Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:18 AM EDT

PDB ID	:	6NHR
Title	:	Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin HA2 I45F mutant
Authors	:	Wu, N.C.; Wilson, I.A.
Deposited on	:	2018-12-23
Resolution	:	2.10 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:

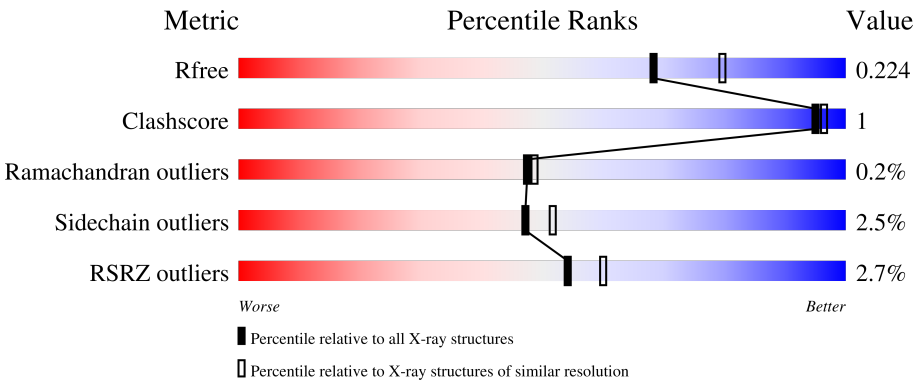
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	321	2% 95%
1	C	321	2% 95%
1	E	321	2% 93% 5%
2	B	176	% 94%
2	D	176	5% 94%

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Mol	Chain	Length	Quality of chain
2	F	176	5% 94%
3	G	3	33% 67%
3	H	3	100%
4	I	2	50% 50%
4	K	2	100%
5	J	4	75% 25%
6	L	4	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
5	MAN	J	4	-	-	-	X
6	MAN	L	4	-	-	-	X
7	NAG	D	201	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12724 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2485	1557	439	476	13	0	1	0
1	C	317	2443	1531	429	470	13	0	0	0
1	E	317	2443	1531	429	470	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP H9XC94
A	10	GLY	-	expression tag	UNP H9XC94
A	145	SER	UNK	variant	UNP H9XC94
A	226	LEU	MET	conflict	UNP H9XC94
C	9	PRO	-	expression tag	UNP H9XC94
C	10	GLY	-	expression tag	UNP H9XC94
C	145	SER	UNK	variant	UNP H9XC94
C	226	LEU	MET	conflict	UNP H9XC94
E	9	PRO	-	expression tag	UNP H9XC94
E	10	GLY	-	expression tag	UNP H9XC94
E	145	SER	UNK	variant	UNP H9XC94
E	226	LEU	MET	conflict	UNP H9XC94

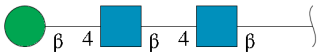
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1405	875	244	280	6	0	1	0
2	D	171	1385	861	241	277	6	0	0	0
2	F	171	1385	861	241	277	6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	PHE	ILE	engineered mutation	UNP Q91MA7
B	123	GLY	ARG	conflict	UNP Q91MA7
D	45	PHE	ILE	engineered mutation	UNP Q91MA7
D	123	GLY	ARG	conflict	UNP Q91MA7
F	45	PHE	ILE	engineered mutation	UNP Q91MA7
F	123	GLY	ARG	conflict	UNP Q91MA7

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(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	G	3	39	22	2	15	0	0	0
3	H	3	39	22	2	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	I	2	28	16	2	10	0	0	0
4	K	2	28	16	2	10	0	0	0

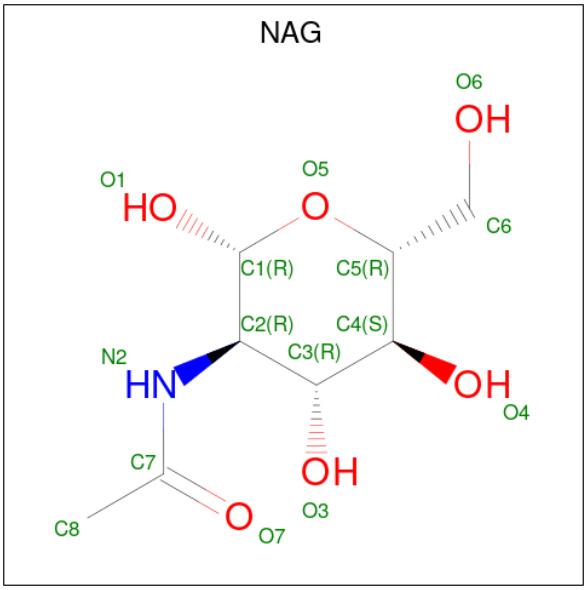
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	J	4	50	28	2	20	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(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			
6	L	4	50	28	2	20	0	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
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	D	1	14	8	1	5	0	0

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

- Molecule 8 is water.

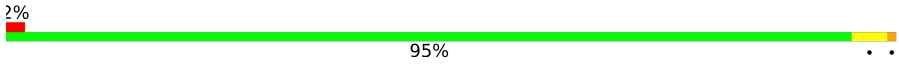
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	186	186	186	0	0
			Total	O		
8	B	94	94	94	0	0
			Total	O		
8	C	180	180	180	0	0
			Total	O		
8	D	93	93	93	0	0
			Total	O		
8	E	219	219	219	0	0
			Total	O		
8	F	74	74	74	0	0

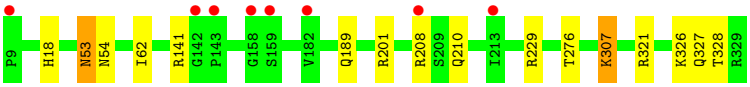
3 Residue-property plots (i)

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: Hemagglutinin HA1 chain

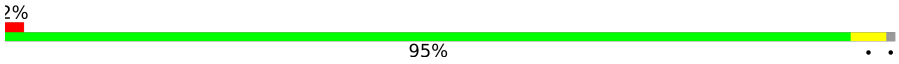
Chain A:





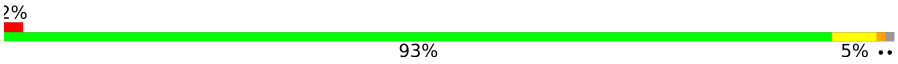
• Molecule 1: Hemagglutinin HA1 chain

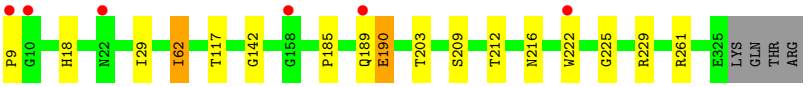
Chain C:



• Molecule 1: Hemagglutinin HA1 chain

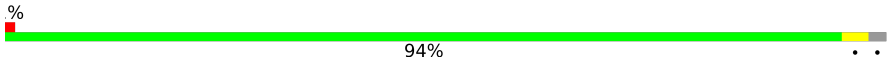
Chain E:





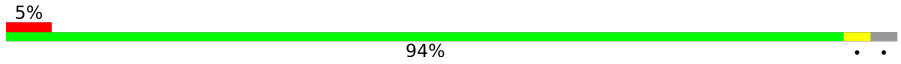
• Molecule 2: Hemagglutinin HA2 chain

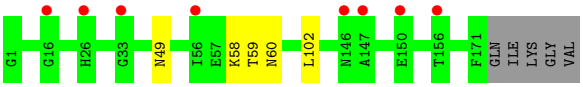
Chain B:



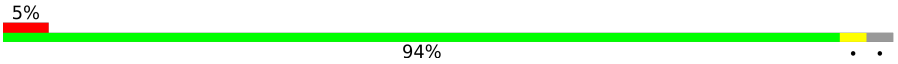
• Molecule 2: Hemagglutinin HA2 chain

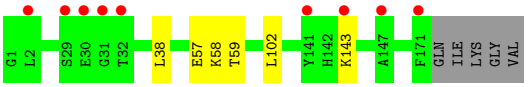
Chain D:





• Molecule 2: Hemagglutinin HA2 chain

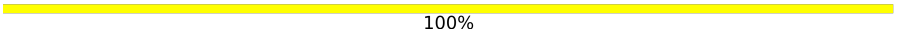
Chain F: 



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

Chain G:

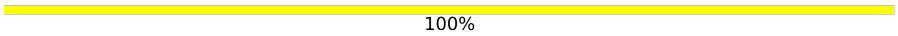
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 

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

Chain I:

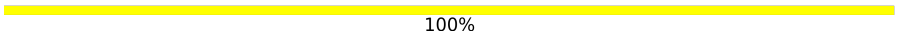
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

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

Chain J:

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

Chain L: 

NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.38Å 131.41Å 72.28Å 90.00° 98.07° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 35.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.10) 97.4 (35.38-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.184 , 0.216 0.191 , 0.224	Depositor DCC
R_{free} test set	5420 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12724	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: NAG, BMA, 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	0.54	0/2545	0.76	3/3465 (0.1%)
1	C	0.53	0/2500	0.73	0/3407
1	E	0.60	0/2500	0.77	1/3407 (0.0%)
2	B	0.51	0/1431	0.70	1/1923 (0.1%)
2	D	0.50	0/1410	0.69	0/1895
2	F	0.50	0/1410	0.69	0/1895
All	All	0.54	0/11796	0.73	5/15992 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	229	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	229	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	B	54	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	321	ARG	CG-CD-NE	-5.10	101.09	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2485	0	2444	6	0
1	C	2443	0	2390	7	1
1	E	2443	0	2390	15	0
2	B	1405	0	1313	1	0
2	D	1385	0	1296	1	1
2	F	1385	0	1297	3	0
3	G	39	0	34	0	0
3	H	39	0	34	0	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
5	J	50	0	43	1	0
6	L	50	0	43	0	0
7	A	14	0	13	0	0
7	C	28	0	26	0	0
7	D	14	0	13	0	0
7	E	42	0	39	0	0
8	A	186	0	0	1	0
8	B	94	0	0	1	0
8	C	180	0	0	0	0
8	D	93	0	0	0	0
8	E	219	0	0	4	0
8	F	74	0	0	0	0
All	All	12724	0	11425	28	1

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 1.

All (28) 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:E:29:ILE:HD11	2:F:102:LEU:HD23	1.71	0.72
1:E:142:GLY:O	8:E:601:HOH:O	2.09	0.70
1:C:29:ILE:HD11	2:D:102:LEU:HD23	1.75	0.69
1:C:212:THR:HG21	1:E:216:ASN:HB3	1.74	0.68
1:E:209:SER:OG	8:E:602:HOH:O	2.11	0.68
1:E:185:PRO:HB3	1:E:190:GLU:CG	2.30	0.62
1:C:141:ARG:HH11	1:C:141:ARG:HG3	1.68	0.59
1:E:261:ARG:NE	8:E:606:HOH:O	2.37	0.58
1:C:212:THR:HB	1:E:216:ASN:CG	2.25	0.57
1:A:141:ARG:HG3	1:A:141:ARG:HH11	1.70	0.55
1:A:327:GLN:OE1	1:A:328:THR:N	2.42	0.52
1:E:203:THR:OG1	1:E:212:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:PRO:HB3	1:E:190:GLU:HG3	1.93	0.51
1:C:141:ARG:HG3	1:C:141:ARG:NH1	2.27	0.50
1:C:167:THR:OG1	5:J:1:NAG:H62	2.11	0.50
1:A:53:ASN:HD22	1:A:54:ASN:N	2.10	0.49
1:A:53:ASN:HD22	1:A:53:ASN:C	2.15	0.49
2:F:57:GLU:O	2:F:59:THR:HG23	2.13	0.49
1:A:141:ARG:HG3	1:A:141:ARG:NH1	2.29	0.46
1:E:185:PRO:HB3	1:E:190:GLU:HG2	2.00	0.43
1:E:29:ILE:HD11	2:F:102:LEU:CD2	2.44	0.43
1:C:141:ARG:HH11	1:C:141:ARG:CG	2.29	0.42
1:E:203:THR:HG23	1:E:212:THR:HG22	2.01	0.42
1:E:203:THR:HG23	1:E:212:THR:CG2	2.49	0.42
1:A:307:LYS:NZ	8:A:508:HOH:O	2.52	0.42
2:B:77:ILE:HG22	8:B:248:HOH:O	2.19	0.42
1:E:117:THR:HG21	8:E:606:HOH:O	2.19	0.41
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.56	0.41

All (1) 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:C:157:SER:OG	2:D:49:ASN:OD1[4_445]	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	320/321 (100%)	315 (98%)	4 (1%)	1 (0%)	41	41
1	C	315/321 (98%)	310 (98%)	4 (1%)	1 (0%)	41	41
1	E	315/321 (98%)	310 (98%)	4 (1%)	1 (0%)	41	41
2	B	171/176 (97%)	163 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	169/176 (96%)	161 (95%)	8 (5%)	0	100	100
2	F	169/176 (96%)	161 (95%)	8 (5%)	0	100	100
All	All	1459/1491 (98%)	1420 (97%)	36 (2%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	62	ILE
1	E	62	ILE
1	A	62	ILE

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	283/282 (100%)	274 (97%)	9 (3%)	39	41
1	C	278/282 (99%)	270 (97%)	8 (3%)	42	46
1	E	278/282 (99%)	273 (98%)	5 (2%)	59	65
2	B	147/149 (99%)	143 (97%)	4 (3%)	44	48
2	D	145/149 (97%)	142 (98%)	3 (2%)	53	59
2	F	145/149 (97%)	142 (98%)	3 (2%)	53	59
All	All	1276/1293 (99%)	1244 (98%)	32 (2%)	47	52

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	ASN
1	A	189	GLN
1	A	201	ARG
1	A	208	ARG
1	A	210	GLN
1	A	276	THR

