wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 01:57 PM BST

PDB ID	:	1IVF
Title	:	STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS NEURAMINIDASE
Authors	:	Jedrzejas, M.J.; Luo, M.
Deposited on	:	1994-12-12
Resolution	:	2.40 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 following versions of software and data (see references (1)) were used in the production of this report:

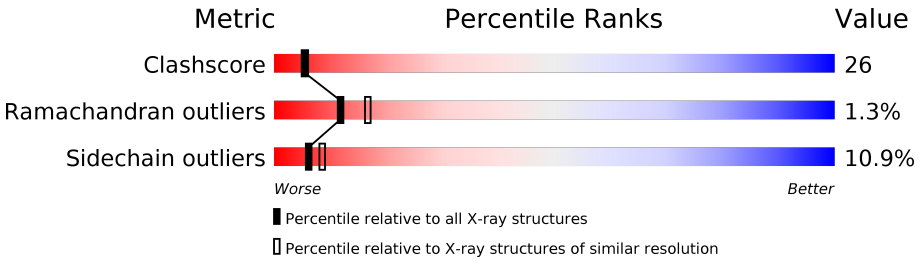
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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	388	47% 46% 7%
1	B	388	48% 45% 7%
2	C	2	100%
2	E	2	100%
2	G	2	100%
2	J	2	100%
3	D	4	75% 25%
4	F	6	67% 33%
4	I	6	67% 33%

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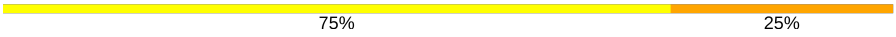
Mol	Chain	Length	Quality of chain
5	H	4	

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
4	NAG	I	1	-	-	X	-
5	FUC	H	4	X	-	-	-
6	CA	A	470	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8629 atoms, of which 2064 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 INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			
1	B	388	Total	C	H	N	O	S	0	0	0
			3745	1866	723	545	588	23			

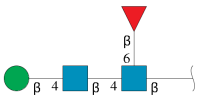
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ASP	ASN	conflict	UNP P06820
B	339	ASP	ASN	conflict	UNP P06820

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

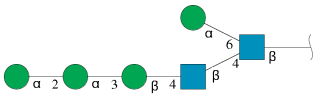
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
2	J	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

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



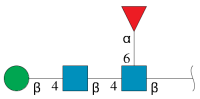
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	4	Total C H N O 96 28 47 2 19	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	6	Total C H N O 139 40 67 2 30	0	0	0
4	I	6	Total C H N O 139 40 67 2 30	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



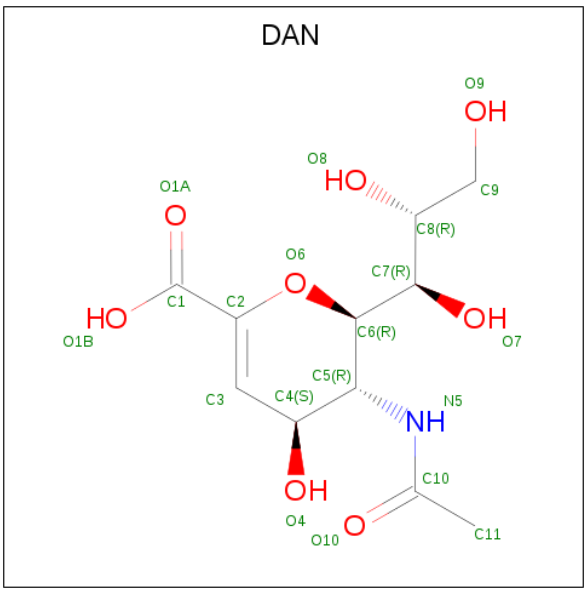
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	4	Total C H N O 96 28 47 2 19	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0

- Molecule 7 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter

code: DAN) (formula: $C_{11}H_{17}NO_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H N O 36 11 16 1 8	0	0
7	B	1	Total C H N O 36 11 16 1 8	0	0

- Molecule 8 is water.

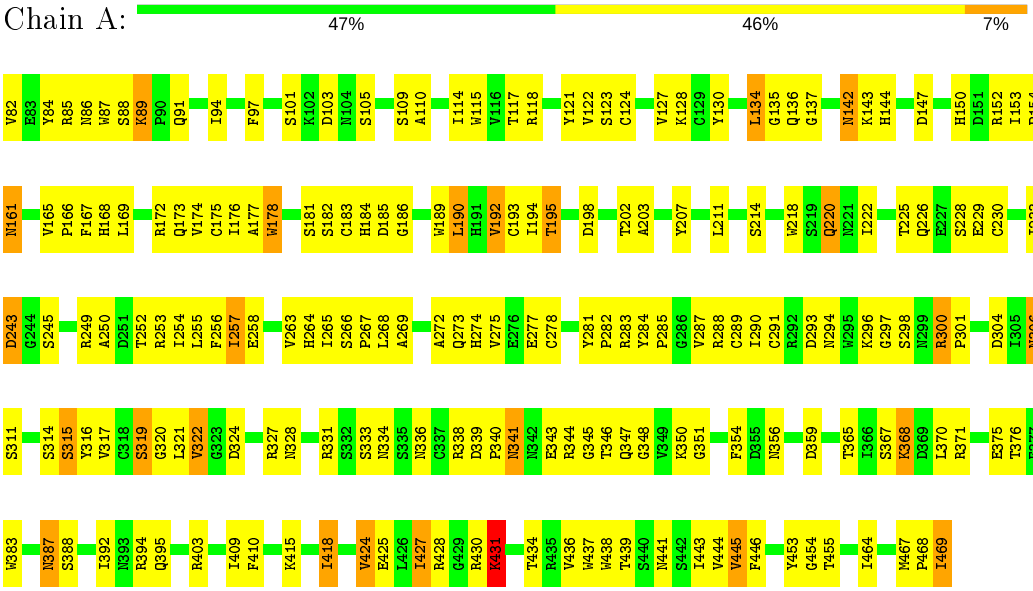
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	119	Total H O 357 238 119	0	0
8	B	6	Total H O 18 12 6	0	0

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.

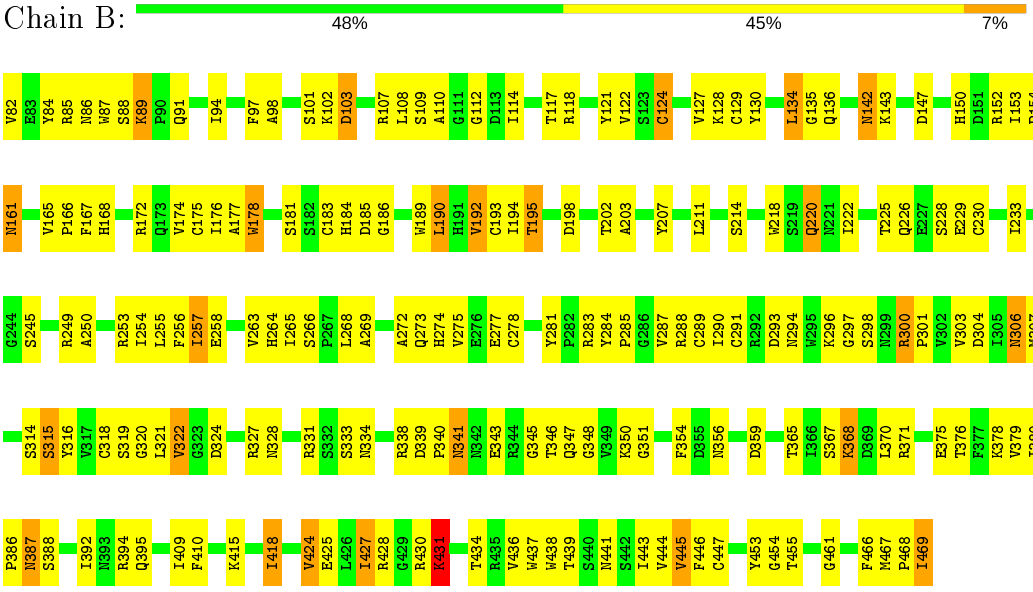
- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain A:



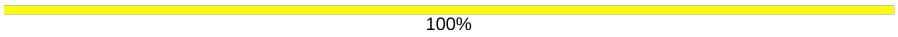
- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain B:



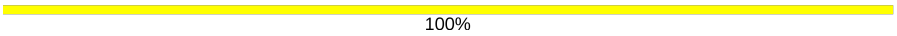
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



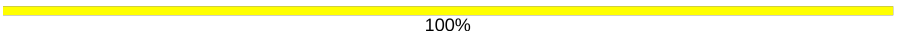
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



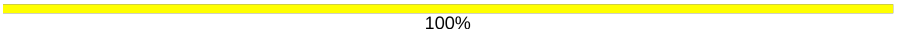
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain J:



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

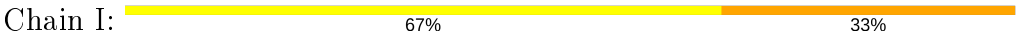
Chain D:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.38Å 139.63Å 140.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.40 25.55 – 2.36	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.40) 47.7 (25.55-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.36Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.163 , (Not available) 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	10.6	Xtriage
Anisotropy	1.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 88.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	8629	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: BMA, NAG, DAN, FUC, FUL, CA, MAN

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	0.59	0/3092	0.90	3/4194 (0.1%)
1	B	0.59	0/3092	0.90	3/4194 (0.1%)
All	All	0.59	0/6184	0.90	6/8388 (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	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	243	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	300	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	300	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	134	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	84	TYR	Sidechain
1	B	121	TYR	Sidechain
1	B	84	TYR	Sidechain

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	3022	723	2851	169	22
1	B	3022	723	2850	172	1
2	C	28	27	25	0	0
2	E	28	27	25	0	0
2	G	28	27	25	0	0
2	J	28	27	25	0	0
3	D	49	47	43	2	0
4	F	72	67	58	9	0
4	I	72	67	61	1	22
5	H	49	47	43	2	0
6	A	1	0	0	2	0
6	B	1	0	0	1	0
7	A	20	16	16	0	0
7	B	20	16	16	0	0
8	A	119	238	0	11	2
8	B	6	12	0	8	0
All	All	6565	2064	6038	327	24

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 26.

