Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 03:09 PM EDT

PDB ID	:	4XJQ
Title	:	The catalytic mechanism of human parainfluenza virus type 3 haemagglutinin-neuraminidase revealed
Authors	:	Dirr, L.; El-Deeb, I.; Guillon, P.; Carroux, C.; Chavas, L.; von Itzstein, M.
Deposited on	:	2015-01-08
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

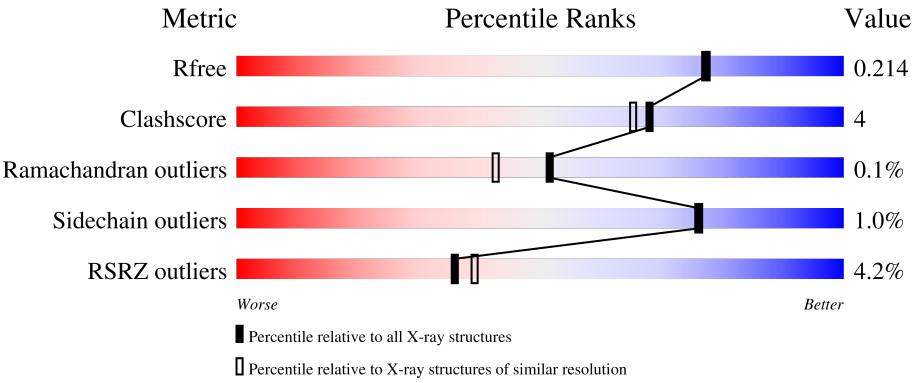
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

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

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	454	3% 85% 9% 5%
1	B	454	5% 89% 6% .
2	C	4	75% 25%
3	D	2	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
7	GOL	A	611	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7603 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-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	18	2	0
			3397	2145	587	645	20			
1	B	434	Total	C	N	O	S	26	2	0
			3406	2154	589	643	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	HIS	-	expression tag	UNP G8G134
A	574	HIS	-	expression tag	UNP G8G134
A	575	HIS	-	expression tag	UNP G8G134
A	576	HIS	-	expression tag	UNP G8G134
A	577	HIS	-	expression tag	UNP G8G134
A	578	HIS	-	expression tag	UNP G8G134
B	573	HIS	-	expression tag	UNP G8G134
B	574	HIS	-	expression tag	UNP G8G134
B	575	HIS	-	expression tag	UNP G8G134
B	576	HIS	-	expression tag	UNP G8G134
B	577	HIS	-	expression tag	UNP G8G134
B	578	HIS	-	expression tag	UNP G8G134

- Molecule 2 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
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

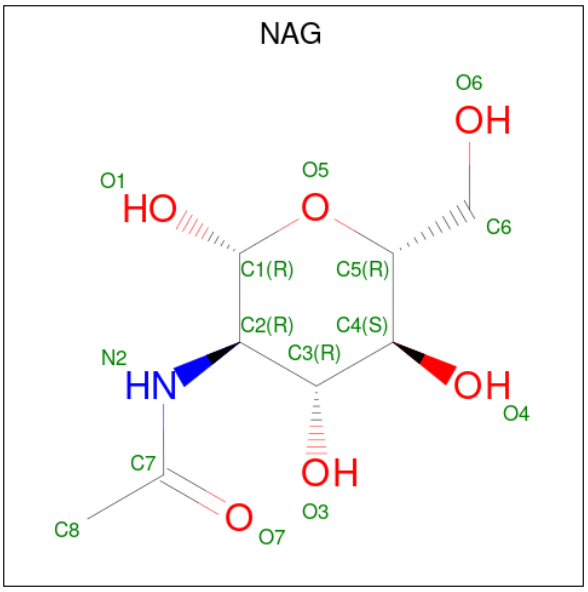
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

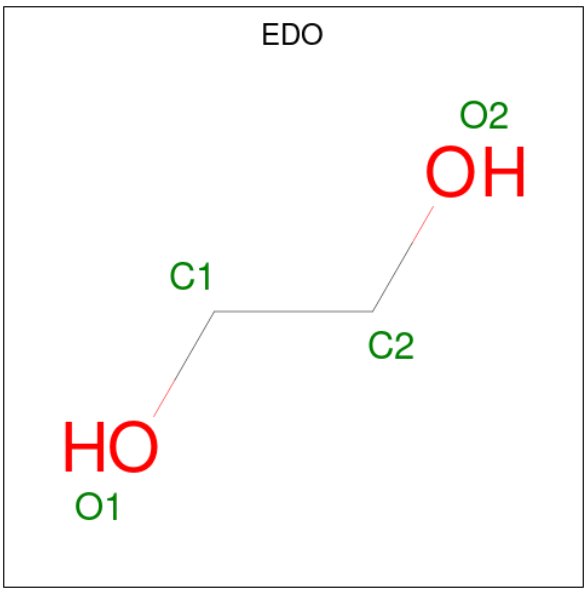
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

