

wwPDB X-ray Structure Validation Summary Report (i)

Oct 30, 2023 – 05:28 PM JST

PDB ID : 4X9H

Title: Crystal structure of Dscam1 isoform 8.4, N-terminal four Ig domains

Authors : Chen, Q. Deposited on : 2014-12-11

Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

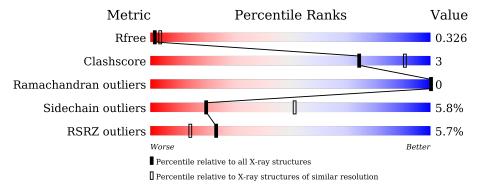
Validation Pipeline (wwPDB-VP) : 2.36

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 2.95 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	y of chain
1	A	400	87%	10%
1	В	400	7%	12% •••
2	С	4	10	00%
2	D	4	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:

	V -				Geometry	Clashes	Electron density
2	MAN	С	4	-	-	-	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6231 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 AP.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	391	Total 3052	C 1925	N 530	O 583	S 1.4	0	2	0
			3032	1923	330	989	14			
1	B	392	Total	\mathbf{C}	Ν	Ο	S	0	1	0
1	D	332	3048	1923	528	583	14		1	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q0E9L0
A	-2	GLY	-	expression tag	UNP Q0E9L0
В	-3	GLY	-	expression tag	UNP Q0E9L0
В	-2	GLY	-	expression tag	UNP Q0E9L0

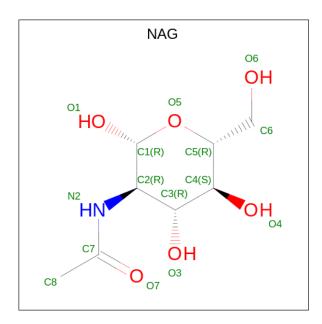
• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
9	С	4	Total	С	N	О	0	0	0
		4	50	28	2	20	0	U	U
9	D	4	Total	С	N	О	0	0	0
2	$\begin{array}{c c} 2 & D \end{array}$	4	50	28	2	20	U	U	U

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





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

• Molecule 4 is water.

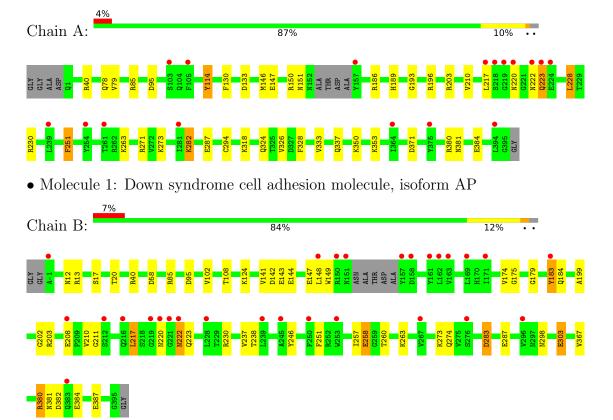
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	В	2	Total O 2 2	0	0



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 AP



• 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: 100%

• 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 D: 50% 50%







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	95.22Å 60.95Å 92.35Å	Depositor
a, b, c, α , β , γ	90.00° 93.56° 90.00°	Depositor
Resolution (Å)	47.52 - 2.95	Depositor
Resolution (A)	47.52 - 2.95	EDS
% Data completeness	99.3 (47.52-2.95)	Depositor
(in resolution range)	99.3 (47.52-2.95)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.93 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.272 , 0.324	Depositor
10, 10 free	0.275 , 0.326	DCC
R_{free} test set	1149 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.25 , 10.4	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6231	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MAN, NAG, 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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.23	0/3119	0.46	0/4228	
1	В	0.24	0/3115	0.46	0/4223	
All	All	0.23	0/6234	0.46	0/8451	

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 maintain group or atoms of a sidechain that are expected to be planar.

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	ASN	Peptide
1	A	223	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	3052	0	3025	18	0
1	В	3048	0	3022	25	0
2	С	50	0	43	0	0
2	D	50	0	43	0	0
3	A	14	0	13	0	0
3	В	14	0	13	0	0
4	A	1	0	0	0	0
4	В	2	0	0	0	0
All	All	6231	0	6159	40	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 3.

