wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 06:19 pm BST

PDB ID	:	3ZK4
Title	:	Structure of purple acid phosphatase PPD1 isolated from yellow lupin (Lupinus luteus) seeds
Authors	:	Antonyuk, S.V.; Strange, R.W.
Deposited on	:	2013-01-21
Resolution	:	1.65 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

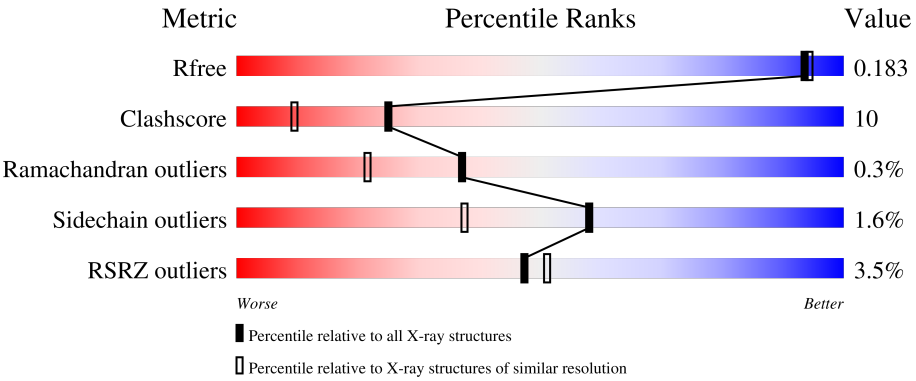
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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	571	94% 5%
1	B	571	91% 8%
1	C	571	8% 80% 18%
2	D	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%
2	J	2	100%
3	I	3	33% 67%
3	K	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
6	GOL	C	1000	-	-	X	-
7	NAG	A	903	-	-	X	-
7	NAG	C	802[B]	-	-	X	-
8	PO4	B	999	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 17881 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.

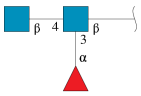
- Molecule 1 is a protein called DIPHOSPHONUCLEOTIDE PHOSPHATASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	20	0
			4652	2986	769	877	20			
1	B	571	Total	C	N	O	S	0	25	0
			4685	3005	775	883	22			
1	C	568	Total	C	N	O	S	0	138	0
			5575	3578	923	1050	24			

- 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	D	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			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

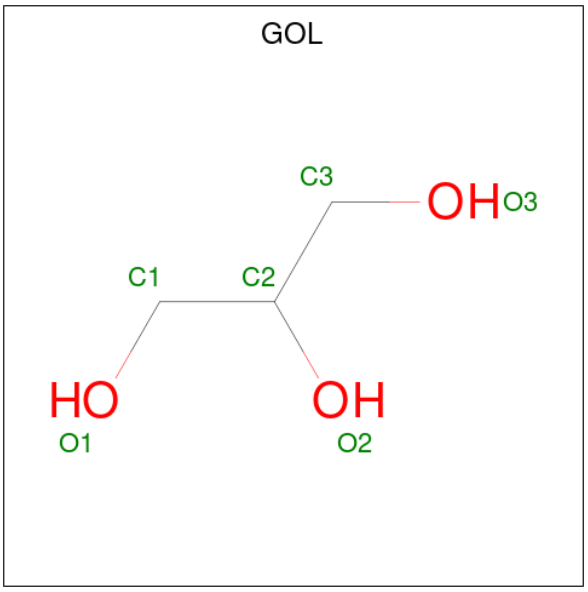
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0
4	B	1	Total Fe 1 1	0	0
4	C	1	Total Fe 1 1	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

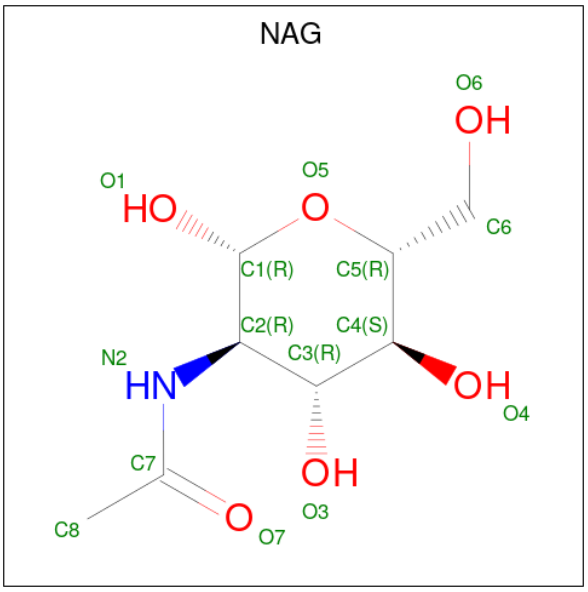
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	B	1	Total Mn 1 1	0	0
5	C	1	Total Mn 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



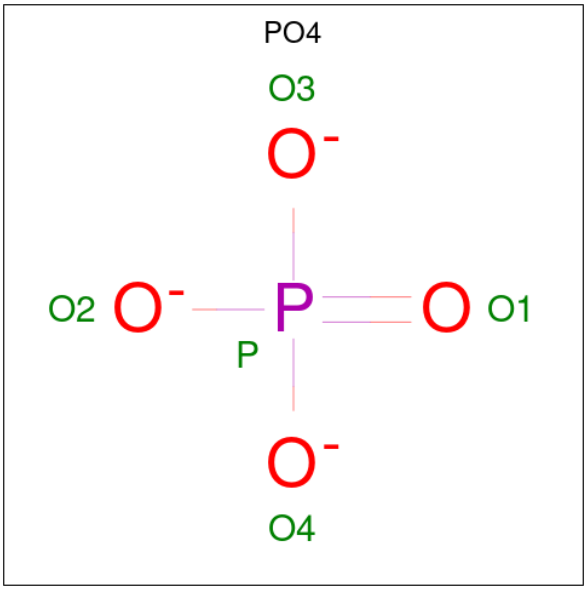
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	A	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 28 16 2 10	0	1
7	C	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 28 16 2 10	0	1

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 9 is water.

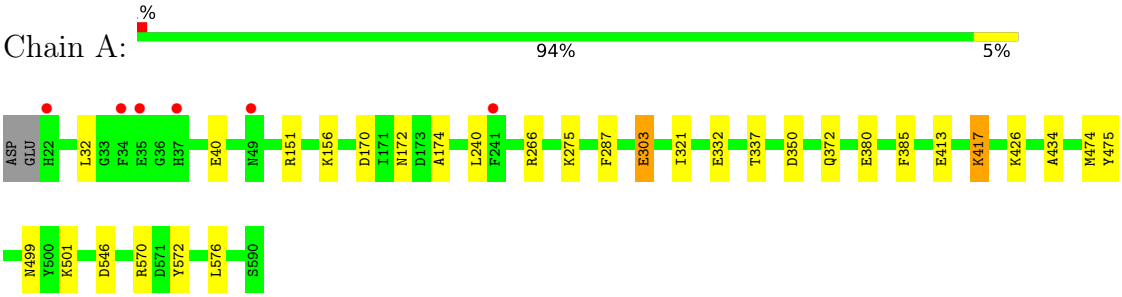
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	997	Total O 1006 1006	0	9
9	B	877	Total O 879 879	0	2
9	C	669	Total O 669 669	0	0

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.

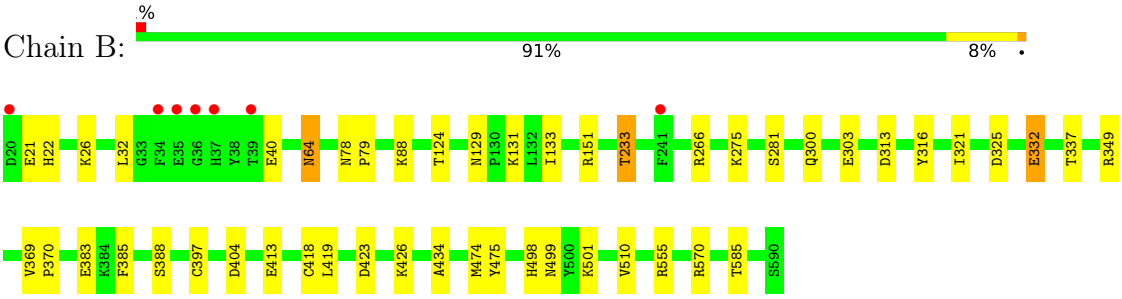
• Molecule 1: DIPHOSPHONUCLEOTIDE PHOSPHATASE 1

Chain A:



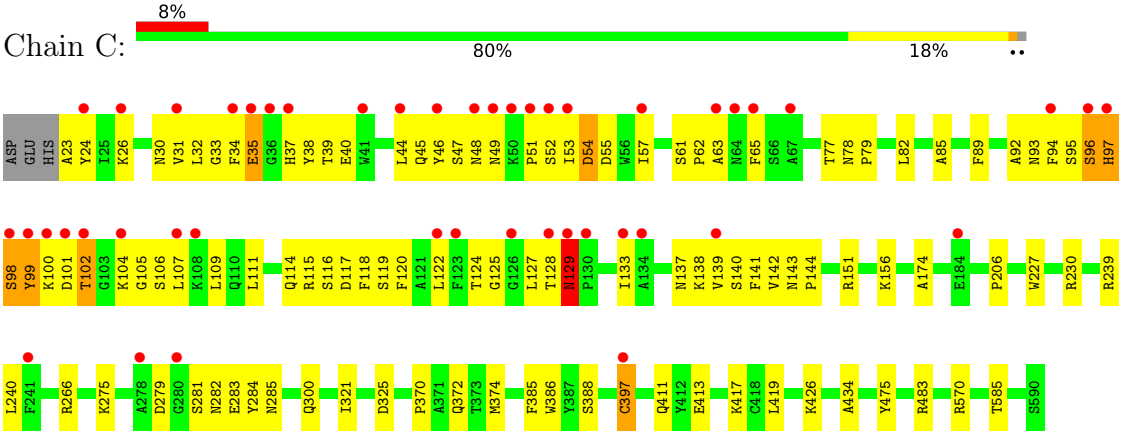
• Molecule 1: DIPHOSPHONUCLEOTIDE PHOSPHATASE 1

