



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:58 PM BST

PDB ID : 2ZHM
Title : Crystal structure of human galectin-9 N-terminal CRD in complex with N-acetyllactosamine trimer (crystal 1)
Authors : Nagae, M.; Nishi, N.; Murata, T.; Usui, T.; Nakamura, T.; Wakatsuki, S.; Kato, R.
Deposited on : 2008-02-06
Resolution : 1.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

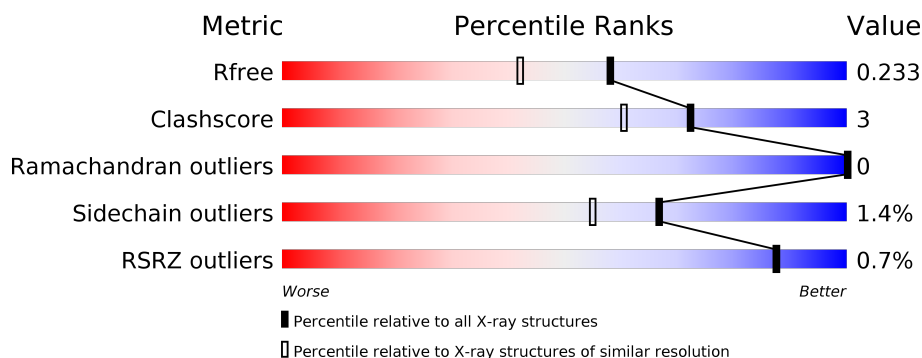
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



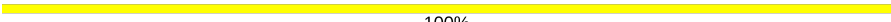
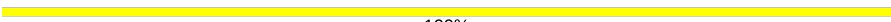
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 on 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 $\leq 5\%$. 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	148	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div> </div>
1	B	148	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	148	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>•</div> </div> </div>
1	D	148	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>• 5%</div> </div> </div>
2	E	6	<div> <div></div> <div>100%</div> </div>
2	F	6	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	5	 100%
4	H	4	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5258 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 Galectin-9.

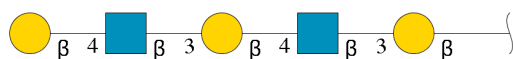
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	2	0
			1123	718	192	207	6			
1	B	142	Total	C	N	O	S	0	4	0
			1125	719	192	208	6			
1	C	142	Total	C	N	O	S	0	0	0
			1115	714	191	205	5			
1	D	141	Total	C	N	O	S	0	0	0
			1105	709	189	202	5			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



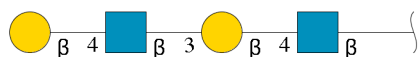
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			76	42	3	31			
2	F	6	Total	C	N	O	0	0	0
			76	42	3	31			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.



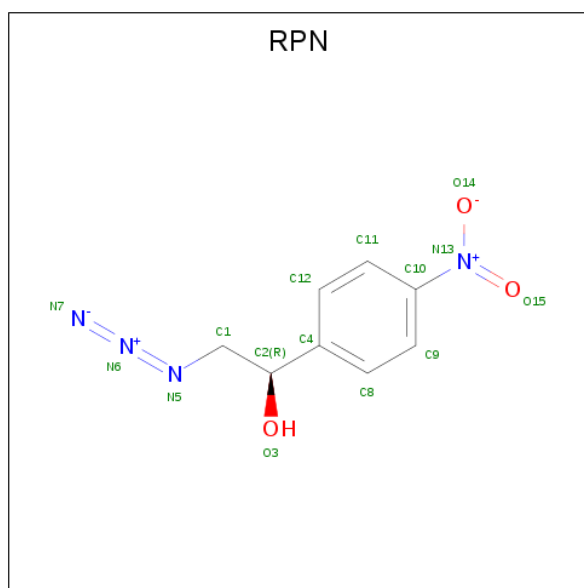
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			62	34	2	26			

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	0	0	0
			51	28	2	21			

- Molecule 5 is (R)-1-PARA-NITRO-PHENYL-2-AZIDO-ETHANOL (three-letter code: RPN) (formula: C₈H₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			9	6	1	2		
5	B	1	Total	C	N	O	0	0
			9	6	1	2		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total 148	O 148	0	0
6	B	140	Total 140	O 140	0	0
6	C	120	Total 120	O 120	0	0
6	D	99	Total 99	O 99	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.

