Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 06:08 AM BST

PDB ID	:	2YP5
Title	:	Haemagglutinin of 2004 Human H3N2 Virus in Complex with Avian Receptor Analogue 3SLN
Authors	:	Xiong, X.; Lin, Y.P.; Wharton, S.A.; Martin, S.R.; Coombs, P.J.; Vachieri, S.G.; Christodoulou, E.; Walker, P.A.; Liu, J.; Skehel, J.J.; Gamblin, S.J.; Hay, A.J.; Daniels, R.S.; McCauley, J.W.
Deposited on	:	2012-10-29
Resolution	:	1.79 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 following versions of software and data (see references (1)) were used in the production of this report:

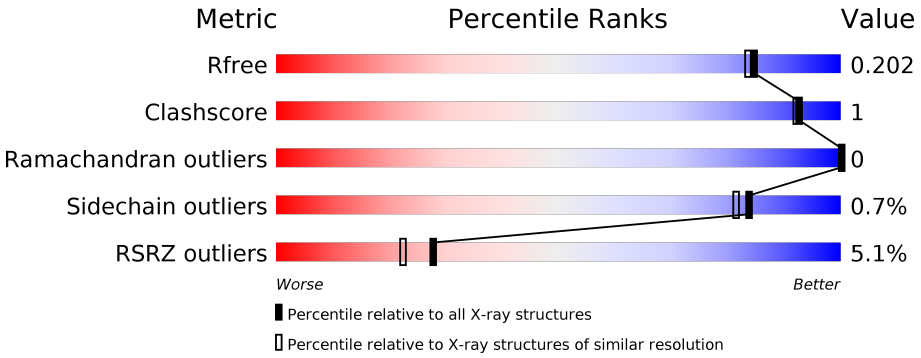
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	503	5% 93%
2	B	3	67% 33%
3	C	2	100%
4	D	2	50% 50%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	803	X	-	-	-
5	NAG	A	810	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4666 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.

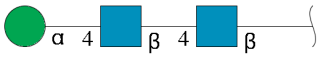
- Molecule 1 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	7	0
			3916	2442	700	756	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	GLN	ARG	engineered mutation	UNP A0FCI1

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



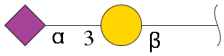
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

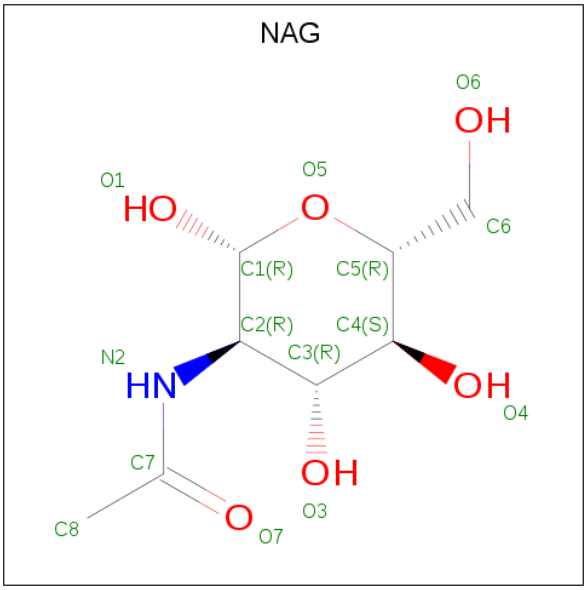
- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto

pyranose.



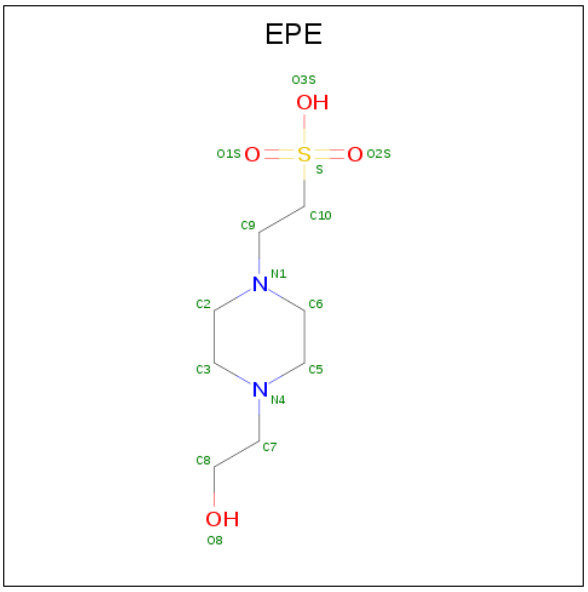
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	2	Total C N O 22 12 1 9	0	0	1

