Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 12:05 AM EDT

PDB ID	:	4HOM
Title	:	Crystal structure of porcine aminopeptidase-N complexed with substance P
Authors	:	Chen, L.; Lin, Y.L.; Peng, G.; Li, F.
Deposited on	:	2012-10-22
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

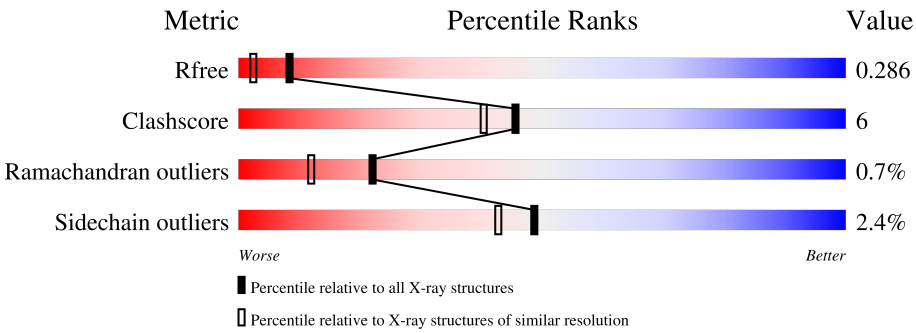
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Mol	Chain	Length	Quality of chain
1	A	908	90% 8% ••
2	B	11	18% 36% 36% 9%
3	C	3	33% 67%
3	D	3	33% 33% 33%
3	G	3	100%
4	E	2	100%
4	F	2	100%

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Mol	Chain	Length	Quality of chain
4	H	2	50% 50%
4	I	2	50% 50%
4	J	2	50% 50%
4	K	2	50% 50%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9093 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	902	7241	4622	1210	1379	30	0	0	0

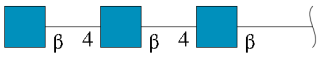
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ASN	PHE	conflict	UNP P15145
A	107	PHE	LEU	conflict	UNP P15145
A	964	SER	-	expression tag	UNP P15145
A	965	HIS	-	expression tag	UNP P15145
A	966	HIS	-	expression tag	UNP P15145
A	967	HIS	-	expression tag	UNP P15145
A	968	HIS	-	expression tag	UNP P15145
A	969	HIS	-	expression tag	UNP P15145
A	970	HIS	-	expression tag	UNP P15145

- Molecule 2 is a protein called substance P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	11	95	63	17	14	1	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	42	24	3	15	0	0	0

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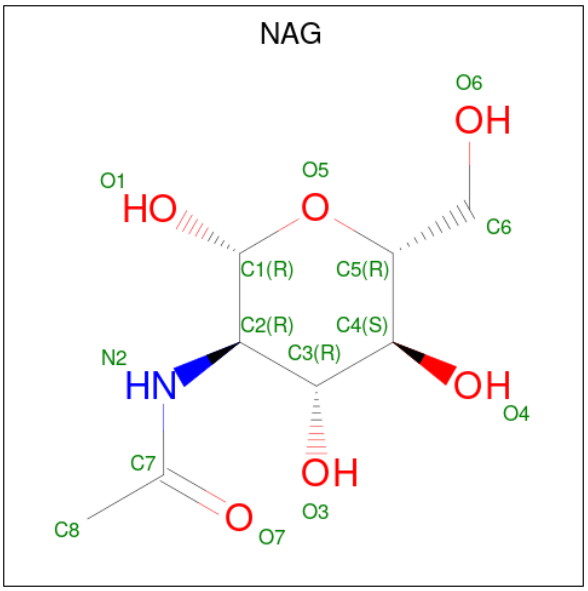
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	42	24	3	15	0	0	0
3	G	3	42	24	3	15	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0
4	F	2	28	16	2	10	0	0	0
4	H	2	28	16	2	10	0	0	0
4	I	2	28	16	2	10	0	0	0
4	J	2	28	16	2	10	0	0	0
4	K	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

- Molecule 7 is water.

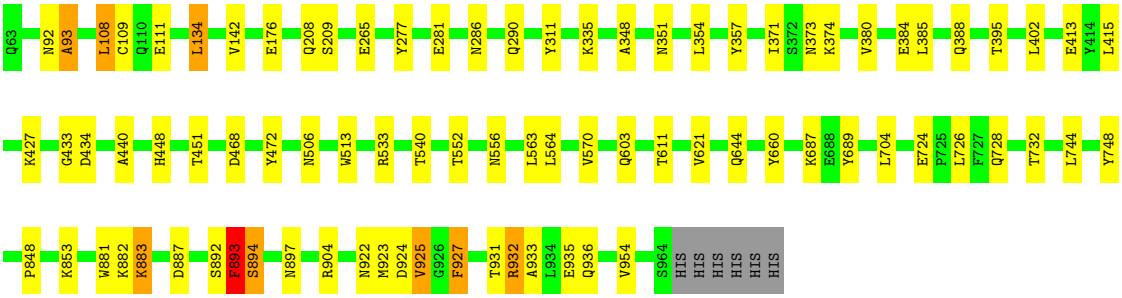
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1423	Total O 1423 1423	0	0
7	B	11	Total O 11 11	0	0

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.

• Molecule 1: Aminopeptidase N

Chain A:



• Molecule 2: substance P

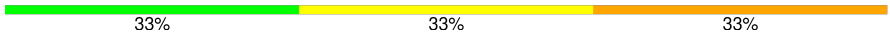
Chain B:

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

Chain C:

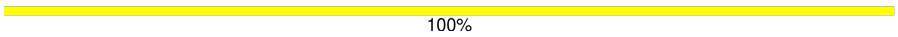
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

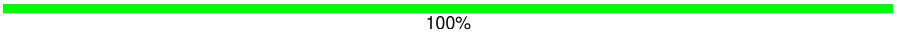


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

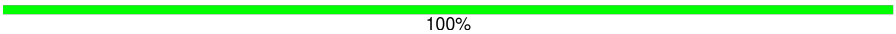
Chain G:



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

Chain E: 

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

Chain F: 

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

Chain H:

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

Chain I:

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

Chain J:

• Molecule 4: 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	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	261.57Å 62.60Å 81.55Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	37.18 – 1.90 37.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (37.18-1.90) 98.0 (37.15-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.147 , 0.201 0.255 , 0.286	Depositor DCC
R_{free} test set	5035 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 71.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9093	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG

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	0.34	0/7429	0.50	0/10124
2	B	0.65	0/98	1.50	4/128 (3.1%)
All	All	0.35	0/7527	0.53	4/10252 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	ARG	C-N-CD	-7.80	103.43	120.60
2	B	2	PRO	N-CA-C	6.73	129.60	112.10
2	B	3	LYS	N-CA-C	6.52	128.60	111.00
2	B	2	PRO	CB-CA-C	-5.78	97.56	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	ARG	Peptide

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	7241	0	6994	80	0
2	B	95	0	99	33	0
3	C	42	0	37	2	0
3	D	42	0	37	1	0
3	G	42	0	37	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
4	K	28	0	25	1	0
5	A	28	0	26	0	0
6	A	1	0	0	0	0
7	A	1423	0	0	18	2
7	B	11	0	0	0	0
All	All	9093	0	7380	96	2

