Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 05:36 PM JST

PDB ID	:	4X9B
Title	:	Crystal structure of Dscam1 isoform 4.44, N-terminal four Ig domains
Authors	:	Chen, Q.; Yu, Y.; Li, S.A.; Cheng, L.
Deposited on	:	2014-12-11
Resolution	:	2.20 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:

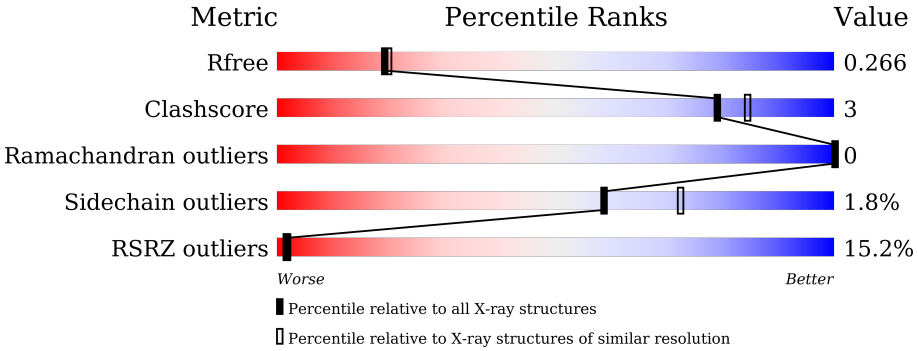
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	397	% 93% 5% •
1	B	397	29% 84% 11% • •
2	C	4	75% 25%
3	D	3	33% 33% 33%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6328 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.

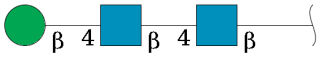
- Molecule 1 is a protein called Down syndrome cell adhesion molecule, isoform 4.44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	3023	1901	523	588	11	0	1	0
1	B	383	2956	1859	512	575	10	0	1	0

- Molecule 2 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.

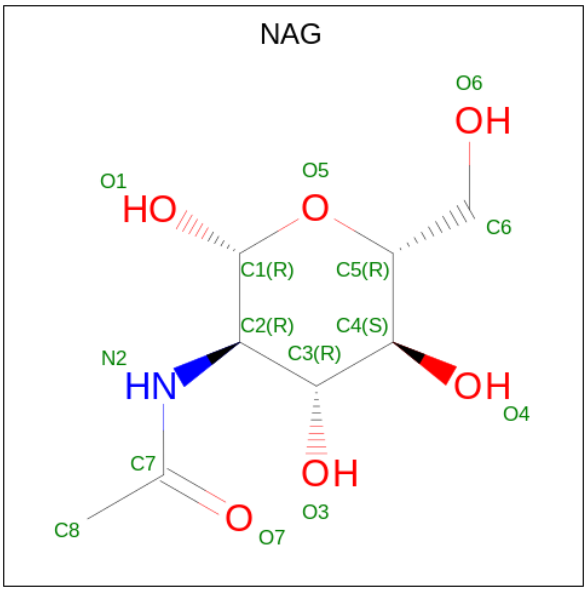
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	50	28	2	20	0	0	0

- 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	D	3	39	22	2	15	0	0	0

- Molecule 4 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		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	2	2	2	0	0

- Molecule 6 is water.

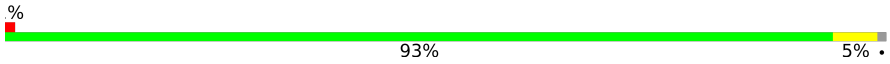
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	174	174	174	0	0
			Total	O		
6	B	56	56	56	0	0

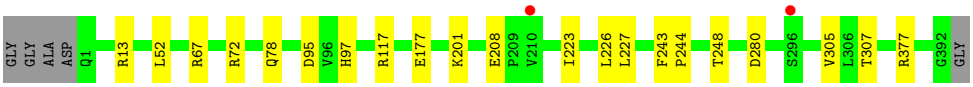
3 Residue-property plots (i)

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: Down syndrome cell adhesion molecule, isoform 4.44