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



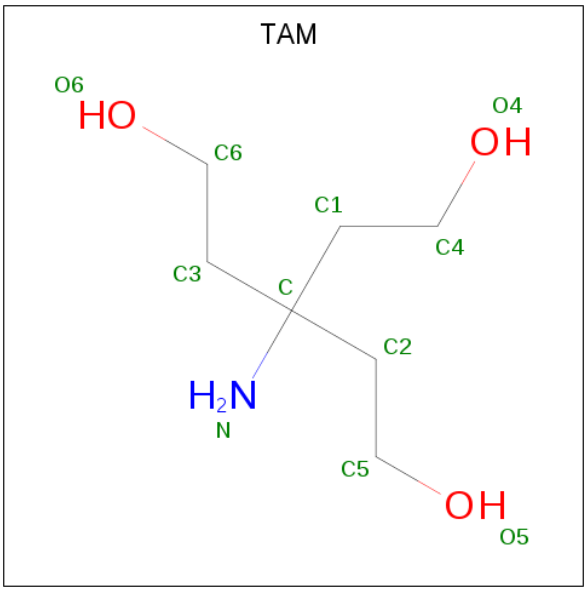
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 8 is water.

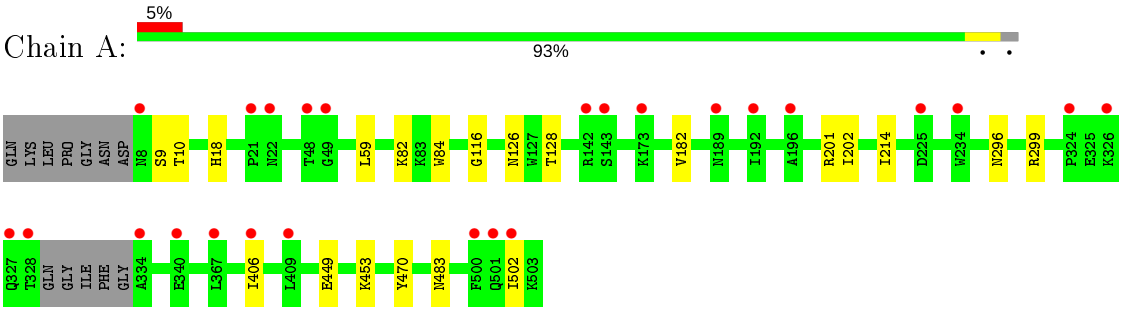
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	535	Total	O	0	0
			535	535		

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

Chain A:

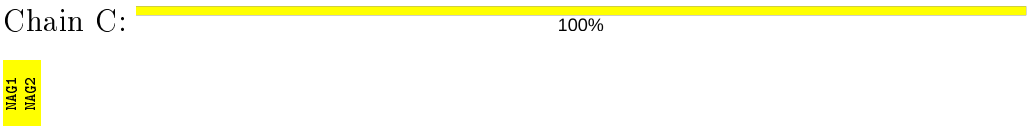


• Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

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

Chain C:



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	100.86Å 100.86Å 386.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	128.84 – 1.79 46.96 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (128.84-1.79) 100.0 (46.96-1.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.172 , 0.196 0.178 , 0.202	Depositor DCC
R_{free} test set	3621 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4666	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SIA, GAL, TAM, EPE, 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	0.52	0/4015	0.62	0/5434

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3916	0	3819	11	0
2	B	39	0	34	0	0
3	C	28	0	25	0	0
4	D	22	0	17	0	0
5	A	70	0	65	2	0
6	A	45	0	54	0	0
7	A	11	0	17	0	0
8	A	535	0	0	4	1
All	All	4666	0	4031	12	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 (12) 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:483:ASN:HB2	5:A:810:NAG:H83	1.84	0.60
1:A:296[B]:ASN:ND2	8:A:901:HOH:O	2.10	0.55
1:A:182:VAL:HG22	1:A:202:ILE:HD12	1.94	0.49
5:A:810:NAG:H81	8:A:1275:HOH:O	2.11	0.49
1:A:449:GLU:O	1:A:453:LYS:HG2	2.15	0.47
1:A:126:ASN:OD1	1:A:128:THR:HG23	2.16	0.45
1:A:59:LEU:HD13	1:A:82:LYS:HE2	1.99	0.43
1:A:10:THR:HG22	1:A:470:TYR:HA	2.00	0.43
1:A:9:SER:HB2	8:A:940:HOH:O	2.18	0.43
1:A:201:ARG:HB3	1:A:214:ILE:HD13	2.01	0.41
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.56	0.40
1:A:406[A]:ILE:HG22	8:A:1253:HOH:O	2.22	0.40

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)
8:A:906:HOH:O	8:A:1333:HOH:O[2_655]	2.16	0.04