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



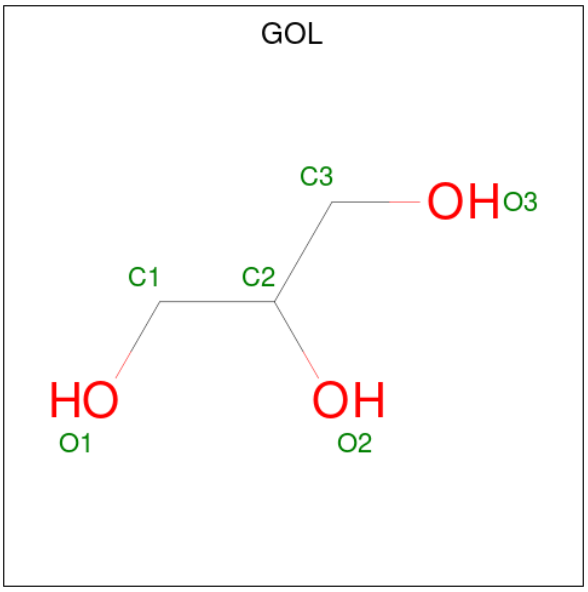
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



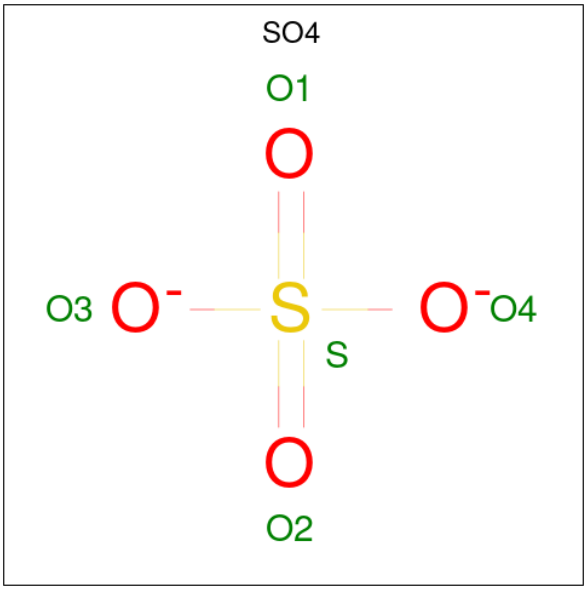
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

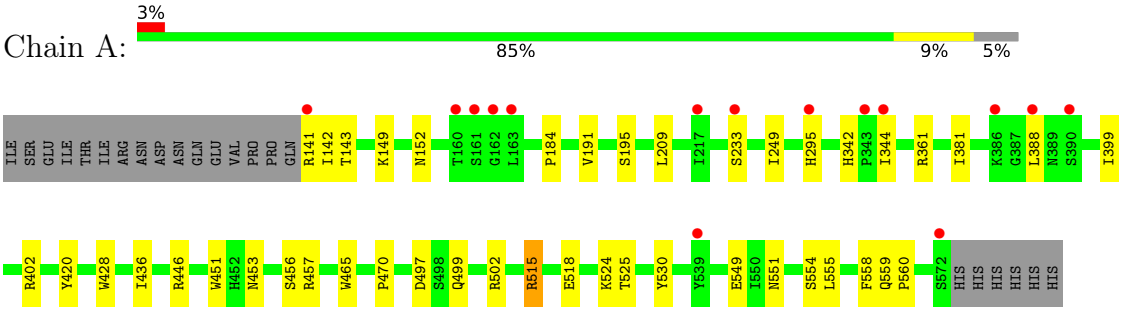
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	320	Total O 320 320	0	0
9	B	318	Total O 318 318	0	0

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.