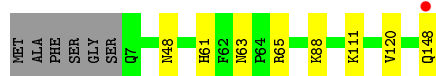
- Molecule 1: Galectin-9

Chain A: 



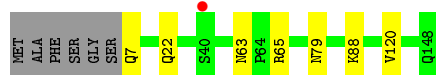
- Molecule 1: Galectin-9

Chain B: 



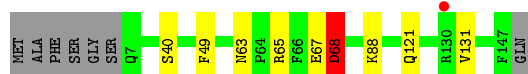
- Molecule 1: Galectin-9

Chain C: 



- Molecule 1: Galectin-9

Chain D: 



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

Chain E: 




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

Chain F:  100%


MAG1
GAL2
MAG3
GAL4
MAG5
GAL6

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

Chain G:  100%

GAL1
MAG2
GAL3
MAG4
GAL5

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

Chain H:  100%

MAG1
GAL2
MAG3
GAL4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	35.22Å 67.96Å 219.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.90 – 1.84 36.93 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.4 (36.90-1.84) 98.4 (36.93-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.235 0.182 , 0.233	Depositor DCC
R_{free} test set	2333 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 37.64 % 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 4.1576e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, NAG, RPN

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	0.59	0/1163	0.67	0/1575
1	B	0.59	0/1173	0.68	0/1589
1	C	0.57	0/1147	0.61	0/1554
1	D	0.58	0/1137	0.66	1/1542 (0.1%)
All	All	0.58	0/4620	0.66	1/6260 (0.0%)

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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68	ASP	N-CA-C	-5.47	96.24	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	67	GLU	Peptide

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	1123	0	1065	8	0
1	B	1125	0	1067	12	0
1	C	1115	0	1062	6	0
1	D	1105	0	1054	5	0
2	E	76	0	65	0	0
2	F	76	0	65	0	0
3	G	62	0	54	0	0
4	H	51	0	45	0	0
5	A	9	0	4	0	0
5	B	9	0	4	0	0
6	A	148	0	0	3	0
6	B	140	0	0	7	0
6	C	120	0	0	1	0
6	D	99	0	0	1	0
All	All	5258	0	4485	31	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.

All (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:A:148:GLN:HA	6:A:1398:HOH:O	1.34	1.25
1:B:148:GLN:HA	6:B:1387:HOH:O	1.56	1.04
1:B:148:GLN:O	6:B:1453:HOH:O	2.10	0.69
1:B:148:GLN:CA	6:B:1387:HOH:O	2.28	0.65
1:D:63:ASN:ND2	1:D:65:ARG:HE	1.96	0.64
1:B:148:GLN:HG3	6:B:1387:HOH:O	1.97	0.64
1:D:63:ASN:HD21	1:D:65:ARG:HE	1.47	0.63
1:A:129:HIS:HD2	6:A:1081:HOH:O	1.83	0.60
1:D:68:ASP:OD2	1:D:68:ASP:N	2.30	0.59
1:C:7:GLN:NE2	1:C:22:GLN:H	2.01	0.58
1:C:63:ASN:ND2	1:C:65:ARG:HE	2.01	0.58
1:B:88:LYS:HG2	1:B:120:VAL:HG11	1.86	0.57
1:B:63:ASN:HD21	1:B:65:ARG:HE	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:ND2	1:B:65:ARG:HE	2.04	0.55
1:C:7:GLN:N	6:C:1442:HOH:O	2.39	0.55
1:B:148:GLN:CG	6:B:1387:HOH:O	2.54	0.53
1:C:7:GLN:HE22	1:C:22:GLN:H	1.56	0.53
1:B:148:GLN:CB	6:B:1387:HOH:O	2.53	0.52
1:C:63:ASN:HD21	1:C:65:ARG:HE	1.59	0.51
1:D:88:LYS:HG3	6:D:1331:HOH:O	2.09	0.51
1:A:30:GLN:HG3	1:A:102[B]:CYS:SG	2.51	0.50
1:A:94:GLN:HG2	6:A:1523:HOH:O	2.10	0.50
1:A:63:ASN:HD21	1:A:65:ARG:HE	1.60	0.48
1:A:63:ASN:ND2	1:A:65:ARG:HE	2.11	0.48
1:B:88:LYS:HG2	1:B:120:VAL:CG1	2.44	0.47
1:B:88:LYS:HE2	6:B:1092:HOH:O	2.13	0.47
1:A:30:GLN:CG	1:A:102[B]:CYS:SG	3.03	0.47
1:A:49:PHE:HB3	1:A:131:VAL:HG11	2.00	0.44
1:B:48:ASN:ND2	1:B:61:HIS:ND1	2.64	0.43
1:D:49:PHE:HB3	1:D:131:VAL:HG11	2.02	0.42
1:C:88:LYS:HD3	1:C:120:VAL:HG12	2.03	0.41

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	143/148 (97%)	141 (99%)	2 (1%)	0	100	100
1	B	144/148 (97%)	142 (99%)	2 (1%)	0	100	100
1	C	140/148 (95%)	136 (97%)	4 (3%)	0	100	100
1	D	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
All	All	566/592 (96%)	556 (98%)	10 (2%)	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	125/127 (98%)	123 (98%)	2 (2%)	62	49
1	B	127/127 (100%)	126 (99%)	1 (1%)	81	75
1	C	123/127 (97%)	122 (99%)	1 (1%)	81	75
1	D	122/127 (96%)	119 (98%)	3 (2%)	47	31
All	All	497/508 (98%)	490 (99%)	7 (1%)	67	55

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	148	GLN
1	B	111	LYS
1	C	79	ASN
1	D	40	SER
1	D	68	ASP
1	D	121	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	63	ASN
1	A	78	GLN
1	A	129	HIS
1	B	48	ASN
1	B	63	ASN
1	B	106	GLN
1	B	129	HIS
1	C	7	GLN
1	C	22	GLN
1	C	63	ASN
1	C	121	GLN

