



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:54 AM BST

PDB ID : 4Q26  
Title : Crystal Structure of Galectin-1 in Complex with N-Acetyllactosamine  
Authors : Grimm, C.; Bertleff-Zieschang, N.  
Deposited on : 2014-04-07  
Resolution : 1.40 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 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

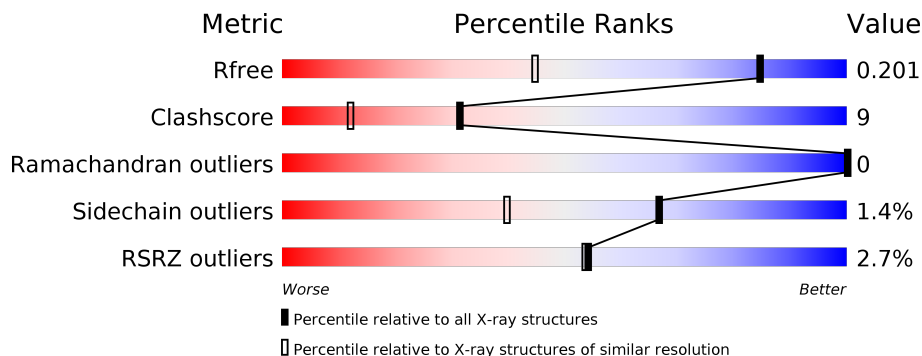
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	136	 86% 10% ..
1	B	136	 86% 11% ..
1	G	136	 79% 16% ...
1	H	136	 76% 21% ..
2	C	2	 100%
2	D	2	 50% 50%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 50% 50%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9095 atoms, of which 4195 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-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	133	2101	680	1025	184	203	9	0	8	0
1	B	133	2084	675	1016	182	202	9	0	5	0
1	G	133	2081	673	1013	183	202	10	0	6	0
1	H	133	2116	684	1033	184	205	10	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P09382
B	-1	GLY	-	expression tag	UNP P09382
G	-1	GLY	-	expression tag	UNP P09382
H	-1	GLY	-	expression tag	UNP P09382

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	51	14	25	1	11	0	0	0
2	D	2	51	14	25	1	11	0	0	0
2	E	2	51	14	25	1	11	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	H	N				O
2	F	2	51	14	25	1	11	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	G	1	14	3	8	3	0	0


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	113	Total	O	0	0
			113	113		
4	G	133	Total	O	0	0
			133	133		
4	H	116	Total	O	0	0
			116	116		

### 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.

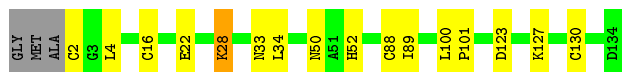
- Molecule 1: Galectin-1

Chain A: 




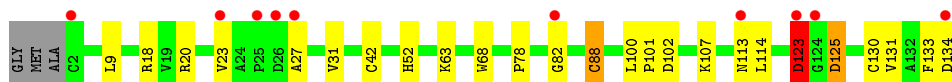
- Molecule 1: Galectin-1

Chain B: 




- Molecule 1: Galectin-1

Chain G: 



- Molecule 1: Galectin-1

Chain H: 



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

Chain C: 



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

Chain D: 

IDG1  
GAL2

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

Chain E:  100%IDG1  
GAL2

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

Chain F:  50% 50%IDG1  
GAL2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.38Å 85.52Å 116.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 1.40 48.02 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.02-1.40) 99.2 (48.02-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 1.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.162 , 0.203 0.161 , 0.201	Depositor DCC
$R_{free}$ test set	2000 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtrriage
Anisotropy	0.624	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 40.39 % 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 2.7560e-04. 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: GOL, CME, GAL, NDG

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	0.85	1/1083 (0.1%)	0.93	2/1464 (0.1%)
1	B	0.78	0/1056	0.87	1/1424 (0.1%)
1	G	0.93	3/1063 (0.3%)	0.99	4/1435 (0.3%)
1	H	0.75	1/1079 (0.1%)	0.87	3/1456 (0.2%)
All	All	0.83	5/4281 (0.1%)	0.91	10/5779 (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	G	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	123	ASP	C-O	6.17	1.35	1.23
1	G	42	CYS	CB-SG	-5.22	1.73	1.81
1	G	125	ASP	CB-CG	5.05	1.62	1.51
1	A	86	GLU	CB-CG	-5.03	1.42	1.52
1	H	105	GLU	CB-CG	-5.00	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	125	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	133	PHE	N-CA-C	-6.05	94.65	111.00
1	G	20	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	B	123	ASP	CB-CG-OD2	-5.65	113.21	118.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	92	ASP	CB-CG-OD1	5.46	123.22	118.30
1	H	123	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	G	123	ASP	O-C-N	5.26	132.15	123.20
1	H	75	ALA	N-CA-C	5.18	124.98	111.00
1	A	123	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	G	107	LYS	CD-CE-NZ	5.03	123.26	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	123	ASP	Peptide
1	G	133	PHE	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1076	1025	1025	19	1
1	B	1068	1016	1033	14	0
1	G	1068	1013	1023	28	1
1	H	1083	1033	1046	30	5
2	C	26	25	21	0	0
2	D	26	25	21	1	0
2	E	26	25	21	0	0
2	F	26	25	21	1	0
3	G	6	8	8	1	0
4	A	133	0	0	3	1
4	B	113	0	0	3	1
4	G	133	0	0	11	0
4	H	116	0	0	5	5
All	All	4900	4195	4219	78	7

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 9.

