



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:29 AM UTC

PDB ID : 2WDB / pdb\_00002wdb  
Title : A family 32 carbohydrate-binding module, from the Mu toxin produced by Clostridium perfringens, in complex with beta-D-glcNAc-beta(1,2) mannose  
Authors : Ficko-Blean, E.; Boraston, A.B.  
Deposited on : 2009-03-23  
Resolution : 2.03 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](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

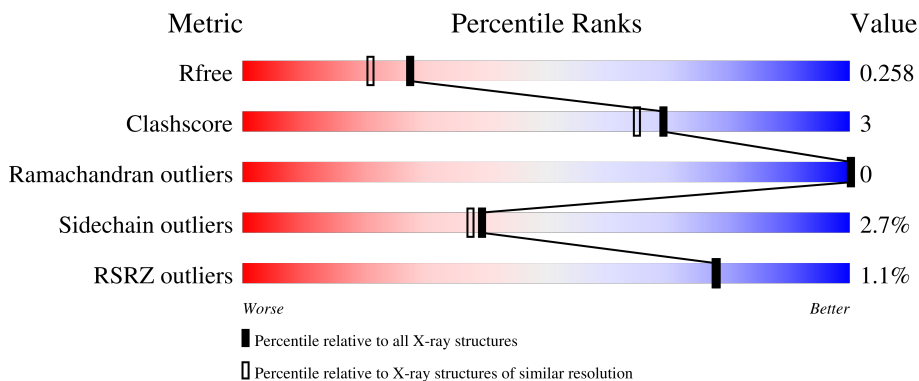
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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.



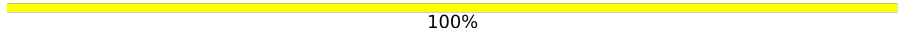
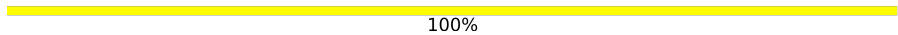

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	192	 2% 65% 6% 27%
1	B	192	 69% 6% 24%
1	C	192	 66% 7% 27%
1	D	192	 69% 5% 26%
2	E	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	E	1	X	-	-	-
2	MAN	F	1	X	-	-	-
2	MAN	G	1	X	-	-	-
2	MAN	H	1	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5090 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.

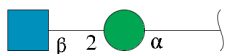
- Molecule 1 is a protein called HYALURONOGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	139	1100	699	177	223	1	17	0	0
1	B	146	1161	734	186	239	2	7	1	0
1	C	141	1117	708	179	229	1	7	0	0
1	D	143	1128	714	181	232	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	944	VAL	ILE	conflict	UNP P26831
B	944	VAL	ILE	conflict	UNP P26831
C	944	VAL	ILE	conflict	UNP P26831
D	944	VAL	ILE	conflict	UNP P26831

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	26	14	1	11	0	0	0
2	F	2	26	14	1	11	0	0	0
2	G	2	26	14	1	11	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	131	Total	O	0	0
			131	131		
4	C	131	Total	O	0	0
			131	131		
4	D	108	Total	O	0	0
			108	108		

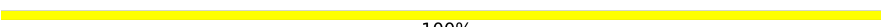


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose

Chain E:  50% 50%

MAN1  
MAG2

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

Chain F:  100%

MAN1  
MAG2

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

Chain G:  100%

MAN1  
MAG2

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

Chain H:  50% 50%

MAN1  
MAG2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.28Å 91.28Å 132.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.06 – 2.03 79.05 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.06-2.03) 99.7 (79.05-2.03)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.70 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.260 0.199 , 0.258	Depositor DCC
$R_{free}$ test set	2110 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.12 % 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 7.5052e-03. 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: MAN, CA, 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	2.36	8/1123 (0.7%)	1.31	8/1518 (0.5%)
1	B	0.75	2/1184 (0.2%)	0.79	1/1600 (0.1%)
1	C	0.88	2/1140 (0.2%)	0.80	2/1541 (0.1%)
1	D	0.61	0/1151	0.75	0/1556
All	All	1.34	12/4598 (0.3%)	0.94	11/6215 (0.2%)

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	A	0	2
1	B	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	916	GLU	CD-OE1	54.28	2.28	1.25
1	A	916	GLU	CD-OE2	40.22	2.01	1.25
1	A	820	GLU	CG-CD	33.26	2.35	1.52
1	C	860	LYS	CG-CD	-15.28	1.06	1.52
1	C	916	GLU	CB-CG	-14.01	1.10	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	GLU	CG-CD-OE2	-31.35	46.29	118.40
1	A	820	GLU	CG-CD-OE1	-12.42	89.83	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	891	GLU	OE1-CD-OE2	-11.67	94.90	122.90
1	C	860	LYS	CB-CG-CD	11.00	136.60	111.30
1	A	891	GLU	CG-CD-OE2	10.07	141.56	118.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	820	GLU	Sidechain
1	A	916	GLU	Sidechain
1	B	916	GLU	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	1100	0	1057	5	0
1	B	1161	0	1108	13	0
1	C	1117	0	1067	7	0
1	D	1128	0	1077	11	0
2	E	26	0	23	0	0
2	F	26	0	23	0	0
2	G	26	0	20	0	0
2	H	26	0	23	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	106	0	0	2	0
4	B	131	0	0	1	1
4	C	131	0	0	0	1
4	D	108	0	0	1	0
All	All	5090	0	4398	31	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.