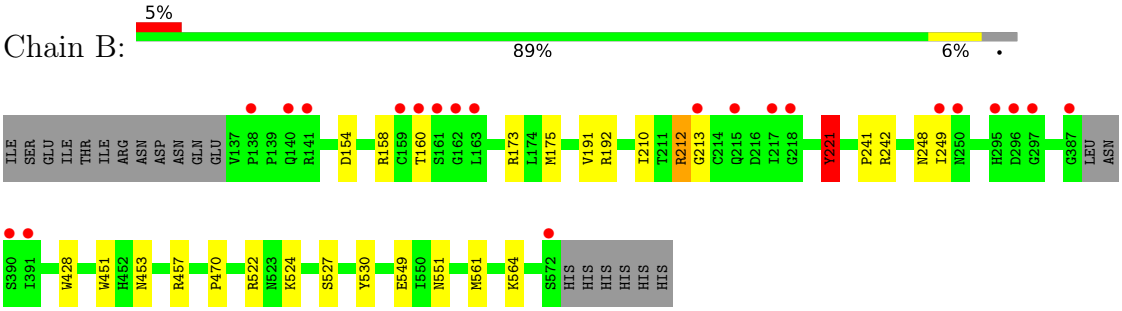
• Molecule 1: Hemagglutinin-neuraminidase

Chain A:



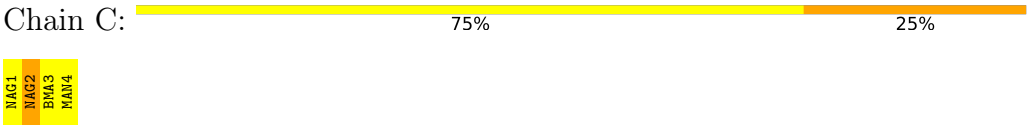
• Molecule 1: Hemagglutinin-neuraminidase

Chain B:



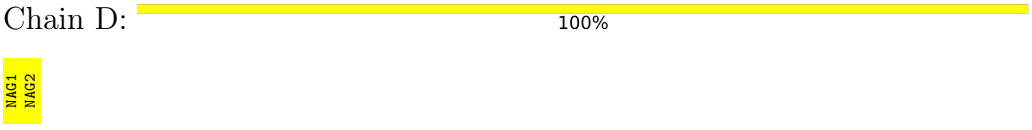
• Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.43Å 94.02Å 105.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.78 – 1.90 19.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.1 (19.78-1.90) 93.2 (19.78-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.162 , 0.209 0.170 , 0.214	Depositor DCC
R_{free} test set	3088 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7603	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: SO4, EDO, MAN, NAG, BMA, CA, GOL

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	0.55	3/3478 (0.1%)	0.92	7/4739 (0.1%)
1	B	0.81	4/3492 (0.1%)	0.80	4/4759 (0.1%)
All	All	0.69	7/6970 (0.1%)	0.86	11/9498 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	ARG	CD-NE	-27.46	0.99	1.46
1	B	212	ARG	CD-NE	-23.13	1.07	1.46
1	A	402	ARG	NE-CZ	-12.12	1.17	1.33
1	B	158	ARG	CG-CD	-6.75	1.35	1.51
1	B	221	TYR	CD2-CE2	-5.81	1.30	1.39
1	A	361	ARG	CB-CG	-5.16	1.38	1.52
1	A	446	ARG	CD-NE	-5.13	1.37	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	402	ARG	NE-CZ-NH1	23.70	132.15	120.30
1	A	402	ARG	NE-CZ-NH2	-23.39	108.61	120.30
1	B	173	ARG	CG-CD-NE	20.03	153.87	111.80
1	A	402	ARG	CD-NE-CZ	18.25	149.15	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	212	ARG	CG-CD-NE	13.09	139.29	111.80
1	B	173	ARG	CD-NE-CZ	11.58	139.81	123.60
1	B	212	ARG	CD-NE-CZ	9.13	136.39	123.60
1	A	515	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	446	ARG	CG-CD-NE	8.16	128.95	111.80
1	A	446	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	515	ARG	NE-CZ-NH1	5.35	122.97	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	212	ARG	Sidechain
1	B	221	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	3397	0	3355	38	0
1	B	3406	0	3366	14	0
2	C	50	0	43	1	0
3	D	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	14	0	13	2	0
5	B	14	0	13	0	0
6	A	16	0	24	1	0
6	B	16	0	24	0	0
7	A	12	0	16	9	0
8	B	10	0	0	0	0
9	A	320	0	0	9	0
9	B	318	0	0	3	0
All	All	7603	0	6879	52	0

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 4.