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 6.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:HB3	2:B:2:PRO:HB3	1.28	1.08
2:B:2:PRO:O	2:B:4:PRO:HD3	1.60	0.99
1:A:384:GLU:OE1	2:B:2:PRO:HA	1.67	0.92
1:A:380:VAL:HG13	7:A:1847:HOH:O	1.70	0.91
1:A:265:GLU:HG3	7:A:1351:HOH:O	1.69	0.91
1:A:451:THR:HG22	7:A:2203:HOH:O	1.75	0.86
7:A:1269:HOH:O	2:B:1:ARG:HB3	1.73	0.86
2:B:3:LYS:HB3	2:B:5:GLN:OE1	1.77	0.83
1:A:556:ASN:HD22	4:J:1:NAG:H83	1.47	0.78
1:A:111:GLU:HG2	7:A:2218:HOH:O	1.85	0.76
1:A:348:ALA:CB	2:B:2:PRO:HB3	2.13	0.75
1:A:384:GLU:OE1	2:B:2:PRO:CA	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1269:HOH:O	2:B:1:ARG:CB	2.31	0.74
2:B:2:PRO:O	2:B:4:PRO:CD	2.36	0.72
1:A:371:ILE:HG13	1:A:744:LEU:HD12	1.75	0.69
1:A:373:ASN:HB3	7:A:2199:HOH:O	1.92	0.68
2:B:1:ARG:HB2	2:B:2:PRO:HD3	1.74	0.68
1:A:371:ILE:CG1	1:A:744:LEU:HD12	2.25	0.67
1:A:472:TYR:CD2	2:B:3:LYS:HB2	2.30	0.66
1:A:433:GLY:HA2	2:B:7:PHE:HA	1.77	0.66
1:A:927:PHE:HD2	1:A:931:THR:HG23	1.60	0.66
1:A:92:ASN:HB3	7:A:2014:HOH:O	1.95	0.65
1:A:564:LEU:HD13	2:B:11:MET:HG3	1.79	0.64
1:A:108:LEU:HD12	1:A:109:CYS:N	2.13	0.63
1:A:704:LEU:HD21	1:A:904:ARG:HG2	1.81	0.63
1:A:176:GLU:OE1	7:A:1512:HOH:O	2.16	0.63
1:A:892:SER:O	1:A:893:PHE:HB2	2.00	0.62
1:A:611:THR:HG21	7:A:1382:HOH:O	2.01	0.61
1:A:208:GLN:HE21	1:A:209:SER:HA	1.67	0.60
1:A:904:ARG:HD2	7:A:1894:HOH:O	2.02	0.60
1:A:932:ARG:N	1:A:932:ARG:HE	2.00	0.59
1:A:552:THR:HB	1:A:611:THR:HG22	1.86	0.58
1:A:448:HIS:HE1	1:A:468:ASP:OD2	1.87	0.57
1:A:92:ASN:O	1:A:93:ALA:HB3	2.05	0.56
1:A:564:LEU:CD1	2:B:11:MET:HG3	2.37	0.55
3:D:2:NAG:H61	3:D:3:NAG:O5	2.08	0.54
1:A:881:TRP:C	1:A:883:LYS:H	2.11	0.54
2:B:3:LYS:CB	2:B:5:GLN:OE1	2.52	0.54
1:A:434:ASP:OD1	2:B:5:GLN:HG3	2.10	0.52
1:A:954:VAL:HG23	7:A:1573:HOH:O	2.10	0.52
1:A:563:LEU:HD11	1:A:570:VAL:CG2	2.40	0.52
1:A:660:TYR:CD1	2:B:10:LEU:HG	2.45	0.51
1:A:660:TYR:HD1	2:B:10:LEU:HG	1.75	0.51
1:A:357:TYR:HE2	1:A:380:VAL:HG12	1.76	0.51
2:B:1:ARG:HB2	2:B:2:PRO:CD	2.42	0.50
2:B:4:PRO:C	2:B:5:GLN:HG2	2.31	0.50
1:A:395:THR:O	1:A:506:ASN:HA	2.12	0.50
1:A:451:THR:HG23	1:A:540:THR:HB	1.94	0.49
1:A:892:SER:O	1:A:893:PHE:CB	2.60	0.49
1:A:848:PRO:HG3	1:A:853:LYS:HE3	1.94	0.49
1:A:281:GLU:OE1	7:A:1541:HOH:O	2.20	0.49
7:A:1441:HOH:O	2:B:10:LEU:HD13	2.13	0.48
1:A:931:THR:HG22	1:A:932:ARG:NE	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ALA:HA	2:B:11:MET:HG2	1.96	0.48
1:A:357:TYR:CE2	1:A:380:VAL:HG12	2.49	0.47
1:A:927:PHE:CD2	1:A:931:THR:HG23	2.46	0.47
1:A:348:ALA:H	2:B:2:PRO:HG3	1.80	0.47
1:A:108:LEU:HD12	1:A:109:CYS:H	1.79	0.46
1:A:371:ILE:HG13	1:A:744:LEU:CD1	2.43	0.46
1:A:348:ALA:N	2:B:2:PRO:HG3	2.30	0.46
7:A:2191:HOH:O	3:C:3:NAG:H83	2.15	0.46
1:A:402:LEU:O	1:A:402:LEU:HG	2.12	0.46
2:B:4:PRO:O	2:B:5:GLN:HG2	2.17	0.45
1:A:448:HIS:CE1	1:A:468:ASP:OD2	2.69	0.45
1:A:208:GLN:HE21	1:A:209:SER:CA	2.29	0.45
1:A:415:LEU:HD22	1:A:427:LYS:HE3	1.97	0.45
1:A:556:ASN:HD22	4:J:1:NAG:C8	2.23	0.45
1:A:440:ALA:HB2	2:B:11:MET:H	1.81	0.45
7:A:2360:HOH:O	2:B:4:PRO:HB3	2.17	0.45
1:A:732:THR:HB	7:A:2161:HOH:O	2.17	0.44
1:A:351:ASN:HB2	1:A:354:LEU:O	2.18	0.44
1:A:563:LEU:HD11	1:A:570:VAL:HG23	2.00	0.44
1:A:924:ASP:O	1:A:925:VAL:HG22	2.18	0.44
7:A:1269:HOH:O	2:B:1:ARG:HB2	2.09	0.44
1:A:371:ILE:HG12	1:A:744:LEU:HD12	1.99	0.43
1:A:92:ASN:O	1:A:93:ALA:CB	2.66	0.43
1:A:208:GLN:HA	1:A:209:SER:HA	1.82	0.43
1:A:932:ARG:HA	1:A:935:GLU:HB2	2.00	0.43
1:A:385:LEU:HA	1:A:388:GLN:HG2	2.01	0.42
1:A:413:GLU:OE1	2:B:4:PRO:HB3	2.19	0.42
1:A:311:TYR:CE1	1:A:374:LYS:HE2	2.55	0.42
1:A:932:ARG:HE	1:A:932:ARG:H	1.67	0.42
1:A:440:ALA:CA	2:B:11:MET:HG2	2.49	0.41
3:C:2:NAG:H4	3:C:3:NAG:H2	1.81	0.41
1:A:472:TYR:CE2	2:B:3:LYS:HB2	2.55	0.41
1:A:621:VAL:HG11	4:K:1:NAG:H82	2.01	0.41
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.56	0.41
1:A:894:SER:OG	1:A:897:ASN:ND2	2.53	0.41
1:A:933:ALA:HA	1:A:936:GLN:OE1	2.21	0.41
1:A:134:LEU:HD13	1:A:142:VAL:CG2	2.51	0.41
1:A:380:VAL:HG22	2:B:4:PRO:HG2	2.03	0.41
1:A:413:GLU:OE2	2:B:4:PRO:HA	2.21	0.41
1:A:883:LYS:HG2	1:A:883:LYS:O	2.20	0.41
1:A:724:GLU:O	1:A:728:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:HG23	1:A:748:TYR:HE1	1.87	0.40
1:A:687:LYS:HA	1:A:726:LEU:HD13	2.03	0.40

All (2) 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:A:2035:HOH:O	7:A:2035:HOH:O[2_556]	1.95	0.25
7:A:2351:HOH:O	7:A:2351:HOH:O[2_556]	1.98	0.22

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	900/908 (99%)	869 (97%)	26 (3%)	5 (1%)	25 15
2	B	9/11 (82%)	2 (22%)	6 (67%)	1 (11%)	0 0
All	All	909/919 (99%)	871 (96%)	32 (4%)	6 (1%)	22 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	LYS
1	A	893	PHE
1	A	925	VAL
2	B	9	GLY
1	A	93	ALA
1	A	894	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	797/803 (99%)	780 (98%)	17 (2%)	53	48
2	B	10/10 (100%)	8 (80%)	2 (20%)	1	0
All	All	807/813 (99%)	788 (98%)	19 (2%)	49	43

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	134	LEU
1	A	277	TYR
1	A	286	ASN
1	A	290	GLN
1	A	335	LYS
1	A	513	TRP
1	A	533	ARG
1	A	603	GLN
1	A	644	GLN
1	A	883	LYS
1	A	887	ASP
1	A	893	PHE
1	A	922	ASN
1	A	923	MET
1	A	927	PHE
1	A	932	ARG
2	B	10	LEU
2	B	11	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	448	HIS
1	A	775	GLN

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Mol	Chain	Res	Type
1	A	782	ASN
1	A	886	GLN
1	A	897	ASN
1	A	921	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)

21 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.56	0	17,19,21	0.79	0
3	NAG	C	2	3	14,14,15	0.49	0	17,19,21	1.35	1 (5%)
3	NAG	C	3	3	14,14,15	0.75	0	17,19,21	1.35	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.57	0	17,19,21	0.84	0
3	NAG	D	2	3	14,14,15	0.72	0	17,19,21	1.56	1 (5%)
3	NAG	D	3	3	14,14,15	0.54	0	17,19,21	0.77	0
4	NAG	E	1	1,4	14,14,15	0.50	0	17,19,21	0.65	0
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	0.83	0
4	NAG	F	1	1,4	14,14,15	0.49	0	17,19,21	0.86	0
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.87	0
3	NAG	G	1	1,3	14,14,15	0.46	0	17,19,21	1.11	2 (11%)
3	NAG	G	2	3	14,14,15	0.55	0	17,19,21	1.18	1 (5%)
3	NAG	G	3	3	14,14,15	0.52	0	17,19,21	1.87	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	H	1	1,4	14,14,15	0.55	0	17,19,21	0.99	0
4	NAG	H	2	4	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.43	0	17,19,21	1.81	3 (17%)
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.89	0
4	NAG	J	1	1,4	14,14,15	0.51	0	17,19,21	1.43	5 (29%)
4	NAG	J	2	4	14,14,15	0.45	0	17,19,21	0.95	0
4	NAG	K	1	1,4	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
4	NAG	K	2	4	14,14,15	0.45	0	17,19,21	0.95	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	C	3	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	3	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	3	3	-	3/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3	NAG	C2-N2-C7	6.29	131.33	122.90
4	I	1	NAG	C1-O5-C5	5.88	120.06	112.19
3	D	2	NAG	C4-C3-C2	4.91	118.22	111.02
3	G	2	NAG	C4-C3-C2	3.82	116.61	111.02
3	C	3	NAG	C4-C3-C2	3.55	116.22	111.02
3	C	2	NAG	C4-C3-C2	3.13	115.60	111.02
3	G	1	NAG	C1-O5-C5	3.04	116.26	112.19
4	H	2	NAG	C1-O5-C5	2.86	116.02	112.19
4	K	1	NAG	C1-O5-C5	2.84	116.00	112.19
4	I	1	NAG	C2-N2-C7	-2.78	119.17	122.90
4	J	1	NAG	O5-C1-C2	-2.67	107.17	111.29
4	K	2	NAG	C1-O5-C5	2.64	115.73	112.19
4	I	1	NAG	C1-C2-N2	-2.55	106.42	110.43
3	G	3	NAG	C3-C4-C5	2.27	114.35	110.23
4	J	1	NAG	C8-C7-N2	2.26	119.87	116.12
4	J	1	NAG	C2-N2-C7	2.24	125.90	122.90
3	C	3	NAG	O5-C1-C2	2.21	114.71	111.29
4	J	1	NAG	C1-O5-C5	2.17	115.10	112.19
3	G	1	NAG	C1-C2-N2	2.14	113.81	110.43
3	G	3	NAG	O7-C7-N2	2.10	125.70	121.98
4	J	1	NAG	O7-C7-C8	-2.04	118.42	122.05