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Mol	Chain	Res	Type
1	D	48	ASN
1	D	63	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 ⓘ

21 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	E	1	2	15,15,15	1.10	1 (6%)	21,21,21	0.81	0
2	GAL	E	2	2	11,11,12	1.20	1 (9%)	15,15,17	1.35	3 (20%)
2	NAG	E	3	2	14,14,15	0.63	0	17,19,21	2.15	3 (17%)
2	GAL	E	4	2	11,11,12	1.11	1 (9%)	15,15,17	1.56	5 (33%)
2	NAG	E	5	2	14,14,15	0.63	0	17,19,21	1.12	2 (11%)
2	GAL	E	6	2	11,11,12	0.51	0	15,15,17	0.85	1 (6%)
2	NAG	F	1	2	15,15,15	1.07	1 (6%)	21,21,21	0.90	0
2	GAL	F	2	2	11,11,12	1.22	1 (9%)	15,15,17	1.03	1 (6%)
2	NAG	F	3	2	14,14,15	0.64	0	17,19,21	1.63	2 (11%)
2	GAL	F	4	2	11,11,12	1.32	1 (9%)	15,15,17	1.68	4 (26%)
2	NAG	F	5	2	14,14,15	0.50	0	17,19,21	1.09	1 (5%)
2	GAL	F	6	2	11,11,12	0.54	0	15,15,17	0.97	1 (6%)
3	GAL	G	1	3	12,12,12	1.21	1 (8%)	17,17,17	1.35	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	2	3	14,14,15	1.11	1 (7%)	17,19,21	1.17	2 (11%)
3	GAL	G	3	3	11,11,12	1.20	1 (9%)	15,15,17	1.02	1 (6%)
3	NAG	G	4	3	14,14,15	0.55	0	17,19,21	1.05	1 (5%)
3	GAL	G	5	3	11,11,12	0.52	0	15,15,17	1.10	1 (6%)
4	NAG	H	1	4	15,15,15	0.90	1 (6%)	21,21,21	1.44	2 (9%)
4	GAL	H	2	4	11,11,12	1.25	1 (9%)	15,15,17	1.04	2 (13%)
4	NAG	H	3	4	14,14,15	0.47	0	17,19,21	1.19	2 (11%)
4	GAL	H	4	4	11,11,12	0.68	0	15,15,17	1.13	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	0/6/26/26	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1
2	GAL	E	4	2	-	1/2/19/22	0/1/1/1
2	NAG	E	5	2	-	0/6/23/26	0/1/1/1
2	GAL	E	6	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	NAG	F	3	2	-	0/6/23/26	0/1/1/1
2	GAL	F	4	2	-	0/2/19/22	0/1/1/1
2	NAG	F	5	2	-	2/6/23/26	0/1/1/1
2	GAL	F	6	2	-	0/2/19/22	0/1/1/1
3	GAL	G	1	3	-	2/2/22/22	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	GAL	G	3	3	-	0/2/19/22	0/1/1/1
3	NAG	G	4	3	-	0/6/23/26	0/1/1/1
3	GAL	G	5	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	4	-	0/6/26/26	0/1/1/1
4	GAL	H	2	4	-	0/2/19/22	0/1/1/1
4	NAG	H	3	4	-	0/6/23/26	0/1/1/1
4	GAL	H	4	4	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	GAL	O3-C3	-4.08	1.33	1.43
3	G	1	GAL	O3-C3	-3.68	1.34	1.43
4	H	2	GAL	O3-C3	-3.65	1.34	1.43
2	E	1	NAG	O4-C4	-3.65	1.34	1.43
2	F	1	NAG	O4-C4	-3.64	1.34	1.43
3	G	3	GAL	O3-C3	-3.52	1.34	1.43
3	G	2	NAG	O4-C4	-3.44	1.34	1.43
2	E	2	GAL	O3-C3	-3.40	1.35	1.43
2	F	2	GAL	O3-C3	-3.31	1.35	1.43
2	E	4	GAL	O3-C3	-3.28	1.35	1.43
4	H	1	NAG	O4-C4	-2.90	1.36	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	NAG	C1-O5-C5	6.31	120.74	112.19
2	F	3	NAG	C1-O5-C5	4.67	118.53	112.19
2	E	3	NAG	C3-C4-C5	4.66	118.54	110.24
2	F	4	GAL	O5-C5-C6	4.38	114.07	107.20
4	H	1	NAG	O4-C4-C5	4.13	119.56	109.30
2	F	5	NAG	O5-C5-C6	3.48	112.66	107.20
4	H	1	NAG	O4-C4-C3	-3.32	102.67	110.35
3	G	3	GAL	O3-C3-C2	-3.27	103.73	109.99
2	F	3	NAG	C3-C4-C5	3.05	115.68	110.24
3	G	4	NAG	O5-C1-C2	-2.86	106.78	111.29
3	G	2	NAG	O4-C4-C5	2.68	115.94	109.30
3	G	5	GAL	C1-O5-C5	2.66	115.79	112.19
2	E	5	NAG	O5-C1-C2	-2.65	107.11	111.29
2	E	4	GAL	O5-C5-C6	2.63	111.33	107.20
2	E	4	GAL	O3-C3-C4	2.62	116.40	110.35
3	G	1	GAL	O3-C3-C4	2.61	116.38	110.35
2	E	2	GAL	O3-C3-C2	-2.59	105.04	109.99
3	G	1	GAL	O5-C5-C6	2.57	112.84	106.44
2	E	2	GAL	C1-C2-C3	2.57	112.83	109.67
2	E	4	GAL	C1-O5-C5	2.57	115.67	112.19
2	F	4	GAL	C6-C5-C4	-2.56	107.00	113.00
2	F	2	GAL	C1-O5-C5	2.55	115.64	112.19
2	F	4	GAL	C1-O5-C5	2.53	115.62	112.19
4	H	3	NAG	O5-C1-C2	-2.50	107.34	111.29
4	H	3	NAG	C1-O5-C5	2.46	115.52	112.19
4	H	4	GAL	C1-O5-C5	2.36	115.38	112.19
4	H	2	GAL	C1-C2-C3	2.35	112.56	109.67
4	H	2	GAL	O3-C3-C2	2.34	114.48	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	4	GAL	C1-C2-C3	2.33	112.53	109.67
2	F	4	GAL	O3-C3-C2	2.30	114.39	109.99
2	E	2	GAL	O3-C3-C4	2.28	115.63	110.35
2	F	6	GAL	O5-C5-C6	2.24	110.72	107.20
2	E	3	NAG	O4-C4-C3	-2.24	105.18	110.35
2	E	6	GAL	O5-C5-C6	2.22	110.69	107.20
3	G	1	GAL	O3-C3-C2	2.19	115.42	110.35
2	E	5	NAG	O5-C5-C6	2.14	110.56	107.20
3	G	2	NAG	O7-C7-C8	-2.07	118.21	122.06
2	E	4	GAL	C1-C2-C3	2.06	112.19	109.67
2	E	4	GAL	O5-C1-C2	2.05	113.93	110.77
3	G	1	GAL	O5-C5-C4	-2.00	106.06	109.69