All (78) 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:G:113:ASN:N	4:G:408:HOH:O	1.97	0.97
1:G:82:GLY:O	4:G:433:HOH:O	1.86	0.94
1:G:113:ASN:CA	4:G:408:HOH:O	2.18	0.91
1:H:120:MET:SD	4:H:389:HOH:O	2.28	0.91
1:A:16:CME:SD	1:A:90[B]:THR:HG23	2.11	0.90
1:A:74:GLU:OE1	4:A:406:HOH:O	1.89	0.88
1:B:50:ASN:OD1	4:B:386:HOH:O	1.92	0.87
1:H:25:PRO:O	1:H:26:ASP:HB2	1.75	0.85
1:B:2:CYS:N	4:B:380:HOH:O	2.12	0.82
1:H:16:CME:SD	1:H:90[B]:THR:CG2	2.68	0.81
1:G:123:ASP:O	1:G:123:ASP:OD2	2.00	0.80
1:A:9:LEU:HD23	1:B:4[A]:LEU:CD1	2.13	0.79
1:G:52:HIS:O	4:G:330:HOH:O	2.02	0.77
1:H:16:CME:SD	1:H:90[B]:THR:HG22	2.25	0.77
1:H:102:ASP:OD2	4:H:366:HOH:O	2.05	0.75
1:G:9:LEU:CD2	1:H:4[A]:LEU:CD1	2.66	0.73
1:G:123:ASP:OD1	4:G:390:HOH:O	2.07	0.72
1:G:114:LEU:N	4:G:408:HOH:O	2.20	0.70
1:G:123:ASP:O	1:G:123:ASP:CG	2.29	0.70
1:G:123:ASP:CG	4:G:390:HOH:O	2.30	0.69
1:H:25:PRO:O	1:H:26:ASP:CB	2.39	0.69
1:G:9:LEU:HD23	1:H:4[A]:LEU:HD12	1.77	0.66
1:H:120:MET:CE	4:H:389:HOH:O	2.43	0.66
1:G:114:LEU:O	4:G:424:HOH:O	2.15	0.65
1:B:34[A]:LEU:HD11	1:B:89:ILE:HD13	1.81	0.62
1:H:16:CME:SD	1:H:90[B]:THR:HG23	2.38	0.62
1:H:4[B]:LEU:C	1:H:4[B]:LEU:HD23	2.21	0.61
1:H:33:ASN:C	1:H:34[B]:LEU:HD12	2.24	0.58
1:A:20:ARG:HH22	1:A:130:CME:HZ3	1.69	0.58
1:H:18:ARG:HB3	1:H:130:CME:OH	2.04	0.58
1:G:9:LEU:HD23	1:H:4[A]:LEU:CD1	2.33	0.57
1:A:16:CME:SD	1:A:90[B]:THR:CG2	2.90	0.57
1:G:18:ARG:NH2	4:G:429:HOH:O	1.85	0.57
1:A:9:LEU:CD2	1:B:4[A]:LEU:HD11	2.34	0.56
1:G:113:ASN:HA	4:G:408:HOH:O	1.96	0.56
1:G:131[B]:VAL:CG2	1:H:131[B]:VAL:HG22	2.36	0.56
1:A:100[A]:LEU:HB3	1:A:101:PRO:HD2	1.87	0.55
1:A:9:LEU:HD22	1:A:133:PHE:CE1	2.42	0.55
1:A:9:LEU:CD2	1:B:4[A]:LEU:CD1	2.84	0.54
1:A:9:LEU:HD23	1:B:4[A]:LEU:HD11	1.88	0.54
3:G:201:GOL:H11	1:H:128:ILE:O	2.08	0.54
1:A:20:ARG:NH2	1:A:130:CME:HZ3	2.22	0.54

