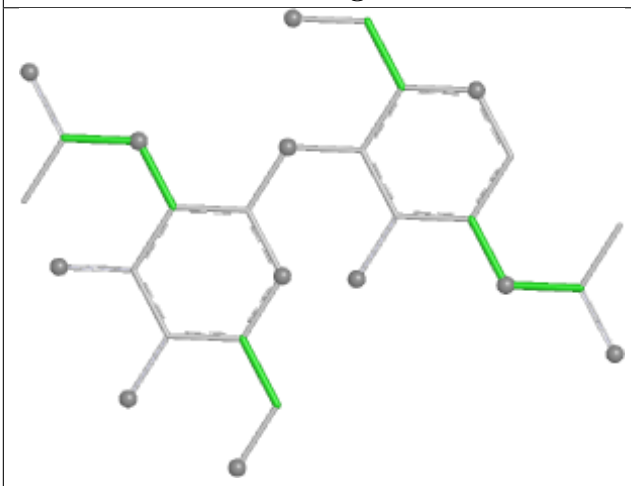
Oligosaccharide Chain F



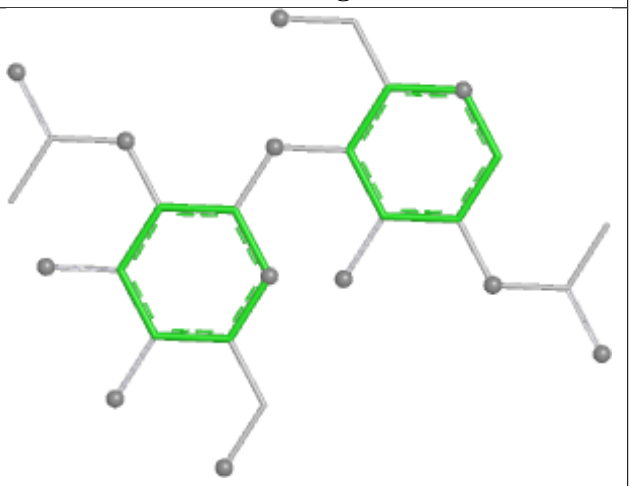
Bond lengths



Bond angles

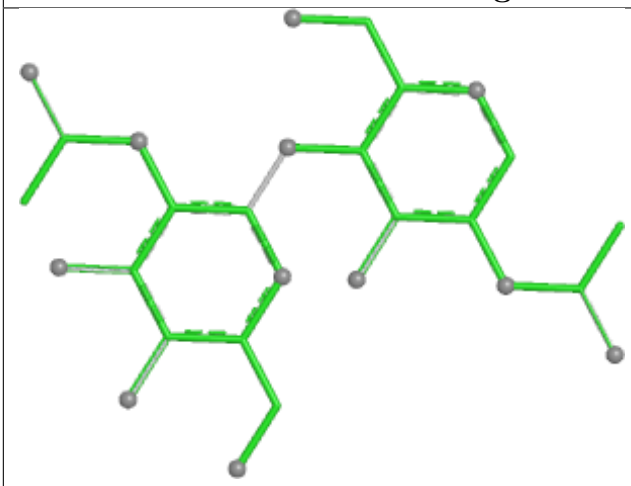


Torsions

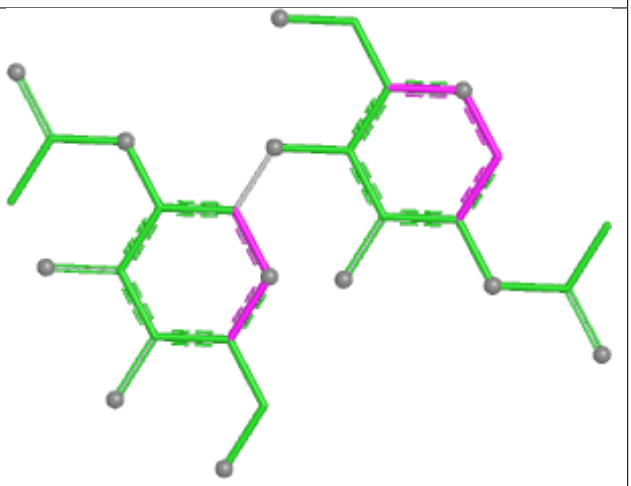


Rings

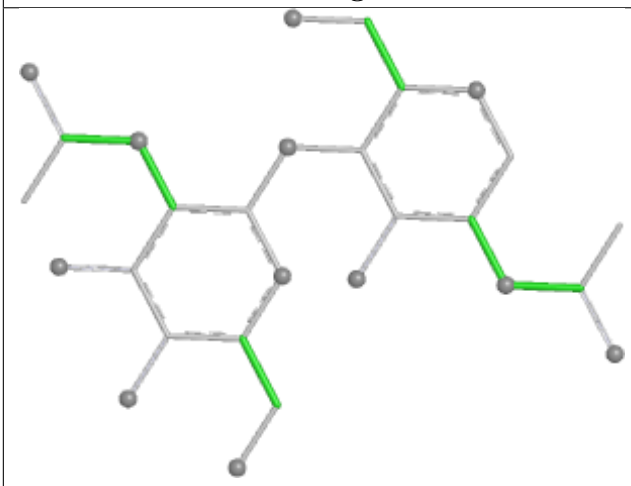
Oligosaccharide Chain G



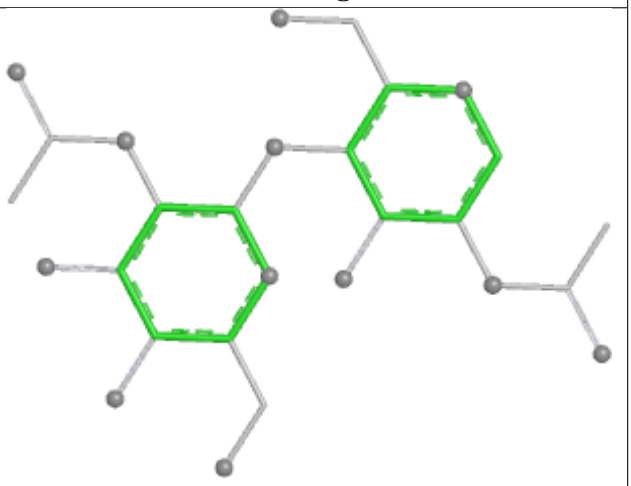
Bond lengths



Bond angles

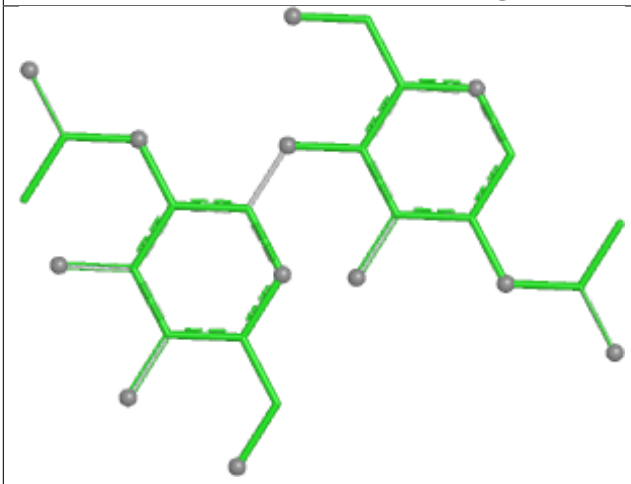


