



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 07:23 PM EDT

PDB ID : 3D11  
Title : Crystal Structures of the Nipah G Attachment Glycoprotein  
Authors : Xu, K.; Rajashankar, K.R.; Chan, Y.P.; Himanen, P.; Broder, C.C.; Nikolov, D.B.  
Deposited on : 2008-05-02  
Resolution : 2.31 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

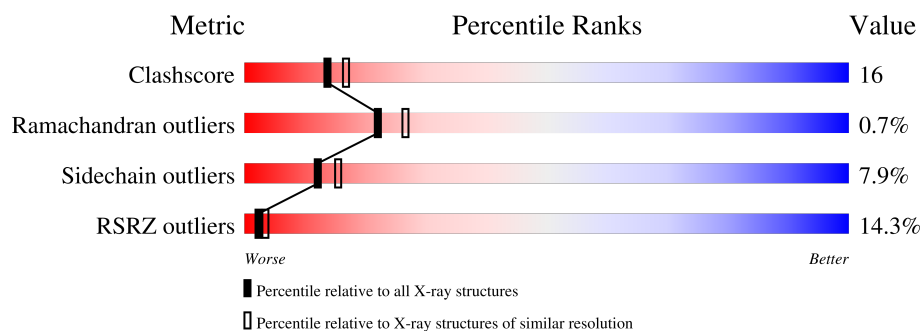
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




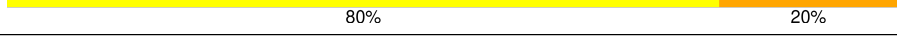
The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	428	
2	B	2	
2	C	2	
3	D	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	2	-	-	-	X
3	NAG	D	1	X	-	-	-
4	NAG	A	1210	X	-	-	X
5	IOD	A	13	-	-	X	-
5	IOD	A	14	-	-	X	-
5	IOD	A	7	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3721 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 Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3361	2141	567	632	21			

There is a discrepancy between the modelled and reference sequences:

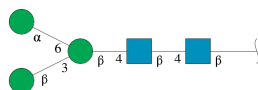
Chain	Residue	Modelled	Actual	Comment	Reference
A	603	ALA	-	expression tag	UNP Q9IH62

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total I	0	0
			19 19		

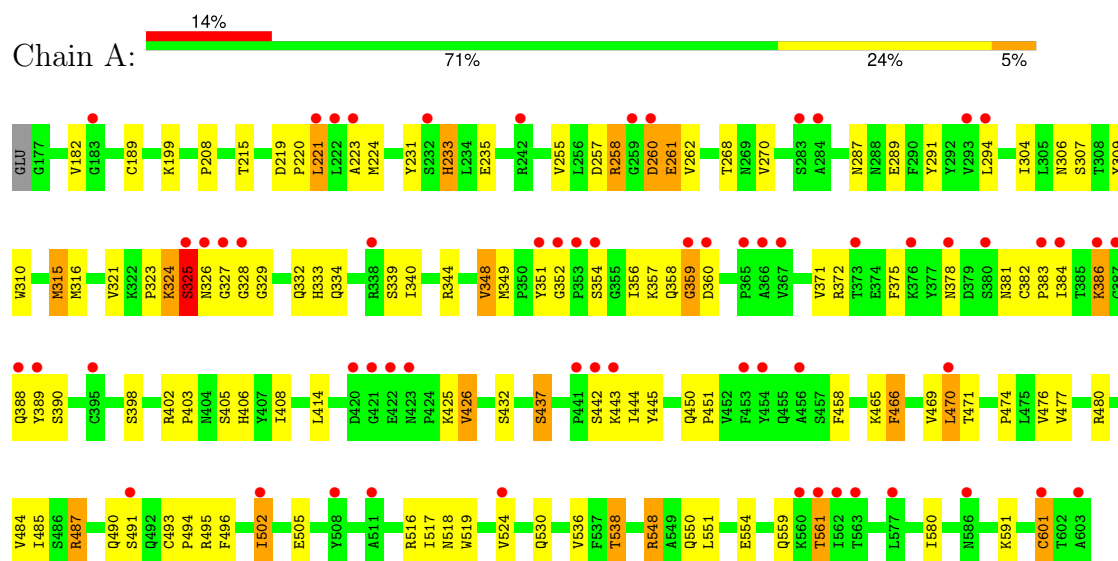
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	210	Total O	0	0
			210 210		

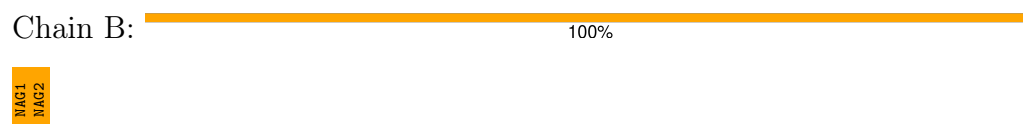
### 3 Residue-property plots [i](#)

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: Hemagglutinin-neuraminidase



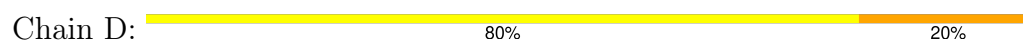
#### • Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



#### • Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.16Å 130.16Å 130.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.24 – 2.31 39.25 – 2.31	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.24-2.31) 90.7 (39.25-2.31)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.31Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.228 , 0.257 0.229 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.37	0/3442	0.55	0/4682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3361	0	3306	99	0
2	B	28	0	25	4	0
2	C	28	0	25	1	0
3	D	61	0	52	1	0
4	A	14	0	13	1	0
5	A	19	0	0	16	0
6	A	210	0	0	16	0
All	All	3721	0	3421	110	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 16.

