



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2024 – 08:22 AM EDT

PDB ID : 5UV6  
Title : Crystal structure of human Opioid Binding Protein/Cell Adhesion Molecule Like (OPCML)  
Authors : Birtley, J.R.; Stern, L.J.; Gabra, H.; Zanini, E.  
Deposited on : 2017-02-19  
Resolution : 2.65 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

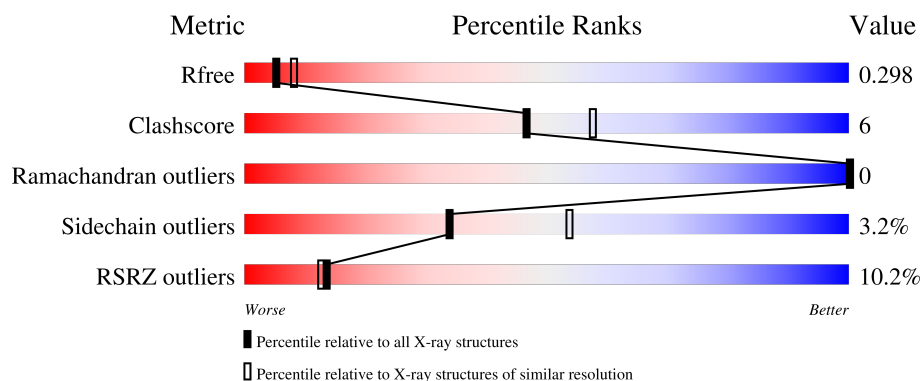
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	286	
1	B	286	
2	C	3	
2	D	3	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4350 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.

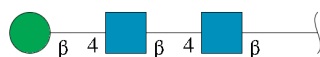
- Molecule 1 is a protein called Opioid-binding protein/cell adhesion molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2065	1294	351	408	12			
1	B	274	Total	C	N	O	S	0	0	0
			2111	1323	361	415	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	317	ALA	-	expression tag	UNP Q14982
A	318	LEU	-	expression tag	UNP Q14982
A	319	VAL	-	expression tag	UNP Q14982
A	320	PRO	-	expression tag	UNP Q14982
A	321	ARG	-	expression tag	UNP Q14982
B	317	ALA	-	expression tag	UNP Q14982
B	318	LEU	-	expression tag	UNP Q14982
B	319	VAL	-	expression tag	UNP Q14982
B	320	PRO	-	expression tag	UNP Q14982
B	321	ARG	-	expression tag	UNP Q14982

- Molecule 2 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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

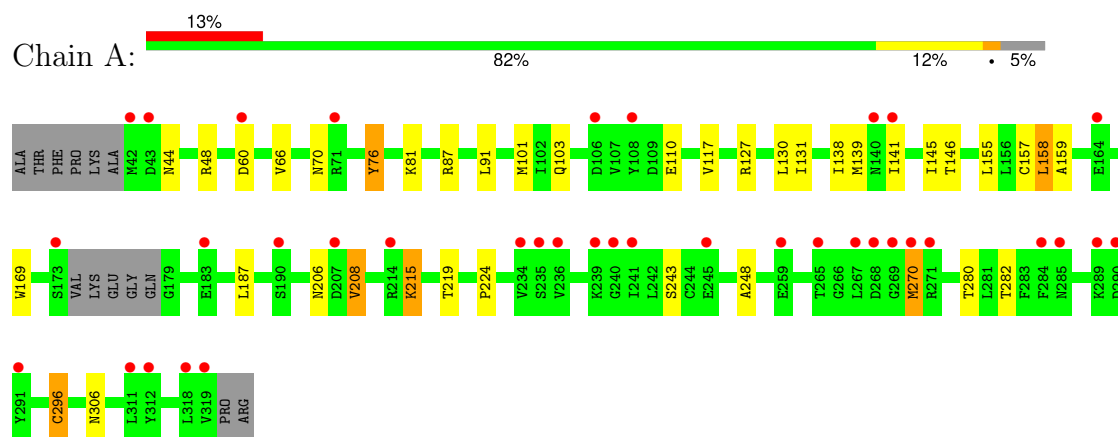
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	23	Total	O	0	0
			23	23		