All (52) 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:524:LYS:HE2	9:A:939:HOH:O	1.52	1.07
1:A:152:ASN:HD22	7:A:611:GOL:H31	1.29	0.94
1:A:152:ASN:HD22	7:A:611:GOL:C3	1.85	0.90
7:A:611:GOL:H11	9:A:753:HOH:O	1.79	0.81
1:A:142:ILE:HG23	1:A:143:THR:HG23	1.68	0.75
1:A:530:TYR:OH	9:A:1020:HOH:O	2.08	0.70
1:A:524:LYS:CE	9:A:939:HOH:O	2.24	0.67
1:A:342:HIS:HB2	1:A:344:ILE:HD11	1.79	0.65
1:A:515:ARG:HD2	1:A:518:GLU:OE1	1.97	0.65
1:A:195:SER:HB2	9:A:954:HOH:O	1.97	0.64
1:A:152:ASN:ND2	7:A:611:GOL:H31	2.08	0.63
1:B:192:ARG:CZ	1:B:210:ILE:HD11	2.29	0.62
1:A:555:LEU:HD12	1:B:561:MET:CE	2.33	0.59
1:A:191:VAL:HG22	1:A:209:LEU:HG	1.84	0.58
1:A:195:SER:CB	9:A:954:HOH:O	2.48	0.56
1:A:152:ASN:ND2	7:A:611:GOL:C3	2.64	0.56
1:A:559:GLN:HG3	9:A:825:HOH:O	2.08	0.54
1:B:249:ILE:O	9:B:962:HOH:O	2.18	0.53
1:A:381:ILE:CD1	1:A:399:ILE:HD11	2.38	0.52
1:B:242:ARG:NH1	9:B:944:HOH:O	2.43	0.52
1:A:551:ASN:HB2	1:A:558:PHE:CE2	2.46	0.51
1:A:191:VAL:HB	1:A:560:PRO:HD3	1.93	0.50
1:B:241:PRO:HD3	9:B:946:HOH:O	2.10	0.50
1:B:527:SER:HB2	1:B:551:ASN:HB3	1.93	0.50
1:A:497:ASP:O	1:A:524:LYS:NZ	2.42	0.49
1:A:524:LYS:HG2	9:A:1005:HOH:O	2.13	0.48
1:A:499:GLN:H	6:A:609:EDO:H22	1.78	0.48
1:A:515:ARG:CD	1:A:518:GLU:OE1	2.63	0.47
1:A:525:THR:HG23	5:A:606:NAG:H82	1.97	0.47
1:A:191:VAL:O	1:A:549:GLU:OE2	2.33	0.46
1:A:451:TRP:CZ2	2:C:2:NAG:H5	2.52	0.45
1:A:428:TRP:CG	1:A:470:PRO:HA	2.53	0.43
1:A:428:TRP:CD2	1:A:470:PRO:HA	2.54	0.43
1:B:530:TYR:HB3	1:B:549:GLU:HG3	2.00	0.43
1:A:152:ASN:HD22	7:A:611:GOL:H32	1.76	0.43
1:B:221:TYR:CD1	1:B:249:ILE:HD12	2.54	0.43
1:A:420:TYR:CE2	1:A:436:ILE:HD11	2.54	0.42
1:B:428:TRP:CG	1:B:470:PRO:HA	2.54	0.42
1:A:149:LYS:NZ	7:A:611:GOL:O3	2.41	0.42
7:A:611:GOL:C2	9:A:713:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:SER:O	1:B:522:ARG:NH2	2.53	0.42
1:B:175:MET:CE	1:B:564:LYS:HB3	2.49	0.42
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.55	0.42
1:B:451:TRP:CZ2	1:B:453:ASN:HB2	2.55	0.42
1:A:184:PRO:HG3	1:A:191:VAL:HG23	2.02	0.41
1:A:381:ILE:HD13	1:A:399:ILE:HD11	2.01	0.41
1:A:502:ARG:HH22	7:A:612:GOL:H2	1.86	0.41
1:A:233:SER:HB2	1:B:248:ASN:HD22	1.86	0.41
1:A:456:SER:HB3	1:A:465:TRP:CE2	2.56	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.82	0.40
5:A:606:NAG:H83	5:A:606:NAG:H3	2.03	0.40
1:B:191:VAL:O	1:B:549:GLU:OE1	2.39	0.40

There are no symmetry-related clashes.

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	432/454 (95%)	413 (96%)	19 (4%)	0	100 100
1	B	431/454 (95%)	413 (96%)	17 (4%)	1 (0%)	47 38
All	All	863/908 (95%)	826 (96%)	36 (4%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	GLY