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131[B]:VAL:HG23	1:H:131[B]:VAL:HG22	1.91	0.53
1:A:16:CME:HA	1:A:90[B]:THR:HG22	1.91	0.52
1:H:10:ASN:OD1	1:H:12:LYS:HE3	2.09	0.52
1:B:22:GLU:OE1	1:B:127:LYS:HE2	2.10	0.51
1:B:28:LYS:NZ	4:B:353:HOH:O	2.42	0.50
1:G:131[B]:VAL:HG22	1:H:131[B]:VAL:CG2	2.41	0.50
1:B:4[B]:LEU:HD23	1:B:4[B]:LEU:C	2.33	0.49
1:A:18:ARG:HB3	1:A:130:CME:HZ2	1.93	0.49
1:G:134:ASP:C	1:H:129:LYS:HE3	2.33	0.49
1:G:131[B]:VAL:CG2	1:H:131[B]:VAL:CG2	2.91	0.48
1:A:130:CME:HZ3	4:A:345:HOH:O	2.13	0.48
1:G:52:HIS:CE1	4:G:343:HOH:O	2.66	0.48
1:H:88:CME:SD	4:H:397:HOH:O	2.60	0.48
1:A:75:ALA:N	4:A:425:HOH:O	2.29	0.47
1:G:88:CME:OH	1:G:101:PRO:HA	2.14	0.47
1:H:34[A]:LEU:HD11	1:H:89:ILE:HD13	1.96	0.46
1:A:100[B]:LEU:HB3	1:A:101:PRO:HD2	1.96	0.46
1:G:9:LEU:CD2	1:H:4[A]:LEU:HD12	2.39	0.46
1:H:16:CME:SD	1:H:88:CME:HB2	2.56	0.46
1:B:88:CME:C	1:B:89:ILE:HG13	2.46	0.45
1:B:52:HIS:HB3	2:D:1:NDG:H3	1.98	0.45
1:A:120:MET:HB3	1:A:120:MET:HE3	1.74	0.45
1:H:34[B]:LEU:HD12	1:H:34[B]:LEU:N	2.32	0.45
1:B:100:LEU:HB3	1:B:101:PRO:HD2	1.98	0.45
1:A:130:CME:C	1:A:130:CME:SD	3.05	0.44
1:B:33:ASN:C	1:B:34[B]:LEU:HD12	2.38	0.43
1:G:23:VAL:HG12	1:G:27:ALA:HB2	2.00	0.43
1:H:112[A]:LEU:HB2	4:H:310:HOH:O	2.19	0.43
1:A:100[A]:LEU:HD23	1:A:100[A]:LEU:HA	1.67	0.43
1:H:100:LEU:HB3	1:H:101:PRO:HD2	2.01	0.43
1:G:63:LYS:HE3	1:G:68:TRP:CE2	2.54	0.42
1:G:78:PRO:HG2	1:G:101:PRO:HD2	2.01	0.42
1:H:52:HIS:HB3	2:F:1:NDG:H3	2.02	0.42
1:G:100:LEU:HB3	1:G:101:PRO:HD2	2.02	0.42
1:H:4[B]:LEU:HD23	1:H:5:VAL:N	2.34	0.41
1:G:31:VAL:HB	1:G:123:ASP:HB3	2.02	0.41

All (7) 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)
1:H:20:ARG:NH2	4:H:321:HOH:O[4_455]	0.72	1.48
1:H:20:ARG:CZ	4:H:321:HOH:O[4_455]	1.33	0.87
1:H:20:ARG:HH22	4:H:321:HOH:O[4_455]	0.95	0.65
1:A:75:ALA:HB1	1:G:102:ASP:HB3[1_655]	1.33	0.27
4:A:375:HOH:O	4:B:361:HOH:O[4_554]	1.96	0.24
1:H:20:ARG:HH21	4:H:321:HOH:O[4_455]	1.40	0.20
1:H:20:ARG:NH1	4:H:321:HOH:O[4_455]	2.06	0.14

## 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	136/136 (100%)	133 (98%)	3 (2%)	0	100	100
1	B	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
1	G	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
1	H	136/136 (100%)	133 (98%)	3 (2%)	0	100	100
All	All	539/544 (99%)	528 (98%)	11 (2%)	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	113/107 (106%)	112 (99%)	1 (1%)	78	58
1	B	110/107 (103%)	109 (99%)	1 (1%)	78	58

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	112/107 (105%)	110 (98%)	2 (2%)	59	28
1	H	114/107 (106%)	112 (98%)	2 (2%)	59	28
All	All	449/428 (105%)	443 (99%)	6 (1%)	67	42

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	B	28	LYS
1	G	123	ASP
1	G	125	ASP
1	H	2	CYS
1	H	109	PRO

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

Mol	Chain	Res	Type
1	B	93	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

12 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	A	16	1	8,9,10	1.13	0	5,9,11	1.69	2 (40%)
1	CME	H	16	1	8,9,10	0.95	0	5,9,11	1.78	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CME	G	88	1	8,9,10	1.12	0	5,9,11	1.26	1 (20%)
1	CME	G	16	1	8,9,10	1.29	0	5,9,11	0.95	0
1	CME	B	130	1	8,9,10	1.21	1 (12%)	5,9,11	3.34	4 (80%)
1	CME	H	88	1	8,9,10	1.10	0	5,9,11	0.64	0
1	CME	H	130	1	8,9,10	1.24	1 (12%)	5,9,11	3.17	4 (80%)
1	CME	G	130	1	8,9,10	0.96	0	5,9,11	2.43	1 (20%)
1	CME	A	130	1	8,9,10	1.05	0	5,9,11	3.30	3 (60%)
1	CME	B	16	1	8,9,10	0.95	0	5,9,11	1.93	1 (20%)
1	CME	B	88	1	8,9,10	1.15	0	5,9,11	0.80	0
1	CME	A	88	1	8,9,10	1.21	0	5,9,11	2.04	2 (40%)