All (110) 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:601:CYS:HB2	5:A:14:IOD:I	2.08	1.23
1:A:601:CYS:CB	5:A:14:IOD:I	2.75	1.03
1:A:601:CYS:SG	5:A:14:IOD:I	2.90	1.00
5:A:9:IOD:I	5:A:14:IOD:I	3.21	0.98
1:A:189:CYS:SG	5:A:14:IOD:I	2.97	0.93
5:A:2:IOD:I	6:A:1366:HOH:O	2.66	0.83
1:A:550:GLN:HE22	1:A:554:GLU:HG2	1.44	0.82
1:A:344:ARG:NH1	5:A:16:IOD:I	2.82	0.82
1:A:471:THR:HG22	1:A:476:VAL:HG22	1.63	0.80
1:A:548:ARG:HB3	1:A:548:ARG:HH11	1.47	0.78
1:A:386:LYS:NZ	1:A:386:LYS:HA	1.98	0.77
1:A:471:THR:HG23	1:A:474:PRO:O	1.86	0.75
1:A:359:GLY:HA2	1:A:360:ASP:OD1	1.87	0.75
1:A:306:ASN:OD1	1:A:309:TYR:HB2	1.90	0.71
6:A:1458:HOH:O	2:B:2:NAG:H61	1.91	0.70
1:A:359:GLY:HA2	1:A:360:ASP:CG	2.13	0.69
1:A:382:CYS:O	1:A:384:ILE:HD13	1.92	0.68
1:A:182:VAL:CG2	5:A:13:IOD:I	3.12	0.67
5:A:15:IOD:I	6:A:1379:HOH:O	2.84	0.66
5:A:12:IOD:I	6:A:1441:HOH:O	2.85	0.65
1:A:182:VAL:HG22	5:A:13:IOD:I	2.66	0.65
2:B:1:NAG:H3	2:B:2:NAG:O5	1.98	0.64
1:A:524:VAL:O	1:A:561:THR:HG21	1.96	0.64
1:A:327:GLY:HA2	6:A:1512:HOH:O	1.97	0.63
1:A:348:VAL:HG11	1:A:414:LEU:HD21	1.80	0.62
1:A:257:ASP:OD1	1:A:258:ARG:O	2.18	0.62
1:A:182:VAL:HG23	5:A:13:IOD:I	2.70	0.61
1:A:375:PHE:HD1	5:A:7:IOD:I	2.54	0.61
1:A:375:PHE:CD1	5:A:7:IOD:I	3.23	0.61
1:A:548:ARG:HH11	1:A:548:ARG:CB	2.13	0.61
1:A:344:ARG:HD2	6:A:1397:HOH:O	2.00	0.61
1:A:386:LYS:HA	1:A:386:LYS:HZ2	1.66	0.59
1:A:494:PRO:HB3	1:A:530:GLN:HE21	1.67	0.59
1:A:580:ILE:HG13	1:A:591:LYS:HD2	1.84	0.59
1:A:332:GLN:O	1:A:333:HIS:HB3	2.02	0.58
1:A:561:THR:CG2	6:A:1364:HOH:O	2.52	0.57
1:A:208:PRO:HG3	5:A:6:IOD:I	2.75	0.56
2:C:1:NAG:H83	2:C:1:NAG:O3	2.06	0.56
1:A:371:VAL:HG23	6:A:1540:HOH:O	2.06	0.55
1:A:339:SER:OG	1:A:425:LYS:HG2	2.07	0.55
1:A:466:PHE:O	1:A:480:ARG:HG2	2.06	0.55
1:A:386:LYS:HA	1:A:386:LYS:HZ3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:CG1	1:A:414:LEU:HD21	2.38	0.54
1:A:372:ARG:NH1	1:A:403:PRO:O	2.42	0.53
1:A:384:ILE:HG13	1:A:390:SER:O	2.08	0.53
1:A:516:ARG:HD2	6:A:1509:HOH:O	2.09	0.52
1:A:258:ARG:HG3	1:A:262:VAL:O	2.10	0.52
1:A:329:GLY:O	1:A:333:HIS:HD2	1.91	0.52
5:A:19:IOD:I	6:A:1366:HOH:O	2.89	0.51
1:A:445:TYR:O	1:A:451:PRO:HA	2.12	0.50
1:A:559:GLN:HG2	6:A:1536:HOH:O	2.12	0.50
1:A:487:ARG:NH2	1:A:493:CYS:O	2.44	0.50
1:A:233:HIS:HE1	1:A:235:GLU:OE2	1.95	0.50
1:A:378:ASN:OD1	4:A:1210:NAG:H5	2.12	0.50
1:A:233:HIS:CE1	1:A:235:GLU:HG3	2.46	0.49
1:A:360:ASP:HB2	6:A:1529:HOH:O	2.11	0.49
1:A:315:MET:HG3	1:A:334:GLN:HE22	1.78	0.48
1:A:324:LYS:HB2	1:A:324:LYS:NZ	2.29	0.48
1:A:536:VAL:HG12	1:A:538:THR:HG22	1.96	0.47
1:A:372:ARG:HH12	1:A:403:PRO:C	2.17	0.47
1:A:294:LEU:HD13	1:A:316:MET:HE2	1.95	0.47
1:A:258:ARG:HH21	1:A:260:ASP:CG	2.18	0.47
1:A:223:ALA:HB2	1:A:354:SER:HB3	1.97	0.46
1:A:325:SER:HB3	1:A:326:ASN:H	1.56	0.46
1:A:324:LYS:O	1:A:324:LYS:HG2	2.15	0.45
1:A:324:LYS:O	1:A:325:SER:C	2.54	0.45
1:A:231:TYR:OH	1:A:233:HIS:HD2	2.00	0.45
1:A:340:ILE:HG12	1:A:426:VAL:CG2	2.47	0.45
1:A:199:LYS:HD3	6:A:1494:HOH:O	2.15	0.45
1:A:268:THR:O	1:A:323:PRO:HG2	2.17	0.45
1:A:469:VAL:HG22	1:A:477:VAL:HG22	1.99	0.45
1:A:224:MET:HE3	1:A:255:VAL:HG21	1.98	0.45
1:A:495:ARG:O	1:A:496:PHE:HB2	2.17	0.45
1:A:372:ARG:HD2	1:A:405:SER:O	2.17	0.44
2:B:1:NAG:H5	2:B:2:NAG:O5	2.17	0.44
1:A:289:GLU:O	1:A:321:VAL:HG22	2.17	0.44
1:A:383:PRO:C	1:A:384:ILE:HD12	2.37	0.44
1:A:470:LEU:HA	1:A:470:LEU:HD12	1.71	0.44
1:A:261:GLU:OE1	1:A:261:GLU:O	2.35	0.44
1:A:443:LYS:HE3	6:A:1373:HOH:O	2.18	0.44
1:A:458:PHE:HA	1:A:505:GLU:O	2.17	0.43
1:A:548:ARG:HH11	1:A:548:ARG:CG	2.30	0.43
1:A:260:ASP:O	1:A:261:GLU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:SER:OG	1:A:502:ILE:HA	2.18	0.43
1:A:219:ASP:N	1:A:220:PRO:CD	2.82	0.43
1:A:260:ASP:O	1:A:261:GLU:CB	2.67	0.43
2:B:1:NAG:C3	2:B:2:NAG:O5	2.63	0.43
1:A:406:HIS:HE1	6:A:1562:HOH:O	2.02	0.42
1:A:450:GLN:HG3	1:A:451:PRO:HD2	2.01	0.42
1:A:287:ASN:HD21	1:A:360:ASP:HB3	1.84	0.42
1:A:378:ASN:HB3	1:A:381:ASN:OD1	2.19	0.42
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.78	0.42
1:A:382:CYS:O	1:A:384:ILE:CD1	2.65	0.42
1:A:517:ILE:HG22	1:A:518:ASN:OD1	2.20	0.42
1:A:304:ILE:HG12	1:A:349:MET:HE1	2.01	0.42
1:A:384:ILE:CG1	1:A:390:SER:O	2.68	0.42
6:A:1406:HOH:O	3:D:5:MAN:C6	2.68	0.42
1:A:310:TRP:CH2	1:A:349:MET:HB3	2.55	0.42
1:A:437:SER:HB2	1:A:465:LYS:NZ	2.34	0.41
1:A:352:GLY:HA3	1:A:442:SER:O	2.21	0.41
1:A:490:GLN:HB3	1:A:491:SER:H	1.73	0.41
1:A:356:ILE:HD13	1:A:444:ILE:HG12	2.02	0.41
1:A:384:ILE:O	1:A:384:ILE:CG2	2.68	0.41
1:A:221:LEU:C	1:A:221:LEU:HD23	2.40	0.41
1:A:403:PRO:HG3	1:A:502:ILE:HD11	2.03	0.41
1:A:357:LYS:O	1:A:357:LYS:HG2	2.21	0.41
1:A:484:VAL:HG23	1:A:485:ILE:HG12	2.03	0.40
1:A:408:ILE:HD12	1:A:408:ILE:C	2.41	0.40
1:A:402:ARG:HA	1:A:403:PRO:HD3	1.93	0.40
1:A:470:LEU:CB	1:A:476:VAL:HG23	2.52	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	425/428 (99%)	384 (90%)	38 (9%)	3 (1%)	22 26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	A	359	GLY
1	A	328	GLY