The worst 5 of 40 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:133:ASP:O	1:B:220:ASN:ND2	2.28	0.67
1:A:271:ARG:NH1	1:A:282:LYS:O	2.30	0.65
1:B:246:TYR:O	1:B:298:ASN:ND2	2.32	0.63
1:B:251:PHE:O	1:B:274:GLN:NE2	2.32	0.62
1:B:183:TYR:O	1:B:202:GLY:N	2.35	0.59

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	389/400 (97%)	370 (95%)	19 (5%)	0	100	100
1	В	389/400 (97%)	366 (94%)	23 (6%)	0	100	100
All	All	778/800 (97%)	736 (95%)	42 (5%)	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	Rotameric Outliers		Percentiles		
1	A	337/338 (100%)	320 (95%)	17 (5%)	24	57		
1	В	336/338 (99%)	314 (94%)	22 (6%)	17	46		
All	All	673/676 (100%)	634 (94%)	39 (6%)	20	51		

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	230	ARG
1	В	367	VAL
1	В	258	GLU
1	В	283	ASP
1	В	384	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	В	225	HIS

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)

8 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	Chain Res	Link	Вс	ond leng	ths	Bond angles		
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	С	1	1,2	14,14,15	0.65	1 (7%)	17,19,21	0.54	0
2	NAG	С	2	2	14,14,15	0.60	1 (7%)	17,19,21	0.57	0
2	BMA	С	3	2	11,11,12	0.72	0	15,15,17	1.92	4 (26%)
2	MAN	С	4	2	11,11,12	0.72	1 (9%)	15,15,17	1.78	4 (26%)
2	NAG	D	1	1,2	14,14,15	0.31	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.40	0
2	BMA	D	3	2	11,11,12	0.82	0	15,15,17	1.27	2 (13%)
2	MAN	D	4	2	11,11,12	1.00	1 (9%)	15,15,17	1.89	3 (20%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	D	4	MAN	O5-C5	2.42	1.48	1.43
2	С	1	NAG	O5-C1	-2.35	1.40	1.43
2	С	4	MAN	C1-C2	2.19	1.57	1.52
2	С	2	NAG	O5-C1	-2.11	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	D	4	MAN	C1-O5-C5	4.76	118.65	112.19
2	С	4	MAN	C1-O5-C5	4.21	117.90	112.19
2	С	3	BMA	C1-O5-C5	4.20	117.89	112.19
2	С	3	BMA	O5-C1-C2	4.05	117.02	110.77
2	С	4	MAN	O5-C1-C2	3.78	116.60	110.77

There are no chirality outliers.

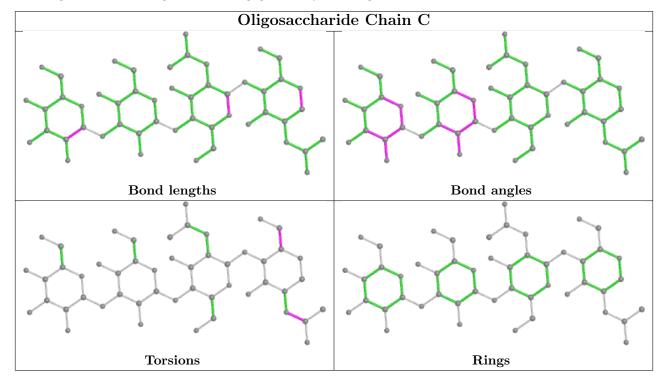
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	1	NAG	C8-C7-N2-C2
2	С	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	С	1	NAG	O5-C5-C6-O6

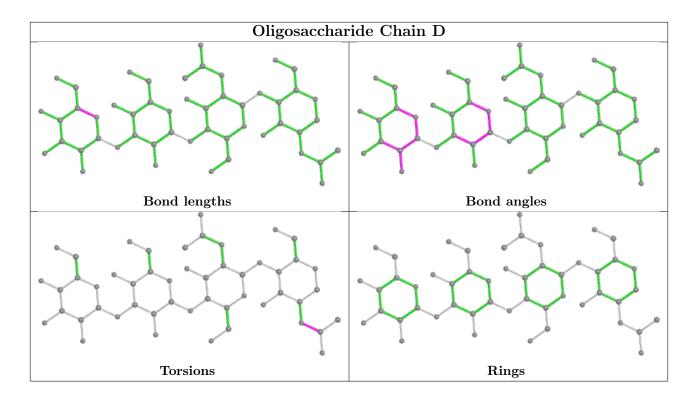
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry (i)

