



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 12:54 PM EDT

PDB ID : 6VSZ  
Title : Crystal structure of a human afucosylated IgG1 Fc expressed in tobacco plants  
(*Nicotiana benthamiana*)  
Authors : Tolbert, W.D.; Pazgier, M.  
Deposited on : 2020-02-12  
Resolution : 2.60 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
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) : 2.23.1

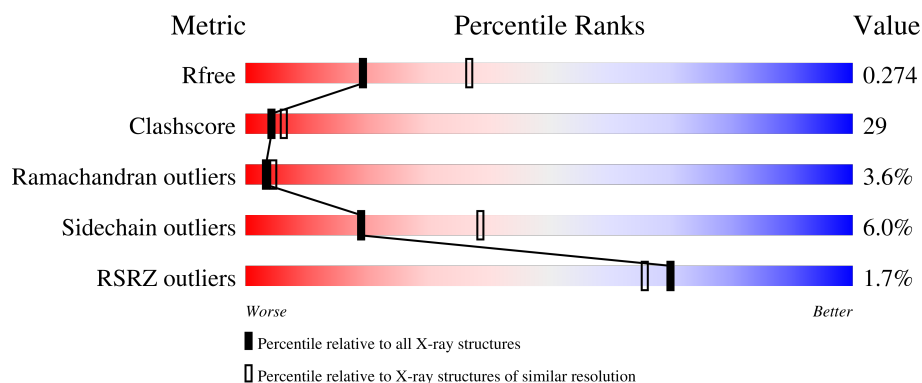
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	<div> <div></div> <div>62%</div> <div>33%</div> <div>..</div> </div>
1	B	211	<div> <div>3%</div> <div></div> <div>55%</div> <div>35%</div> <div>7%</div> <div>..</div> </div>
2	C	8	<div> <div>12%</div> <div>50%</div> <div>38%</div> </div>
2	D	8	<div> <div>12%</div> <div>38%</div> <div>50%</div> </div>

## 2 Entry composition [i](#)

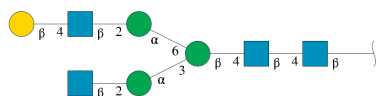
There are 3 unique types of molecules in this entry. The entry contains 3555 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1673	1064	284	319	6			
1	B	208	Total	C	N	O	S	0	0	0
			1662	1058	280	318	6			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			100	56	4	40			
2	D	8	Total	C	N	O	0	0	0
			100	56	4	40			

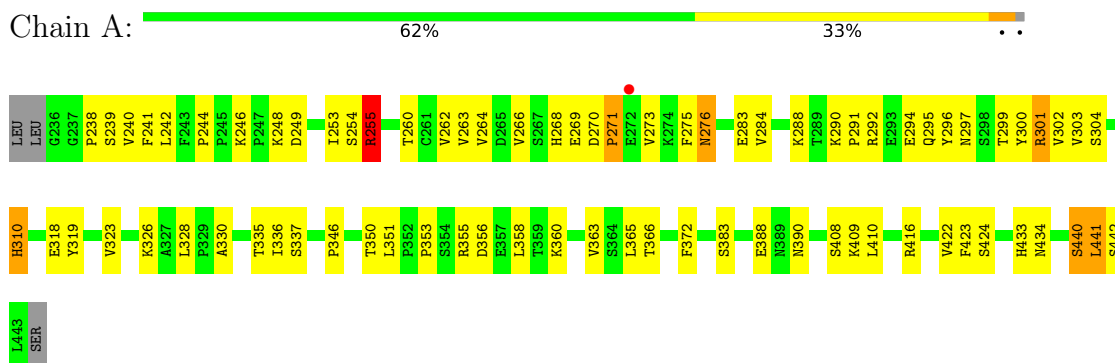
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	11	Total	O	0	0
			11	11		

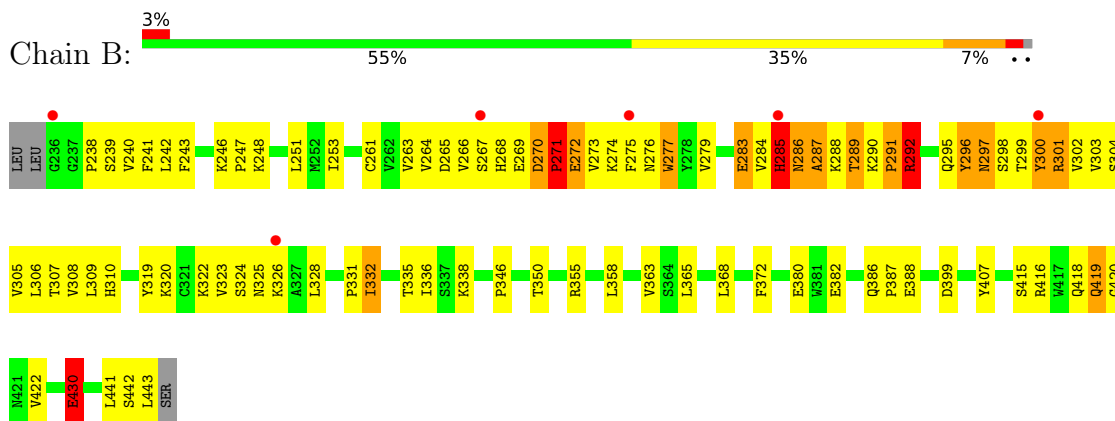
### 3 Residue-property plots

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.