Chain B:



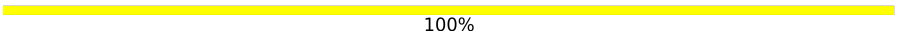
• Molecule 1: DIPHOSPHONUCLEOTIDE PHOSPHATASE 1

Chain C:



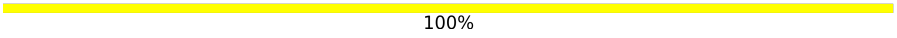
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



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

Chain E:

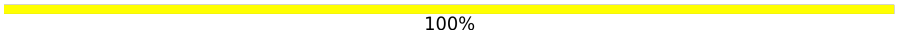


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

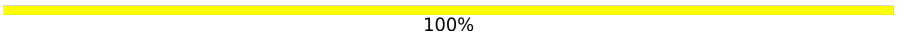
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



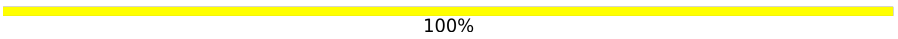
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



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

Chain J:

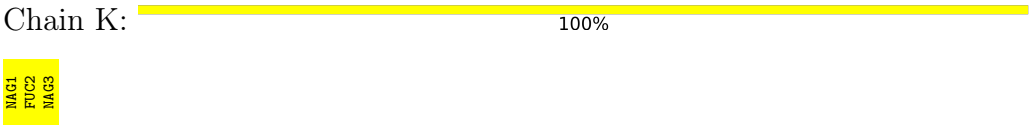


• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: alpha-L-fucopyranose-(1-3)-[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 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.93Å 223.93Å 111.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.62 – 1.65 41.62 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (41.62-1.65) 98.4 (41.62-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.150 , 0.175 0.161 , 0.183	Depositor DCC
R_{free} test set	16796 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17881	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, FUC, FE, MN, GOL, PO4

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	1.01	2/4858 (0.0%)	0.88	8/6603 (0.1%)
1	B	0.72	1/4899 (0.0%)	0.81	4/6659 (0.1%)
1	C	0.71	2/5791 (0.0%)	0.85	5/7871 (0.1%)
All	All	0.82	5/15548 (0.0%)	0.85	17/21133 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	C	0	1
All	All	1	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	417[A]	LYS	CG-CD	34.76	2.70	1.52
1	A	417[B]	LYS	CG-CD	34.76	2.70	1.52
1	C	129[A]	ASN	C-N	7.44	1.48	1.34
1	C	129[B]	ASN	C-N	7.44	1.48	1.34
1	B	233	THR	CB-CG2	-5.20	1.35	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417[A]	LYS	CB-CG-CD	-17.14	67.05	111.60
1	A	417[B]	LYS	CB-CG-CD	-17.14	67.05	111.60
1	C	128[A]	THR	O-C-N	13.10	143.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	128[B]	THR	O-C-N	13.10	143.65	122.70
1	A	417[A]	LYS	CG-CD-CE	12.35	148.94	111.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	233	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	129[A]	ASN	Mainchain

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	4652	0	4423	24	0
1	B	4685	0	4468	35	0
1	C	5575	0	5308	211	0
2	D	28	0	25	0	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	J	28	0	25	0	0
3	I	38	0	34	1	0
3	K	38	0	34	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	18	0	24	1	0
6	C	6	0	8	4	0
7	A	28	0	26	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	28	0	26	2	0
7	C	70	0	65	25	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
8	C	5	0	0	0	0
9	A	1006	0	0	22	2
9	B	879	0	0	21	1
9	C	669	0	0	36	3
All	All	17881	0	14566	288	3

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 10.

The worst 5 of 288 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)
7:A:903:NAG:H82	9:A:2835:HOH:O	1.19	1.35
1:C:26[B]:LYS:CD	9:C:2003:HOH:O	1.74	1.33
1:C:96[A]:SER:OG	1:C:105[A]:GLY:HA3	1.07	1.24
1:C:96[A]:SER:OG	1:C:105[A]:GLY:CA	1.88	1.21
1:C:125[A]:GLY:O	1:C:129[A]:ASN:CB	1.93	1.16

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:2747:HOH:O	9:C:2135:HOH:O[4_455]	2.04	0.16
9:A:2375:HOH:O	9:C:2473:HOH:O[8_556]	2.12	0.08
9:A:2111:HOH:O	9:C:2524:HOH:O[1_556]	2.18	0.02

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	587/571 (103%)	569 (97%)	18 (3%)	0	100	100
1	B	594/571 (104%)	575 (97%)	19 (3%)	0	100	100
1	C	703/571 (123%)	668 (95%)	25 (4%)	10 (1%)	9	1
All	All	1884/1713 (110%)	1812 (96%)	62 (3%)	10 (0%)	37	11

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96[A]	SER
1	C	96[B]	SER
1	C	97[A]	HIS
1	C	97[B]	HIS
1	C	35[A]	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	508/490 (104%)	499 (98%)	9 (2%)	54	32
1	B	514/490 (105%)	507 (99%)	7 (1%)	62	43
1	C	609/490 (124%)	596 (98%)	13 (2%)	48	26
All	All	1631/1470 (111%)	1602 (98%)	29 (2%)	58	32

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	385	PHE
1	C	397[B]	CYS
1	C	54[B]	ASP
1	C	275	LYS
1	C	54[A]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	326	GLN
1	B	64	ASN
1	C	326	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	D	1	2,1	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	2.16	4 (23%)
2	NAG	E	1	2,1	14,14,15	0.87	1 (7%)	17,19,21	0.89	1 (5%)
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	1.03	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.64	0	17,19,21	1.05	2 (11%)
2	NAG	F	2	2	14,14,15	0.54	0	17,19,21	0.79	0
2	NAG	G	1	2,1	14,14,15	1.17	1 (7%)	17,19,21	1.05	1 (5%)
2	NAG	G	2	2	14,14,15	0.77	1 (7%)	17,19,21	0.87	0
2	NAG	H	1	2,1	14,14,15	0.96	0	17,19,21	1.41	1 (5%)
2	NAG	H	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.79	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.82	1 (7%)	17,19,21	0.73	0
3	FUC	I	2	3	10,10,11	0.70	0	14,14,16	1.24	2 (14%)
3	NAG	I	3	3	14,14,15	0.55	0	17,19,21	1.36	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	J	1	2,1	14,14,15	0.78	0	17,19,21	1.12	2 (11%)
2	NAG	J	2	2	14,14,15	0.67	0	17,19,21	2.43	8 (47%)
3	NAG	K	1	3,1	14,14,15	0.49	0	17,19,21	2.47	4 (23%)
3	FUC	K	2	3	10,10,11	0.63	0	14,14,16	1.18	2 (14%)
3	NAG	K	3	3	14,14,15	0.46	0	17,19,21	1.88	6 (35%)

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	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	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	2,1	-	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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	FUC	I	2	3	-	-	0/1/1/1
3	NAG	I	3	3	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	K	2	3	-	-	0/1/1/1
3	NAG	K	3	3	-	5/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	NAG	O5-C1	-3.95	1.37	1.43
3	I	1	NAG	O5-C1	-2.53	1.39	1.43
2	E	1	NAG	O5-C1	-2.31	1.40	1.43
2	H	2	NAG	O5-C1	-2.26	1.40	1.43
2	G	2	NAG	O5-C1	-2.13	1.40	1.43

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	1	NAG	C1-O5-C5	8.16	123.24	112.19
2	D	2	NAG	C2-N2-C7	5.84	131.22	122.90
2	J	2	NAG	C1-O5-C5	5.07	119.06	112.19
2	H	2	NAG	C2-N2-C7	4.97	129.98	122.90
2	J	2	NAG	C2-N2-C7	4.57	129.41	122.90

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
3	K	3	NAG	O5-C5-C6-O6
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	J	2	NAG	C8-C7-N2-C2

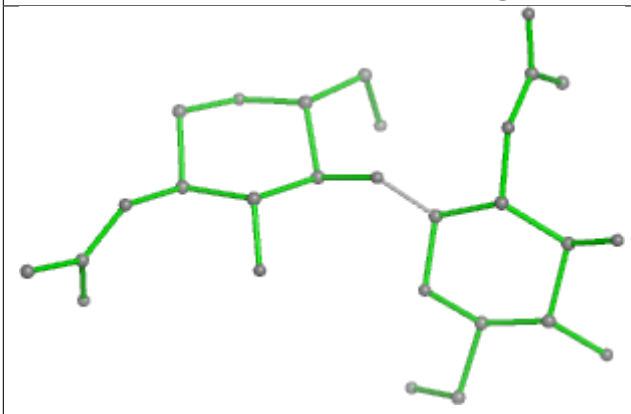
There are no ring outliers.