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	494/503 (98%)	474 (96%)	20 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	436/438 (100%)	432 (99%)	4 (1%)	78 75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	299[A]	ARG
1	A	299[B]	ARG
1	A	502	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

7 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	B	1	1,2	14,14,15	0.54	0	17,19,21	0.75	0
2	NAG	B	2	2	14,14,15	0.48	0	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	B	3	2	11,11,12	0.38	0	15,15,17	1.14	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
3	NAG	C	2	3	14,14,15	0.50	0	17,19,21	0.88	1 (5%)
4	GAL	D	1	4	1,1,12	0.31	0	-		
4	SIA	D	2	4	17,20,21	0.43	0	21,28,31	1.10	2 (9%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	1/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	SIA	D	2	4	-	0/14/34/38	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	MAN	C1-O5-C5	3.59	117.06	112.19
3	C	1	NAG	C1-O5-C5	2.58	115.69	112.19
4	D	2	SIA	C4-C5-N5	-2.36	105.71	110.38
4	D	2	SIA	C6-O6-C2	2.23	116.12	111.34
3	C	2	NAG	O5-C5-C6	2.21	110.67	107.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

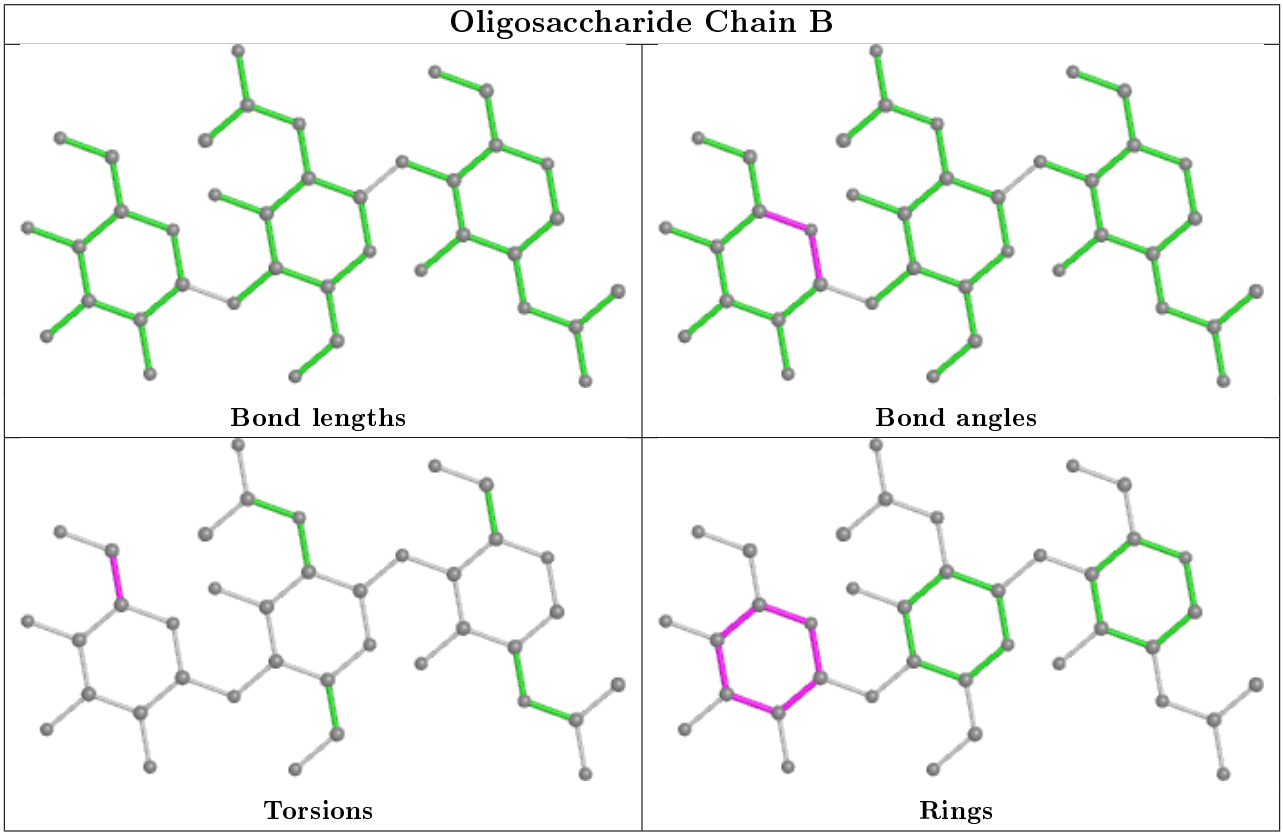
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

All (1) ring outliers are listed below:

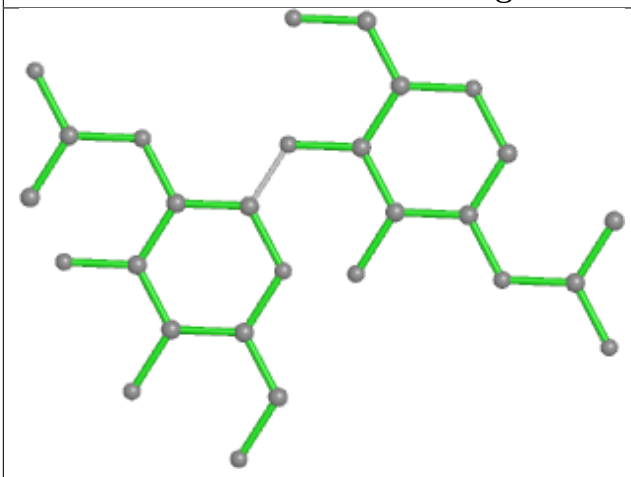
Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

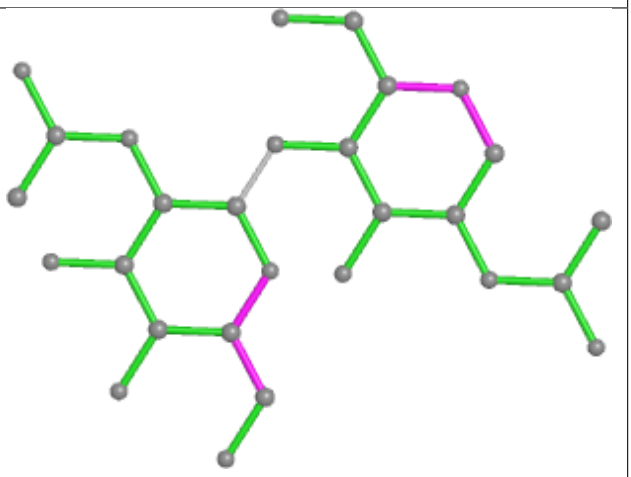
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