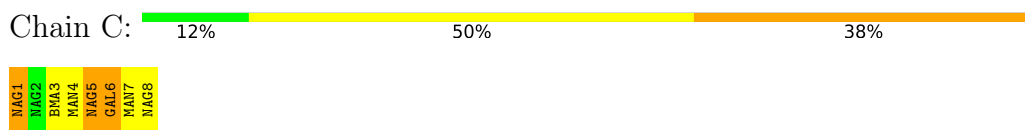
- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  12% 38% 50%

NAG1  
NAG2  
BNA3  
MAN4  
NAG5  
GAL6  
MAN7  
NAG8

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.70Å 80.32Å 136.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 68.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	87.1 (50.00-2.60) 87.1 (68.50-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.62Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???), REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.221 , 0.276 0.220 , 0.274	Depositor DCC
$R_{free}$ test set	769 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3555	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	0/1719	0.81	0/2341
1	B	0.67	2/1708 (0.1%)	0.76	1/2327 (0.0%)
All	All	0.66	2/3427 (0.1%)	0.78	1/4668 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	430	GLU	CD-OE2	-5.91	1.19	1.25
1	B	430	GLU	CD-OE1	-5.46	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	PRO	N-CA-C	5.60	126.66	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255[A]	ARG	Mainchain

## 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	1673	0	1640	81	0
1	B	1662	0	1628	124	0
2	C	100	0	85	4	0
2	D	100	0	84	8	0
3	A	9	0	0	2	0
3	B	11	0	0	0	0
All	All	3555	0	3437	204	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 29.