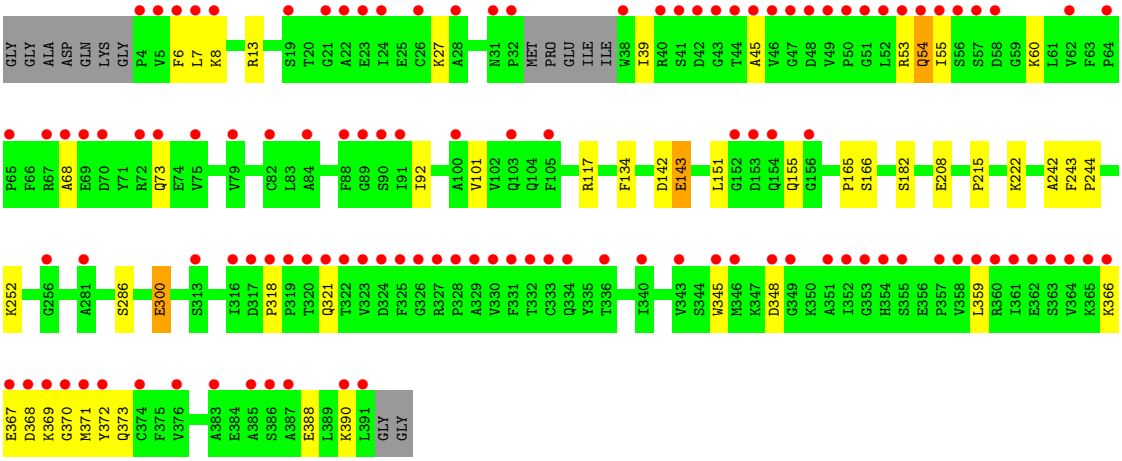
Chain A:





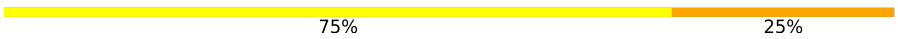
• Molecule 1: Down syndrome cell adhesion molecule, isoform 4.44

Chain B:



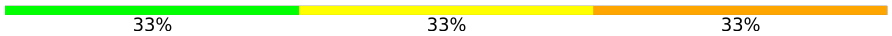
• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain D:



NAG1
NAG2
BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.90Å 59.81Å 89.56Å 90.00° 109.06° 90.00°	Depositor
Resolution (Å)	48.85 – 2.20 48.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.85-2.20) 99.8 (48.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.207 , 0.261 0.213 , 0.266	Depositor DCC
R_{free} test set	1007 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6328	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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, MAN, NA, BMA

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	0.31	0/3086	0.52	0/4184
1	B	0.27	0/3017	0.50	0/4090
All	All	0.29	0/6103	0.51	0/8274

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	155	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	2998	11	1
1	B	2956	0	2921	22	0
2	C	50	0	43	1	1
3	D	39	0	34	2	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	2	0	0	0	0
6	A	174	0	0	2	0
6	B	56	0	0	0	0
All	All	6328	0	6022	34	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 3.