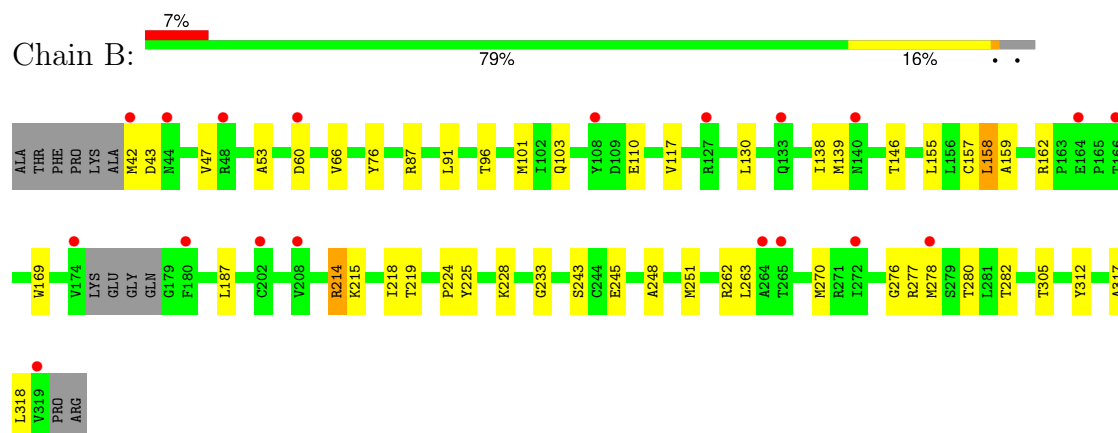
### 3 Residue-property plots [i](#)

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.

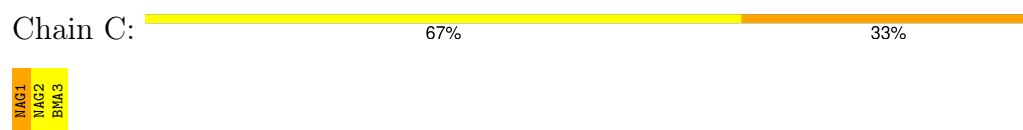
- Molecule 1: Opioid-binding protein/cell adhesion molecule




- Molecule 1: Opioid-binding protein/cell adhesion molecule



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



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

Chain D:  100%

MAG1  
MAG2  
BGLA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.56Å 93.56Å 262.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.44 – 2.65 18.44 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.2 (18.44-2.65) 80.4 (18.44-2.65)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.284 , 0.300 0.281 , 0.298	Depositor DCC
$R_{free}$ test set	1805 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4629e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: BMA, NAG

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	0.36	1/2102 (0.0%)	0.56	0/2871
1	B	0.34	0/2148	0.56	0/2924
All	All	0.35	1/4250 (0.0%)	0.56	0/5795

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	CYS	CB-SG	-5.70	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	1993	22	0
1	B	2111	0	2083	26	0
2	C	39	0	34	1	0
2	D	39	0	34	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	17	0	0	0	0
4	B	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4350	0	4196	48	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 6.

