wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 09:03 pm BST

PDB ID	:	2W1U
Title	:	A family 32 carbohydrate-binding module, from the Mu toxin produced by Clostridium perfringens, in complex with beta-D-glcNAc-beta(1,3) galNAc
Authors	:	Ficko-Blean, E.; Boraston, A.B.
Deposited on	:	2008-10-20
Resolution	:	2.00 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 (i)) were used in the production of this report:

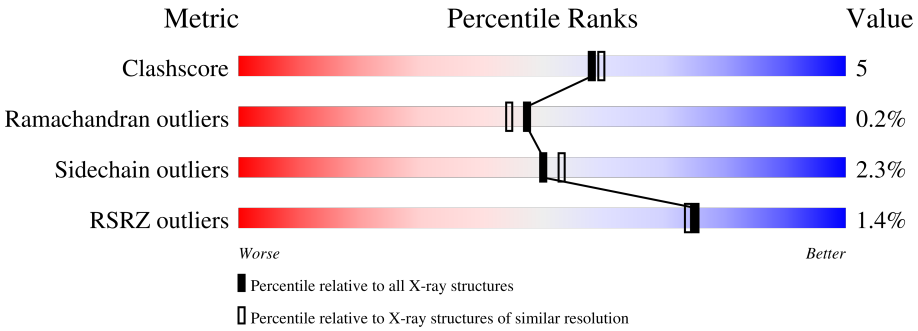
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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	192	65% 7% 28%
1	B	192	67% 8% 24%
1	C	192	67% 6% 27%
1	D	192	65% 9% 25%
2	E	2	50% 50%
2	F	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	100%
3	G	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5331 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.

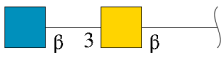
- Molecule 1 is a protein called HYALURONOGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1100	699	177	223	1			
1	B	146	Total	C	N	O	S	0	0	0
			1153	730	184	237	2			
1	C	140	Total	C	N	O	S	0	0	0
			1109	704	177	227	1			
1	D	144	Total	C	N	O	S	3	0	0
			1136	719	182	233	2			

There are 4 discrepancies between the modelled and reference sequences:

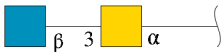
Chain	Residue	Modelled	Actual	Comment	Reference
A	944	VAL	ILE	variant	UNP P26831
B	944	VAL	ILE	variant	UNP P26831
C	944	VAL	ILE	variant	UNP P26831
D	944	VAL	ILE	variant	UNP P26831

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	F	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	H	2	Total	C	N	O	0	0	0
			29	16	2	11			

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

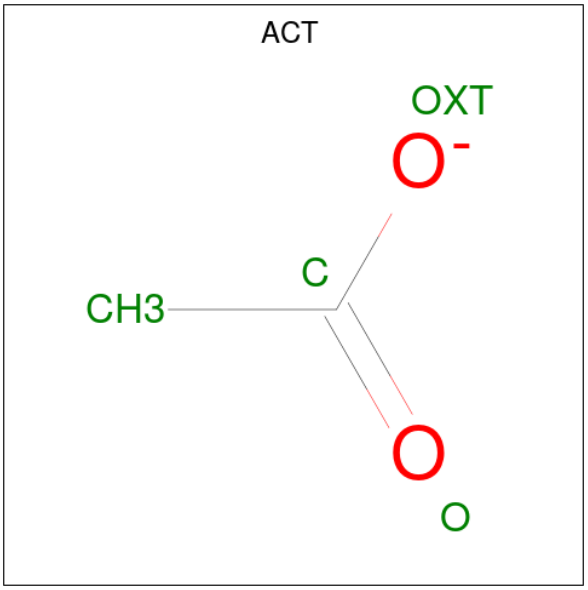


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	2	Total C N O 29 16 2 11	0	0	0

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

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

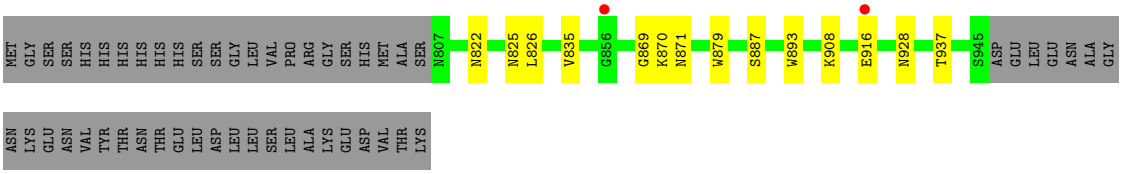
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	154	Total O 154 154	0	0
6	B	171	Total O 171 171	0	0
6	C	197	Total O 197 197	0	0
6	D	179	Total O 179 179	0	0

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.

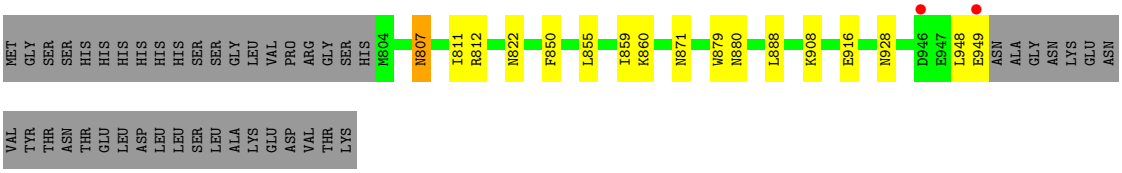
• Molecule 1: HYALURONOGLUCOSAMINIDASE

Chain A:



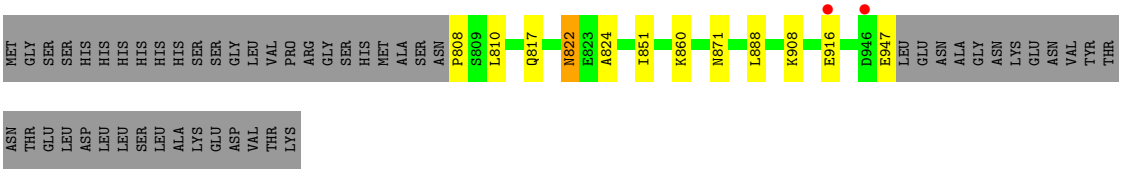
• Molecule 1: HYALURONOGLUCOSAMINIDASE

Chain B:



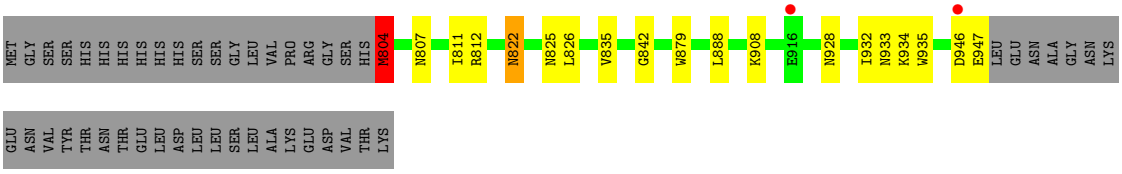
• Molecule 1: HYALURONOGLUCOSAMINIDASE

Chain C:



• Molecule 1: HYALURONOGLUCOSAMINIDASE

Chain D:

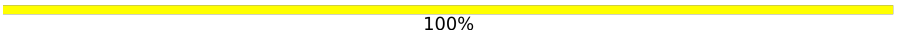


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain E:

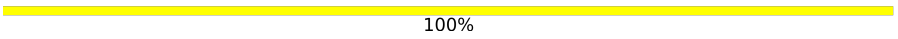
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain F:



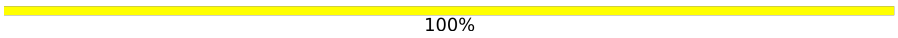
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose

Chain H:



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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.17Å 91.17Å 132.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.00) 98.5 (19.89-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.75 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.169 , 0.213 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5331	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2G, ACT, NAG, CA, NGA

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	0.74	0/1123	0.71	0/1518
1	B	0.80	0/1176	0.72	0/1589
1	C	0.75	0/1132	0.72	0/1529
1	D	0.82	1/1159 (0.1%)	1.01	2/1566 (0.1%)
All	All	0.78	1/4590 (0.0%)	0.80	2/6202 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	804	MET	CB-CG	-7.35	1.27	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	804	MET	CA-CB-CG	27.76	160.49	113.30
1	D	804	MET	CB-CG-SD	5.87	130.02	112.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1058	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1153	0	1103	16	0
1	C	1109	0	1062	7	0
1	D	1136	0	1086	15	0
2	E	29	0	27	0	0
2	F	29	0	27	0	0
2	H	29	0	27	0	0
3	G	29	0	24	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	4	0	3	0	0
5	C	4	0	3	1	0
5	D	4	0	3	1	0
6	A	154	0	0	0	1
6	B	171	0	0	1	1
6	C	197	0	0	1	1
6	D	179	0	0	4	1
All	All	5331	0	4423	43	2

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 5.

The worst 5 of 43 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:C:808:PRO:N	6:C:2001:HOH:O	2.05	0.89
1:C:822:ASN:HD22	1:C:824:ALA:H	1.29	0.80
1:B:807:ASN:H	1:B:807:ASN:HD22	1.33	0.77
1:A:826:LEU:HD21	1:A:835:VAL:HG12	1.74	0.69
1:B:871:ASN:ND2	1:B:908:LYS:HE2	2.11	0.64

All (2) 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)
6:A:2099:HOH:O	6:D:2136:HOH:O[2_445]	1.89	0.31
6:B:2107:HOH:O	6:C:2112:HOH:O[2_545]	2.05	0.15

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%)	132 (96%)	5 (4%)	0	100	100
1	B	144/192 (75%)	141 (98%)	3 (2%)	0	100	100
1	C	138/192 (72%)	133 (96%)	5 (4%)	0	100	100
1	D	142/192 (74%)	139 (98%)	2 (1%)	1 (1%)	22	16
All	All	561/768 (73%)	545 (97%)	15 (3%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	935	TRP

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%)	118 (99%)	1 (1%)	81	86
1	B	125/165 (76%)	121 (97%)	4 (3%)	39	38
1	C	120/165 (73%)	117 (98%)	3 (2%)	47	49
1	D	123/165 (74%)	120 (98%)	3 (2%)	49	51
All	All	487/660 (74%)	476 (98%)	11 (2%)	50	53

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	916	GLU
1	D	804	MET
1	D	888	LEU
1	D	822	ASN
1	B	888	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	807	ASN
1	D	822	ASN
1	D	880	ASN
1	B	880	ASN
1	C	822	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	NGA	E	1	2	15,15,15	0.53	0	21,21,21	1.84	2 (9%)
2	NAG	E	2	2	14,14,15	0.53	0	17,19,21	0.69	0
2	NGA	F	1	2	15,15,15	0.52	0	21,21,21	1.43	4 (19%)
2	NAG	F	2	2	14,14,15	0.66	0	17,19,21	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A2G	G	1	3	15,15,15	0.60	0	21,21,21	0.80	1 (4%)
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	1.12	1 (5%)
2	NGA	H	1	2	15,15,15	0.57	0	21,21,21	1.18	2 (9%)
2	NAG	H	2	2	14,14,15	0.85	1 (7%)	17,19,21	1.04	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	NGA	E	1	2	-	0/6/26/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NGA	F	1	2	-	0/6/26/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
3	A2G	G	1	3	-	0/6/26/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
2	NGA	H	1	2	-	0/6/26/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	O5-C1	-2.02	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NGA	C1-C2-N2	-6.29	103.44	110.73
2	E	1	NGA	C3-C2-N2	3.34	116.92	110.62
2	F	1	NGA	C1-C2-N2	-3.30	106.91	110.73
2	F	1	NGA	O5-C1-C2	3.08	112.61	109.52
2	H	1	NGA	C1-C2-N2	-2.89	107.38	110.73

There are no chirality outliers.