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	NAG	C3-C2-N2-C7
3	C	3	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
3	C	3	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	G	3	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	3	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

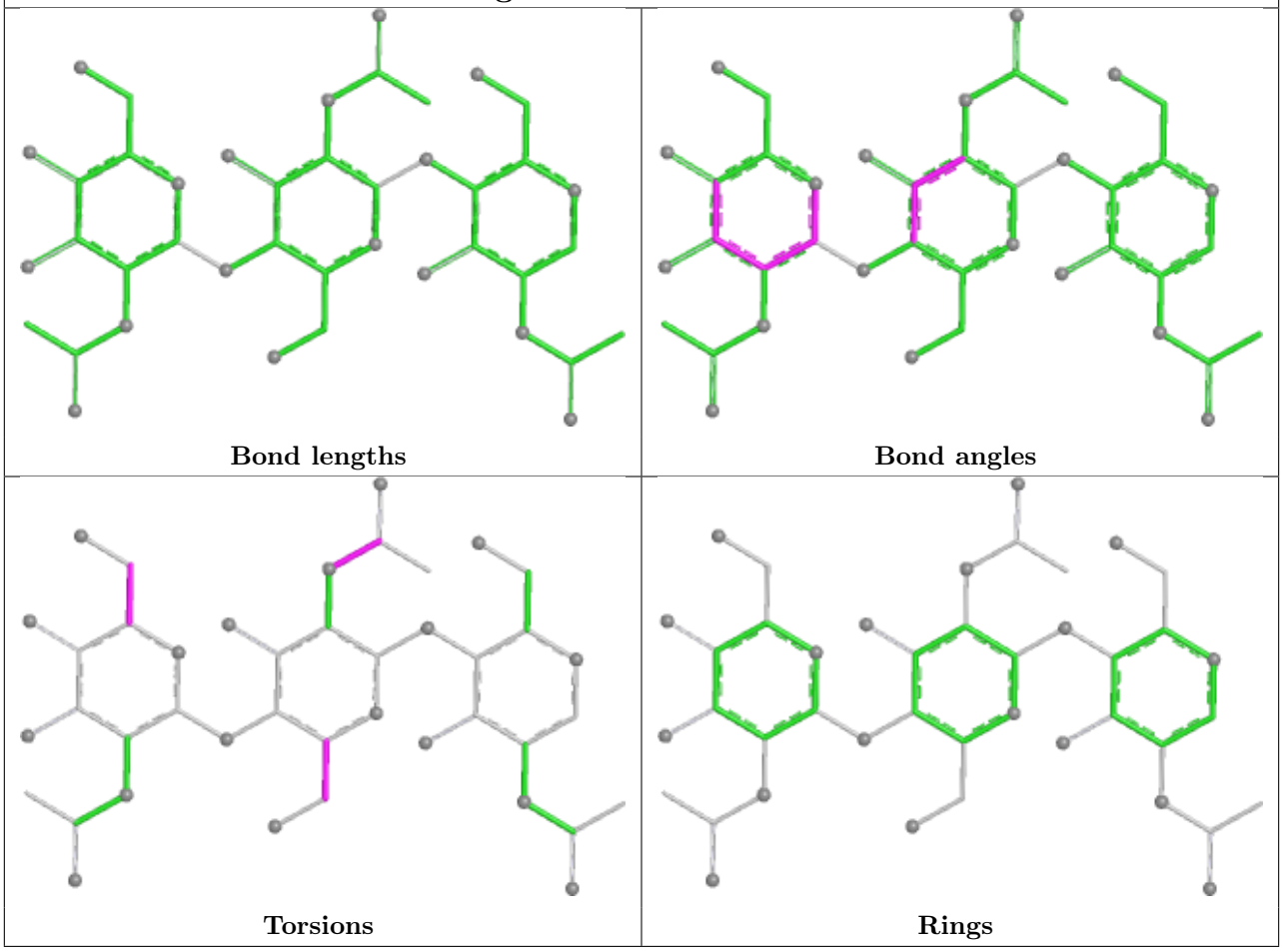
There are no ring outliers.

6 monomers are involved in 6 short contacts:

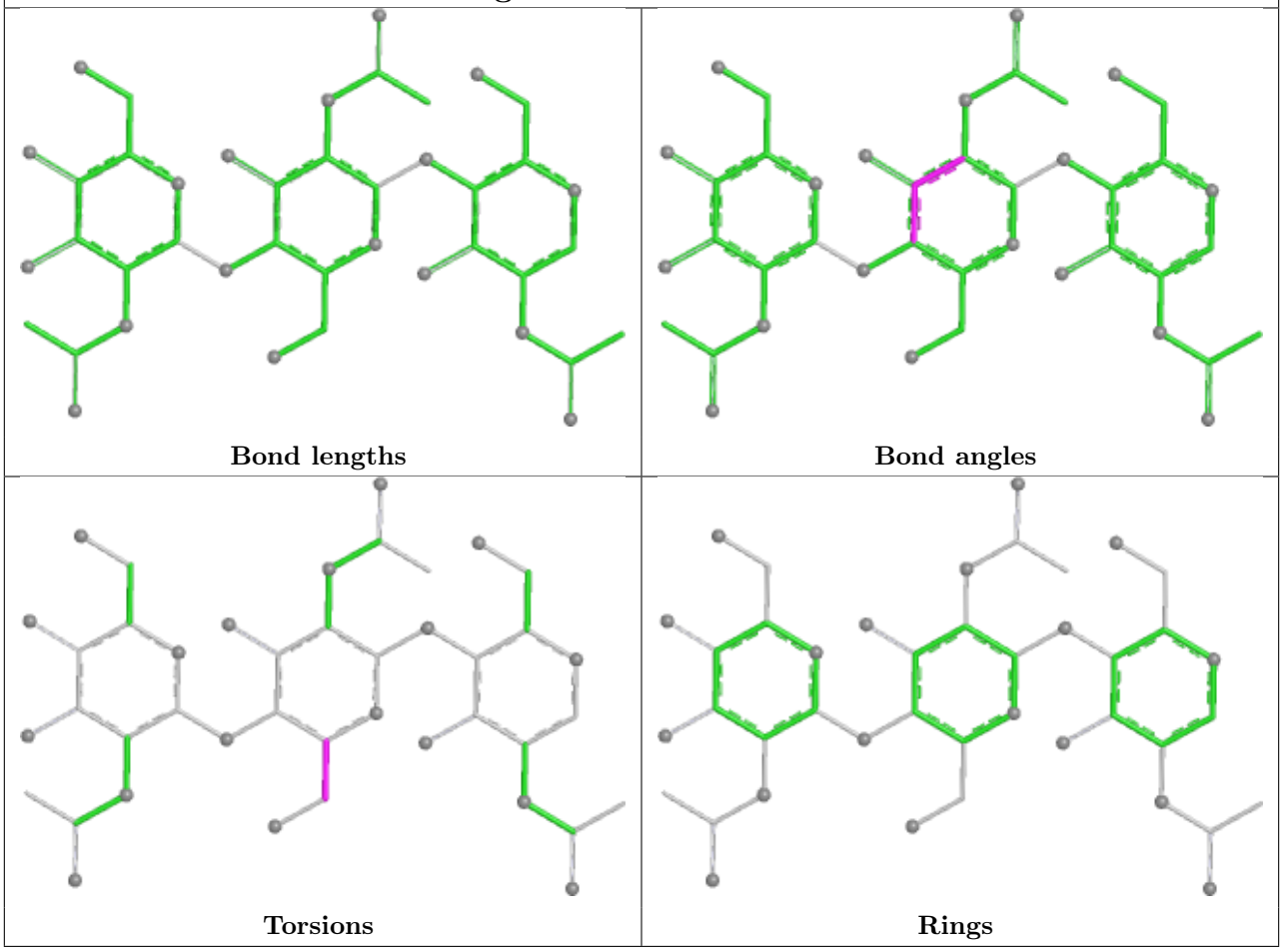
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
4	J	1	NAG	2	0
3	C	2	NAG	1	0
4	K	1	NAG	1	0
3	C	3	NAG	2	0
3	D	3	NAG	1	0