All (204) 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:B:270:ASP:H	1:B:271:PRO:HD2	1.00	1.14
1:B:266:VAL:CG1	1:B:300:TYR:HB2	1.76	1.13
1:B:277:TRP:CE3	1:B:306:LEU:CD2	2.31	1.13
1:B:266:VAL:HG11	1:B:300:TYR:HB2	1.33	1.10
1:B:277:TRP:CE3	1:B:306:LEU:HD23	1.86	1.09
1:B:323:VAL:CG1	1:B:332:ILE:HG22	1.89	1.02
1:B:270:ASP:N	1:B:271:PRO:HD2	1.82	0.95
1:A:358:LEU:HD23	1:A:363:VAL:HG11	1.53	0.90
1:A:350:THR:HG22	1:A:441:LEU:HD13	1.53	0.88
1:B:323:VAL:HG12	1:B:332:ILE:HG22	1.55	0.88
1:B:267:SER:O	1:B:271:PRO:HG3	1.74	0.87
1:B:241:PHE:HE2	2:D:2:NAG:H4	1.39	0.86
1:B:276:ASN:HB3	1:B:283:GLU:OE1	1.76	0.86
1:B:277:TRP:CZ3	1:B:306:LEU:HD23	2.12	0.85
1:B:277:TRP:CD2	1:B:306:LEU:HD23	2.12	0.84
1:B:325:ASN:HB3	1:B:328:LEU:HG	1.60	0.83
1:B:270:ASP:H	1:B:271:PRO:CD	1.85	0.82
1:B:240:VAL:HG21	1:B:323:VAL:HG11	1.62	0.81
1:B:274:LYS:HD3	1:B:275:PHE:H	1.46	0.81
1:B:241:PHE:CE2	2:D:2:NAG:H4	2.17	0.79
1:B:253:ILE:H	1:B:253:ILE:HD12	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:SER:HG	1:A:440:SER:HG	1.30	0.79
1:A:318:GLU:HG3	1:A:337:SER:OG	1.83	0.78
1:B:292:ARG:HB2	1:B:292:ARG:NH1	1.97	0.78
1:B:277:TRP:CD1	1:B:287:ALA:HB2	2.19	0.77
1:A:383:SER:HB2	1:A:423:PHE:HA	1.67	0.75
1:A:249:ASP:OD1	1:A:255[A]:ARG:NH1	2.20	0.75
1:A:255[B]:ARG:HB2	1:A:255[B]:ARG:HH11	1.52	0.75
1:B:264:VAL:HG22	1:B:265:ASP:H	1.52	0.74
1:B:338:LYS:NZ	1:B:430:GLU:OE2	2.20	0.74
1:A:409:LYS:NZ	1:B:399:ASP:OD2	2.21	0.73
1:B:287:ALA:HB1	1:B:304:SER:OG	1.89	0.72
1:B:292:ARG:HD2	1:B:300:TYR:HD2	1.54	0.72
1:B:350:THR:HB	1:B:441:LEU:HD13	1.71	0.72
1:A:295:GLN:HG2	2:C:1:NAG:H62	1.69	0.72
1:B:269:GLU:O	1:B:270:ASP:OD2	2.07	0.72
1:B:266:VAL:HG12	1:B:300:TYR:HB2	1.69	0.72
1:B:277:TRP:CZ3	1:B:306:LEU:CD2	2.71	0.72
1:B:285:HIS:O	1:B:286:ASN:ND2	2.23	0.71
1:A:275:PHE:CD2	1:A:304:SER:HB2	2.26	0.70
1:B:248:LYS:NZ	1:B:380:GLU:OE1	2.23	0.70
1:B:273:VAL:HG21	1:B:302:VAL:HG11	1.74	0.69
1:B:246:LYS:HG2	2:D:6:GAL:O4	1.94	0.68
1:B:267:SER:O	1:B:271:PRO:HD3	1.92	0.68
1:B:292:ARG:HD2	1:B:300:TYR:CD2	2.28	0.68
1:B:242:LEU:HD22	1:B:336:ILE:HG21	1.75	0.68
1:B:267:SER:O	1:B:271:PRO:CG	2.42	0.68
1:B:306:LEU:HD12	1:B:307:THR:O	1.95	0.67
1:B:277:TRP:CD2	1:B:306:LEU:CD2	2.75	0.67
1:B:274:LYS:HB3	1:B:324:SER:HB2	1.76	0.67
1:B:292:ARG:HB2	1:B:292:ARG:HH11	1.58	0.67
1:B:290:LYS:NZ	1:B:305:VAL:HG11	2.10	0.66
1:B:306:LEU:HD11	1:B:308:VAL:HG12	1.80	0.64
1:B:277:TRP:CE3	1:B:306:LEU:HD21	2.32	0.64
1:A:366:THR:HG1	1:B:407:TYR:HH	1.43	0.64
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.34	0.63
1:A:240:VAL:HG21	1:A:323:VAL:HG11	1.79	0.62
1:B:295:GLN:NE2	1:B:301:ARG:HB2	2.14	0.62
1:B:267:SER:C	1:B:271:PRO:HD3	2.19	0.62
1:B:264:VAL:HG21	2:D:1:NAG:O4	2.00	0.62
1:A:276:ASN:ND2	1:A:283:GLU:OE2	2.32	0.62
1:B:287:ALA:O	1:B:289:THR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:OE1	1:B:326:LYS:HD3	2.00	0.61
1:B:365:LEU:HD23	1:B:441:LEU:HD23	1.82	0.61
1:A:292:ARG:HE	1:A:300:TYR:HE1	1.46	0.61
1:B:322:LYS:HE2	1:B:331:PRO:CB	2.31	0.60
1:A:350:THR:CG2	1:A:441:LEU:HD13	2.27	0.60
1:B:306:LEU:CD1	1:B:308:VAL:HG12	2.32	0.60
1:B:284:VAL:O	1:B:285:HIS:O	2.20	0.60
1:B:274:LYS:HD3	1:B:275:PHE:N	2.17	0.60
1:B:272:GLU:OE1	1:B:326:LYS:CD	2.51	0.59
1:B:267:SER:O	1:B:271:PRO:CD	2.51	0.58
1:A:249:ASP:OD1	1:A:255[B]:ARG:HD2	2.04	0.58
1:B:290:LYS:HZ3	1:B:305:VAL:HG11	1.68	0.58
1:B:242:LEU:CD2	1:B:336:ILE:HG21	2.34	0.57
1:B:322:LYS:HE2	1:B:331:PRO:HB2	1.85	0.57
1:B:355:ARG:HA	1:B:358:LEU:HD12	1.85	0.57
1:B:266:VAL:CG1	1:B:300:TYR:CB	2.69	0.57
1:A:238:PRO:HA	1:A:264:VAL:O	2.04	0.57
1:B:240:VAL:HG21	1:B:332:ILE:HG21	1.87	0.57
1:B:320:LYS:HG2	1:B:335:THR:HG23	1.86	0.56
1:B:270:ASP:N	1:B:271:PRO:CD	2.58	0.56
1:A:266:VAL:HG21	1:A:273:VAL:HG21	1.88	0.56
1:B:242:LEU:HD22	1:B:336:ILE:CG2	2.36	0.56
1:A:260:THR:HG21	2:C:5:NAG:H61	1.87	0.56
1:B:415:SER:OG	1:B:416:ARG:N	2.39	0.55
1:A:255[A]:ARG:NH1	1:A:255[A]:ARG:HG2	2.22	0.55
1:B:323:VAL:CG1	1:B:332:ILE:CG2	2.77	0.55
1:A:297:ASN:CG	1:A:299:THR:HG23	2.27	0.55
1:B:238:PRO:HG2	1:B:328:LEU:HD21	1.88	0.55
1:A:388:GLU:HG3	1:A:410:LEU:HD21	1.88	0.55
1:B:368:LEU:HG	1:B:407:TYR:CE2	2.41	0.55
1:A:422:VAL:HG22	1:A:442:SER:HB3	1.89	0.54
1:A:255[A]:ARG:CG	1:A:255[A]:ARG:HH11	2.20	0.54
1:A:422:VAL:HA	1:A:442:SER:HB3	1.90	0.54
1:A:288:LYS:O	1:A:288:LYS:HG3	2.06	0.54
1:B:264:VAL:HG21	2:D:2:NAG:C1	2.37	0.54
1:B:253:ILE:H	1:B:253:ILE:CD1	2.14	0.54
1:A:292:ARG:HD2	1:A:300:TYR:HD1	1.72	0.54
1:B:266:VAL:HG12	1:B:300:TYR:H	1.73	0.53
1:A:284:VAL:O	3:A:601:HOH:O	2.19	0.53