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
1	CME	A	16	1	-	0/5/8/10	-
1	CME	H	16	1	-	1/5/8/10	-
1	CME	G	88	1	-	0/5/8/10	-
1	CME	G	16	1	-	0/5/8/10	-
1	CME	B	130	1	-	1/5/8/10	-
1	CME	H	88	1	-	1/5/8/10	-
1	CME	H	130	1	-	2/5/8/10	-
1	CME	G	130	1	-	2/5/8/10	-
1	CME	A	130	1	-	1/5/8/10	-
1	CME	B	16	1	-	0/5/8/10	-
1	CME	B	88	1	-	1/5/8/10	-
1	CME	A	88	1	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	130	CME	CA-N	-2.40	1.40	1.48
1	B	130	CME	CA-N	-2.38	1.41	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	CME	CE-SD-SG	6.18	131.93	103.45

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	CME	CE-SD-SG	4.99	126.45	103.45
1	G	130	CME	CE-SD-SG	4.89	126.00	103.45
1	H	130	CME	CZ-CE-SD	-4.54	97.60	113.37
1	B	130	CME	CZ-CE-SD	-3.81	100.15	113.37
1	B	16	CME	CB-SG-SD	3.69	113.38	103.82
1	H	130	CME	CE-SD-SG	3.60	120.02	103.45
1	H	16	CME	CB-SG-SD	3.45	112.76	103.82
1	B	130	CME	OH-CZ-CE	3.45	124.43	110.83
1	A	88	CME	CE-SD-SG	3.23	118.35	103.45
1	H	130	CME	OH-CZ-CE	3.20	123.44	110.83
1	A	130	CME	OH-CZ-CE	2.98	122.58	110.83
1	A	88	CME	OH-CZ-CE	-2.87	99.52	110.83
1	H	130	CME	CB-SG-SD	2.56	110.45	103.82
1	A	16	CME	OH-CZ-CE	2.55	120.88	110.83
1	A	16	CME	CZ-CE-SD	-2.54	104.54	113.37
1	A	130	CME	CB-SG-SD	-2.49	97.36	103.82
1	G	88	CME	CB-SG-SD	2.31	109.82	103.82
1	B	130	CME	CB-SG-SD	-2.11	98.36	103.82

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	130	CME	SD-CE-CZ-OH
1	A	88	CME	SD-CE-CZ-OH
1	H	130	CME	CE-SD-SG-CB
1	H	16	CME	SD-CE-CZ-OH
1	B	130	CME	SD-CE-CZ-OH
1	G	130	CME	SD-CE-CZ-OH
1	A	130	CME	SD-CE-CZ-OH
1	G	130	CME	CE-SD-SG-CB
1	B	88	CME	SD-CE-CZ-OH
1	H	88	CME	CA-CB-SG-SD

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	16	CME	3	0
1	H	16	CME	4	0
1	G	88	CME	1	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	88	CME	2	0
1	H	130	CME	1	0
1	A	130	CME	5	0
1	B	88	CME	1	0

## 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	NDG	C	1	2	15,15,15	1.59	4 (26%)	21,21,21	1.17	3 (14%)
2	GAL	C	2	2	11,11,12	2.19	2 (18%)	15,15,17	1.33	2 (13%)
2	NDG	D	1	2	15,15,15	2.21	5 (33%)	21,21,21	1.99	5 (23%)
2	GAL	D	2	2	11,11,12	1.98	3 (27%)	15,15,17	1.73	4 (26%)
2	NDG	E	1	2	15,15,15	2.32	6 (40%)	21,21,21	1.51	5 (23%)
2	GAL	E	2	2	11,11,12	1.75	3 (27%)	15,15,17	1.51	3 (20%)
2	NDG	F	1	2	15,15,15	1.63	4 (26%)	21,21,21	1.75	4 (19%)
2	GAL	F	2	2	11,11,12	1.57	2 (18%)	15,15,17	1.55	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	C	1	2	-	0/6/26/26	0/1/1/1
2	GAL	C	2	2	-	0/2/19/22	0/1/1/1
2	NDG	D	1	2	-	0/6/26/26	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	NDG	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	NDG	F	1	2	-	0/6/26/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GAL	O5-C5	5.79	1.55	1.43
2	D	1	NDG	C1-C2	5.10	1.59	1.52
2	E	1	NDG	O5-C1	4.21	1.53	1.42
2	D	2	GAL	O5-C1	-4.01	1.37	1.43
2	E	1	NDG	C3-C2	-3.99	1.45	1.53
2	E	1	NDG	C4-C5	3.80	1.61	1.53
2	F	2	GAL	O5-C5	3.49	1.50	1.43
2	D	2	GAL	C4-C3	-3.47	1.43	1.52
2	E	1	NDG	O3-C3	3.32	1.50	1.43
2	D	1	NDG	C4-C3	-3.21	1.44	1.52
2	D	1	NDG	C4-C5	-3.12	1.46	1.53
2	F	1	NDG	C8-C7	3.10	1.57	1.50
2	D	1	NDG	O3-C3	2.95	1.49	1.43
2	C	1	NDG	C3-C2	-2.89	1.47	1.53
2	E	2	GAL	O5-C5	2.84	1.49	1.43
2	E	2	GAL	C4-C3	-2.79	1.45	1.52
2	E	1	NDG	O5-C5	-2.73	1.37	1.44
2	F	1	NDG	O3-C3	2.69	1.49	1.43
2	E	1	NDG	C4-C3	-2.61	1.45	1.52
2	E	2	GAL	C2-C3	2.60	1.56	1.52
2	C	2	GAL	C2-C3	2.57	1.56	1.52
2	C	1	NDG	C1-C2	2.55	1.56	1.52
2	D	1	NDG	C3-C2	-2.54	1.48	1.53
2	C	1	NDG	O3-C3	2.48	1.48	1.43
2	F	1	NDG	C4-C5	-2.46	1.47	1.53
2	D	2	GAL	C4-C5	2.41	1.58	1.53
2	F	1	NDG	C4-C3	-2.24	1.46	1.52
2	C	1	NDG	C4-C3	-2.12	1.46	1.52
2	F	2	GAL	C4-C5	2.00	1.57	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NDG	O3-C3-C2	-5.01	99.54	109.66
2	D	1	NDG	O3-C3-C2	-4.86	99.86	109.66
2	E	2	GAL	O3-C3-C2	-3.72	102.88	109.99
2	D	1	NDG	O7-C7-C8	3.63	128.79	122.06