All (48) 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:215:LYS:HB3	1:A:215:LYS:NZ	2.05	0.71
1:B:110:GLU:OE2	1:B:162:ARG:NH2	2.27	0.67
1:A:270:MET:HA	1:A:282:THR:O	1.93	0.67
1:B:66:VAL:HG23	1:B:117:VAL:HG12	1.76	0.66
1:B:228:LYS:HB2	1:B:245:GLU:HB3	1.77	0.66
1:B:139:MET:HB2	1:B:158:LEU:HD12	1.81	0.62
1:B:251:MET:SD	1:B:277:ARG:HG3	2.39	0.62
1:B:270:MET:HA	1:B:282:THR:O	1.99	0.61
1:A:296:CYS:O	1:A:306:ASN:HA	2.00	0.61
1:B:224:PRO:HB3	1:B:248:ALA:HB2	1.83	0.60
1:B:243:SER:HB2	1:B:280:THR:HG22	1.85	0.59
1:A:139:MET:HB2	1:A:158:LEU:HD12	1.85	0.56
1:A:127:ARG:HH11	1:A:127:ARG:HG2	1.72	0.55
1:A:215:LYS:HB3	1:A:215:LYS:HZ3	1.71	0.55
1:A:224:PRO:HB3	1:A:248:ALA:HB2	1.90	0.54
1:B:263:LEU:HB3	1:B:270:MET:HE3	1.88	0.54
1:B:263:LEU:HB3	1:B:270:MET:CE	2.38	0.54
1:A:66:VAL:HG23	1:A:117:VAL:HG12	1.91	0.52
1:A:91:LEU:HD11	1:A:101:MET:HB2	1.92	0.52
1:B:91:LEU:HD11	1:B:101:MET:HB2	1.92	0.52
1:B:262:ARG:HG3	1:B:263:LEU:N	2.25	0.50
1:B:146:THR:HG22	1:B:219:THR:OG1	2.10	0.50
1:A:138:ILE:HD13	1:A:159:ALA:HB2	1.93	0.49
1:B:157:CYS:HB2	1:B:169:TRP:CZ2	2.48	0.49
1:A:243:SER:HB2	1:A:280:THR:HG22	1.94	0.48
1:A:110:GLU:HG3	1:A:130:LEU:O	2.13	0.48
1:A:146:THR:HG22	1:A:219:THR:OG1	2.14	0.48
1:A:157:CYS:HB2	1:A:169:TRP:CZ2	2.49	0.47
1:B:317:ALA:C	1:B:318:LEU:HD12	2.34	0.47
1:B:87:ARG:O	1:B:103:GLN:HG2	2.15	0.46
1:B:276:GLY:O	1:B:278:MET:N	2.47	0.46
1:A:206:ASN:OD1	1:A:208:VAL:HG13	2.16	0.45
1:A:70:ASN:HD22	2:C:1:NAG:H83	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HD12	1:A:157:CYS:SG	2.57	0.44
1:A:155:LEU:HD12	1:A:187:LEU:HD23	1.98	0.44
1:B:155:LEU:HD12	1:B:187:LEU:HD23	1.98	0.44
1:A:141:ILE:HD11	1:A:169:TRP:CH2	2.53	0.43
1:A:44:ASN:HB3	1:A:131:ILE:HD12	2.00	0.42
1:B:155:LEU:HD11	1:B:218:ILE:HD11	2.01	0.42
1:B:214:ARG:NH2	1:B:215:LYS:HG2	2.35	0.42
1:A:87:ARG:O	1:A:103:GLN:HG2	2.20	0.41
1:A:76:TYR:CZ	1:A:81:LYS:HB2	2.55	0.41
1:B:47:VAL:HG21	1:B:53:ALA:HA	2.01	0.41
1:B:110:GLU:HG3	1:B:130:LEU:O	2.20	0.41
1:B:214:ARG:NE	1:B:214:ARG:HA	2.35	0.41
1:B:233:GLY:HA2	1:B:312:TYR:O	2.21	0.41
1:B:138:ILE:HD13	1:B:159:ALA:HB2	2.03	0.40
1:B:225:TYR:HA	1:B:305:THR:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	269/286 (94%)	258 (96%)	11 (4%)	0	100	100
1	B	270/286 (94%)	256 (95%)	14 (5%)	0	100	100
All	All	539/572 (94%)	514 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	227/250 (91%)	219 (96%)	8 (4%)	31	50
1	B	238/250 (95%)	231 (97%)	7 (3%)	37	58
All	All	465/500 (93%)	450 (97%)	15 (3%)	34	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	60	ASP
1	A	76	TYR
1	A	145	ILE
1	A	158	LEU
1	A	208	VAL
1	A	215	LYS
1	A	270	MET
1	B	42	MET
1	B	43	ASP
1	B	60	ASP
1	B	76	TYR
1	B	96	THR
1	B	158	LEU
1	B	214	ARG