All (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:O	1:B:372:TYR:OH	2.03	0.76
1:B:142:ASP:OD1	1:B:143:GLU:N	2.27	0.67
1:B:117:ARG:NH2	1:B:208:GLU:OE1	2.34	0.60
1:B:92:ILE:O	1:B:373:GLN:NE2	2.36	0.58
1:A:117:ARG:NH1	1:A:208:GLU:OE2	2.37	0.57
3:D:1:NAG:O7	3:D:1:NAG:O3	2.20	0.56
1:B:215:PRO:HA	1:B:242:ALA:HB2	1.93	0.51
1:B:68:ALA:HB3	3:D:1:NAG:H82	1.92	0.51
1:B:151:LEU:HD11	1:B:165:PRO:HA	1.94	0.49
1:A:95:ASP:OD2	1:A:377:ARG:NH1	2.47	0.47
1:A:243:PHE:HA	1:A:244:PRO:C	2.34	0.47
1:B:252:LYS:NZ	1:B:286:SER:O	2.46	0.47
1:B:366:LYS:HG3	1:B:369:LYS:HB3	1.97	0.46
1:A:201:LYS:NZ	6:A:506:HOH:O	2.40	0.45
1:A:13:ARG:HD2	1:A:97:HIS:HB2	1.98	0.45
1:B:388:GLU:OE2	1:B:390:LYS:NZ	2.50	0.45
1:B:54:GLN:HG3	1:B:55:ILE:N	2.33	0.44
1:B:222:LYS:NZ	1:B:300:GLU:OE2	2.45	0.44
1:B:345:TRP:CG	1:B:359:LEU:HD11	2.53	0.44
1:B:318:PRO:HB2	1:B:321:GLN:NE2	2.33	0.43
1:B:348:ASP:OD1	1:B:371:MET:N	2.47	0.43
1:B:369:LYS:HD2	1:B:370:GLY:N	2.34	0.43
1:A:227:LEU:HD12	1:A:307:THR:HB	2.00	0.42
1:B:39:ILE:HG22	1:B:45:ALA:HB2	2.01	0.42
1:A:248:THR:HG21	6:A:618:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:H	1:A:177:GLU:CD	2.22	0.42
1:A:223:ILE:HD11	1:A:305:VAL:HG23	2.01	0.42
1:B:243:PHE:HA	1:B:244:PRO:C	2.39	0.42
1:A:67:ARG:HA	2:C:1:NAG:H83	2.02	0.42
1:B:143:GLU:HG3	1:B:182:SER:HB2	2.02	0.42
1:B:367:GLU:OE1	1:B:367:GLU:N	2.51	0.42
1:B:8:LYS:HB3	1:B:27:LYS:HB2	2.01	0.41
1:A:52:LEU:CD1	1:A:72:ARG:HD3	2.50	0.41
1:B:101:VAL:HG21	1:B:134:PHE:CE2	2.55	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:A:78:GLN:OE1	2:C:4:MAN:O6[2_546]	2.19	0.01

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	391/397 (98%)	384 (98%)	7 (2%)	0	100	100
1	B	380/397 (96%)	363 (96%)	17 (4%)	0	100	100
All	All	771/794 (97%)	747 (97%)	24 (3%)	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	335/335 (100%)	333 (99%)	2 (1%)	86 93
1	B	327/335 (98%)	317 (97%)	10 (3%)	40 51
All	All	662/670 (99%)	650 (98%)	12 (2%)	59 72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	LEU
1	A	280	ASP
1	B	6	PHE
1	B	7	LEU
1	B	13	ARG
1	B	53	ARG
1	B	54	GLN
1	B	60	LYS
1	B	73	GLN
1	B	143	GLU
1	B	166	SER
1	B	300	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	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)

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	C	1	2,1	14,14,15	0.31	0	17,19,21	0.72	0
2	NAG	C	2	2	14,14,15	0.72	1 (7%)	17,19,21	0.56	0
2	BMA	C	3	2	11,11,12	0.61	0	15,15,17	1.03	1 (6%)
2	MAN	C	4	2	11,11,12	0.78	0	15,15,17	1.18	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.73	1 (7%)	17,19,21	0.61	0
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.48	0
3	BMA	D	3	3	11,11,12	0.93	0	15,15,17	1.13	2 (13%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-2.59	1.39	1.43
3	D	1	NAG	C1-C2	2.25	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C1-O5-C5	3.42	116.83	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	BMA	O2-C2-C3	-3.10	103.92	110.14
2	C	3	BMA	C1-O5-C5	2.36	115.39	112.19
2	C	4	MAN	O2-C2-C3	-2.22	105.69	110.14
3	D	3	BMA	O2-C2-C1	2.14	113.53	109.15

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
3	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7

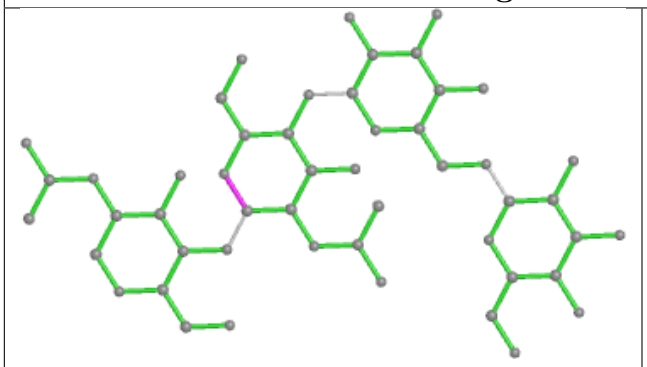
There are no ring outliers.