The worst 5 of 327 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:B:124:CYS:SG	8:B:518:HOH:O	1.94	1.19
1:B:453:TYR:O	4:F:1:NAG:O7	1.61	1.15
1:B:454:GLY:O	8:B:512:HOH:O	1.69	1.08
1:B:107:ARG:HD2	8:B:501:HOH:O	0.76	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LYS:HA	1:B:431:LYS:HZ2	1.34	0.91

The worst 5 of 24 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)
1:A:454:GLY:CA	4:I:1:NAG:C8[4_555]	0.63	1.57
1:A:454:GLY:CA	4:I:1:NAG:C7[4_555]	0.91	1.29
1:A:454:GLY:N	4:I:1:NAG:C8[4_555]	1.31	0.89
1:A:454:GLY:H	4:I:1:NAG:H81[4_555]	0.74	0.86
1:A:454:GLY:N	4:I:1:NAG:H81[4_555]	0.76	0.84

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	386/388 (100%)	327 (85%)	54 (14%)	5 (1%)	12	17
1	B	386/388 (100%)	327 (85%)	54 (14%)	5 (1%)	12	17
All	All	772/776 (100%)	654 (85%)	108 (14%)	10 (1%)	12	17

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	B	431	LYS
1	A	89	LYS
1	A	322	VAL
1	A	341	ASN

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	338/338 (100%)	301 (89%)	37 (11%)	6 8
1	B	338/338 (100%)	301 (89%)	37 (11%)	6 8
All	All	676/676 (100%)	602 (89%)	74 (11%)	6 8

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	LYS
1	B	134	LEU
1	B	427	ILE
1	A	443	ILE
1	B	82	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	ASN
1	B	104	ASN
1	B	358	ASN
1	A	393	ASN
1	B	131	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)

28 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.84	0	17,19,21	1.20	1 (5%)
2	NAG	C	2	2	14,14,15	1.68	5 (35%)	17,19,21	1.96	3 (17%)
3	NAG	D	1	1,3	14,14,15	0.79	0	17,19,21	3.15	7 (41%)
3	NAG	D	2	3	14,14,15	1.84	5 (35%)	17,19,21	1.91	4 (23%)
3	BMA	D	3	3	11,11,12	1.72	4 (36%)	15,15,17	2.25	1 (6%)
3	FUL	D	4	3	10,10,11	1.95	3 (30%)	14,14,16	1.44	3 (21%)
2	NAG	E	1	1,2	14,14,15	0.89	0	17,19,21	1.83	3 (17%)
2	NAG	E	2	2	14,14,15	1.52	2 (14%)	17,19,21	2.10	4 (23%)
4	NAG	F	1	1,4	14,14,15	2.50	6 (42%)	17,19,21	2.33	6 (35%)
4	NAG	F	2	4	14,14,15	1.40	2 (14%)	17,19,21	3.76	7 (41%)
4	BMA	F	3	4	11,11,12	1.50	1 (9%)	15,15,17	3.46	5 (33%)
4	MAN	F	4	4	11,11,12	2.36	6 (54%)	15,15,17	3.17	6 (40%)
4	MAN	F	5	4	11,11,12	2.86	6 (54%)	15,15,17	3.72	6 (40%)
4	MAN	F	6	4	11,11,12	1.53	1 (9%)	15,15,17	2.57	6 (40%)
2	NAG	G	1	1,2	14,14,15	0.84	0	17,19,21	1.20	1 (5%)
2	NAG	G	2	2	14,14,15	1.68	5 (35%)	17,19,21	1.96	3 (17%)
5	NAG	H	1	1,5	14,14,15	0.79	0	17,19,21	3.15	7 (41%)
5	NAG	H	2	5	14,14,15	1.84	5 (35%)	17,19,21	1.91	4 (23%)
5	BMA	H	3	5	11,11,12	1.72	4 (36%)	15,15,17	2.25	1 (6%)
5	FUC	H	4	5	10,10,11	1.95	3 (30%)	14,14,16	1.44	3 (21%)
4	NAG	I	1	1,4	14,14,15	2.50	6 (42%)	17,19,21	2.33	6 (35%)
4	NAG	I	2	4	14,14,15	1.40	2 (14%)	17,19,21	3.76	7 (41%)
4	BMA	I	3	4	11,11,12	1.50	1 (9%)	15,15,17	3.46	5 (33%)
4	MAN	I	4	4	11,11,12	2.36	6 (54%)	15,15,17	3.17	6 (40%)
4	MAN	I	5	4	11,11,12	2.86	6 (54%)	15,15,17	3.72	6 (40%)
4	MAN	I	6	4	11,11,12	1.53	1 (9%)	15,15,17	2.57	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	J	1	1,2	14,14,15	0.89	0	17,19,21	1.83	3 (17%)
2	NAG	J	2	2	14,14,15	1.52	2 (14%)	17,19,21	2.10	4 (23%)

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

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

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5	MAN	C4-C5	5.33	1.64	1.53
4	F	5	MAN	C4-C5	5.33	1.64	1.53
4	F	4	MAN	C4-C5	4.94	1.63	1.53
4	I	4	MAN	C4-C5	4.94	1.63	1.53
4	F	1	NAG	O5-C1	4.85	1.51	1.43

The worst 5 of 124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	3	BMA	O3-C3-C2	10.65	130.38	109.99
4	F	3	BMA	O3-C3-C2	10.65	130.38	109.99
3	D	1	NAG	C1-O5-C5	9.82	125.50	112.19
5	H	1	NAG	C1-O5-C5	9.82	125.50	112.19
4	I	5	MAN	C1-O5-C5	8.84	124.16	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	H	4	FUC	C1

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7
5	H	1	NAG	C1-C2-N2-C7
2	J	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	I	6	MAN	O5-C5-C6-O6

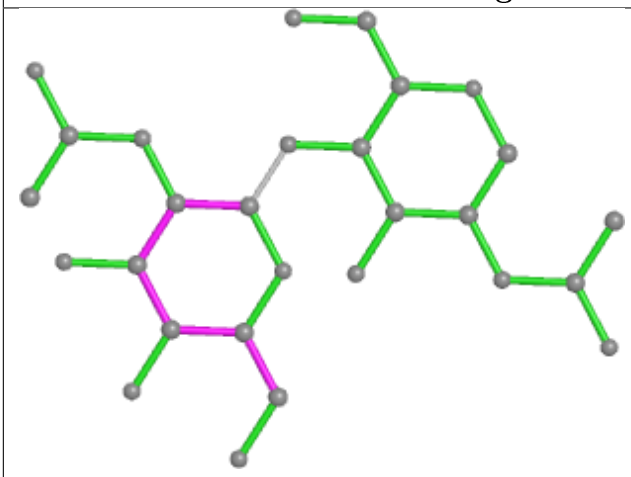
There are no ring outliers.

6 monomers are involved in 36 short contacts:

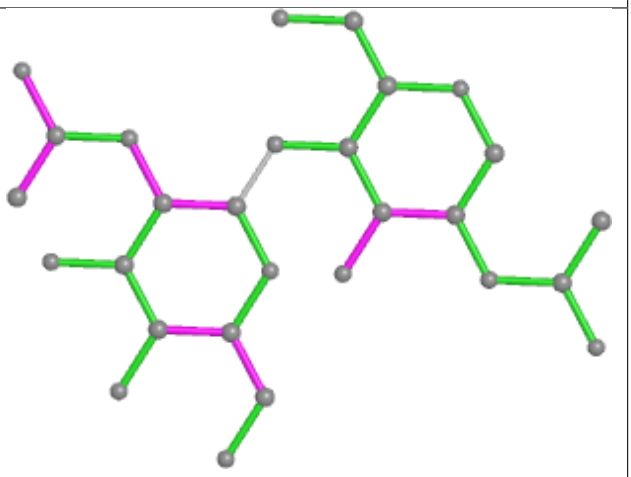
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	5	MAN	0	1
4	F	1	NAG	5	0
4	F	5	MAN	4	0
3	D	1	NAG	2	0
4	I	1	NAG	1	21
5	H	1	NAG	2	0