The worst 5 of 31 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:D:805:ALA:N	4:D:2001:HOH:O	2.10	0.82
1:B:807:ASN:ND2	1:D:812:ARG:H	1.82	0.77
1:B:871:ASN:HD21	1:B:908:LYS:HE2	1.53	0.74
1:D:822:ASN:C	1:D:822:ASN:HD22	1.97	0.72
1:A:811:ILE:HD12	4:A:2060:HOH:O	1.89	0.72

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)
4:B:2082:HOH:O	4:C:2075:HOH:O[2_655]	2.03	0.17

## 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	137/192 (71%)	130 (95%)	7 (5%)	0	100	100
1	B	145/192 (76%)	139 (96%)	6 (4%)	0	100	100
1	C	139/192 (72%)	135 (97%)	4 (3%)	0	100	100
1	D	141/192 (73%)	139 (99%)	2 (1%)	0	100	100
All	All	562/768 (73%)	543 (97%)	19 (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	119/165 (72%)	117 (98%)	2 (2%)	53	53
1	B	126/165 (76%)	120 (95%)	6 (5%)	23	15
1	C	121/165 (73%)	118 (98%)	3 (2%)	42	40
1	D	122/165 (74%)	120 (98%)	2 (2%)	55	56
All	All	488/660 (74%)	475 (97%)	13 (3%)	39	37

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	916	GLU
1	C	888	LEU
1	D	888	LEU
1	C	916	GLU
1	D	822	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	871	ASN
1	C	880	ASN
1	D	880	ASN
1	D	822	ASN
1	D	832	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](#)

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	E	1	2	12,12,12	2.14	3 (25%)	17,17,17	2.34	6 (35%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	0.74	0
2	MAN	F	1	2	12,12,12	2.13	5 (41%)	17,17,17	2.09	4 (23%)
2	NAG	F	2	2	14,14,15	0.84	1 (7%)	17,19,21	1.15	1 (5%)
2	MAN	G	1	2	12,12,12	2.49	4 (33%)	17,17,17	2.62	8 (47%)
2	NAG	G	2	2	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
2	MAN	H	1	2	12,12,12	1.94	3 (25%)	17,17,17	2.06	4 (23%)
2	NAG	H	2	2	14,14,15	0.54	0	17,19,21	0.99	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
2	MAN	E	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	MAN	F	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	MAN	G	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	MAN	H	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	MAN	O1-C1	-6.38	1.19	1.39
2	E	1	MAN	O5-C5	-5.88	1.30	1.44
2	H	1	MAN	O5-C5	-4.51	1.33	1.44
2	F	1	MAN	O5-C5	-3.96	1.34	1.44
2	F	1	MAN	O1-C1	-3.35	1.29	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	MAN	C1-C2-C3	-5.74	98.65	110.36
2	E	1	MAN	O1-C1-C2	5.71	125.56	108.98
2	H	1	MAN	O1-C1-C2	5.09	123.75	108.98
2	F	1	MAN	O1-C1-O5	4.85	124.81	110.41
2	F	1	MAN	C1-C2-C3	-4.64	100.90	110.36

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	MAN	C1
2	F	1	MAN	C1
2	G	1	MAN	C1
2	H	1	MAN	C1