2 monomers are involved in 1 short contact:

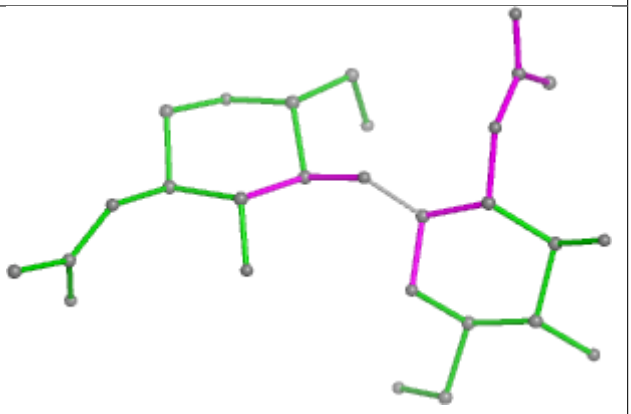
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	NAG	1	0
3	I	2	FUC	1	0

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

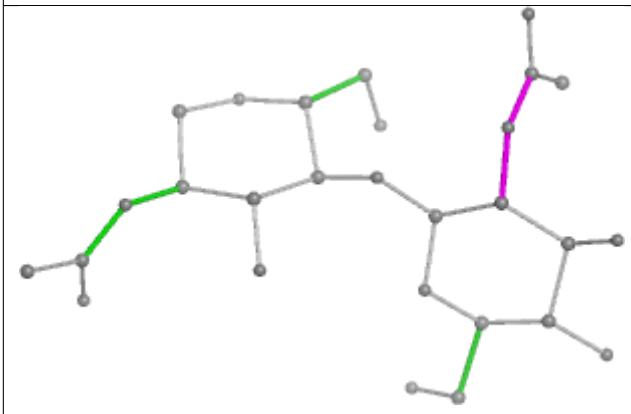
Oligosaccharide Chain D



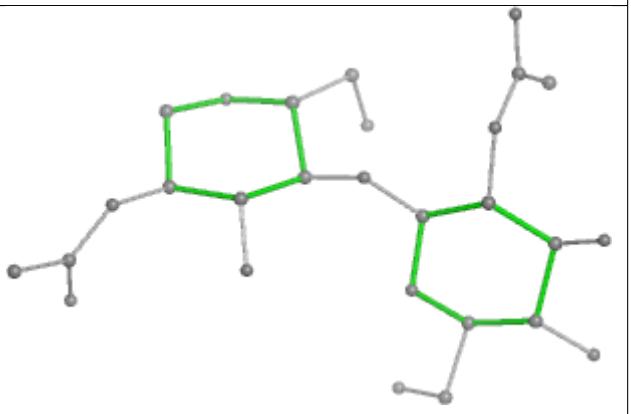
Bond lengths



Bond angles

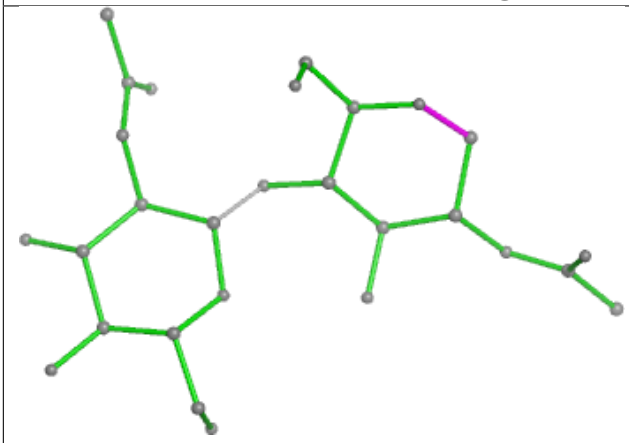


Torsions

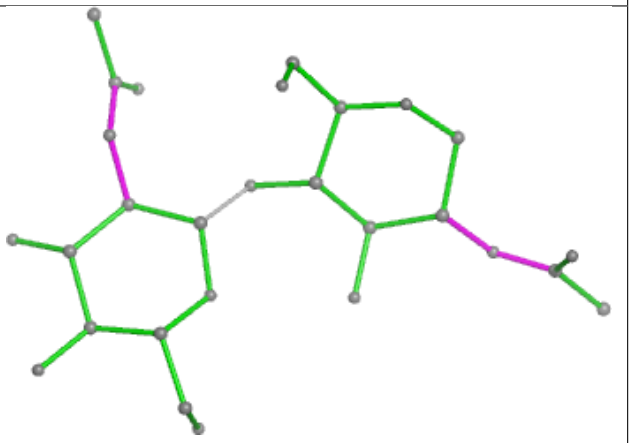


Rings

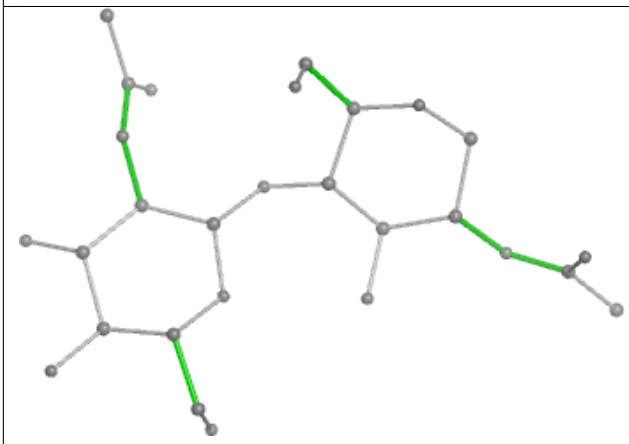
Oligosaccharide Chain E



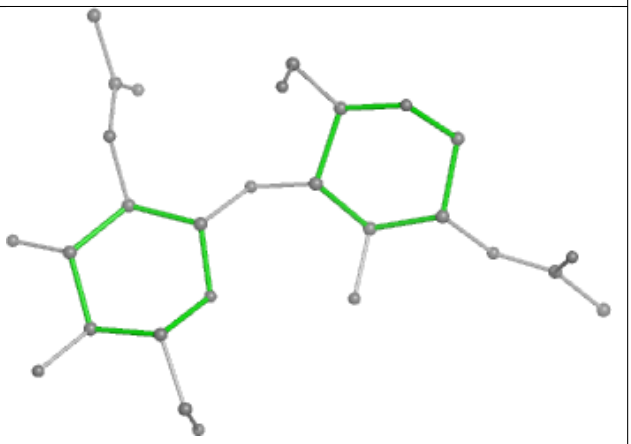
Bond lengths



Bond angles

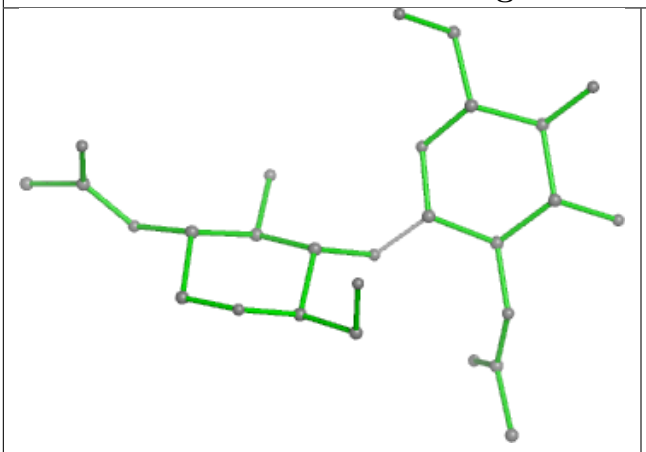


Torsions

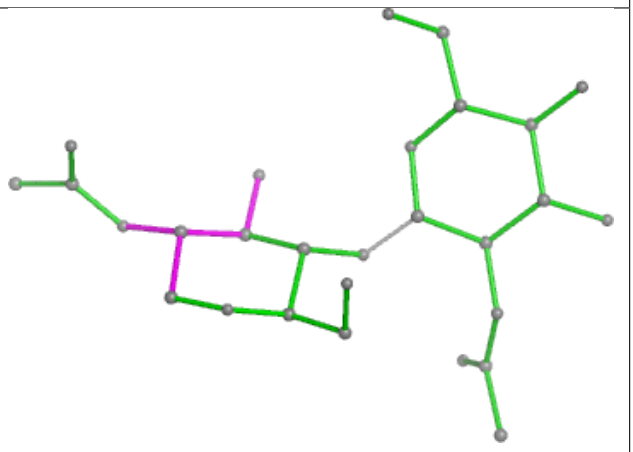


Rings

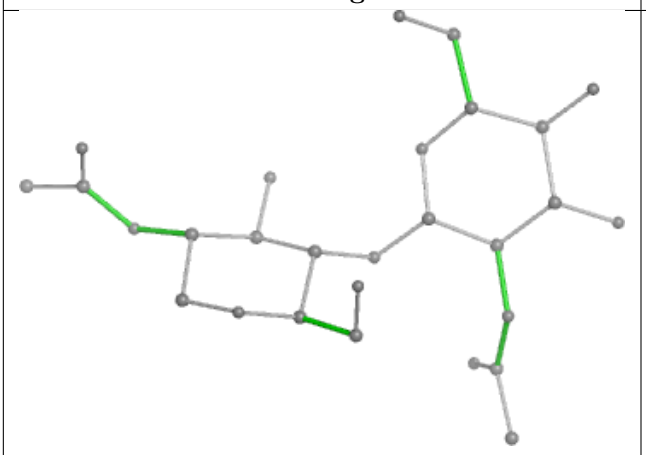
Oligosaccharide Chain F



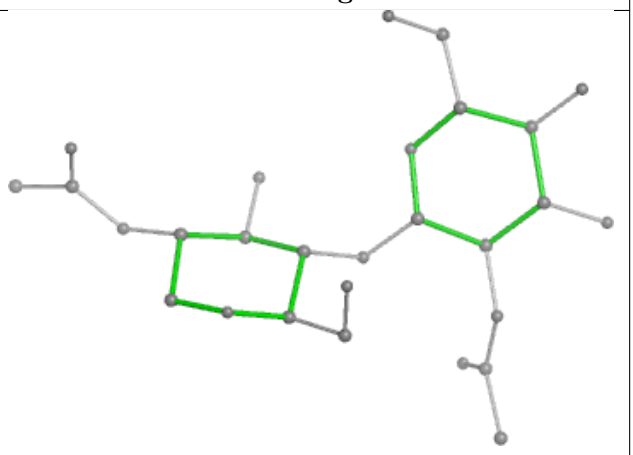
Bond lengths



Bond angles

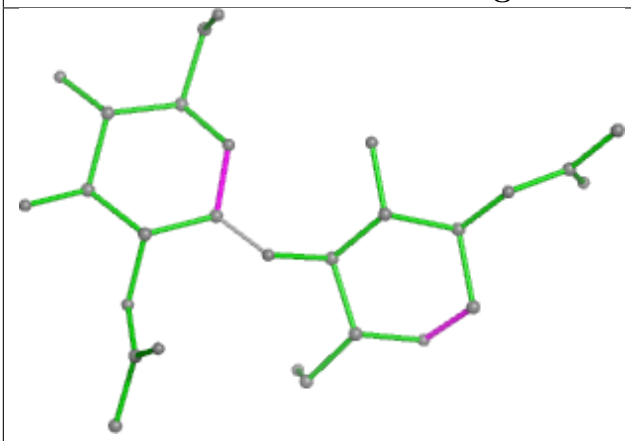


Torsions

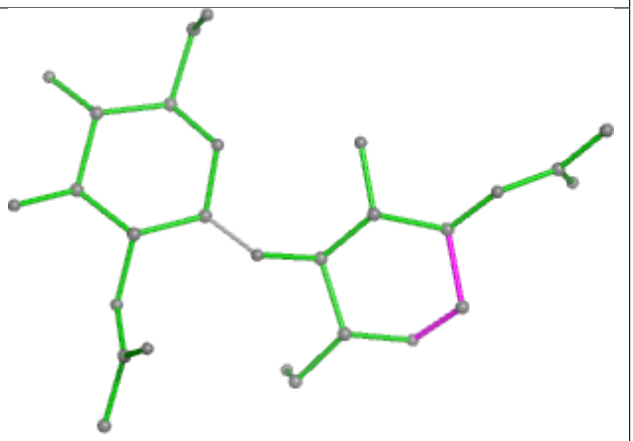


Rings

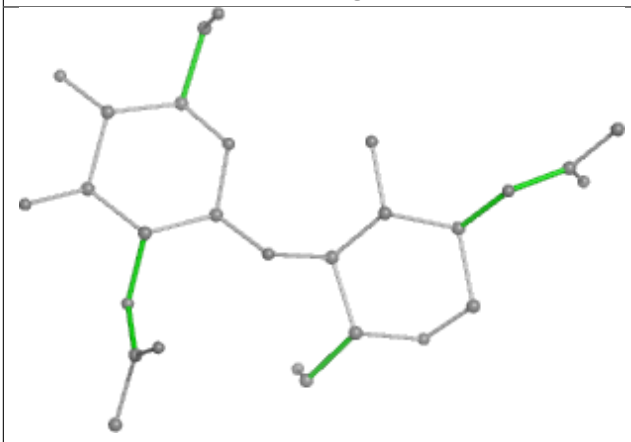
Oligosaccharide Chain G



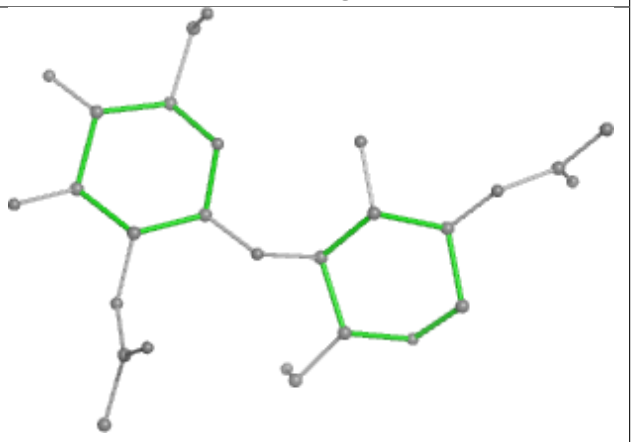
Bond lengths



Bond angles

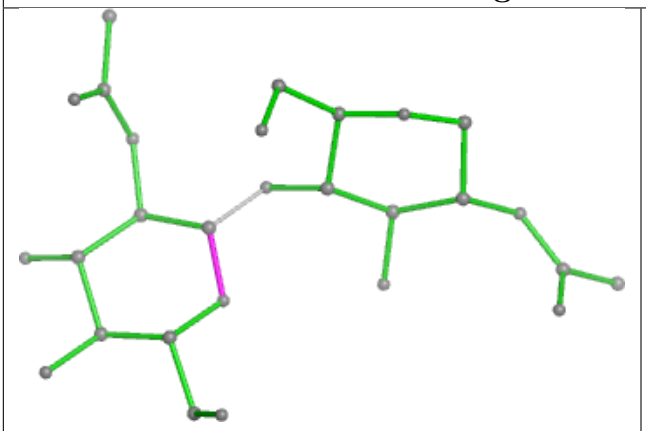