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

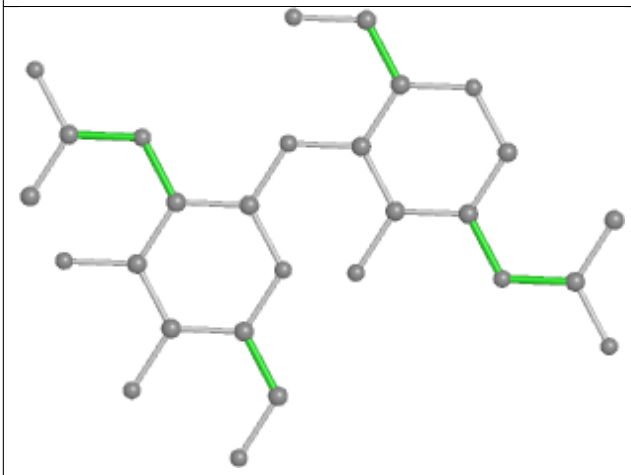
Oligosaccharide Chain C



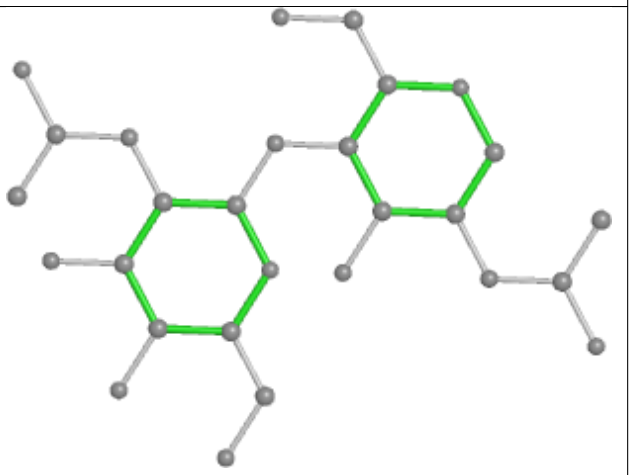
Bond lengths



Bond angles

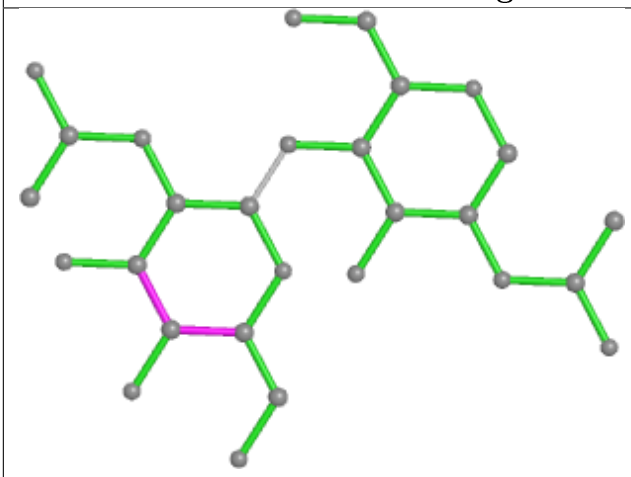


Torsions

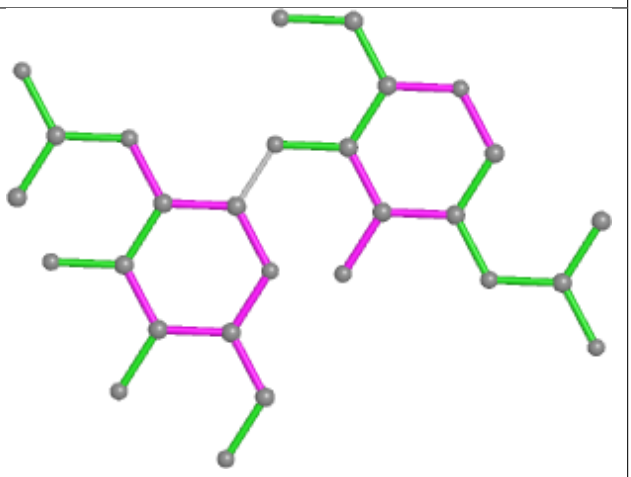


Rings

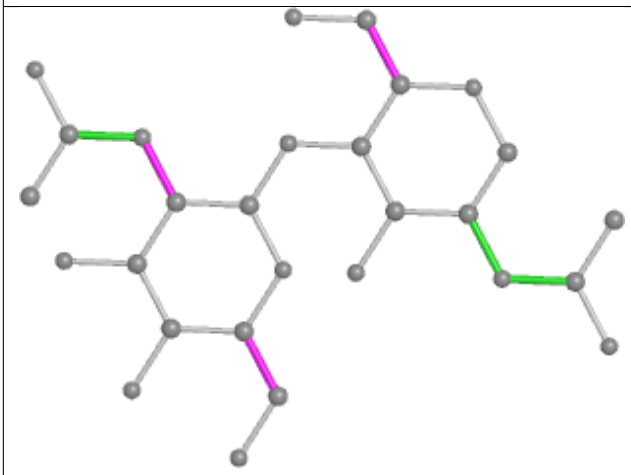
Oligosaccharide Chain E



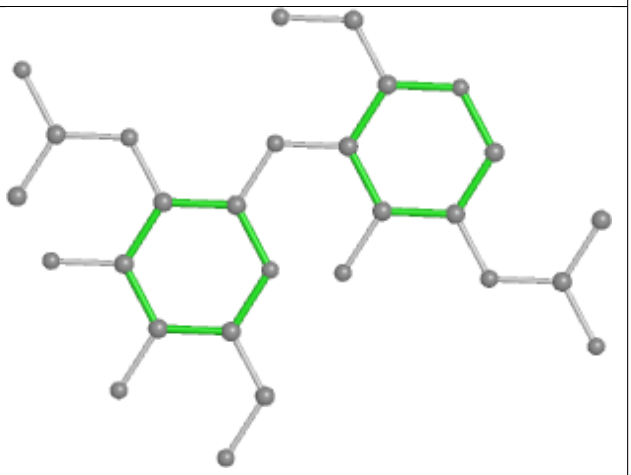
Bond lengths



Bond angles

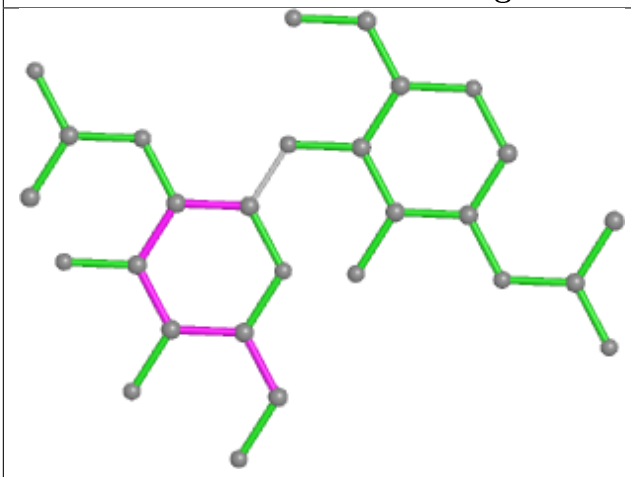


Torsions

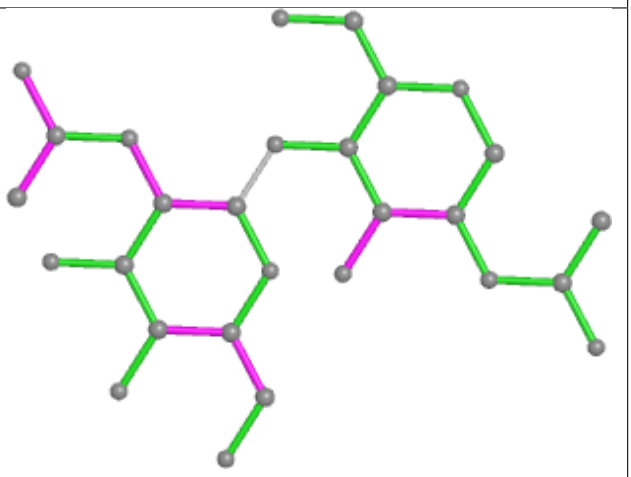


Rings

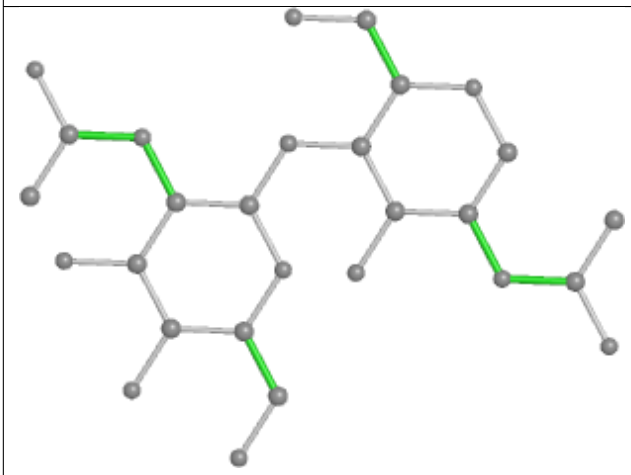
Oligosaccharide Chain G



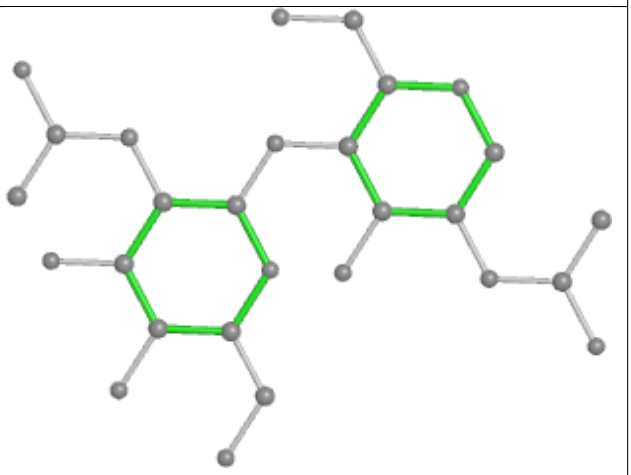
Bond lengths



Bond angles

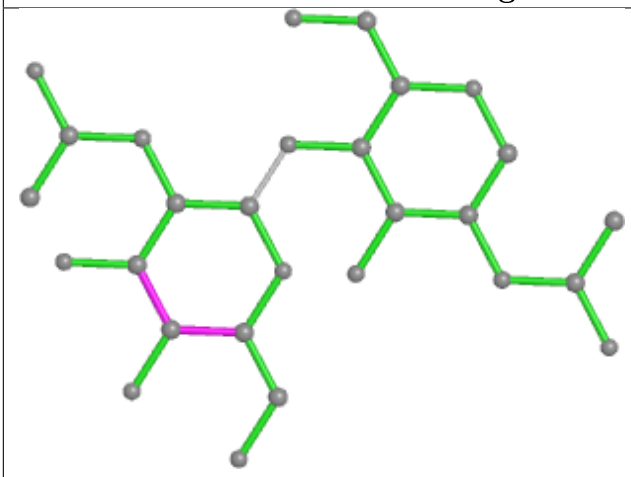


Torsions

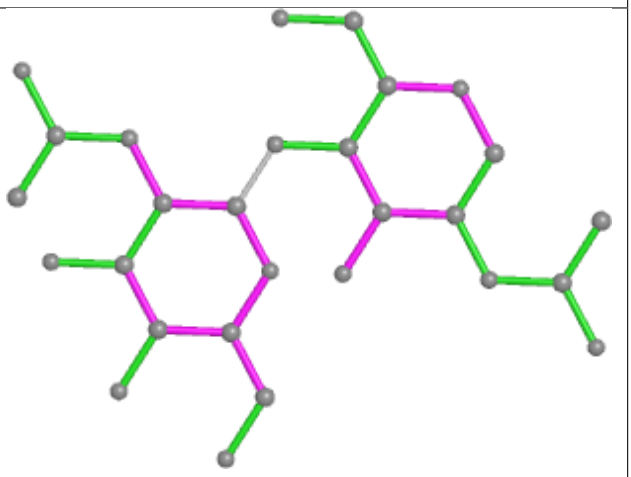


Rings

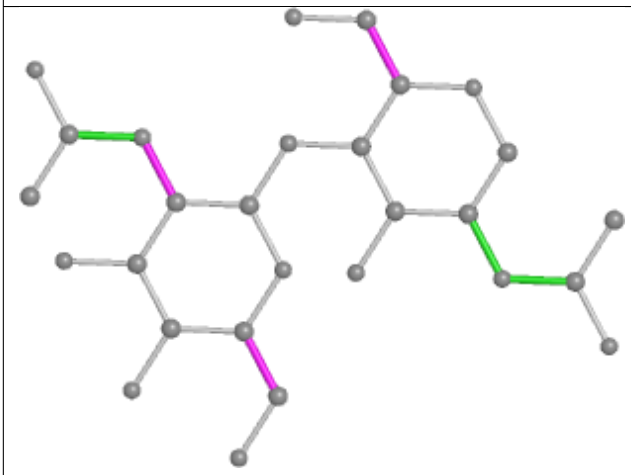
Oligosaccharide Chain J



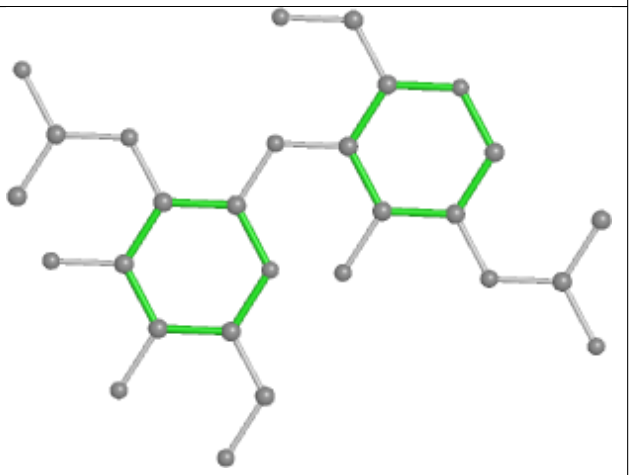
Bond lengths



Bond angles

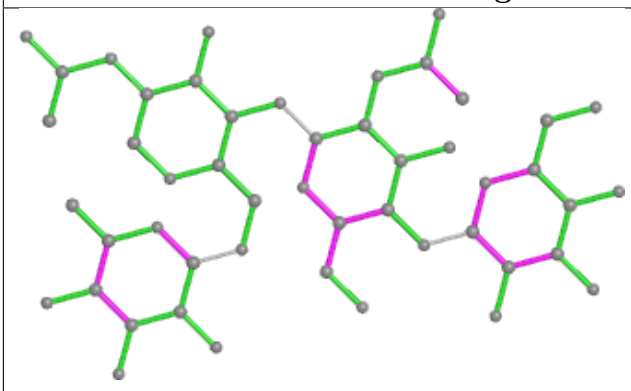


Torsions

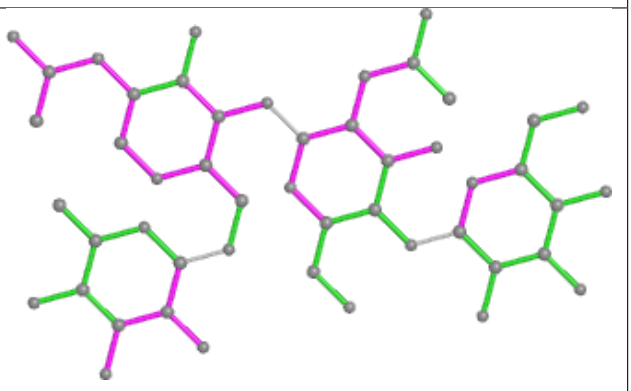