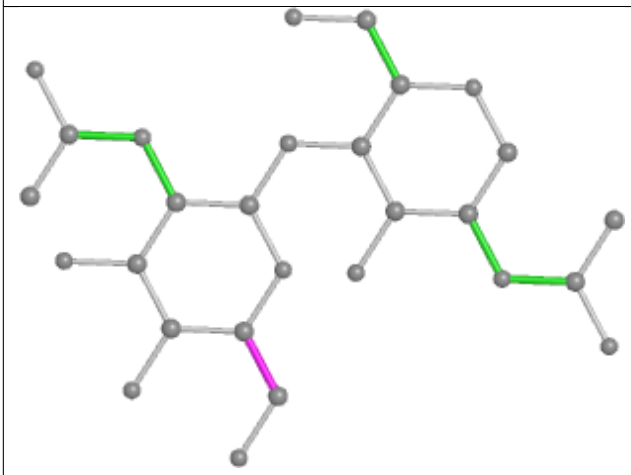
Oligosaccharide Chain C



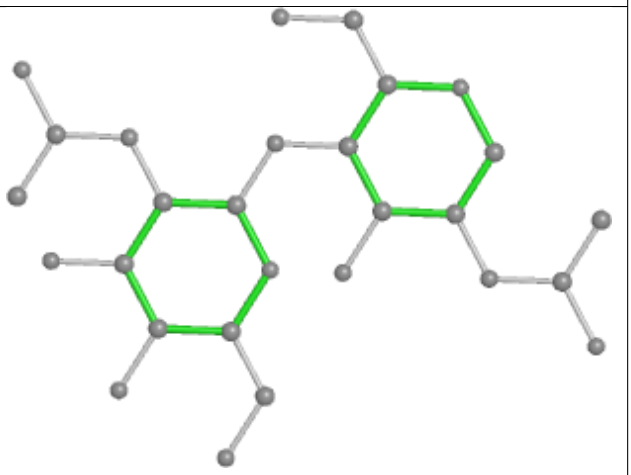
Bond lengths



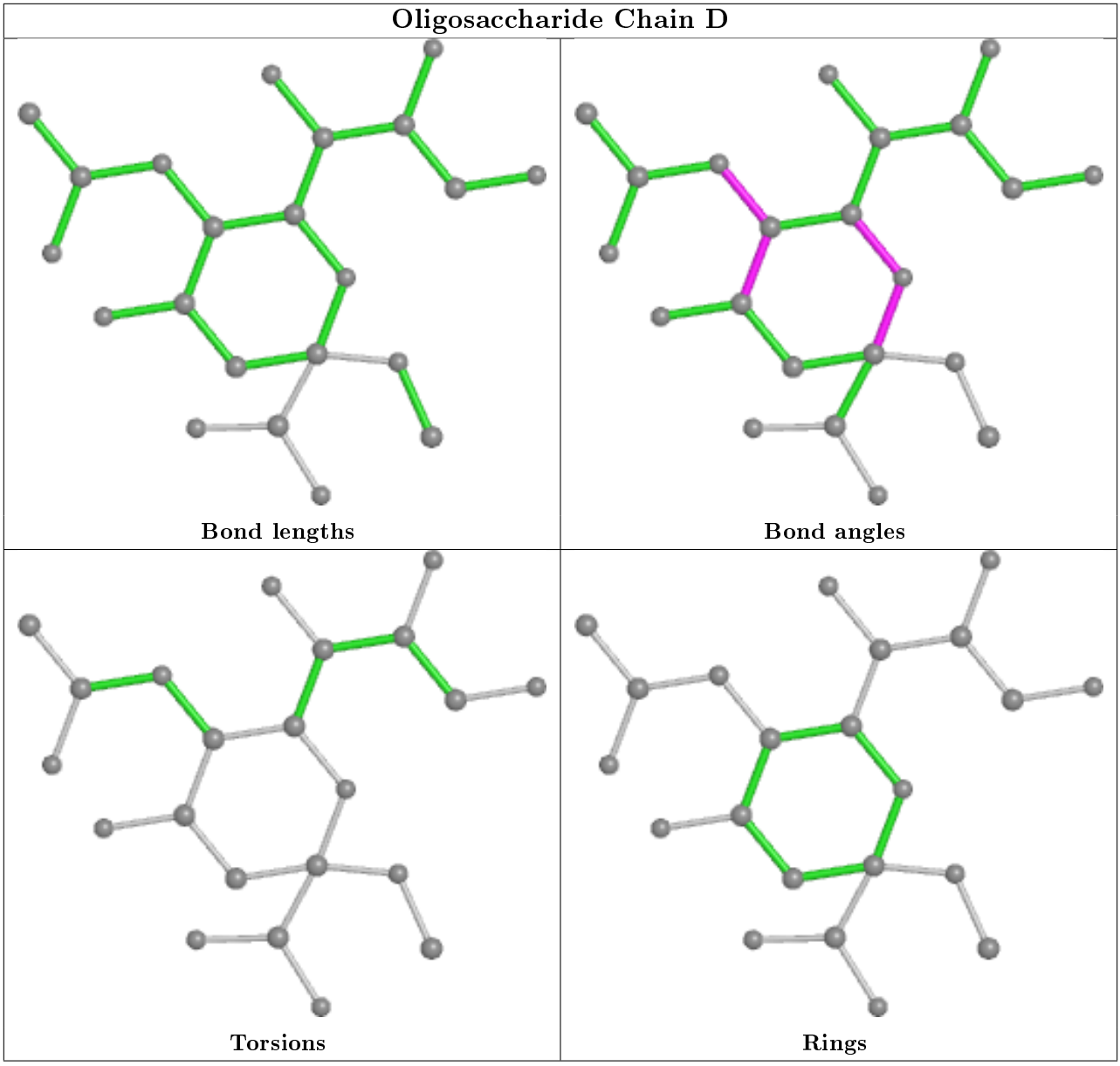
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 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	$\#\|Z\|>2$
5	NAG	A	801	1	14,14,15	0.38	0	17,19,21	1.12	1 (5%)
6	EPE	A	811	-	15,15,15	2.18	2 (13%)	18,20,20	5.84	5 (27%)
5	NAG	A	810	1	14,14,15	0.59	0	17,19,21	1.34	2 (11%)
5	NAG	A	802	1	14,14,15	0.48	0	17,19,21	0.68	0
7	TAM	A	816	-	7,10,10	0.61	0	9,12,12	0.49	0
6	EPE	A	813	-	15,15,15	2.10	2 (13%)	18,20,20	1.17	2 (11%)
5	NAG	A	803	1	14,14,15	0.65	0	17,19,21	0.99	1 (5%)
5	NAG	A	809	1	14,14,15	0.74	1 (7%)	17,19,21	1.06	1 (5%)
6	EPE	A	812	-	15,15,15	2.03	2 (13%)	18,20,20	1.11	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	801	1	-	0/6/23/26	0/1/1/1
6	EPE	A	811	-	-	6/9/19/19	0/1/1/1
6	EPE	A	812	-	-	3/9/19/19	0/1/1/1
5	NAG	A	810	1	-	2/6/23/26	0/1/1/1
5	NAG	A	802	1	-	0/6/23/26	0/1/1/1
7	TAM	A	816	-	-	5/12/12/12	-
6	EPE	A	813	-	-	6/9/19/19	0/1/1/1
5	NAG	A	809	1	-	0/6/23/26	0/1/1/1
5	NAG	A	803	1	1/1/5/7	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	811	EPE	C10-S	-6.80	1.67	1.77
6	A	813	EPE	C10-S	-6.39	1.68	1.77
6	A	812	EPE	C10-S	-6.14	1.68	1.77
6	A	811	EPE	O3S-S	4.73	1.64	1.47
6	A	813	EPE	O3S-S	4.68	1.64	1.47
6	A	812	EPE	O3S-S	4.60	1.63	1.47
5	A	809	NAG	O5-C1	-2.04	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	811	EPE	O3S-S-C10	-12.00	86.37	105.77
6	A	811	EPE	O3S-S-O2S	-11.26	83.75	111.27
6	A	811	EPE	O2S-S-C10	10.55	119.61	106.92
6	A	811	EPE	O3S-S-O1S	-10.52	85.57	111.27
6	A	811	EPE	O1S-S-C10	10.25	119.26	106.92
5	A	801	NAG	C1-O5-C5	3.69	117.19	112.19