Torsions

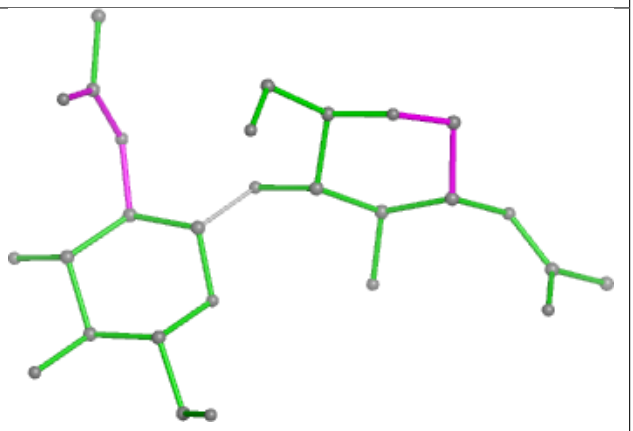


Rings

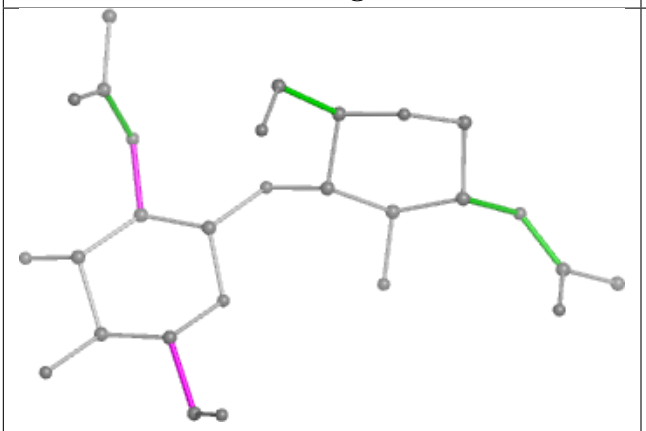
Oligosaccharide Chain H



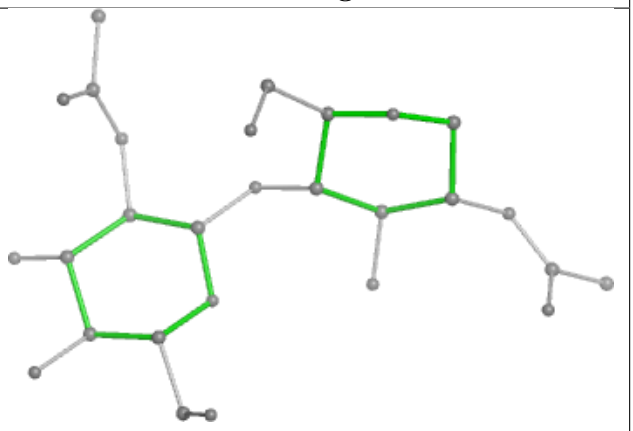
Bond lengths



Bond angles

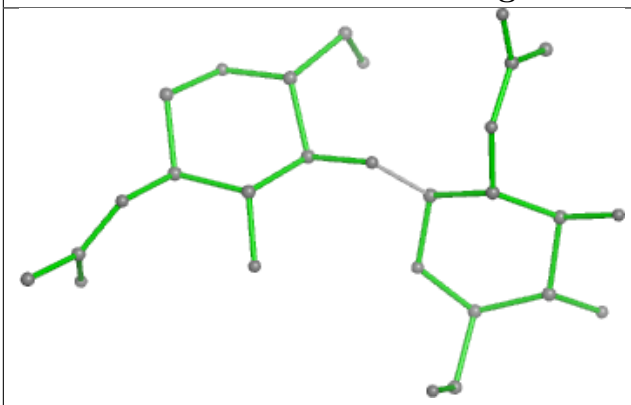


Torsions

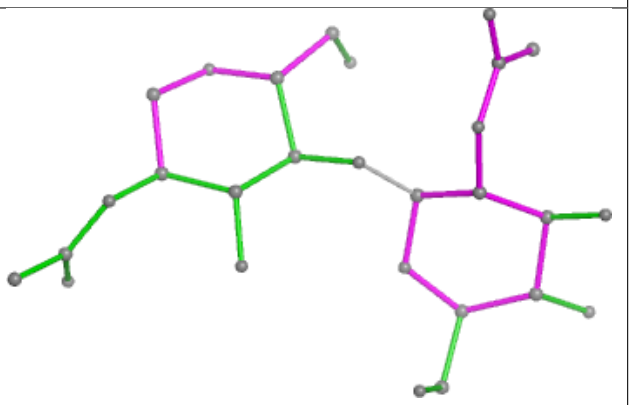


Rings

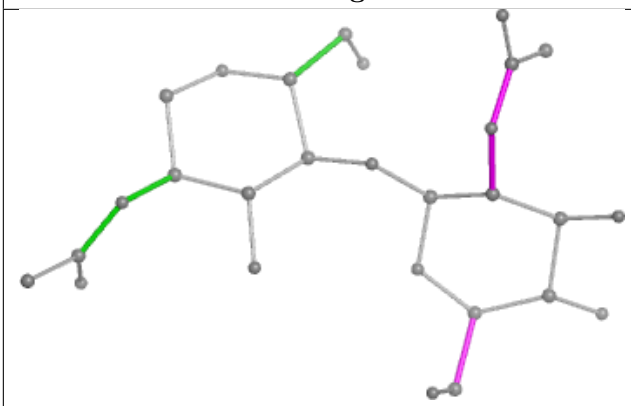
Oligosaccharide Chain J



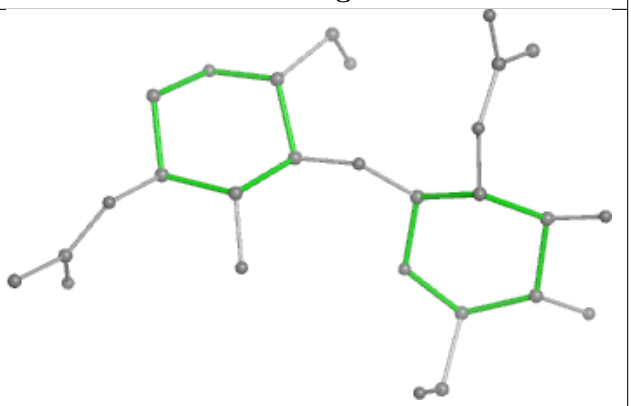
Bond lengths



Bond angles

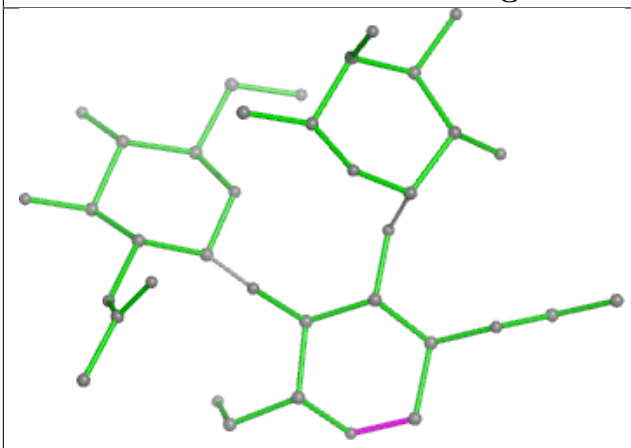


Torsions

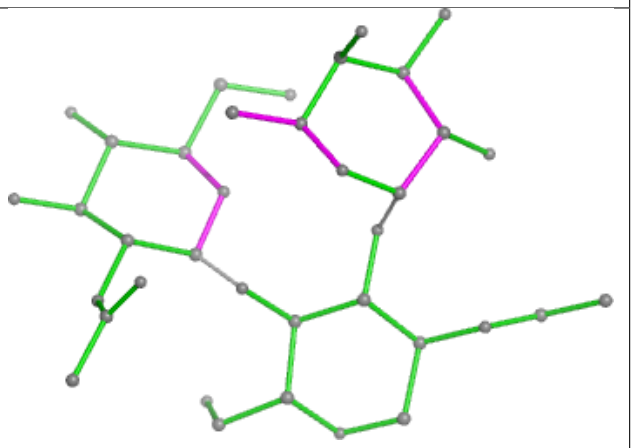


Rings

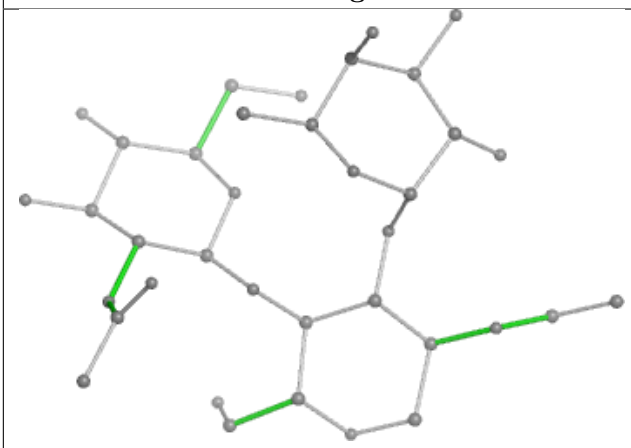
Oligosaccharide Chain I



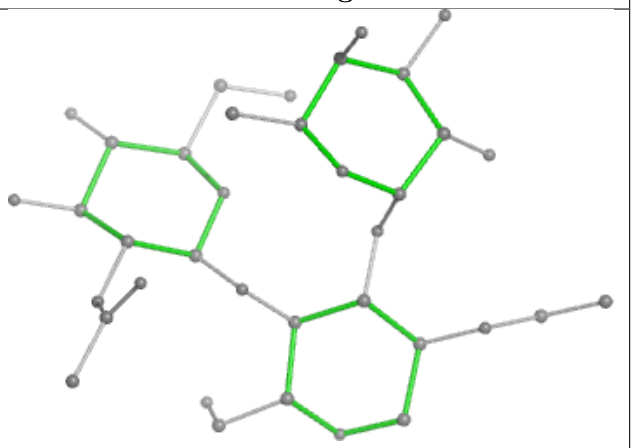
Bond lengths



Bond angles

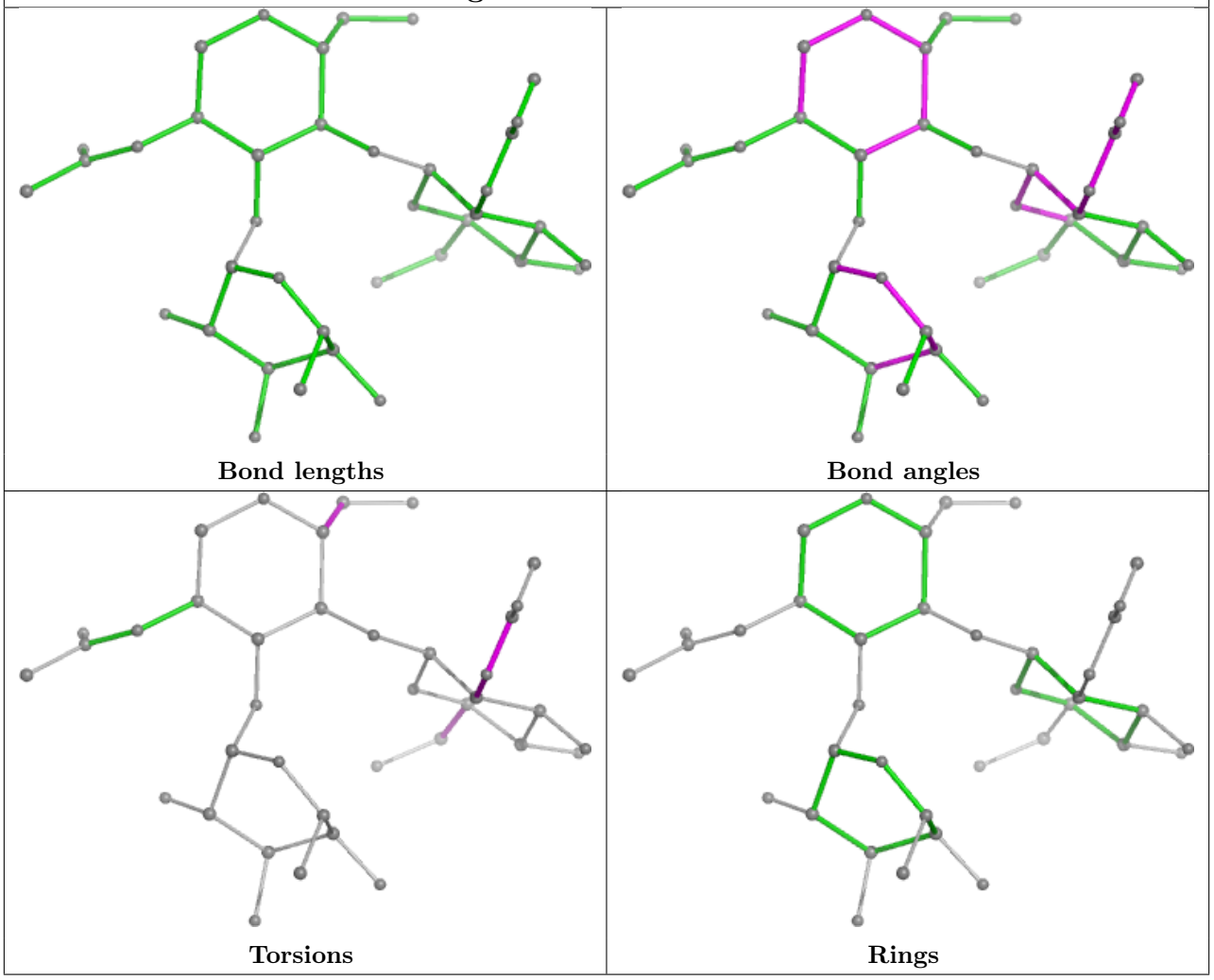


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	PO4	B	999	4,5	4,4,4	1.99	1 (25%)	6,6,6	2.17	3 (50%)
6	GOL	A	1001	-	5,5,5	0.20	0	5,5,5	0.55	0
7	NAG	C	802[B]	-	14,14,15	0.59	0	17,19,21	1.94	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	C	814	1	14,14,15	0.49	0	17,19,21	1.54	4 (23%)
7	NAG	B	903	1	14,14,15	0.57	0	17,19,21	2.89	5 (29%)
6	GOL	A	901	-	5,5,5	0.42	0	5,5,5	0.58	0
