wwPDB X-ray Structure Validation Summary Report (i)

Mar 31, 2025 – 08:27 PM JST

PDB ID	:	5EGE / pdb_00005ege
Title	:	Structure of ENPP6, a choline-specific glycerophosphodiester-phosphodiesterase
Authors	:	Morita, J.; Kano, K.; Kato, K.; Takita, H.; Ishitani, R.; Nishimasu, H.; Nureki, O.; Aoki, J.
Deposited on	:	2015-10-27
Resolution	:	2.00 Å(reported)

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

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

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

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

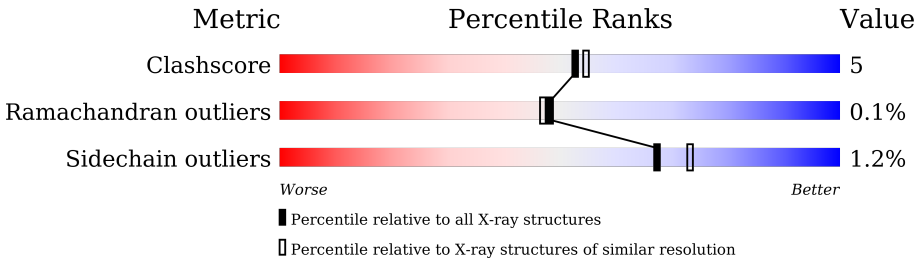
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.00 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))
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	429	84% 7% 9%
1	B	429	80% 11% 9%
1	C	429	81% 10% 9%
1	D	429	81% 10% 9%
2	E	3	33% 33% 33%
2	G	3	67% 33%
2	I	3	33% 67%
2	K	3	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	2	100%
3	H	2	50% 50%
3	J	2	50% 50%
3	L	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15249 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 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3201	2059	548	575	19			
1	B	392	Total	C	N	O	S	0	0	0
			3201	2059	548	575	19			
1	C	392	Total	C	N	O	S	0	1	0
			3204	2061	548	576	19			
1	D	392	Total	C	N	O	S	0	0	0
			3201	2059	548	575	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	ALA	CYS	engineered mutation	UNP Q8BGN3
A	412	SER	CYS	engineered mutation	UNP Q8BGN3
A	422	SER	-	expression tag	UNP Q8BGN3
A	423	ARG	-	expression tag	UNP Q8BGN3
A	424	GLU	-	expression tag	UNP Q8BGN3
A	425	ASN	-	expression tag	UNP Q8BGN3
A	426	LEU	-	expression tag	UNP Q8BGN3
A	427	TYR	-	expression tag	UNP Q8BGN3
A	428	PHE	-	expression tag	UNP Q8BGN3
A	429	GLN	-	expression tag	UNP Q8BGN3
B	393	ALA	CYS	engineered mutation	UNP Q8BGN3
B	412	SER	CYS	engineered mutation	UNP Q8BGN3
B	422	SER	-	expression tag	UNP Q8BGN3
B	423	ARG	-	expression tag	UNP Q8BGN3
B	424	GLU	-	expression tag	UNP Q8BGN3
B	425	ASN	-	expression tag	UNP Q8BGN3
B	426	LEU	-	expression tag	UNP Q8BGN3
B	427	TYR	-	expression tag	UNP Q8BGN3
B	428	PHE	-	expression tag	UNP Q8BGN3
B	429	GLN	-	expression tag	UNP Q8BGN3

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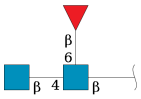
Chain	Residue	Modelled	Actual	Comment	Reference
C	393	ALA	CYS	engineered mutation	UNP Q8BGN3
C	412	SER	CYS	engineered mutation	UNP Q8BGN3
C	422	SER	-	expression tag	UNP Q8BGN3
C	423	ARG	-	expression tag	UNP Q8BGN3
C	424	GLU	-	expression tag	UNP Q8BGN3
C	425	ASN	-	expression tag	UNP Q8BGN3
C	426	LEU	-	expression tag	UNP Q8BGN3
C	427	TYR	-	expression tag	UNP Q8BGN3
C	428	PHE	-	expression tag	UNP Q8BGN3
C	429	GLN	-	expression tag	UNP Q8BGN3
D	393	ALA	CYS	engineered mutation	UNP Q8BGN3
D	412	SER	CYS	engineered mutation	UNP Q8BGN3
D	422	SER	-	expression tag	UNP Q8BGN3
D	423	ARG	-	expression tag	UNP Q8BGN3
D	424	GLU	-	expression tag	UNP Q8BGN3
D	425	ASN	-	expression tag	UNP Q8BGN3
D	426	LEU	-	expression tag	UNP Q8BGN3
D	427	TYR	-	expression tag	UNP Q8BGN3
D	428	PHE	-	expression tag	UNP Q8BGN3
D	429	GLN	-	expression tag	UNP Q8BGN3

- Molecule 2 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.

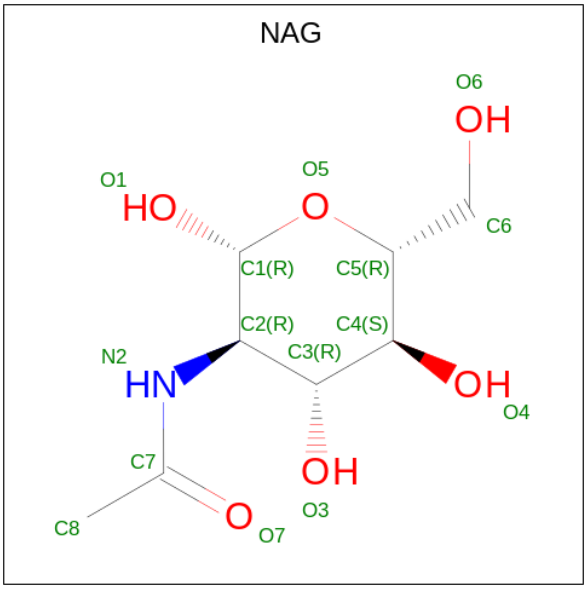


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	F	2	Total C N O 28 16 2 10	0	0	0
3	H	2	Total C N O 28 16 2 10	0	0	0
3	J	2	Total C N O 28 16 2 10	0	0	0
3	L	2	Total C N O 28 16 2 10	0	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	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

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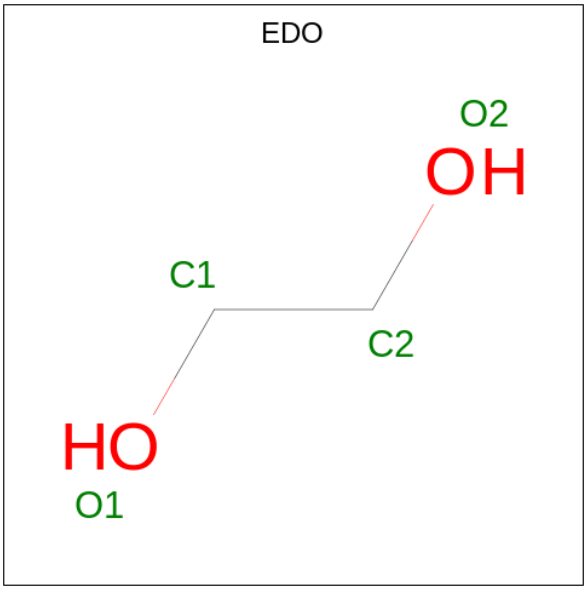
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	C	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	526	Total O 526 526	0	0
7	B	551	Total O 551 551	0	0
7	C	467	Total O 467 467	0	0
7	D	504	Total O 504 504	0	0

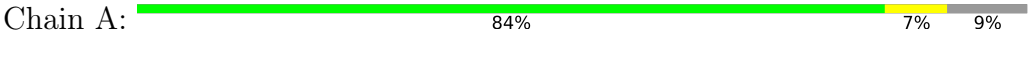
3 Residue-property plots (i)

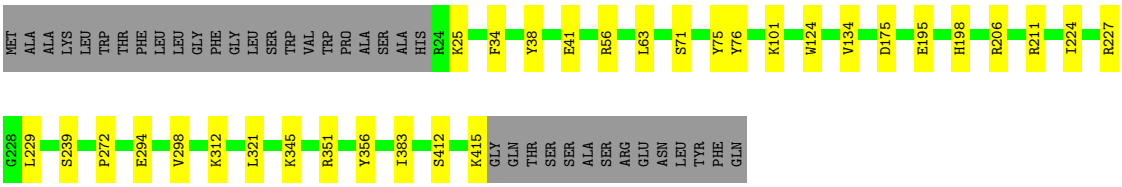
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6

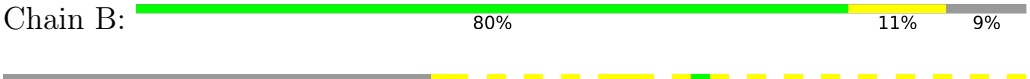
Chain A:

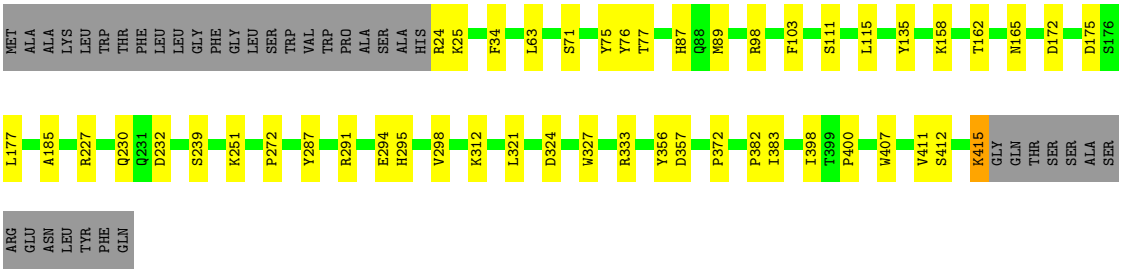




• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6

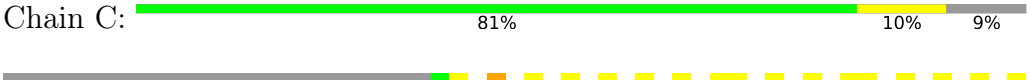
Chain B:





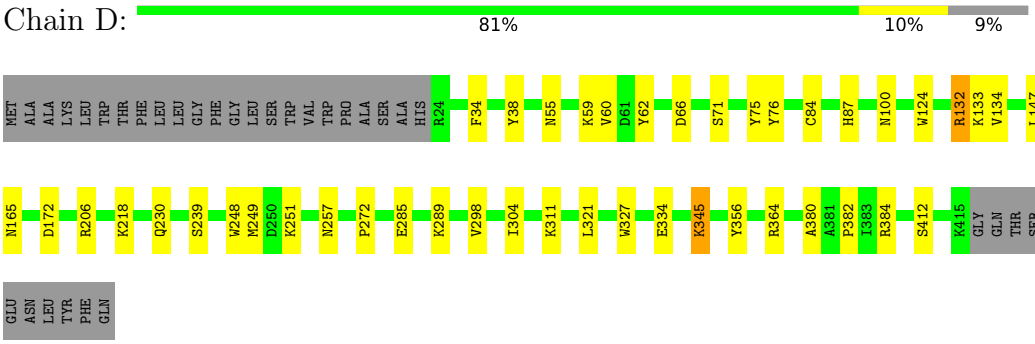
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6

Chain C:



• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 6

Chain D:



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

Chain E:

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

Chain G:

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

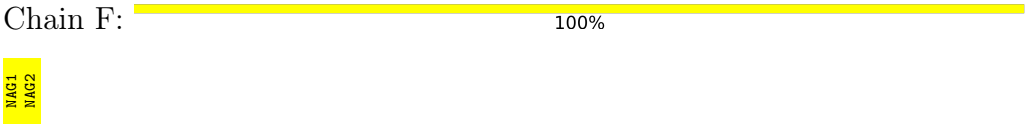
Chain I:

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

Chain K:

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

Chain F:



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

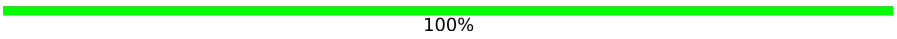
Chain H:

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

Chain J:

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

Chain L:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.29Å 78.24Å 103.64Å 90.04° 89.98° 114.61°	Depositor
Resolution (Å)	41.90 – 2.00	Depositor
% Data completeness (in resolution range)	96.8 (41.90-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10_2155: 000)	Depositor
R, R_{free}	0.167 , 0.206	Depositor
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.566	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l 0.437 for -h,-k,l 0.021 for -h,h+k,-l	Xtriage
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: ZN, EDO, NAG, FUL

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	0.37	0/3294	0.55	0/4473
1	B	0.38	0/3294	0.55	0/4473
1	C	0.39	1/3300 (0.0%)	0.54	0/4481
1	D	0.37	0/3294	0.53	0/4473
All	All	0.37	1/13182 (0.0%)	0.54	0/17900

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	336	LEU	C-N	6.51	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3201	0	3130	23	0
1	B	3201	0	3130	32	0
1	C	3204	0	3133	32	0
1	D	3201	0	3131	33	0
2	E	38	0	34	1	0
2	G	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	38	0	33	5	0
2	K	38	0	34	2	0
3	F	28	0	25	1	0
3	H	28	0	25	1	0
3	J	28	0	25	1	0
3	L	28	0	25	0	0
4	A	28	0	26	0	0
4	B	28	0	26	1	0
4	C	28	0	26	0	0
4	D	14	0	13	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	8	0	12	2	0
6	B	4	0	6	0	0
6	C	8	0	12	2	0
6	D	4	0	6	0	0
7	A	526	0	0	12	1
7	B	551	0	0	12	4
7	C	467	0	0	15	1
7	D	504	0	0	14	4
All	All	15249	0	12886	128	5

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 128 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:218:LYS:NZ	7:C:604:HOH:O	2.02	0.92
1:A:198:HIS:HE2	6:A:511:EDO:HO2	0.95	0.88
1:C:285:GLU:OE1	7:C:601:HOH:O	1.91	0.88
1:C:415:LYS:O	7:C:603:HOH:O	2.00	0.79
1:B:291:ARG:NH1	1:B:298:VAL:O	2.16	0.78

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:646:HOH:O	7:D:819:HOH:O[1_545]	2.05	0.15
7:B:1021:HOH:O	7:D:897:HOH:O[1_445]	2.09	0.11
7:A:929:HOH:O	7:B:1023:HOH:O[1_556]	2.14	0.06
7:C:991:HOH:O	7:D:960:HOH:O[1_546]	2.16	0.04
7:B:982:HOH:O	7:D:740:HOH:O[1_655]	2.19	0.01

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	390/429 (91%)	375 (96%)	15 (4%)	0	100	100
1	B	390/429 (91%)	376 (96%)	13 (3%)	1 (0%)	37	35
1	C	391/429 (91%)	375 (96%)	15 (4%)	1 (0%)	37	35
1	D	390/429 (91%)	376 (96%)	14 (4%)	0	100	100
All	All	1561/1716 (91%)	1502 (96%)	57 (4%)	2 (0%)	48	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	ASP
1	C	344	GLY

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	348/377 (92%)	346 (99%)	2 (1%)	84	88
1	B	348/377 (92%)	344 (99%)	4 (1%)	70	76
1	C	349/377 (93%)	343 (98%)	6 (2%)	56	61
1	D	348/377 (92%)	343 (99%)	5 (1%)	62	68
All	All	1393/1508 (92%)	1376 (99%)	17 (1%)	67	73

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	132	ARG
1	D	345	LYS
1	C	66	ASP
1	C	76	TYR
1	C	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	165	ASN
1	C	288	HIS
1	D	165	ASN
1	B	165	ASN
1	B	87	HIS

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)

20 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	0.45	0	17,19,21	1.33	1 (5%)
2	NAG	E	2	2	14,14,15	0.25	0	17,19,21	0.41	0
2	FUL	E	3	2	10,10,11	1.35	1 (10%)	14,14,16	1.86	2 (14%)
3	NAG	F	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	1.20	1 (5%)
3	NAG	F	2	3	14,14,15	0.22	0	17,19,21	0.52	0
2	NAG	G	1	1,2	14,14,15	0.53	0	17,19,21	0.72	0
2	NAG	G	2	2	14,14,15	0.21	0	17,19,21	0.54	0
2	FUL	G	3	2	10,10,11	1.58	2 (20%)	14,14,16	1.77	2 (14%)
3	NAG	H	1	1,3	14,14,15	0.44	0	17,19,21	0.59	0
3	NAG	H	2	3	14,14,15	0.34	0	17,19,21	0.60	0
2	NAG	I	1	1,2	14,14,15	0.51	0	17,19,21	1.61	2 (11%)
2	NAG	I	2	2	14,14,15	0.18	0	17,19,21	0.39	0
2	FUL	I	3	1,2	10,10,11	1.31	1 (10%)	14,14,16	1.77	4 (28%)
3	NAG	J	1	1,3	14,14,15	0.53	0	17,19,21	0.61	0
3	NAG	J	2	3	14,14,15	0.34	0	17,19,21	0.51	0
2	NAG	K	1	1,2	14,14,15	0.41	0	17,19,21	0.67	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.34	0
2	FUL	K	3	2	10,10,11	1.44	3 (30%)	14,14,16	1.75	4 (28%)
3	NAG	L	1	1,3	14,14,15	0.42	0	17,19,21	0.55	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.46	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	E	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	FUL	E	3	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	FUL	G	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	FUL	I	3	1,2	-	-	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	FUL	K	3	2	-	-	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	FUL	C4-C3	3.15	1.60	1.52
3	F	1	NAG	O5-C1	-3.06	1.38	1.43
2	E	3	FUL	C4-C3	3.03	1.60	1.52
2	K	3	FUL	C4-C5	2.90	1.59	1.52
2	G	3	FUL	O5-C1	-2.87	1.39	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	FUL	C1-C2-C3	-5.38	103.06	109.67
2	G	3	FUL	C1-C2-C3	-5.06	103.45	109.67
2	I	1	NAG	C2-N2-C7	5.04	130.08	122.90
2	I	3	FUL	C1-C2-C3	-4.69	103.90	109.67
2	E	1	NAG	C2-N2-C7	4.23	128.93	122.90