6	A	813	EPE	O1S-S-C10	3.48	111.10	106.92
5	A	810	NAG	O5-C5-C6	2.84	111.65	107.20
5	A	809	NAG	C1-C2-N2	2.60	114.93	110.49
5	A	810	NAG	C8-C7-N2	2.22	119.86	116.10
6	A	812	EPE	C9-N1-C6	2.20	116.86	111.23
5	A	803	NAG	O5-C1-C2	-2.15	107.89	111.29
6	A	813	EPE	O2S-S-C10	2.06	109.40	106.92
6	A	812	EPE	O1S-S-C10	2.04	109.37	106.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	803	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	811	EPE	N4-C7-C8-O8
6	A	811	EPE	S-C10-C9-N1
6	A	811	EPE	C9-C10-S-O2S
6	A	811	EPE	C9-C10-S-O3S
7	A	816	TAM	N-C-C2-C5
7	A	816	TAM	C-C2-C5-O5
6	A	813	EPE	C10-C9-N1-C2
6	A	813	EPE	C10-C9-N1-C6
6	A	813	EPE	C9-C10-S-O1S
6	A	813	EPE	C9-C10-S-O2S
6	A	813	EPE	C9-C10-S-O3S
6	A	812	EPE	C10-C9-N1-C6
5	A	803	NAG	C8-C7-N2-C2
5	A	803	NAG	O7-C7-N2-C2
5	A	810	NAG	C8-C7-N2-C2
5	A	810	NAG	O7-C7-N2-C2
6	A	812	EPE	C10-C9-N1-C2
7	A	816	TAM	C3-C-C2-C5
7	A	816	TAM	C1-C-C3-C6
6	A	813	EPE	N4-C7-C8-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	812	EPE	N4-C7-C8-O8
7	A	816	TAM	N-C-C3-C6
6	A	811	EPE	C8-C7-N4-C3
6	A	811	EPE	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	810	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	491/503 (97%)	0.04	25 (5%) 28 22	10, 25, 44, 89	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	THR	7.5
1	A	502	ILE	5.9
1	A	8	ASN	5.7
1	A	327	GLN	5.6
1	A	196	ALA	5.1
1	A	334	ALA	5.1
1	A	48	THR	4.7
1	A	501	GLN	3.7
1	A	326	LYS	3.4
1	A	142	ARG	3.1
1	A	500	PHE	2.7
1	A	189	ASN	2.7
1	A	22	ASN	2.7
1	A	225	ASP	2.6
1	A	143	SER	2.6
1	A	192	ILE	2.5
1	A	367	LEU	2.5
1	A	406[A]	ILE	2.4
1	A	324	PRO	2.4
1	A	49	GLY	2.4
1	A	21	PRO	2.3
1	A	409	LEU	2.3
1	A	173	LYS	2.2
1	A	234	TRP	2.1
1	A	340	GLU	2.1