8	PO4	C	999	4,5	4,4,4	0.54	0	6,6,6	1.60	2 (33%)
8	PO4	A	999	4,5	4,4,4	1.09	0	6,6,6	1.17	0
7	NAG	A	905	1	14,14,15	0.55	0	17,19,21	2.17	3 (17%)
6	GOL	C	1000	-	5,5,5	0.94	0	5,5,5	1.44	1 (20%)
7	NAG	B	925	1	14,14,15	0.48	0	17,19,21	1.39	3 (17%)
7	NAG	C	802[A]	-	14,14,15	0.50	0	17,19,21	1.82	3 (17%)
7	NAG	C	903[B]	-	14,14,15	0.80	1 (7%)	17,19,21	1.94	5 (29%)
7	NAG	A	903	1	14,14,15	0.74	1 (7%)	17,19,21	1.59	3 (17%)
6	GOL	A	1000	-	5,5,5	0.39	0	5,5,5	0.81	0
7	NAG	C	903[A]	-	14,14,15	0.96	1 (7%)	17,19,21	2.37	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1001	-	-	2/4/4/4	-
7	NAG	C	802[B]	-	-	3/6/23/26	0/1/1/1
7	NAG	C	814	1	-	2/6/23/26	0/1/1/1
7	NAG	B	903	1	-	2/6/23/26	0/1/1/1
6	GOL	A	901	-	-	0/4/4/4	-
7	NAG	A	905	1	-	2/6/23/26	0/1/1/1
6	GOL	C	1000	-	-	3/4/4/4	-
7	NAG	B	925	1	-	0/6/23/26	0/1/1/1
7	NAG	C	802[A]	-	-	3/6/23/26	0/1/1/1
7	NAG	C	903[B]	-	-	2/6/23/26	0/1/1/1
7	NAG	A	903	1	-	2/6/23/26	0/1/1/1
6	GOL	A	1000	-	-	2/4/4/4	-
7	NAG	C	903[A]	-	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	999	PO4	P-O1	3.35	1.58	1.50
7	A	903	NAG	O5-C1	-2.49	1.39	1.43
7	C	903[A]	NAG	C2-N2	-2.17	1.42	1.46
7	C	903[B]	NAG	C2-N2	-2.11	1.42	1.46