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6

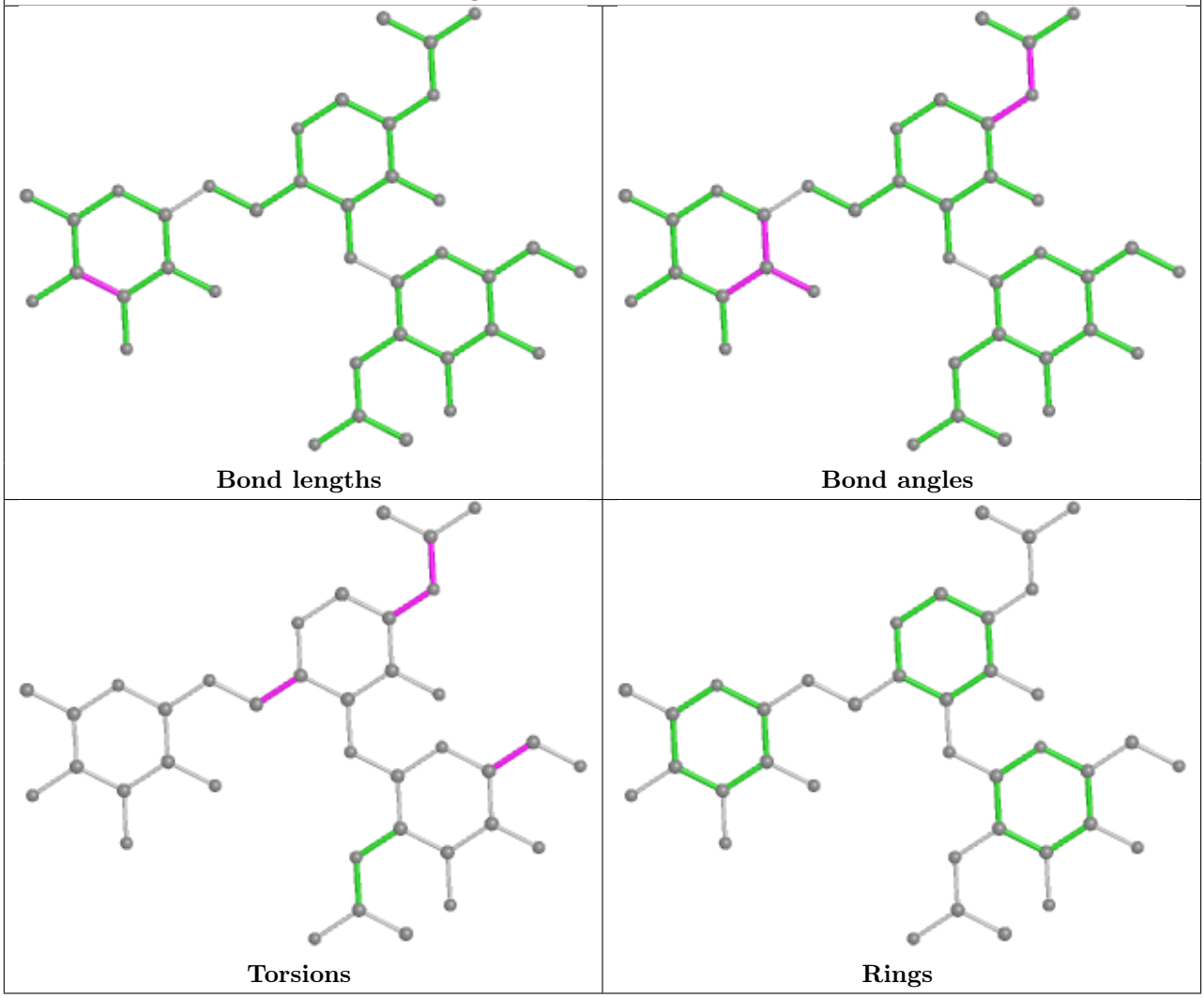
There are no ring outliers.

8 monomers are involved in 11 short contacts:

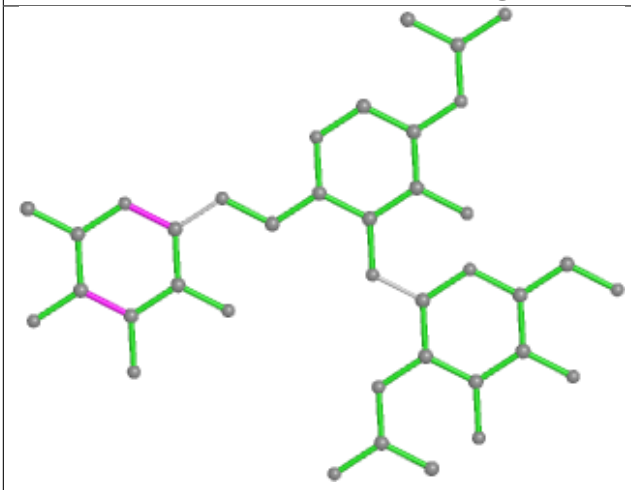
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	3	FUL	1	0
3	F	2	NAG	1	0
3	J	2	NAG	1	0
3	H	2	NAG	1	0
2	E	1	NAG	1	0
2	I	1	NAG	3	0
2	K	2	NAG	2	0
2	I	2	NAG	1	0