There are no chirality outliers.

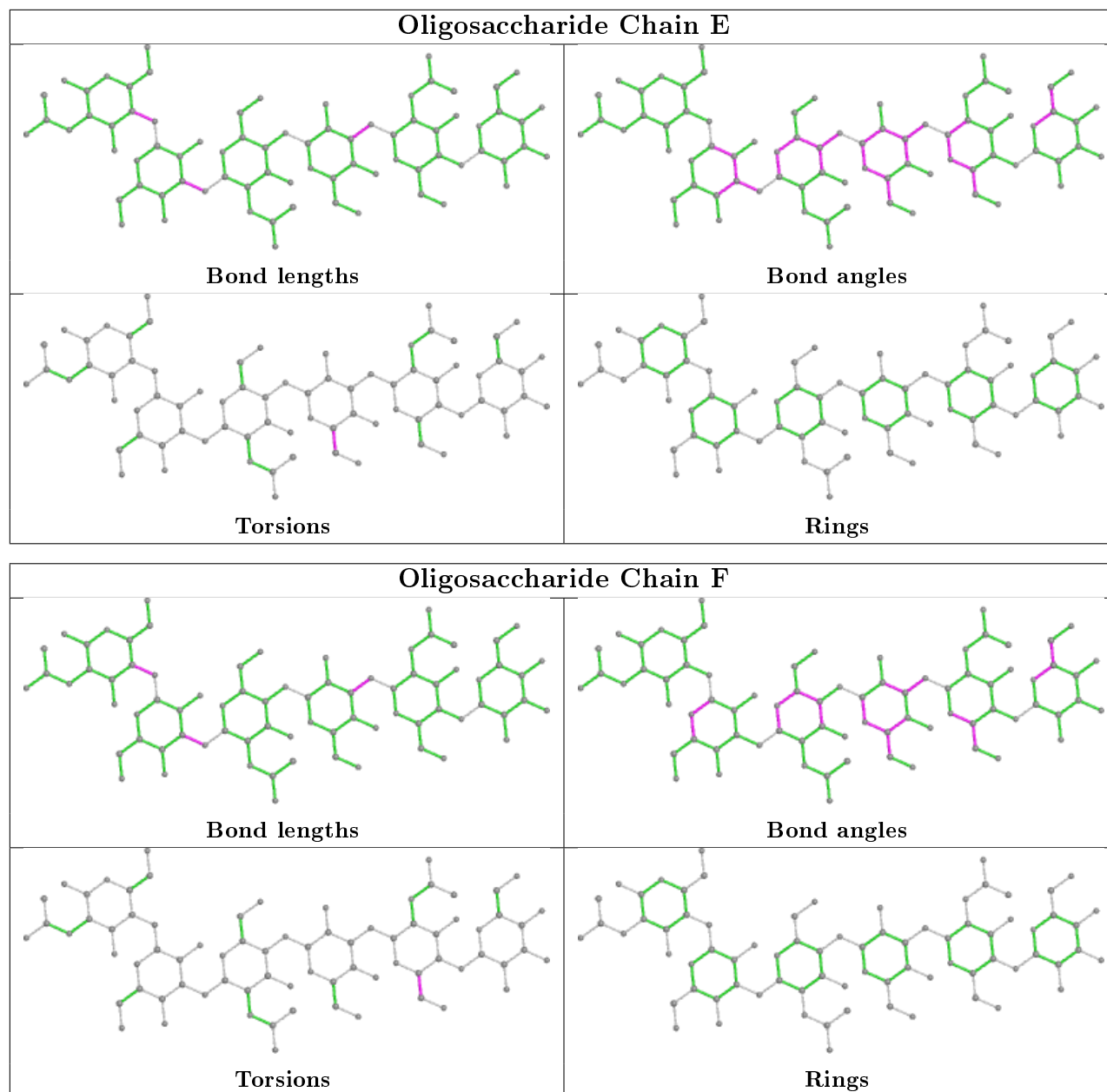
All (7) torsion outliers are listed below:

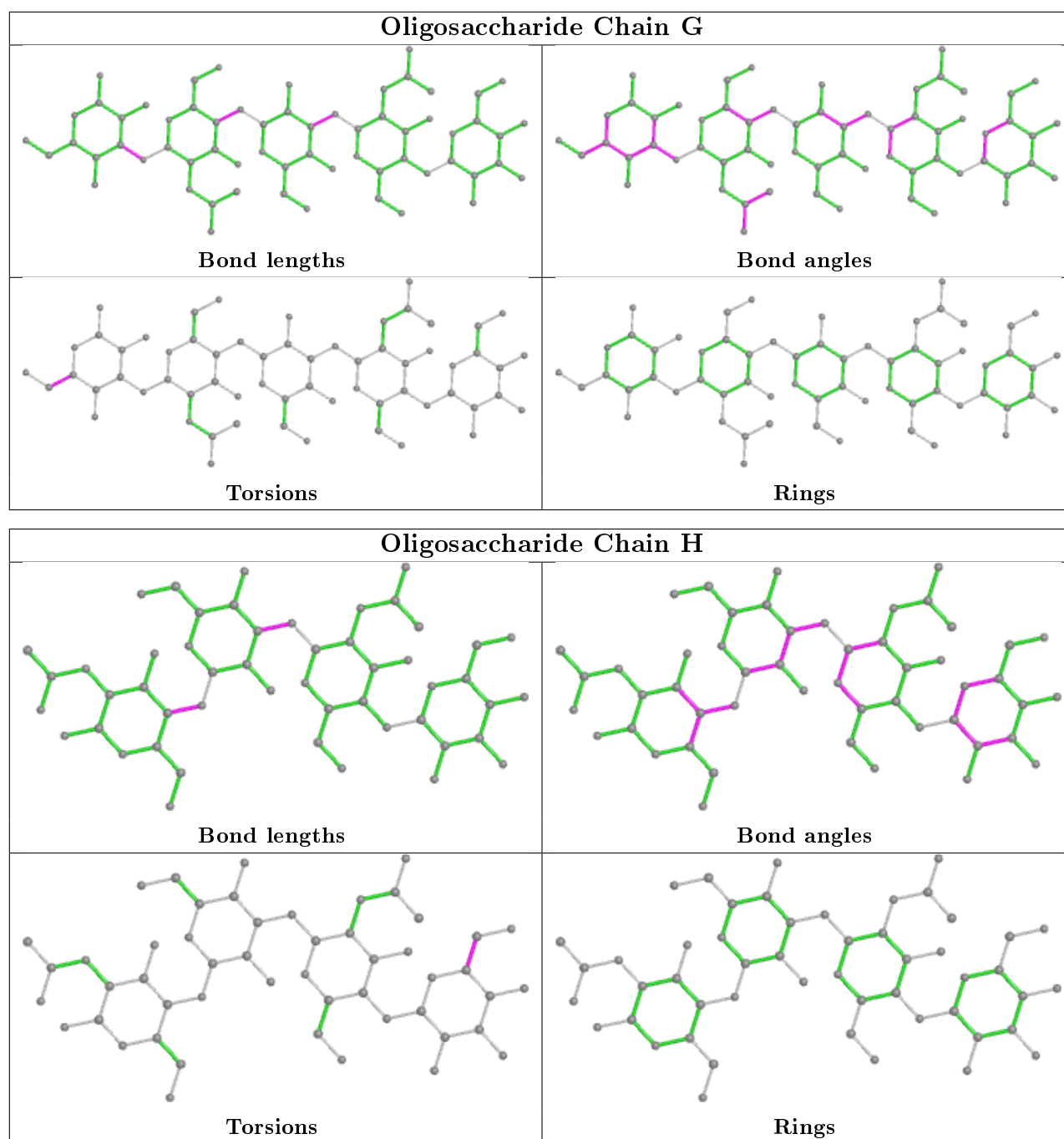
Mol	Chain	Res	Type	Atoms
4	H	4	GAL	C4-C5-C6-O6
3	G	1	GAL	O5-C5-C6-O6
4	H	4	GAL	O5-C5-C6-O6
3	G	1	GAL	C4-C5-C6-O6
2	F	5	NAG	C4-C5-C6-O6
2	F	5	NAG	O5-C5-C6-O6
2	E	4	GAL	O5-C5-C6-O6