### 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	381/382 (100%)	351 (92%)	30 (8%)	12 15

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	221	LEU
1	A	233	HIS
1	A	258	ARG
1	A	260	ASP
1	A	261	GLU
1	A	270	VAL
1	A	291	TYR
1	A	307	SER
1	A	315	MET
1	A	324	LYS
1	A	325	SER
1	A	348	VAL
1	A	351	TYR
1	A	358	GLN
1	A	386	LYS
1	A	388	GLN
1	A	389	TYR

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Mol	Chain	Res	Type
1	A	426	VAL
1	A	432	SER
1	A	437	SER
1	A	466	PHE
1	A	470	LEU
1	A	487	ARG
1	A	502	ILE
1	A	519	TRP
1	A	538	THR
1	A	548	ARG
1	A	561	THR
1	A	601	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	233	HIS
1	A	287	ASN
1	A	333	HIS
1	A	334	GLN
1	A	434	GLN
1	A	492	GLN
1	A	497	ASN
1	A	530	GLN
1	A	550	GLN
1	A	586	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 ⓘ

9 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	B	1	2,1	14,14,15	0.38	0	17,19,21	1.25	1 (5%)
2	NAG	B	2	2	14,14,15	0.52	0	17,19,21	1.56	1 (5%)
2	NAG	C	1	2,1	14,14,15	0.49	0	17,19,21	1.39	3 (17%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	1.33	1 (5%)
3	NAG	D	1	1,3	14,14,15	1.46	2 (14%)	17,19,21	2.68	7 (41%)
3	NAG	D	2	3	14,14,15	1.29	1 (7%)	17,19,21	1.75	4 (23%)
3	BMA	D	3	3	11,11,12	0.79	0	15,15,17	1.30	1 (6%)
3	BMA	D	4	3	11,11,12	0.91	0	15,15,17	2.26	5 (33%)
3	MAN	D	5	3	11,11,12	0.86	0	15,15,17	1.53	4 (26%)