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

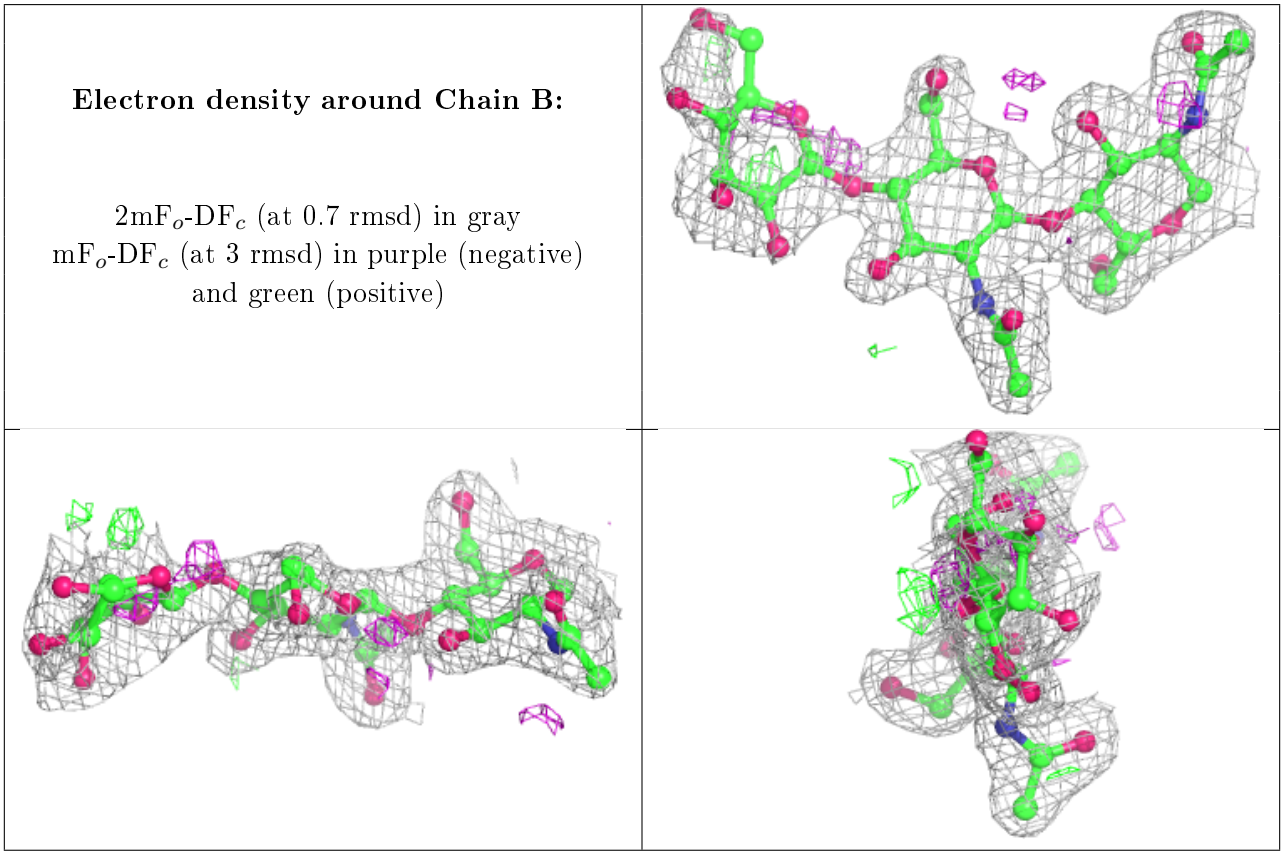
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

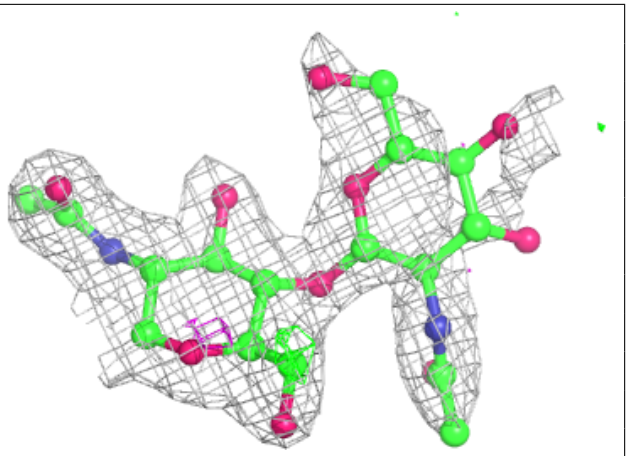
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	B	3	11/12	0.53	0.40	67,74,78,80	0
3	NAG	C	2	14/15	0.73	0.33	62,70,75,77	0
3	NAG	C	1	14/15	0.85	0.17	42,46,53,61	0
2	NAG	B	2	14/15	0.85	0.21	36,43,50,58	0
4	GAL	D	1	2/12	0.86	0.16	52,52,52,53	0
4	SIA	D	2	20/21	0.89	0.24	43,51,53,55	0
2	NAG	B	1	14/15	0.95	0.13	34,38,44,45	0

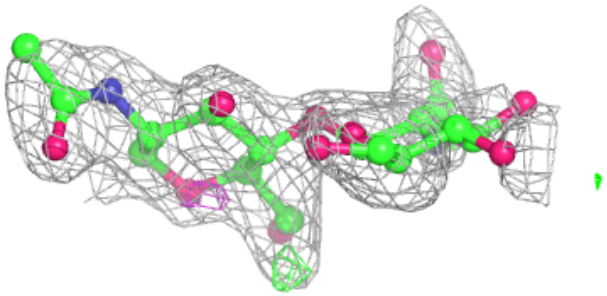
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