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	RPN	B	1008	-	8,9,15	0.72	0	9,11,19	0.61	0
5	RPN	A	1001	-	8,9,15	0.79	0	9,11,19	1.01	1 (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
5	RPN	B	1008	-	-	0/2/4/12	0/1/1/1
5	RPN	A	1001	-	-	0/2/4/12	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	1001	RPN	O15-N13-C10	2.33	122.09	118.80

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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	143/148 (96%)	-0.49	1 (0%) 87 87	11, 17, 24, 34	0
1	B	142/148 (95%)	-0.42	1 (0%) 87 87	11, 16, 24, 32	0
1	C	142/148 (95%)	-0.38	1 (0%) 87 87	15, 21, 29, 35	0
1	D	141/148 (95%)	-0.26	1 (0%) 87 87	14, 23, 31, 39	0
All	All	568/592 (95%)	-0.39	4 (0%) 87 87	11, 19, 29, 39	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	GLN	3.5
1	B	148	GLN	3.2
1	C	40	SER	2.4
1	D	130	ARG	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

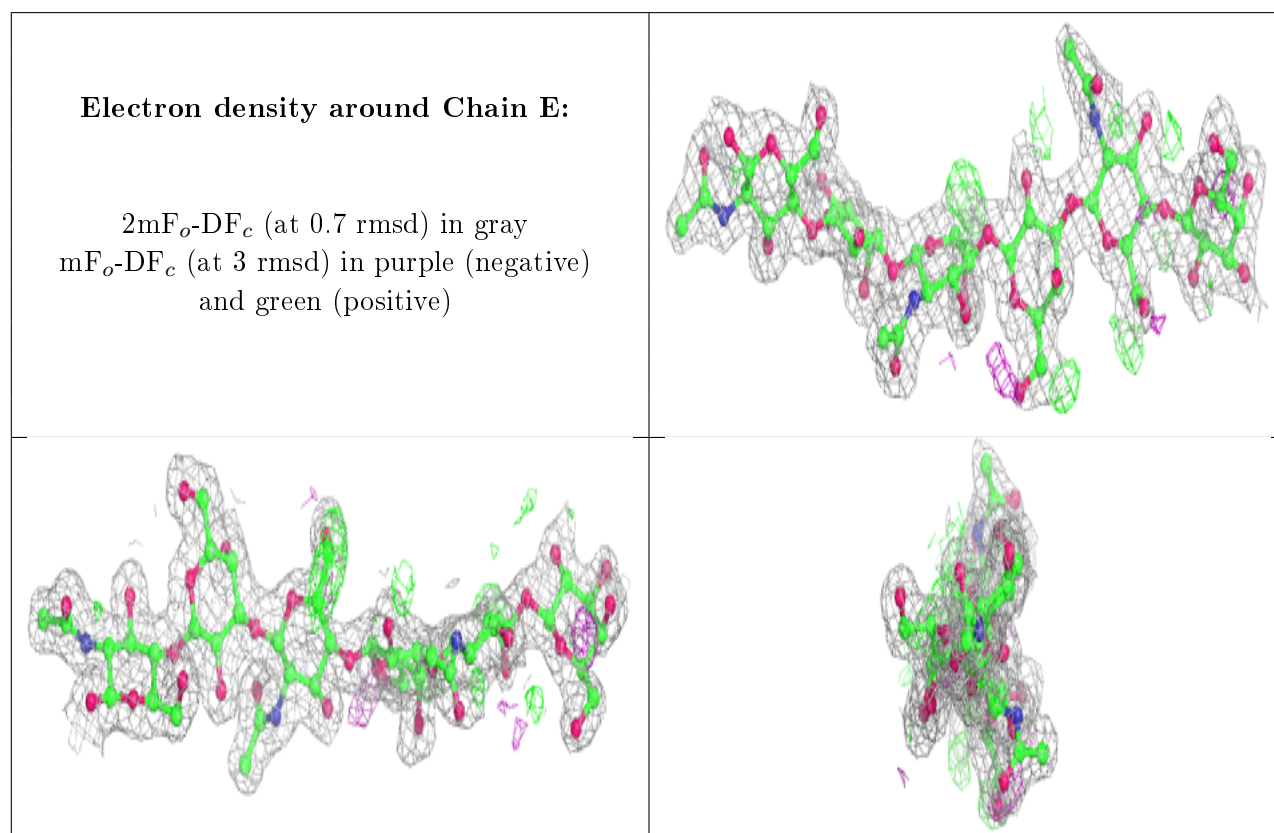
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	E	6	11/12	0.79	0.17	31,35,36,37	0
2	NAG	F	5	14/15	0.80	0.21	40,42,45,46	0
3	GAL	G	5	11/12	0.84	0.16	33,35,37,39	0