There are no torsion outliers.

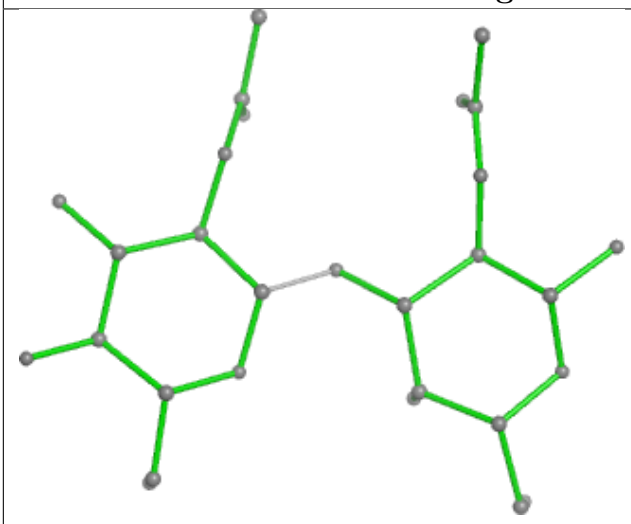
There are no ring outliers.

No monomer is involved in short contacts.

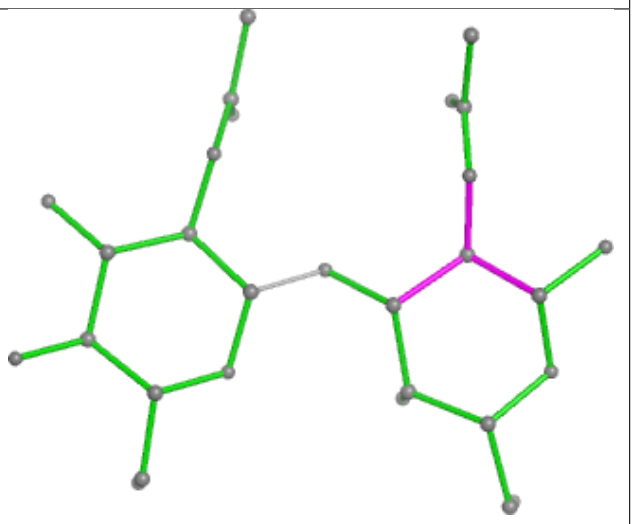
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