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	392/412 (95%)	388 (99%)	4 (1%)	76	76
1	B	393/412 (95%)	389 (99%)	4 (1%)	76	76
All	All	785/824 (95%)	777 (99%)	8 (1%)	76	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	249	ILE
1	A	295	HIS
1	A	457	ARG
1	B	154	ASP
1	B	160	THR
1	B	457	ARG
1	B	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	433	GLN
1	A	551	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 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	2,1	14,14,15	0.64	0	17,19,21	1.25	2 (11%)
2	NAG	C	2	2	14,14,15	0.40	0	17,19,21	1.06	1 (5%)
2	BMA	C	3	2	11,11,12	0.32	0	15,15,17	0.95	1 (6%)
2	MAN	C	4	2	11,11,12	0.57	0	15,15,17	1.29	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.56	0	17,19,21	1.60	2 (11%)
3	NAG	D	2	3	14,14,15	0.42	0	17,19,21	1.19	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	O5-C1-C2	-4.25	104.58	111.29
2	C	4	MAN	C1-O5-C5	3.89	117.46	112.19
3	D	1	NAG	C1-O5-C5	3.77	117.29	112.19
2	C	2	NAG	O5-C5-C6	3.21	112.24	107.20
2	C	1	NAG	C1-O5-C5	2.67	115.81	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	C8-C7-N2	2.48	120.30	116.10
2	C	3	BMA	O5-C5-C6	2.41	110.99	107.20
3	D	2	NAG	O5-C1-C2	-2.22	107.79	111.29
2	C	1	NAG	C6-C5-C4	-2.16	107.95	113.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

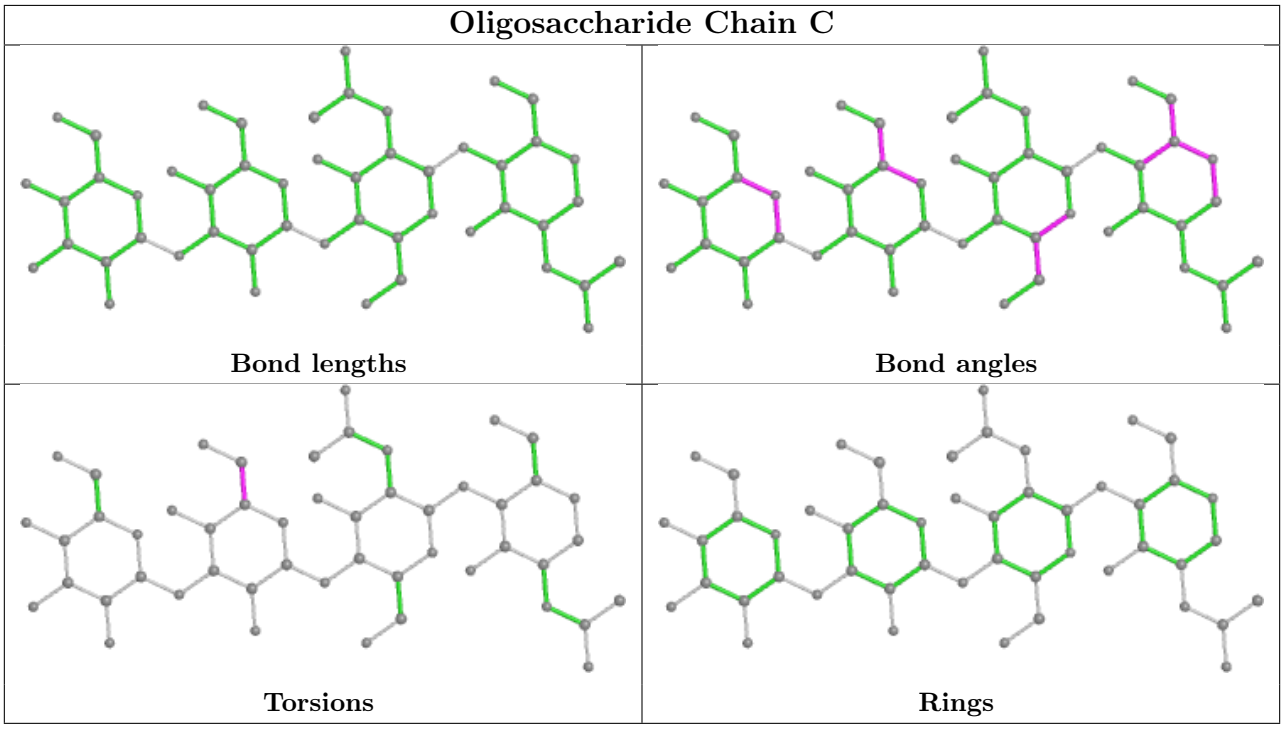
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