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

Mol	Chain	Res	Type
1	A	44	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	1.94	4 (28%)	17,19,21	1.27	2 (11%)
2	NAG	C	2	2	14,14,15	1.96	4 (28%)	17,19,21	1.14	2 (11%)
2	BMA	C	3	2	11,11,12	1.69	2 (18%)	15,15,17	1.18	3 (20%)
2	NAG	D	1	2,1	14,14,15	1.85	4 (28%)	17,19,21	1.06	1 (5%)
2	NAG	D	2	2	14,14,15	1.93	4 (28%)	17,19,21	1.61	4 (23%)
2	BMA	D	3	2	11,11,12	1.92	3 (27%)	15,15,17	1.49	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	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	BMA	O5-C1	4.92	1.52	1.43
2	C	3	BMA	O5-C1	4.54	1.51	1.43
2	C	1	NAG	O5-C1	4.12	1.50	1.43
2	C	2	NAG	O5-C1	3.98	1.50	1.43
2	C	2	NAG	C7-N2	3.93	1.47	1.34
2	D	1	NAG	O5-C1	3.90	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C7-N2	3.84	1.46	1.34
2	C	1	NAG	C7-N2	3.83	1.46	1.34
2	D	2	NAG	O5-C1	3.79	1.50	1.43
2	D	1	NAG	C7-N2	3.73	1.46	1.34
2	D	3	BMA	O5-C5	2.74	1.48	1.43
2	D	2	NAG	C2-N2	2.66	1.50	1.46
2	C	2	NAG	C2-N2	2.55	1.50	1.46
2	C	1	NAG	C2-N2	2.41	1.50	1.46
2	C	1	NAG	O5-C5	2.29	1.47	1.43
2	D	1	NAG	C2-N2	2.29	1.50	1.46
2	D	2	NAG	O5-C5	2.26	1.47	1.43
2	D	3	BMA	C2-C3	-2.19	1.49	1.52
2	C	3	BMA	O5-C5	2.07	1.47	1.43
2	C	2	NAG	O5-C5	2.06	1.47	1.43
2	D	1	NAG	O5-C5	2.04	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C4-C3-C2	4.03	116.93	111.02
2	D	3	BMA	C1-O5-C5	-3.55	107.43	112.19
2	C	2	NAG	C8-C7-N2	2.59	120.42	116.12
2	D	3	BMA	C3-C4-C5	2.40	114.59	110.23
2	D	2	NAG	O4-C4-C3	-2.40	104.73	110.38
2	D	2	NAG	C8-C7-N2	2.39	120.09	116.12
2	C	3	BMA	C1-O5-C5	-2.36	109.03	112.19
2	D	1	NAG	C4-C3-C2	2.34	114.45	111.02
2	C	3	BMA	C1-C2-C3	2.18	112.83	109.64
2	C	1	NAG	C1-C2-N2	-2.18	107.00	110.43
2	C	3	BMA	C2-C3-C4	2.16	114.67	110.86
2	C	1	NAG	C8-C7-N2	2.14	119.67	116.12
2	D	2	NAG	C2-N2-C7	-2.13	120.05	122.90
2	C	2	NAG	C2-N2-C7	-2.13	120.05	122.90

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

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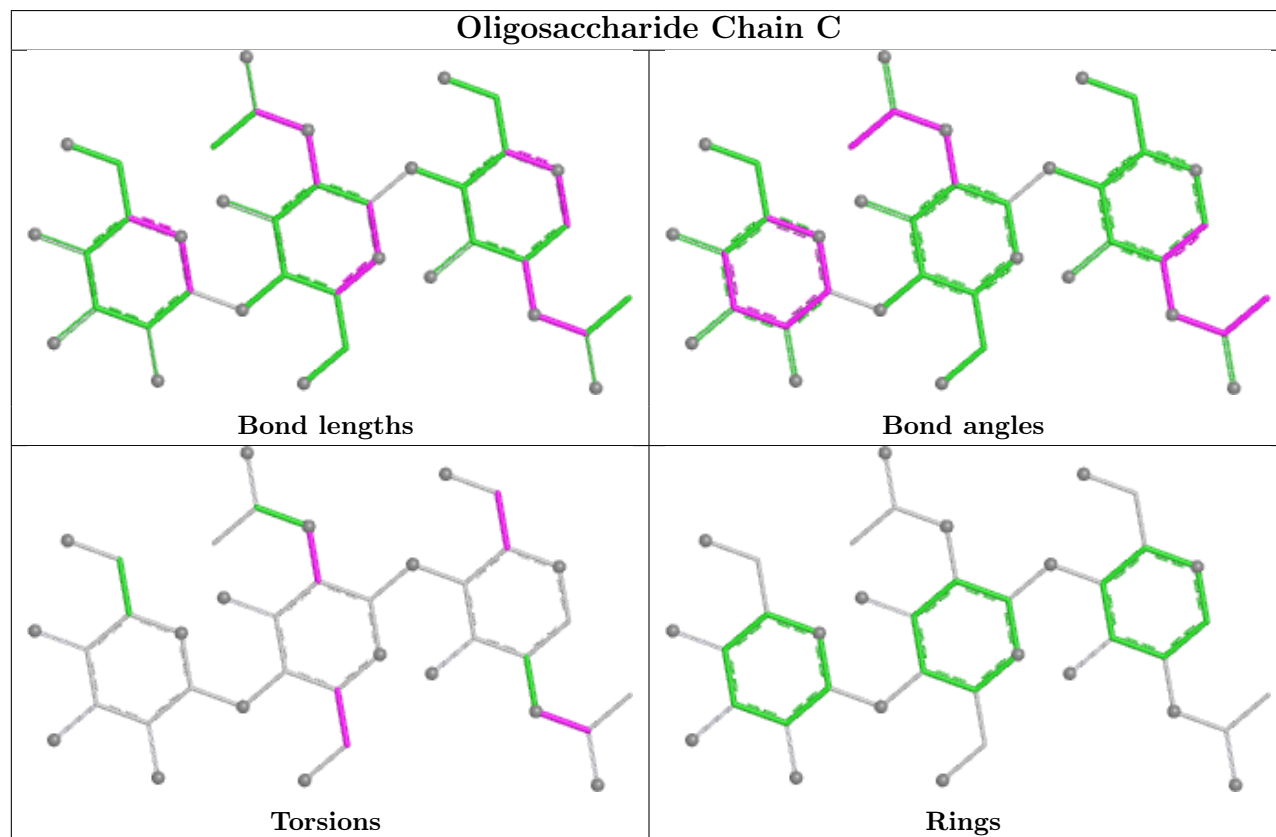
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7