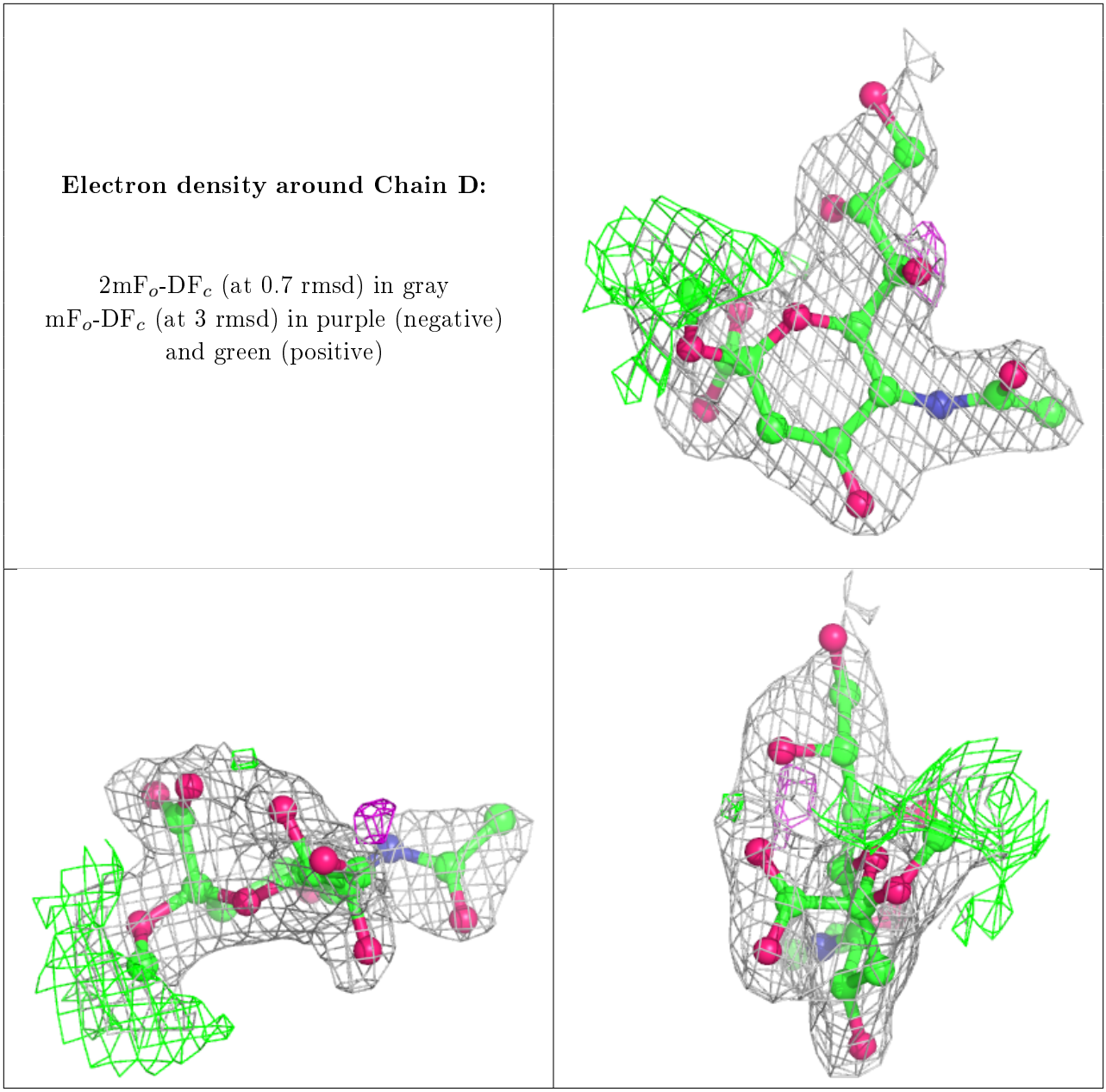
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Chain D:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	810	14/15	0.62	0.41	61,68,72,74	0
6	EPE	A	811	15/15	0.66	0.24	30,53,77,78	0
7	TAM	A	816	11/11	0.72	0.21	60,61,62,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	803	14/15	0.73	0.22	50,61,68,68	0
5	NAG	A	801	14/15	0.75	0.27	43,52,55,57	0
6	EPE	A	813	15/15	0.84	0.22	39,46,52,53	0
5	NAG	A	809	14/15	0.85	0.24	29,37,44,44	0
5	NAG	A	802	14/15	0.86	0.23	35,42,47,48	0
6	EPE	A	812	15/15	0.93	0.14	34,47,53,55	0

6.5 Other polymers

There are no such residues in this entry.