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Mol	Chain	Res	Type
1	A	307	LYS
1	A	326	LYS
2	B	39	LYS
2	B	60	ASN
2	B	139	LYS
2	B	143	LYS
1	C	18	HIS
1	C	167	THR
1	C	189	GLN
1	C	201	ARG
1	C	208	ARG
1	C	210	GLN
1	C	219	SER
1	C	222	TRP
2	D	58	LYS
2	D	59	THR
2	D	60	ASN
1	E	9	PRO
1	E	18	HIS
1	E	62	ILE
1	E	189	GLN
1	E	190	GLU
2	F	38	LEU
2	F	58	LYS
2	F	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	54	ASN
2	B	53	ASN
2	B	125	GLN
1	C	54	ASN
2	D	53	ASN
2	D	125	GLN
1	E	54	ASN
2	F	53	ASN
2	F	125	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	$\#\|Z\| > 2$
3	NAG	G	1	3,1	14,14,15	0.34	0	17,19,21	1.18	1 (5%)
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	2.44	3 (17%)
3	BMA	G	3	3	11,11,12	0.50	0	15,15,17	0.80	0
3	NAG	H	1	3,1	14,14,15	0.51	0	17,19,21	1.31	2 (11%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
3	BMA	H	3	3	11,11,12	0.50	0	15,15,17	1.21	3 (20%)
4	NAG	I	1	1,4	14,14,15	0.52	0	17,19,21	0.62	0
4	NAG	I	2	4	14,14,15	0.31	0	17,19,21	1.16	1 (5%)
5	NAG	J	1	5,1	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
5	NAG	J	2	5	14,14,15	0.36	0	17,19,21	1.20	1 (5%)
5	BMA	J	3	5	11,11,12	0.36	0	15,15,17	1.20	3 (20%)
5	MAN	J	4	5	11,11,12	0.62	0	15,15,17	2.42	3 (20%)
4	NAG	K	1	1,4	14,14,15	0.33	0	17,19,21	0.86	1 (5%)
4	NAG	K	2	4	14,14,15	0.60	0	17,19,21	2.07	2 (11%)
6	NAG	L	1	6,1	14,14,15	0.37	0	17,19,21	1.12	1 (5%)
6	NAG	L	2	6	14,14,15	0.33	0	17,19,21	1.26	2 (11%)
6	BMA	L	3	6	11,11,12	0.44	0	15,15,17	1.86	3 (20%)
6	MAN	L	4	6	11,11,12	0.39	0	15,15,17	1.21	1 (6%)

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	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	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
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C1-O5-C5	8.37	123.53	112.19
5	J	4	MAN	C1-O5-C5	7.39	122.20	112.19
4	K	2	NAG	C1-O5-C5	7.32	122.10	112.19
5	J	4	MAN	C1-C2-C3	4.64	115.37	109.67
6	L	3	BMA	C1-O5-C5	4.21	117.89	112.19
6	L	4	MAN	C1-O5-C5	4.17	117.84	112.19
6	L	2	NAG	C1-O5-C5	3.82	117.37	112.19
4	I	2	NAG	C1-O5-C5	3.81	117.36	112.19
3	G	1	NAG	C1-O5-C5	3.47	116.89	112.19
3	H	1	NAG	C1-C2-N2	3.39	116.28	110.49
5	J	2	NAG	C1-C2-N2	3.39	116.27	110.49
6	L	3	BMA	C3-C4-C5	3.37	116.24	110.24
3	G	2	NAG	O5-C5-C4	3.02	118.19	110.83
5	J	4	MAN	O5-C1-C2	2.94	115.31	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	3	BMA	C1-C2-C3	2.93	113.26	109.67
3	H	2	NAG	O5-C5-C6	2.91	111.77	107.20
3	G	2	NAG	C3-C4-C5	2.79	115.22	110.24
6	L	1	NAG	O5-C1-C2	-2.79	106.89	111.29
5	J	1	NAG	O3-C3-C4	-2.63	104.27	110.35
3	H	3	BMA	C1-C2-C3	2.63	112.89	109.67
5	J	3	BMA	C1-O5-C5	2.60	115.71	112.19
4	K	2	NAG	C4-C3-C2	-2.50	107.36	111.02
3	H	3	BMA	C1-O5-C5	2.48	115.55	112.19
3	H	1	NAG	C1-O5-C5	2.47	115.53	112.19
6	L	2	NAG	C1-C2-N2	2.44	114.65	110.49
5	J	3	BMA	O5-C5-C6	2.39	110.95	107.20
4	K	1	NAG	C1-C2-N2	2.35	114.51	110.49
5	J	3	BMA	C6-C5-C4	-2.18	107.89	113.00
3	H	3	BMA	O5-C5-C6	2.12	110.52	107.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
6	L	4	MAN	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6

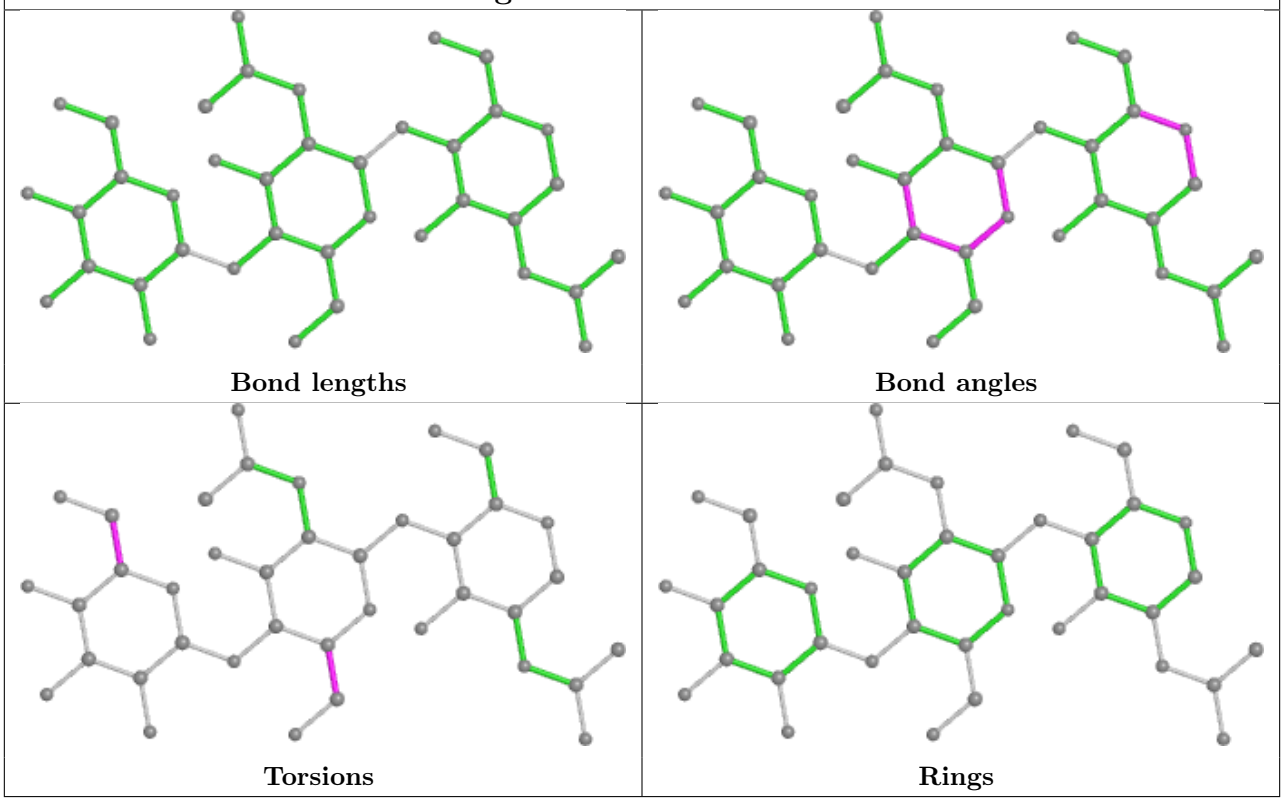
There are no ring outliers.