3 monomers are involved in 4 short contacts:

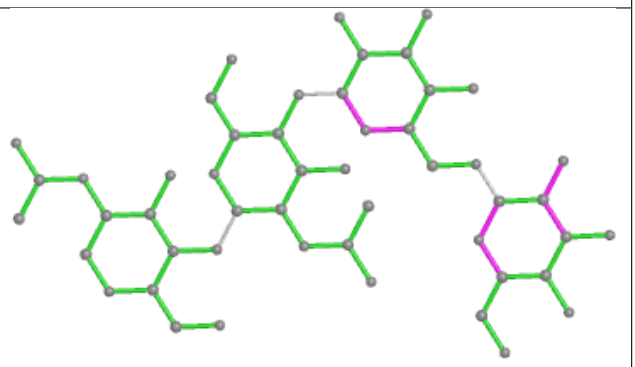
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	2	0
2	C	4	MAN	0	1
2	C	1	NAG	1	0

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

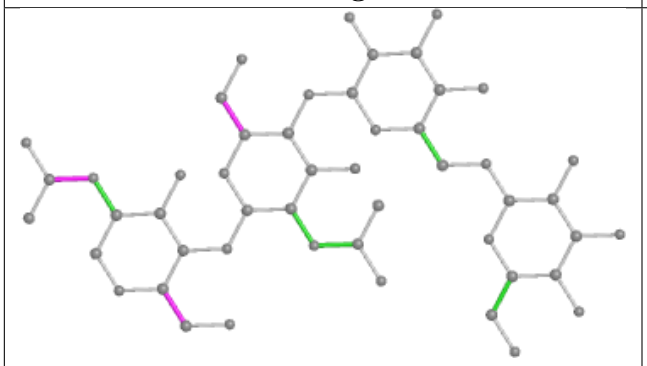
Oligosaccharide Chain C



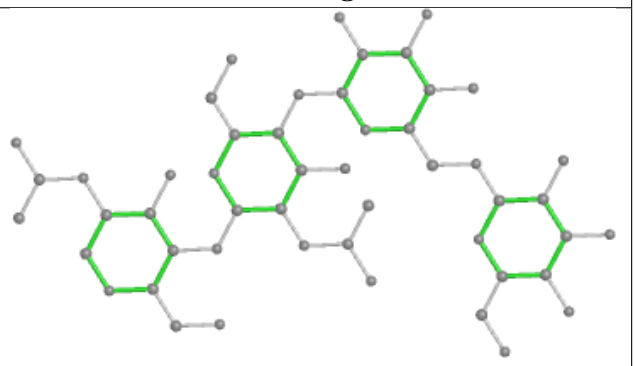
Bond lengths



Bond angles

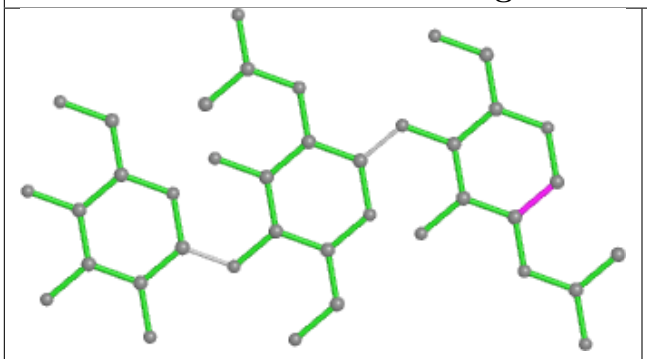


Torsions

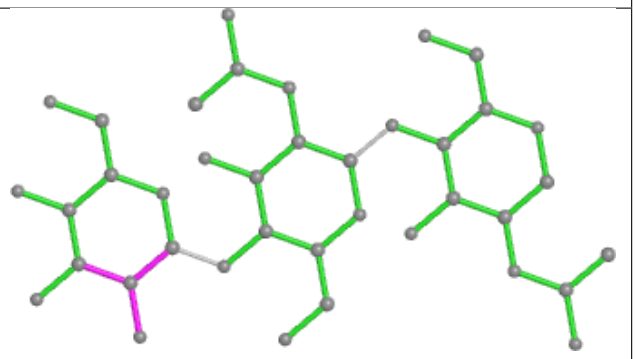


Rings

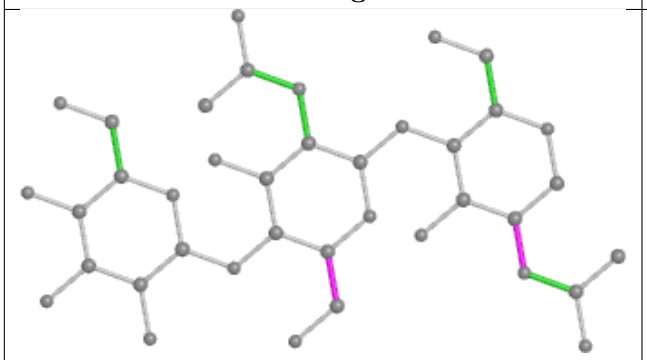
Oligosaccharide Chain D



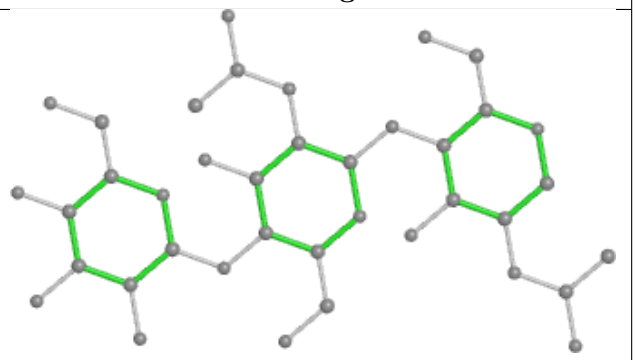
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	405	1	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	B	404	1	14,14,15	0.24	0	17,19,21	0.52	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
4	NAG	A	405	1	-	2/6/23/26	0/1/1/1
4	NAG	B	404	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	NAG	C4-C5-C6-O6
4	A	405	NAG	O5-C5-C6-O6
4	B	404	NAG	C4-C5-C6-O6
4	B	404	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	392/397 (98%)	0.19	2 (0%)	91	90	18, 31, 53, 78	0
1	B	383/397 (96%)	1.73	116 (30%)	0	0	27, 65, 135, 215	0
All	All	775/794 (97%)	0.95	118 (15%)	2	2	18, 40, 113, 215	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	328	PRO	13.3
1	B	355	SER	13.3
1	B	330	VAL	13.0
1	B	325	PHE	11.9
1	B	332	THR	11.7
1	B	329	ALA	9.6
1	B	57	SER	9.5
1	B	357	PRO	9.2
1	B	352	ILE	8.6
1	B	361	ILE	8.3
1	B	354	HIS	8.1
1	B	321	GLN	7.9
1	B	331	PHE	7.8
1	B	362	GLU	7.6
1	B	323	VAL	7.3
1	B	47	GLY	6.9
1	B	54	GLN	6.8
1	B	368	ASP	6.5
1	B	370	GLY	6.5
1	B	55	ILE	6.4
1	B	154	GLN	6.2
1	B	68	ALA	6.1
1	B	320	THR	6.1