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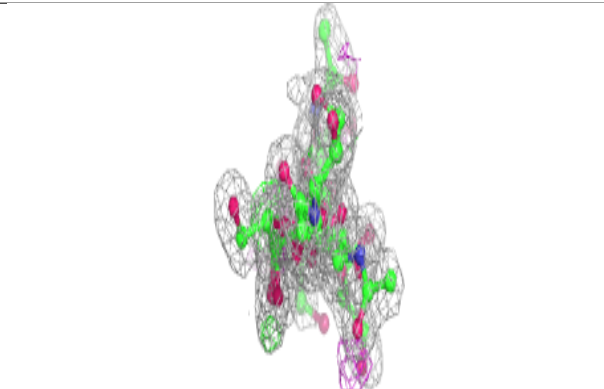
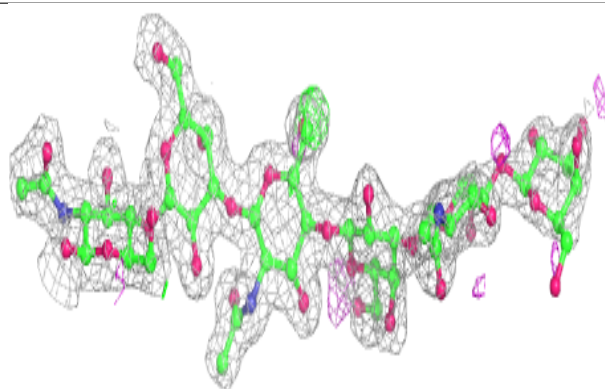
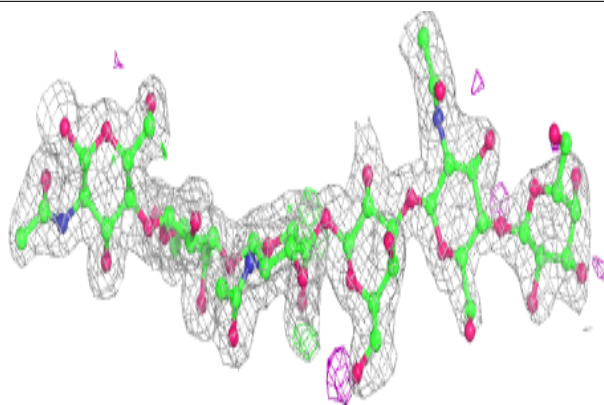
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAL	G	1	12/12	0.85	0.15	29,40,41,42	0
2	NAG	E	3	14/15	0.85	0.12	21,23,26,26	0
2	GAL	F	6	11/12	0.85	0.23	47,49,51,52	0
4	GAL	H	4	11/12	0.87	0.15	33,35,38,40	0
2	GAL	E	4	11/12	0.88	0.11	25,27,31,34	0
2	GAL	F	4	11/12	0.88	0.12	29,31,36,38	0
2	NAG	F	3	14/15	0.88	0.10	19,22,27,27	0
2	NAG	E	5	14/15	0.89	0.12	33,35,37,40	0
3	GAL	G	3	11/12	0.91	0.10	16,20,22,23	0
4	NAG	H	3	14/15	0.92	0.11	22,28,31,31	0
4	NAG	H	1	15/15	0.93	0.08	21,25,29,32	0
3	NAG	G	4	14/15	0.94	0.10	20,26,29,31	0
4	GAL	H	2	11/12	0.95	0.07	17,20,22,23	0
2	NAG	F	1	15/15	0.95	0.08	14,17,22,23	0
3	NAG	G	2	14/15	0.95	0.08	23,25,30,31	0
2	NAG	E	1	15/15	0.96	0.07	18,22,25,26	0
2	GAL	E	2	11/12	0.97	0.07	16,19,21,23	0
2	GAL	F	2	11/12	0.98	0.06	13,16,20,22	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.