1 monomer is involved in 1 short contact:

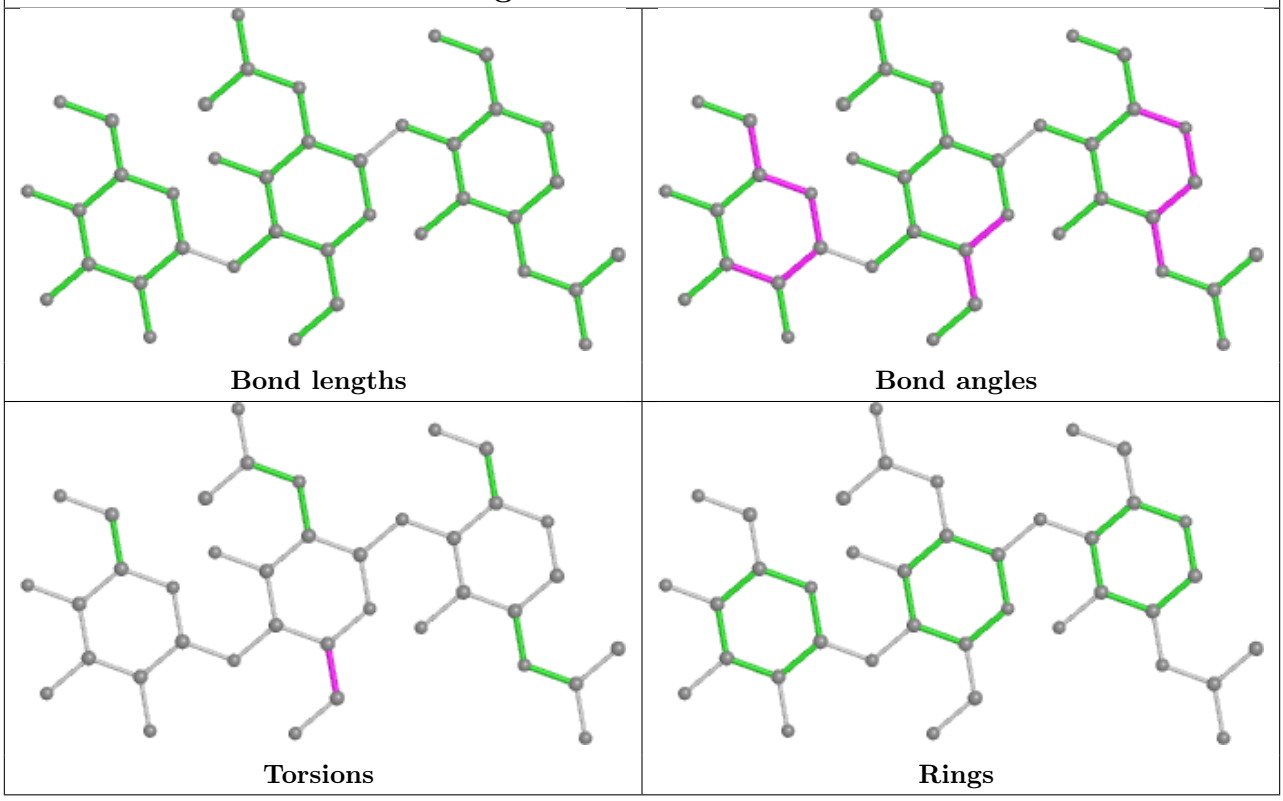
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1	NAG	1	0