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

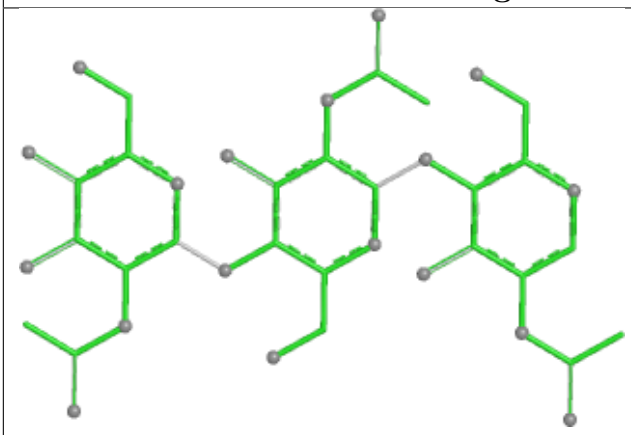
Oligosaccharide Chain C



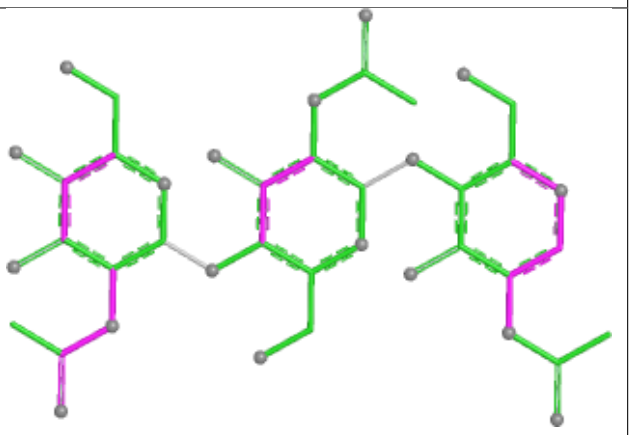
Oligosaccharide Chain D



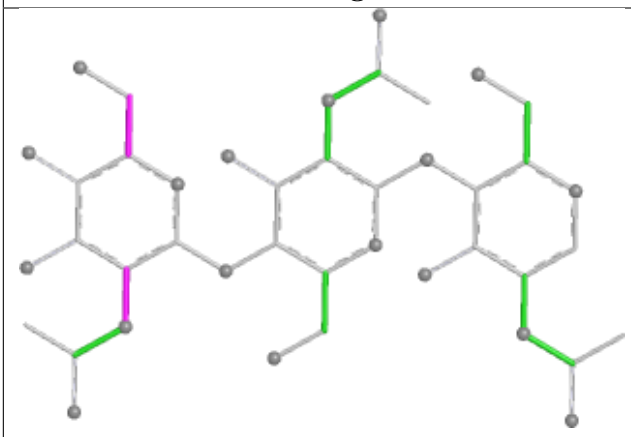
Oligosaccharide Chain G



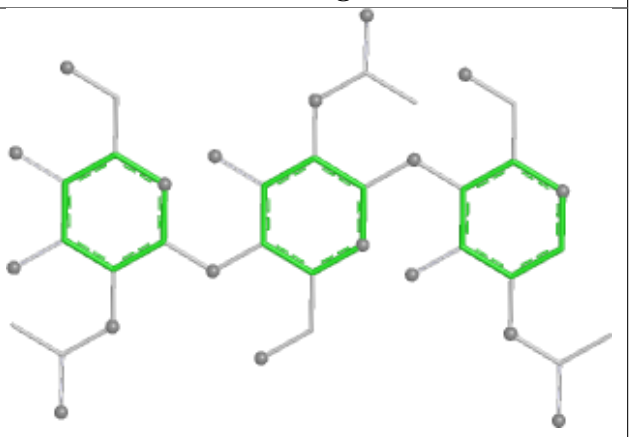
Bond lengths



Bond angles

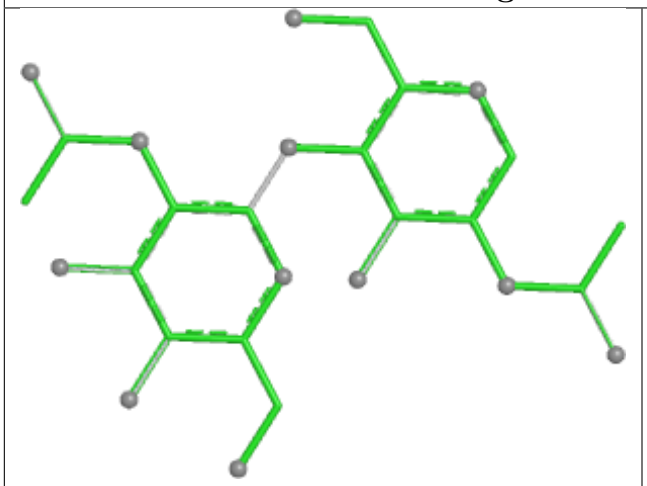


Torsions

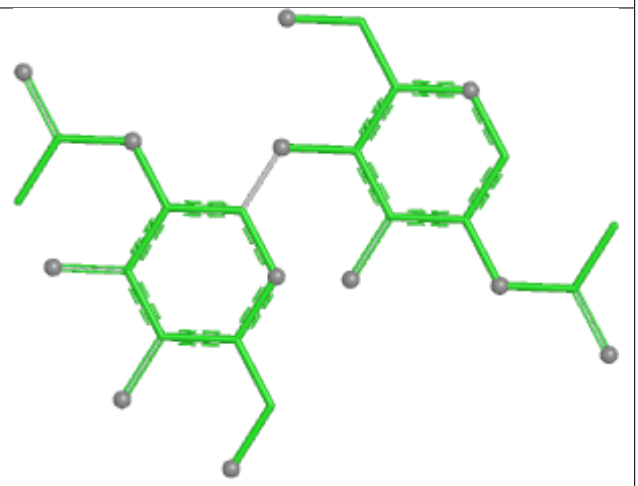


Rings

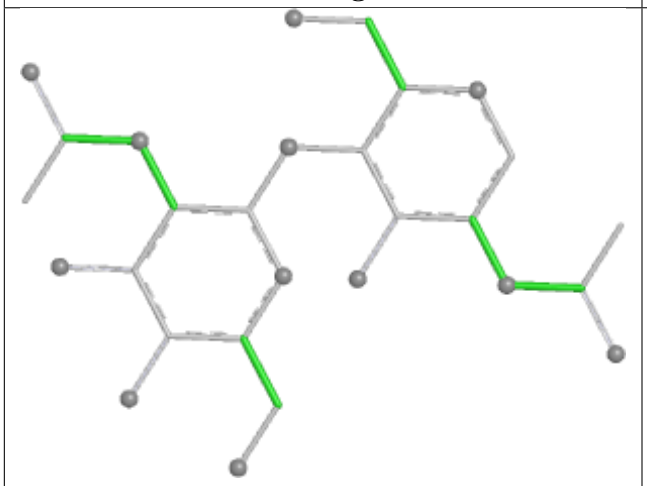
Oligosaccharide Chain E



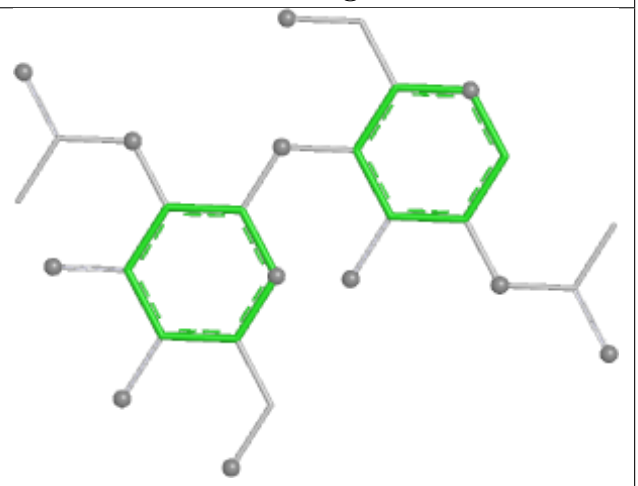
Bond lengths



Bond angles

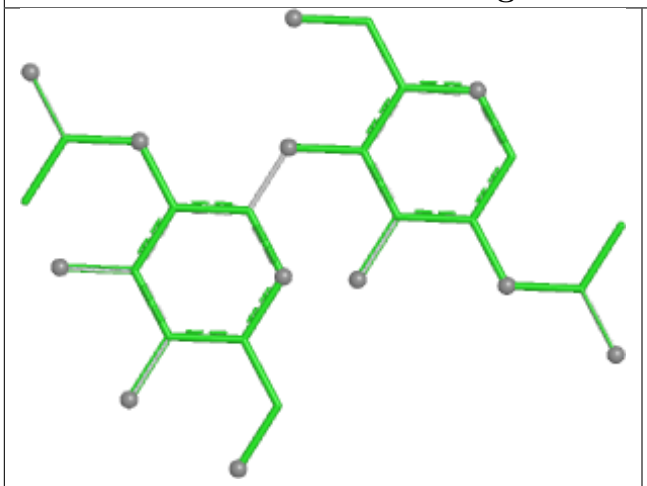


Torsions

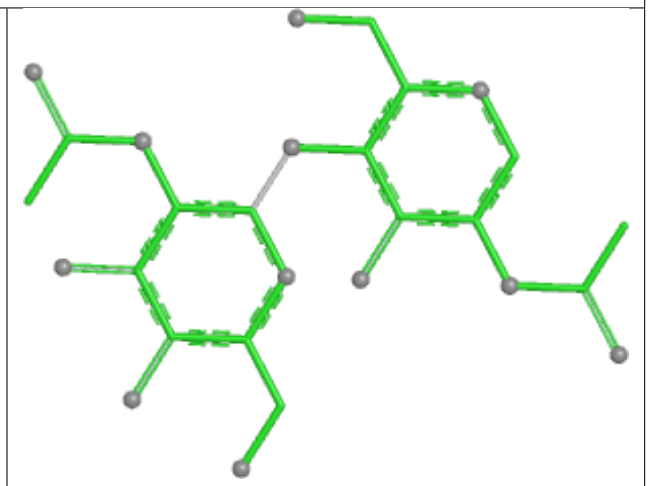