1:B:289:THR:HA	1:B:304:SER:HA	1.90	0.53
1:B:297:ASN:OD1	1:B:299:THR:OG1	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:TRP:CE3	1:B:306:LEU:HD22	2.40	0.53
1:A:292:ARG:HB3	1:A:302:VAL:HG22	1.91	0.53
1:A:294:GLU:HB3	1:A:300:TYR:CE2	2.44	0.53
1:B:418:GLN:HA	1:B:443:LEU:HD12	1.91	0.52
1:A:295:GLN:OE1	1:A:301:ARG:HB3	2.09	0.52
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.91	0.52
1:B:323:VAL:HG13	1:B:332:ILE:HG22	1.86	0.52
1:A:350:THR:HG21	1:A:441:LEU:HB2	1.92	0.52
1:B:287:ALA:HB1	1:B:304:SER:HG	1.75	0.52
1:A:248:LYS:HZ1	1:A:255[B]:ARG:HH21	1.57	0.52
1:A:270:ASP:HB3	1:A:326:LYS:NZ	2.25	0.52
1:A:248:LYS:NZ	1:A:255[B]:ARG:HH21	2.08	0.51
1:A:388:GLU:OE1	1:A:416:ARG:NH2	2.29	0.51
1:A:239:SER:HB2	1:A:264:VAL:CG1	2.40	0.51
1:A:292:ARG:NE	1:A:300:TYR:CE1	2.78	0.51
1:A:390:ASN:O	1:A:410:LEU:HD12	2.11	0.51
1:B:301:ARG:HH21	1:B:303:VAL:HG21	1.77	0.50
1:A:239:SER:HB2	1:A:264:VAL:HG12	1.93	0.50
1:A:255[B]:ARG:HH11	1:A:255[B]:ARG:CB	2.20	0.50
1:A:262:VAL:HG12	1:A:303:VAL:HG22	1.92	0.50
1:A:292:ARG:HD2	1:A:300:TYR:CD1	2.47	0.50
1:A:246:LYS:HG2	2:C:6:GAL:O4	2.12	0.50
1:A:270:ASP:HB2	1:A:326:LYS:HE3	1.94	0.50
1:B:309:LEU:HD23	1:B:310:HIS:N	2.27	0.50
1:A:275:PHE:CE2	1:A:304:SER:HB2	2.47	0.49
1:B:266:VAL:HG12	1:B:300:TYR:CB	2.40	0.49
1:B:292:ARG:CD	1:B:300:TYR:HD2	2.22	0.49
1:B:264:VAL:HG22	1:B:265:ASP:N	2.25	0.49
1:B:267:SER:OG	1:B:271:PRO:HD3	2.12	0.49
1:A:269:GLU:H	1:A:269:GLU:CD	2.15	0.49
1:A:244:PRO:HB3	1:A:336:ILE:HD11	1.94	0.49
1:B:382:GLU:HA	1:B:388:GLU:H	1.79	0.48
1:B:239:SER:HB2	1:B:264:VAL:HG12	1.95	0.48
1:A:330:ALA:HA	3:A:602:HOH:O	2.14	0.48
1:A:296:TYR:CE1	1:A:297:ASN:ND2	2.82	0.47
1:B:297:ASN:O	1:B:298:SER:OG	2.26	0.47
1:A:255[A]:ARG:NH1	1:A:255[A]:ARG:CG	2.72	0.47
1:B:297:ASN:O	1:B:299:THR:HG23	2.14	0.47
1:B:291:PRO:O	1:B:292:ARG:O	2.32	0.47
1:A:263:VAL:HG23	1:A:302:VAL:H	1.79	0.47
1:A:422:VAL:HG22	1:A:442:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:HG11	2:D:2:NAG:H61	1.96	0.47
1:A:240:VAL:CG2	1:A:323:VAL:HG11	2.43	0.47
1:B:247:PRO:O	1:B:251:LEU:HG	2.15	0.47
1:A:296:TYR:CZ	1:A:297:ASN:HB3	2.50	0.47
1:B:285:HIS:N	1:B:285:HIS:ND1	2.63	0.47
1:B:240:VAL:HG22	1:B:263:VAL:HG13	1.96	0.47
1:B:296:TYR:O	1:B:296:TYR:CG	2.68	0.46
1:B:274:LYS:HB3	1:B:324:SER:CB	2.45	0.46
1:A:253:ILE:HA	1:A:310:HIS:CD2	2.51	0.46
1:B:240:VAL:CG2	1:B:332:ILE:HG21	2.45	0.46
1:B:422:VAL:HG23	1:B:442:SER:HB3	1.98	0.46
1:A:296:TYR:CG	1:A:297:ASN:N	2.85	0.45
1:B:295:GLN:HE22	1:B:301:ARG:HB2	1.81	0.45
1:A:297:ASN:OD1	1:A:299:THR:HG23	2.16	0.45
1:B:291:PRO:O	1:B:292:ARG:C	2.55	0.44
1:A:290:LYS:HB2	1:A:290:LYS:HE2	1.90	0.44
1:B:266:VAL:HG12	1:B:300:TYR:N	2.32	0.44
1:A:310:HIS:ND1	1:A:310:HIS:N	2.65	0.44
1:B:358:LEU:HD23	1:B:363:VAL:HG11	1.99	0.44
1:A:275:PHE:CD2	1:A:304:SER:CB	2.98	0.44
1:B:265:ASP:OD2	2:D:1:NAG:H3	2.18	0.44
1:A:269:GLU:O	1:A:271:PRO:HD3	2.18	0.44
1:B:386:GLN:HG3	1:B:387:PRO:HD2	2.00	0.44
1:A:350:THR:O	1:A:351:LEU:HD23	2.18	0.43
1:B:296:TYR:CD1	1:B:296:TYR:C	2.90	0.43
1:B:242:LEU:HD23	1:B:243:PHE:N	2.33	0.43
1:B:268:HIS:CD2	1:B:268:HIS:O	2.71	0.43
1:B:279:VAL:HG22	1:B:319:TYR:CD2	2.54	0.43
1:B:277:TRP:CZ3	1:B:306:LEU:HD21	2.51	0.43
1:B:266:VAL:HG12	1:B:300:TYR:CA	2.49	0.42
1:A:238:PRO:HG2	1:A:328:LEU:HG	2.01	0.42
1:A:358:LEU:CD2	1:A:363:VAL:HG11	2.38	0.42
1:A:292:ARG:NE	1:A:300:TYR:HE1	2.13	0.42
1:B:269:GLU:N	1:B:269:GLU:OE1	2.52	0.42
1:A:244:PRO:HB3	1:A:336:ILE:CD1	2.50	0.42
1:A:319:TYR:O	1:A:335:THR:HA	2.19	0.42
1:A:248:LYS:NZ	1:A:255[B]:ARG:NH2	2.67	0.42
1:A:270:ASP:OD2	1:A:270:ASP:N	2.53	0.42
1:A:350:THR:HB	1:A:441:LEU:HD12	2.02	0.42
1:B:292:ARG:NH1	1:B:292:ARG:CB	2.77	0.42
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:HB2	1:A:366:THR:HB	2.02	0.41
1:B:292:ARG:CB	1:B:292:ARG:CZ	2.98	0.41
1:B:415:SER:O	1:B:419:GLN:HG3	2.19	0.41
1:A:241:PHE:HB2	1:A:262:VAL:HG22	2.03	0.41
1:B:238:PRO:HA	1:B:265:ASP:O	2.20	0.41
1:A:255[A]:ARG:HH11	1:A:255[A]:ARG:CB	2.34	0.41
1:B:322:LYS:HE2	1:B:331:PRO:HB3	2.00	0.41
2:C:6:GAL:O4	2:C:6:GAL:O6	2.29	0.41
1:A:353:PRO:HG3	1:A:365:LEU:HD23	2.02	0.41
1:A:273:VAL:CG1	1:A:323:VAL:HG23	2.51	0.41
1:A:433:HIS:O	1:A:434:ASN:HB2	2.21	0.41
1:B:253:ILE:HD12	1:B:253:ILE:N	2.25	0.41
1:B:269:GLU:O	1:B:270:ASP:CG	2.58	0.41
1:B:386:GLN:HA	1:B:387:PRO:HD3	1.95	0.41
1:B:422:VAL:HA	1:B:442:SER:HB3	2.02	0.41
1:A:239:SER:O	1:A:264:VAL:HG12	2.21	0.41
1:A:238:PRO:HG2	1:A:328:LEU:CD1	2.51	0.40
1:B:346:PRO:HB3	1:B:372:PHE:HB3	2.03	0.40
1:B:243:PHE:HE1	2:D:3:BMA:H62	1.86	0.40