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	903	NAG	C1-O5-C5	9.89	125.59	112.19
7	C	903[A]	NAG	C1-O5-C5	7.51	122.37	112.19
7	A	905	NAG	C1-O5-C5	7.02	121.71	112.19
7	C	802[A]	NAG	O5-C1-C2	-4.60	104.03	111.29
7	C	903[A]	NAG	C1-C2-N2	-4.50	102.80	110.49

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	GOL	O1-C1-C2-C3
6	C	1000	GOL	C1-C2-C3-O3
7	C	802[A]	NAG	C3-C2-N2-C7
7	A	903	NAG	O5-C5-C6-O6
7	A	905	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	GOL	1	0
7	C	802[B]	NAG	20	0
7	B	903	NAG	1	0
6	C	1000	GOL	4	0
7	B	925	NAG	1	0
7	C	802[A]	NAG	5	0
7	A	903	NAG	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	569/571 (99%)	-0.45	6 (1%)	77	81	9, 17, 28, 54	27 (4%)
1	B	571/571 (100%)	-0.41	7 (1%)	76	80	7, 17, 29, 67	35 (6%)
1	C	568/571 (99%)	0.23	46 (8%)	19	20	8, 18, 28, 52	140 (24%)
All	All	1708/1713 (99%)	-0.21	59 (3%)	47	51	7, 17, 28, 67	202 (11%)

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	HIS	7.6
1	C	51[A]	PRO	6.9
1	C	53[A]	ILE	6.4
1	C	102[A]	THR	6.0
1	C	129[A]	ASN	5.8

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
3	NAG	K	3	14/15	0.49	0.19	84,91,100,100	0
2	NAG	J	2	14/15	0.65	0.17	50,57,70,77	0
3	FUC	K	2	10/11	0.66	0.17	59,71,75,80	0

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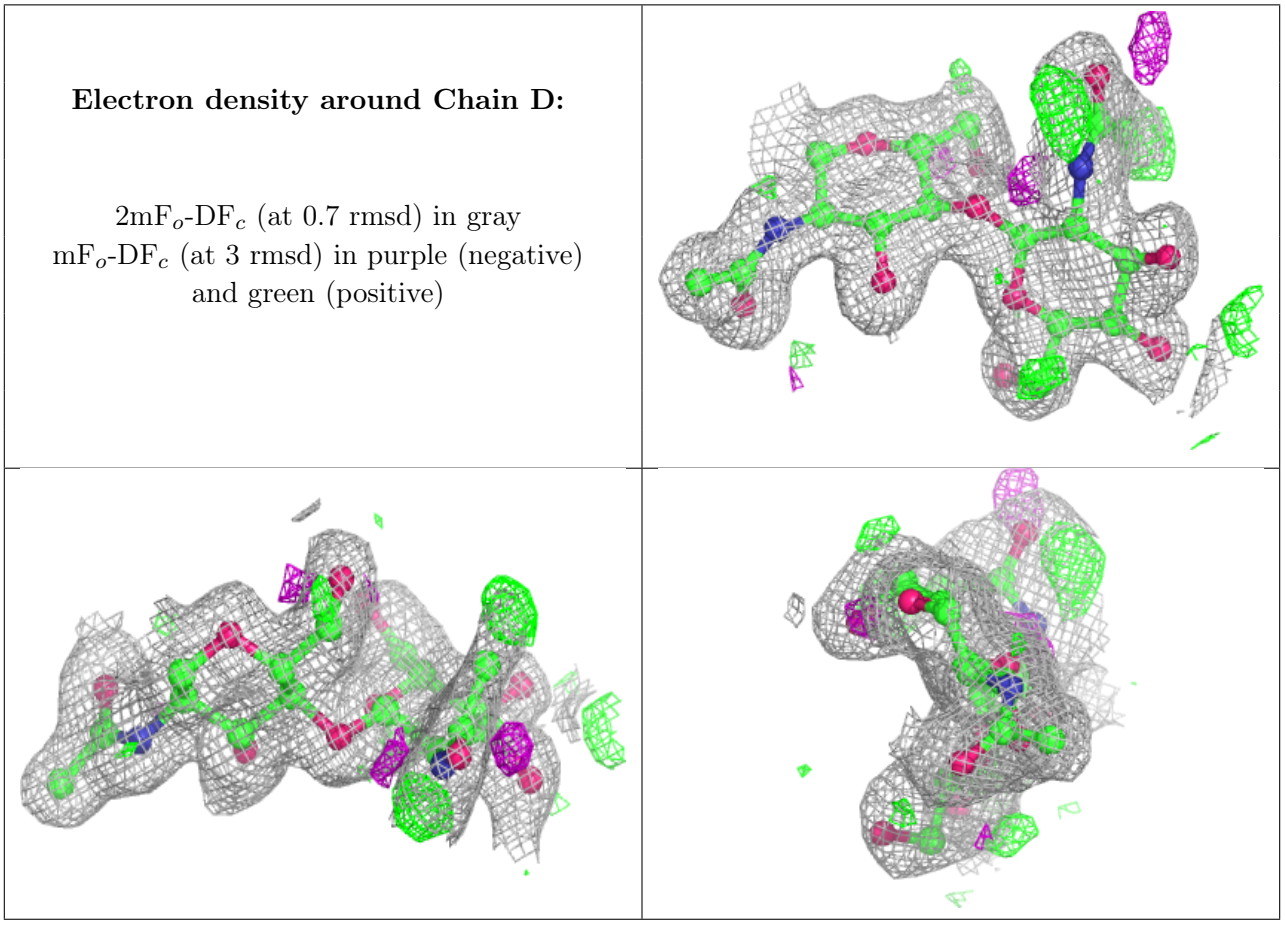
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	I	3	14/15	0.71	0.20	72,84,89,93	0
2	NAG	F	2	14/15	0.72	0.16	60,70,78,79	0
3	FUC	I	2	10/11	0.77	0.13	60,67,72,76	0
3	NAG	K	1	14/15	0.79	0.14	46,56,68,81	0
2	NAG	D	2	14/15	0.80	0.14	37,47,54,60	0
2	NAG	H	2	14/15	0.80	0.14	41,52,61,62	0
2	NAG	E	2	14/15	0.83	0.13	35,38,47,48	0
3	NAG	I	1	14/15	0.86	0.12	42,50,56,62	0
2	NAG	G	2	14/15	0.86	0.12	34,39,49,54	0
2	NAG	F	1	14/15	0.88	0.10	40,47,52,57	0
2	NAG	J	1	14/15	0.92	0.09	25,29,37,41	0
2	NAG	G	1	14/15	0.94	0.09	24,27,29,33	0
2	NAG	E	1	14/15	0.96	0.07	21,23,26,30	0
2	NAG	D	1	14/15	0.96	0.06	18,20,25,27	0
2	NAG	H	1	14/15	0.96	0.07	22,24,28,32	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.

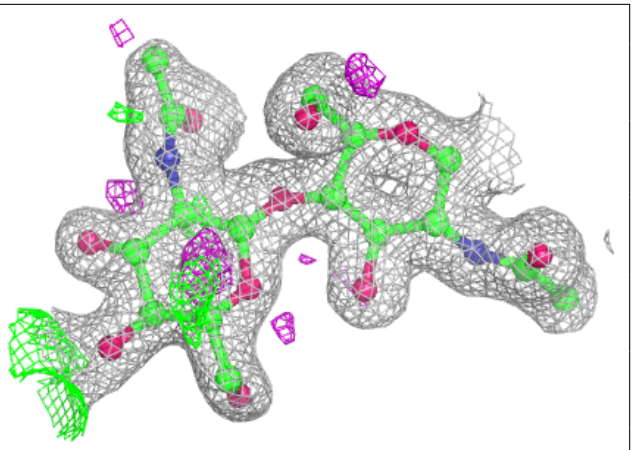
Electron density around Chain D:

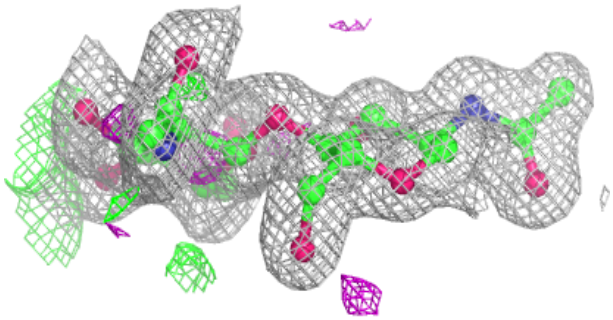
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

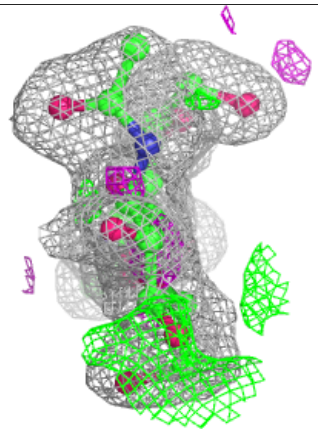


Electron density around Chain E:

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

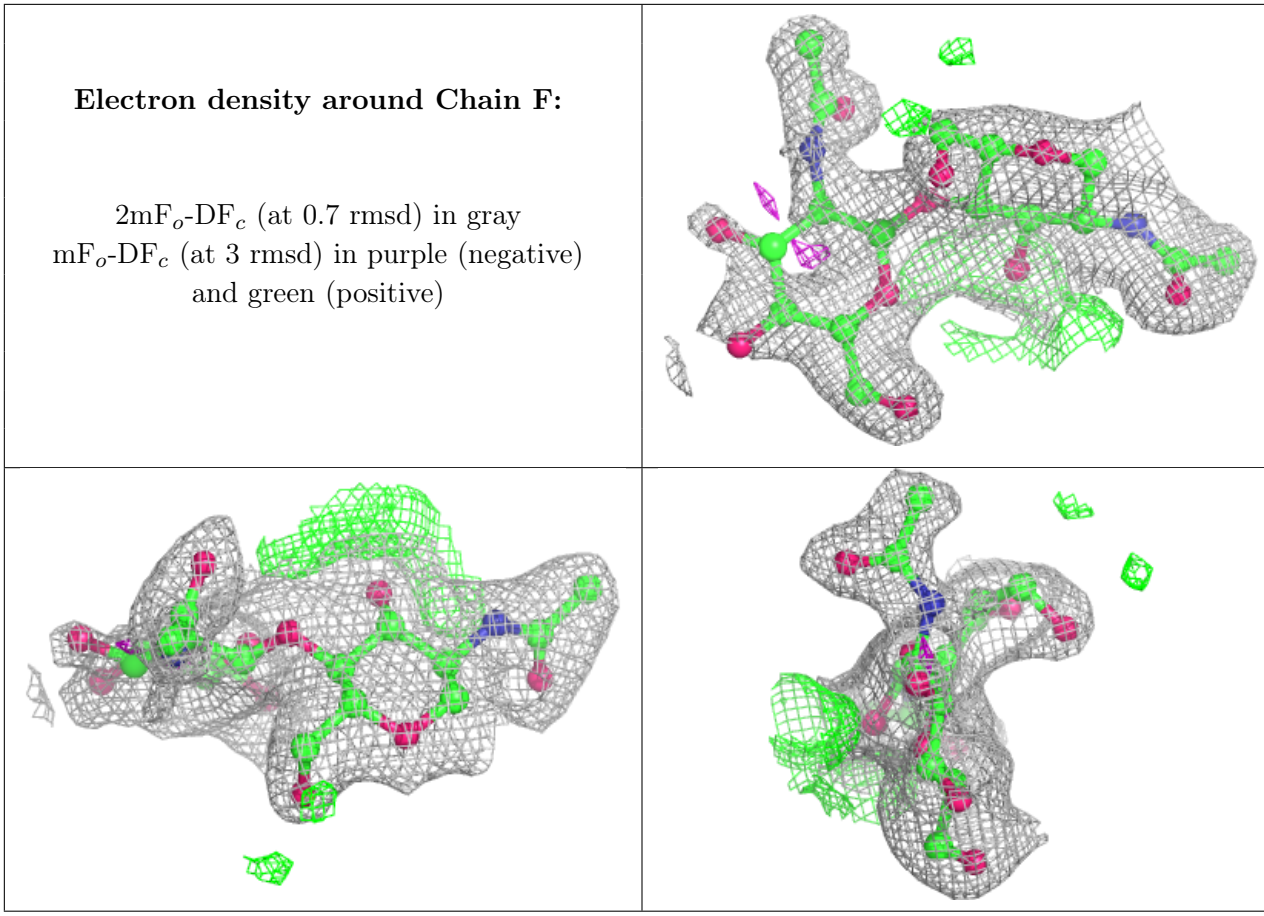






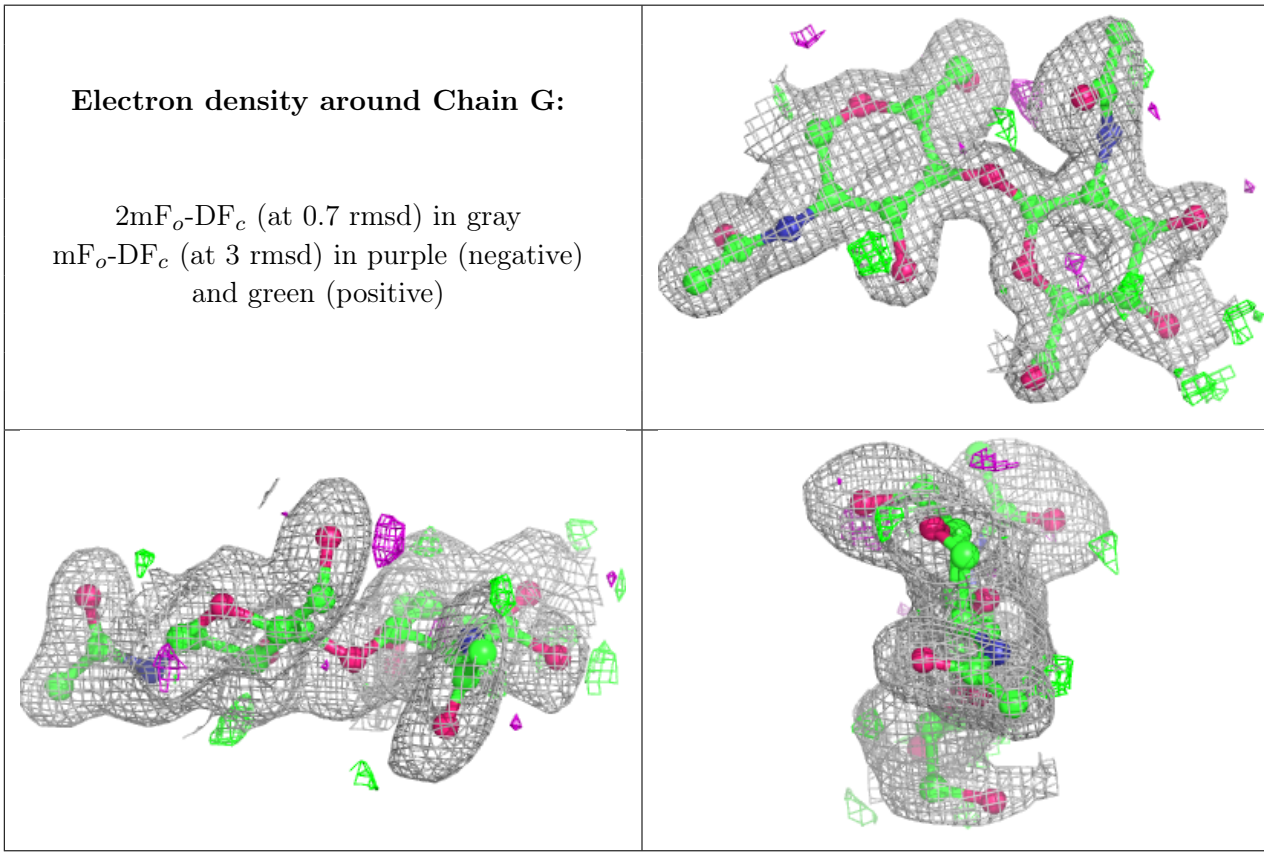
Electron density around Chain F:

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



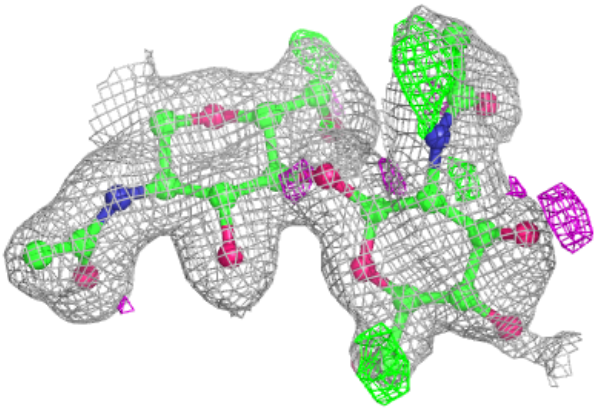
Electron density around Chain G:

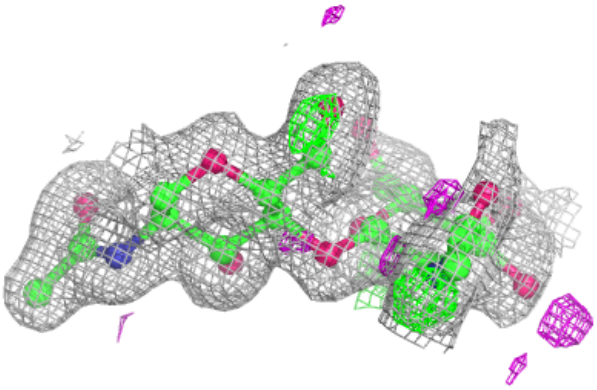
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

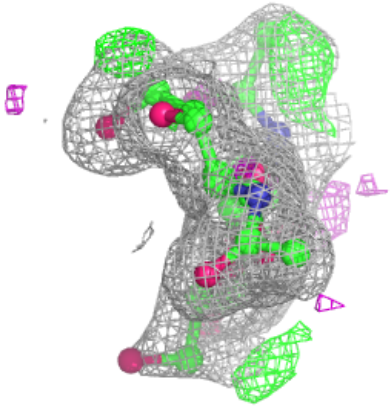


Electron density around Chain H:

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

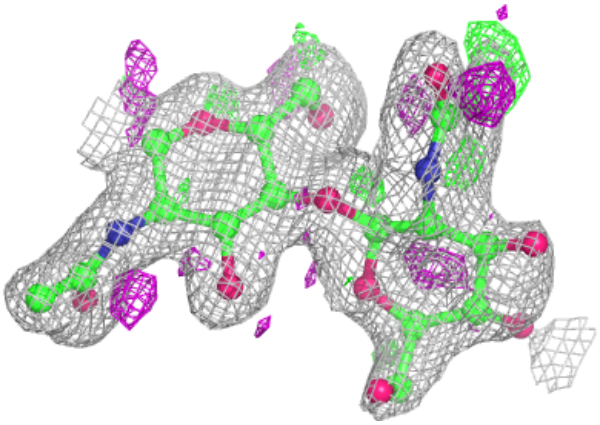


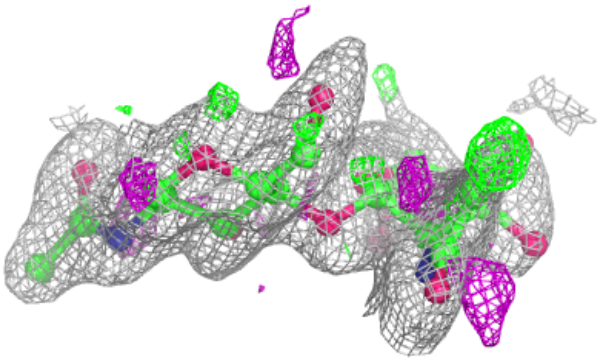


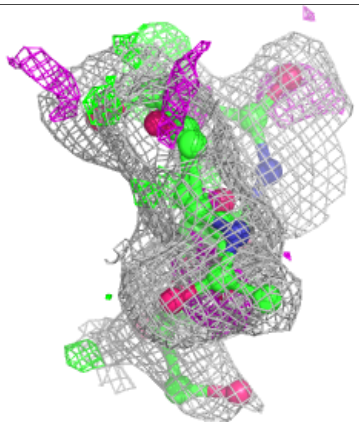


Electron density around Chain J:

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

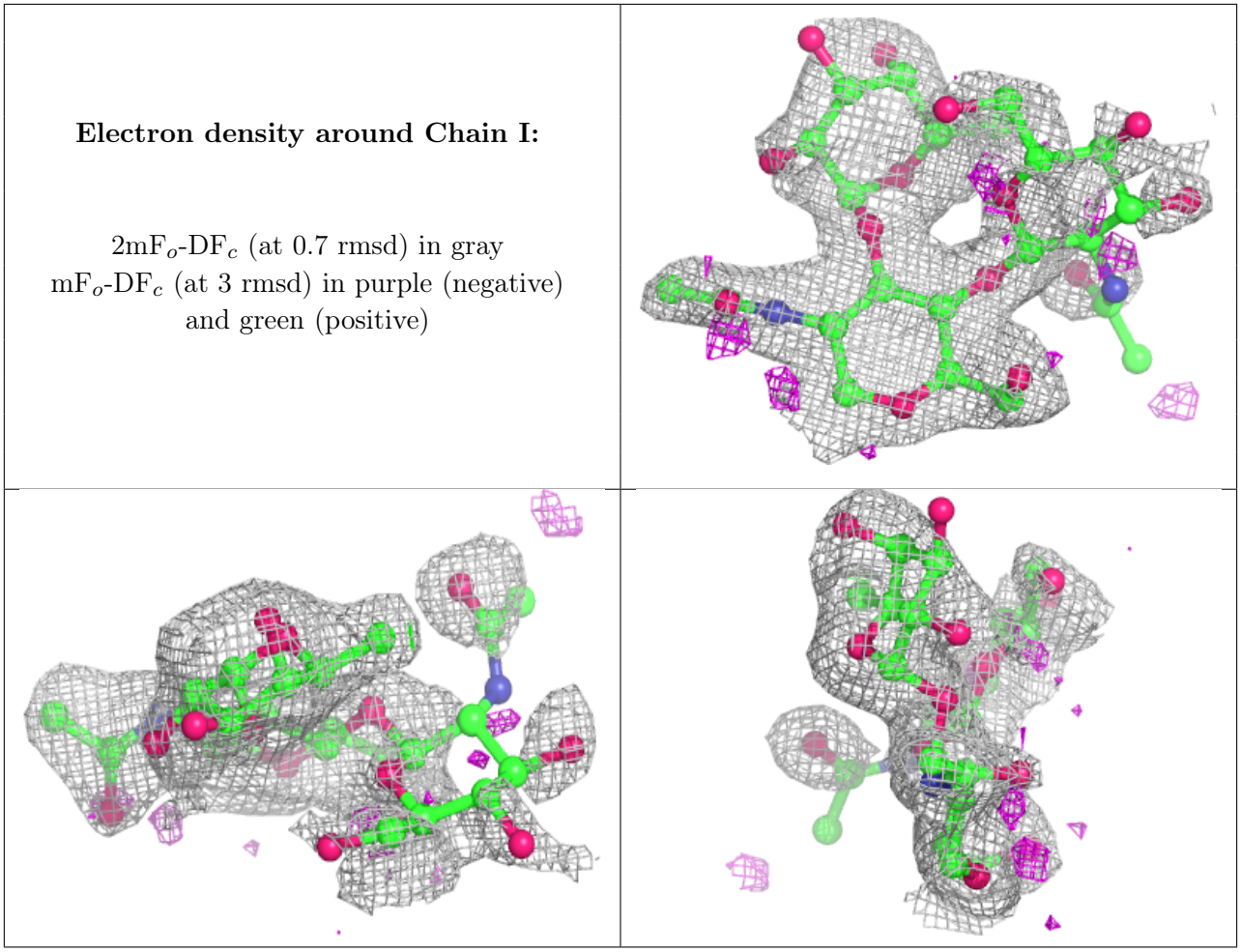






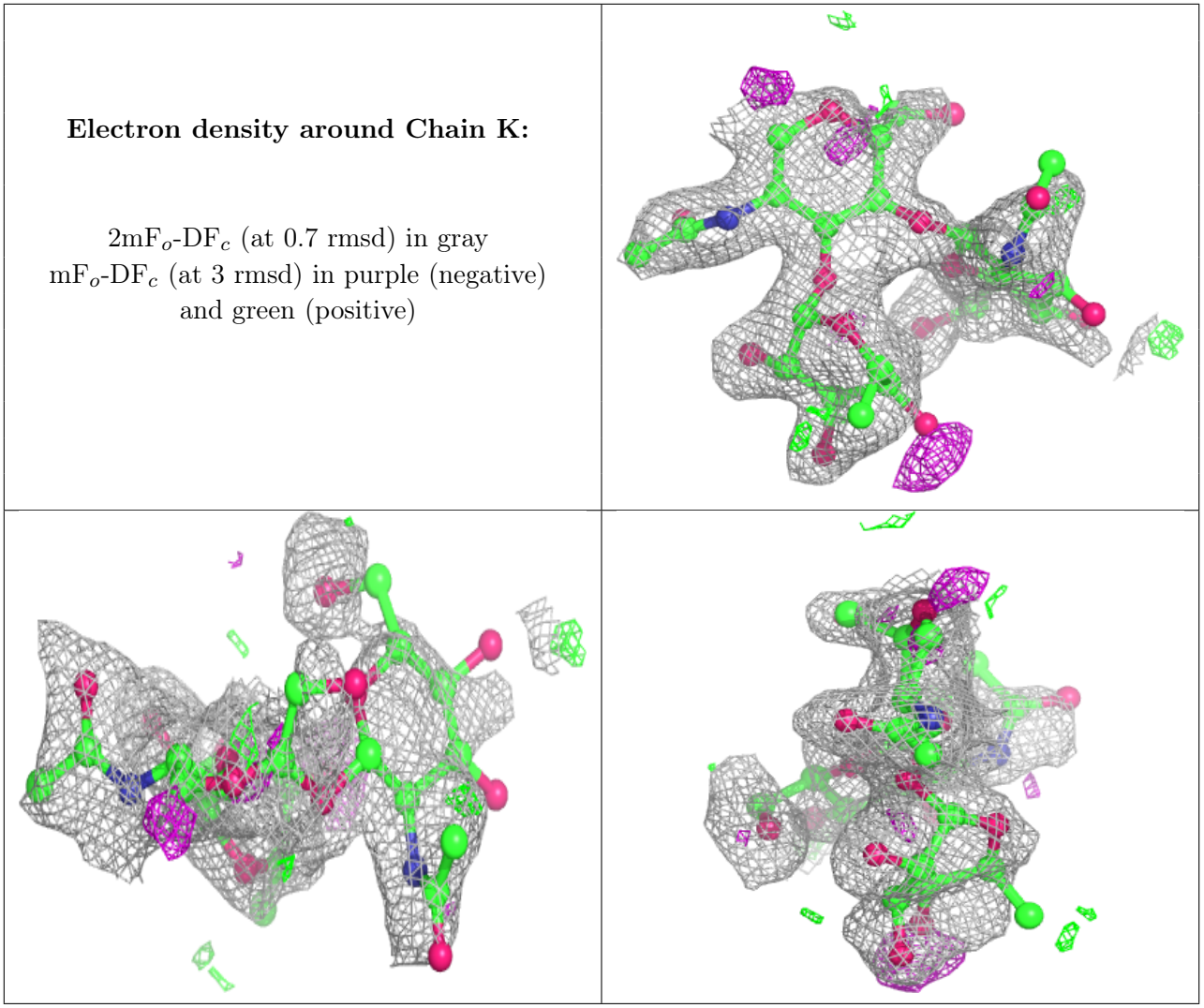
Electron density around Chain I:

$2mF_o$-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)



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
7	NAG	A	905	14/15	0.74	0.16	50,58,70,76	0
7	NAG	C	903[A]	14/15	0.75	0.25	31,36,40,41	14
7	NAG	C	903[B]	14/15	0.75	0.25	24,27,31,32	14
7	NAG	B	903	14/15	0.77	0.18	42,58,67,74	0
6	GOL	C	1000	6/6	0.80	0.21	43,45,49,53	0
7	NAG	C	814	14/15	0.81	0.13	48,52,60,67	0
6	GOL	A	1001	6/6	0.81	0.17	41,43,44,45	0
7	NAG	A	903	14/15	0.81	0.21	30,34,40,40	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	A	1000	6/6	0.82	0.17	35,45,48,53	0
7	NAG	B	925	14/15	0.83	0.13	40,50,59,69	0
7	NAG	C	802[A]	14/15	0.83	0.17	28,32,42,47	14
7	NAG	C	802[B]	14/15	0.83	0.17	26,31,38,39	14
6	GOL	A	901	6/6	0.92	0.12	22,24,25,28	0
8	PO4	B	999	5/5	0.97	0.08	18,20,22,23	0
8	PO4	C	999	5/5	0.97	0.07	19,24,27,29	0
4	FE	C	800	1/1	0.98	0.06	21,21,21,21	0
8	PO4	A	999	5/5	0.98	0.06	18,19,22,23	0
4	FE	B	800	1/1	0.99	0.05	19,19,19,19	0
5	MN	C	801	1/1	0.99	0.03	17,17,17,17	0
5	MN	B	801	1/1	1.00	0.01	14,14,14,14	0
4	FE	A	800	1/1	1.00	0.04	17,17,17,17	0
5	MN	A	801	1/1	1.00	0.01	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.