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	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1	1,3	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	BMA	D	4	3	-	1/2/19/22	1/1/1/1
3	MAN	D	5	3	-	2/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C7-N2	3.53	1.45	1.34
3	D	2	NAG	C7-N2	3.51	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.03	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	6.37	120.72	112.19
3	D	4	BMA	C1-C2-C3	6.28	118.79	109.64
2	B	2	NAG	C1-O5-C5	5.47	119.51	112.19
2	C	2	NAG	C2-N2-C7	-4.89	116.34	122.90
3	D	1	NAG	C2-N2-C7	-4.85	116.40	122.90
3	D	2	NAG	C1-O5-C5	4.40	118.08	112.19
3	D	1	NAG	O5-C1-C2	4.00	117.48	111.29
2	B	1	NAG	C1-O5-C5	3.62	117.04	112.19
3	D	3	BMA	C1-O5-C5	3.53	116.92	112.19
3	D	1	NAG	O5-C5-C4	3.43	119.16	110.83
3	D	4	BMA	O2-C2-C1	3.18	116.50	109.22
2	C	1	NAG	C2-N2-C7	-2.98	118.91	122.90
3	D	2	NAG	C2-N2-C7	-2.81	119.13	122.90
3	D	4	BMA	O5-C5-C4	2.70	117.40	110.83
2	C	1	NAG	C1-O5-C5	2.58	115.64	112.19
2	C	1	NAG	O4-C4-C3	-2.57	104.31	110.38
3	D	5	MAN	O3-C3-C2	-2.48	104.99	110.05
3	D	1	NAG	C8-C7-N2	2.40	120.09	116.12
3	D	4	BMA	C6-C5-C4	-2.39	107.14	113.02
3	D	1	NAG	C6-C5-C4	-2.37	107.21	113.02
3	D	2	NAG	O4-C4-C3	-2.36	104.81	110.38
3	D	5	MAN	O3-C3-C4	-2.34	104.87	110.38
3	D	4	BMA	C1-O5-C5	2.31	115.28	112.19
3	D	2	NAG	C6-C5-C4	-2.26	107.47	113.02
3	D	1	NAG	C1-C2-N2	-2.15	107.05	110.43
3	D	5	MAN	C6-C5-C4	-2.09	107.88	113.02
3	D	5	MAN	C1-O5-C5	2.04	114.92	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1	NAG	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	5	MAN	C4-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	4	BMA	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7

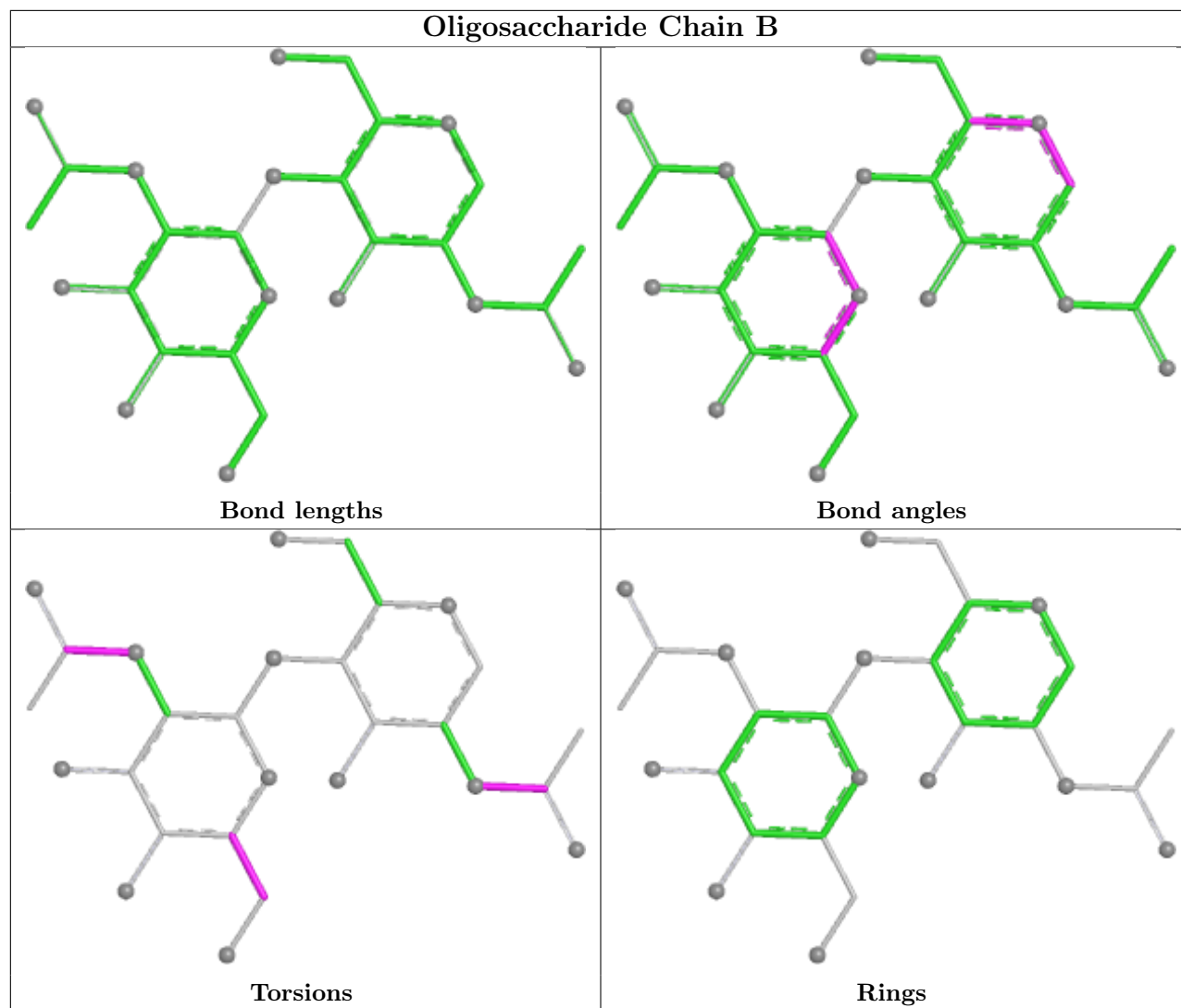
All (2) ring outliers are listed below:

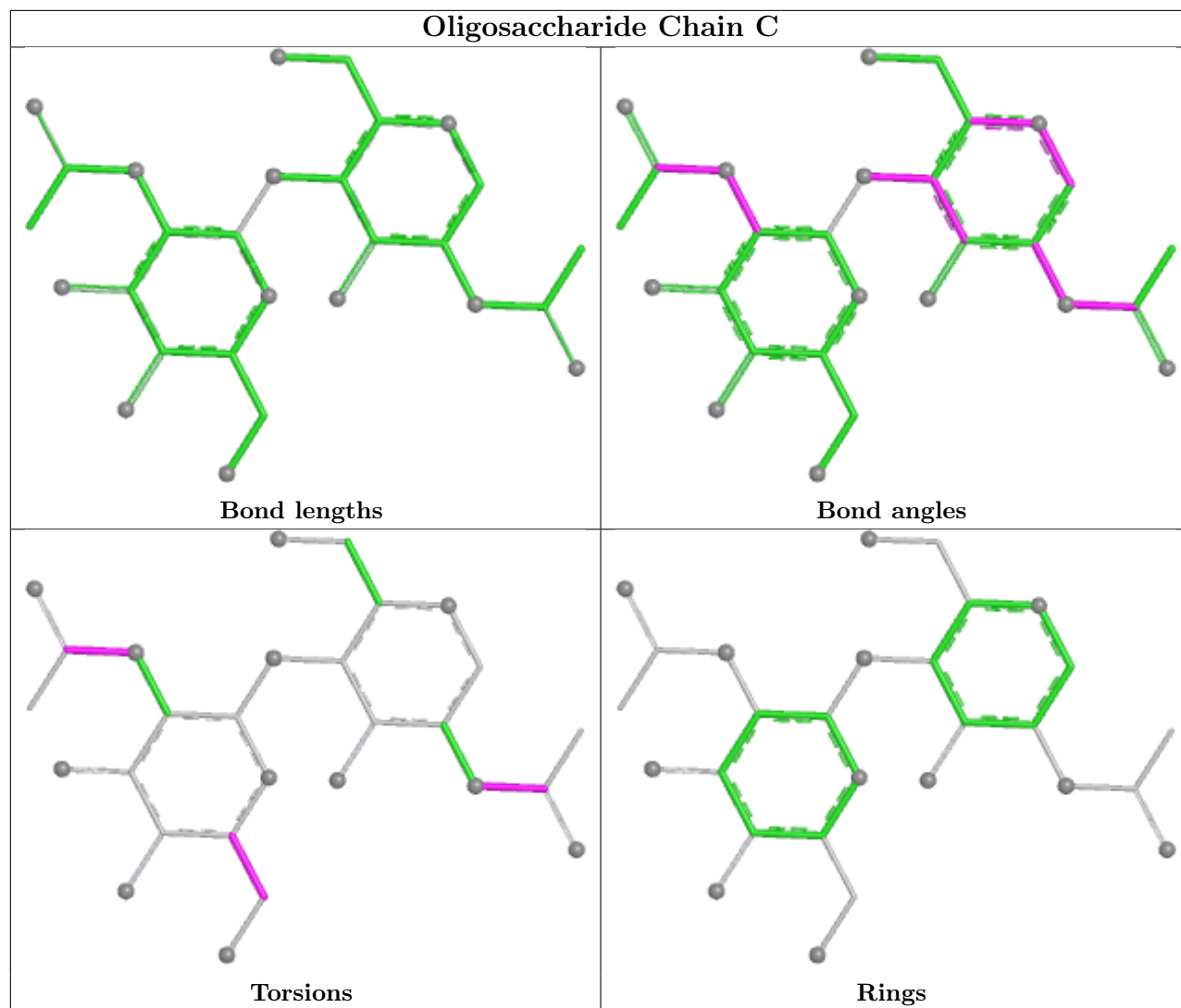
Mol	Chain	Res	Type	Atoms
3	D	5	MAN	C1-C2-C3-C4-C5-O5
3	D	4	BMA	C1-C2-C3-C4-C5-O5