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

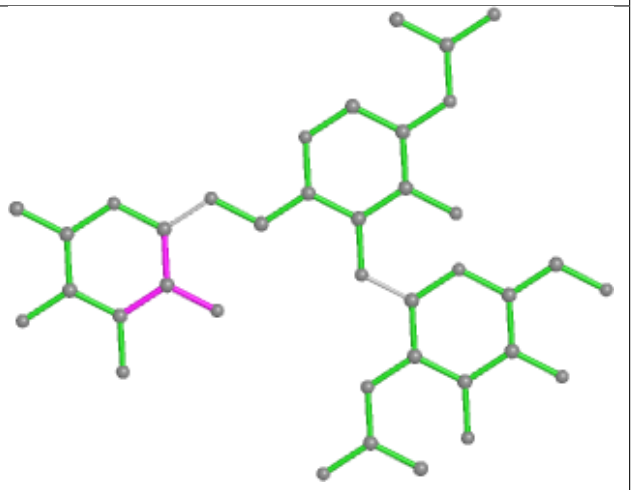
Oligosaccharide Chain E



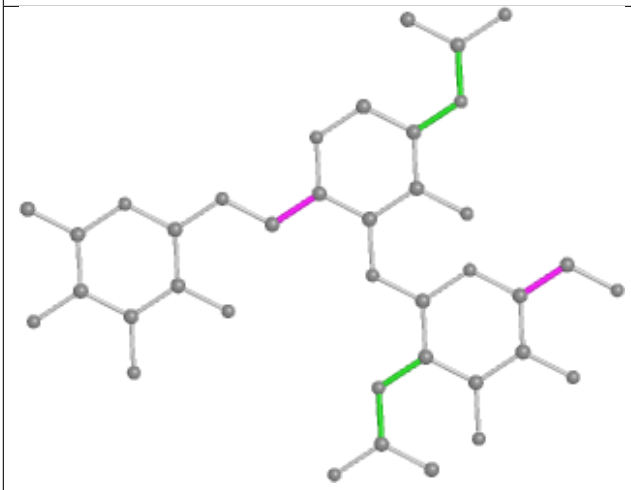
Oligosaccharide Chain G



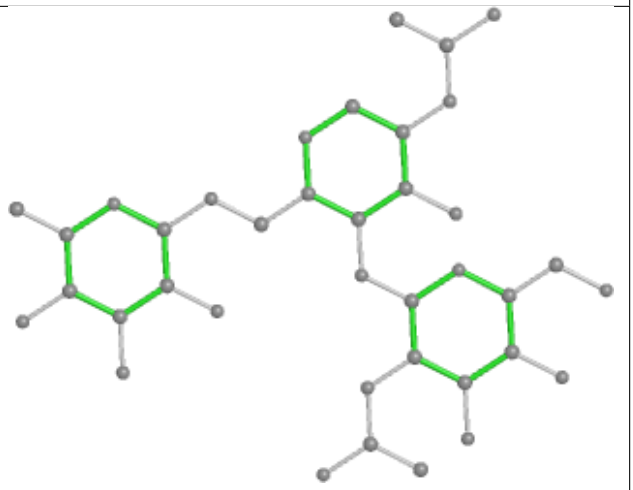
Bond lengths



Bond angles

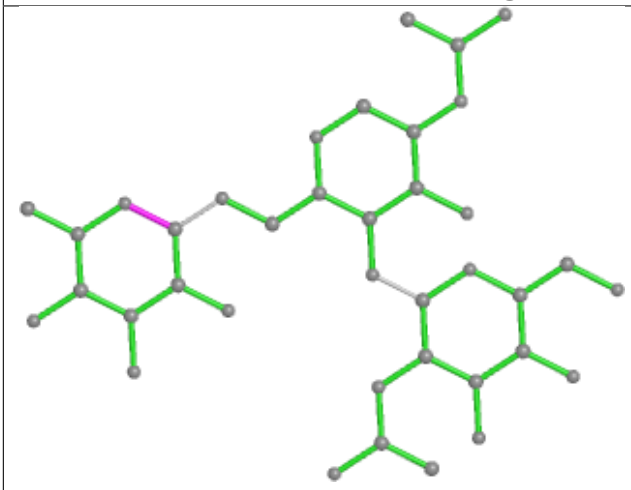


Torsions

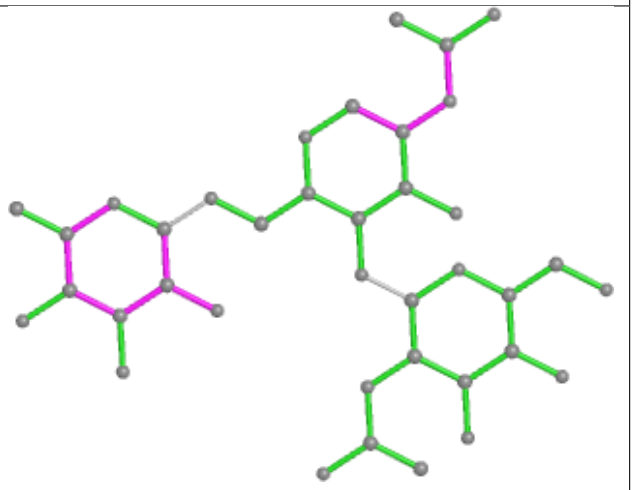


Rings

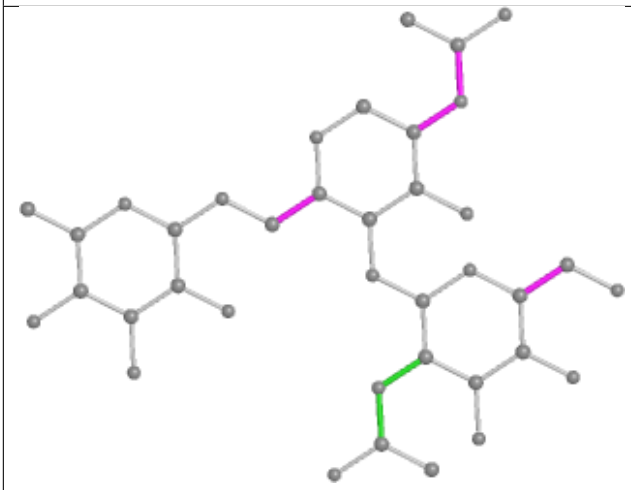
Oligosaccharide Chain I



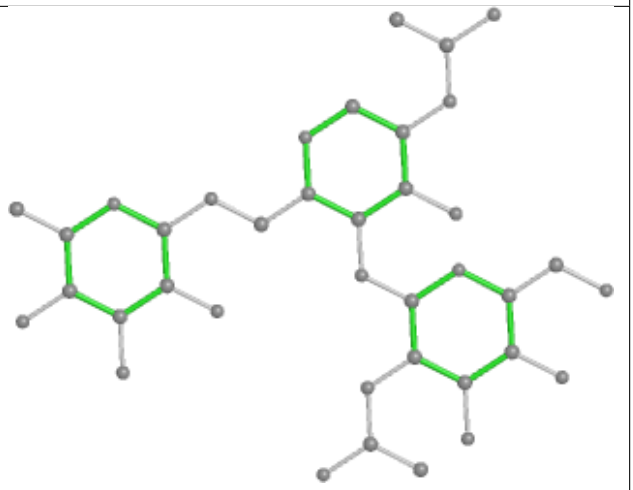
Bond lengths



Bond angles

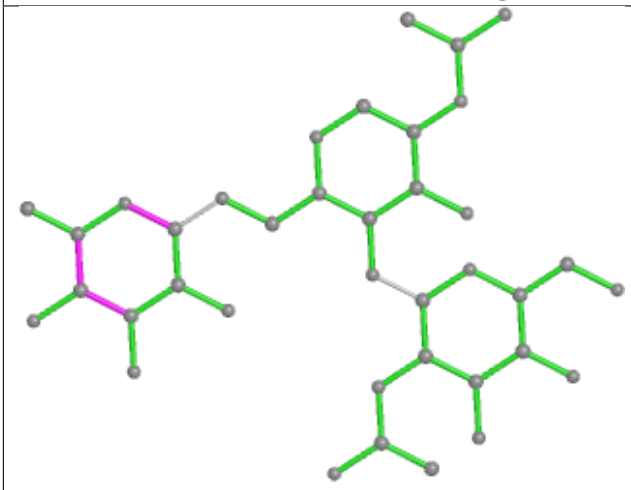


Torsions

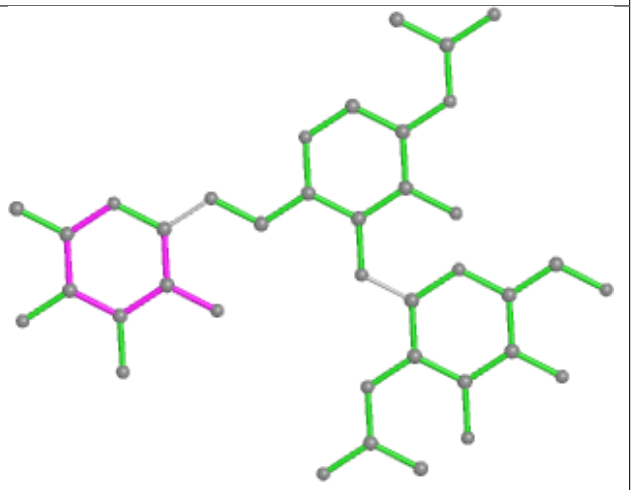


Rings

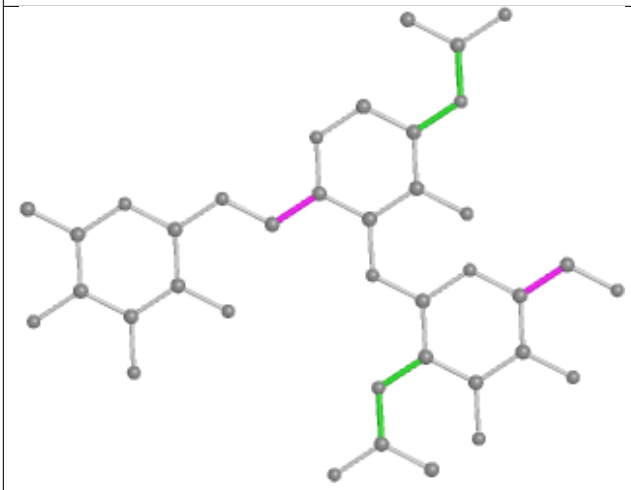
Oligosaccharide Chain K



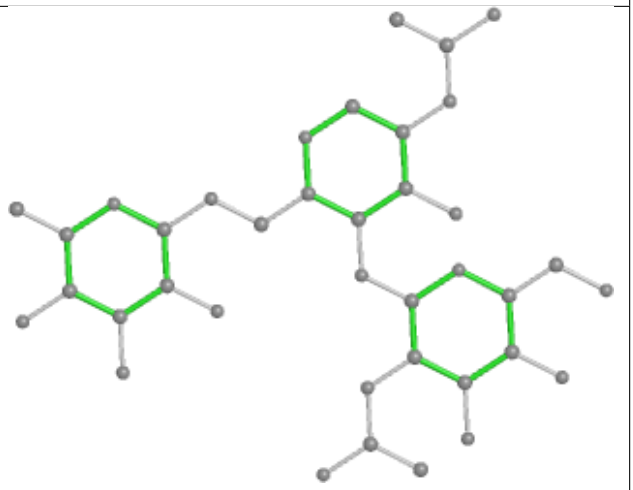
Bond lengths



Bond angles

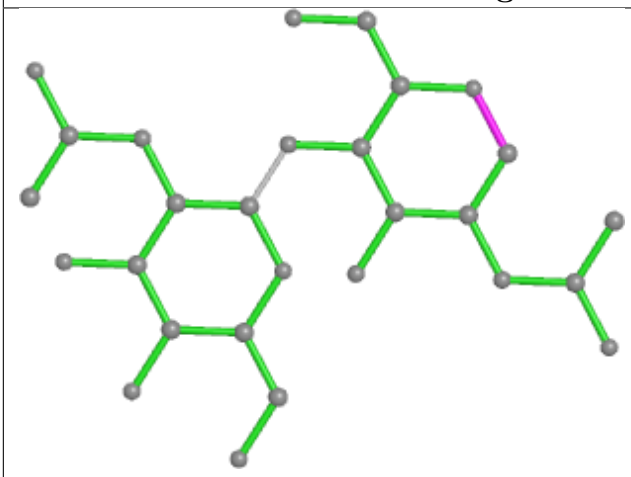


Torsions

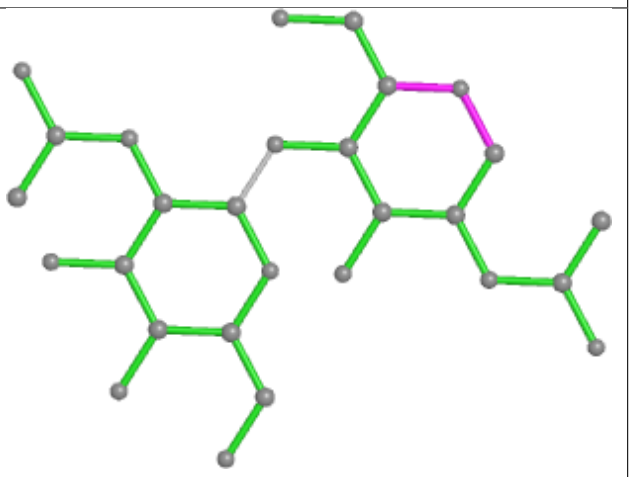


Rings

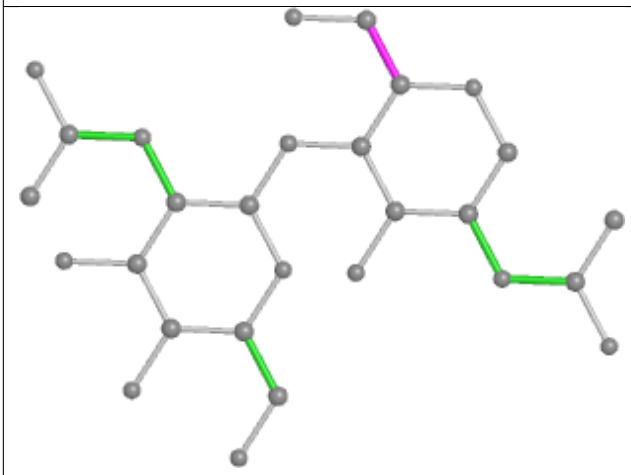
Oligosaccharide Chain F



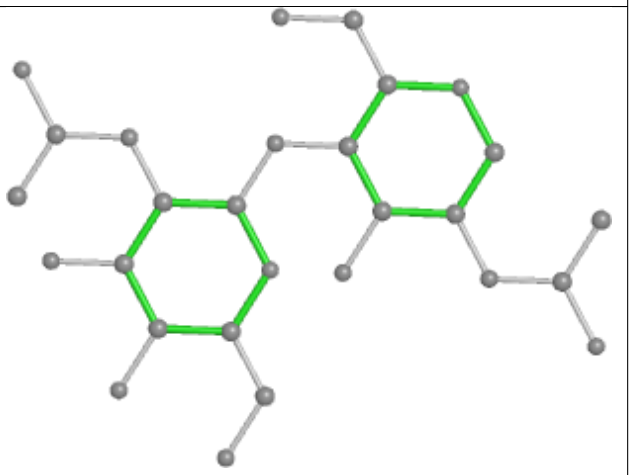
Bond lengths



Bond angles

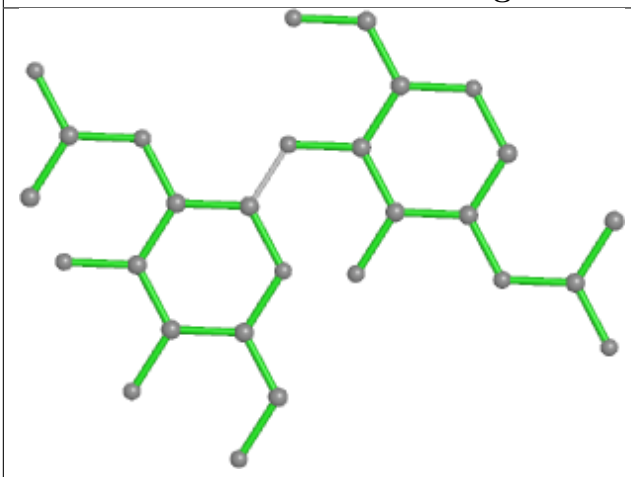


Torsions

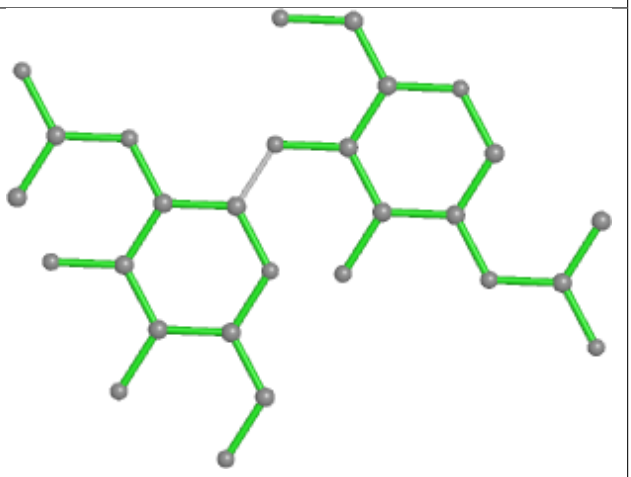


Rings