Rings

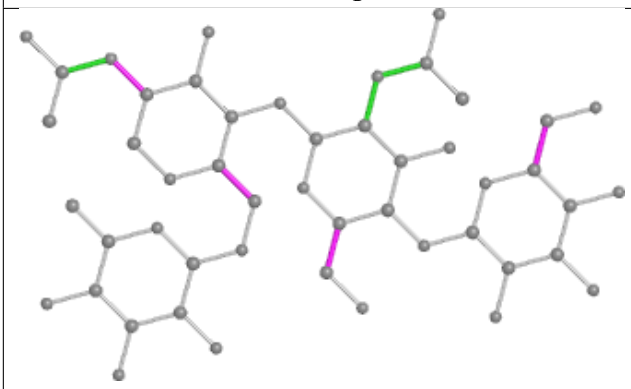
Oligosaccharide Chain D



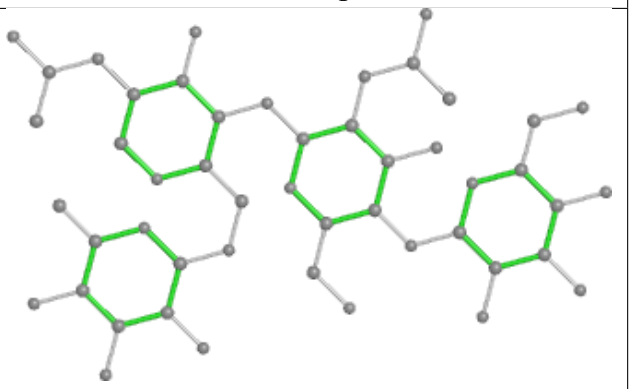
Bond lengths



Bond angles

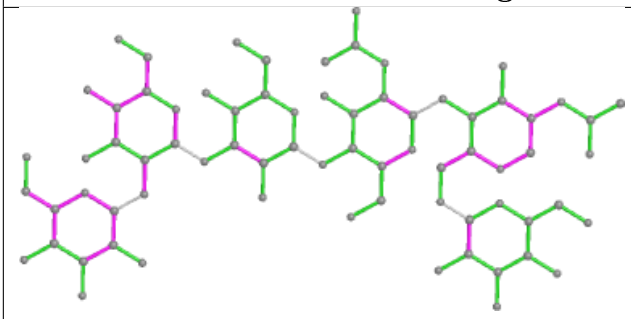


Torsions

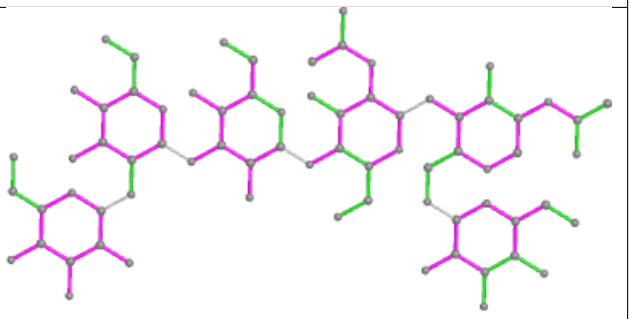


Rings

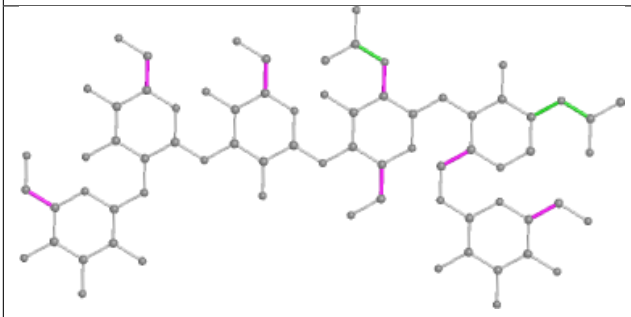
Oligosaccharide Chain F



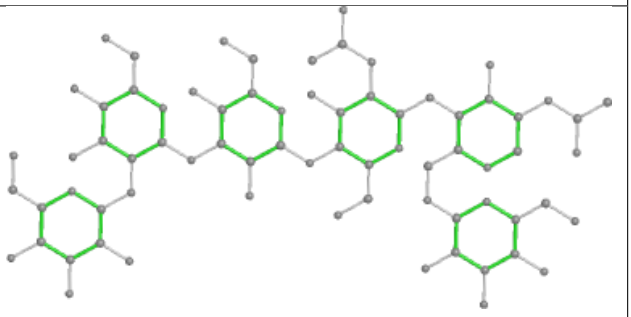
Bond lengths



Bond angles

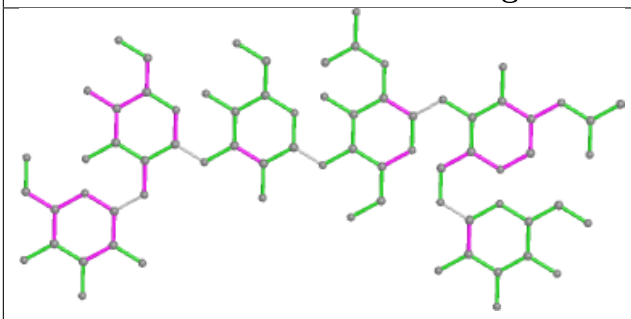


Torsions

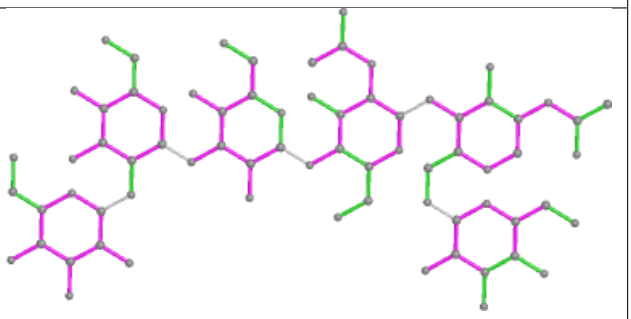


Rings

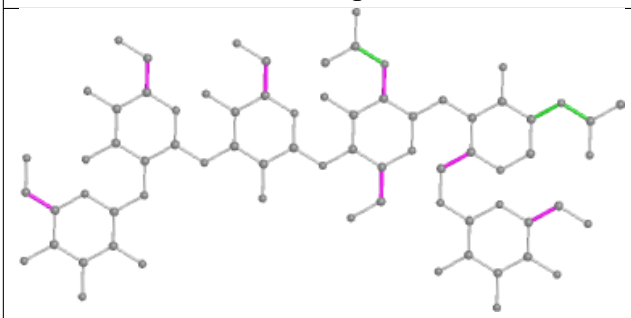
Oligosaccharide Chain I



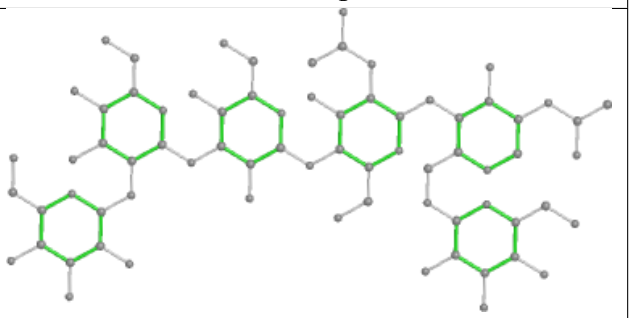
Bond lengths



Bond angles

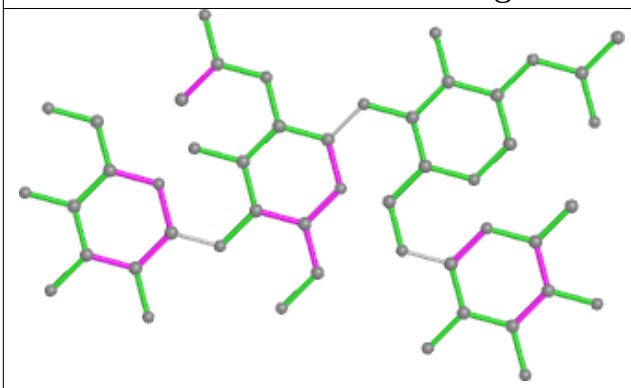


Torsions

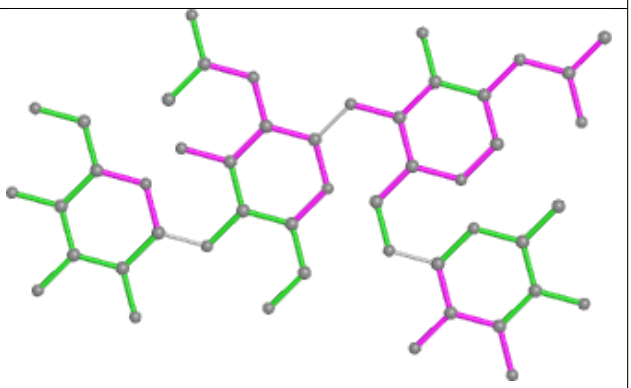


Rings

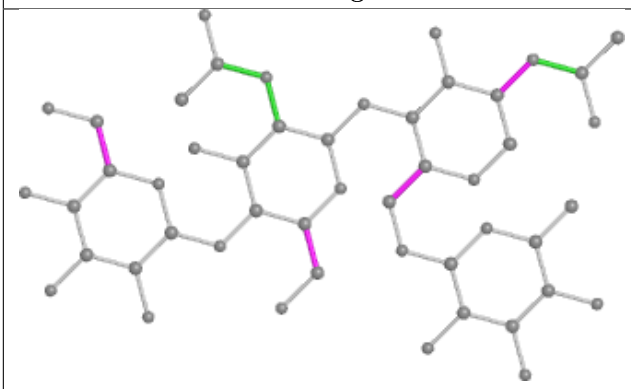
Oligosaccharide Chain H



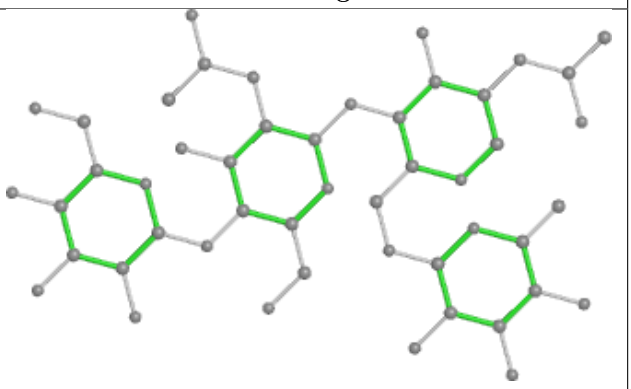
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
7	DAN	A	471	-	17,20,20	2.90	9 (52%)	18,28,28	2.16	7 (38%)