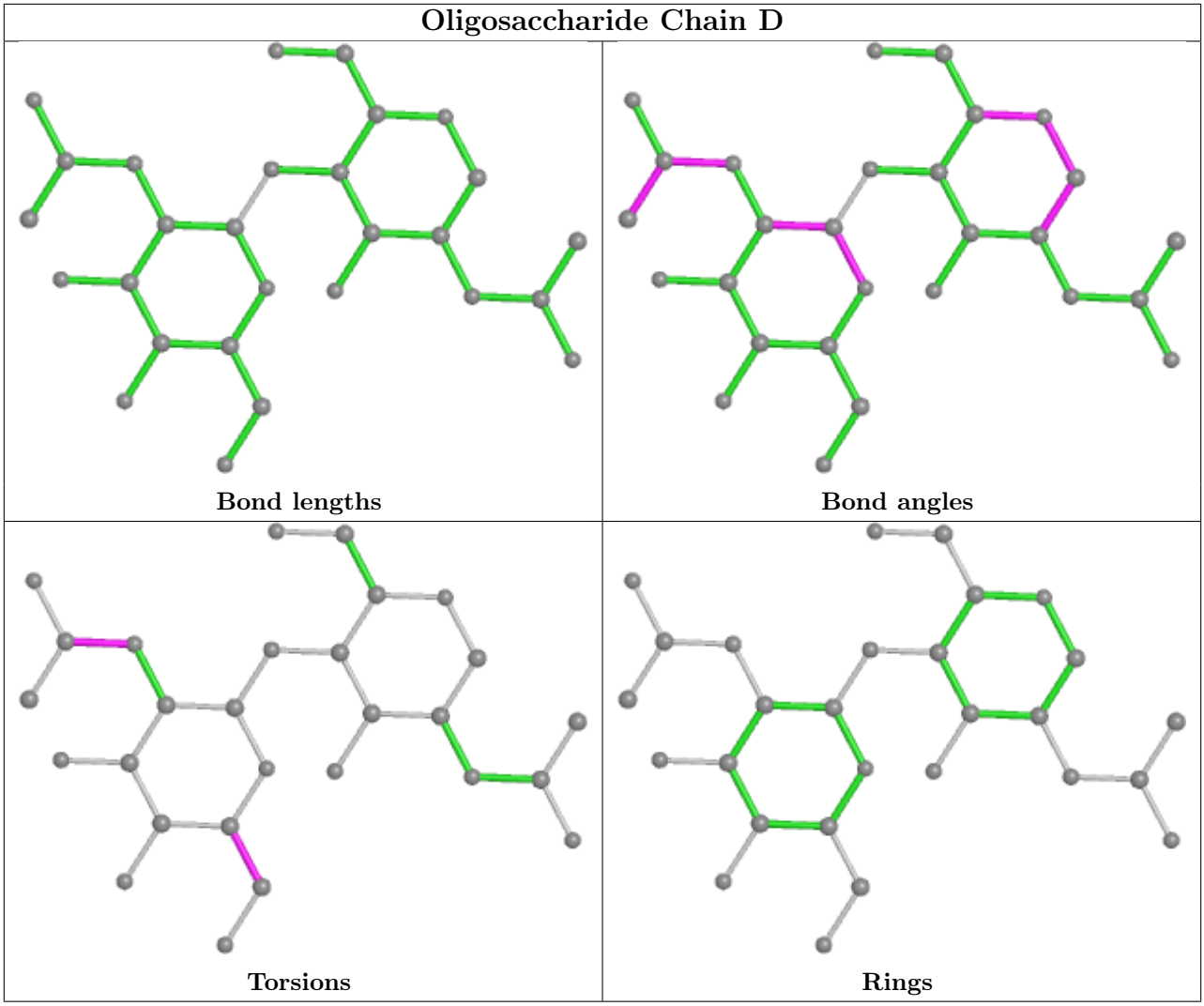
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	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.





5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	GOL	A	612	-	5,5,5	0.40	0	5,5,5	0.56	0
6	EDO	A	610	-	3,3,3	0.37	0	2,2,2	0.48	0
8	SO4	B	602	-	4,4,4	0.27	0	6,6,6	0.14	0
6	EDO	A	607	-	3,3,3	0.94	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	EDO	B	609	-	3,3,3	0.36	0	2,2,2	0.80	0
6	EDO	A	609	-	3,3,3	0.41	0	2,2,2	0.38	0
6	EDO	B	606	-	3,3,3	0.75	0	2,2,2	0.11	0
8	SO4	B	607	-	4,4,4	0.32	0	6,6,6	0.51	0
5	NAG	A	606	1	14,14,15	0.48	0	17,19,21	1.96	5 (29%)
5	NAG	B	605	1	14,14,15	0.51	0	17,19,21	2.02	3 (17%)
6	EDO	A	608	-	3,3,3	0.48	0	2,2,2	0.30	0
6	EDO	B	610	-	3,3,3	0.49	0	2,2,2	0.42	0
6	EDO	B	608	-	3,3,3	0.48	0	2,2,2	0.31	0
7	GOL	A	611	-	5,5,5	0.35	0	5,5,5	0.83	0