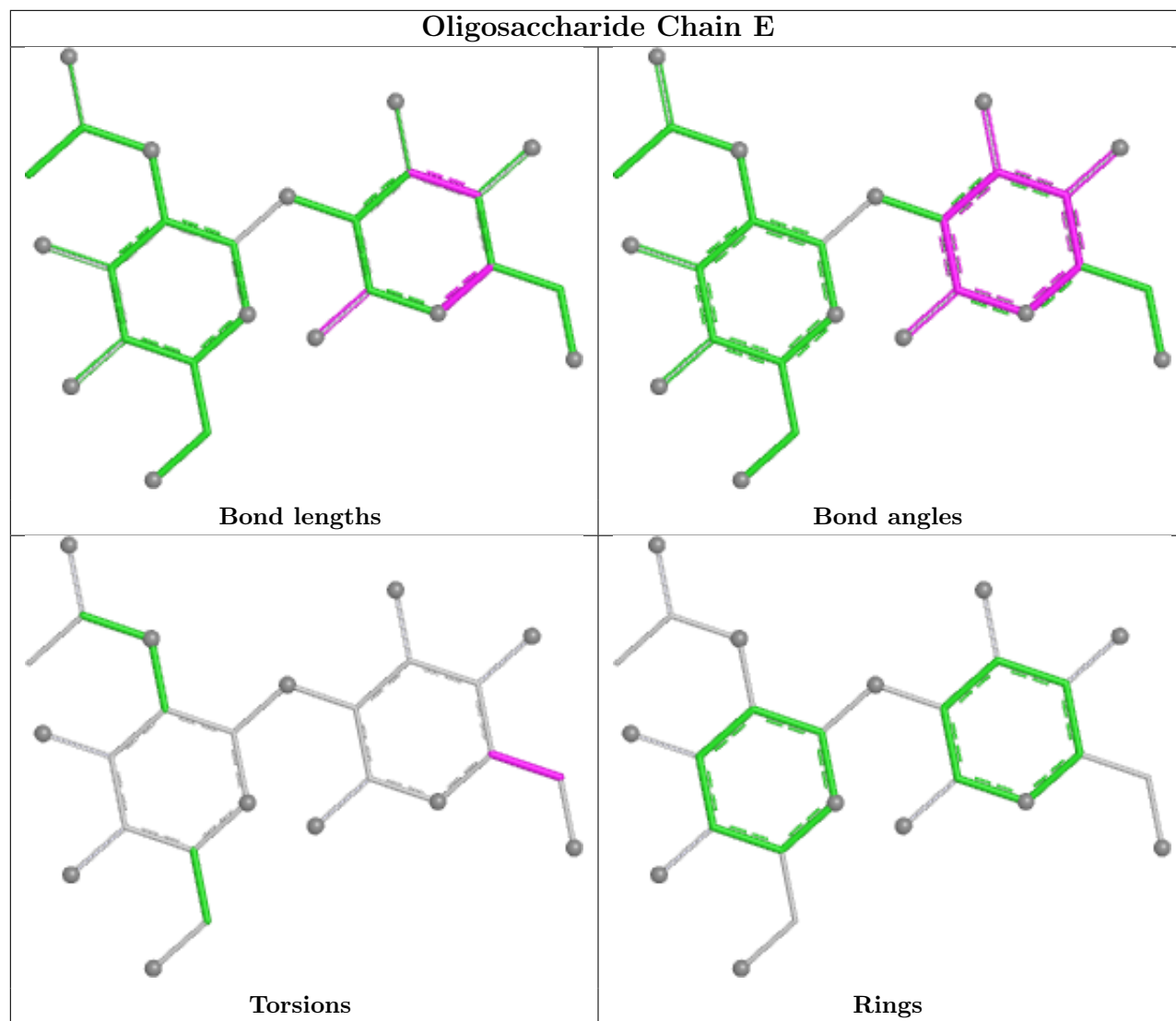
All (3) torsion outliers are listed below:

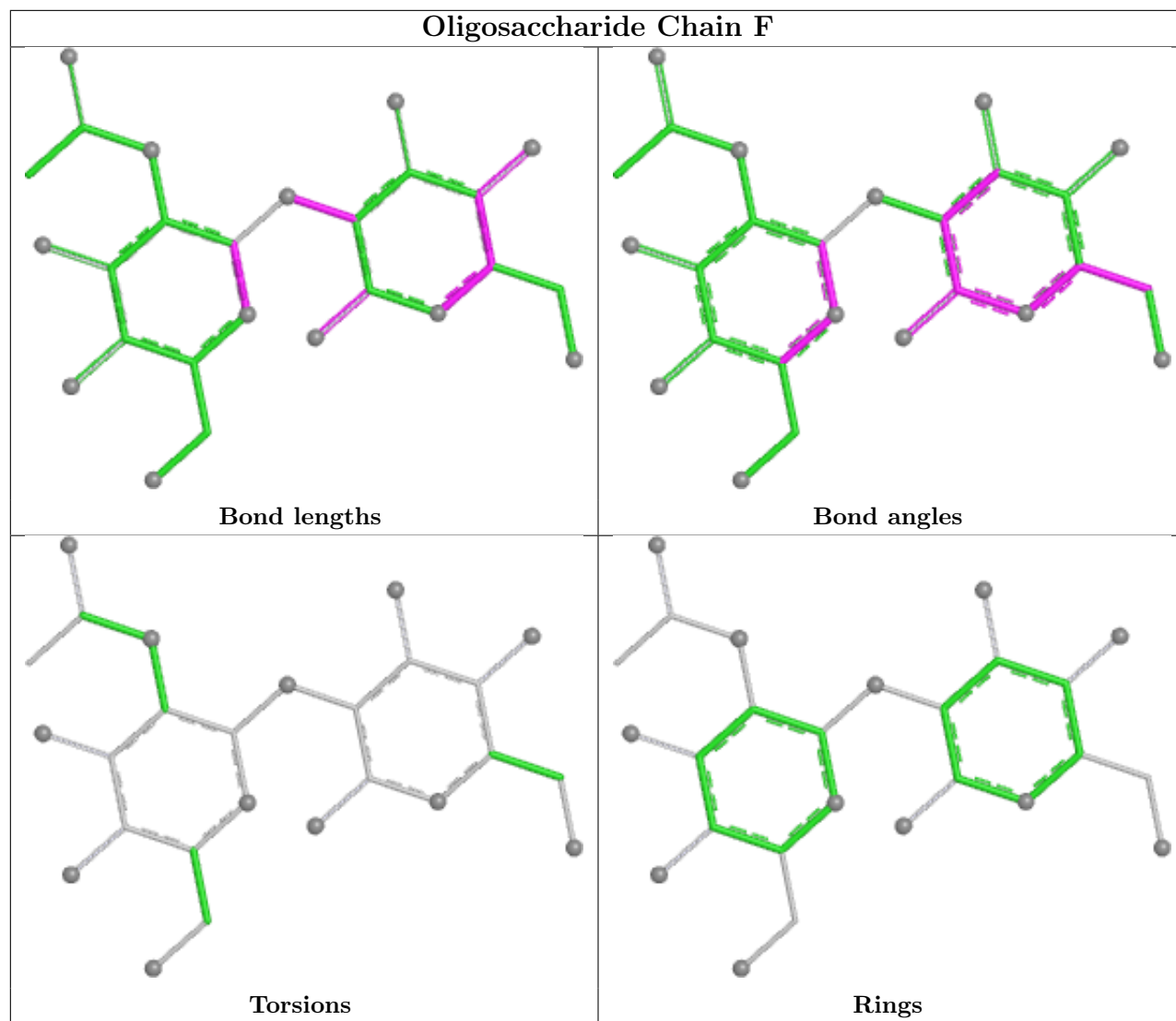
Mol	Chain	Res	Type	Atoms
2	E	1	MAN	O5-C5-C6-O6
2	H	1	MAN	O5-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7