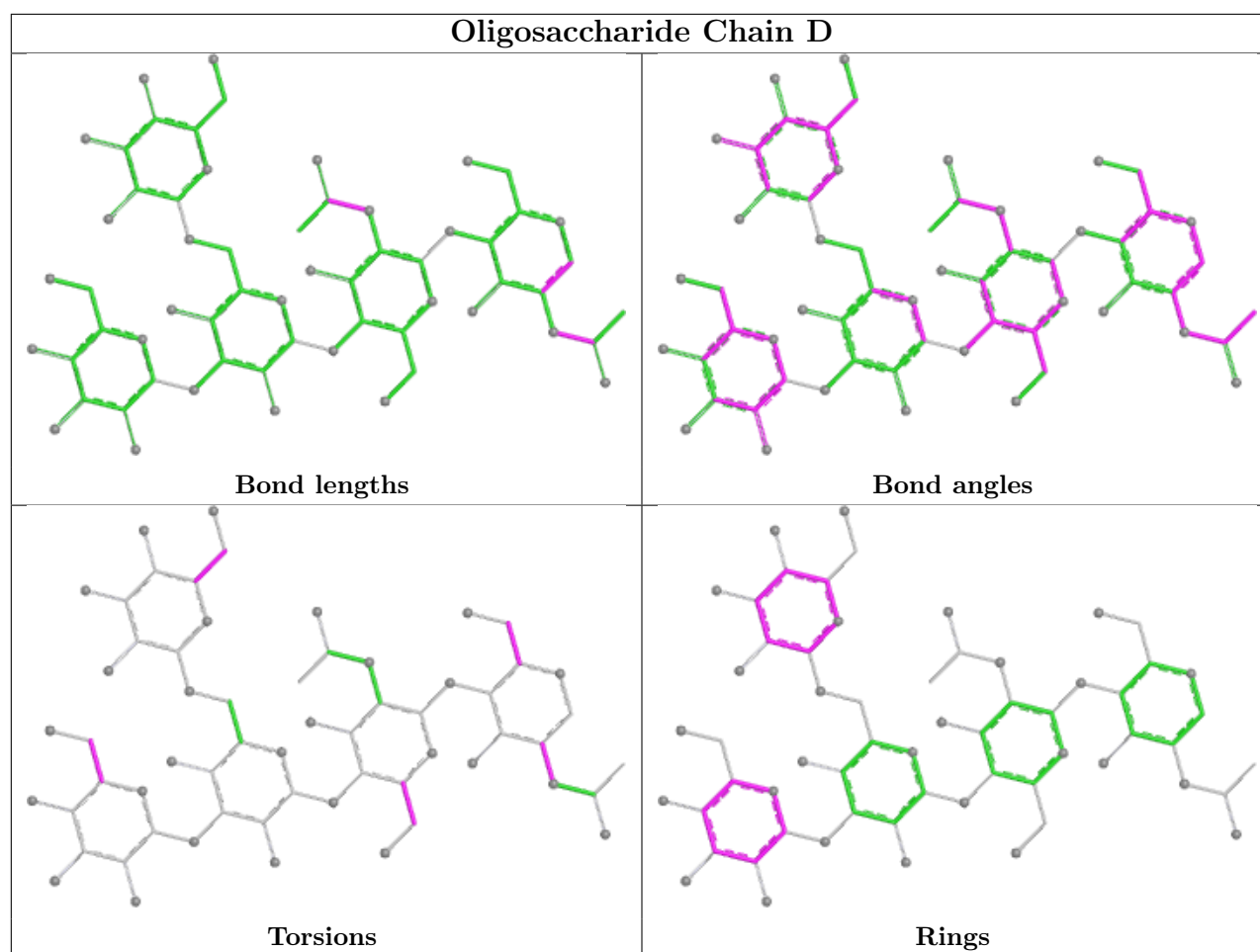
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	4	0
2	B	1	NAG	3	0
2	C	1	NAG	1	0
3	D	5	MAN	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](#)

Of 20 ligands modelled in this entry, 19 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	1210	1	14,14,15	0.46	0	17,19,21	1.32	3 (17%)

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
4	NAG	A	1210	1	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1210	NAG	C1-O5-C5	2.97	116.16	112.19
4	A	1210	NAG	C3-C4-C5	2.33	114.45	110.23
4	A	1210	NAG	O5-C1-C2	-2.12	108.02	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1210	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1210	NAG	C3-C2-N2-C7
4	A	1210	NAG	C8-C7-N2-C2
4	A	1210	NAG	O7-C7-N2-C2
4	A	1210	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1210	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	427/428 (99%)	0.77	61 (14%) 2 3	28, 40, 59, 72	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	ARG	6.0
1	A	259	GLY	4.7
1	A	389	TYR	4.6
1	A	603	ALA	4.6
1	A	562	ILE	4.3
1	A	442	SER	4.3
1	A	441	PRO	4.0
1	A	508	TYR	4.0
1	A	326	ASN	3.9
1	A	422	GLU	3.8
1	A	395	CYS	3.8
1	A	387	CYS	3.8
1	A	423	ASN	3.8
1	A	365	PRO	3.6
1	A	222	LEU	3.6
1	A	454	TYR	3.5
1	A	221	LEU	3.5
1	A	359	GLY	3.4
1	A	601	CYS	3.4
1	A	586	ASN	3.4
1	A	388	GLN	3.3
1	A	328	GLY	3.3
1	A	384	ILE	3.1
1	A	421	GLY	3.1
1	A	351	TYR	3.1
1	A	456	ALA	3.0
1	A	242	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	383	PRO	2.9
1	A	283	SER	2.9
1	A	360	ASP	2.9
1	A	354	SER	2.9
1	A	223	ALA	2.9
1	A	524	VAL	2.8
1	A	577	LEU	2.7
1	A	327	GLY	2.7
1	A	386	LYS	2.7
1	A	502	ILE	2.7
1	A	380	SER	2.6
1	A	366	ALA	2.6
1	A	443	LYS	2.6
1	A	353	PRO	2.6
1	A	561	THR	2.5
1	A	453	PHE	2.5
1	A	260	ASP	2.5
1	A	293	VAL	2.5
1	A	420	ASP	2.5
1	A	511	ALA	2.4
1	A	491	SER	2.4
1	A	294	LEU	2.4
1	A	352	GLY	2.4
1	A	284	ALA	2.4
1	A	376	LYS	2.4
1	A	367	VAL	2.3
1	A	325	SER	2.2
1	A	563	THR	2.2
1	A	378	ASN	2.2
1	A	560	LYS	2.2
1	A	183	GLY	2.2
1	A	470	LEU	2.1
1	A	373	THR	2.1
1	A	232	SER	2.0