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GAL	O3-C3-C2	-3.53	103.23	109.99
2	E	1	NDG	O3-C3-C2	-3.53	102.53	109.66
2	F	2	GAL	O3-C3-C2	-3.43	103.43	109.99
2	D	1	NDG	C1-C2-C3	-3.30	106.04	110.54
2	F	2	GAL	O5-C5-C4	-2.80	104.02	110.83
2	C	2	GAL	O3-C3-C2	-2.74	104.75	109.99
2	D	1	NDG	C8-C7-N2	-2.65	111.61	116.10
2	E	1	NDG	C2-N2-C7	-2.62	116.80	123.18
2	D	2	GAL	O4-C4-C3	2.60	116.37	110.35
2	F	1	NDG	C8-C7-N2	-2.54	111.80	116.10
2	F	1	NDG	O7-C7-C8	2.51	126.71	122.06
2	F	2	GAL	O5-C5-C6	2.47	111.08	107.20
2	C	1	NDG	C1-C2-N2	-2.44	107.90	110.73
2	F	1	NDG	O5-C5-C6	-2.44	100.36	106.44
2	C	2	GAL	C6-C5-C4	2.40	118.62	113.00
2	E	1	NDG	C1-C2-N2	-2.39	107.96	110.73
2	D	2	GAL	C3-C4-C5	-2.38	105.99	110.24
2	D	1	NDG	O3-C3-C4	-2.35	104.91	110.35
2	E	1	NDG	O7-C7-N2	2.26	126.11	121.95
2	E	1	NDG	C1-O5-C5	-2.16	109.59	113.66
2	C	1	NDG	O7-C7-N2	2.13	125.86	121.95
2	C	1	NDG	C8-C7-N2	-2.11	112.52	116.10
2	E	2	GAL	C1-C2-C3	-2.05	107.15	109.67
2	D	2	GAL	O5-C5-C6	2.03	110.39	107.20
2	E	2	GAL	C6-C5-C4	2.00	117.69	113.00

There are no chirality outliers.