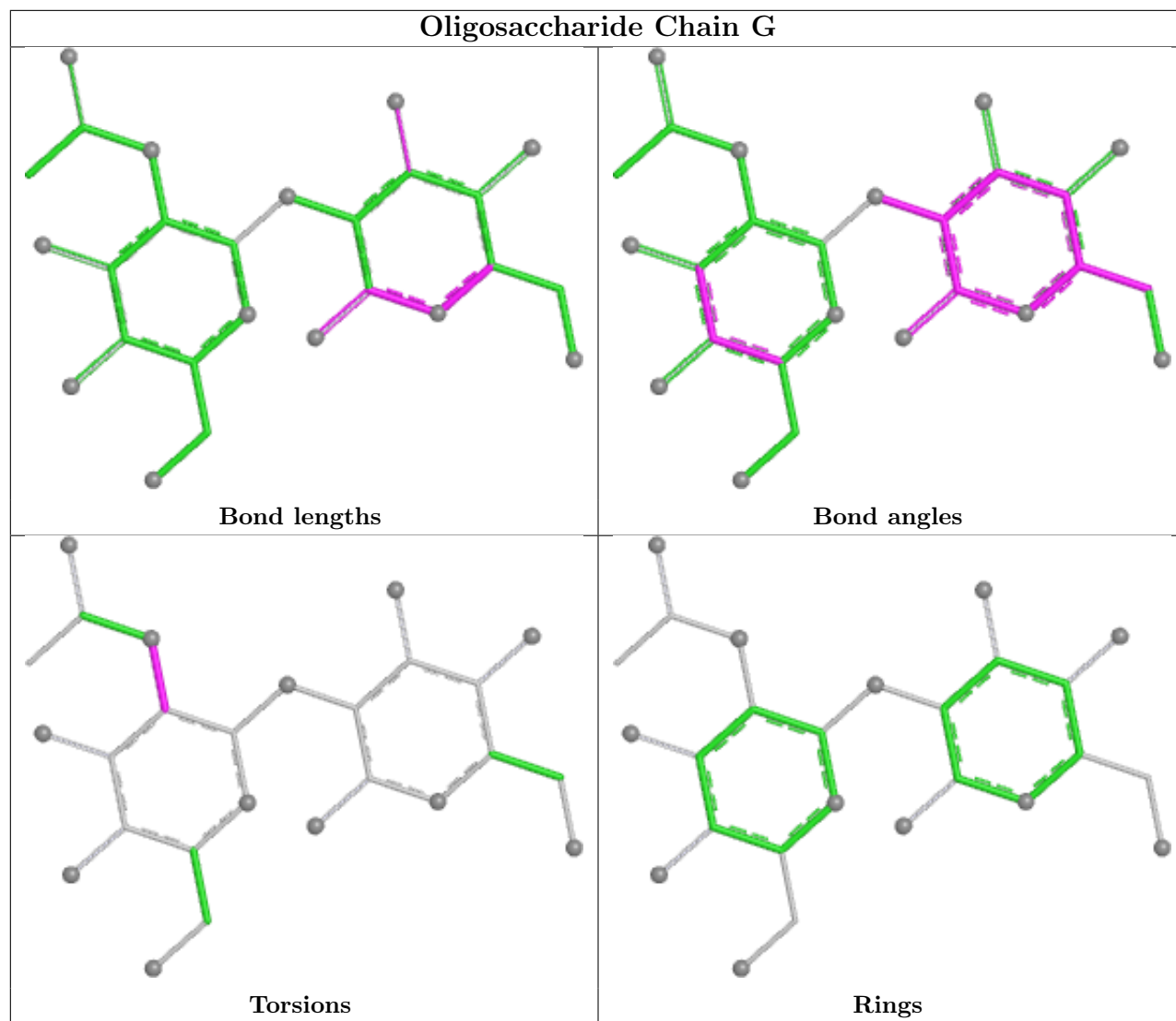
There are no ring outliers.