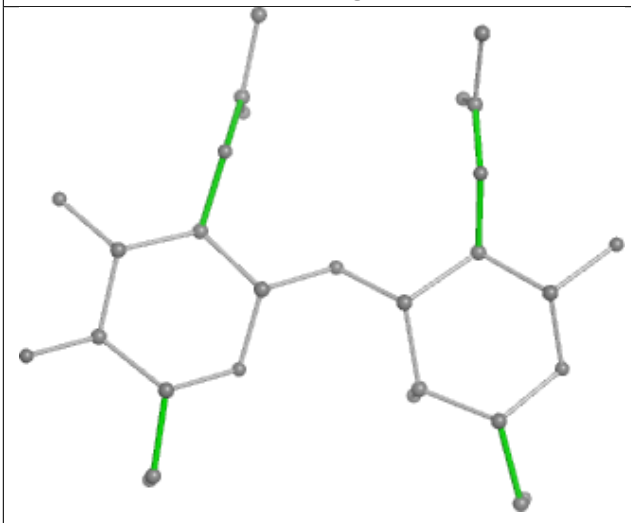
Oligosaccharide Chain E



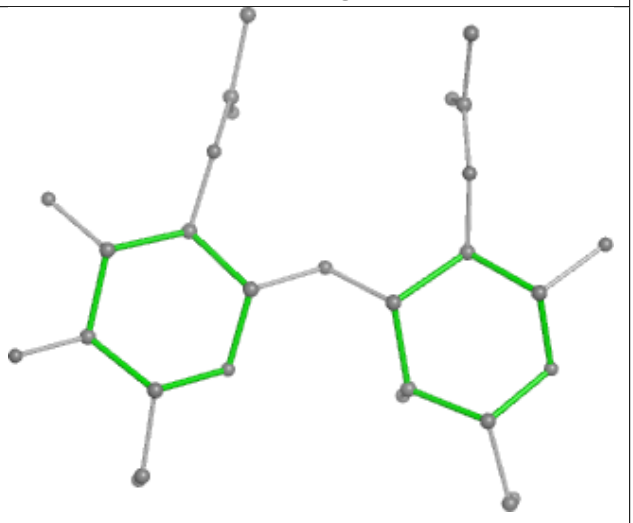
Bond lengths



Bond angles

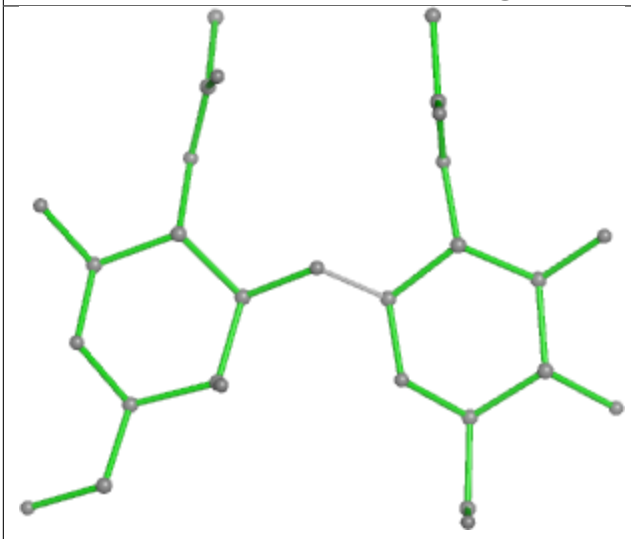


Torsions

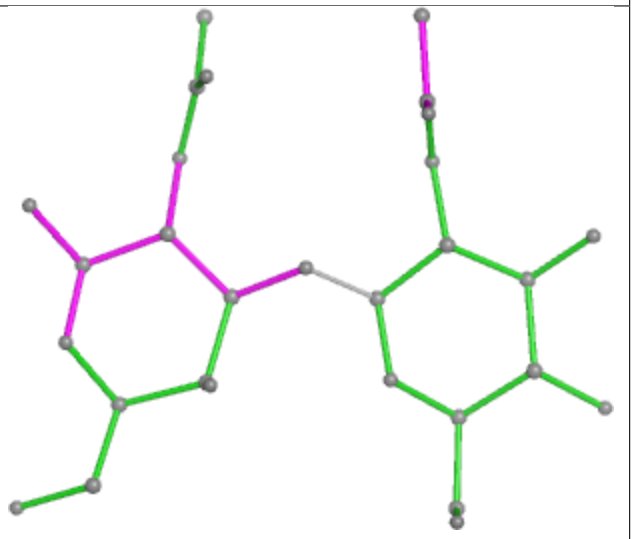


Rings

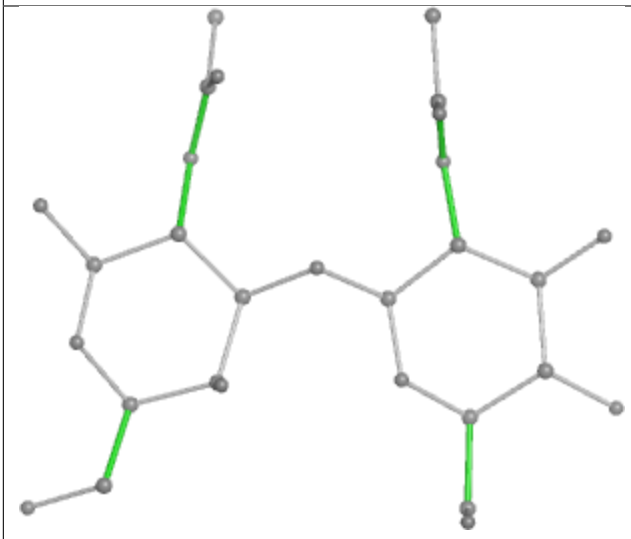
Oligosaccharide Chain F



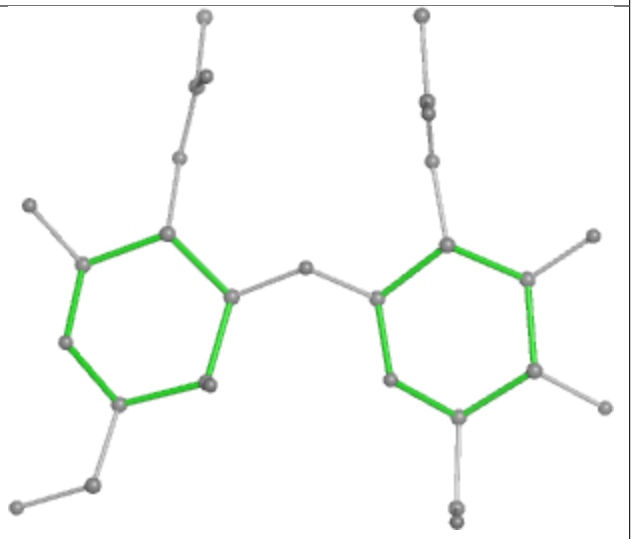
Bond lengths



Bond angles

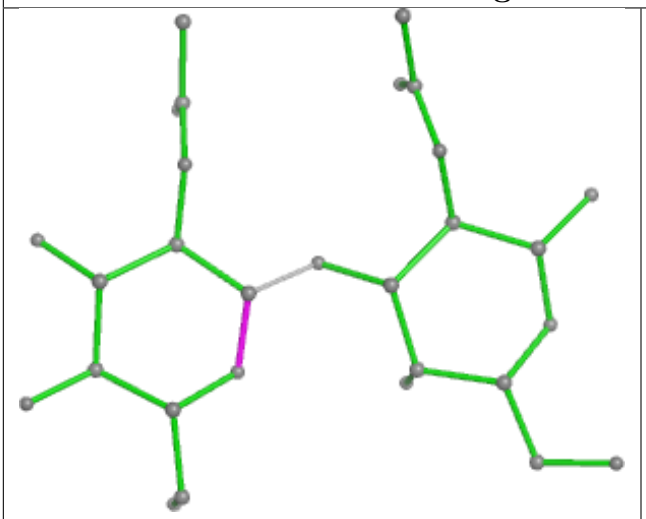


Torsions

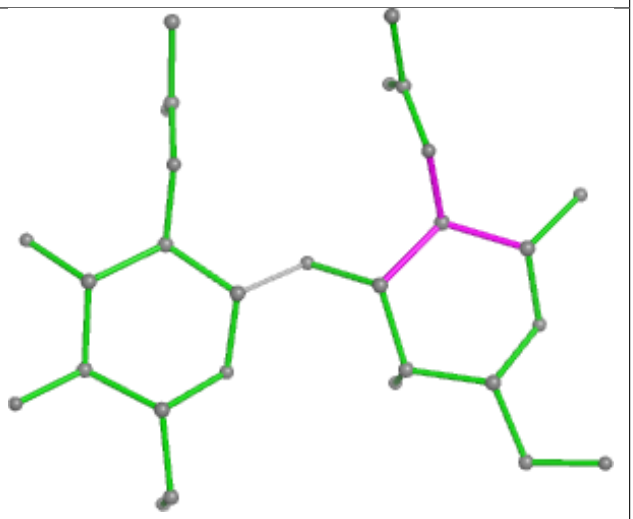


Rings

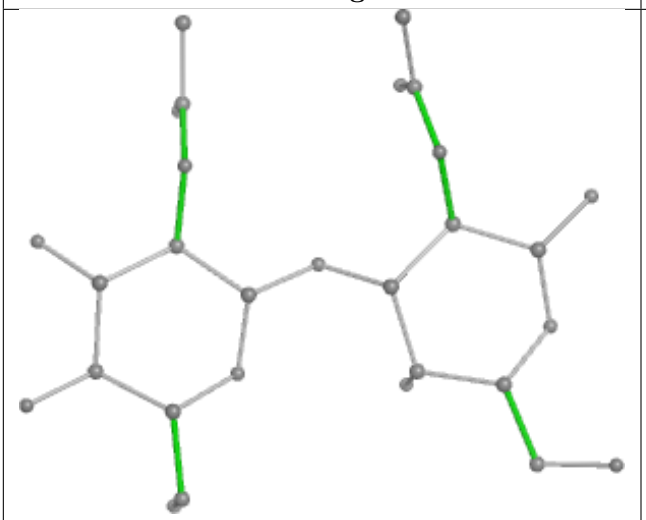
Oligosaccharide Chain H



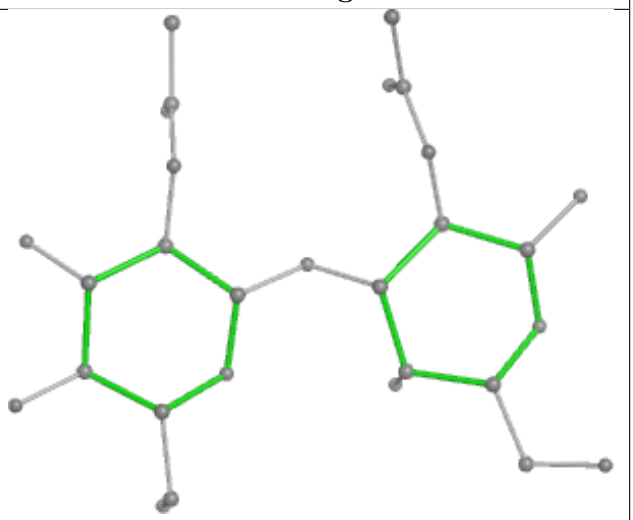
Bond lengths



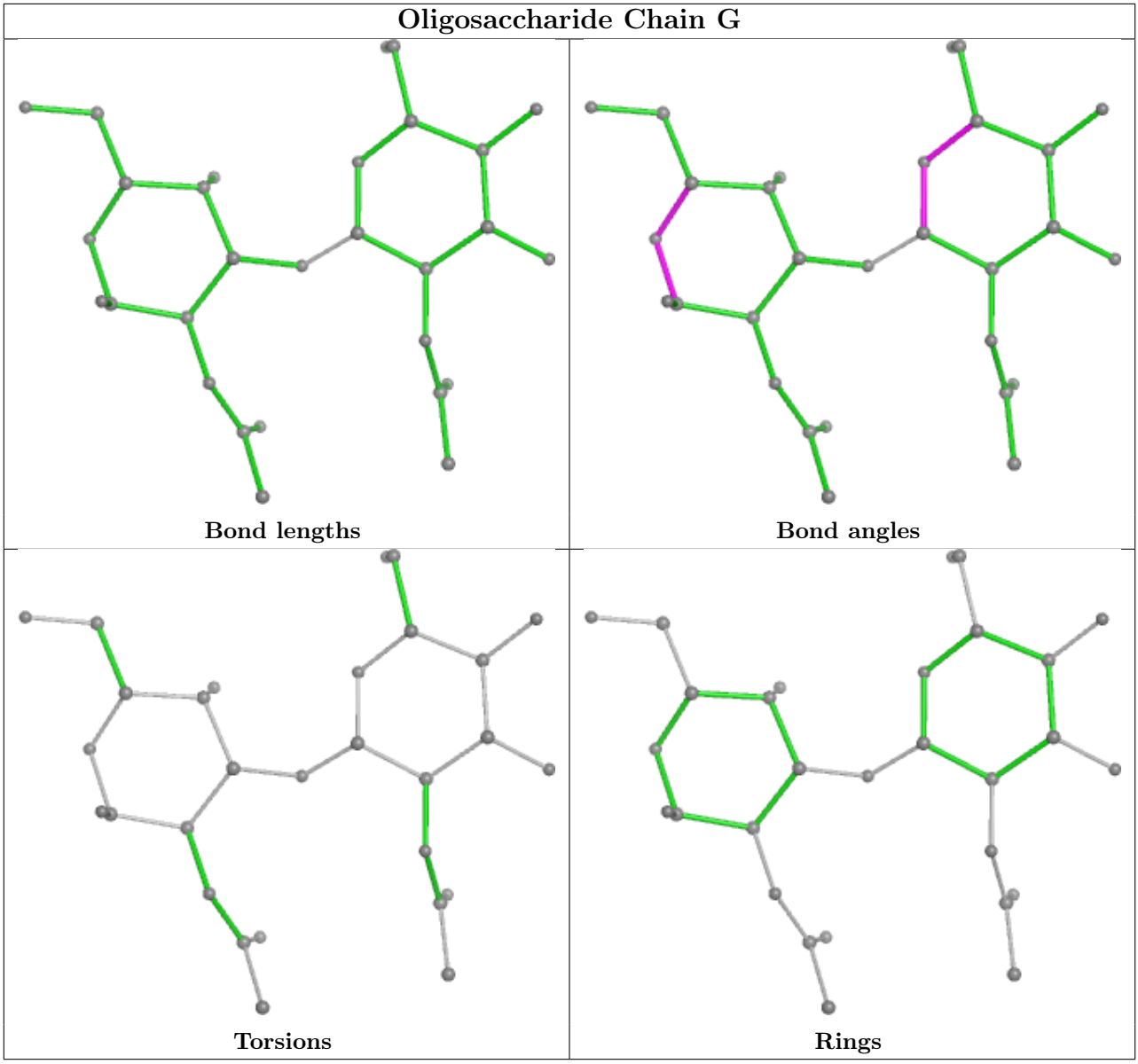
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	ACT	B	1953	-	3,3,3	0.78	0	3,3,3	1.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ACT	C	1951	-	3,3,3	0.77	0	3,3,3	1.35	0
5	ACT	D	1951	-	3,3,3	0.96	0	3,3,3	1.08	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1951	ACT	1	0
5	D	1951	ACT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	139/192 (72%)	-0.37	2 (1%)	75	74	12, 20, 35, 39	0
1	B	146/192 (76%)	-0.60	2 (1%)	75	74	10, 15, 28, 53	0
1	C	140/192 (72%)	-0.59	2 (1%)	75	74	11, 15, 32, 44	0
1	D	144/192 (75%)	-0.65	2 (1%)	75	74	11, 16, 25, 43	1 (0%)
All	All	569/768 (74%)	-0.56	8 (1%)	75	74	10, 16, 32, 53	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	916	GLU	3.4
1	A	916	GLU	2.7
1	A	856	GLY	2.7
1	B	949	GLU	2.3
1	C	916	GLU	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NGA	H	1	15/15	0.88	0.17	24,30,36,37	0
2	NGA	F	1	15/15	0.90	0.14	19,22,28,32	0