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

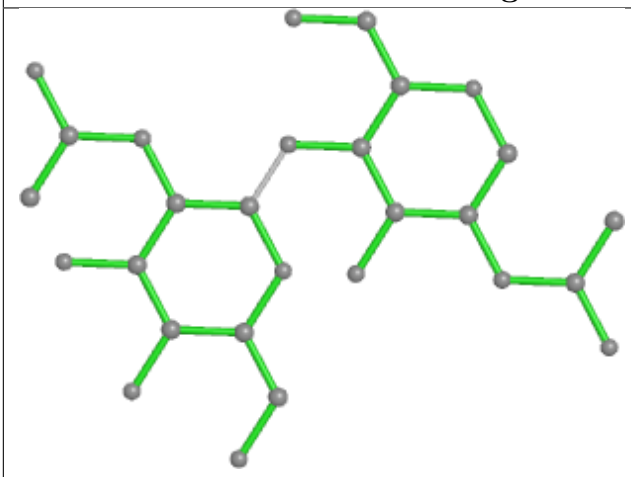
Oligosaccharide Chain G



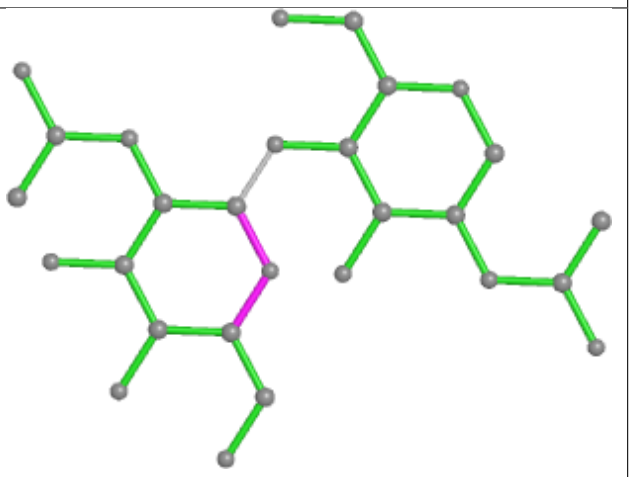
Oligosaccharide Chain H



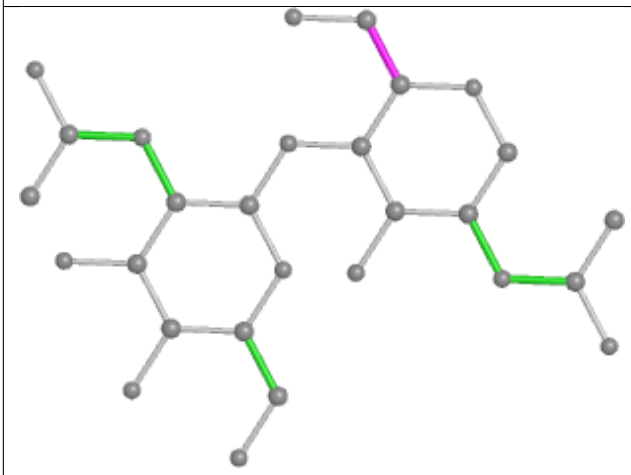
Oligosaccharide Chain I



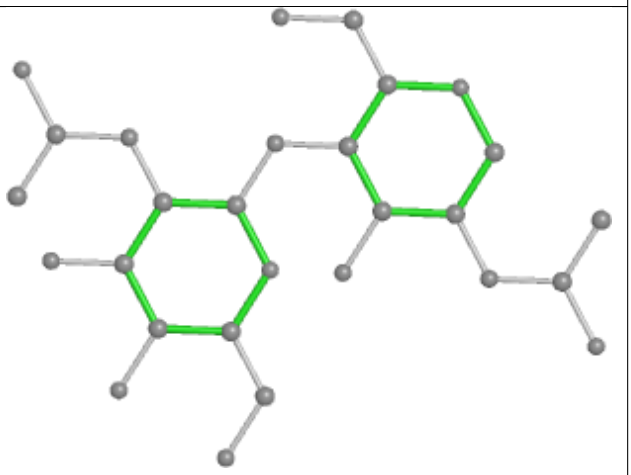
Bond lengths



Bond angles

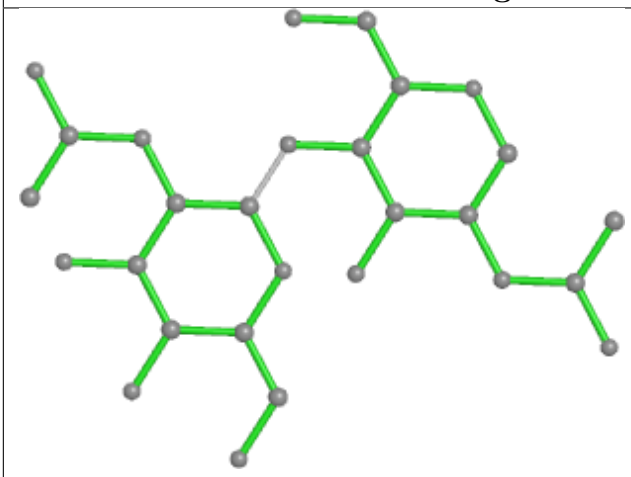


Torsions

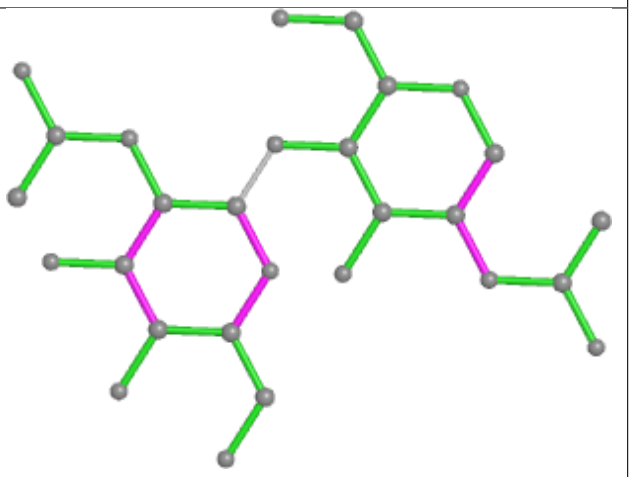


Rings

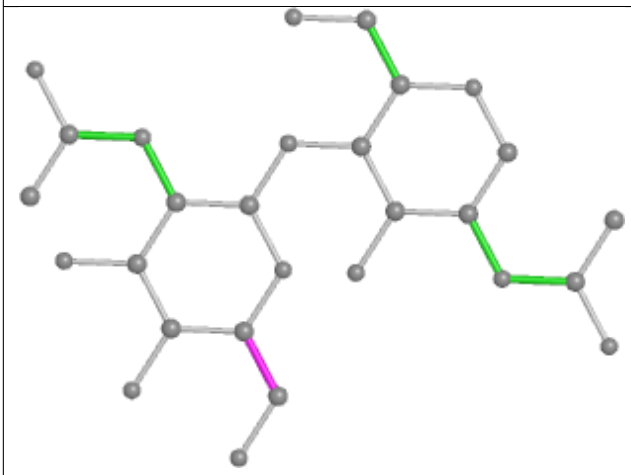
Oligosaccharide Chain K



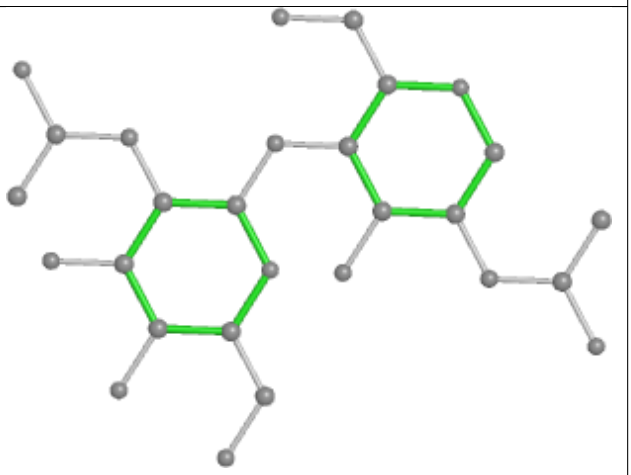
Bond lengths



Bond angles

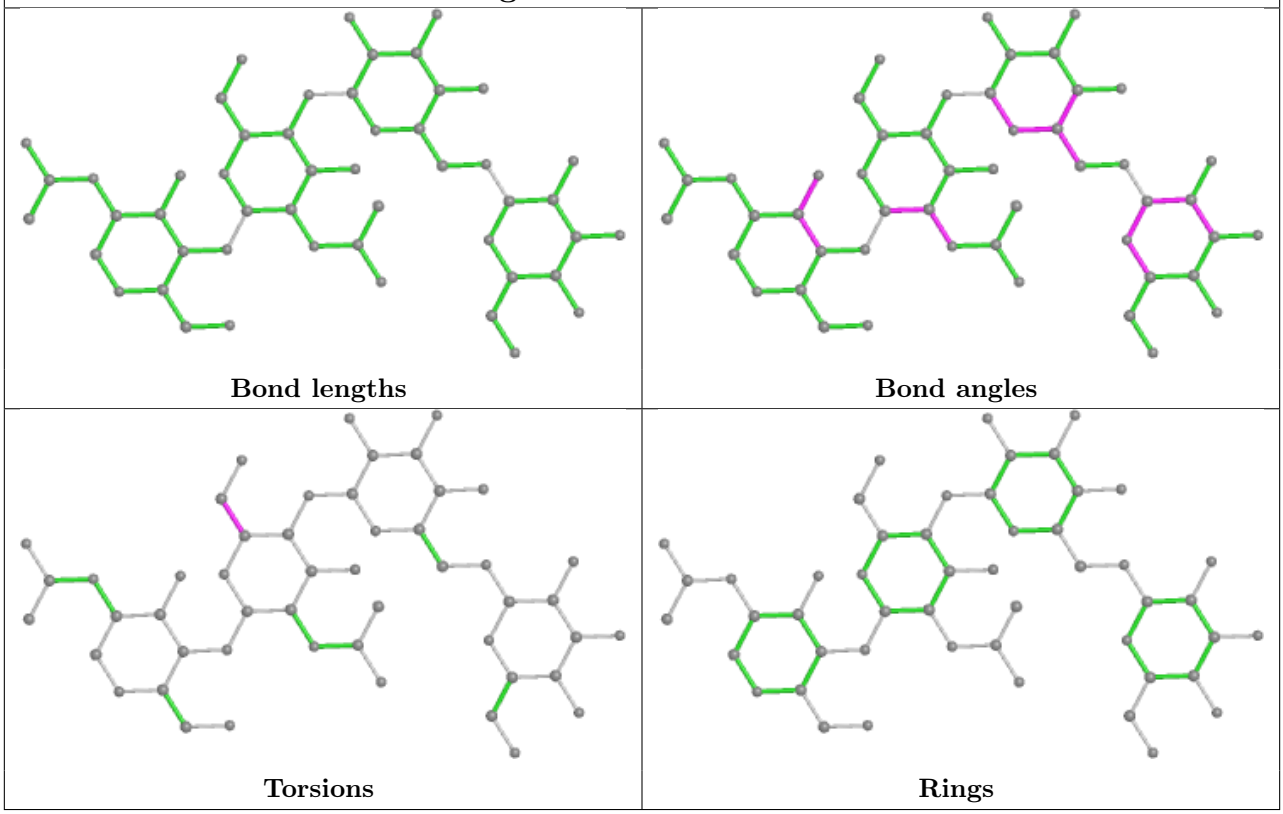


Torsions

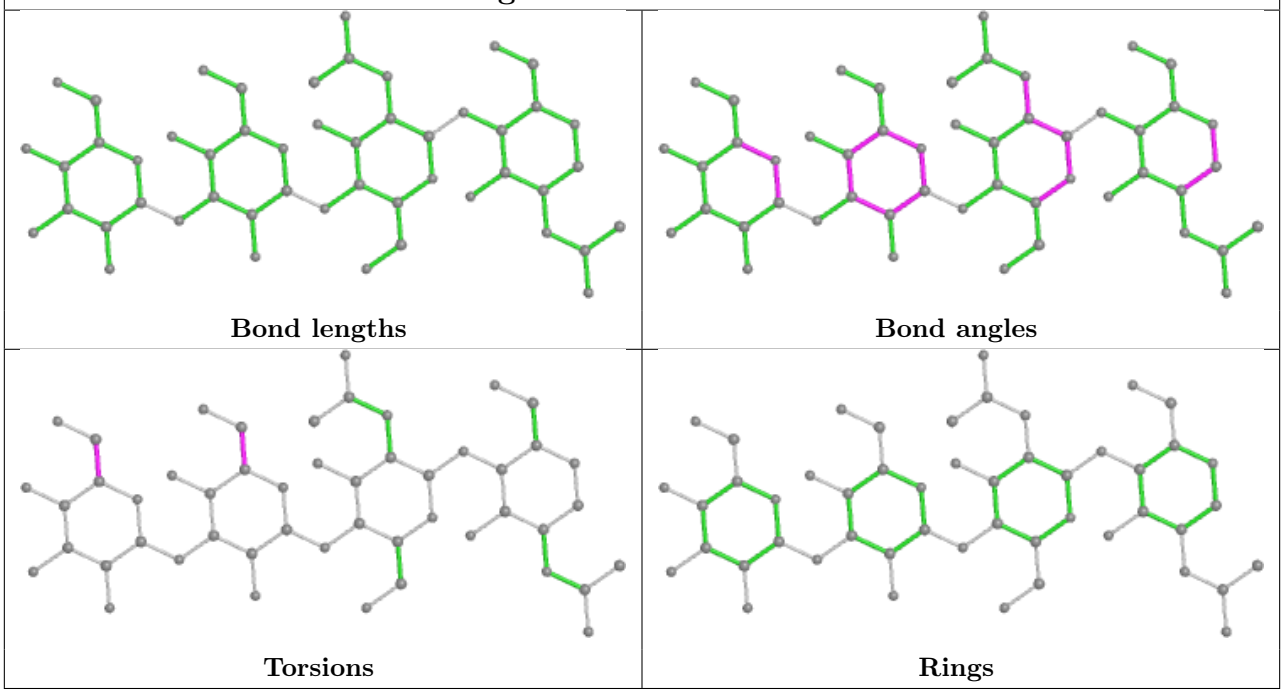


Rings

Oligosaccharide Chain J



Oligosaccharide Chain L



5.6 Ligand geometry (i)

7 ligands 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	$\#\|Z\| > 2$
7	NAG	E	501	1	14,14,15	0.58	0	17,19,21	1.49	1 (5%)
7	NAG	C	502	1	14,14,15	0.61	0	17,19,21	1.55	2 (11%)
7	NAG	E	507	1	14,14,15	0.51	0	17,19,21	1.13	2 (11%)
7	NAG	C	501	1	14,14,15	0.57	0	17,19,21	2.27	3 (17%)
7	NAG	A	404	1	14,14,15	0.58	0	17,19,21	1.25	3 (17%)
7	NAG	E	506	1	14,14,15	0.49	0	17,19,21	1.25	2 (11%)
7	NAG	D	201	2	14,14,15	0.77	1 (7%)	17,19,21	2.17	5 (29%)

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	NAG	E	501	1	-	0/6/23/26	0/1/1/1
7	NAG	C	502	1	-	2/6/23/26	0/1/1/1
7	NAG	E	507	1	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	0/6/23/26	0/1/1/1
7	NAG	A	404	1	-	2/6/23/26	0/1/1/1
7	NAG	E	506	1	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	201	NAG	C1-C2	2.19	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	501	NAG	C1-O5-C5	8.16	123.25	112.19
7	E	501	NAG	C1-O5-C5	5.12	119.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	201	NAG	C2-N2-C7	5.09	130.16	122.90
7	C	502	NAG	C1-O5-C5	4.77	118.65	112.19
7	D	201	NAG	C1-O5-C5	4.03	117.66	112.19
7	D	201	NAG	O5-C1-C2	3.83	117.34	111.29