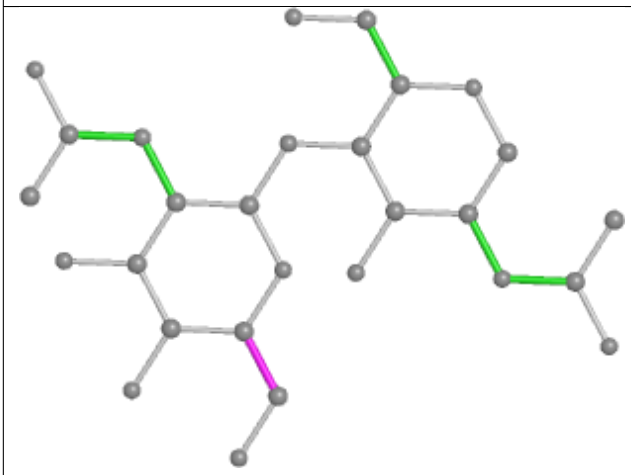
Oligosaccharide Chain H



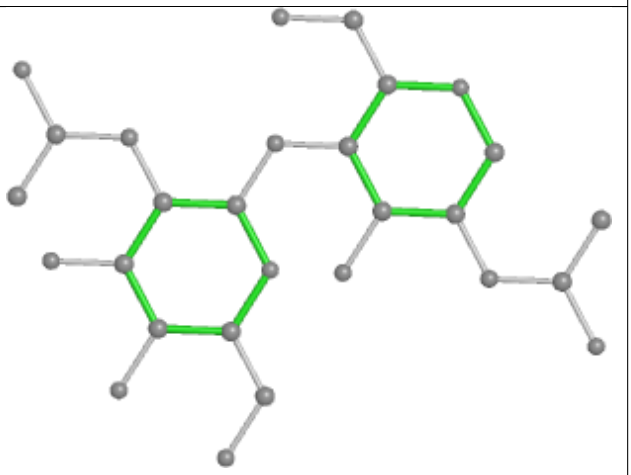
Bond lengths



Bond angles

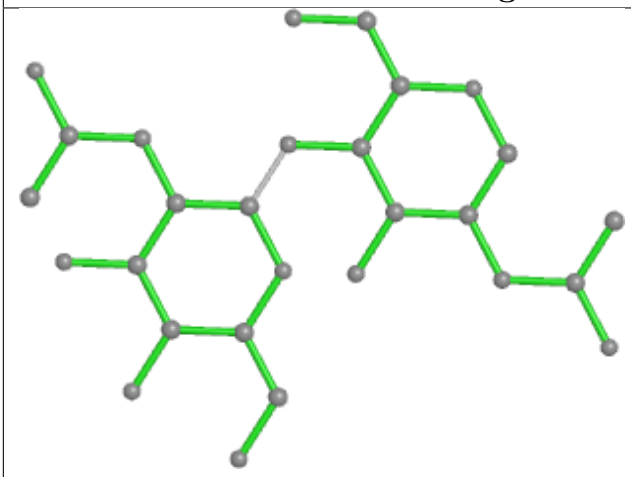


Torsions

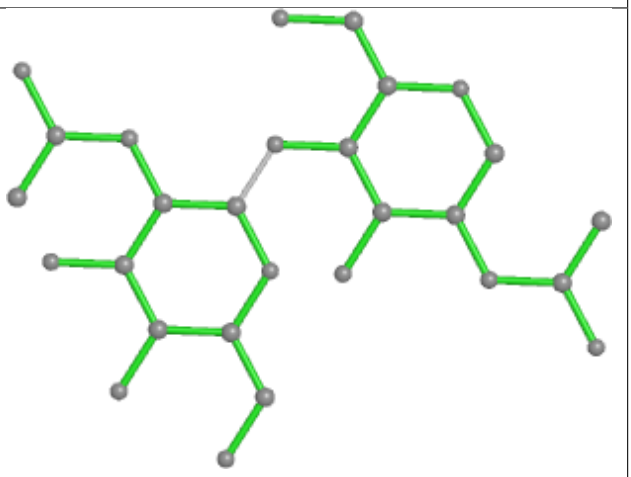


Rings

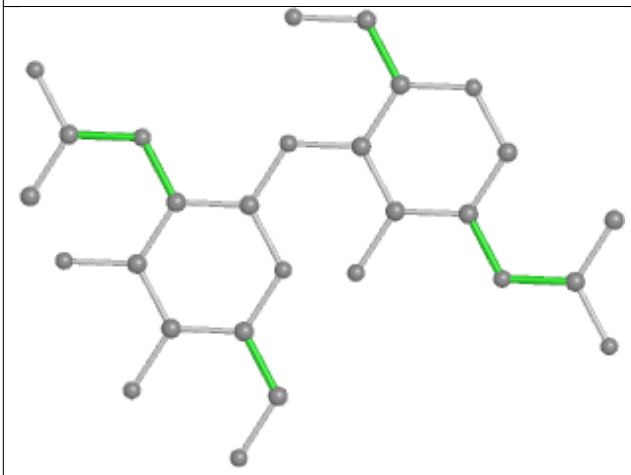
Oligosaccharide Chain J



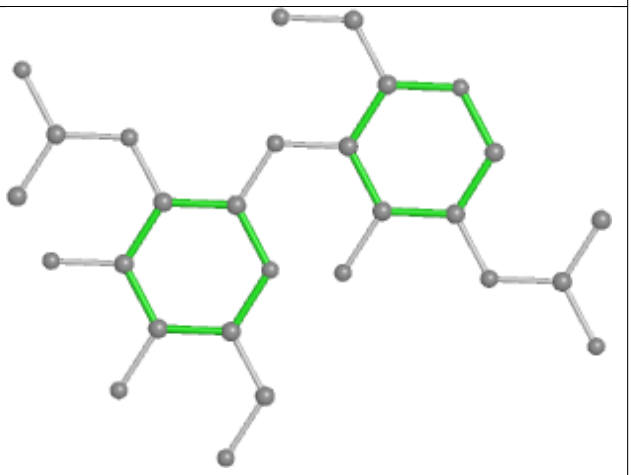
Bond lengths



Bond angles

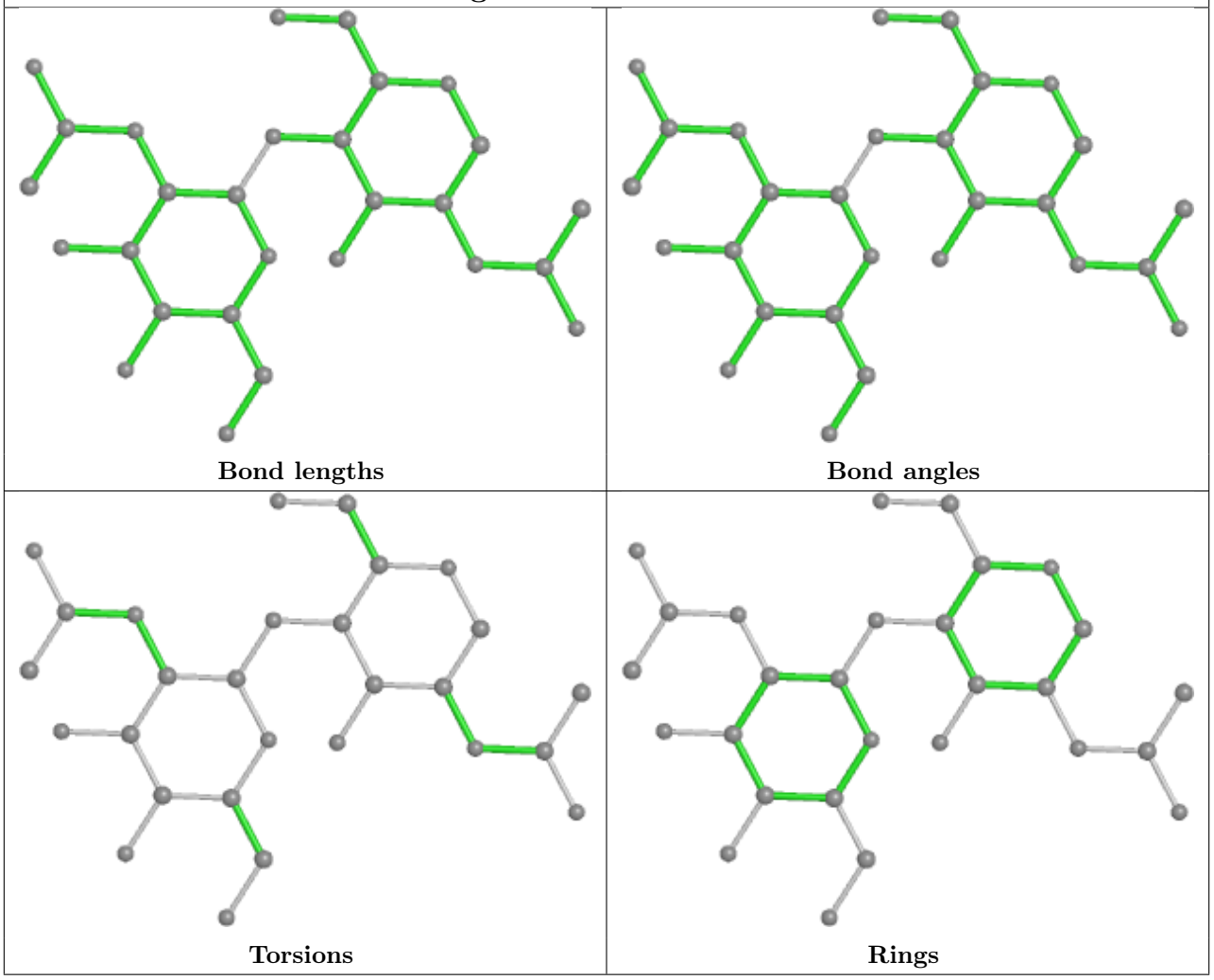


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	C	502	1	14,14,15	0.33	0	17,19,21	0.86	1 (5%)
4	NAG	B	501	1	14,14,15	0.36	0	17,19,21	0.49	0
6	EDO	D	509	-	3,3,3	0.48	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	B	510	-	3,3,3	0.50	0	2,2,2	0.35	0
6	EDO	A	510	-	3,3,3	0.50	0	2,2,2	0.26	0
6	EDO	C	511	-	3,3,3	0.50	0	2,2,2	0.26	0
6	EDO	A	511	-	3,3,3	0.44	0	2,2,2	0.51	0
4	NAG	A	502	1	14,14,15	0.20	0	17,19,21	0.69	1 (5%)
4	NAG	C	501	1	14,14,15	0.20	0	17,19,21	0.50	0
6	EDO	C	510	-	3,3,3	0.55	0	2,2,2	0.26	0
4	NAG	B	502	1	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	A	501	1	14,14,15	0.37	0	17,19,21	0.45	0