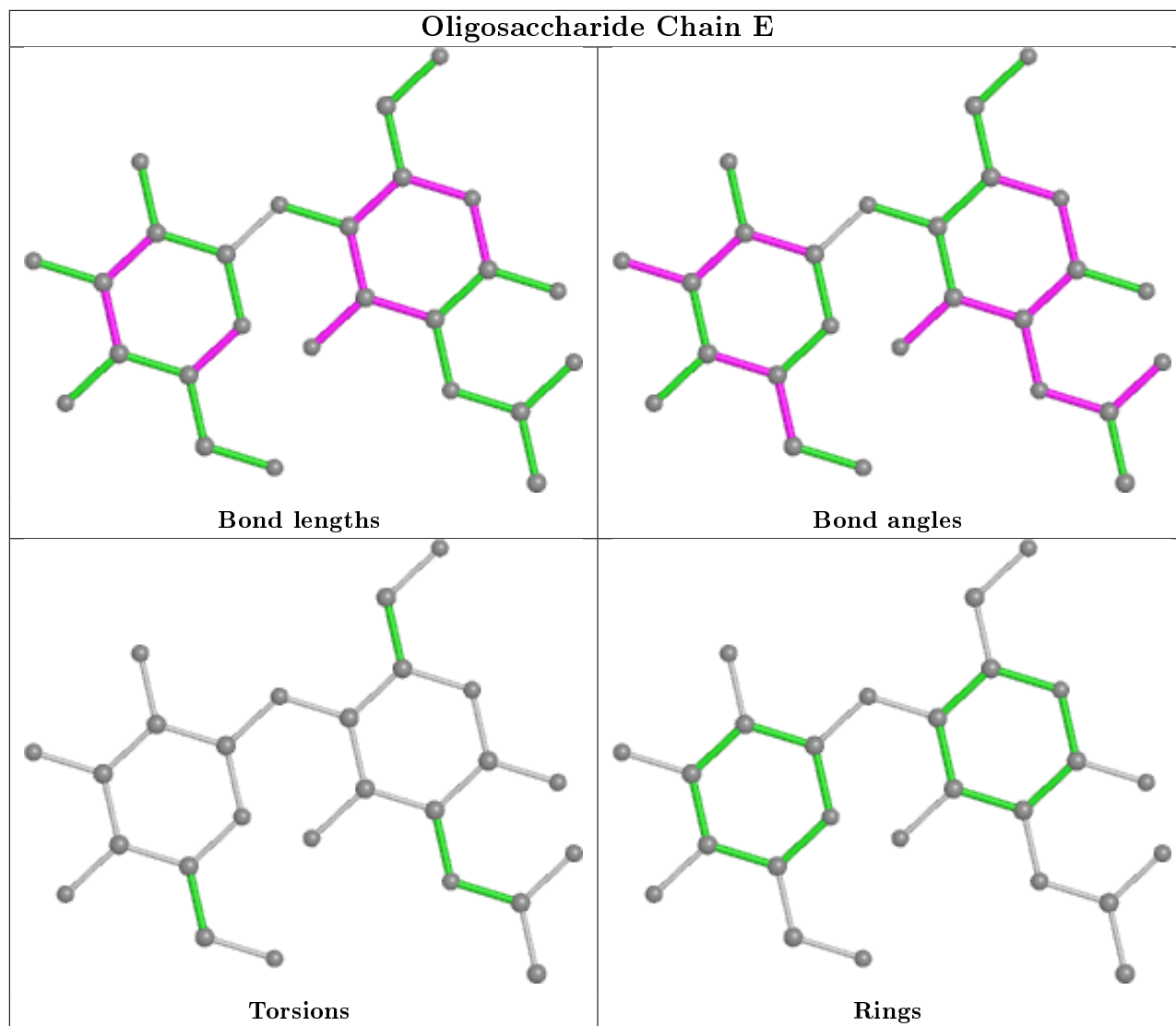
There are no torsion outliers.

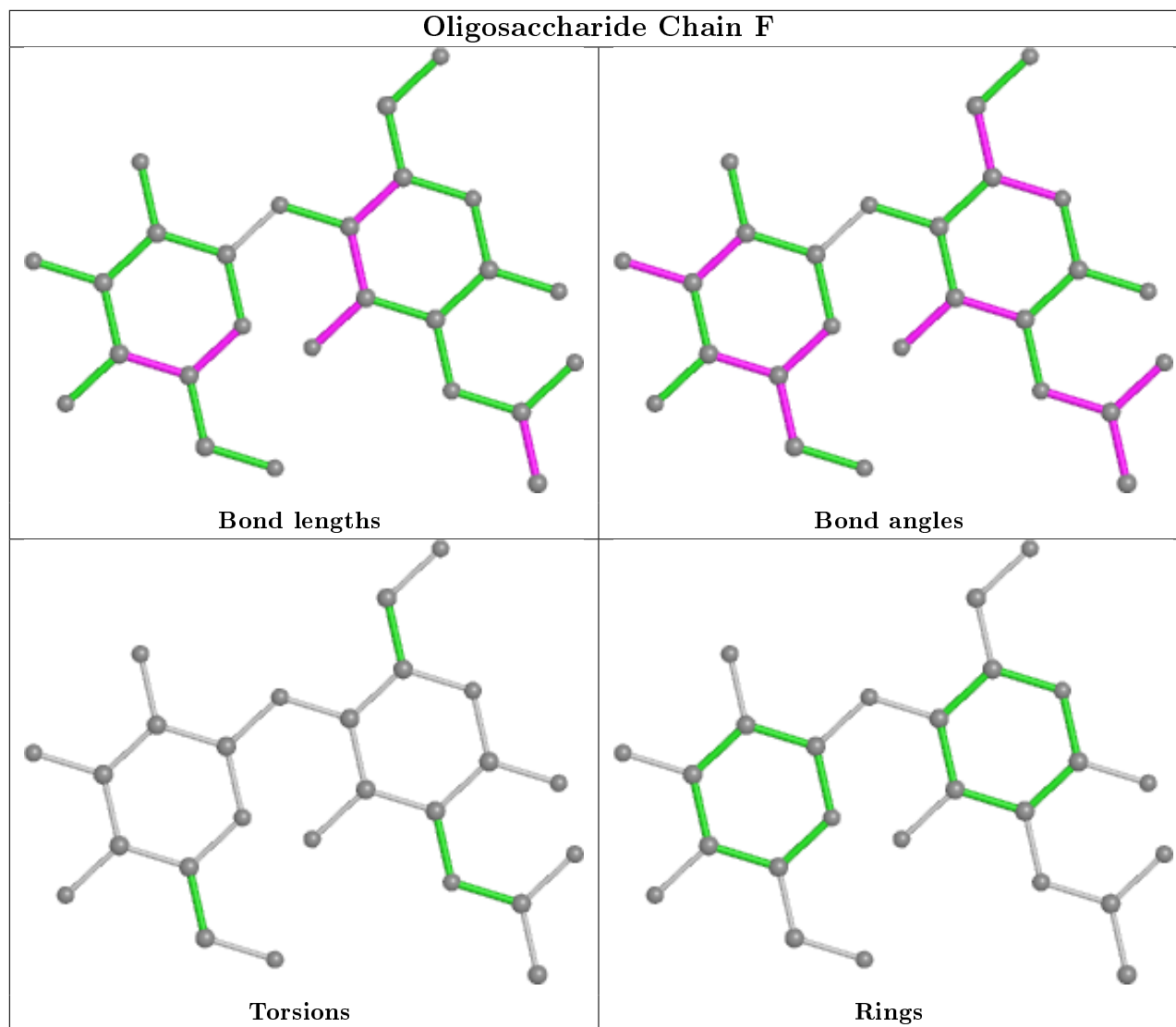
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NDG	1	0
2	D	1	NDG	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](#)