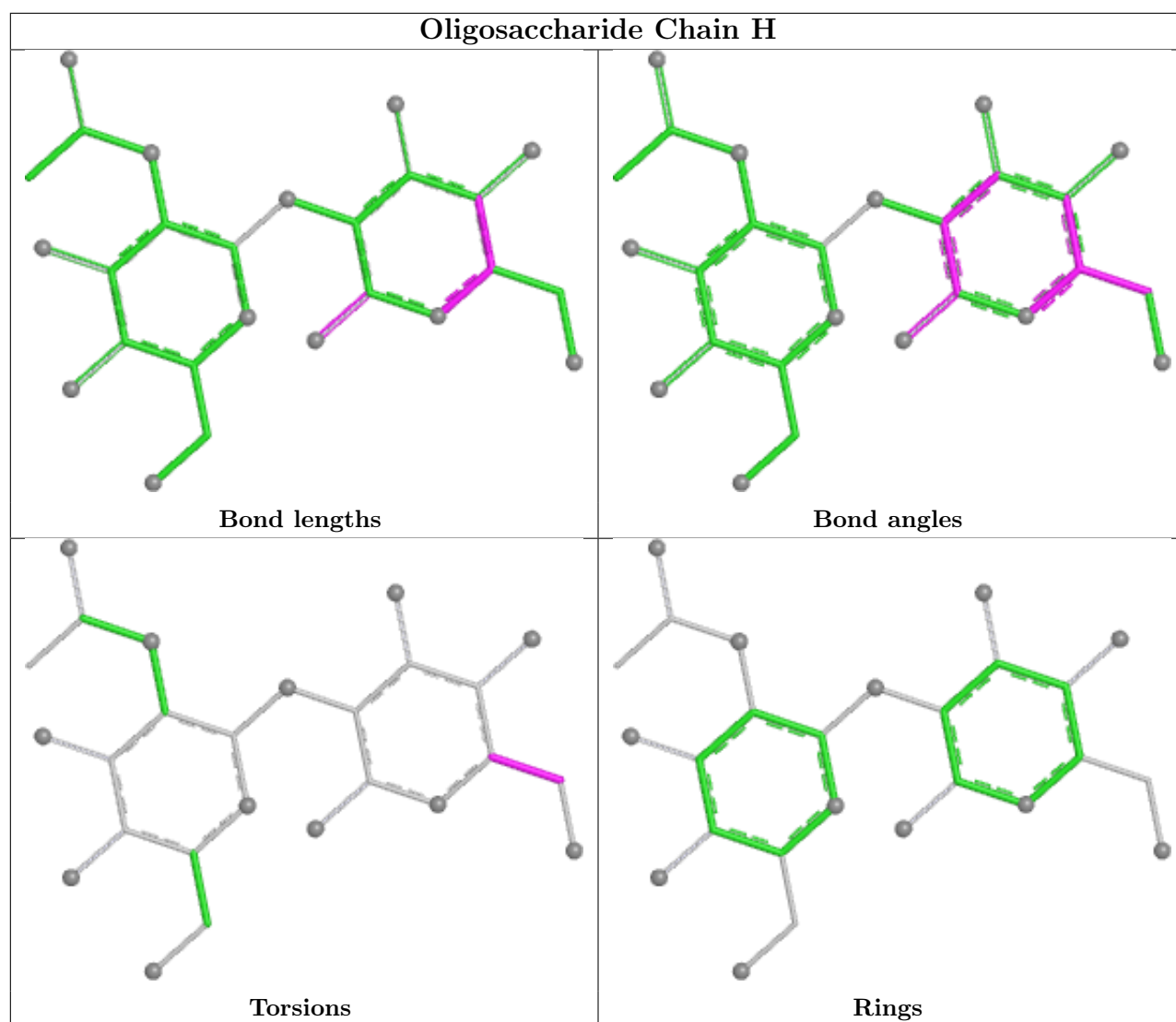
No monomer is involved in short contacts.