There are no symmetry-related clashes.

## 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	207/211 (98%)	197 (95%)	8 (4%)	2 (1%)	15	32
1	B	206/211 (98%)	175 (85%)	18 (9%)	13 (6%)	1	1
All	All	413/422 (98%)	372 (90%)	26 (6%)	15 (4%)	3	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	ASP
1	B	271	PRO
1	B	285	HIS
1	B	292	ARG
1	B	297	ASN
1	B	288	LYS
1	B	289	THR
1	B	286	ASN
1	B	419	GLN
1	B	420	GLY
1	A	291	PRO
1	B	287	ALA
1	A	271	PRO
1	B	277	TRP
1	B	291	PRO

### 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	194/196 (99%)	180 (93%)	14 (7%)	14	29
1	B	193/196 (98%)	183 (95%)	10 (5%)	23	46
All	All	387/392 (99%)	363 (94%)	24 (6%)	19	37

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	LEU
1	A	254	SER
1	A	255[A]	ARG
1	A	255[B]	ARG
1	A	268	HIS
1	A	276	ASN
1	A	301	ARG
1	A	310	HIS
1	A	355	ARG

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Mol	Chain	Res	Type
1	A	356	ASP
1	A	360	LYS
1	A	408	SER
1	A	440	SER
1	A	441	LEU
1	B	271	PRO
1	B	272	GLU
1	B	283	GLU
1	B	285	HIS
1	B	292	ARG
1	B	296	TYR
1	B	300	TYR
1	B	301	ARG
1	B	332	ILE
1	B	430	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	B	276	ASN
1	B	286	ASN
1	B	295	GLN
1	B	384	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](#)

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	1.22	1 (7%)	17,19,21	0.75	0
2	NAG	C	2	2	14,14,15	0.17	0	17,19,21	0.58	0
2	BMA	C	3	2	11,11,12	0.91	0	15,15,17	1.10	2 (13%)
2	MAN	C	4	2	11,11,12	1.27	2 (18%)	15,15,17	1.13	1 (6%)
2	NAG	C	5	2	14,14,15	0.56	0	17,19,21	0.84	1 (5%)
2	GAL	C	6	2	11,11,12	0.73	0	15,15,17	0.94	1 (6%)
2	MAN	C	7	2	11,11,12	1.40	2 (18%)	15,15,17	1.26	1 (6%)
2	NAG	C	8	2	14,14,15	0.55	0	17,19,21	0.79	1 (5%)
2	NAG	D	1	1,2	14,14,15	1.47	2 (14%)	17,19,21	0.71	0
2	NAG	D	2	2	14,14,15	0.39	0	17,19,21	1.09	1 (5%)
2	BMA	D	3	2	11,11,12	0.69	0	15,15,17	1.31	1 (6%)
2	MAN	D	4	2	11,11,12	1.75	2 (18%)	15,15,17	0.97	0
2	NAG	D	5	2	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
2	GAL	D	6	2	11,11,12	1.28	2 (18%)	15,15,17	1.10	1 (6%)
2	MAN	D	7	2	11,11,12	1.15	1 (9%)	15,15,17	1.25	1 (6%)
2	NAG	D	8	2	14,14,15	0.33	0	17,19,21	0.55	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	NAG	C	5	2	-	0/6/23/26	0/1/1/1
2	GAL	C	6	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	1/2/19/22	0/1/1/1
2	NAG	C	8	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	NAG	D	5	2	-	0/6/23/26	0/1/1/1
2	GAL	D	6	2	-	2/2/19/22	0/1/1/1
2	MAN	D	7	2	-	1/2/19/22	0/1/1/1
2	NAG	D	8	2	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	4.11	1.50	1.43
2	D	4	MAN	C2-C3	3.92	1.58	1.52
2	D	4	MAN	O5-C1	-3.73	1.37	1.43
2	D	1	NAG	O5-C1	3.57	1.49	1.43
2	D	1	NAG	C1-C2	3.26	1.57	1.52
2	D	7	MAN	O5-C1	-3.00	1.38	1.43
2	C	4	MAN	C4-C5	2.83	1.59	1.53
2	C	7	MAN	O5-C1	-2.82	1.39	1.43
2	D	6	GAL	O4-C4	-2.68	1.36	1.43
2	C	7	MAN	O2-C2	-2.64	1.37	1.43
2	D	6	GAL	O5-C1	-2.29	1.40	1.43
2	C	4	MAN	O5-C1	-2.00	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	MAN	O2-C2-C3	-3.71	102.70	110.14
2	D	2	NAG	C3-C4-C5	3.37	116.24	110.24
2	C	7	MAN	O2-C2-C3	-3.19	103.75	110.14
2	C	4	MAN	O2-C2-C3	-3.06	104.01	110.14
2	C	8	NAG	C1-O5-C5	2.74	115.91	112.19
2	C	3	BMA	C1-O5-C5	2.47	115.54	112.19
2	D	6	GAL	O5-C5-C6	-2.32	103.56	107.20
2	C	3	BMA	O2-C2-C3	-2.32	105.50	110.14
2	C	6	GAL	C1-C2-C3	2.31	112.50	109.67
2	D	3	BMA	O2-C2-C3	-2.18	105.76	110.14
2	D	5	NAG	C1-O5-C5	2.16	115.12	112.19
2	C	5	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