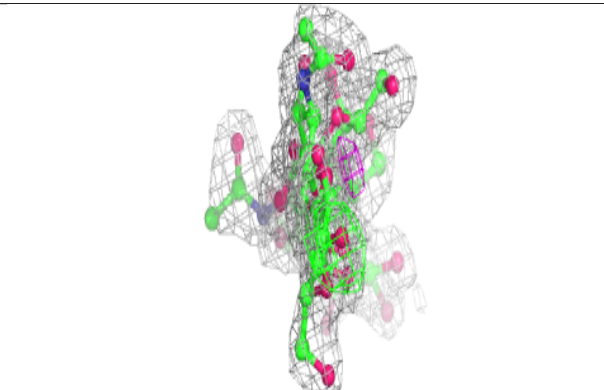
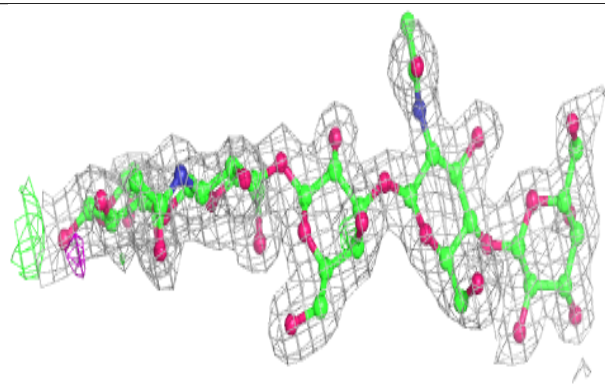
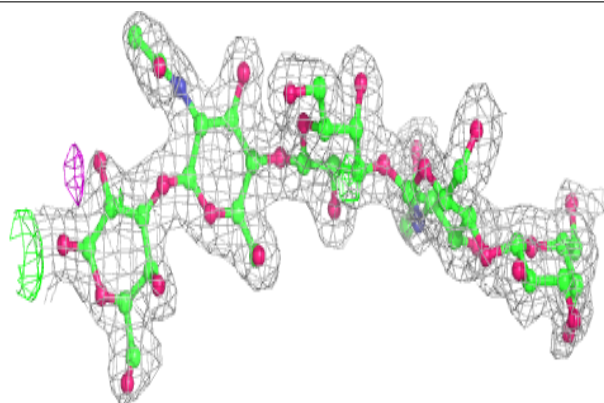


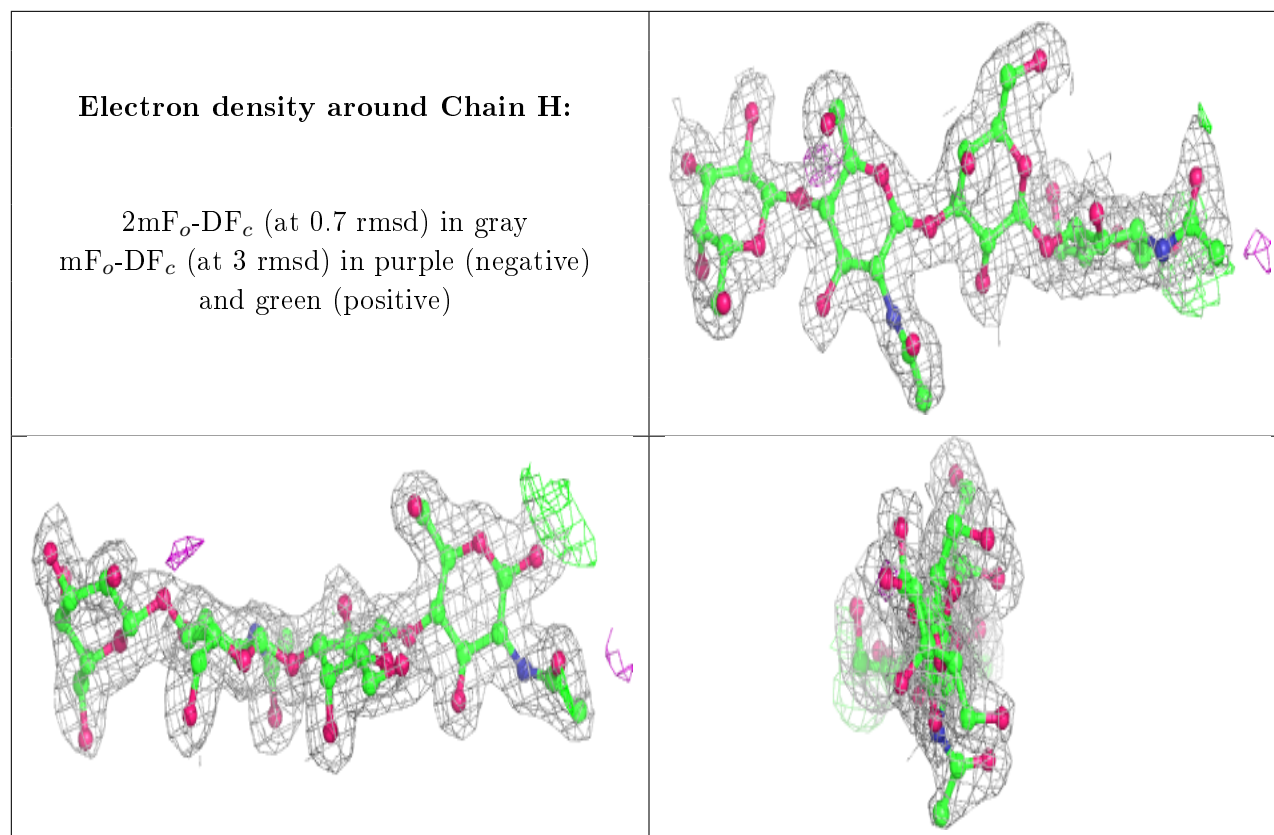
Electron density around Chain F:

$2mF_o-DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	RPN	A	1001	9/15	0.74	0.18	31,33,35,37	0
5	RPN	B	1008	9/15	0.85	0.16	26,28,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.