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	139/192 (72%)	0.39	3 (2%) 62 62	20, 30, 46, 54	7 (5%)
1	B	146/192 (76%)	-0.20	1 (0%) 84 84	9, 22, 36, 57	3 (2%)
1	C	141/192 (73%)	-0.26	1 (0%) 84 84	14, 22, 41, 54	2 (1%)
1	D	143/192 (74%)	0.09	1 (0%) 84 84	19, 27, 38, 53	0
All	All	569/768 (74%)	0.00	6 (1%) 78 78	9, 25, 42, 57	12 (2%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	862	ASP	2.9
1	A	859	ILE	2.8
1	B	804	MET	2.7
1	A	818	VAL	2.5
1	C	856	GLY	2.4

### 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.

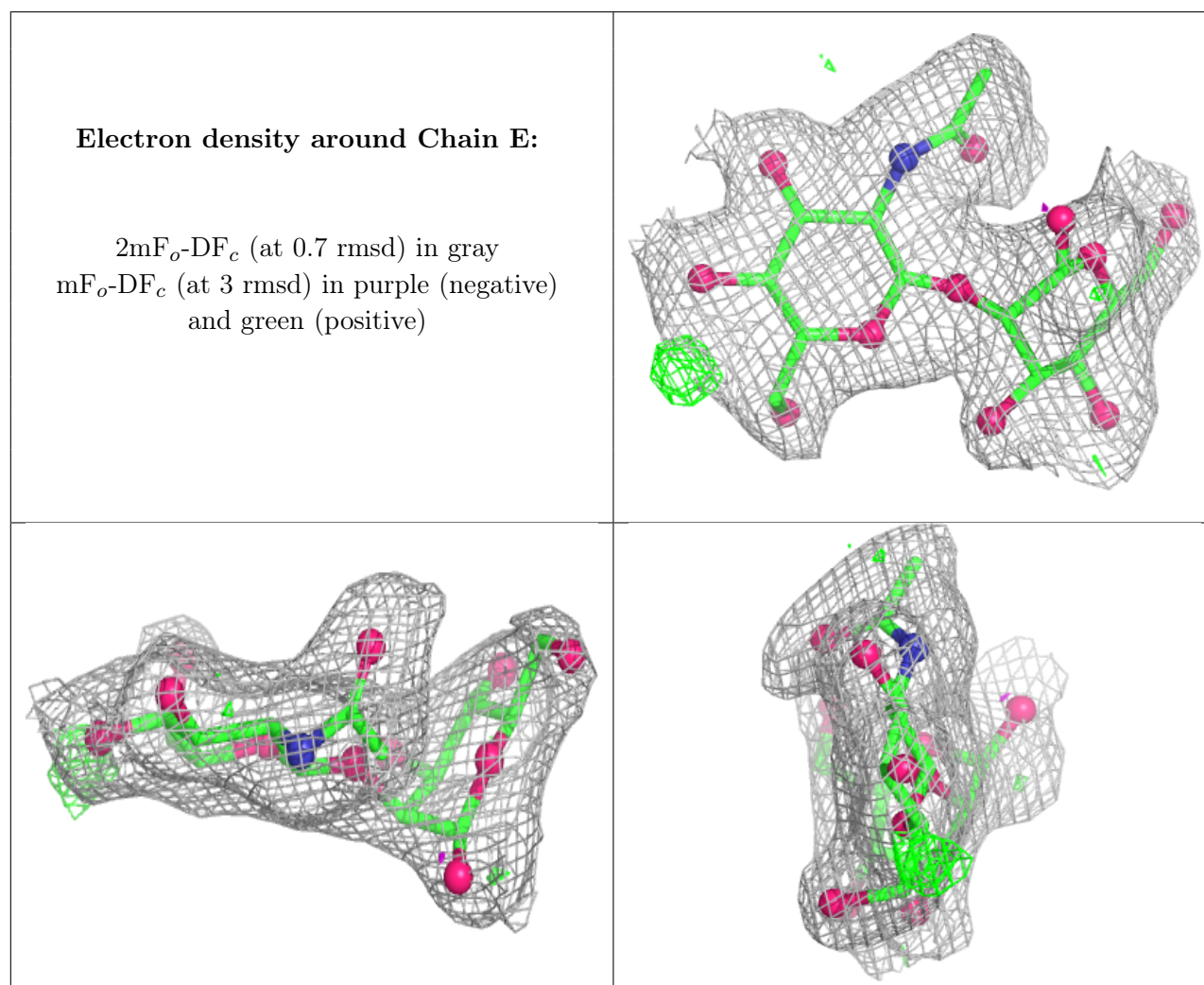
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	H	1	12/12	0.81	0.12	35,43,45,46	0
2	MAN	E	1	12/12	0.82	0.12	47,54,56,57	0

