



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2021 – 12:13 AM EDT

PDB ID : 1U65  
Title : Ache W. CPT-11  
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Deposited on : 2004-07-29  
Resolution : 2.61 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 : 2.18  
buster-report : 1.1.7 (2018)  
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) : 2.18

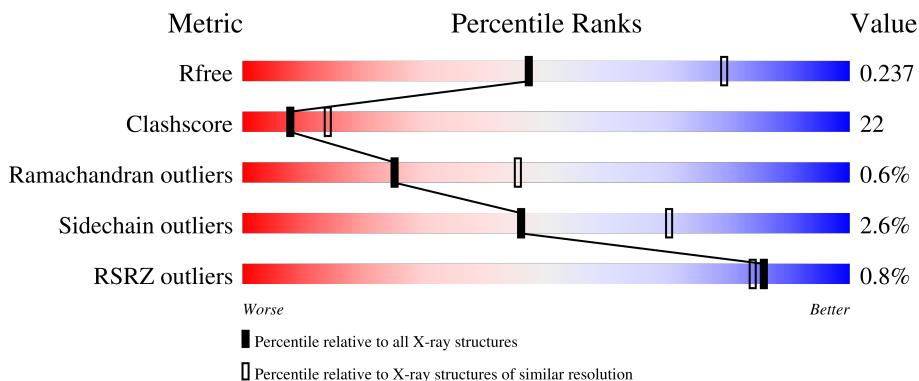
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	543	
2	B	2	
3	C	2	
4	D	2	

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	1	X	-	X	-
3	NAG	C	1	-	-	X	-
3	FUC	C	2	X	-	X	-
4	NAG	D	1	-	-	X	X
7	IOD	A	604	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4635 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	533	4249	2724	721	782	22	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	24	14	1	9	0	0	0

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



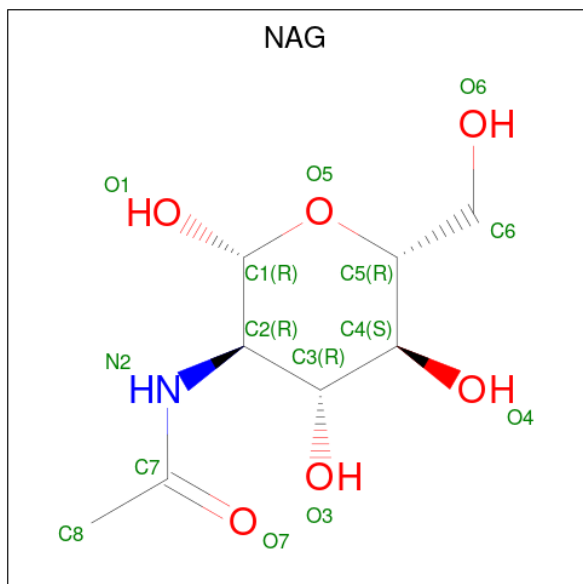
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	24	14	1	9	0	0	0

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



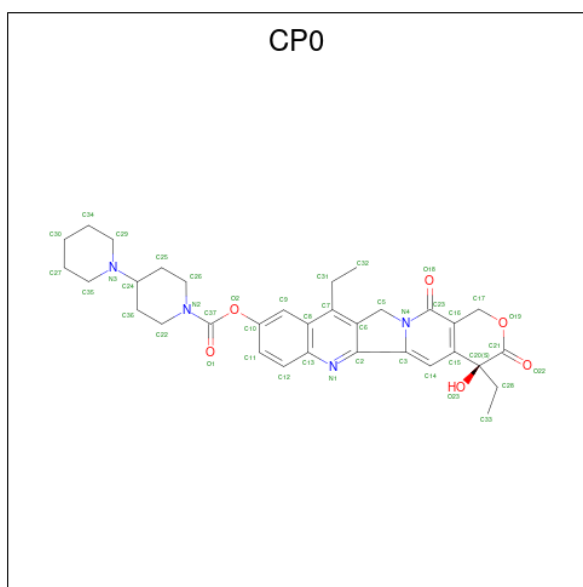
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	25	14	1	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is (4S)-4,11-DIETHYL-4-HYDROXY-3,14-DIOXO-3,4,12,14-TETRAHYDRO-1H-PYRANO[3',4':6,7]INDOLIZINO[1,2-B]QUINOLIN-9-YL 1,4'-BIPIPERIDINE-1'-CARBOXYLATE (three-letter code: CP0) (formula:  $C_{33}H_{38}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	43	33	4	6	0	0