Rings

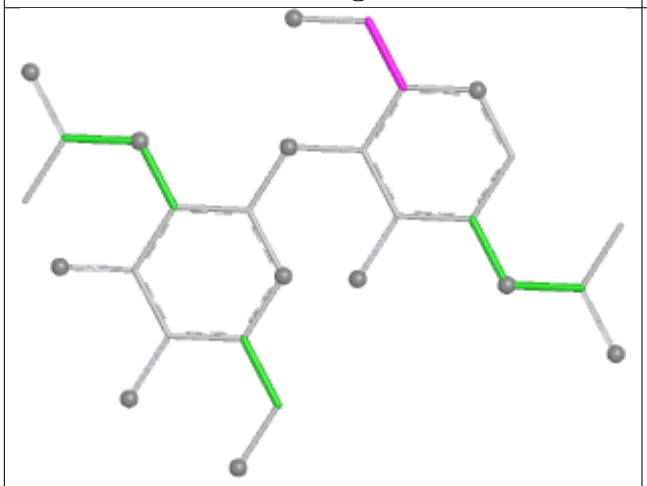
Oligosaccharide Chain F



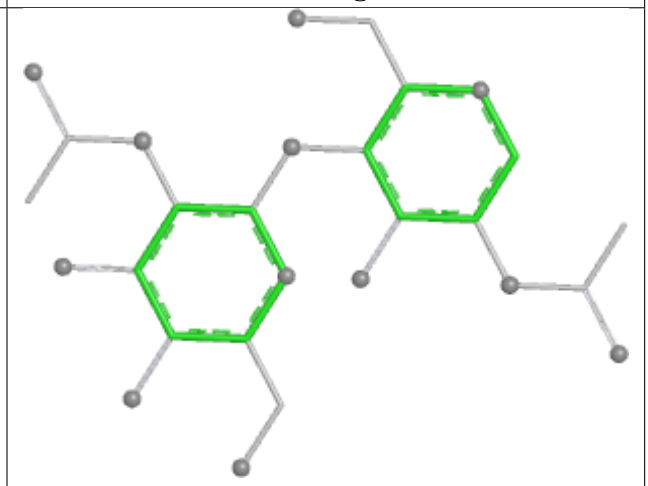
Bond lengths



Bond angles

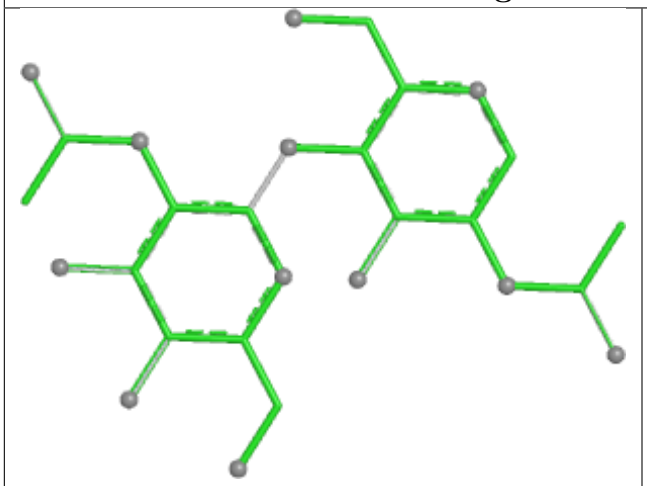


Torsions

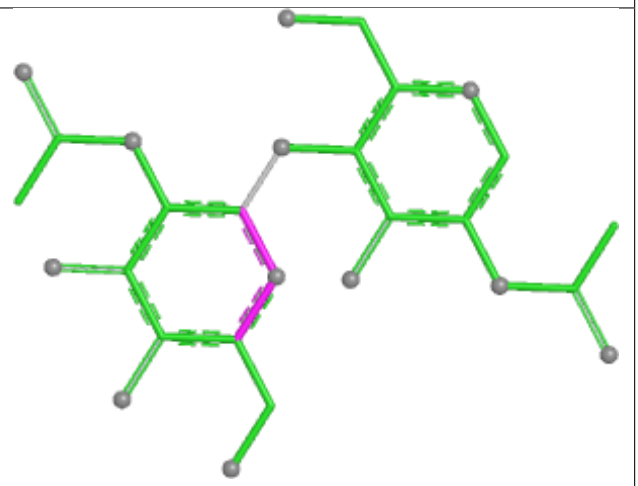


Rings

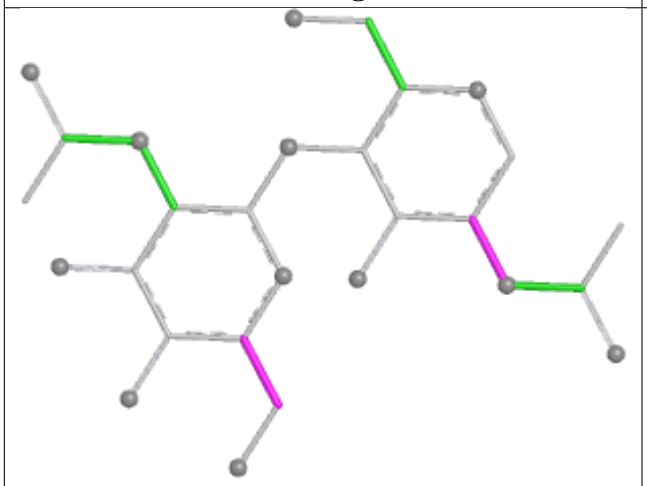
Oligosaccharide Chain H



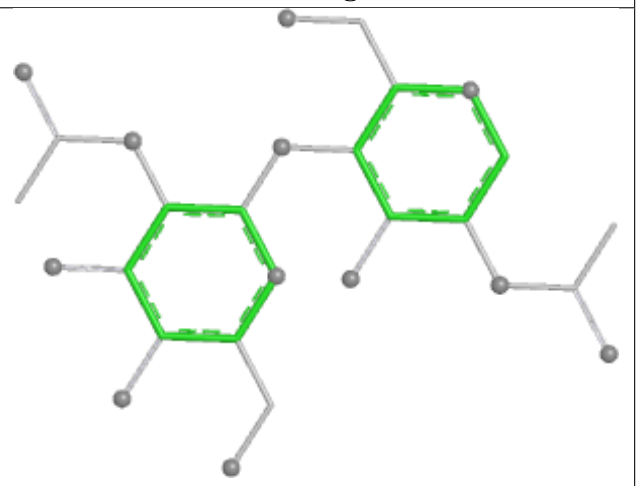
Bond lengths



Bond angles

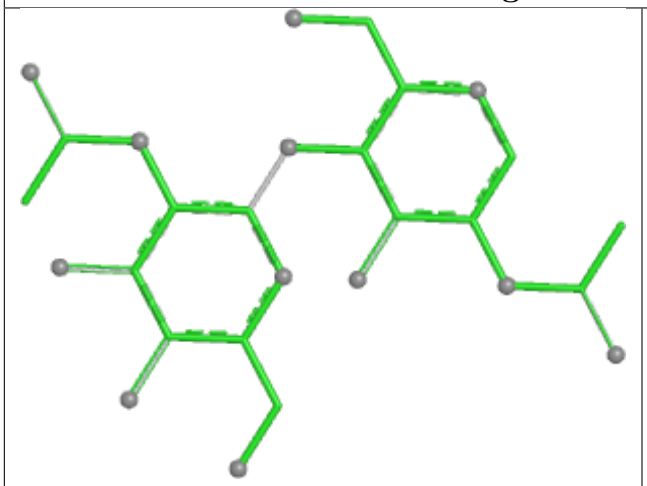


Torsions

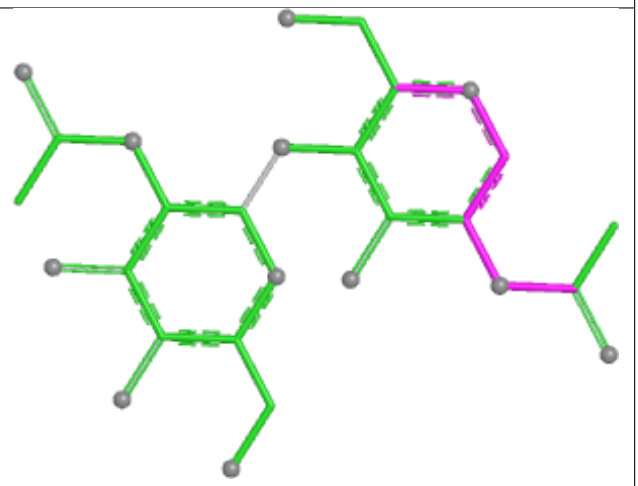


Rings

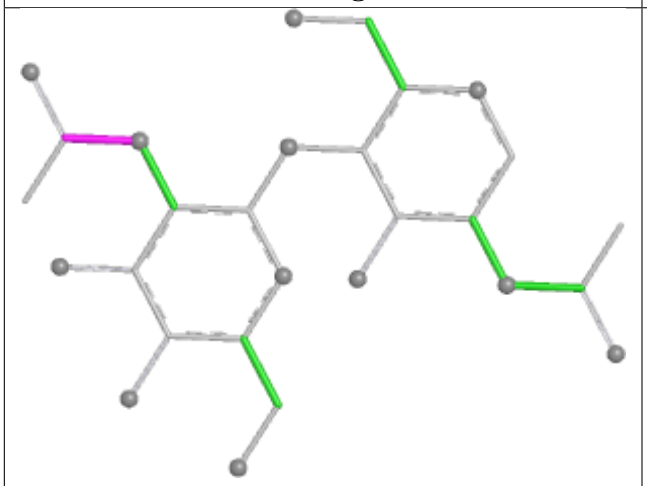
Oligosaccharide Chain I



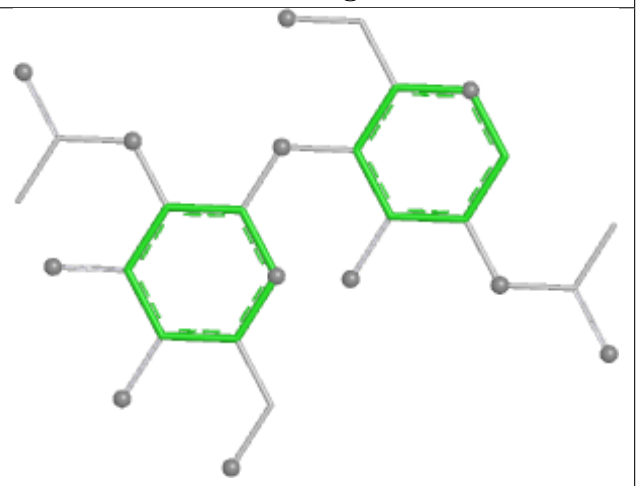
Bond lengths



Bond angles