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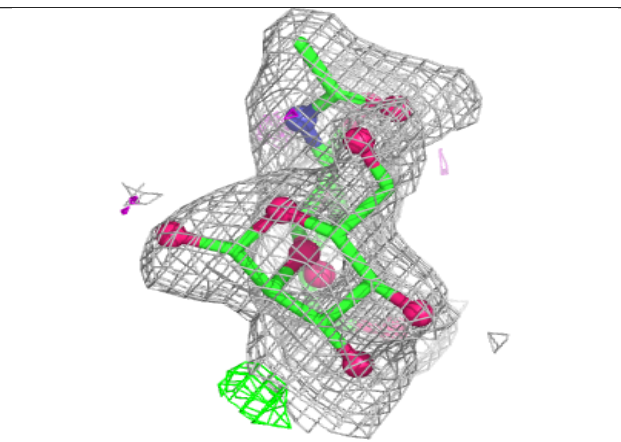
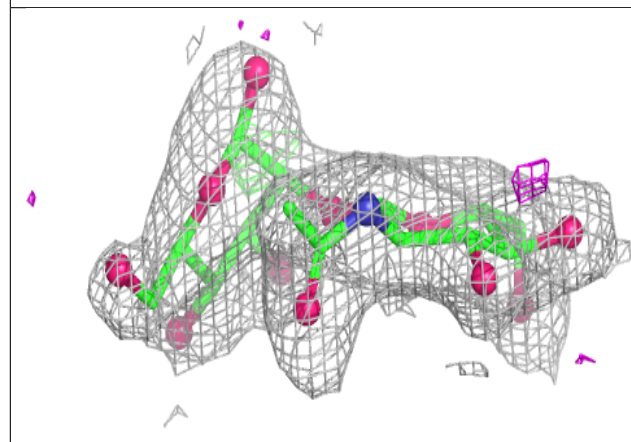
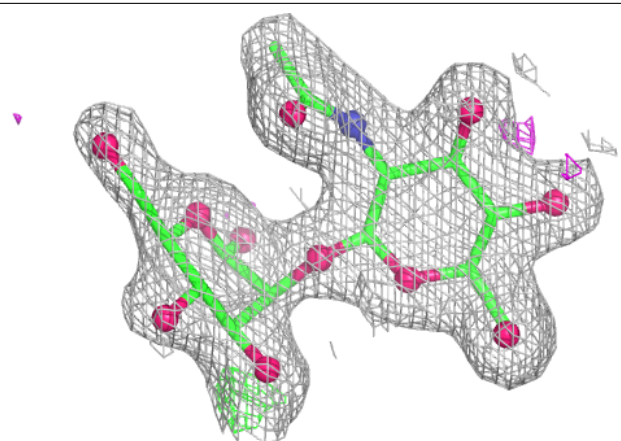
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	F	1	12/12	0.84	0.12	33,43,46,46	0
2	MAN	G	1	12/12	0.88	0.09	27,29,31,33	0
2	NAG	E	2	14/15	0.91	0.10	35,37,40,41	0
2	NAG	H	2	14/15	0.93	0.07	24,27,29,30	0
2	NAG	G	2	14/15	0.94	0.06	19,22,24,24	0
2	NAG	F	2	14/15	0.96	0.07	25,26,27,28	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.



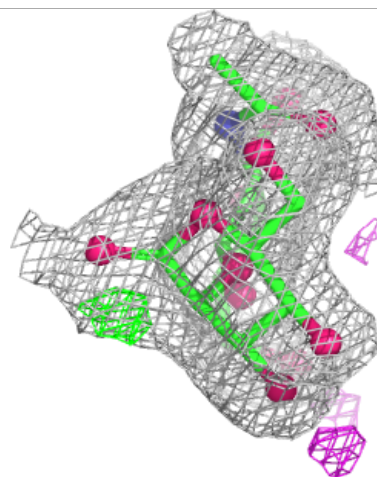
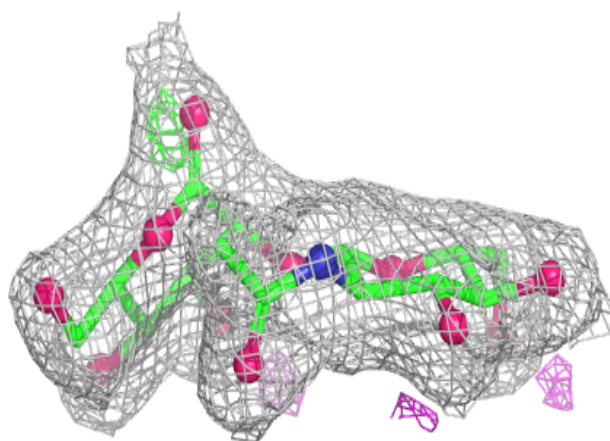
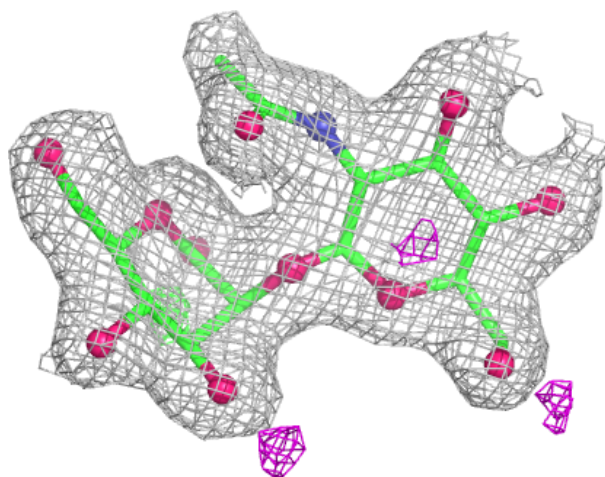
**Electron density around Chain F:**