4	NAG	D	501	1	14,14,15	0.34	0	17,19,21	0.84	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	C	502	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	0/6/23/26	0/1/1/1
6	EDO	D	509	-	-	0/1/1/1	-
6	EDO	B	510	-	-	0/1/1/1	-
6	EDO	A	510	-	-	0/1/1/1	-
6	EDO	C	511	-	-	1/1/1/1	-
6	EDO	A	511	-	-	0/1/1/1	-
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	C	501	1	-	2/6/23/26	0/1/1/1
6	EDO	C	510	-	-	1/1/1/1	-
4	NAG	B	502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	D	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	502	NAG	C1-O5-C5	3.03	116.30	112.19
4	D	501	NAG	C1-O5-C5	2.56	115.66	112.19
4	A	502	NAG	C1-O5-C5	2.24	115.23	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	501	NAG	O5-C5-C6-O6
4	C	501	NAG	C4-C5-C6-O6
6	C	511	EDO	O1-C1-C2-O2
6	C	510	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	511	EDO	2	0
6	A	511	EDO	2	0
4	B	502	NAG	1	0
4	D	501	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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

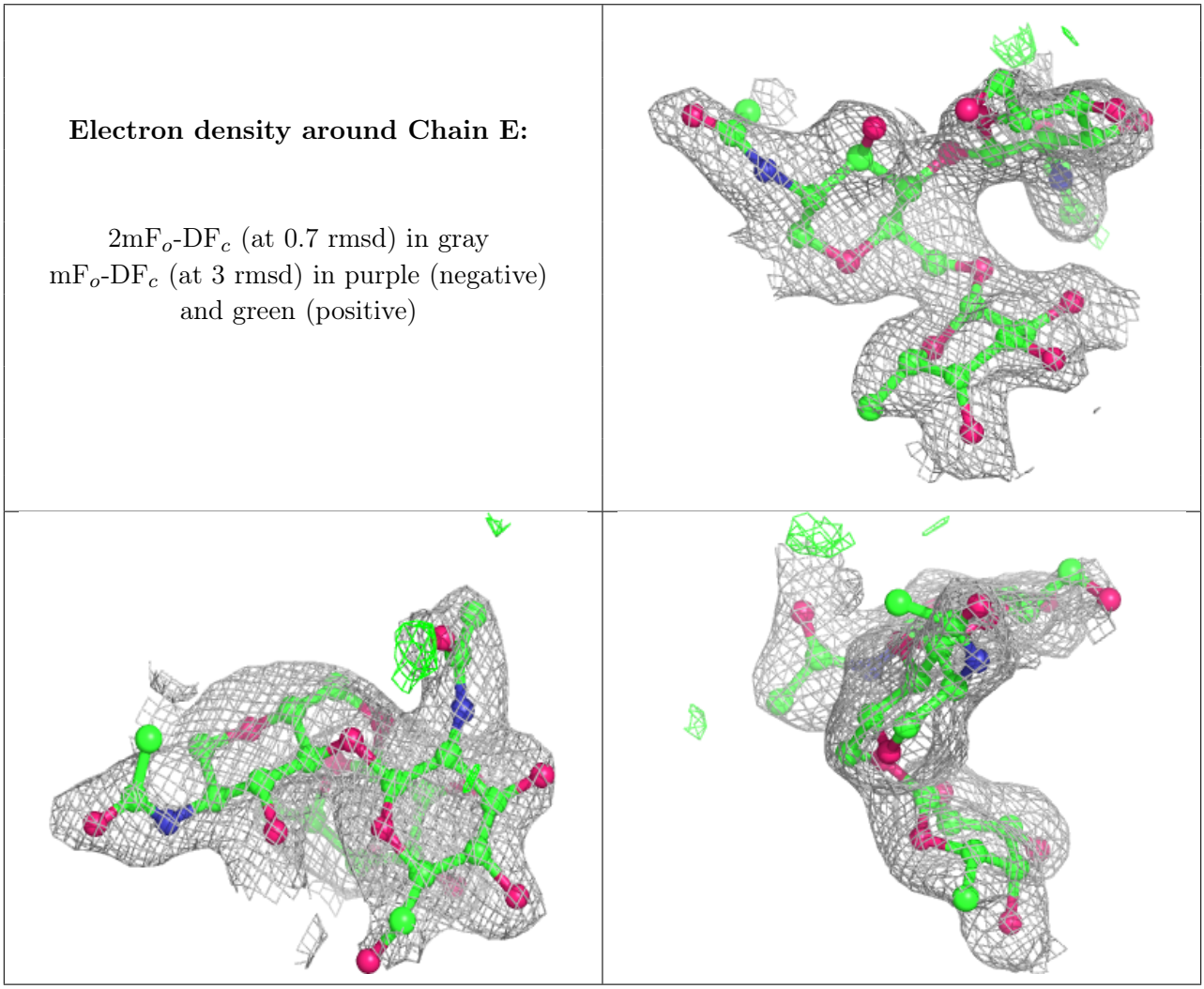
6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

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.