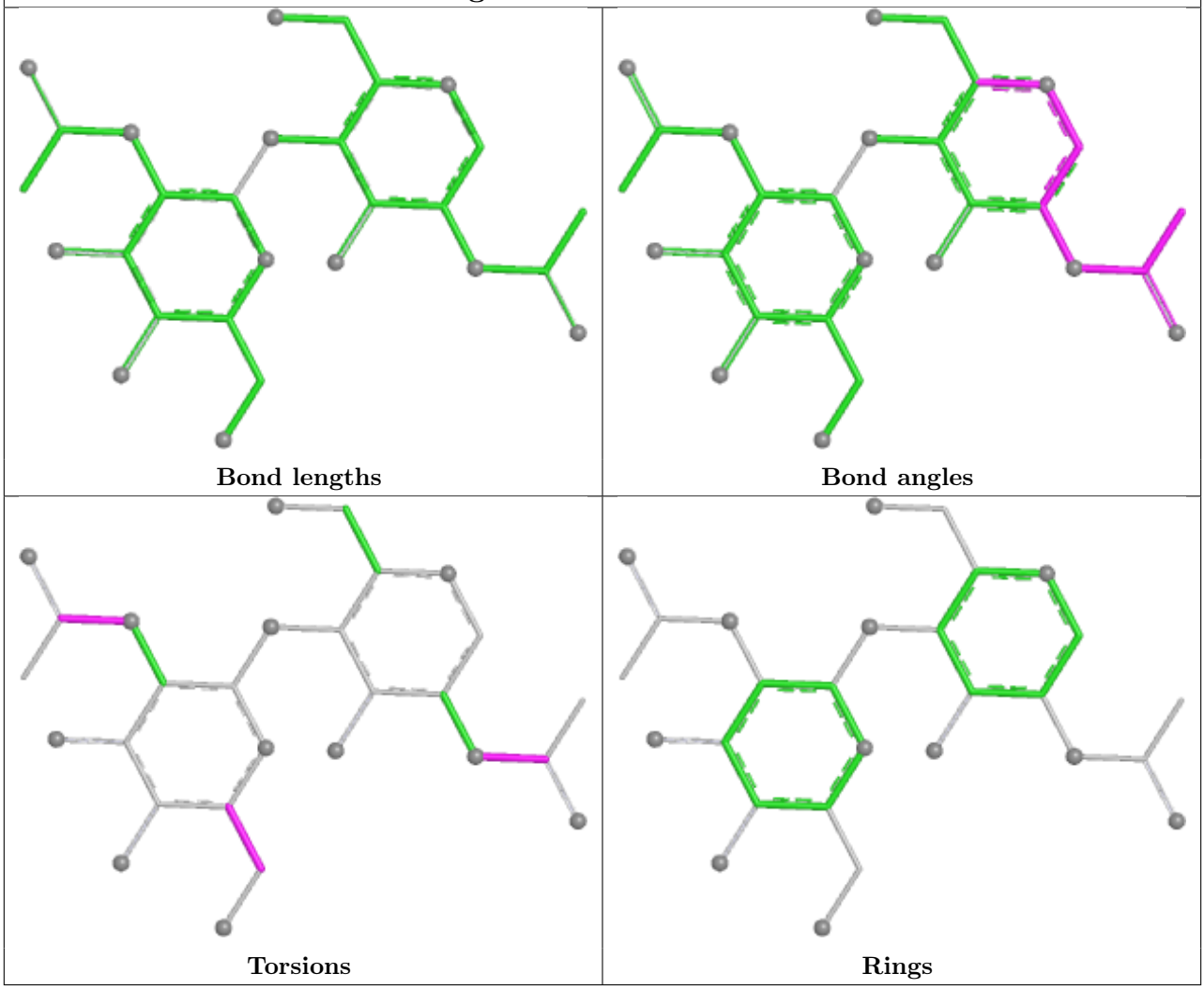


Torsions

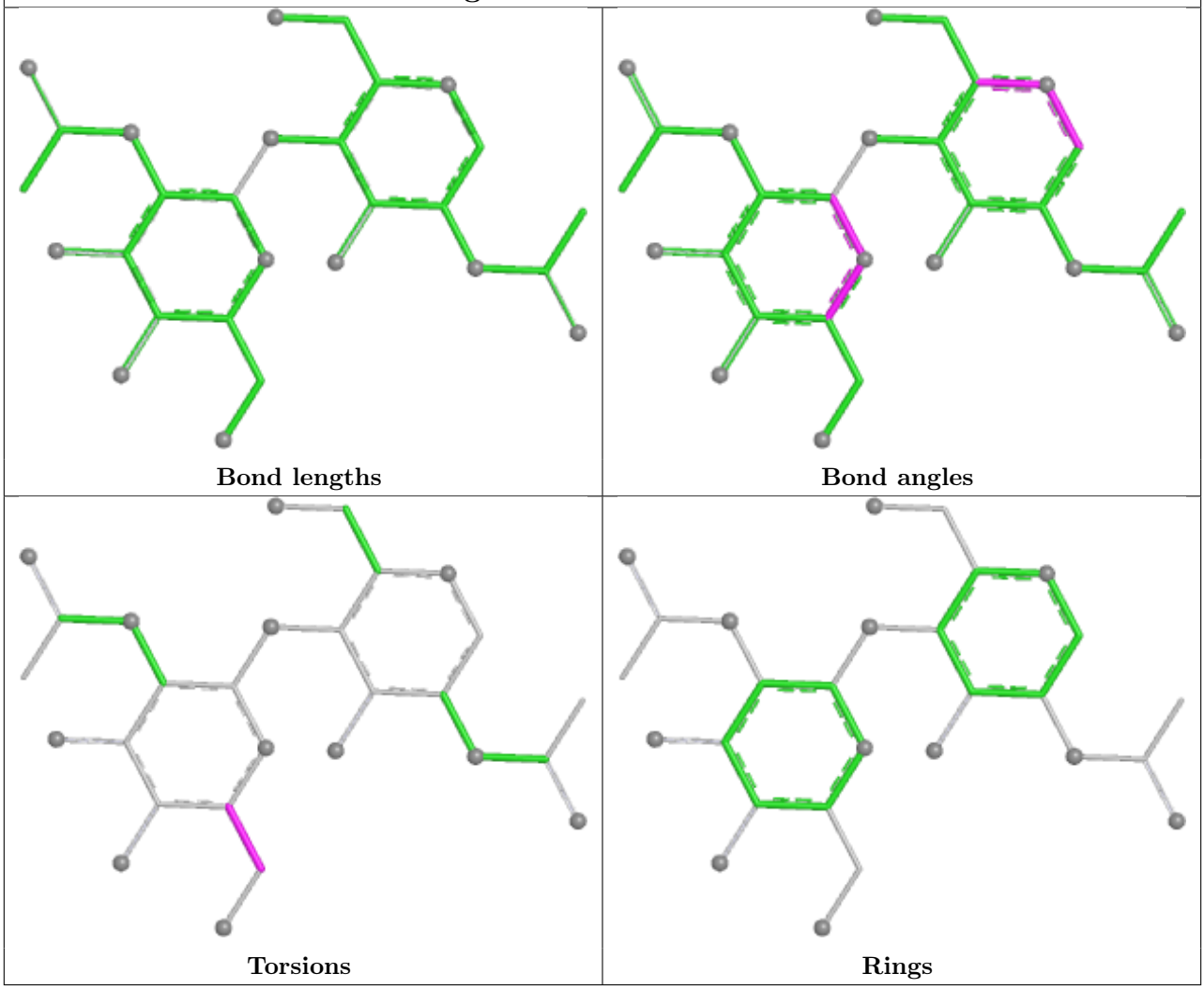


Rings

Oligosaccharide Chain J



Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	NAG	A	1023	1	14,14,15	0.55	0	17,19,21	0.73	0
5	NAG	A	1020	1	14,14,15	0.50	0	17,19,21	1.42	2 (11%)

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
5	NAG	A	1023	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1020	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1020	NAG	C2-N2-C7	3.90	128.13	122.90
5	A	1020	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1020	NAG	C3-C2-N2-C7
5	A	1020	NAG	C4-C5-C6-O6
5	A	1020	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