Torsions

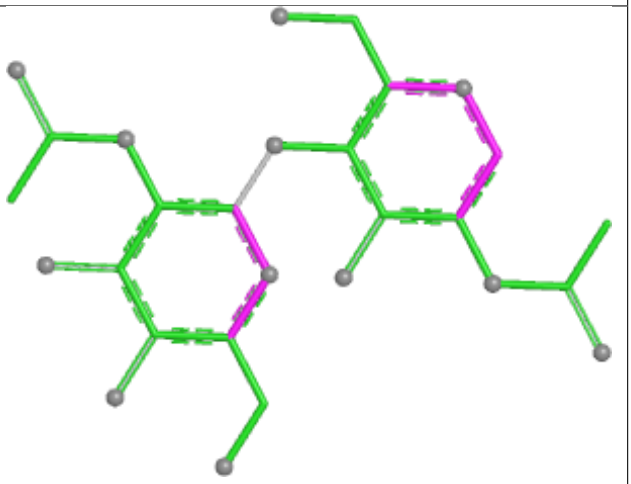


Rings

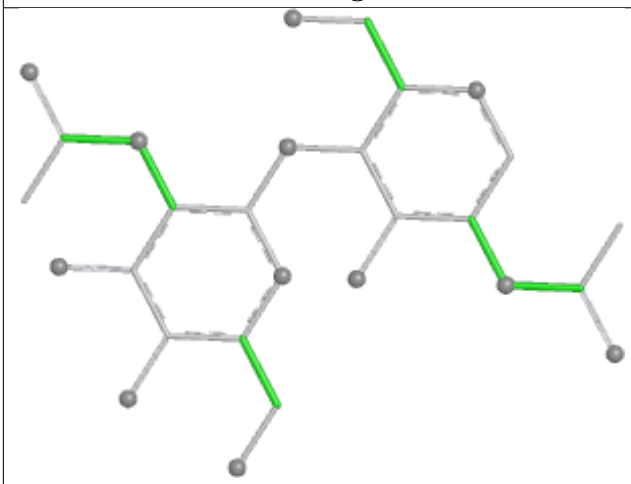
Oligosaccharide Chain H



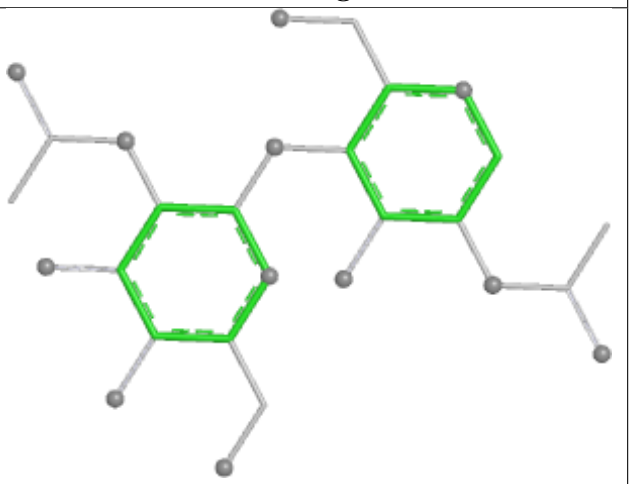
Bond lengths



Bond angles

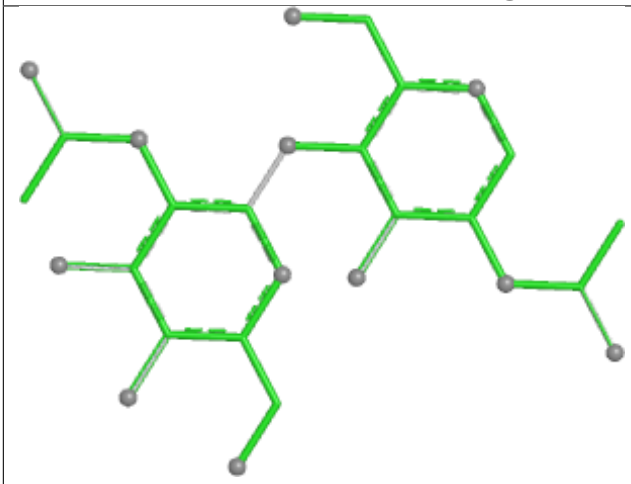


Torsions

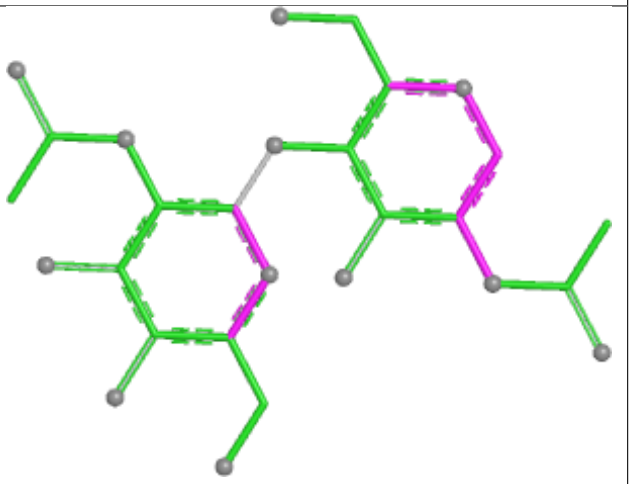


Rings

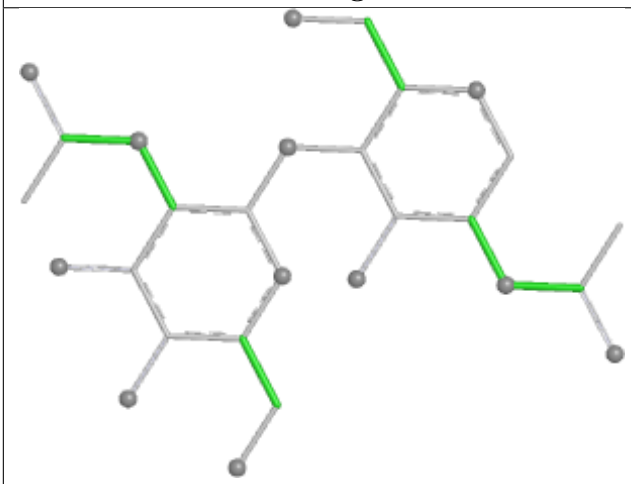
Oligosaccharide Chain I



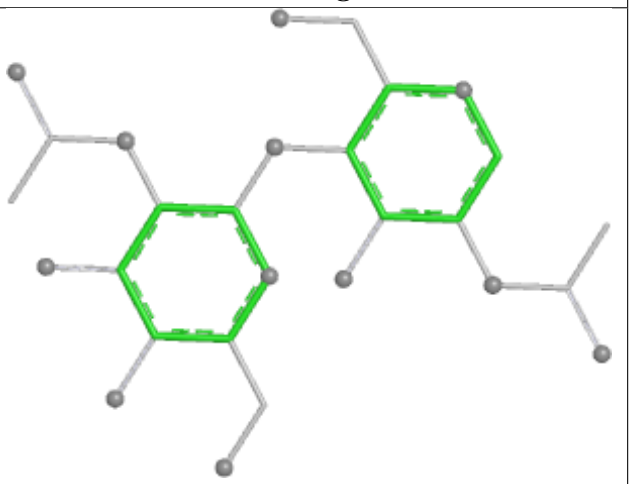