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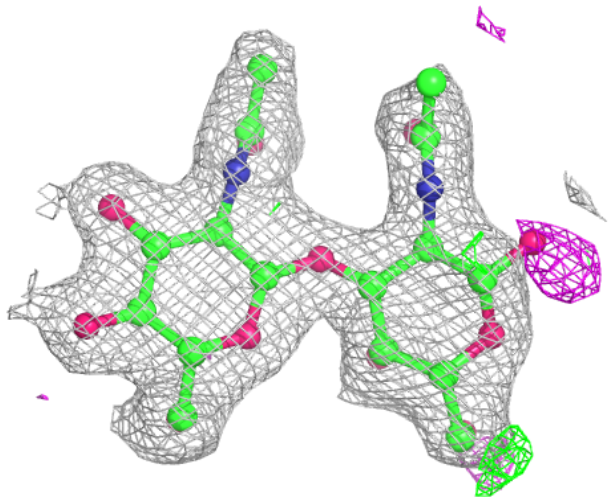
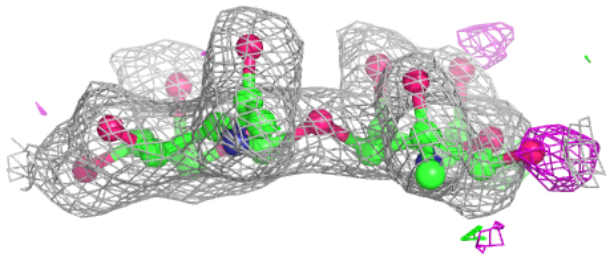
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NGA	E	1	15/15	0.90	0.17	30,36,42,44	0
3	A2G	G	1	15/15	0.92	0.09	13,16,19,22	0
2	NAG	E	2	14/15	0.96	0.07	19,23,27,28	0
2	NAG	H	2	14/15	0.96	0.07	12,17,19,19	0
2	NAG	F	2	14/15	0.96	0.07	13,16,17,18	0
3	NAG	G	2	14/15	0.97	0.07	11,13,17,20	0

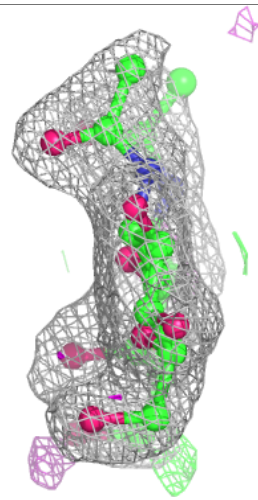
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