7	DAN	B	471	-	17,20,20	2.90	9 (52%)	18,28,28	2.16	7 (38%)

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
7	DAN	A	471	-	-	3/14/34/34	0/1/1/1
7	DAN	B	471	-	-	3/14/34/34	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	471	DAN	C3-C2	6.35	1.40	1.32
7	B	471	DAN	C3-C2	6.35	1.40	1.32
7	A	471	DAN	C4-C5	-4.80	1.47	1.53
7	B	471	DAN	C4-C5	-4.80	1.47	1.53
7	A	471	DAN	C7-C6	4.58	1.58	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	471	DAN	O6-C2-C3	-5.28	117.20	124.33
7	B	471	DAN	O6-C2-C3	-5.28	117.20	124.33
7	A	471	DAN	O4-C4-C5	-3.59	106.11	112.61
7	B	471	DAN	O4-C4-C5	-3.59	106.11	112.61
7	A	471	DAN	C6-C5-N5	2.98	115.87	110.91

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

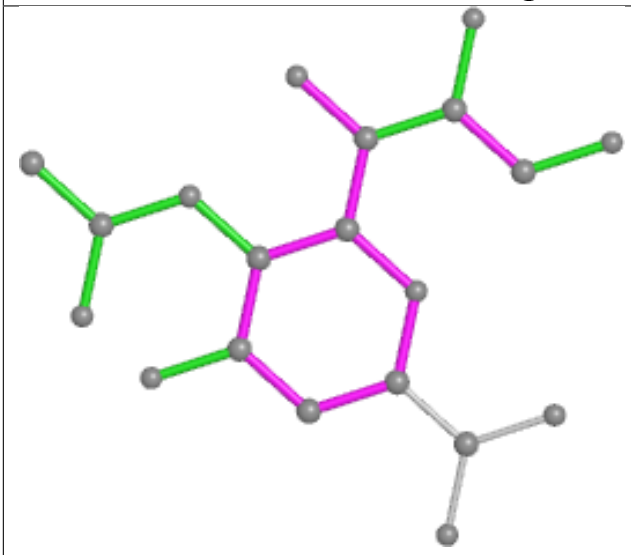
Mol	Chain	Res	Type	Atoms
7	A	471	DAN	C7-C8-C9-O9
7	A	471	DAN	O8-C8-C9-O9
7	B	471	DAN	C7-C8-C9-O9
7	B	471	DAN	O8-C8-C9-O9
7	A	471	DAN	O6-C6-C7-O7

There are no ring outliers.

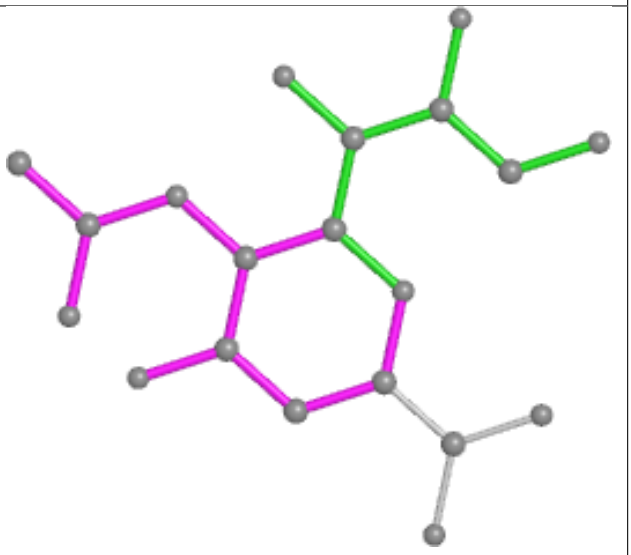
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