Bond lengths



Bond angles

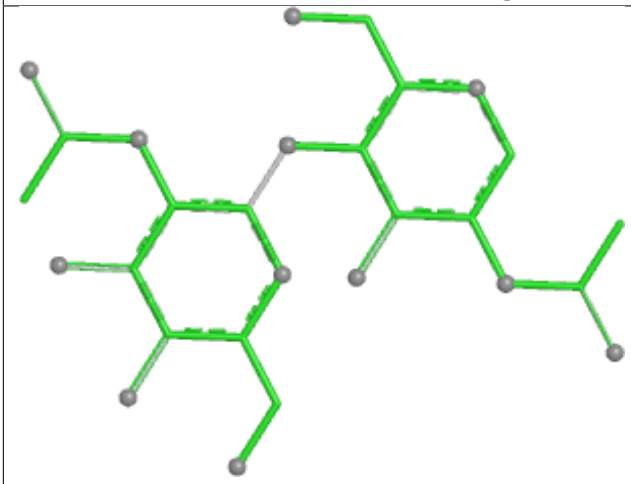


Torsions

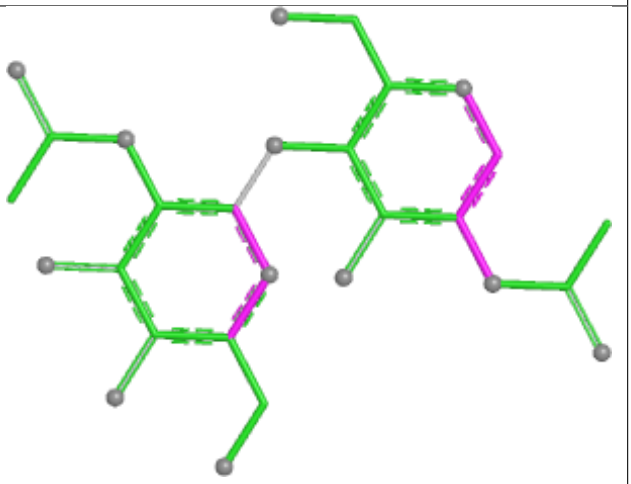


Rings

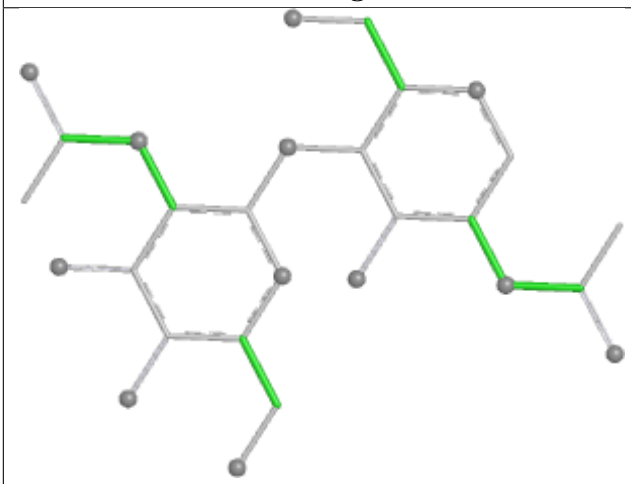
Oligosaccharide Chain J



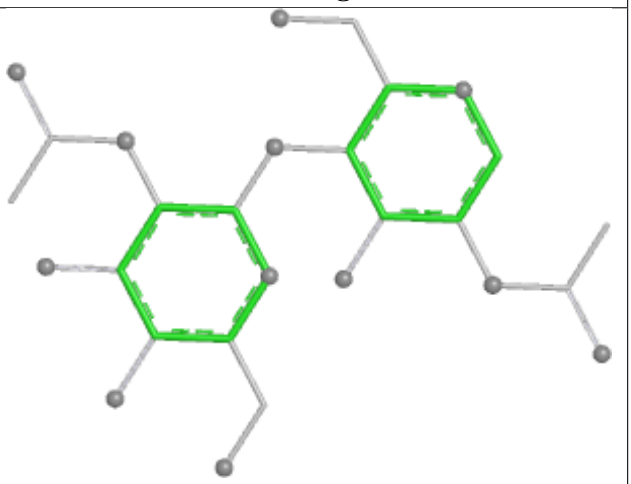
Bond lengths



Bond angles

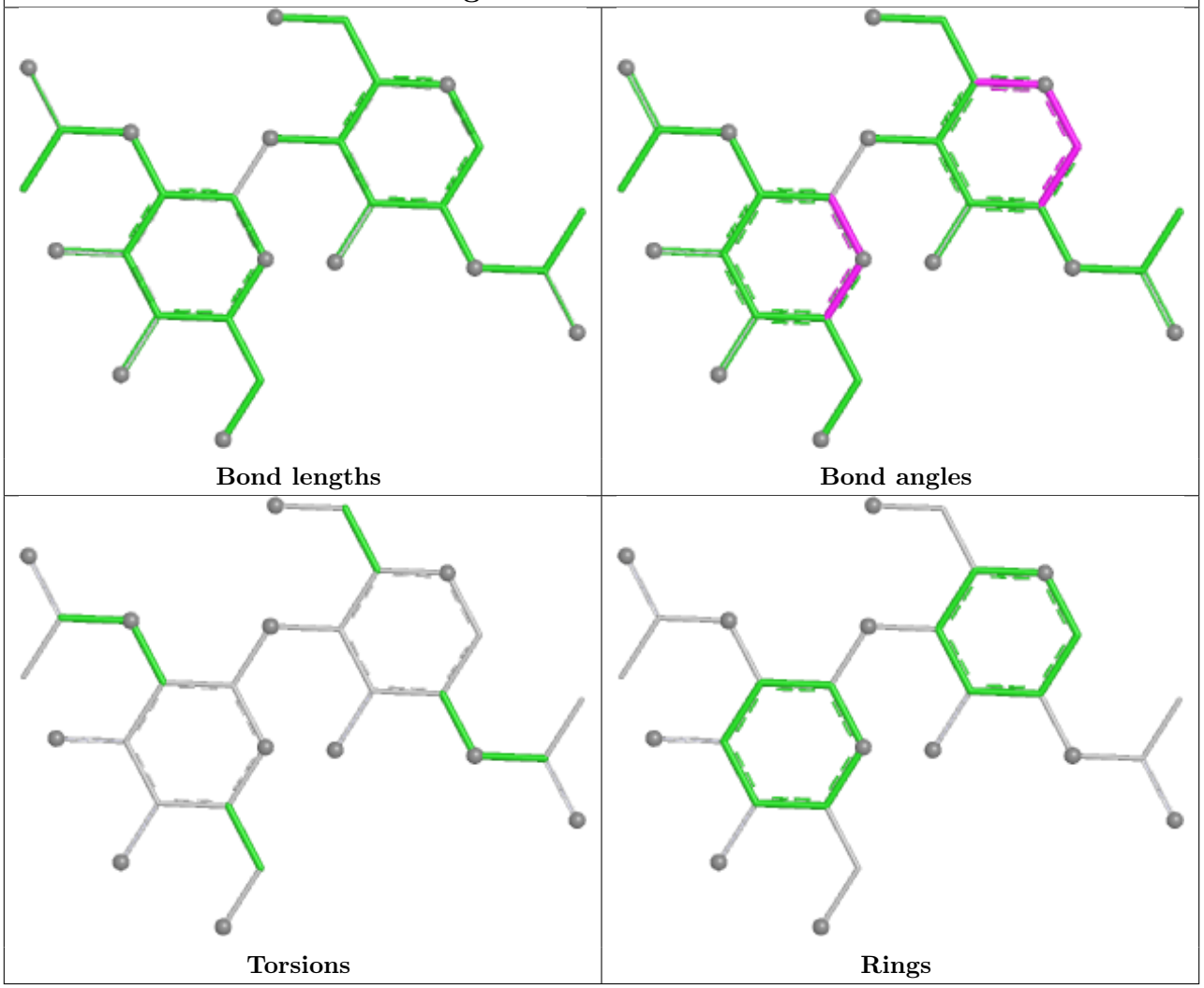


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	NAG	A	908	1	14,14,15	0.41	0	17,19,21	1.29	3 (17%)
4	NAG	B	904	1	14,14,15	0.32	0	17,19,21	1.10	2 (11%)
4	NAG	D	907	1	14,14,15	0.41	0	17,19,21	1.38	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	905	1	14,14,15	0.33	0	17,19,21	1.09	2 (11%)
4	NAG	D	904	1	14,14,15	0.30	0	17,19,21	1.15	2 (11%)
4	NAG	C	904	1	14,14,15	0.33	0	17,19,21	1.12	2 (11%)
4	NAG	A	904	1	14,14,15	0.32	0	17,19,21	1.19	3 (17%)
4	NAG	A	905	1	14,14,15	0.39	0	17,19,21	1.21	1 (5%)