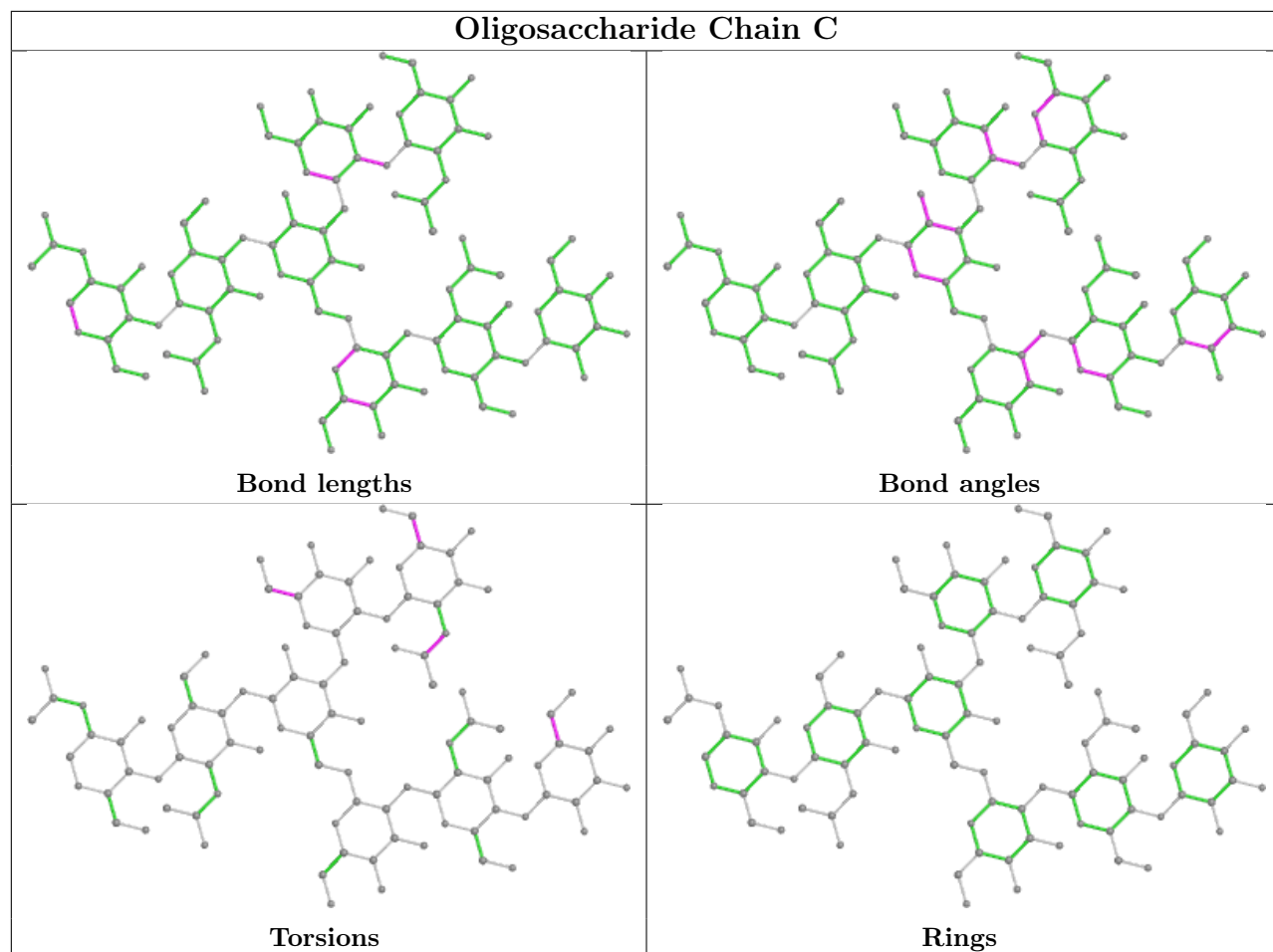
Mol	Chain	Res	Type	Atoms
2	C	6	GAL	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
2	C	8	NAG	C8-C7-N2-C2
2	C	8	NAG	O7-C7-N2-C2
2	D	8	NAG	C8-C7-N2-C2
2	D	8	NAG	O7-C7-N2-C2
2	D	6	GAL	O5-C5-C6-O6
2	C	6	GAL	O5-C5-C6-O6
2	C	8	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	6	GAL	C4-C5-C6-O6
2	C	8	NAG	C4-C5-C6-O6
2	D	7	MAN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6