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
7	A	1	1	1	0	0

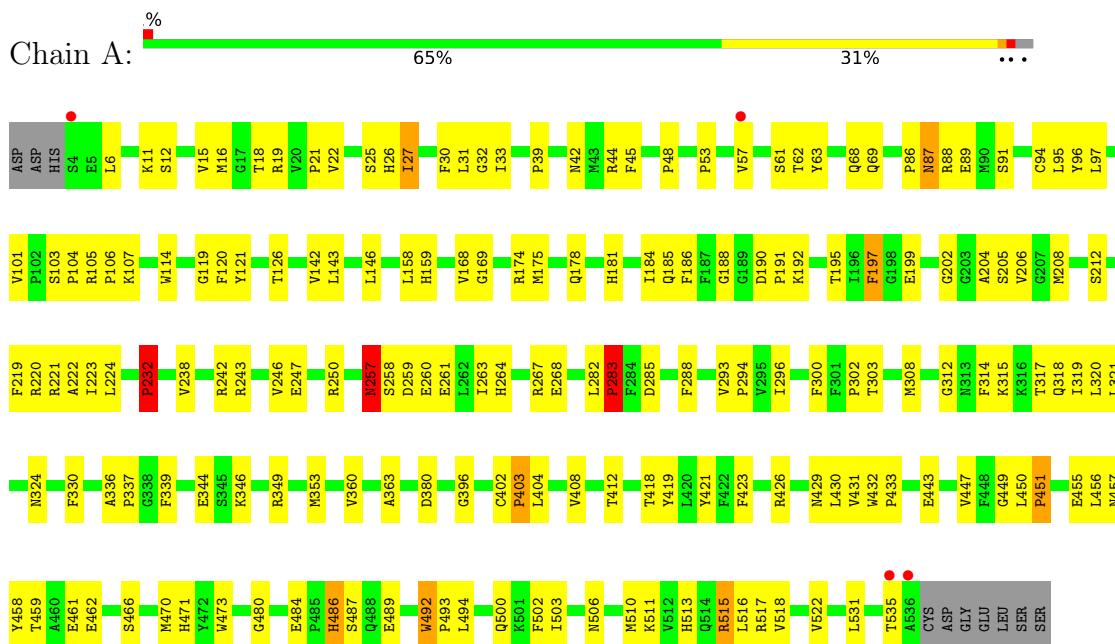
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	241	241	241	0	0

### 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.

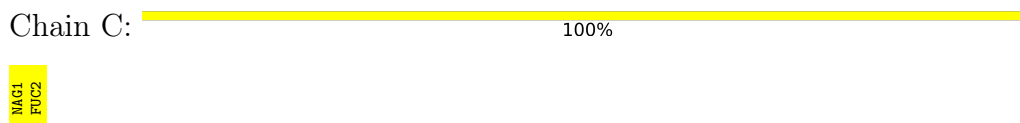
- Molecule 1: Acetylcholinesterase



- Molecule 2: beta-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



MAG1  
MAY2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.87Å 137.87Å 70.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.88 – 2.61 27.87 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.2 (27.88-2.61) 99.3 (27.87-2.61)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.187 , 0.237 0.188 , 0.237	Depositor DCC
$R_{free}$ test set	2382 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: MAN, FUC, NAG, FUL, CP0, IOD

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	0.50	3/4372 (0.1%)	0.73	8/5936 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	403	PRO	N-CD	-18.02	1.22	1.47
1	A	451	PRO	N-CD	5.34	1.55	1.47
1	A	493	PRO	N-CD	5.34	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PRO	CA-N-CD	-18.49	85.61	111.50
1	A	337	PRO	CA-N-CD	-16.06	89.02	111.50
1	A	232	PRO	CA-N-CD	-11.97	94.74	111.50
1	A	283	PRO	N-CA-CB	6.30	110.86	103.30
1	A	283	PRO	N-CD-CG	6.13	112.39	103.20
1	A	337	PRO	N-CA-CB	5.71	110.15	103.30
1	A	403	PRO	N-CD-CG	5.51	111.47	103.20
1	A	283	PRO	CB-CA-C	-5.26	98.85	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	ARG	Sidechain

## 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	4249	0	4099	167	1
2	B	24	0	22	8	0
3	C	24	0	22	7	0
4	D	25	0	22	12	0
5	A	28	0	26	2	0
6	A	43	0	38	4	0
7	A	1	0	0	5	0
8	A	241	0	0	21	0
All	All	4635	0	4229	186	1

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 22.