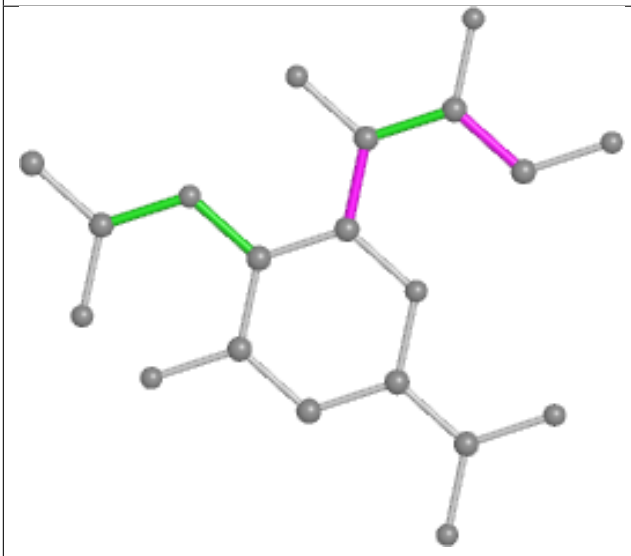
Ligand DAN A 471



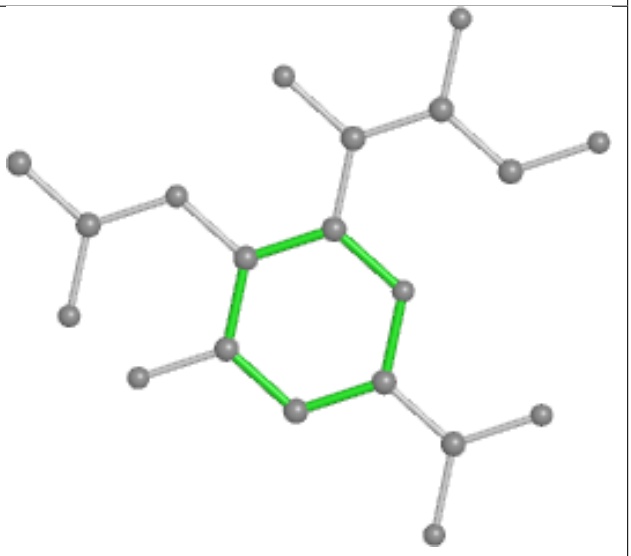
Bond lengths



Bond angles

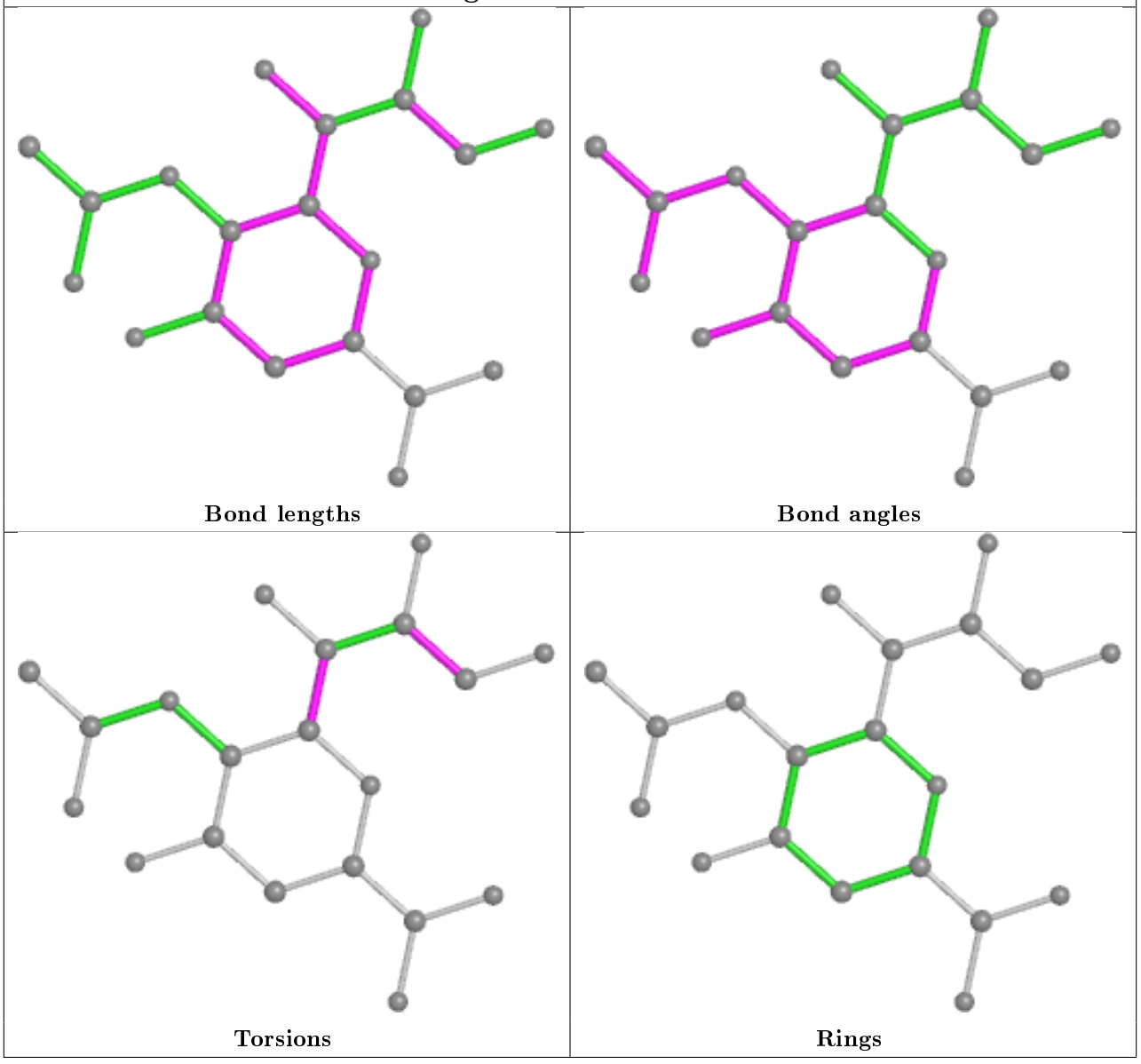


Torsions



Rings

Ligand DAN B 471



5.7 Other polymers

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

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

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

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

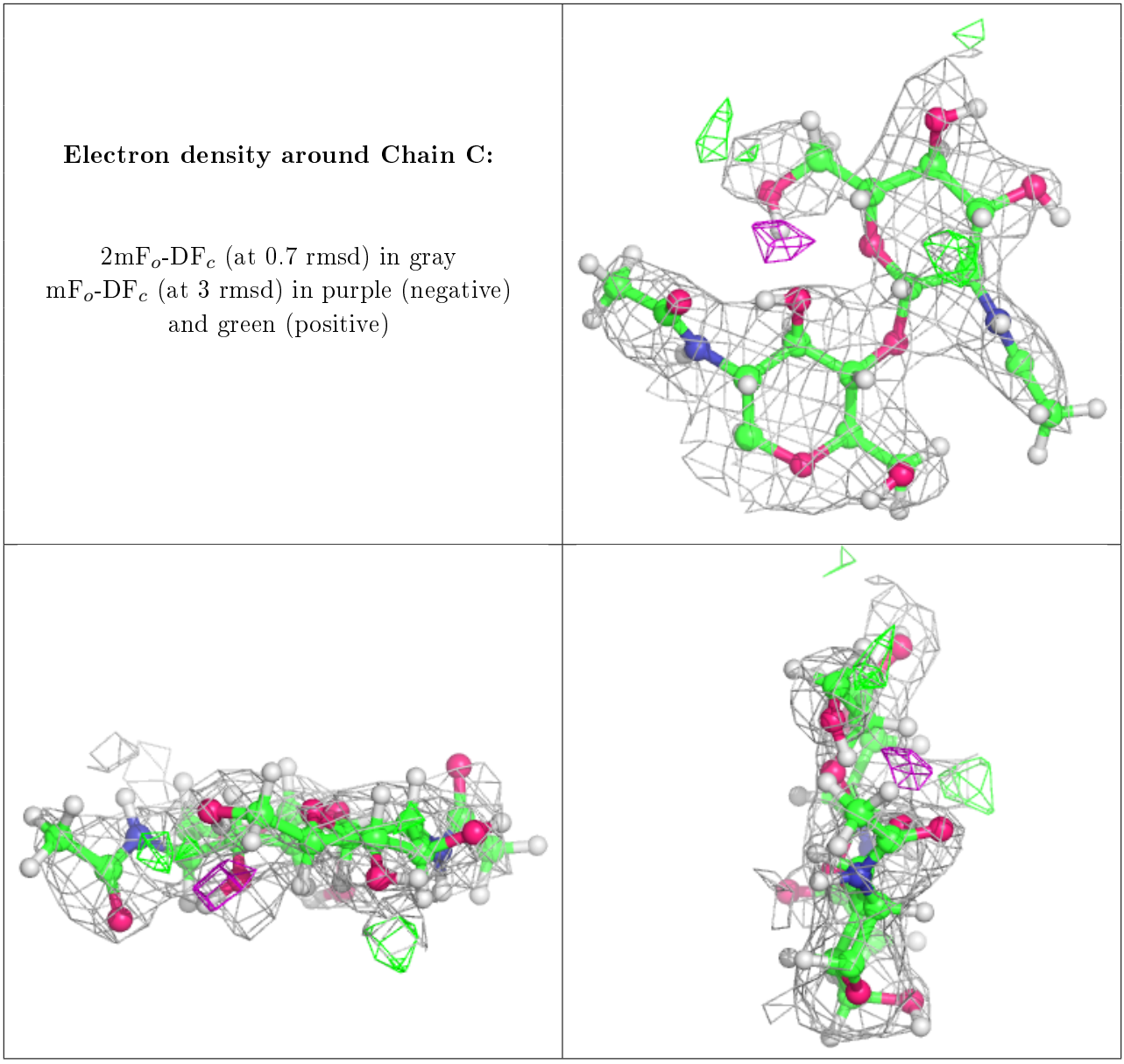
6.3 Carbohydrates

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.

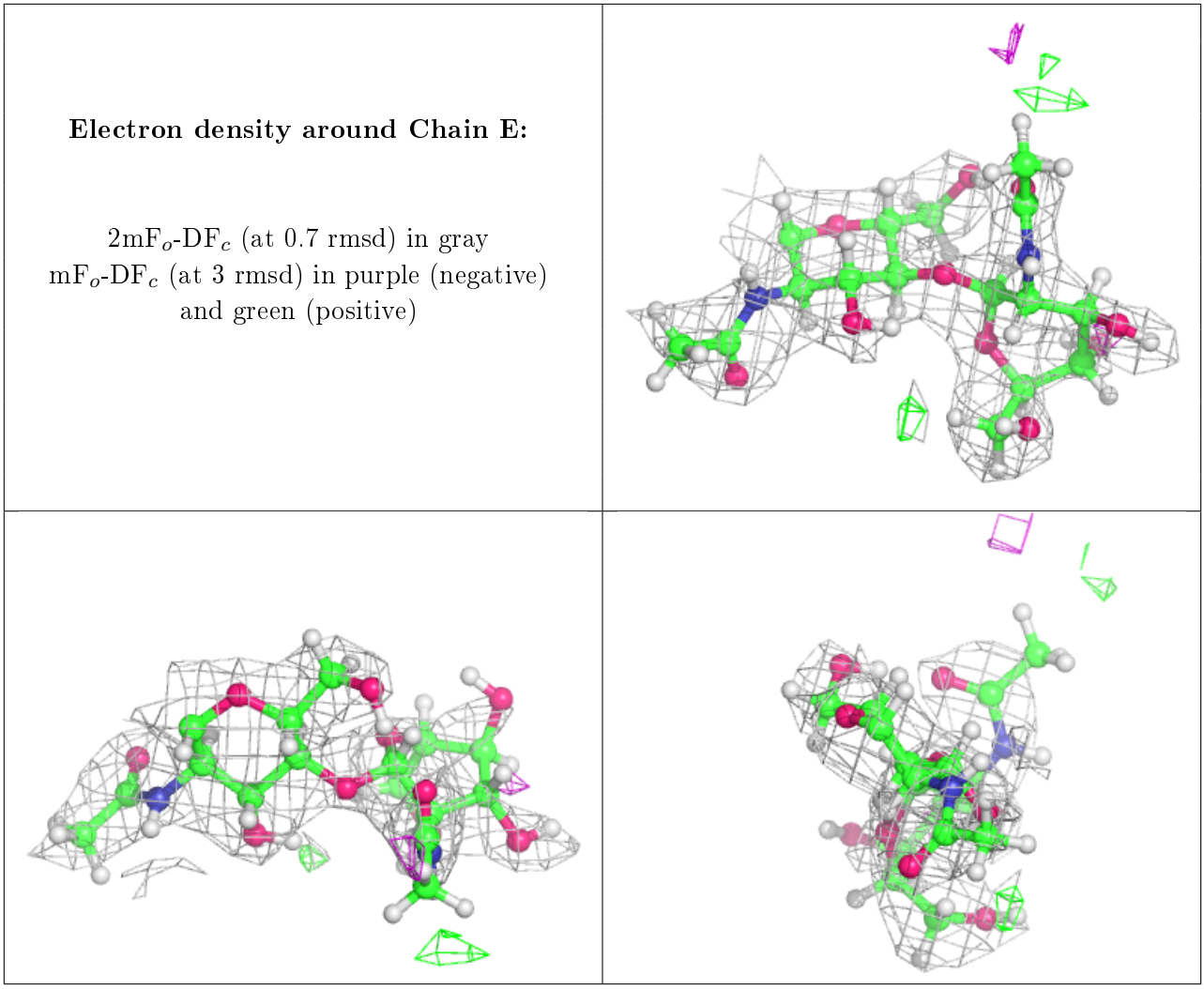
Electron density around Chain C:

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



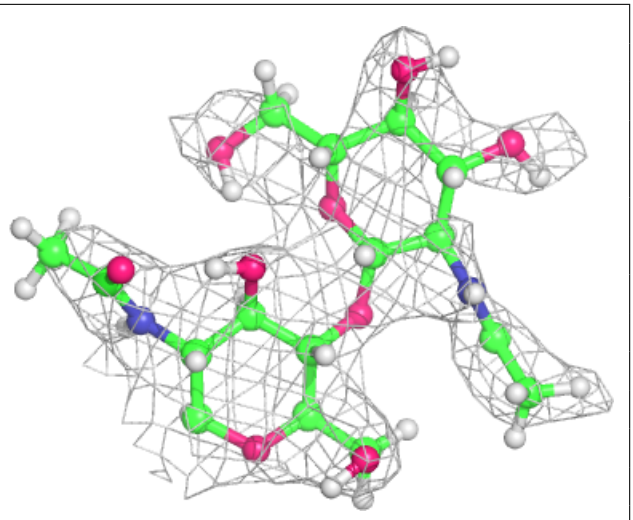
Electron density around Chain E:

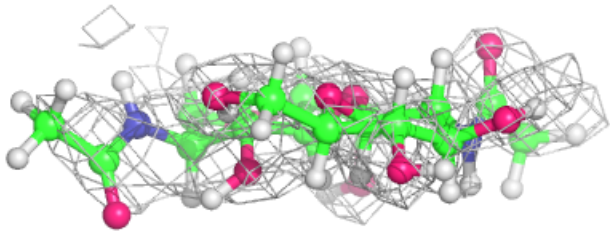
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

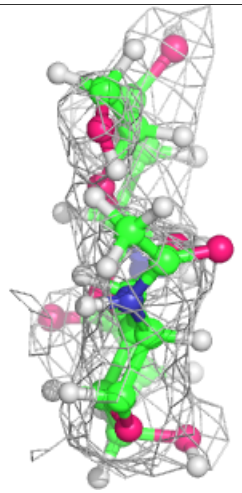


Electron density around Chain G:

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

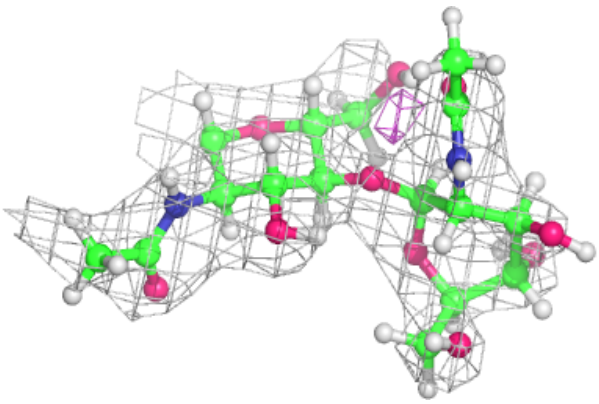


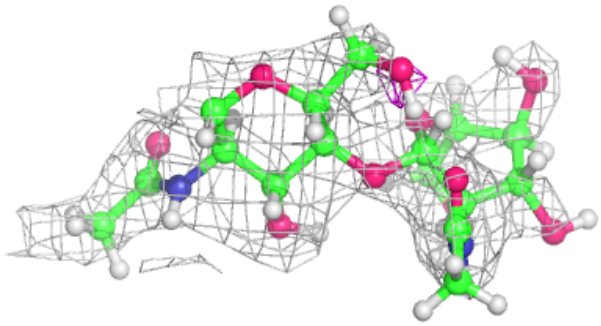


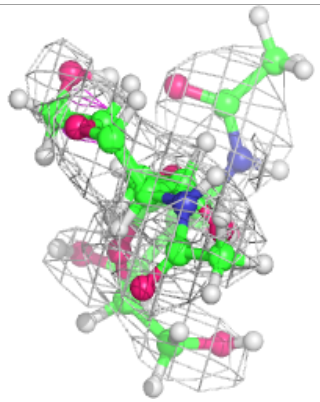


Electron density around Chain J:

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

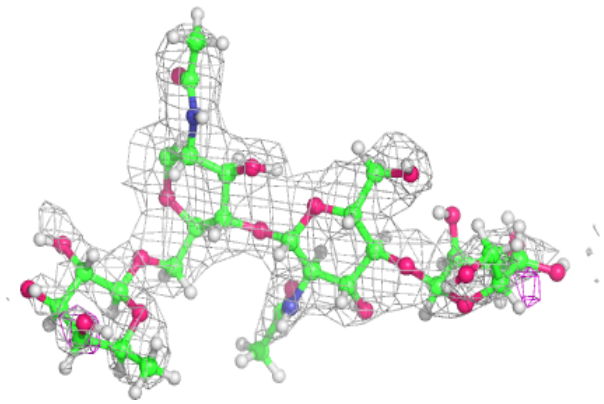


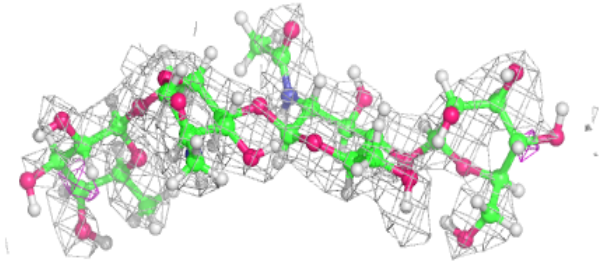


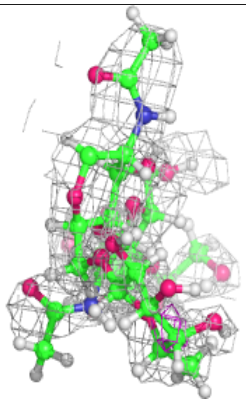


Electron density around Chain D:

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

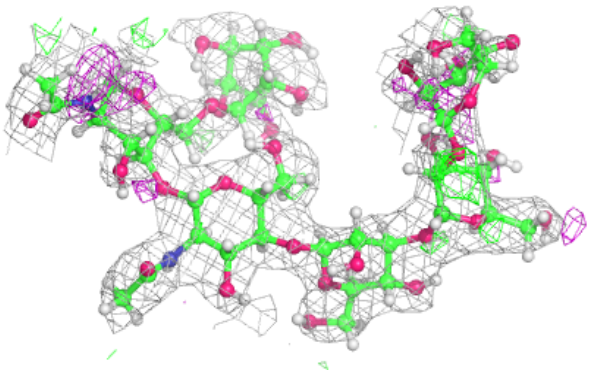


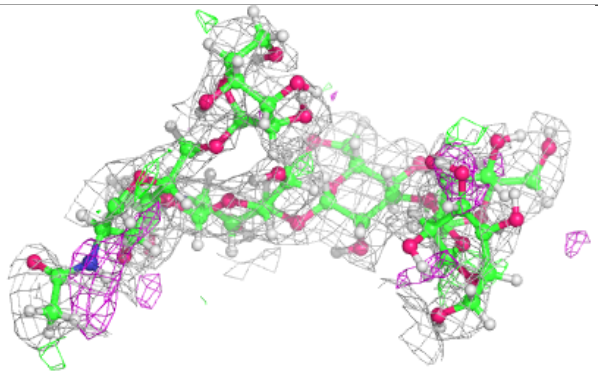


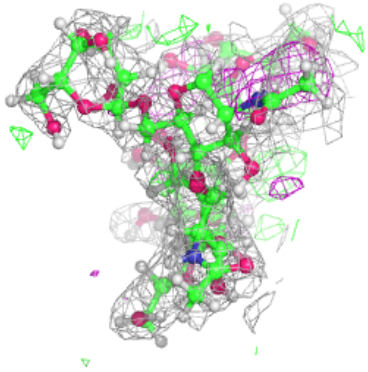


Electron density around Chain F:

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

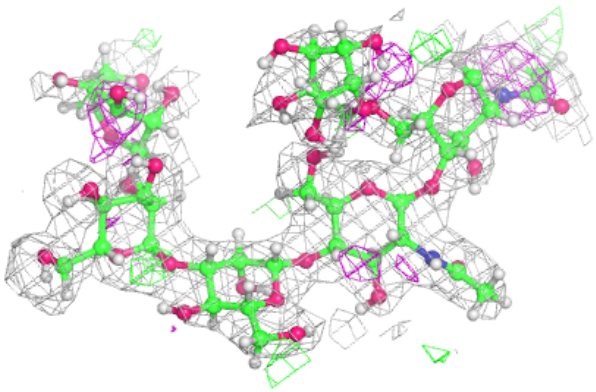


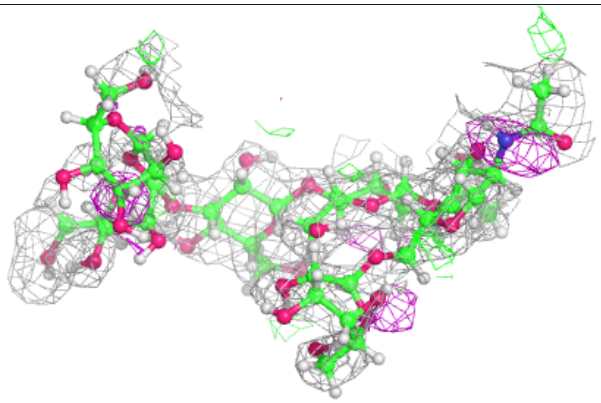


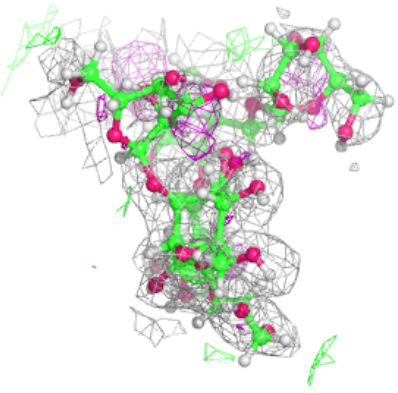


Electron density around Chain I:

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

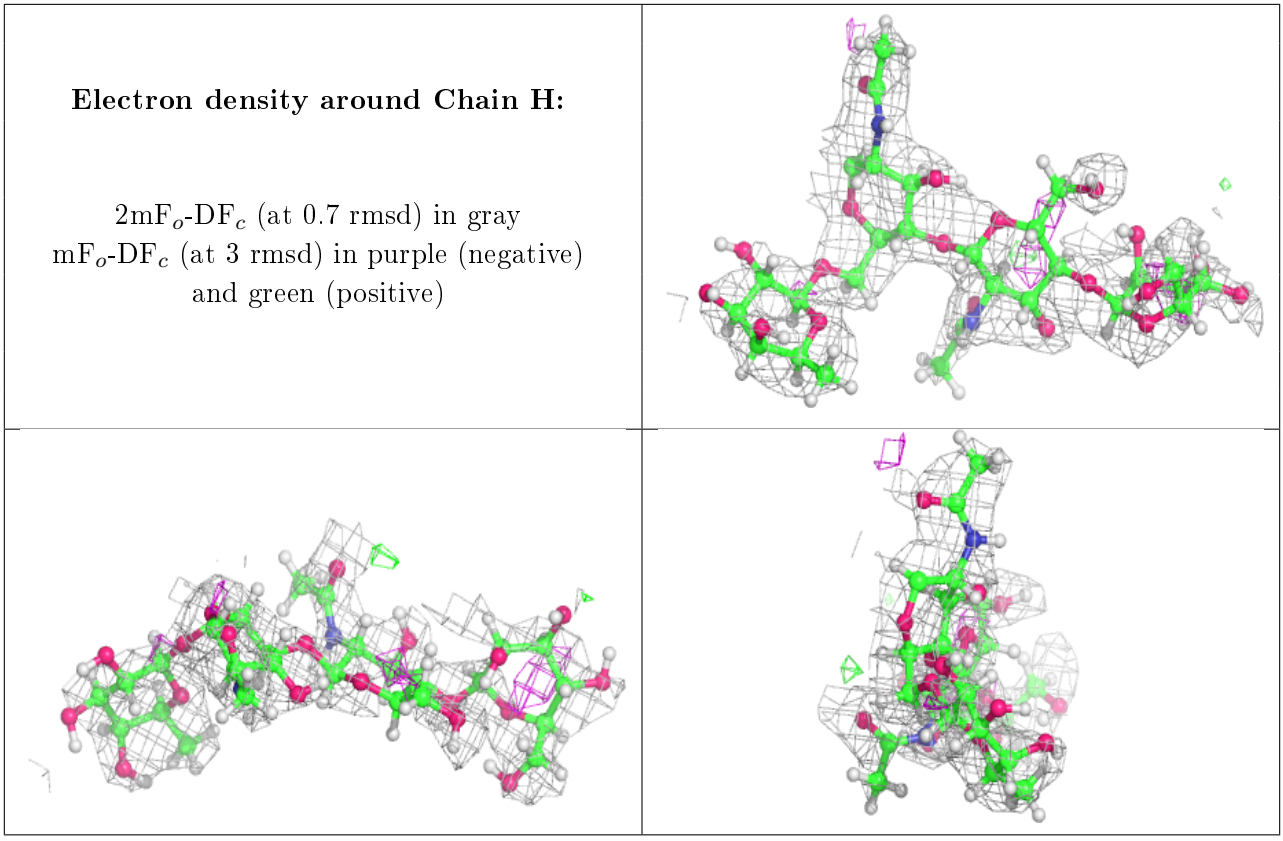






Electron density around Chain H:

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



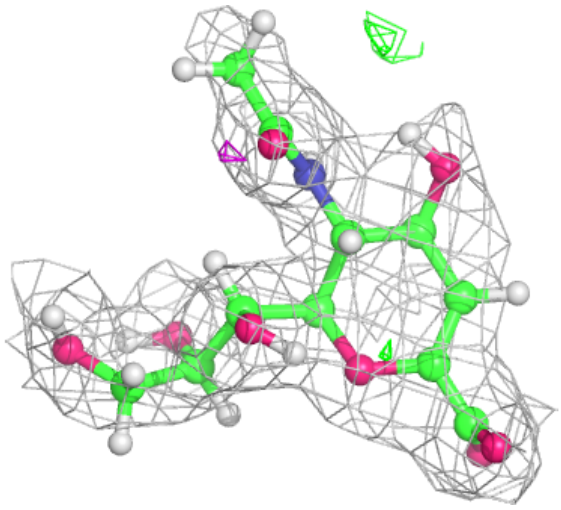
6.4 Ligands

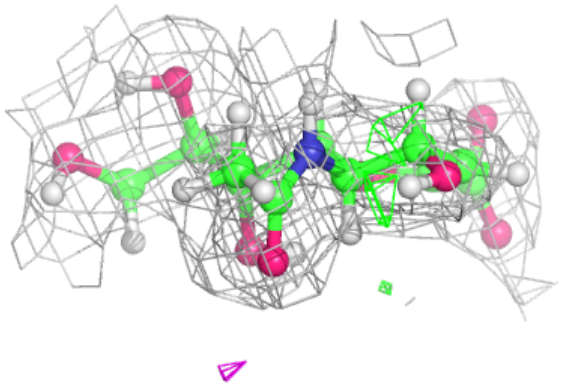
Unable to reproduce the depositors R factor - this section is therefore empty.

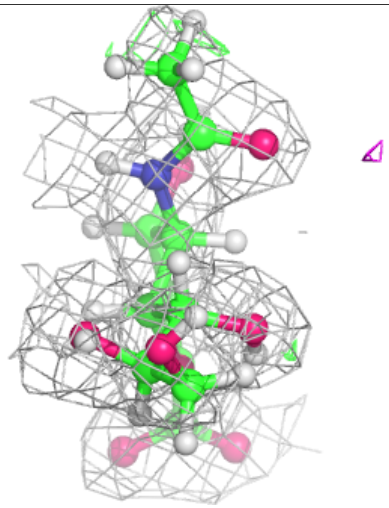
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DAN A 471:

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

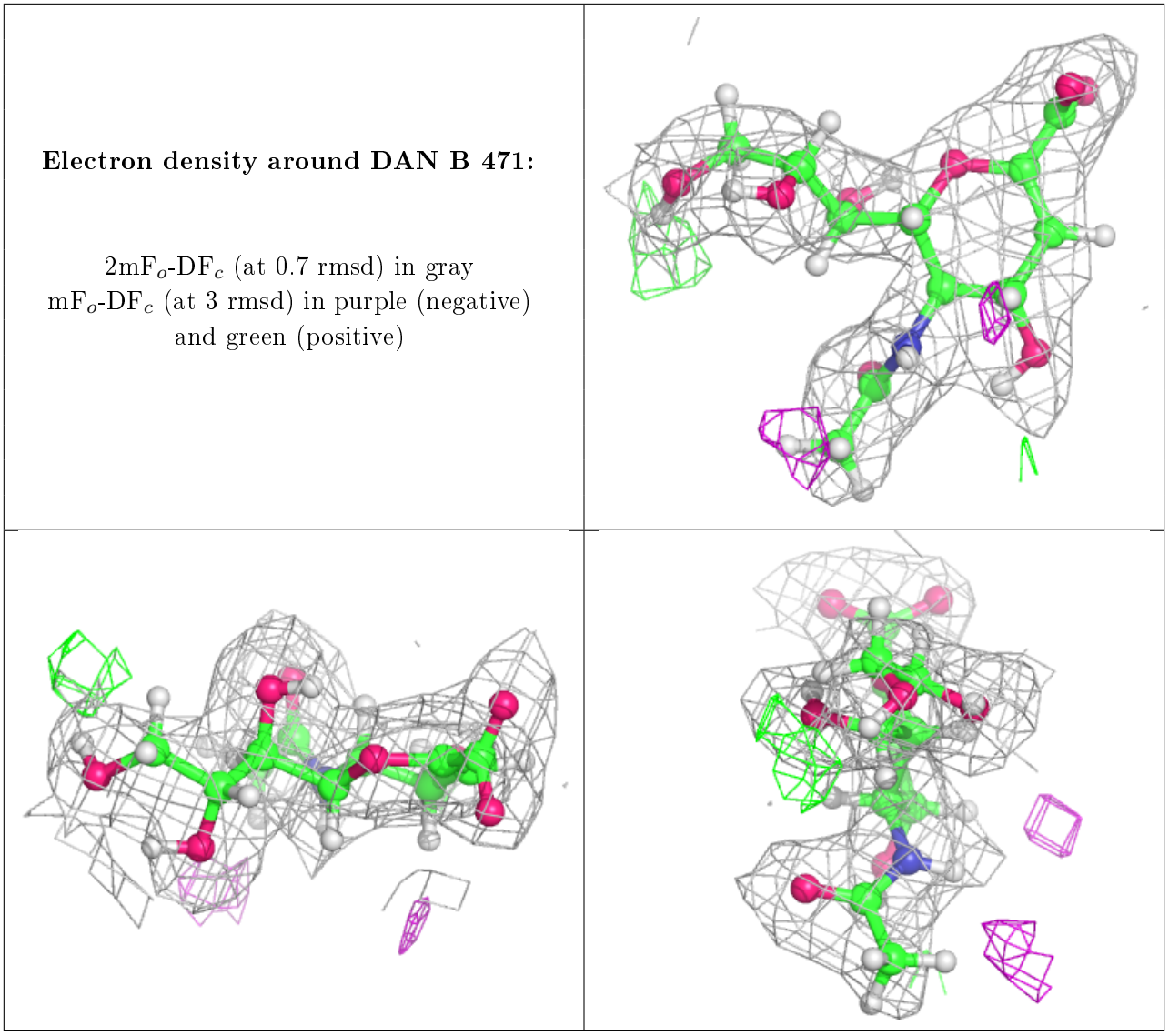






Electron density around DAN B 471:

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



6.5 Other polymers (i)

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