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	405	1	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	В	405	1	14,14,15	0.27	0	17,19,21	0.41	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
3	NAG	A	405	1	-	1/6/23/26	0/1/1/1
3	NAG	В	405	1	-	0/6/23/26	0/1/1/1



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	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, 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			$OWAB(Å^2)$	Q < 0.9	
1	A	391/400 (97%)	0.30	17 (4%) 35 22	48, 71, 97, 118	0
1	В	392/400 (98%)	0.48	28 (7%) 16 9	52, 77, 111, 150	0
All	All	783/800 (97%)	0.39	45 (5%) 23 14	48, 73, 108, 150	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	220	ASN	8.6
1	В	161	TYR	5.8
1	В	216	GLN	5.0
1	В	250	PHE	4.8
1	В	150	ARG	4.8

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	$\operatorname{B-factors}({\c A}^2)$	Q < 0.9
2	BMA	С	3	11/12	0.50	0.37	120,128,137,144	0
2	MAN	С	4	11/12	0.66	0.58	115,137,142,142	0
2	MAN	D	4	11/12	0.68	0.35	78,84,91,93	0
2	NAG	С	2	14/15	0.85	0.22	81,93,106,114	0
2	BMA	D	3	11/12	0.86	0.17	73,80,86,87	0

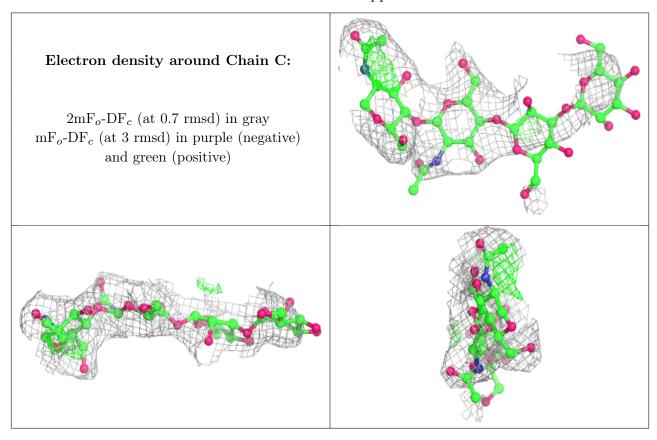
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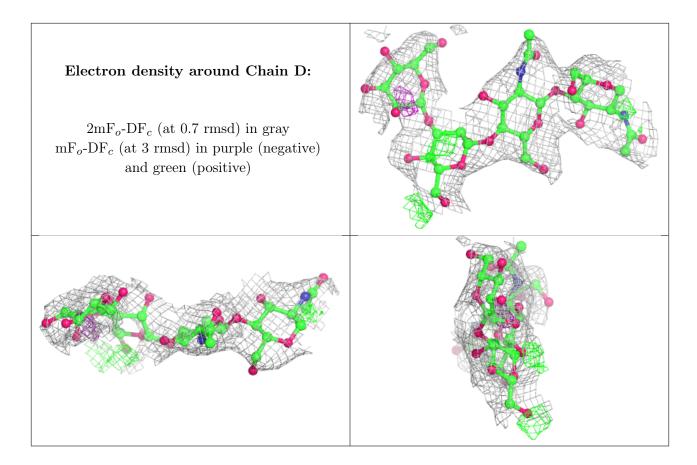
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	NAG	D	1	14/15	0.89	0.22	63,72,77,83	0
2	NAG	С	1	14/15	0.90	0.18	54,66,74,76	0
2	NAG	D	2	14/15	0.92	0.17	73,78,82,85	0

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.







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.

$ box{ ho}$	/Iol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
	3	NAG	A	405	14/15	0.77	0.34	83,88,92,94	0
	3	NAG	В	405	14/15	0.80	0.31	106,117,121,121	0

6.5 Other polymers (i)

There are no such residues in this entry.