1 ligand is 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	GOL	G	201	-	5,5,5	0.60	0	5,5,5	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	G	201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	201	GOL	C1-C2-C3-O3
3	G	201	GOL	O2-C2-C3-O3
3	G	201	GOL	O1-C1-C2-O2
3	G	201	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	201	GOL	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 [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	130/136 (95%)	-0.26	1 (0%) 86 84	18, 25, 41, 60	0
1	B	130/136 (95%)	-0.20	0 100 100	16, 26, 43, 58	0
1	G	130/136 (95%)	0.10	10 (7%) 13 12	18, 27, 55, 71	0
1	H	130/136 (95%)	-0.19	3 (2%) 60 60	18, 29, 45, 60	0
All	All	520/544 (95%)	-0.14	14 (2%) 54 54	16, 26, 46, 71	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	27	ALA	4.7
1	G	134	ASP	4.5
1	G	25	PRO	4.4
1	G	113	ASN	4.1
1	H	2	CYS	3.2
1	G	2	CYS	3.1
1	G	124	GLY	3.0
1	G	23	VAL	2.9
1	G	123	ASP	2.8
1	H	93	GLN	2.4
1	G	82	GLY	2.3
1	A	134	ASP	2.2
1	G	26	ASP	2.2
1	H	75	ALA	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CME	B	130	10/11	0.90	0.12	14,30,61,66	0
1	CME	G	16	10/11	0.92	0.10	29,36,57,58	0
1	CME	H	16	10/11	0.92	0.15	28,38,69,72	0
1	CME	H	88	10/11	0.92	0.10	22,28,59,62	0
1	CME	H	130	10/11	0.93	0.13	21,31,77,81	0
1	CME	B	16	10/11	0.93	0.12	20,29,55,64	0
1	CME	G	130	10/11	0.94	0.12	18,24,66,67	0
1	CME	A	130	10/11	0.94	0.13	15,21,61,75	0
1	CME	G	88	10/11	0.94	0.11	19,29,67,69	0
1	CME	A	88	10/11	0.94	0.10	20,26,44,56	0
1	CME	B	88	10/11	0.96	0.07	20,26,47,54	0
1	CME	A	16	10/11	0.96	0.07	27,38,49,59	0

### 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.

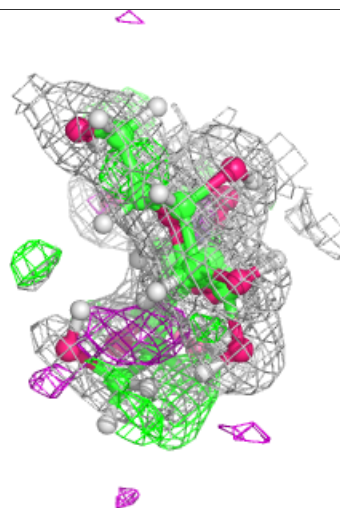
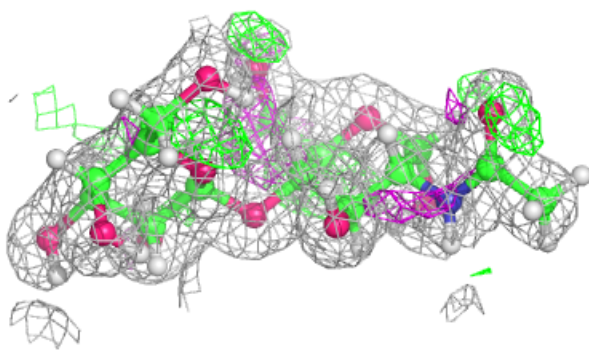
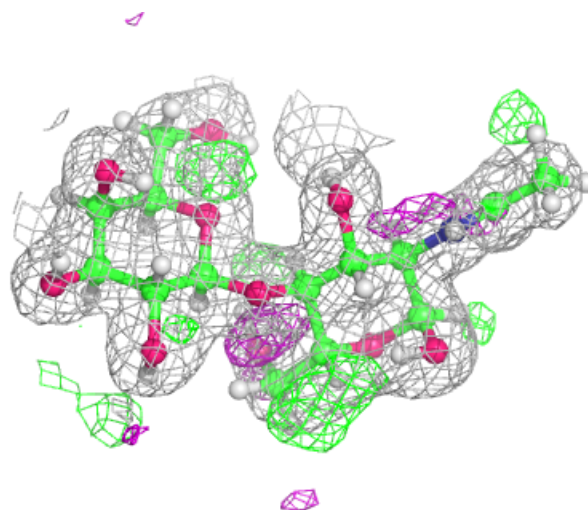
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDG	E	1	15/15	0.91	0.12	23,29,41,49	0
2	GAL	C	2	11/12	0.94	0.07	19,25,33,36	0
2	NDG	C	1	15/15	0.94	0.11	21,30,36,42	0
2	GAL	E	2	11/12	0.95	0.07	18,23,30,36	0
2	GAL	F	2	11/12	0.96	0.08	18,23,28,31	0
2	NDG	D	1	15/15	0.97	0.06	14,19,23,28	0
2	GAL	D	2	11/12	0.97	0.07	16,20,24,28	0
2	NDG	F	1	15/15	0.97	0.06	15,20,25,30	0