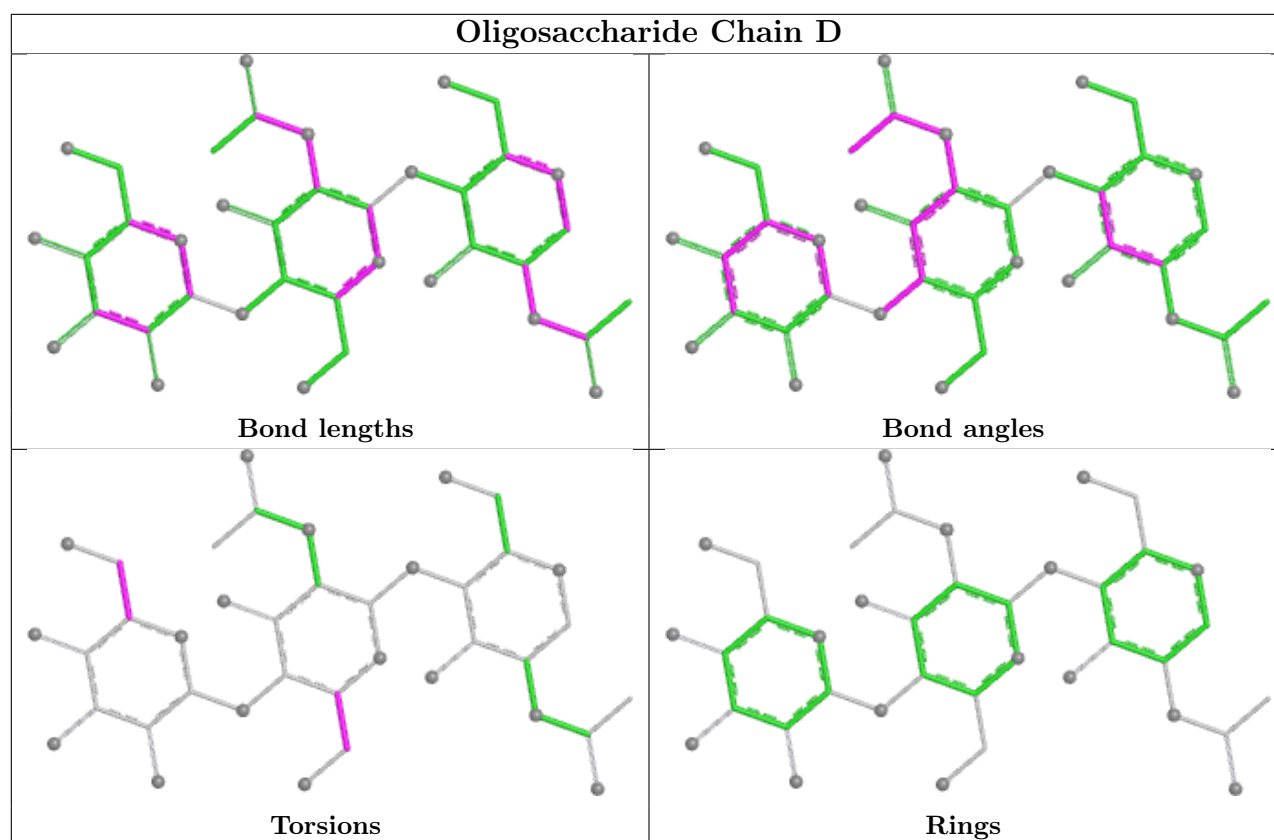
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.





## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
3	NAG	A	1004	1	14,14,15	2.15	4 (28%)	17,19,21	1.24	2 (11%)
3	NAG	B	2005	1	14,14,15	2.13	4 (28%)	17,19,21	1.00	1 (5%)
3	NAG	A	1005	1	14,14,15	2.03	5 (35%)	17,19,21	1.36	4 (23%)
3	NAG	B	2004	1	14,14,15	1.88	4 (28%)	17,19,21	1.24	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
3	NAG	A	1004	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1005	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2004	1	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	NAG	O5-C1	4.56	1.51	1.43
3	B	2005	NAG	O5-C1	4.54	1.51	1.43
3	A	1004	NAG	C7-N2	4.46	1.48	1.34
3	A	1005	NAG	O5-C1	4.23	1.50	1.43
3	B	2005	NAG	C7-N2	4.17	1.47	1.34
3	B	2004	NAG	O5-C1	4.04	1.50	1.43
3	B	2004	NAG	C7-N2	3.63	1.46	1.34
3	A	1005	NAG	C7-N2	3.61	1.46	1.34
3	B	2005	NAG	C2-N2	3.12	1.51	1.46
3	A	1005	NAG	C2-N2	2.99	1.51	1.46
3	A	1004	NAG	C2-N2	2.99	1.51	1.46
3	A	1005	NAG	O5-C5	2.36	1.48	1.43
3	B	2005	NAG	O5-C5	2.32	1.48	1.43
3	A	1004	NAG	O5-C5	2.24	1.47	1.43
3	B	2004	NAG	C2-N2	2.22	1.49	1.46
3	A	1005	NAG	C3-C2	-2.07	1.48	1.52
3	B	2004	NAG	O5-C5	2.01	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	NAG	C2-N2-C7	-3.32	118.45	122.90
3	B	2004	NAG	C2-N2-C7	-2.76	119.20	122.90
3	A	1004	NAG	C8-C7-N2	2.65	120.52	116.12
3	A	1005	NAG	O5-C1-C2	-2.54	107.36	111.29
3	A	1005	NAG	C1-C2-N2	2.40	114.22	110.43
3	B	2005	NAG	C8-C7-N2	2.39	120.09	116.12
3	A	1005	NAG	C6-C5-C4	-2.22	107.57	113.02
3	A	1005	NAG	C4-C3-C2	-2.17	107.84	111.02
3	B	2004	NAG	C8-C7-N2	2.06	119.53	116.12

There are no chirality outliers.

All (6) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	1005	NAG	O5-C5-C6-O6
3	A	1005	NAG	C4-C5-C6-O6
3	A	1004	NAG	C4-C5-C6-O6
3	A	1004	NAG	O5-C5-C6-O6
3	A	1005	NAG	C1-C2-N2-C7
3	A	1005	NAG	C3-C2-N2-C7

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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/286 (95%)	0.75	37 (13%) 8 7	46, 84, 131, 164	0
1	B	274/286 (95%)	0.60	19 (6%) 24 22	45, 83, 120, 142	0
All	All	547/572 (95%)	0.68	56 (10%) 13 13	45, 84, 125, 164	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	VAL	4.9
1	B	42	MET	4.7
1	B	108	TYR	4.3
1	A	42	MET	4.2
1	B	60	ASP	4.0
1	A	291	TYR	3.8
1	A	234	VAL	3.6
1	A	289	LYS	3.4
1	A	240	GLY	3.3
1	A	239	LYS	3.3
1	A	311	LEU	3.3
1	A	312	TYR	3.2
1	B	48	ARG	3.1
1	A	71	ARG	3.0
1	A	108	TYR	2.9
1	A	318	LEU	2.8
1	A	60	ASP	2.8
1	A	268	ASP	2.8
1	A	285	ASN	2.8
1	A	207	ASP	2.7
1	B	265	THR	2.6
1	B	166	THR	2.6
1	A	43	ASP	2.6
1	A	141	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	270	MET	2.5
1	B	127	ARG	2.5
1	B	140	ASN	2.5
1	A	106	ASP	2.5
1	B	264	ALA	2.5
1	B	164	GLU	2.4
1	A	290	ASP	2.4
1	A	190	SER	2.4
1	B	133	GLN	2.4
1	A	319	VAL	2.3
1	A	173	SER	2.3
1	A	245	GLU	2.3
1	B	278	MET	2.3
1	A	140	ASN	2.3
1	A	214	ARG	2.3
1	B	202	CYS	2.3
1	A	236	VAL	2.3
1	B	319	VAL	2.3
1	A	267	LEU	2.3
1	A	269	GLY	2.2
1	A	235	SER	2.2
1	A	164	GLU	2.2
1	A	284	PHE	2.2
1	B	180	PHE	2.2
1	B	208	VAL	2.1
1	A	259	GLU	2.1
1	A	183	GLU	2.1
1	A	241	ILE	2.1
1	B	44	ASN	2.1
1	B	272	ILE	2.0
1	A	271	ARG	2.0
1	A	265	THR	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.