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
4	NAG	A	908	1	-	1/6/23/26	0/1/1/1
4	NAG	B	904	1	-	1/6/23/26	0/1/1/1
4	NAG	D	907	1	-	3/6/23/26	0/1/1/1
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
4	NAG	D	904	1	-	1/6/23/26	0/1/1/1
4	NAG	C	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	905	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	907	NAG	C1-O5-C5	4.60	118.35	112.19
4	A	908	NAG	O5-C1-C2	-3.99	105.11	111.29
4	A	905	NAG	C1-O5-C5	3.64	117.07	112.19
4	D	904	NAG	O5-C1-C2	-3.25	106.26	111.29
4	A	904	NAG	O5-C1-C2	-3.16	106.40	111.29

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	907	NAG	O5-C5-C6-O6
4	D	907	NAG	C4-C5-C6-O6
4	A	905	NAG	O5-C5-C6-O6
4	A	905	NAG	C4-C5-C6-O6
4	A	908	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	907	NAG	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	765/840 (91%)	-0.04	17 (2%)	62	52	28, 66, 114, 148	1 (0%)
1	B	759/840 (90%)	0.39	20 (2%)	57	47	56, 93, 127, 150	1 (0%)
1	C	742/840 (88%)	0.26	24 (3%)	50	40	43, 82, 126, 168	1 (0%)
1	D	781/840 (92%)	-0.07	16 (2%)	65	56	30, 61, 102, 130	1 (0%)
All	All	3047/3360 (90%)	0.13	77 (2%)	58	48	28, 76, 121, 168	4 (0%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	669	VAL	5.0
1	B	652	GLY	4.8
1	C	101	SER	4.5
1	D	474	GLY	4.3
1	D	110	GLU	4.0

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
2	NAG	G	2	14/15	0.76	0.12	112,115,124,125	0
2	NAG	J	2	14/15	0.76	0.15	109,112,119,119	0

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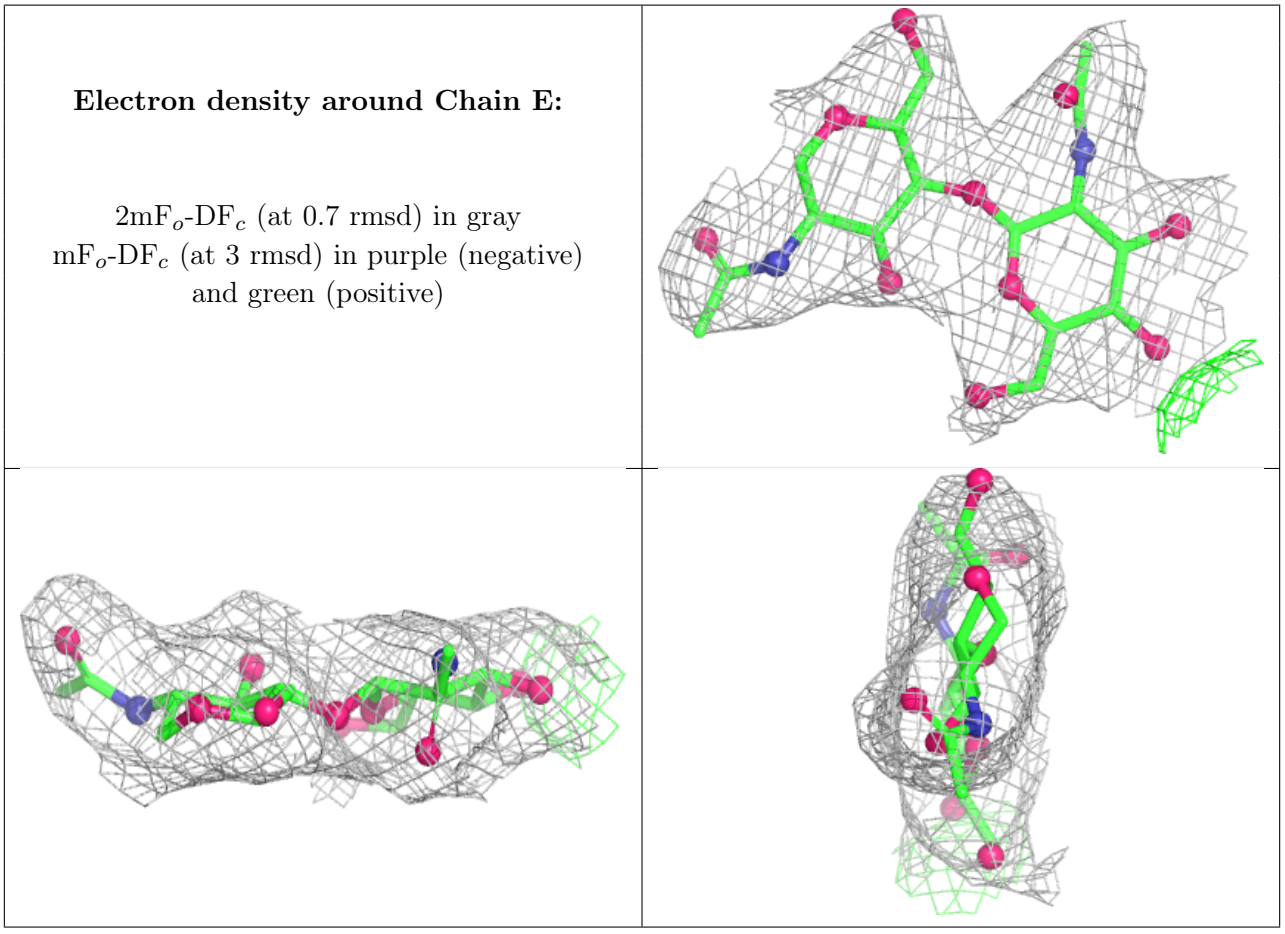
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	H	2	14/15	0.80	0.12	103,108,111,113	0
2	NAG	K	2	14/15	0.83	0.12	63,71,78,82	0
2	NAG	I	2	14/15	0.84	0.09	68,72,82,87	0
2	NAG	E	2	14/15	0.85	0.09	79,86,96,98	0
2	NAG	G	1	14/15	0.86	0.09	95,101,108,111	0
2	NAG	H	1	14/15	0.90	0.10	87,92,99,101	0
2	NAG	J	1	14/15	0.91	0.13	90,96,100,103	0
2	NAG	E	1	14/15	0.93	0.08	56,62,69,74	0
2	NAG	K	1	14/15	0.94	0.10	43,55,60,63	0
2	NAG	F	2	14/15	0.94	0.08	49,61,67,67	0
2	NAG	F	1	14/15	0.96	0.06	36,43,51,57	0
2	NAG	I	1	14/15	0.97	0.06	53,58,62,63	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.