1	B	7	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	364	VAL	5.9
1	B	316	ILE	5.9
1	B	358	VAL	5.8
1	B	324	ASP	5.7
1	B	372	TYR	5.7
1	B	44	THR	5.6
1	B	327	ARG	5.6
1	B	333	CYS	5.5
1	B	367	GLU	5.4
1	B	387	ALA	5.3
1	B	326	GLY	5.2
1	B	365	LYS	5.1
1	B	353	GLY	5.0
1	B	318	PRO	5.0
1	B	366	LYS	4.7
1	B	42	ASP	4.7
1	B	56	SER	4.7
1	B	88	PHE	4.6
1	B	391	LEU	4.5
1	B	22	ALA	4.4
1	B	322	THR	4.3
1	B	317	ASP	4.2
1	B	386	SER	4.2
1	B	390	LYS	4.2
1	B	336	THR	4.1
1	B	105	PHE	4.1
1	B	31	ASN	4.1
1	B	64	PRO	4.0
1	B	363	SER	4.0
1	B	72	ARG	3.9
1	B	82	CYS	3.9
1	B	67	ARG	3.9
1	B	153	ASP	3.8
1	B	340	ILE	3.8
1	B	313[A]	SER	3.7
1	B	79	VAL	3.7
1	B	49	VAL	3.6
1	B	28	ALA	3.6
1	B	43	GLY	3.6
1	B	38	TRP	3.5
1	A	210	VAL	3.5
1	B	50	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	359	LEU	3.5
1	B	5	VAL	3.5
1	B	69	GLU	3.4
1	B	360	ARG	3.4
1	B	152	GLY	3.4
1	B	52	LEU	3.4
1	B	156	GLY	3.3
1	B	90	SER	3.3
1	B	89	GLY	3.2
1	B	4	PRO	3.2
1	B	345	TRP	3.1
1	B	349	GLY	3.1
1	B	369	LYS	3.1
1	B	48	ASP	3.0
1	B	385	ALA	3.0
1	B	46	VAL	3.0
1	B	348	ASP	2.9
1	B	84	ALA	2.9
1	B	75	VAL	2.9
1	B	374	CYS	2.9
1	B	319	PRO	2.8
1	B	26	CYS	2.8
1	B	24	ILE	2.8
1	B	371	MET	2.7
1	B	343	VAL	2.7
1	B	51	GLY	2.7
1	B	8	LYS	2.6
1	B	21	GLY	2.6
1	B	346	MET	2.6
1	B	62	VAL	2.5
1	B	45	ALA	2.5
1	B	91	ILE	2.5
1	B	334	GLN	2.4
1	B	65	PRO	2.4
1	B	73	GLN	2.4
1	B	19	SER	2.4
1	B	70	ASP	2.3
1	B	351	ALA	2.3
1	B	58	ASP	2.2
1	B	6	PHE	2.2
1	B	23	GLU	2.2
1	B	53	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	32	PRO	2.2
1	B	383	ALA	2.2
1	B	100	ALA	2.1
1	A	296	SER	2.1
1	B	41	SER	2.1
1	B	40	ARG	2.1
1	B	103	GLN	2.1
1	B	376	VAL	2.1
1	B	256	GLY	2.1
1	B	281	ALA	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)