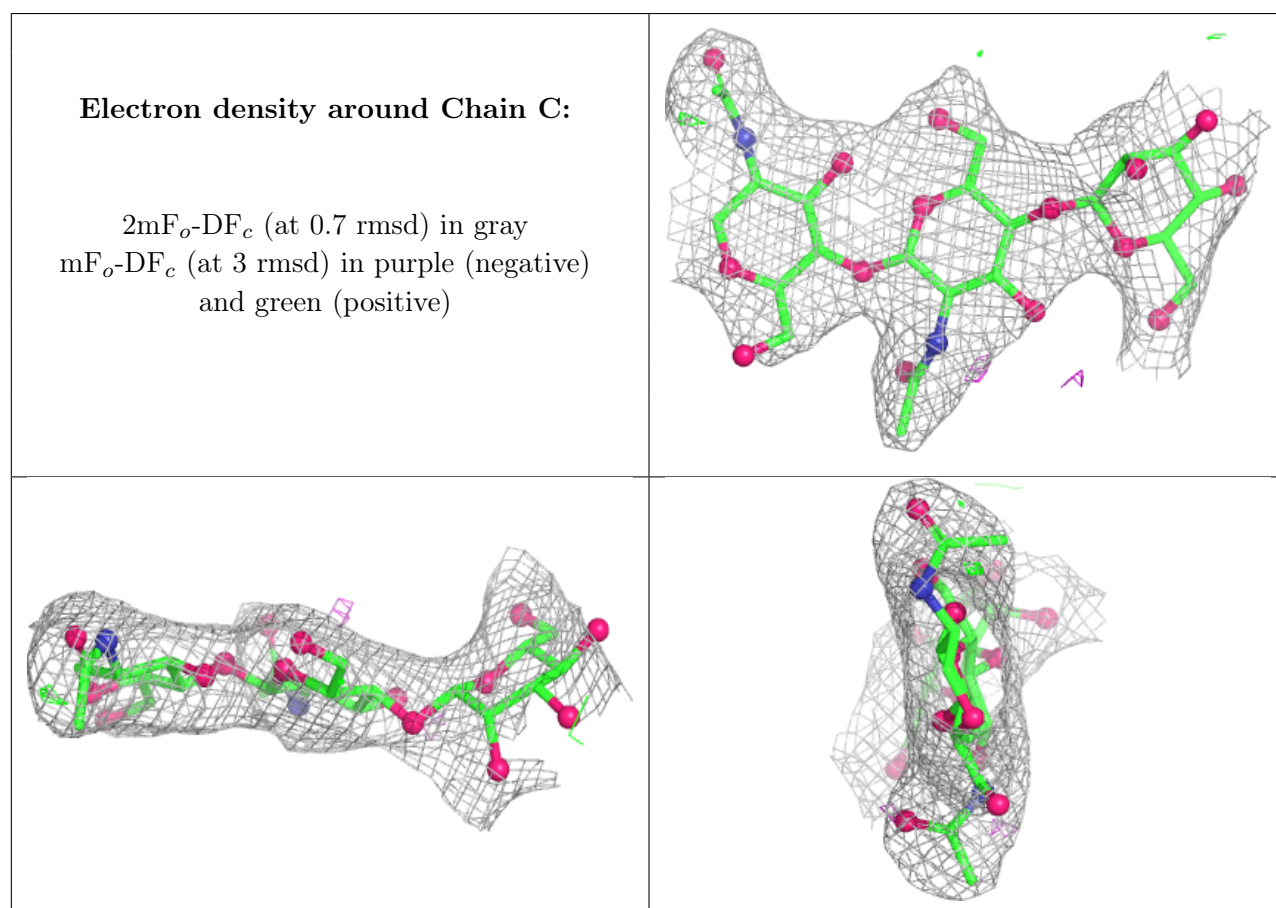
## 6.3 Carbohydrates [i](#)