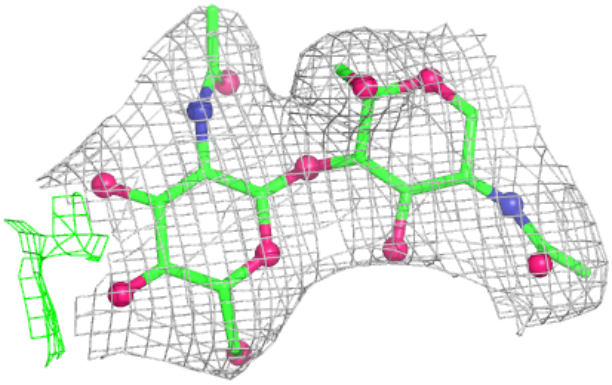
Electron density around Chain E:

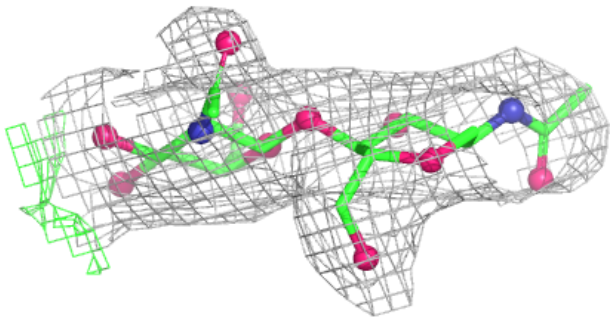
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

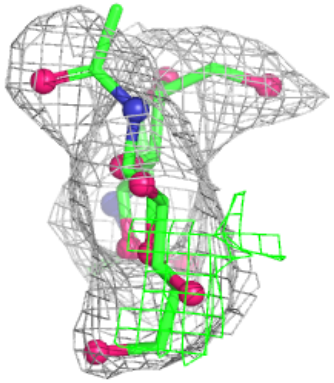


Electron density around Chain F:

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

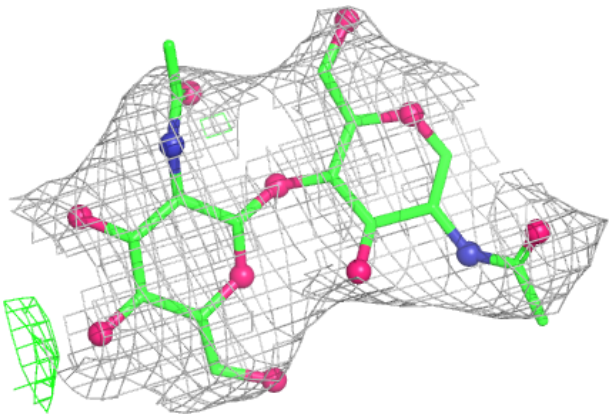


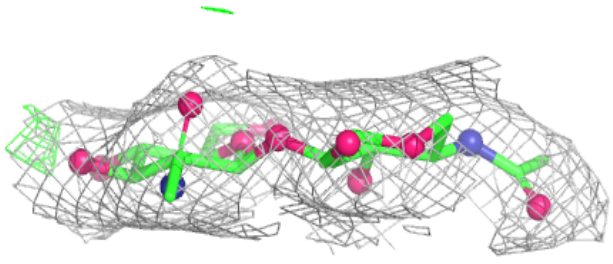


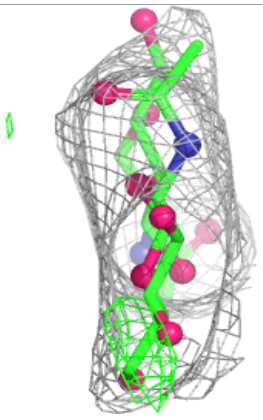


Electron density around Chain G:

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

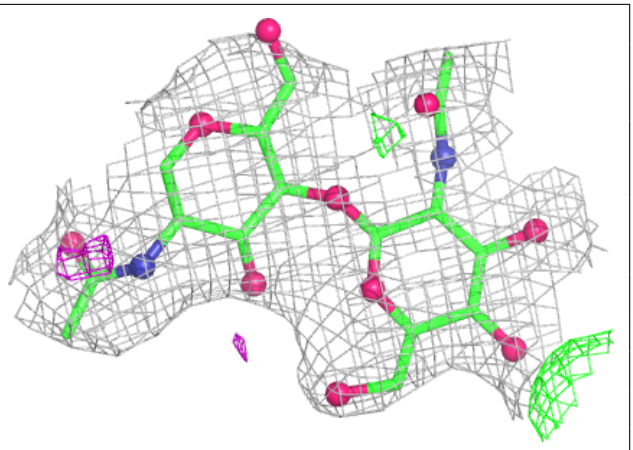


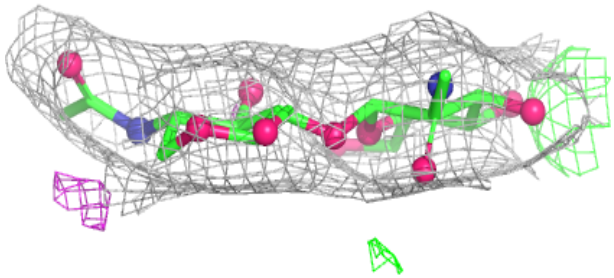


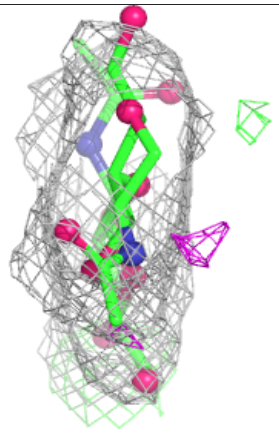


Electron density around Chain H:

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

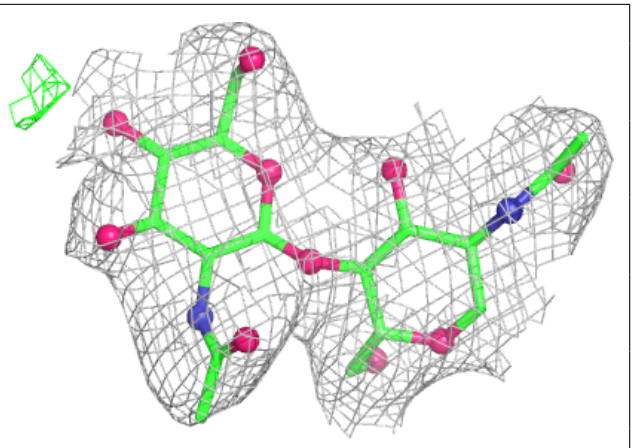


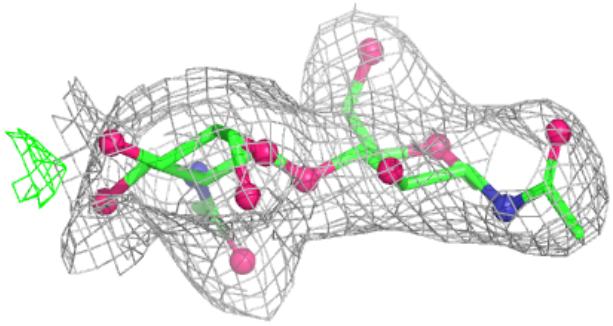


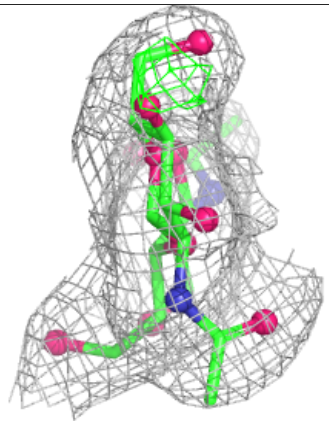


Electron density around Chain I:

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

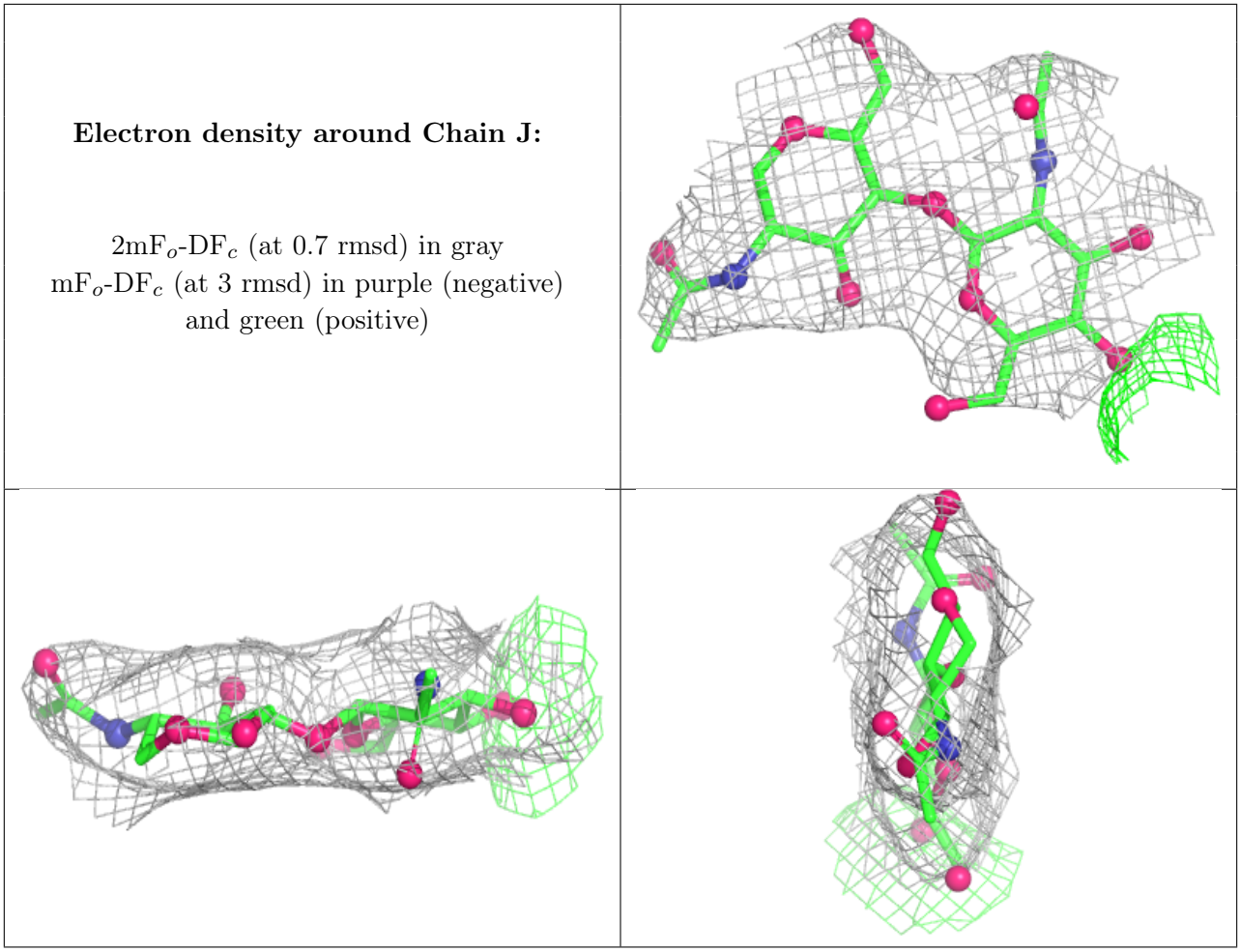






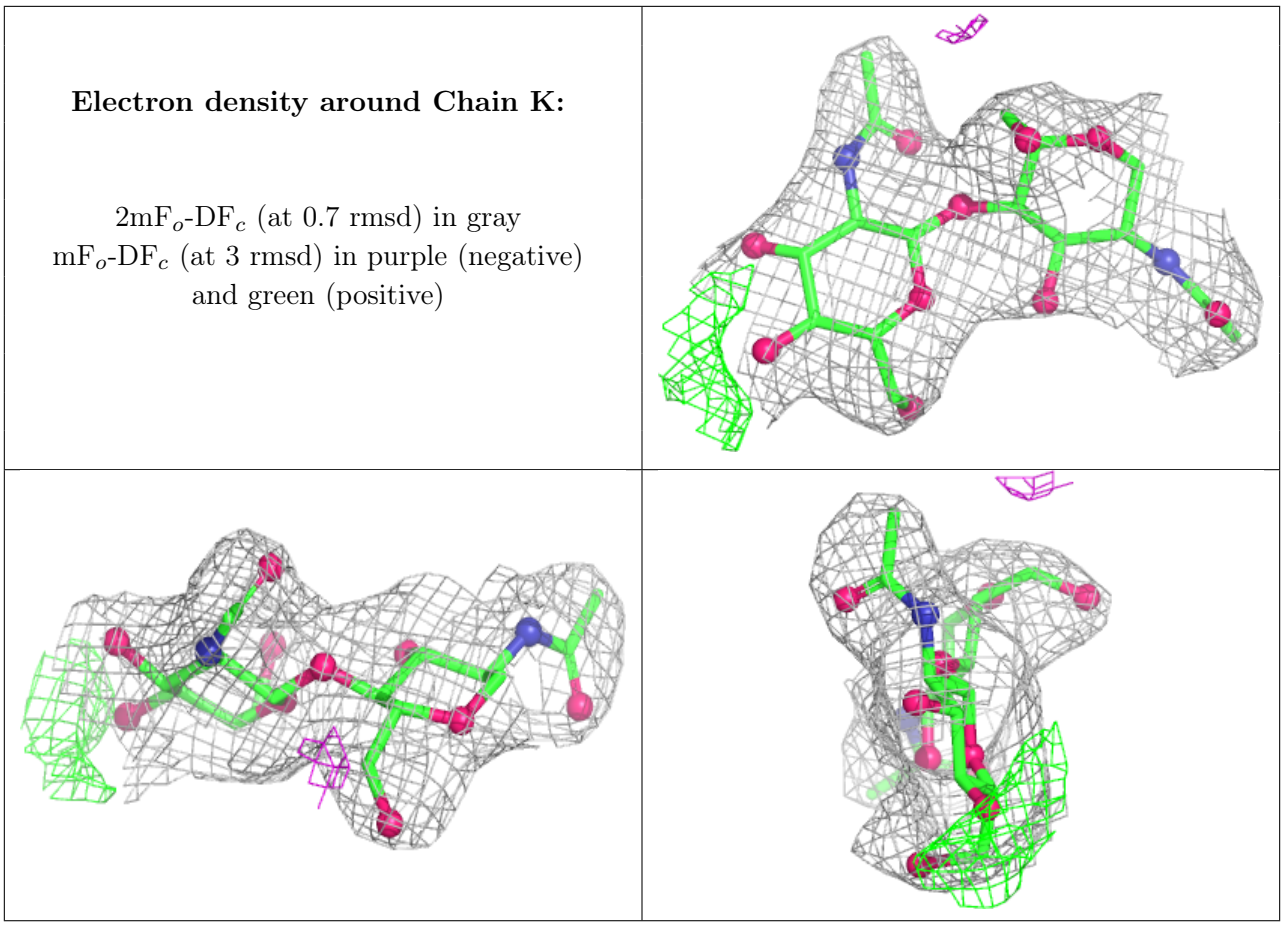
Electron density around Chain J:

$2mF_o$-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, 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	NAG	A	908	14/15	0.67	0.11	96,103,112,113	0
4	NAG	D	907	14/15	0.76	0.11	77,84,89,91	0
4	NAG	A	905	14/15	0.81	0.10	45,62,74,75	0
4	NAG	B	904	14/15	0.82	0.13	117,120,124,124	0
4	NAG	C	904	14/15	0.84	0.11	74,86,94,97	0
4	NAG	B	905	14/15	0.84	0.13	79,85,91,92	0
4	NAG	D	904	14/15	0.87	0.12	58,65,73,76	0
4	NAG	A	904	14/15	0.90	0.10	63,70,73,75	0
3	CA	D	901	1/1	0.91	0.07	102,102,102,102	0
3	CA	B	901	1/1	0.97	0.03	95,95,95,95	0
3	CA	A	901	1/1	0.97	0.04	72,72,72,72	0
3	CA	C	901	1/1	0.98	0.07	87,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.