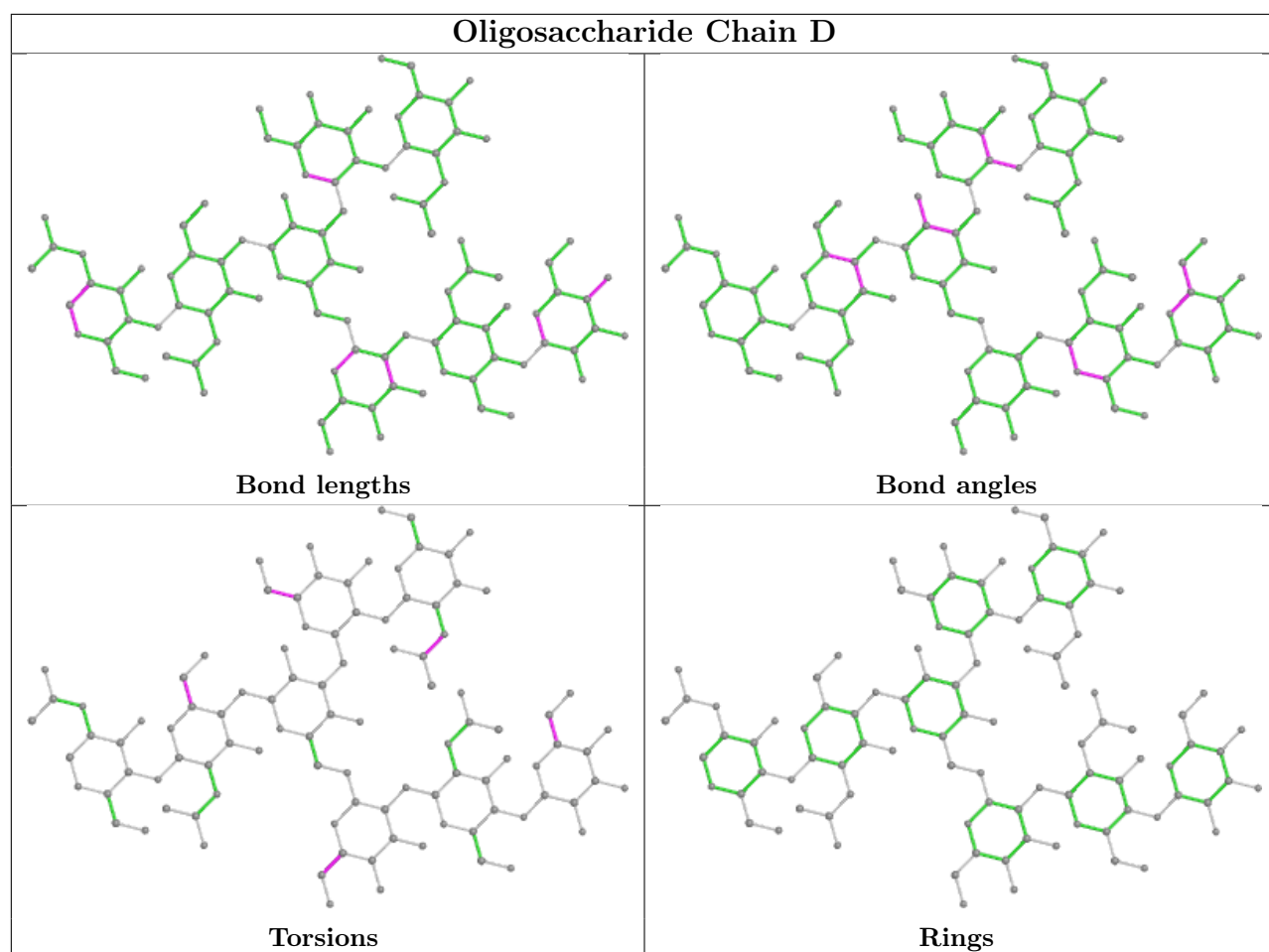
There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	GAL	2	0
2	C	5	NAG	1	0
2	D	1	NAG	2	0
2	D	2	NAG	4	0
2	D	6	GAL	1	0
2	D	3	BMA	1	0
2	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	208/211 (98%)	-0.24	1 (0%) 91 89	37, 71, 122, 149	0
1	B	208/211 (98%)	-0.19	6 (2%) 51 45	36, 78, 145, 179	0
All	All	416/422 (98%)	-0.21	7 (1%) 70 66	36, 75, 140, 179	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	SER	3.7
1	B	326	LYS	2.7
1	B	300	TYR	2.5
1	A	272	GLU	2.5
1	B	275	PHE	2.5
1	B	236	GLY	2.5
1	B	285	HIS	2.4

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.70	0.32	121,128,134,136	0
2	NAG	D	1	14/15	0.76	0.24	123,133,137,139	0