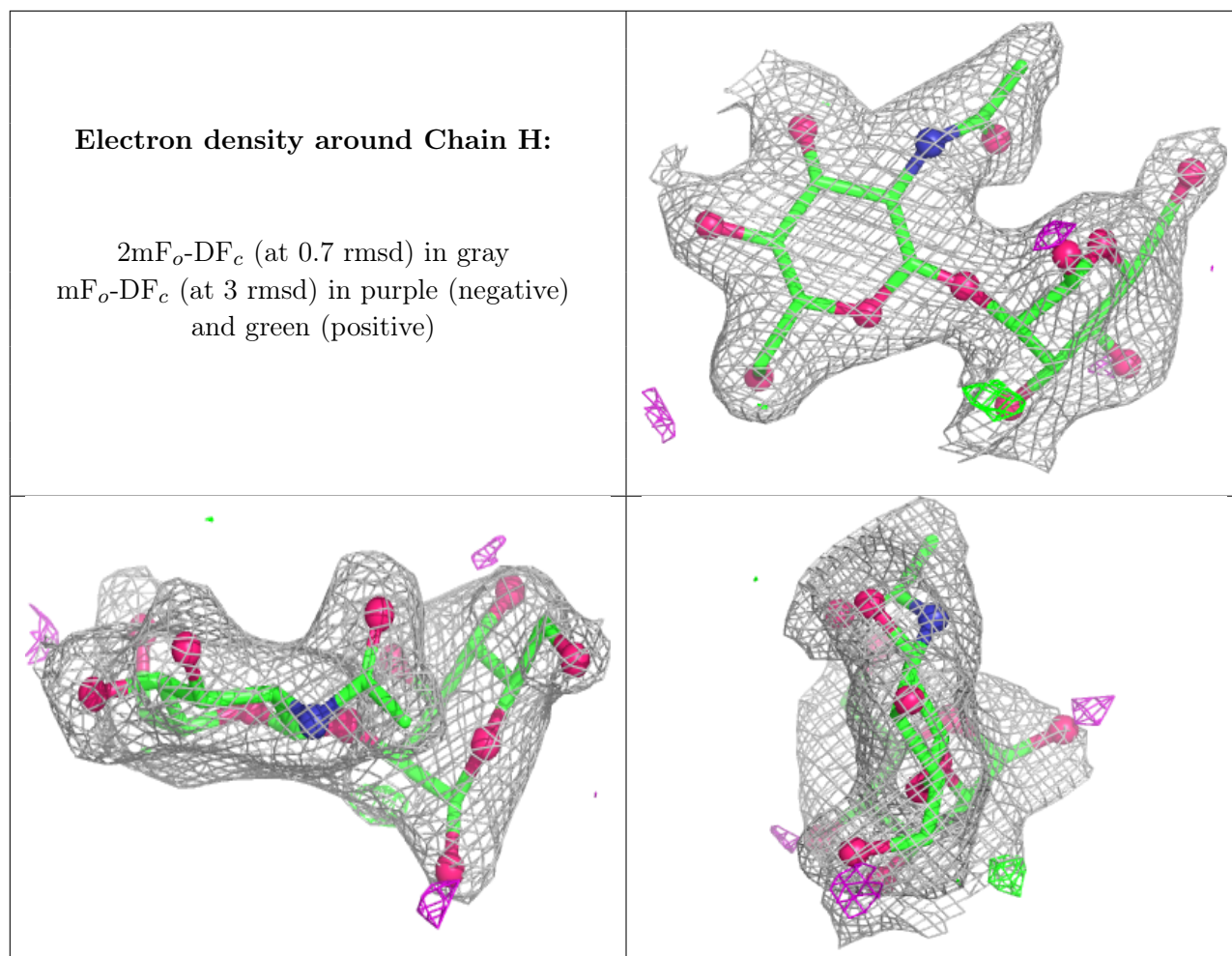
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

$2mF_o-DF_c$  (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<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	CA	A	1948	1/1	0.97	0.04	31,31,31,31	0
3	CA	B	1952	1/1	0.99	0.02	20,20,20,20	0
3	CA	C	1950	1/1	0.99	0.02	19,19,19,19	0
3	CA	D	1950	1/1	0.99	0.02	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.