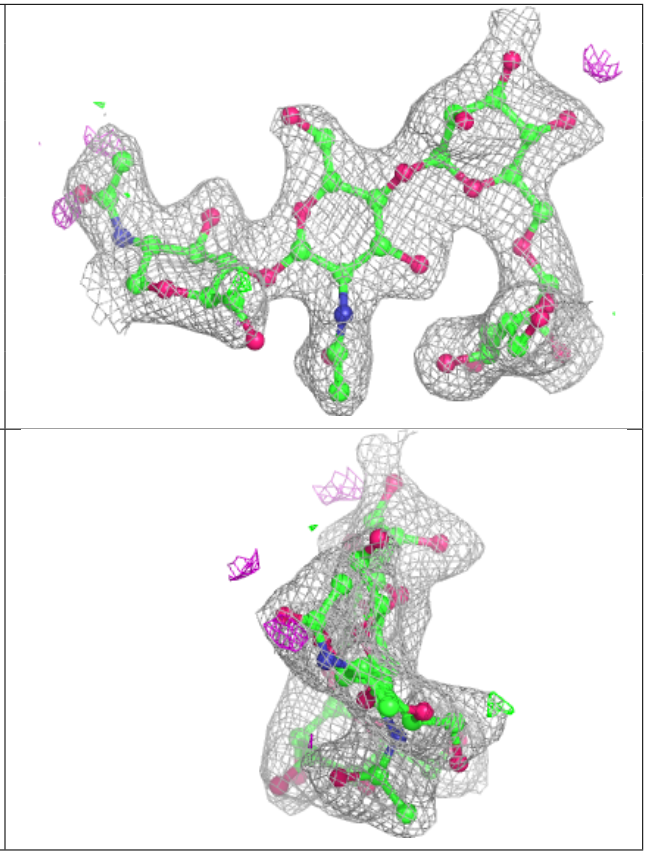
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