All (186) 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:243:ARG:NH2	1:A:283:PRO:HD3	1.56	1.19
2:B:1:NAG:H5	4:D:1:NAG:H62	1.40	1.02
1:A:243:ARG:HH22	1:A:283:PRO:HD3	1.29	0.95
1:A:243:ARG:NH2	1:A:283:PRO:CD	2.35	0.88
2:B:1:NAG:H4	2:B:2:FUL:C6	2.07	0.84
1:A:107:LYS:HD2	1:A:188:GLY:HA2	1.59	0.84
2:B:1:NAG:C5	4:D:1:NAG:H62	2.08	0.82
1:A:268:GLU:OE1	7:A:604:IOD:I	2.69	0.81
2:B:1:NAG:H4	2:B:2:FUL:H63	1.64	0.79
1:A:449:GLY:HA2	1:A:466:SER:OG	1.81	0.79
1:A:458:TYR:OH	4:D:2:MAN:H61	1.84	0.76
3:C:1:NAG:N2	3:C:2:FUC:H2	2.00	0.76
1:A:158:LEU:HD12	1:A:263:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:O	1:A:408:VAL:HG23	1.88	0.73
1:A:268:GLU:OE2	7:A:604:IOD:I	2.78	0.72
1:A:264:HIS:NE2	7:A:604:IOD:I	2.93	0.72
1:A:426:ARG:NH1	1:A:430:LEU:HD23	2.05	0.72
1:A:19:ARG:CZ	1:A:26:HIS:HB2	2.20	0.71
1:A:450:LEU:N	1:A:451:PRO:CD	2.54	0.70
1:A:303:THR:HA	8:A:770:HOH:O	1.92	0.70
1:A:42:ASN:HB2	8:A:884:HOH:O	1.92	0.69
1:A:268:GLU:CD	7:A:604:IOD:I	3.00	0.69
1:A:500:GLN:NE2	1:A:515:ARG:HG2	2.09	0.68
1:A:178:GLN:O	1:A:181:HIS:HB3	1.94	0.67
1:A:259:ASP:O	1:A:263:ILE:HG12	1.95	0.67
1:A:87:ASN:HD22	1:A:87:ASN:C	1.99	0.66
2:B:1:NAG:C4	2:B:2:FUL:H63	2.25	0.66
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.32	0.65
1:A:402:CYS:N	1:A:403:PRO:HD2	2.12	0.64
1:A:107:LYS:HB3	8:A:791:HOH:O	1.97	0.64
3:C:1:NAG:H83	3:C:2:FUC:H2	1.80	0.64
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.98	0.64
1:A:204:ALA:O	1:A:208:MET:HG3	1.98	0.63
1:A:506:ASN:HB2	8:A:778:HOH:O	1.98	0.62
1:A:471:HIS:HB3	8:A:730:HOH:O	1.99	0.62
1:A:285:ASP:HA	6:A:603:CP0:H282	1.81	0.61
1:A:264:HIS:CD2	7:A:604:IOD:I	3.23	0.61
1:A:451:PRO:HG2	1:A:466:SER:HB2	1.81	0.61
1:A:220:ARG:HH22	1:A:318:GLN:HE22	1.48	0.60
1:A:31:LEU:HB2	1:A:62:THR:O	2.01	0.60
1:A:457:ASN:HB2	4:D:1:NAG:C5	2.31	0.60
5:A:601:NAG:C1	5:A:602:NAG:H61	2.32	0.60
3:C:1:NAG:N2	3:C:2:FUC:C2	2.64	0.60
1:A:48:PRO:HG2	1:A:175:MET:HE3	1.83	0.59
1:A:243:ARG:HH21	1:A:283:PRO:CD	2.15	0.59
1:A:302:PRO:HD2	1:A:308:MET:CE	2.32	0.59
1:A:344:GLU:OE1	1:A:346:LYS:HE3	2.01	0.59
1:A:457:ASN:HB2	4:D:1:NAG:H5	1.84	0.59
1:A:264:HIS:HE1	8:A:756:HOH:O	1.85	0.59
1:A:426:ARG:CZ	1:A:430:LEU:HD23	2.32	0.59
2:B:1:NAG:C6	4:D:1:NAG:H62	2.32	0.59
1:A:6:LEU:HB3	1:A:16:MET:HE3	1.85	0.58
1:A:232:PRO:HD3	8:A:869:HOH:O	2.03	0.58
1:A:22:VAL:HG11	1:A:27:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HB	1:A:294:PRO:HD2	1.86	0.58
3:C:1:NAG:C8	3:C:2:FUC:H2	2.34	0.58
1:A:44:ARG:O	1:A:45:PHE:HB2	2.05	0.57
1:A:221:ARG:HE	1:A:480:GLY:HA2	1.69	0.57
2:B:1:NAG:H4	2:B:2:FUL:H61	1.87	0.57
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.86	0.57
1:A:317:THR:OG1	1:A:318:GLN:N	2.38	0.57
1:A:89:GLU:HG3	8:A:888:HOH:O	2.05	0.57
1:A:402:CYS:N	1:A:403:PRO:CD	2.68	0.56
1:A:450:LEU:N	1:A:451:PRO:HD3	2.20	0.56
1:A:159:HIS:CB	1:A:238:VAL:HG13	2.34	0.56
1:A:199:GLU:HG3	1:A:443:GLU:OE2	2.05	0.56
1:A:257:ASN:HD22	1:A:257:ASN:N	2.03	0.56
1:A:146:LEU:C	1:A:146:LEU:HD12	2.26	0.56
1:A:45:PHE:O	1:A:168:VAL:HG11	2.06	0.56
1:A:19:ARG:NH2	1:A:26:HIS:HB2	2.22	0.55
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.42	0.55
3:C:1:NAG:C7	3:C:2:FUC:H2	2.37	0.54
1:A:257:ASN:HD22	1:A:258:SER:H	1.56	0.54
1:A:103:SER:HA	1:A:104:PRO:C	2.28	0.54
1:A:451:PRO:HD2	1:A:466:SER:OG	2.08	0.53
1:A:518:VAL:O	1:A:522:VAL:HG23	2.09	0.53
1:A:16:MET:HB2	1:A:57:VAL:CG1	2.39	0.53
1:A:159:HIS:HB3	1:A:238:VAL:HG13	1.90	0.53
1:A:336:ALA:HB3	1:A:339:PHE:CD1	2.43	0.53
1:A:466:SER:O	1:A:470:MET:HG3	2.09	0.53
1:A:455:GLU:OE2	1:A:455:GLU:N	2.37	0.52
1:A:431:VAL:HG22	8:A:814:HOH:O	2.09	0.52
1:A:39:PRO:HD3	1:A:95:LEU:HD12	1.90	0.52
1:A:447:VAL:O	1:A:470:MET:HG2	2.10	0.52
1:A:531:LEU:C	1:A:531:LEU:HD23	2.28	0.52
1:A:293:VAL:HB	1:A:294:PRO:CD	2.39	0.52
1:A:106:PRO:HB3	8:A:817:HOH:O	2.09	0.52
1:A:107:LYS:HE3	1:A:185:GLN:O	2.10	0.52
1:A:16:MET:HG2	8:A:731:HOH:O	2.10	0.52
1:A:87:ASN:C	1:A:87:ASN:ND2	2.63	0.52
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.40	0.51
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.45	0.51