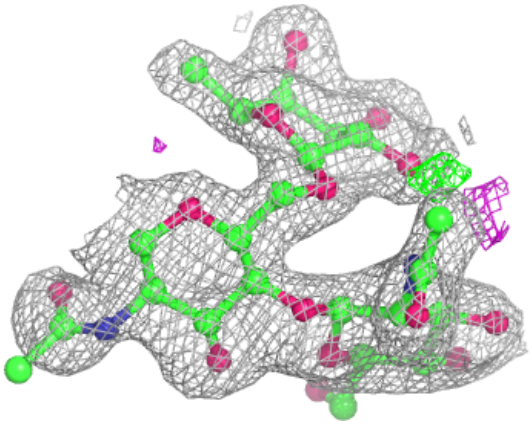
Electron density around Chain E:

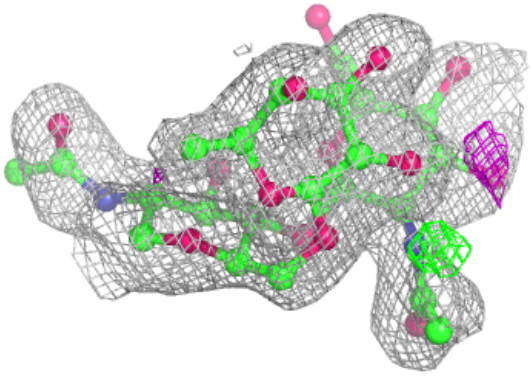
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

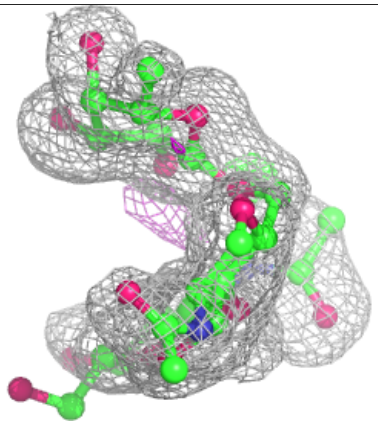


Electron density around Chain G:

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

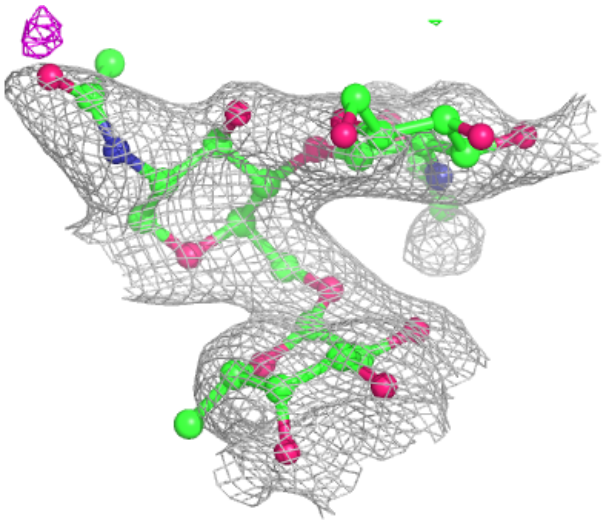


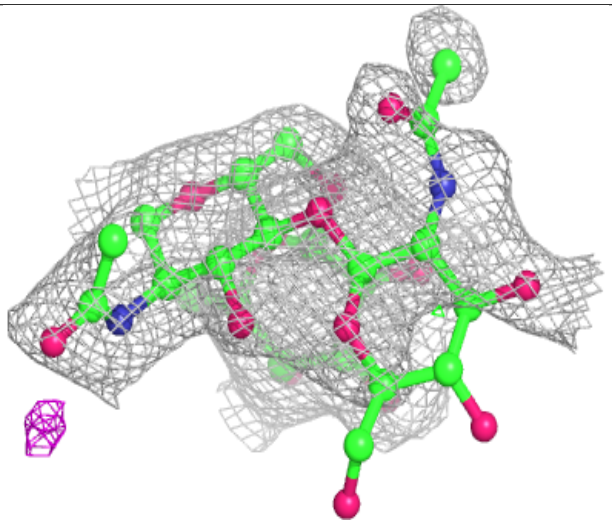


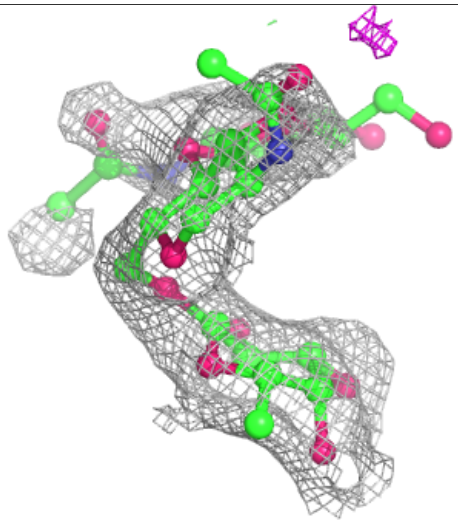


Electron density around Chain I:

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

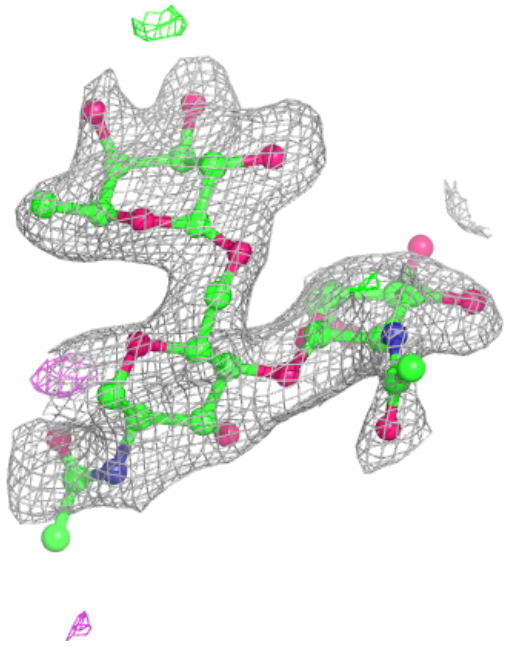


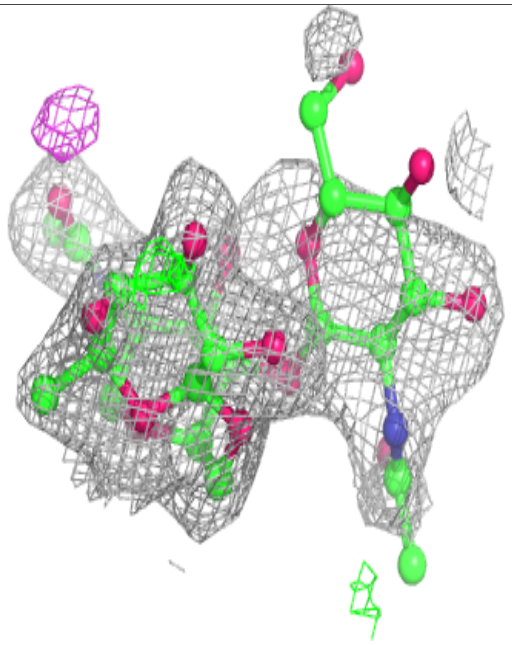


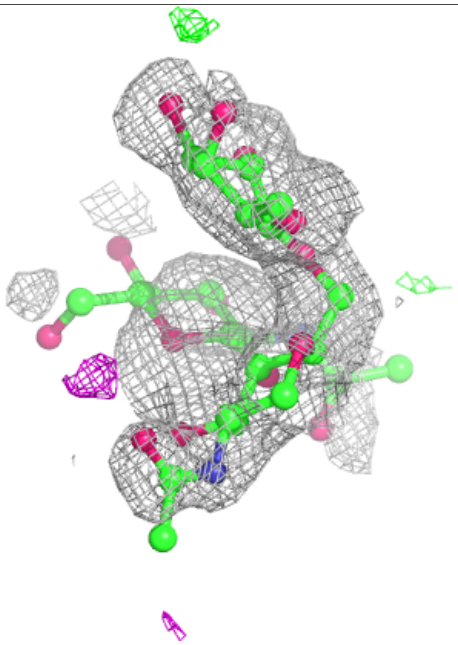


Electron density around Chain K:

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

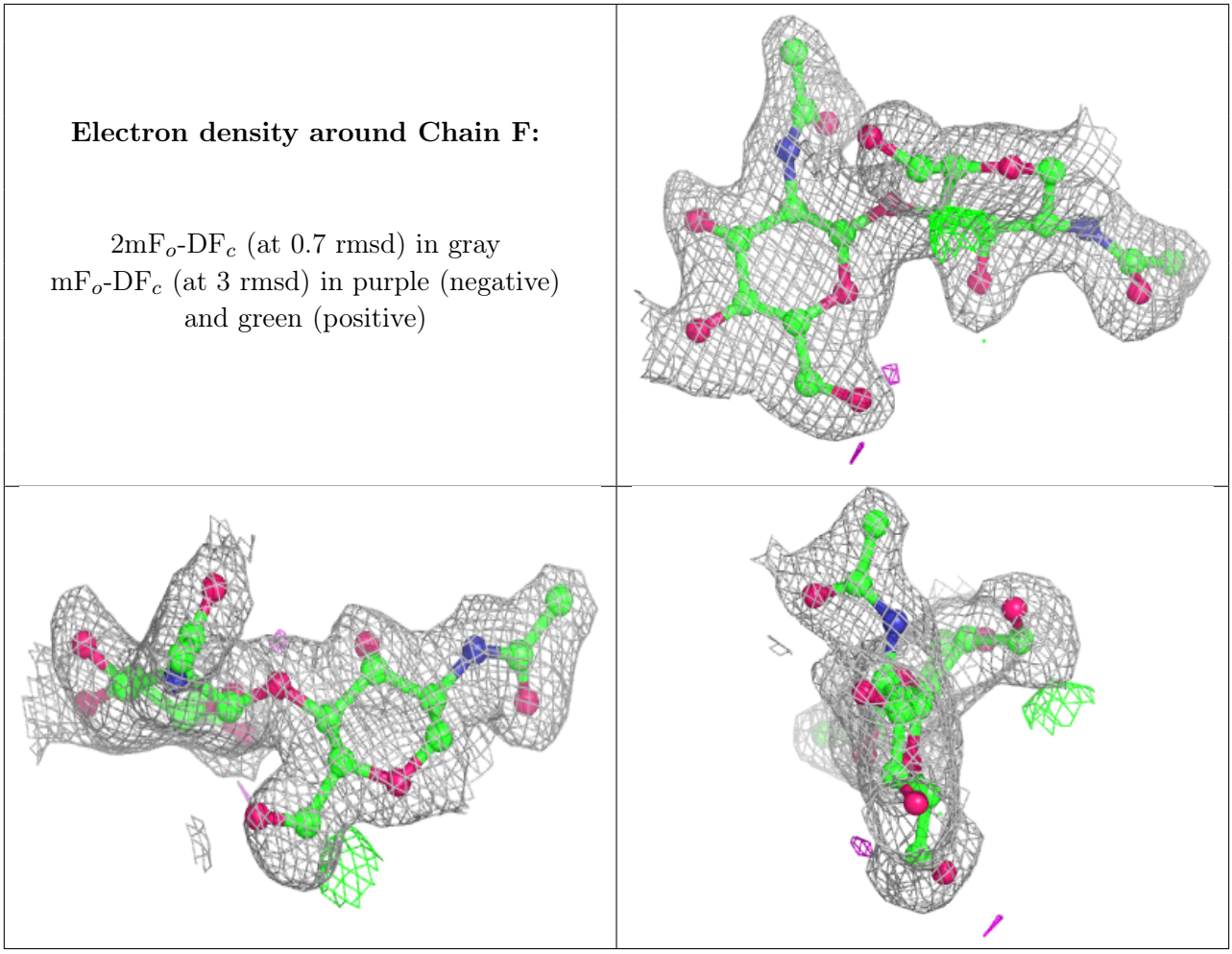






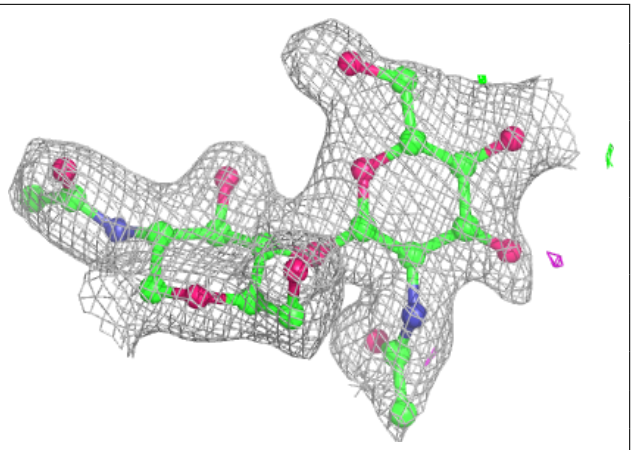
Electron density around Chain F:

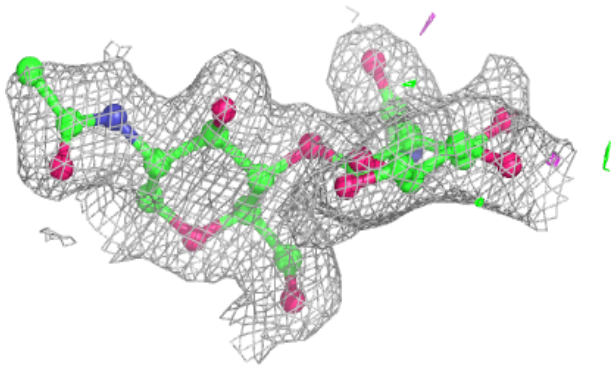
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

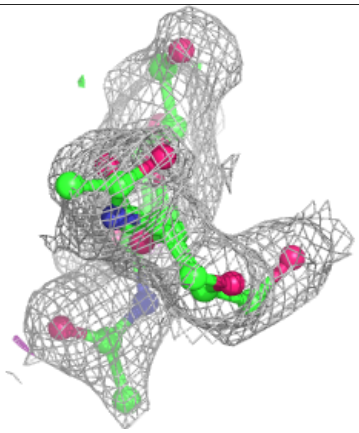


Electron density around Chain H:

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

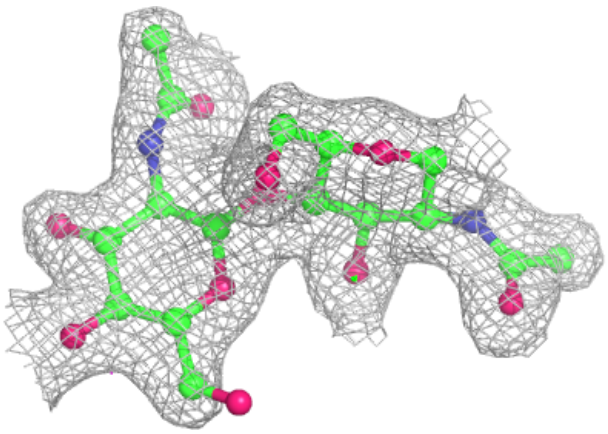


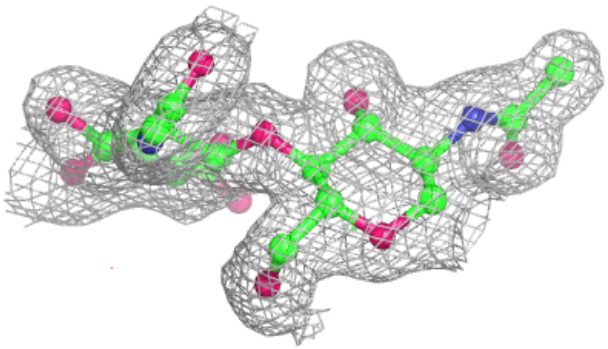


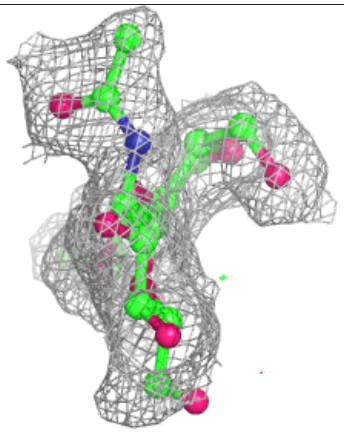


Electron density around Chain J:

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

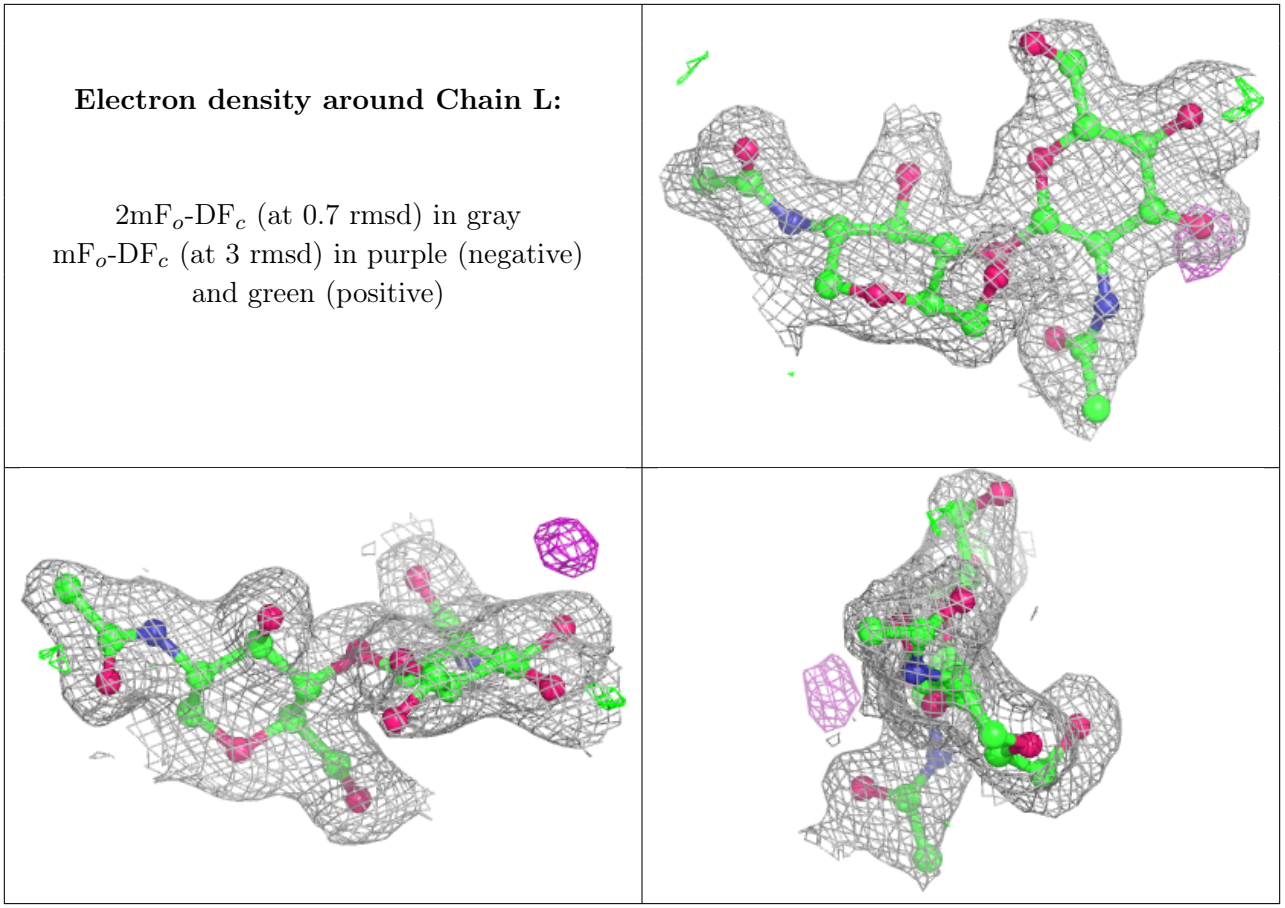






Electron density around Chain L:

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



6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.