7	A	404	NAG	O5-C5-C6	3.23	112.26	107.20
7	C	501	NAG	O5-C5-C4	2.58	117.09	110.83
7	D	201	NAG	C1-C2-N2	-2.53	106.16	110.49
7	E	506	NAG	C1-C2-N2	2.53	114.81	110.49
7	C	502	NAG	C3-C4-C5	2.52	114.73	110.24
7	E	507	NAG	C1-O5-C5	2.52	115.60	112.19
7	C	501	NAG	C4-C3-C2	-2.36	107.55	111.02
7	A	404	NAG	O5-C1-C2	-2.30	107.66	111.29
7	A	404	NAG	C1-O5-C5	2.28	115.28	112.19
7	E	507	NAG	O5-C5-C6	2.27	110.76	107.20
7	E	506	NAG	C3-C4-C5	-2.18	106.36	110.24
7	D	201	NAG	O7-C7-N2	2.06	125.74	121.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	201	NAG	C3-C2-N2-C7
7	A	404	NAG	O5-C5-C6-O6
7	C	502	NAG	C4-C5-C6-O6
7	A	404	NAG	C4-C5-C6-O6
7	C	502	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)

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, 95th 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	321/321 (100%)	0.12	8 (2%)	57	62	27, 45, 74, 111	0
1	C	317/321 (98%)	-0.04	7 (2%)	62	66	29, 44, 65, 94	0
1	E	317/321 (98%)	-0.13	6 (1%)	66	71	23, 35, 56, 103	0
2	B	172/176 (97%)	0.21	2 (1%)	79	82	25, 53, 82, 114	0
2	D	171/176 (97%)	0.44	8 (4%)	31	37	25, 54, 91, 105	0
2	F	171/176 (97%)	0.43	9 (5%)	26	32	25, 55, 87, 101	0
All	All	1469/1491 (98%)	0.12	40 (2%)	54	60	23, 44, 81, 114	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	7.5
1	E	9	PRO	5.2
1	C	9	PRO	4.7
2	D	33	GLY	4.4
2	F	171	PHE	4.4
1	A	159	SER	3.8
1	C	22	ASN	3.8
1	A	143	PRO	3.7
2	F	143	LYS	3.6
2	D	147	ALA	3.4
1	E	189	GLN	3.4
2	F	31	GLY	3.3
2	F	30	GLU	3.1
1	C	212	THR	3.1
1	E	222	TRP	3.1
2	F	2	LEU	2.9
2	F	29	SER	2.8
1	A	142	GLY	2.7
1	C	222	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	168	ASN	2.7
1	A	182	VAL	2.5
2	B	172	GLN	2.4
1	A	213	ILE	2.4
1	C	21	PRO	2.4
1	E	158	GLY	2.4
1	C	10	GLY	2.3
1	A	158	GLY	2.3
2	D	156	THR	2.3
1	E	22	ASN	2.3
1	A	208	ARG	2.3
1	C	208	ARG	2.3
2	F	32	THR	2.1
2	D	146	ASN	2.1
2	F	141	TYR	2.1
2	D	16	GLY	2.1
2	D	56	ILE	2.0
2	D	150	GLU	2.0
2	D	26	HIS	2.0
2	F	147	ALA	2.0
1	E	10	GLY	2.0