1:A:486:HIS:HB3	8:A:767:HOH:O	2.10	0.51
1:A:15:VAL:HG11	1:A:33:ILE:HD12	1.91	0.51
6:A:603:CP0:O1	6:A:603:CP0:H11	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD12	1:A:263:ILE:CD1	2.38	0.51
1:A:242:ARG:O	1:A:246:VAL:HG23	2.11	0.51
1:A:302:PRO:HD2	1:A:308:MET:HE1	1.93	0.51
1:A:471:HIS:ND1	8:A:703:HOH:O	2.34	0.51
1:A:457:ASN:HB2	4:D:1:NAG:H61	1.93	0.51
1:A:263:ILE:O	1:A:267:ARG:HG3	2.10	0.51
1:A:487:SER:OG	1:A:489:GLU:HG3	2.12	0.51
1:A:432:TRP:HB3	1:A:433:PRO:HD2	1.92	0.50
1:A:6:LEU:HB3	1:A:16:MET:CE	2.41	0.50
1:A:114:TRP:HB2	1:A:197:PHE:CE1	2.46	0.50
1:A:471:HIS:NE2	1:A:484:GLU:OE1	2.45	0.50
1:A:142:VAL:HG11	1:A:184:ILE:HD11	1.94	0.49
1:A:260:GLU:H	1:A:260:GLU:CD	2.15	0.49
1:A:30:PHE:CD1	1:A:30:PHE:N	2.81	0.49
1:A:219:PHE:O	1:A:315:LYS:HE3	2.13	0.49
1:A:419:TYR:CZ	1:A:494:LEU:HD13	2.48	0.49
1:A:257:ASN:HD21	1:A:261:GLU:CB	2.25	0.49
1:A:429:ASN:HB2	4:D:1:NAG:O4	2.13	0.49
6:A:603:CP0:H352	8:A:811:HOH:O	2.12	0.48
1:A:221:ARG:HE	1:A:480:GLY:CA	2.25	0.48
1:A:324:ASN:OD1	1:A:423:PHE:HB3	2.13	0.48
1:A:68:GLN:NE2	1:A:68:GLN:HA	2.28	0.48
1:A:458:TYR:OH	4:D:2:MAN:C6	2.57	0.48
1:A:6:LEU:HD22	1:A:18:THR:N	2.29	0.48
1:A:257:ASN:N	1:A:257:ASN:ND2	2.61	0.48
3:C:1:NAG:H83	3:C:2:FUC:O4	2.13	0.48
1:A:202:GLY:O	1:A:205:SER:HB2	2.14	0.48
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.13	0.48
1:A:21:PRO:HA	1:A:25:SER:O	2.14	0.47
1:A:238:VAL:HG23	1:A:296:ILE:O	2.13	0.47
1:A:268:GLU:HG2	8:A:868:HOH:O	2.14	0.47
1:A:22:VAL:CG1	1:A:27:ILE:HD12	2.42	0.47
1:A:11:LYS:HG3	1:A:186:PHE:HE2	1.80	0.47
1:A:456:LEU:C	4:D:1:NAG:H61	2.35	0.47
3:C:1:NAG:HN2	3:C:2:FUC:C2	2.27	0.47
1:A:15:VAL:HG11	1:A:33:ILE:CD1	2.45	0.47
1:A:486:HIS:ND1	8:A:704:HOH:O	2.35	0.47
1:A:516:LEU:HD12	1:A:517:ARG:HG3	1.96	0.47
1:A:302:PRO:HD2	1:A:308:MET:SD	2.55	0.46
1:A:107:LYS:HD2	1:A:107:LYS:HA	1.75	0.46
1:A:91:SER:O	1:A:94:CYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NE	1:A:480:GLY:HA2	2.31	0.46
1:A:450:LEU:H	1:A:451:PRO:HD3	1.80	0.46
1:A:119:GLY:O	1:A:120:PHE:HB2	2.16	0.46
1:A:16:MET:HB2	1:A:57:VAL:HG11	1.98	0.45
1:A:396:GLY:HA3	8:A:825:HOH:O	2.15	0.45
1:A:459:THR:HG23	1:A:462:GLU:OE1	2.15	0.45
1:A:44:ARG:O	1:A:45:PHE:CB	2.63	0.45
1:A:510:MET:HG2	1:A:511:LYS:N	2.31	0.45
1:A:69:GLN:CD	1:A:86:PRO:HG3	2.36	0.45
1:A:412:THR:HG22	1:A:412:THR:O	2.15	0.45
1:A:257:ASN:HD22	1:A:258:SER:N	2.15	0.45
1:A:486:HIS:CE1	8:A:704:HOH:O	2.69	0.45
1:A:121:TYR:HB3	8:A:813:HOH:O	2.16	0.45
1:A:212:SER:HB2	1:A:300:PHE:CE1	2.51	0.44
1:A:247:GLU:HA	1:A:250:ARG:NH1	2.31	0.44
1:A:349:ARG:O	1:A:353:MET:HG2	2.17	0.44
1:A:344:GLU:CD	1:A:346:LYS:HE3	2.37	0.44
1:A:282:LEU:HD12	6:A:603:CP0:O23	2.17	0.44
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.53	0.44
2:B:1:NAG:H5	4:D:1:NAG:C6	2.28	0.44
1:A:22:VAL:O	1:A:22:VAL:HG13	2.17	0.44
1:A:511:LYS:HE3	8:A:904:HOH:O	2.18	0.44
1:A:206:VAL:HG11	1:A:222:ALA:HB1	1.99	0.43
1:A:257:ASN:HD21	1:A:261:GLU:HG3	1.83	0.43
1:A:223:ILE:HA	1:A:320:LEU:O	2.19	0.43
1:A:12:SER:O	1:A:53:PRO:HA	2.18	0.43
1:A:264:HIS:CE1	8:A:756:HOH:O	2.67	0.43
1:A:174:ARG:NH2	1:A:212:SER:OG	2.52	0.43
1:A:195:THR:OG1	1:A:221:ARG:HG3	2.19	0.43
1:A:88:ARG:HD3	1:A:88:ARG:HA	1.94	0.42
1:A:190:ASP:OD1	1:A:192:LYS:CG	2.67	0.42
1:A:461:GLU:H	1:A:461:GLU:CD	2.21	0.42
1:A:101:VAL:HG11	1:A:105:ARG:HG3	2.02	0.42
1:A:360:VAL:HG12	1:A:363:ALA:HB2	2.00	0.42
1:A:18:THR:CG2	1:A:61:SER:HA	2.50	0.42
1:A:168:VAL:HG23	1:A:169:GLY:N	2.34	0.42
1:A:421:TYR:C	1:A:421:TYR:CD1	2.92	0.42
1:A:457:ASN:HB2	4:D:1:NAG:C6	2.49	0.42
1:A:319:ILE:O	1:A:319:ILE:HG13	2.20	0.42
1:A:492:TRP:CD2	1:A:503:ILE:HD11	2.55	0.41
1:A:190:ASP:HA	1:A:191:PRO:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:O	1:A:96:TYR:HD2	2.03	0.41
1:A:404:LEU:C	1:A:404:LEU:HD23	2.41	0.41
1:A:418:THR:O	1:A:494:LEU:HD12	2.21	0.41
1:A:97:LEU:HD12	1:A:97:LEU:C	2.41	0.41
1:A:224:LEU:HD12	1:A:224:LEU:N	2.35	0.41
1:A:257:ASN:ND2	1:A:261:GLU:HG3	2.36	0.41
5:A:601:NAG:C1	5:A:602:NAG:O4	2.69	0.41
1:A:221:ARG:NE	1:A:480:GLY:CA	2.85	0.40
1:A:461:GLU:OE1	1:A:461:GLU:N	2.48	0.40