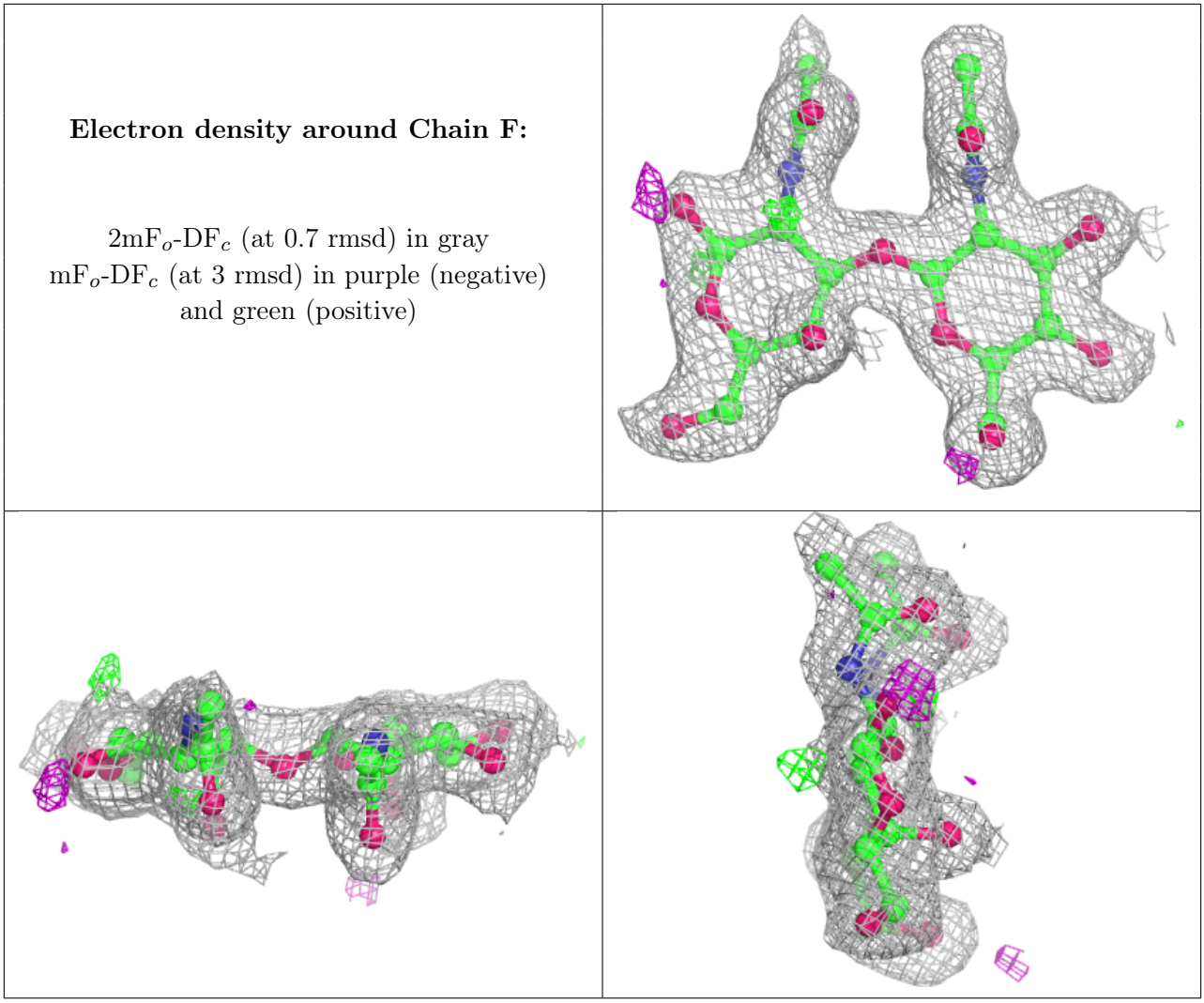






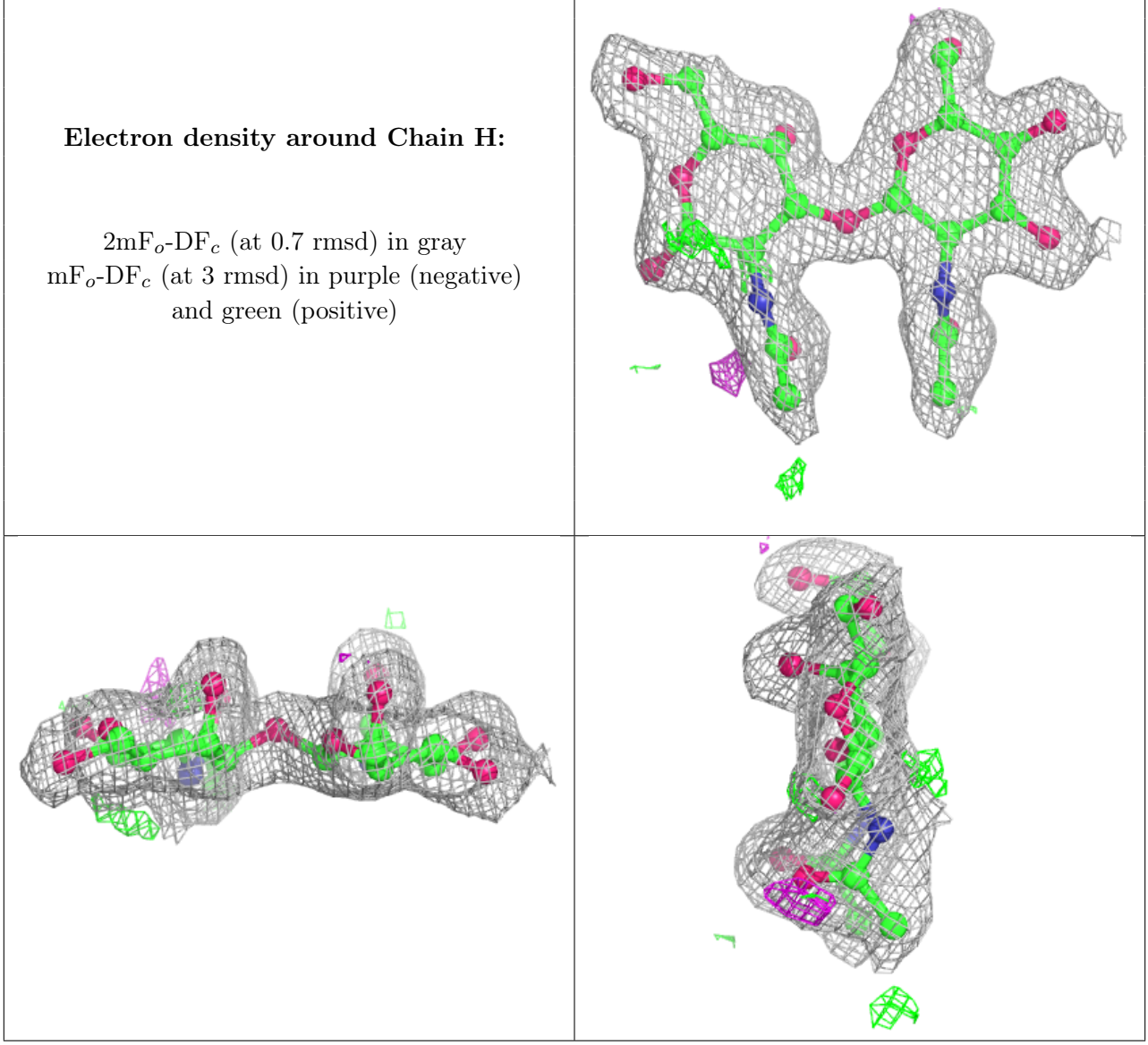
Electron density around Chain F:

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



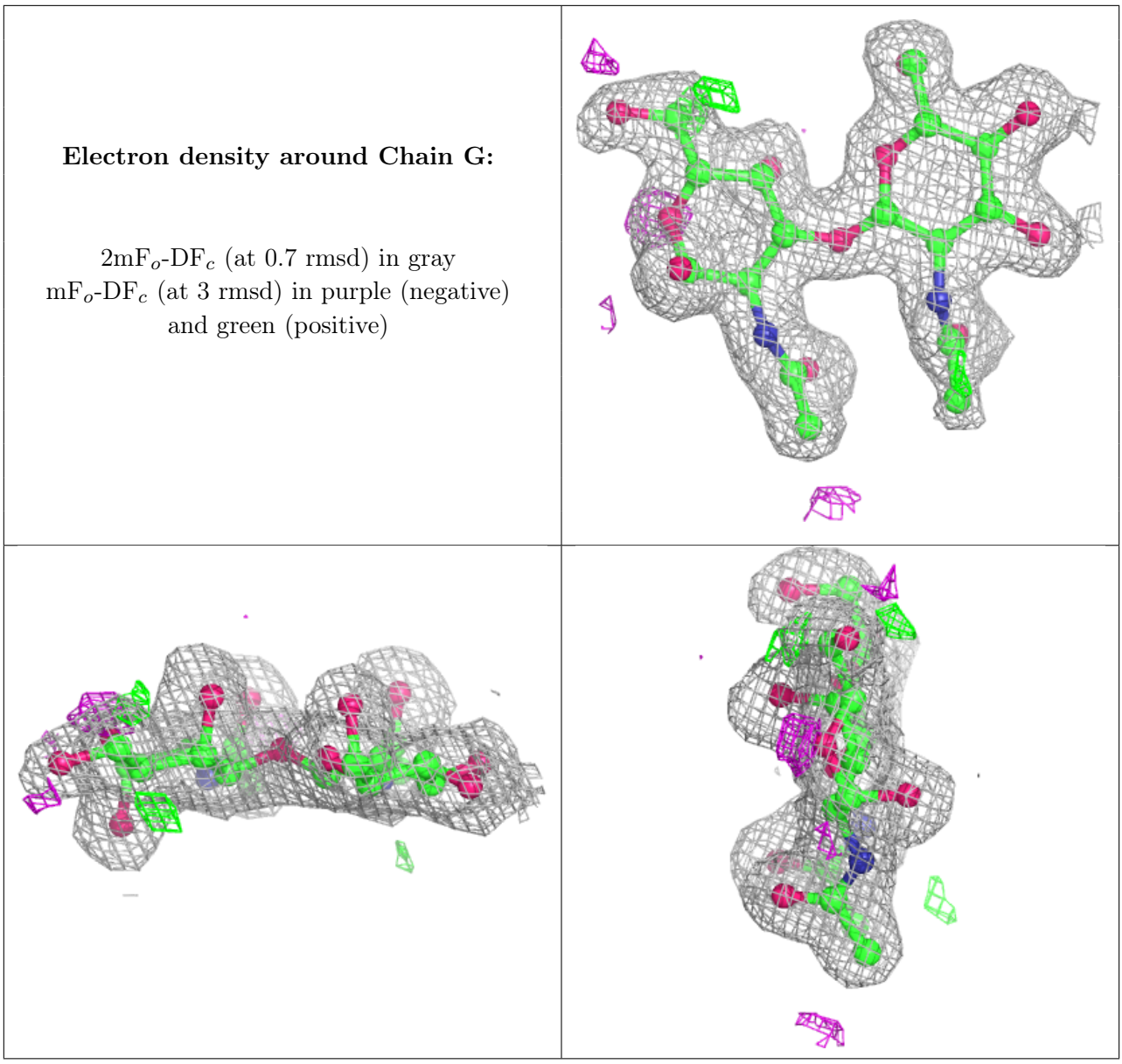
Electron density around Chain H:

$2mF_o$-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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	B	1953	4/4	0.53	0.28	47,47,47,48	0
5	ACT	C	1951	4/4	0.76	0.28	19,21,22,22	0
5	ACT	D	1951	4/4	0.88	0.22	27,27,27,29	0
4	CA	A	1948	1/1	0.98	0.03	19,19,19,19	0
4	CA	B	1952	1/1	0.99	0.04	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	D	1950	1/1	1.00	0.04	17,17,17,17	0
4	CA	C	1950	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.