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

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

6.3 Carbohydrates (i)

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, 95th 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	BMA	G	3	11/12	0.39	0.29	96,101,103,105	0
4	NAG	I	2	14/15	0.58	0.35	63,77,84,87	0
5	MAN	J	4	11/12	0.61	0.55	100,104,105,108	0
4	NAG	K	2	14/15	0.72	0.29	69,74,81,83	0
6	BMA	L	3	11/12	0.77	0.18	75,80,87,96	0
6	MAN	L	4	11/12	0.77	0.41	105,107,109,109	0
3	BMA	H	3	11/12	0.81	0.27	82,86,87,90	0

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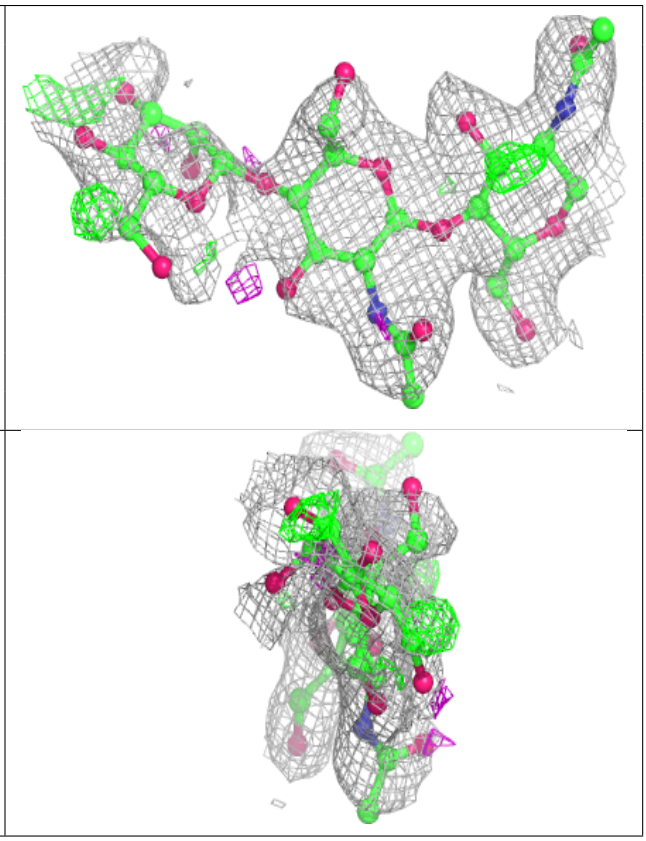
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.85	0.31	73,79,90,96	0
5	BMA	J	3	11/12	0.87	0.19	76,82,87,94	0
3	NAG	H	2	14/15	0.90	0.21	69,74,81,81	0
3	NAG	G	1	14/15	0.91	0.16	48,55,60,64	0
6	NAG	L	1	14/15	0.92	0.14	48,52,55,58	0
6	NAG	L	2	14/15	0.92	0.14	49,58,66,66	0
4	NAG	K	1	14/15	0.93	0.10	40,47,51,59	0
3	NAG	H	1	14/15	0.93	0.20	61,68,76,78	0
5	NAG	J	2	14/15	0.93	0.11	51,54,62,69	0
5	NAG	J	1	14/15	0.95	0.10	44,48,54,60	0
4	NAG	I	1	14/15	0.95	0.19	39,43,52,63	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

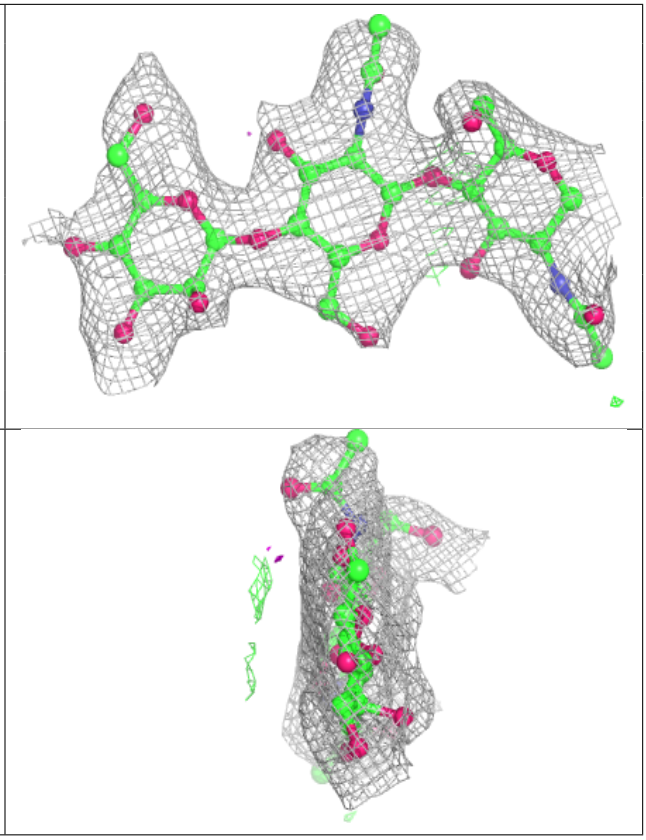
Electron density around Chain G:

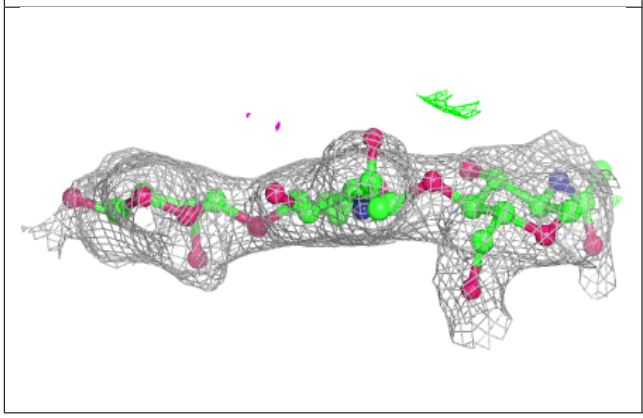
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