All (1) 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:A:535:THR:CG2	1:A:535:THR:CG2[5_675]	2.08	0.12

## 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	531/543 (98%)	480 (90%)	48 (9%)	3 (1%)	25 45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	486	HIS
1	A	380	ASP



### 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	465/474 (98%)	453 (97%)	12 (3%)	46 70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ILE
1	A	87	ASN
1	A	143	LEU
1	A	197	PHE
1	A	232	PRO
1	A	257	ASN
1	A	283	PRO
1	A	288	PHE
1	A	321	LEU
1	A	330	PHE
1	A	473	TRP
1	A	492	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	66	ASN
1	A	68	GLN
1	A	87	ASN
1	A	181	HIS
1	A	257	ASN
1	A	280	ASN
1	A	382	ASN
1	A	500	GLN
1	A	519	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](#)

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

### 5.5 Carbohydrates [i](#)

6 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	0.71	0	17,19,21	0.76	0
2	FUL	B	2	2	10,10,11	0.84	0	14,14,16	1.19	3 (21%)
3	NAG	C	1	1,3	14,14,15	0.69	0	17,19,21	0.59	0
3	FUC	C	2	3	10,10,11	0.53	0	14,14,16	0.54	0
4	NAG	D	1	4	14,14,15	0.61	0	17,19,21	0.92	1 (5%)
4	MAN	D	2	4	11,11,12	0.39	0	15,15,17	0.60	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	B	1	2,1	1/1/5/7	3/6/23/26	0/1/1/1
2	FUL	B	2	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	3/6/23/26	0/1/1/1
3	FUC	C	2	3	1/1/4/5	-	0/1/1/1
4	NAG	D	1	4	-	4/6/23/26	0/1/1/1
4	MAN	D	2	4	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	FUL	C1-C2-C3	2.51	112.75	109.67
4	D	1	NAG	C4-C3-C2	-2.49	107.36	111.02
2	B	2	FUL	C1-O5-C5	2.36	118.12	112.78
2	B	2	FUL	O5-C5-C4	2.02	113.15	109.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1
3	C	2	FUC	C1

All (12) torsion outliers are listed below:

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

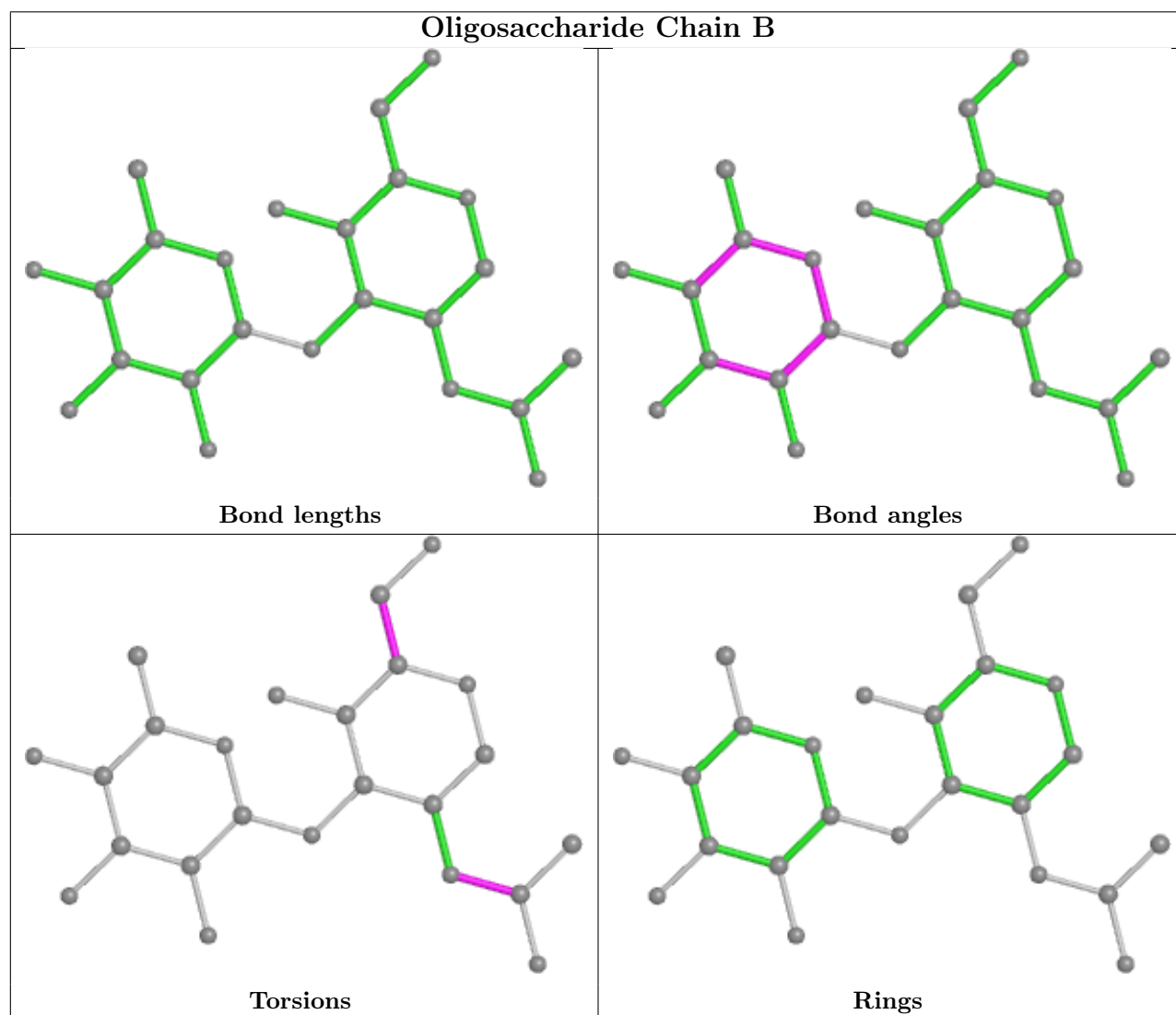
All (1) ring outliers are listed below:

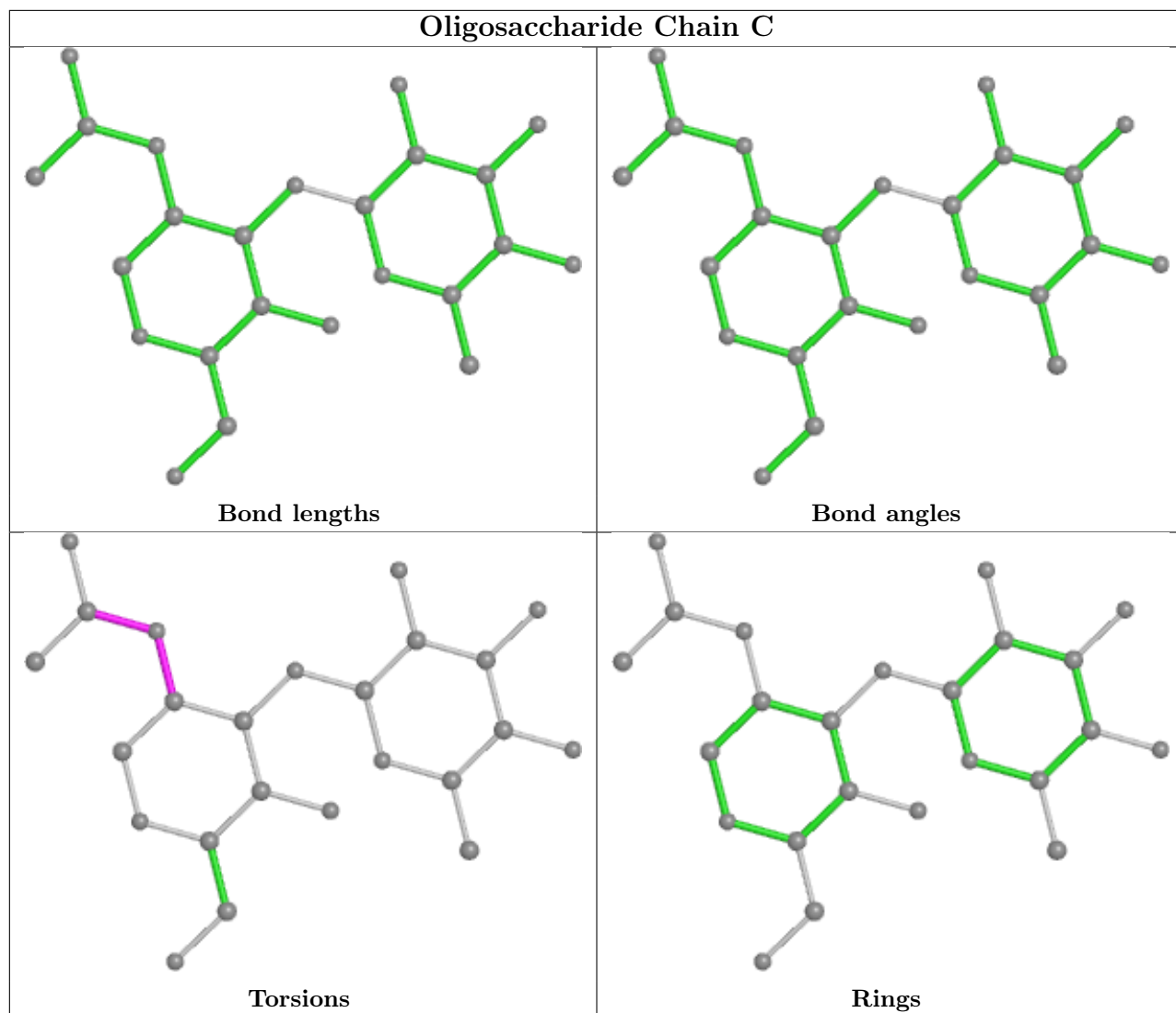
Mol	Chain	Res	Type	Atoms
4	D	2	MAN	C1-C2-C3-C4-C5-O5