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

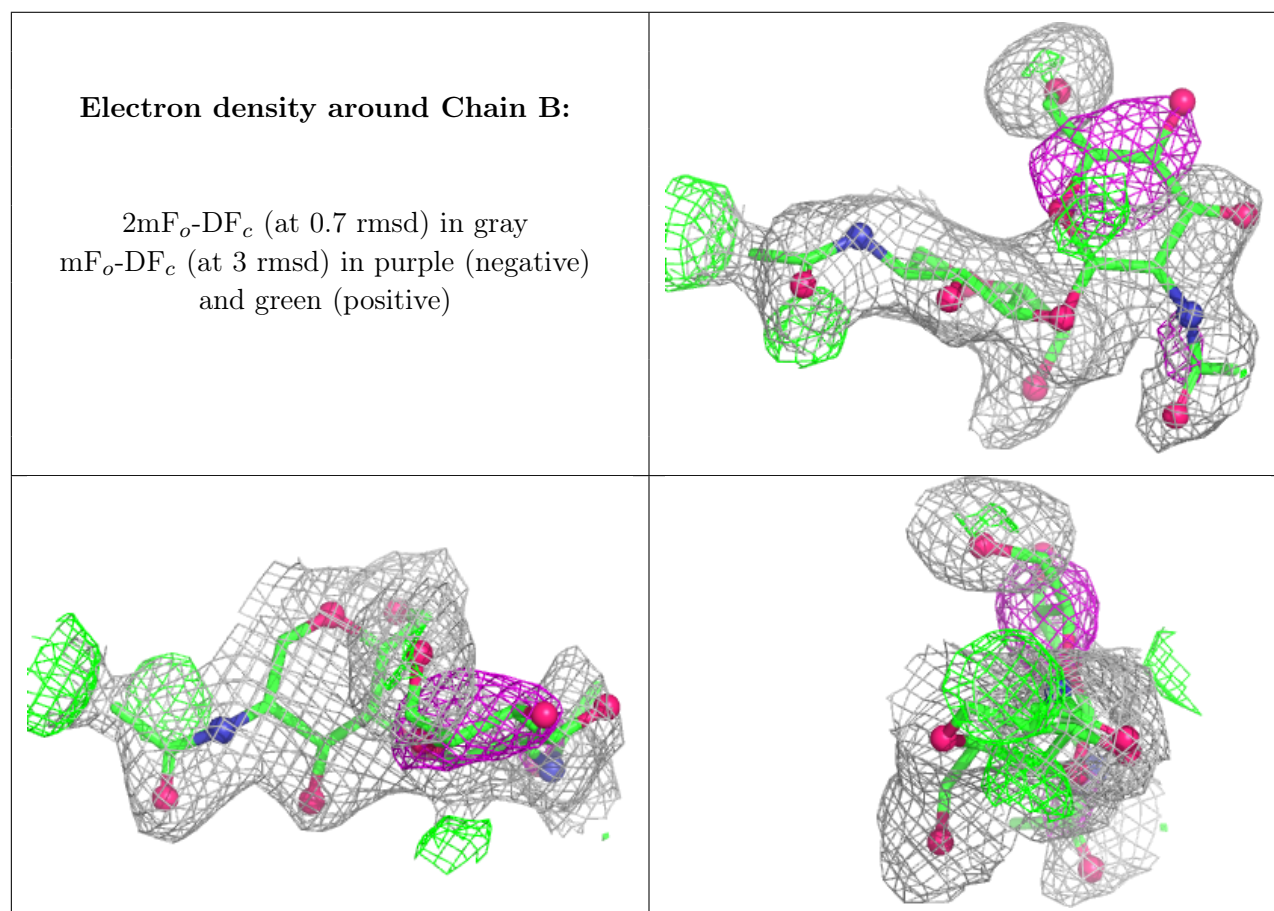
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B	2	14/15	0.30	0.54	51,63,65,65	0
2	NAG	B	1	14/15	0.76	0.22	49,56,60,60	0
3	MAN	D	5	11/12	0.79	0.21	49,51,53,56	0
2	NAG	C	2	14/15	0.83	0.30	58,59,61,61	0
2	NAG	C	1	14/15	0.86	0.24	54,56,59,59	0
3	BMA	D	4	11/12	0.88	0.17	44,48,50,52	0
3	BMA	D	3	11/12	0.90	0.08	47,50,52,52	0
3	NAG	D	1	14/15	0.92	0.12	38,39,41,42	0
3	NAG	D	2	14/15	0.96	0.15	40,42,45,47	0

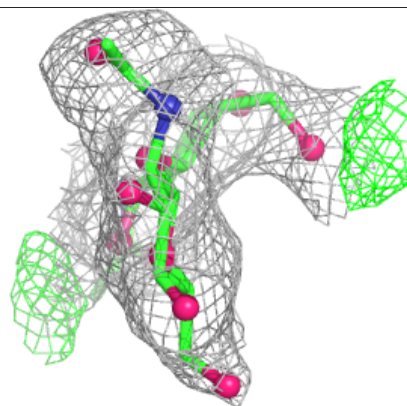
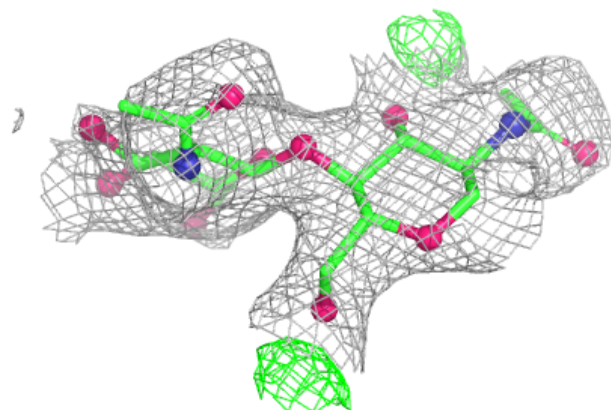
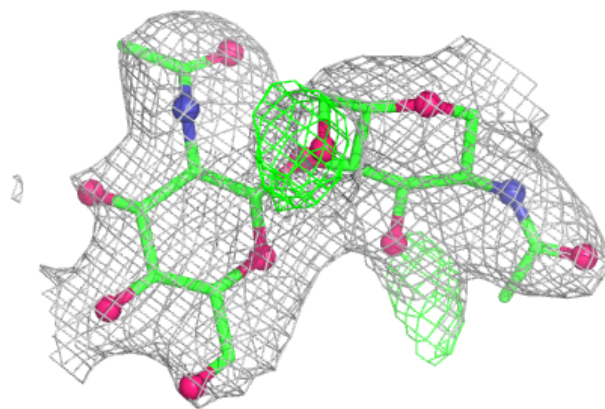
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