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	GOL	A	612	-	-	4/4/4/4	-
6	EDO	A	610	-	-	1/1/1/1	-
6	EDO	A	607	-	-	0/1/1/1	-
6	EDO	B	609	-	-	1/1/1/1	-
6	EDO	A	609	-	-	1/1/1/1	-
6	EDO	B	606	-	-	0/1/1/1	-
5	NAG	A	606	1	-	3/6/23/26	0/1/1/1
5	NAG	B	605	1	-	2/6/23/26	0/1/1/1
6	EDO	A	608	-	-	0/1/1/1	-
6	EDO	B	610	-	-	0/1/1/1	-
6	EDO	B	608	-	-	0/1/1/1	-
7	GOL	A	611	-	-	3/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	605	NAG	C1-O5-C5	5.41	119.52	112.19
5	B	605	NAG	O5-C5-C6	4.46	114.20	107.20
5	A	606	NAG	O5-C1-C2	-4.26	104.56	111.29
5	A	606	NAG	C2-N2-C7	3.39	127.72	122.90
5	B	605	NAG	C1-C2-N2	-3.15	105.11	110.49
5	A	606	NAG	C1-O5-C5	3.14	116.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	606	NAG	C8-C7-N2	2.89	120.99	116.10
5	A	606	NAG	O5-C5-C4	2.05	115.82	110.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	612	GOL	O1-C1-C2-C3
7	A	612	GOL	C1-C2-C3-O3
5	B	605	NAG	C4-C5-C6-O6
5	A	606	NAG	C8-C7-N2-C2
5	A	606	NAG	O7-C7-N2-C2
7	A	611	GOL	C1-C2-C3-O3
7	A	612	GOL	O2-C2-C3-O3
5	B	605	NAG	O5-C5-C6-O6
7	A	611	GOL	O2-C2-C3-O3
7	A	612	GOL	O1-C1-C2-O2
6	A	610	EDO	O1-C1-C2-O2
5	A	606	NAG	C3-C2-N2-C7
6	A	609	EDO	O1-C1-C2-O2
7	A	611	GOL	O1-C1-C2-C3
6	B	609	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	612	GOL	1	0
6	A	609	EDO	1	0
5	A	606	NAG	2	0
7	A	611	GOL	8	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	432/454 (95%)	-0.05	15 (3%)	44	47	11, 20, 41, 61	4 (0%)
1	B	434/454 (95%)	0.01	21 (4%)	30	33	13, 21, 41, 55	5 (1%)
All	All	866/908 (95%)	-0.02	36 (4%)	36	39	11, 21, 41, 61	9 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	ILE	5.1
1	B	160	THR	5.1
1	A	141	ARG	5.0
1	B	217	ILE	4.6
1	B	163	LEU	4.6
1	B	215	GLN	4.5
1	A	163	LEU	4.5
1	A	390	SER	4.5
1	B	161	SER	4.4
1	B	218	GLY	4.0
1	A	161	SER	3.9
1	B	387	GLY	3.8
1	A	160	THR	3.7
1	A	343	PRO	3.6
1	B	159	CYS	3.5
1	B	296	ASP	3.2
1	B	572	SER	3.2
1	A	295	HIS	3.1
1	B	391	ILE	3.1
1	A	162	GLY	3.0
1	B	213	GLY	3.0
1	A	388	LEU	2.9
1	B	140	GLN	2.8
1	B	390	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	250	ASN	2.7
1	A	217	ILE	2.5
1	B	162	GLY	2.5
1	A	233	SER	2.5
1	B	295	HIS	2.3
1	A	386	LYS	2.2
1	B	138	PRO	2.2
1	B	141	ARG	2.2
1	A	572	SER	2.1
1	A	539	TYR	2.1
1	B	249	ILE	2.1
1	B	297	GLY	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)

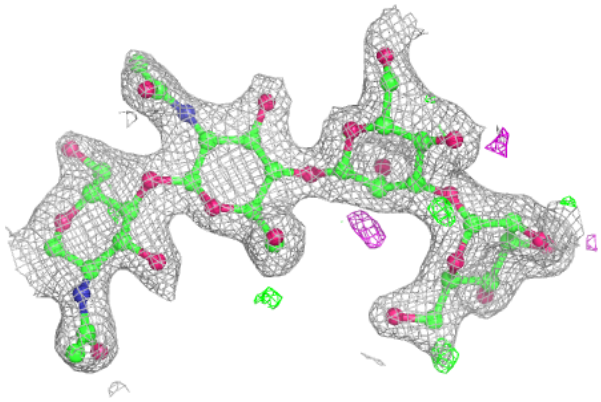
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