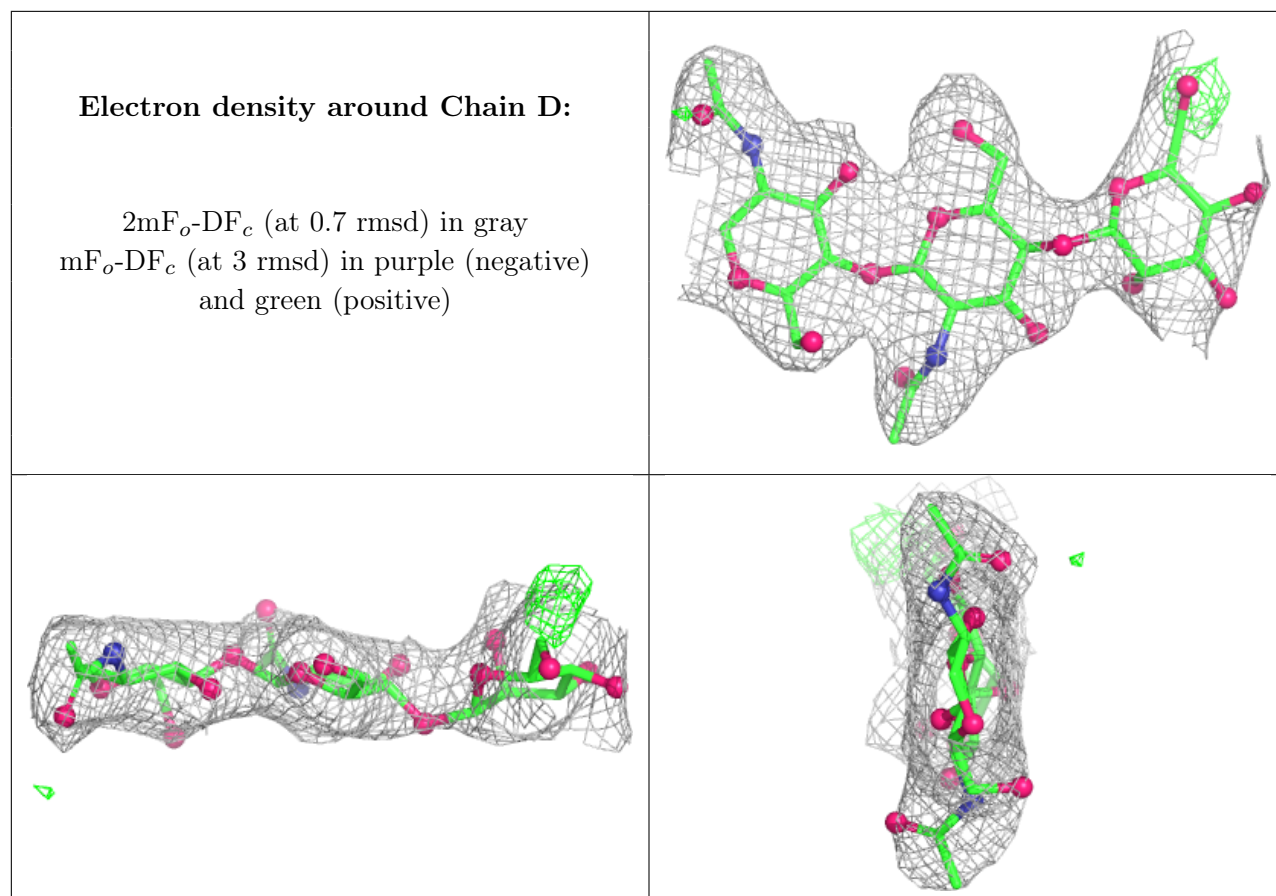
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BMA	D	3	11/12	0.39	0.20	118,118,118,118	0
2	BMA	C	3	11/12	0.68	0.14	102,102,102,102	0
2	NAG	C	2	14/15	0.88	0.11	62,78,95,100	0
2	NAG	D	2	14/15	0.89	0.15	75,96,119,120	0
2	NAG	D	1	14/15	0.90	0.13	63,77,90,91	0
2	NAG	C	1	14/15	0.92	0.13	58,64,85,96	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1004	14/15	0.44	0.26	78,114,167,196	0
3	NAG	B	2005	14/15	0.64	0.19	71,88,116,125	0
3	NAG	A	1005	14/15	0.90	0.12	61,71,91,93	0
3	NAG	B	2004	14/15	0.94	0.09	65,76,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.