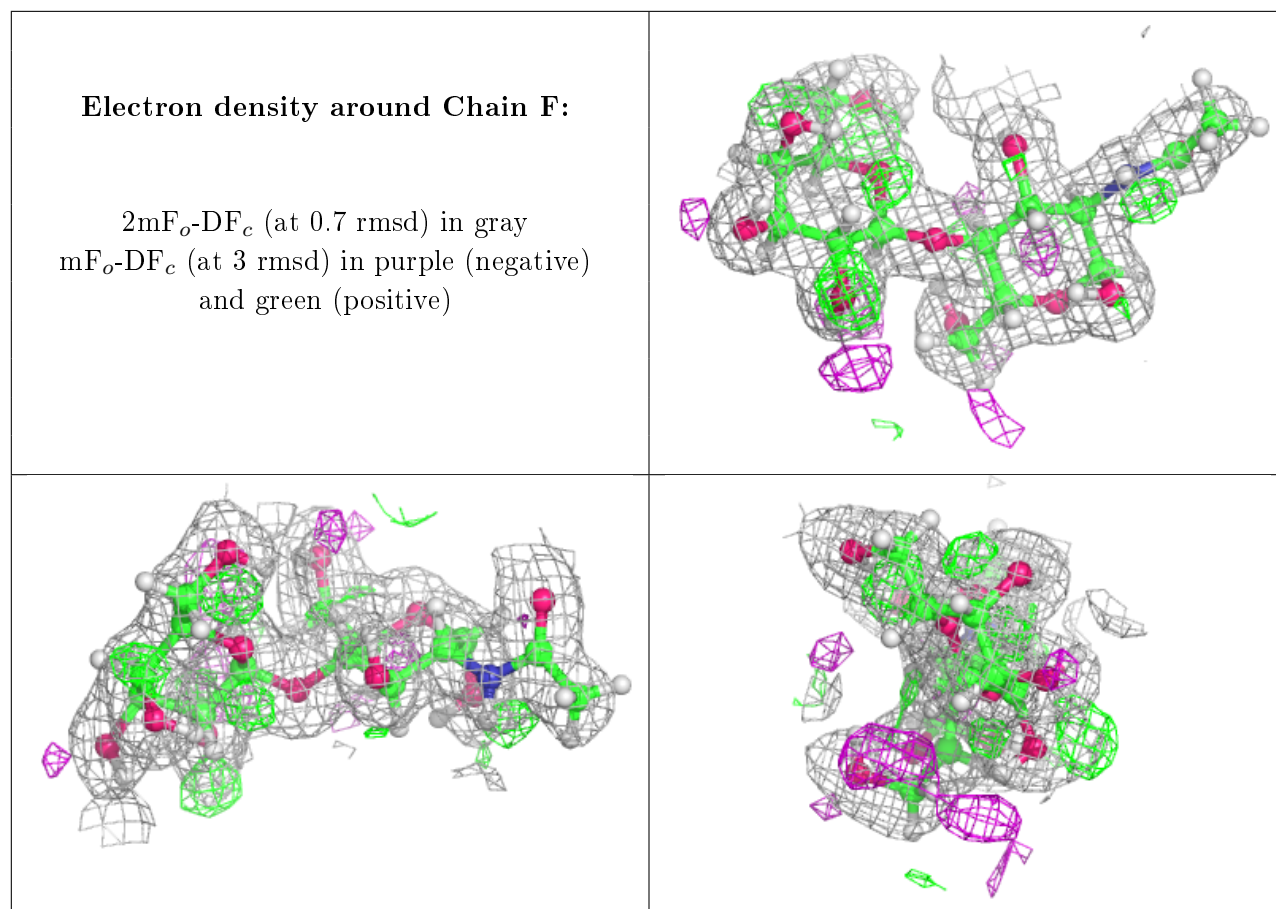
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 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(Å <sup>2</sup> )	Q<0.9
3	GOL	G	201	6/6	0.80	0.16	34,43,63,66	11

## 6.5 Other polymers [i](#)

There are no such residues in this entry.