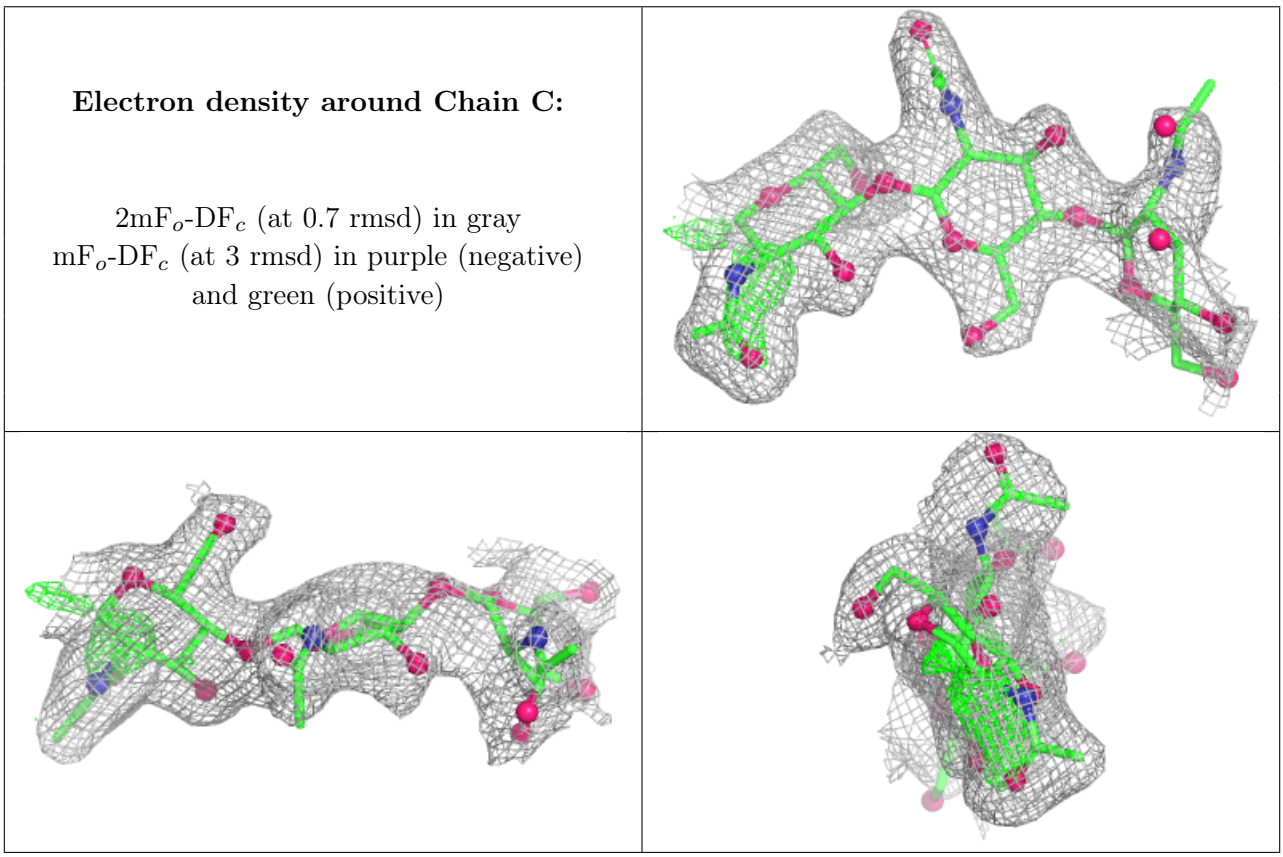
6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

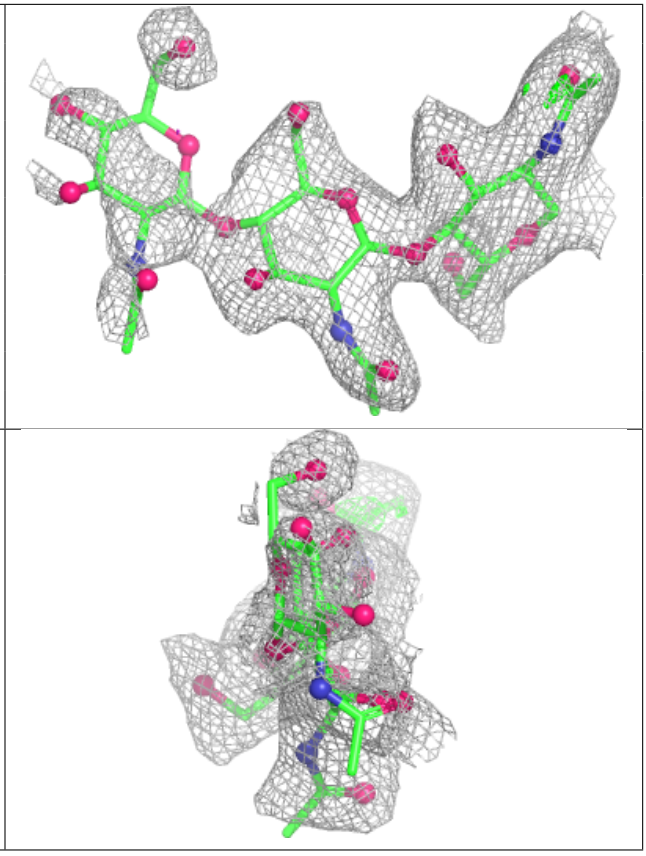
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



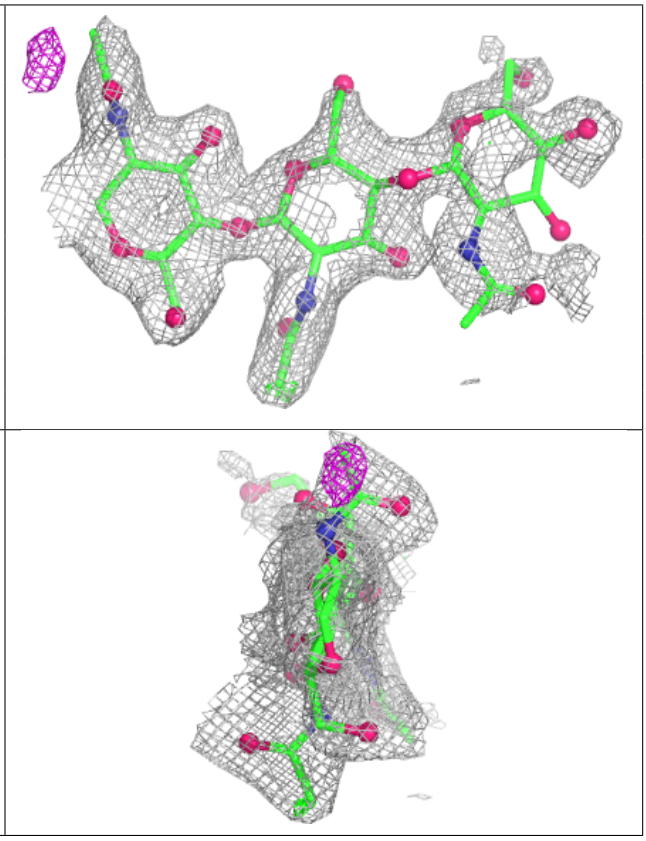
Electron density around Chain D:

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



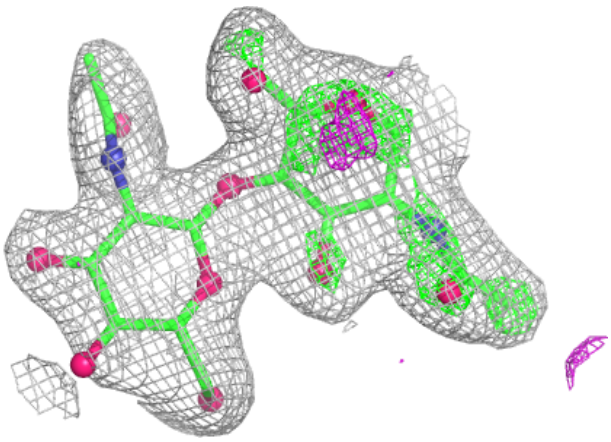
Electron density around Chain G:

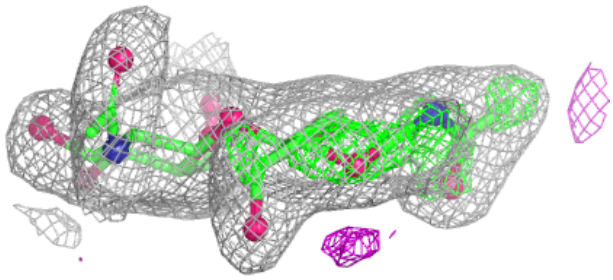
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

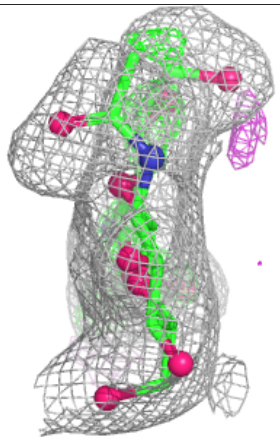


Electron density around Chain E:

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

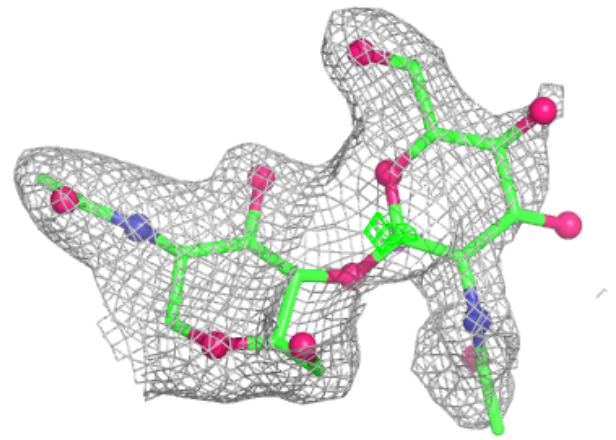


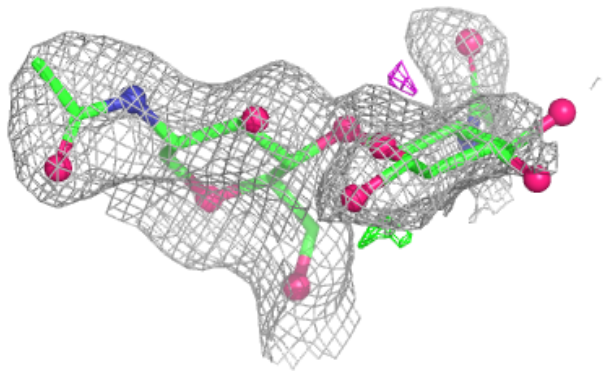


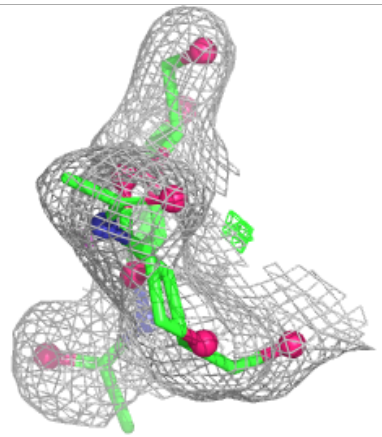


Electron density around Chain F:

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

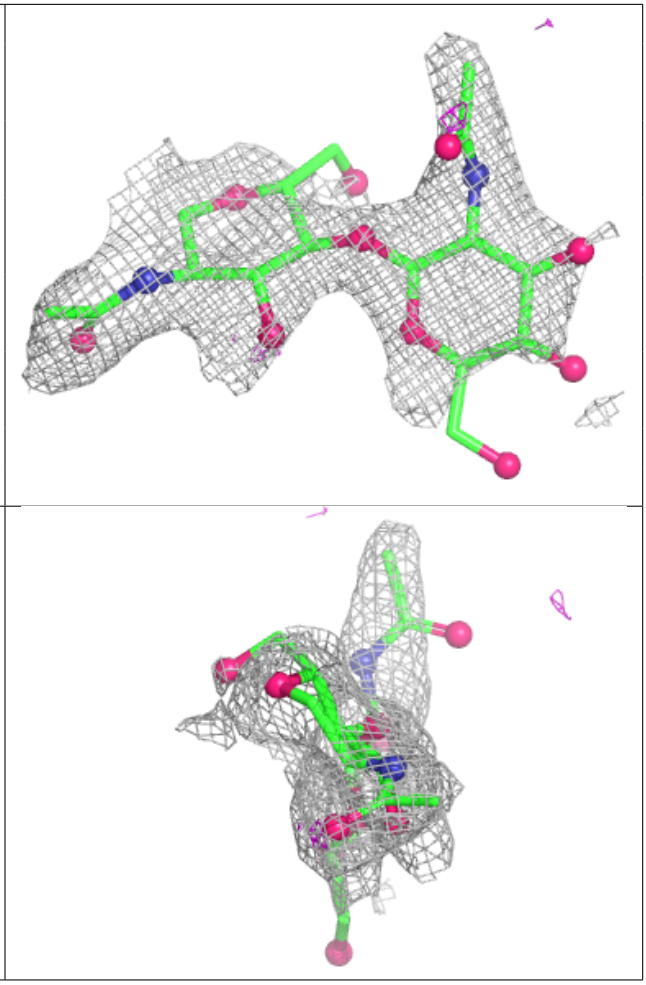






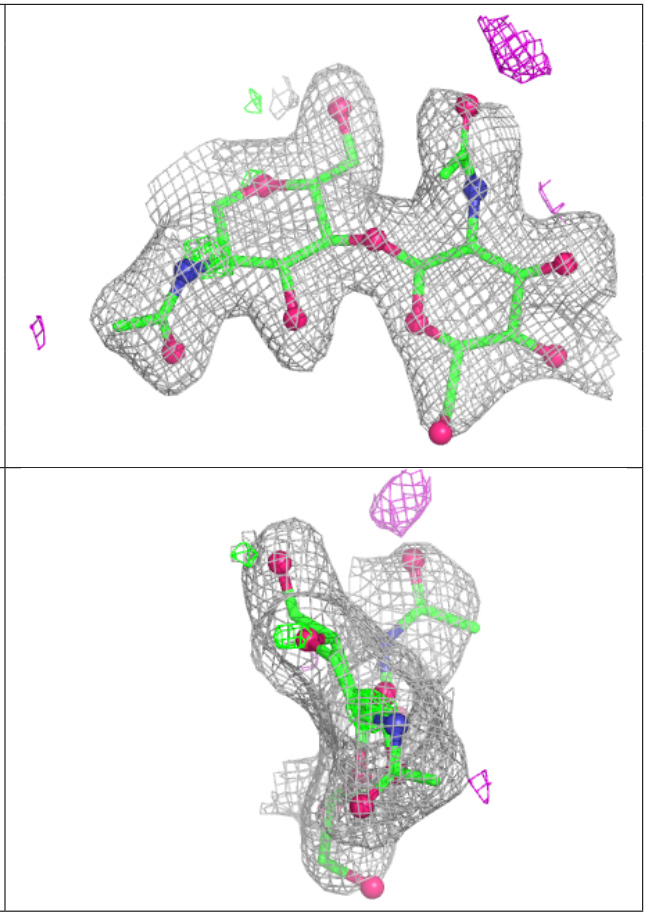
Electron density around Chain H:

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



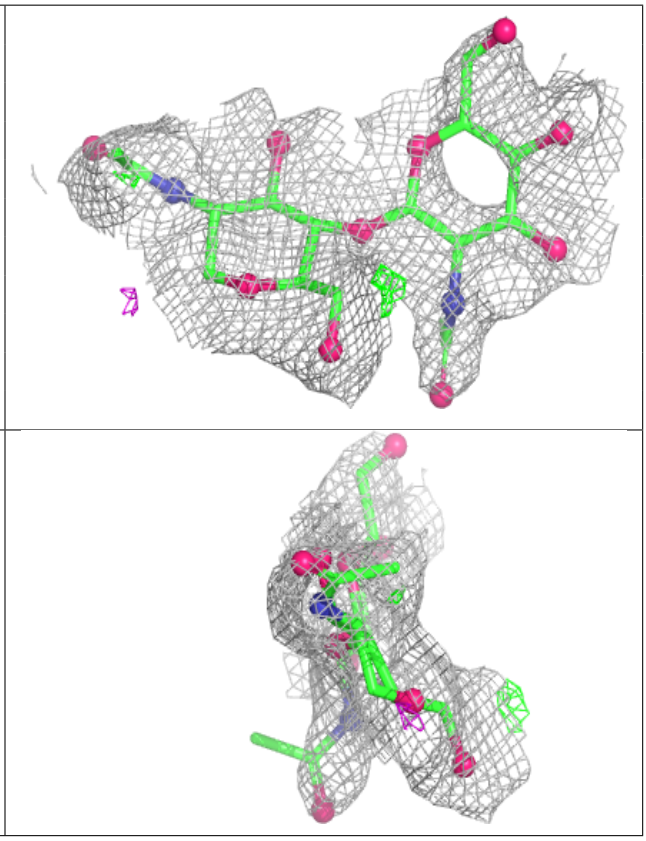
Electron density around Chain I:

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



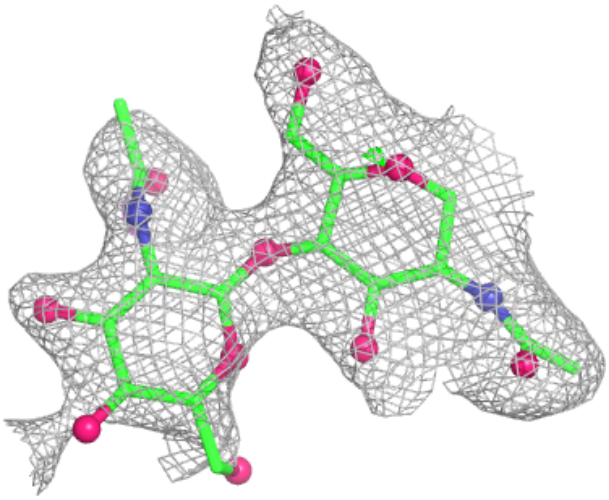
Electron density around Chain J:

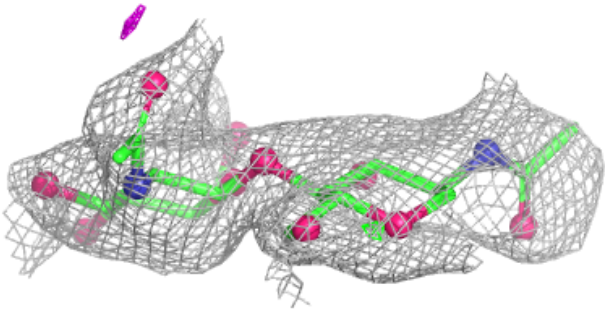
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.