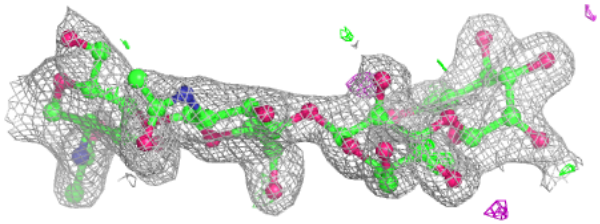
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.80	0.28	52,57,60,61	0
2	BMA	C	3	11/12	0.84	0.23	36,40,43,45	0
2	MAN	C	4	11/12	0.87	0.23	32,36,39,41	0
2	NAG	C	1	14/15	0.88	0.14	36,39,43,47	0
3	NAG	D	1	14/15	0.90	0.21	45,49,54,54	0
2	NAG	C	2	14/15	0.91	0.20	35,36,38,39	0

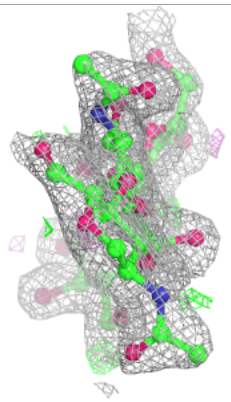
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

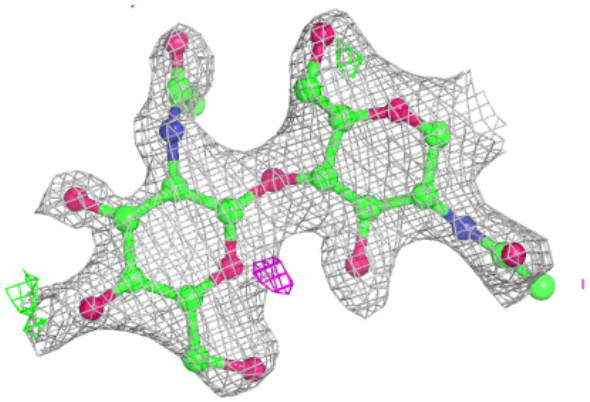


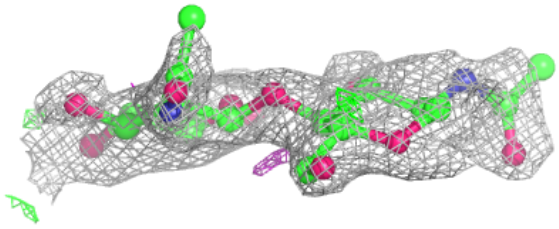


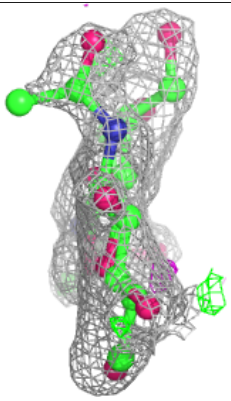


Electron density around Chain D:

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







6.4 Ligands (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
6	EDO	A	609	4/4	0.72	0.14	41,44,44,46	0
5	NAG	B	605	14/15	0.77	0.30	46,51,56,61	0
5	NAG	A	606	14/15	0.80	0.26	38,44,46,53	0
7	GOL	A	612	6/6	0.80	0.13	51,52,53,54	0
6	EDO	B	608	4/4	0.85	0.17	26,29,30,33	0
7	GOL	A	611	6/6	0.87	0.16	33,34,35,35	0
6	EDO	B	610	4/4	0.87	0.12	43,46,46,48	0
6	EDO	A	610	4/4	0.88	0.11	34,35,36,38	0
6	EDO	B	609	4/4	0.93	0.14	35,37,37,40	0
6	EDO	A	607	4/4	0.94	0.12	15,18,18,19	0
6	EDO	B	606	4/4	0.95	0.10	16,17,17,18	0
6	EDO	A	608	4/4	0.95	0.08	28,28,29,30	0
8	SO4	B	602	5/5	0.95	0.18	58,61,62,64	0
8	SO4	B	607	5/5	0.98	0.07	27,29,29,31	0
4	CA	A	601	1/1	0.99	0.03	18,18,18,18	0
4	CA	B	601	1/1	0.99	0.03	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.