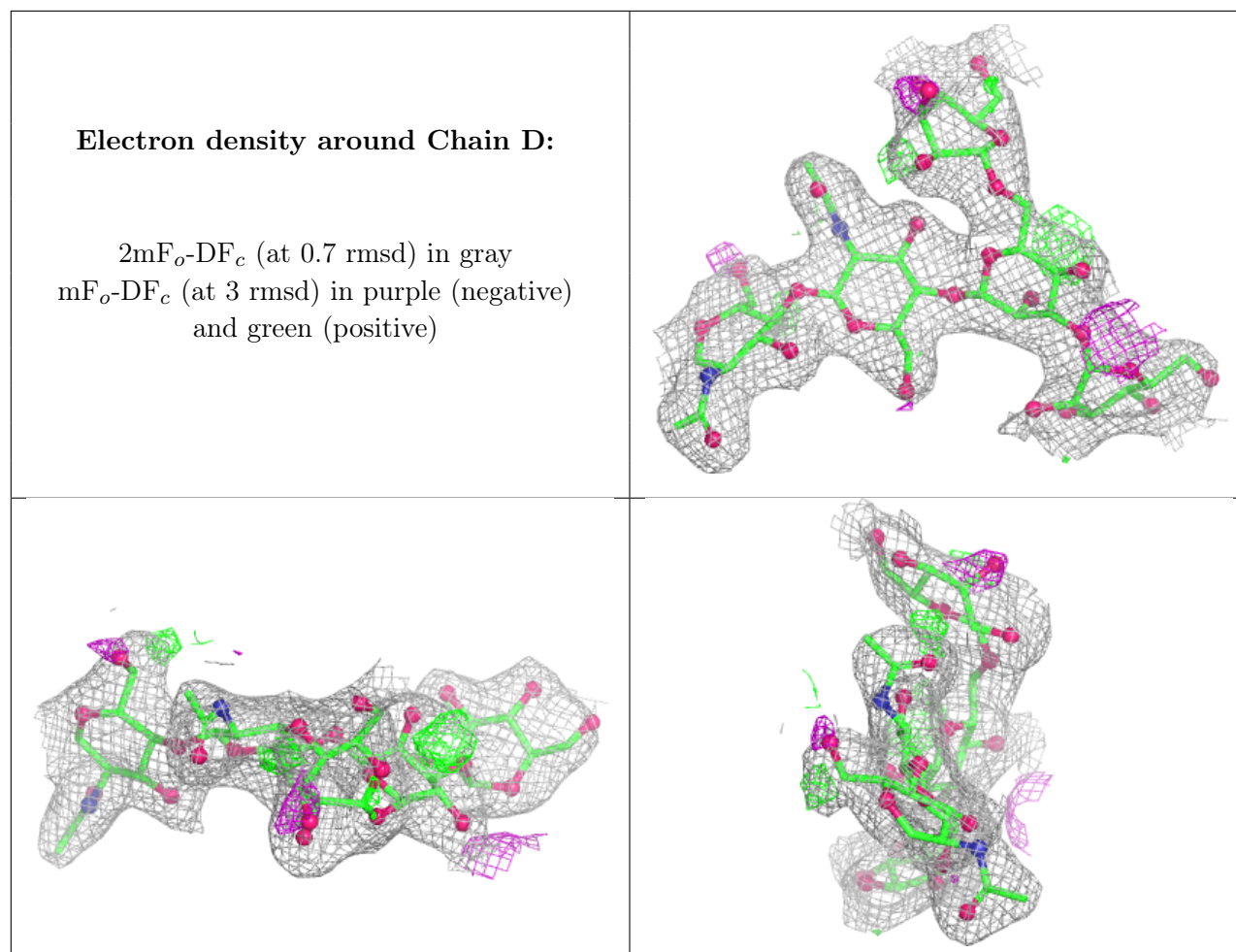




**Electron density around Chain C:**

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





## 6.4 Ligands [i](#)

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
4	NAG	A	1210	14/15	0.73	0.53	74,76,78,80	0
5	IOD	A	14	1/1	0.87	0.61	95,95,95,95	0
5	IOD	A	13	1/1	0.91	0.20	92,92,92,92	0
5	IOD	A	16	1/1	0.91	0.32	105,105,105,105	0
5	IOD	A	15	1/1	0.94	0.11	82,82,82,82	0
5	IOD	A	19	1/1	0.94	0.18	96,96,96,96	0
5	IOD	A	9	1/1	0.95	0.17	79,79,79,79	0
5	IOD	A	8	1/1	0.97	0.07	74,74,74,74	0
5	IOD	A	5	1/1	0.97	0.05	57,57,57,57	0
5	IOD	A	10	1/1	0.97	0.07	81,81,81,81	0
5	IOD	A	18	1/1	0.97	0.21	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	IOD	A	7	1/1	0.97	0.11	78,78,78,78	0
5	IOD	A	1	1/1	0.98	0.08	44,44,44,44	0
5	IOD	A	11	1/1	0.98	0.19	85,85,85,85	0
5	IOD	A	12	1/1	0.98	0.19	80,80,80,80	0
5	IOD	A	3	1/1	0.99	0.07	47,47,47,47	0
5	IOD	A	17	1/1	0.99	0.22	91,91,91,91	0
5	IOD	A	2	1/1	0.99	0.08	43,43,43,43	0
5	IOD	A	6	1/1	0.99	0.03	61,61,61,61	0
5	IOD	A	4	1/1	1.00	0.16	47,47,47,47	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.