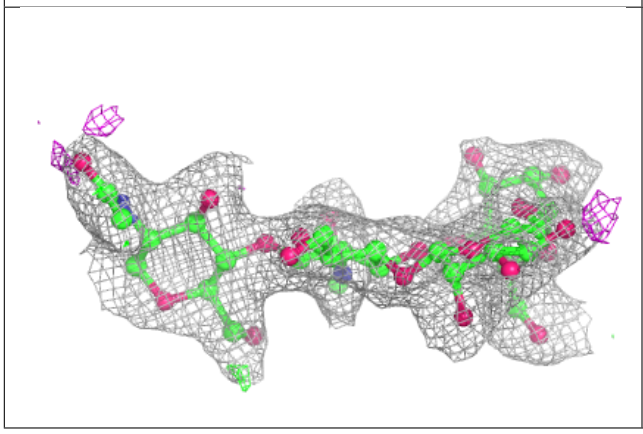
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	D	3	11/12	0.62	0.32	94,109,118,122	0
3	NAG	D	2	14/15	0.66	0.37	112,126,149,149	0
3	NAG	D	1	14/15	0.72	0.31	94,102,120,123	0
2	NAG	C	1	14/15	0.91	0.16	24,31,41,65	0
2	MAN	C	4	11/12	0.93	0.15	23,38,49,56	0
2	BMA	C	3	11/12	0.93	0.14	36,45,49,61	0
2	NAG	C	2	14/15	0.94	0.12	34,42,47,56	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:

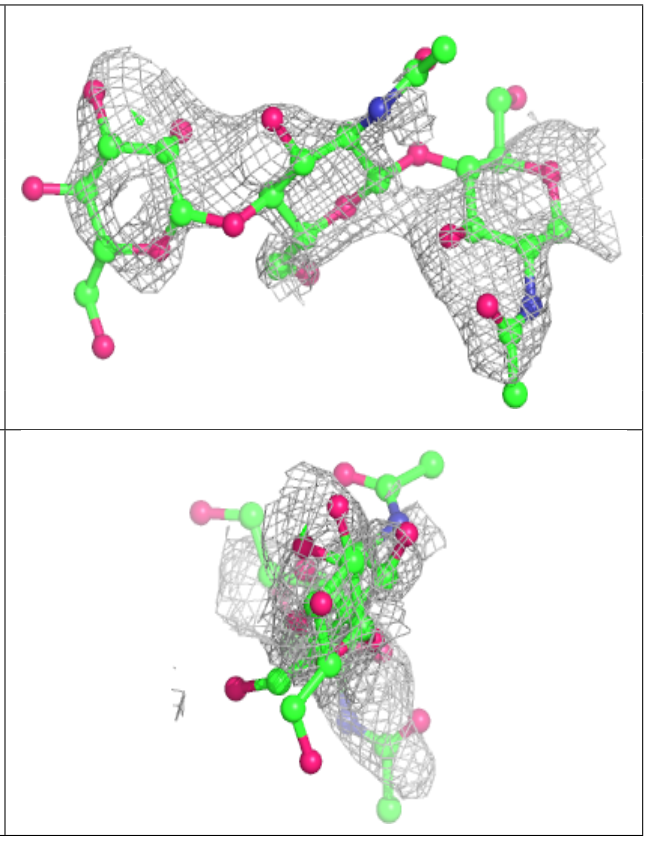
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

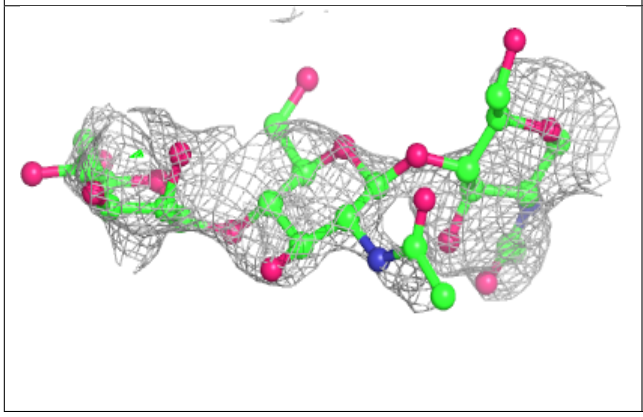




Electron density around Chain D:

$2mF_o$-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, 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
5	NA	A	406	1/1	0.83	0.19	66,66,66,66	0
4	NAG	B	404	14/15	0.84	0.19	52,61,77,77	0
4	NAG	A	405	14/15	0.89	0.23	53,61,84,93	0
5	NA	A	407	1/1	0.90	0.14	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.