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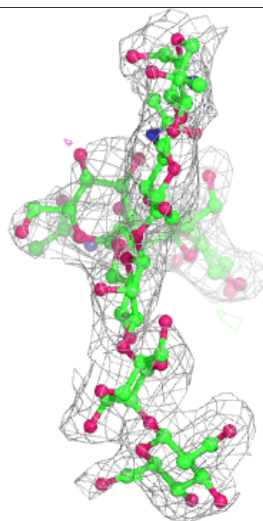
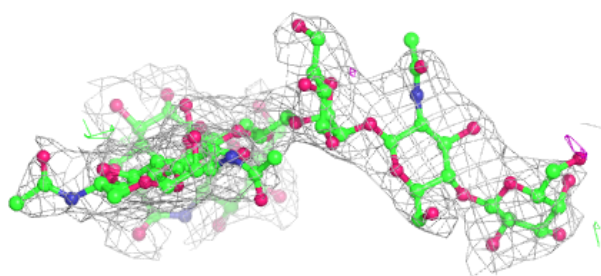
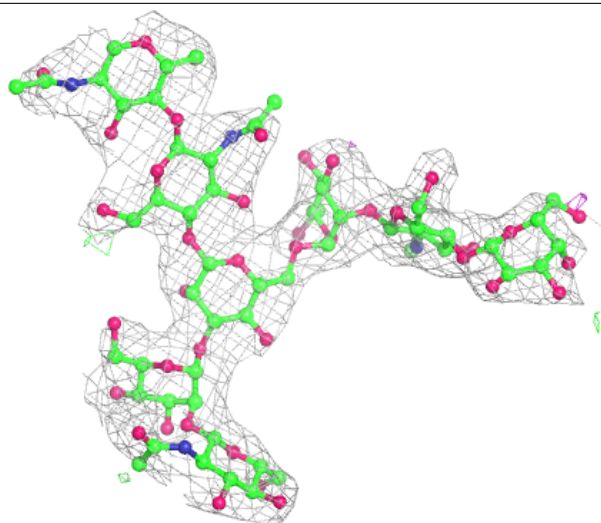
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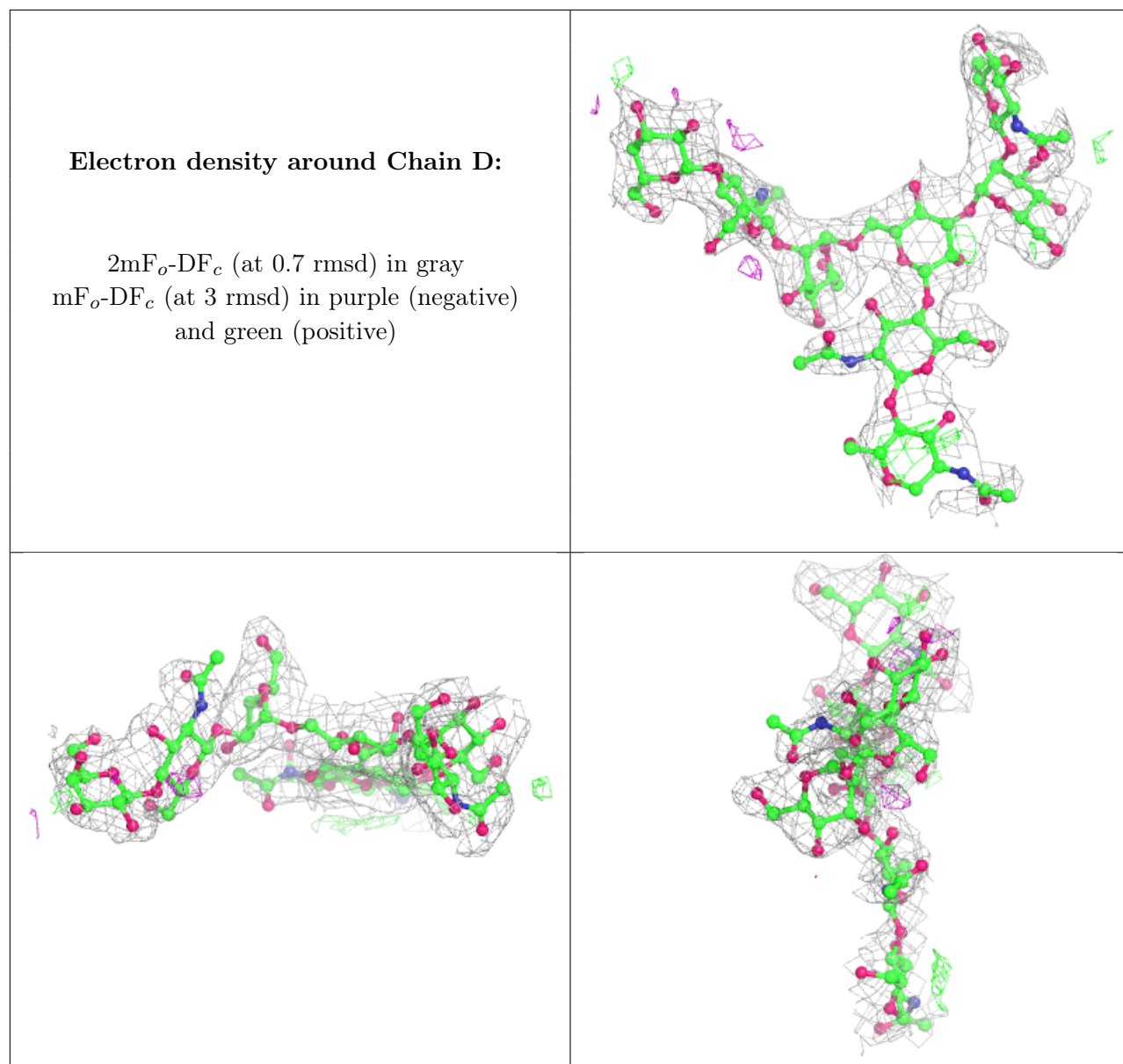
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	8	14/15	0.83	0.16	99,104,106,106	0
2	BMA	D	3	11/12	0.85	0.11	104,109,115,118	0
2	NAG	D	8	14/15	0.85	0.14	98,101,109,111	0
2	GAL	D	6	11/12	0.86	0.25	92,98,102,104	0
2	BMA	C	3	11/12	0.86	0.12	92,93,96,96	0
2	NAG	C	1	14/15	0.88	0.14	73,80,88,91	0
2	NAG	C	5	14/15	0.88	0.22	85,91,95,99	0
2	GAL	C	6	11/12	0.88	0.32	90,99,106,109	0
2	MAN	D	7	11/12	0.89	0.12	94,101,107,107	0
2	MAN	C	4	11/12	0.89	0.18	83,92,95,95	0
2	NAG	D	5	14/15	0.92	0.21	98,103,106,106	0
2	NAG	C	2	14/15	0.93	0.16	87,91,96,96	0
2	MAN	D	4	11/12	0.93	0.14	93,98,103,104	0
2	MAN	C	7	11/12	0.95	0.12	88,91,96,99	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 C:**

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





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.