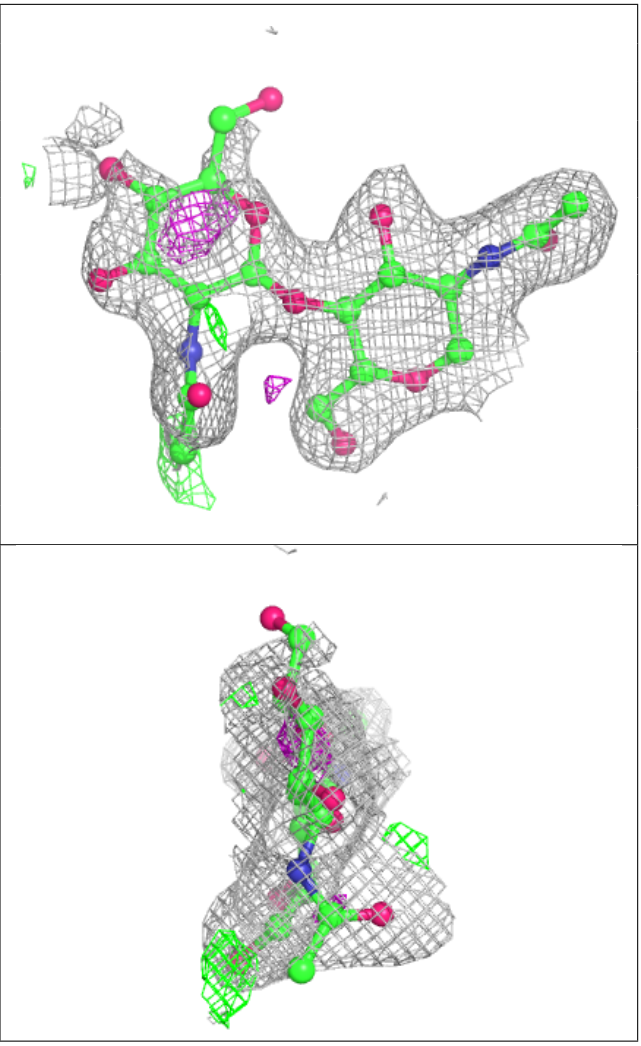
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





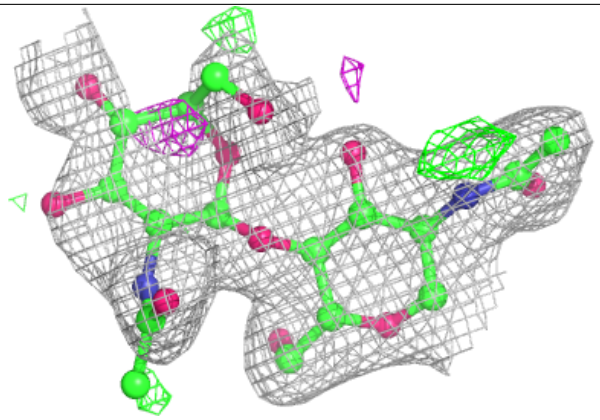
Electron density around Chain I:

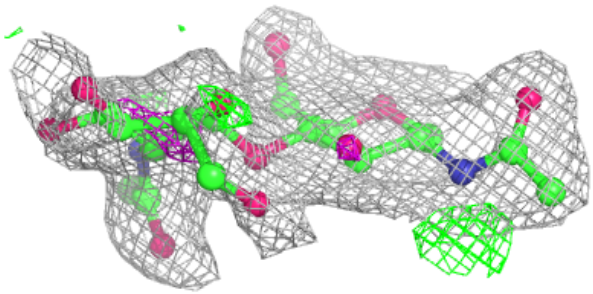
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

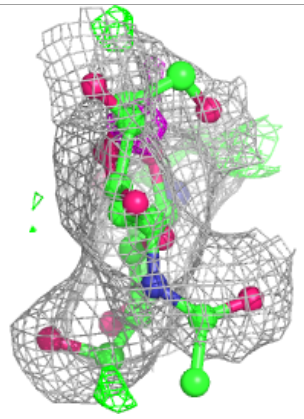


Electron density around Chain K:

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

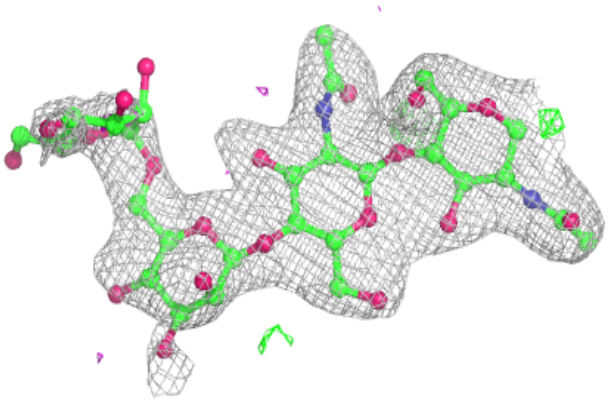


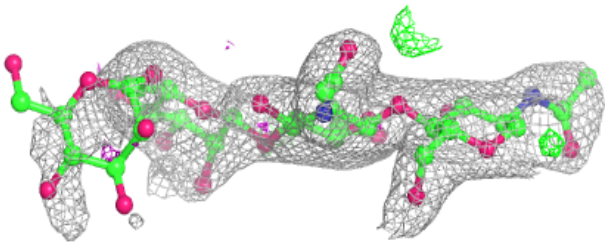


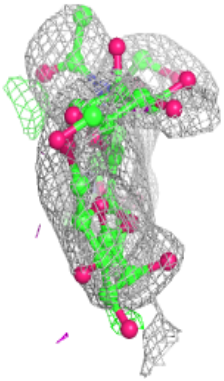


Electron density around Chain J:

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

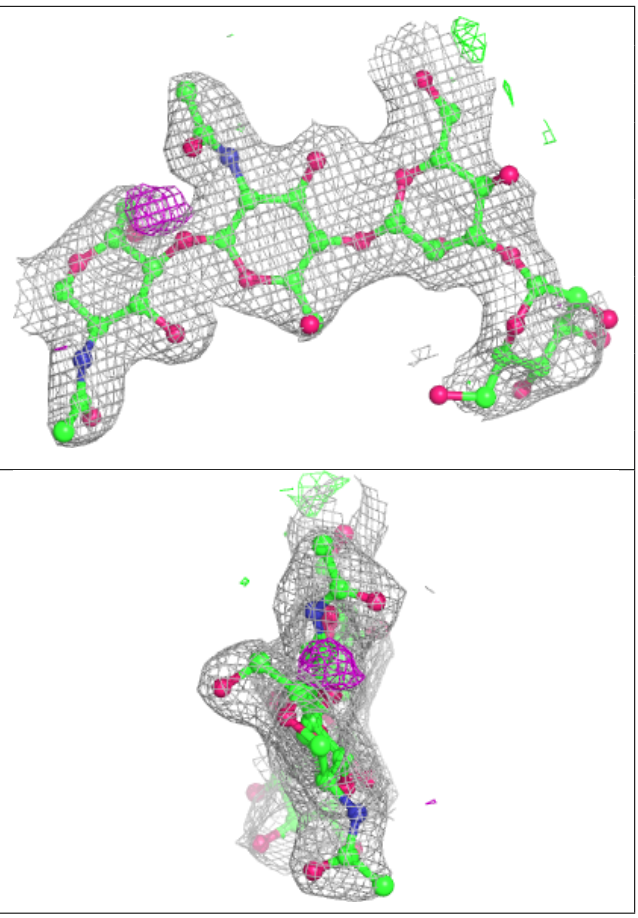






Electron density around Chain L:

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



6.4 Ligands (i)

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, 95th 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	D	201	14/15	0.67	0.40	87,97,103,106	0
7	NAG	C	501	14/15	0.73	0.29	63,72,79,79	0
7	NAG	E	501	14/15	0.73	0.33	68,76,80,85	0
7	NAG	C	502	14/15	0.76	0.26	68,77,82,83	0
7	NAG	A	404	14/15	0.84	0.16	56,65,71,72	0
7	NAG	E	507	14/15	0.85	0.15	47,50,54,56	0
7	NAG	E	506	14/15	0.93	0.13	40,46,52,56	0

6.5 Other polymers (i)

There are no such residues in this entry.