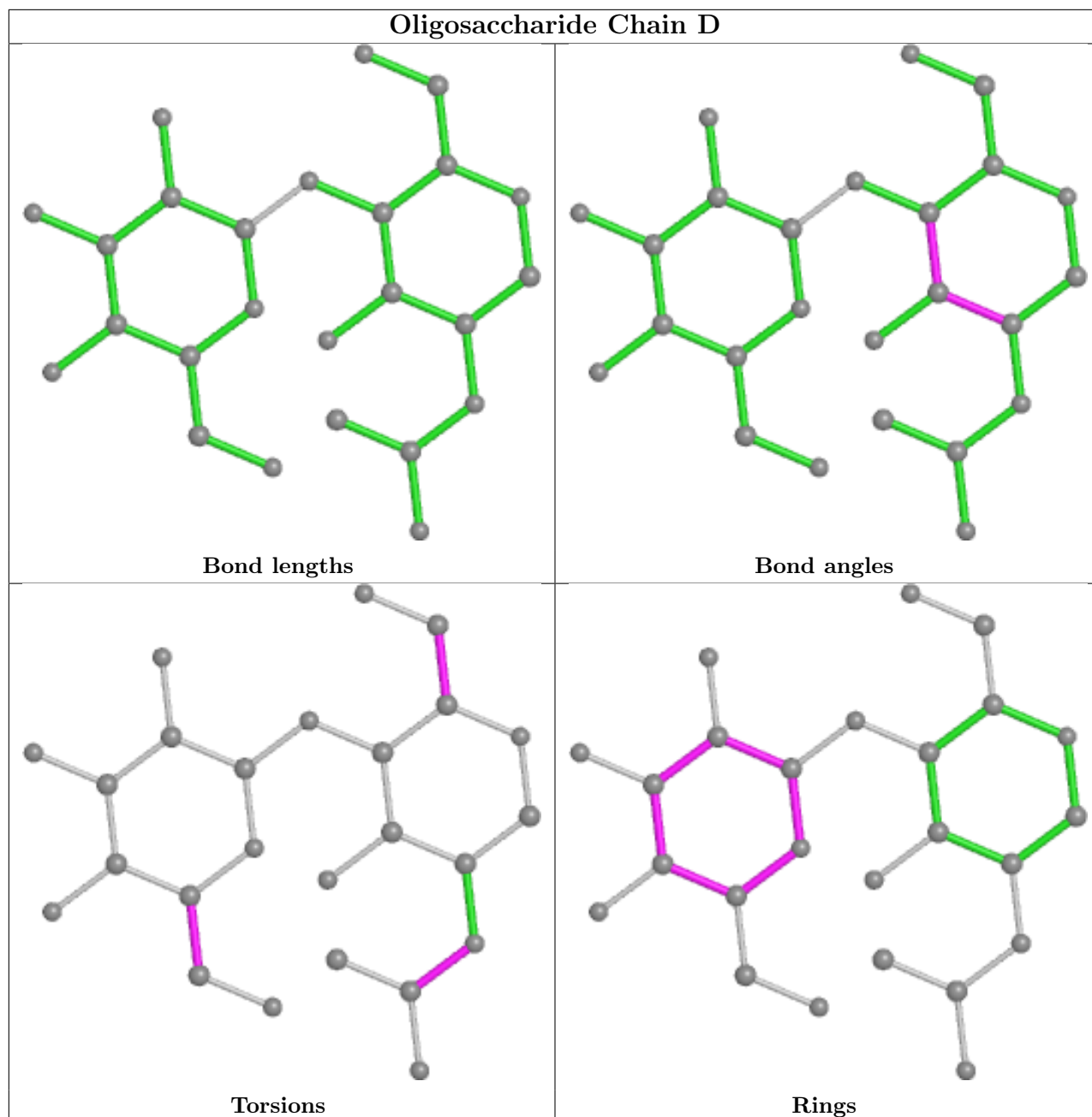
6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	7	0
2	B	1	NAG	8	0
4	D	1	NAG	10	0
4	D	2	MAN	2	0
3	C	2	FUC	7	0
2	B	2	FUL	4	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	602	1	14,14,15	0.54	0	17,19,21	0.68	1 (5%)
6	CP0	A	603	-	47,49,49	3.53	27 (57%)	51,74,74	2.86	20 (39%)
5	NAG	A	601	-	14,14,15	0.64	0	17,19,21	0.66	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
5	NAG	A	602	1	-	4/6/23/26	0/1/1/1
6	CP0	A	603	-	-	7/17/60/60	0/7/7/7
5	NAG	A	601	-	-	5/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	CP0	C23-N4	8.88	1.51	1.38
6	A	603	CP0	C11-C10	7.64	1.54	1.38
6	A	603	CP0	C6-C7	7.10	1.47	1.38
6	A	603	CP0	C8-C13	6.59	1.53	1.42
6	A	603	CP0	C29-N3	6.25	1.59	1.47
6	A	603	CP0	C14-C15	6.07	1.48	1.39
6	A	603	CP0	C12-C13	5.60	1.51	1.41
6	A	603	CP0	C23-C16	5.02	1.52	1.41
6	A	603	CP0	O2-C37	4.51	1.46	1.36
6	A	603	CP0	C3-N4	4.38	1.45	1.36
6	A	603	CP0	C13-N1	4.05	1.44	1.37
6	A	603	CP0	C7-C8	3.90	1.49	1.43
6	A	603	CP0	C9-C8	3.74	1.49	1.42
6	A	603	CP0	C3-C2	-3.54	1.40	1.47
6	A	603	CP0	O19-C21	3.53	1.38	1.34
6	A	603	CP0	C20-C15	3.24	1.59	1.53
6	A	603	CP0	C36-C22	3.14	1.61	1.52
6	A	603	CP0	C17-C16	2.99	1.56	1.51
6	A	603	CP0	C36-C24	2.88	1.59	1.52
6	A	603	CP0	C9-C10	2.70	1.41	1.37
6	A	603	CP0	C24-N3	2.56	1.55	1.48
6	A	603	CP0	C16-C15	2.51	1.42	1.38
6	A	603	CP0	C30-C27	2.43	1.61	1.51
6	A	603	CP0	O1-C37	-2.40	1.17	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	CP0	C22-N2	2.33	1.51	1.47
6	A	603	CP0	O23-C20	2.16	1.45	1.42
6	A	603	CP0	O19-C17	2.14	1.48	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	CP0	C22-N2-C37	7.89	144.35	121.77
6	A	603	CP0	C16-C23-N4	-6.77	112.88	120.23
6	A	603	CP0	C36-C22-N2	-6.45	101.01	110.82
6	A	603	CP0	C26-N2-C37	-6.44	103.36	121.77
6	A	603	CP0	C11-C12-C13	-5.68	113.68	120.84
6	A	603	CP0	O2-C37-N2	4.83	115.45	110.75
6	A	603	CP0	C10-O2-C37	4.74	126.11	117.27
6	A	603	CP0	C12-C13-C8	4.30	124.06	119.13
6	A	603	CP0	C25-C26-N2	-4.27	104.33	110.82
6	A	603	CP0	C12-C11-C10	4.01	125.55	120.17
6	A	603	CP0	C12-C13-N1	-3.67	113.09	118.69
6	A	603	CP0	C9-C8-C7	3.07	127.53	121.84
6	A	603	CP0	C14-C3-C2	2.78	130.75	124.70
6	A	603	CP0	C34-C29-N3	-2.74	106.66	111.28
6	A	603	CP0	C3-C2-N1	2.47	121.79	118.19
6	A	603	CP0	O2-C37-O1	-2.26	119.39	123.74
6	A	603	CP0	C33-C28-C20	2.23	116.79	114.07
6	A	603	CP0	O19-C17-C16	2.22	114.17	111.51
6	A	603	CP0	C5-C6-C7	2.12	133.07	128.96
6	A	603	CP0	C7-C8-C13	-2.03	115.90	118.31
5	A	602	NAG	C2-N2-C7	-2.03	120.02	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	C3-C2-N2-C7
5	A	601	NAG	C8-C7-N2-C2
5	A	601	NAG	O7-C7-N2-C2
5	A	602	NAG	C8-C7-N2-C2
5	A	602	NAG	O7-C7-N2-C2
6	A	603	CP0	C11-C10-O2-C37
6	A	603	CP0	O1-C37-N2-C22
6	A	603	CP0	O1-C37-N2-C26
6	A	603	CP0	O2-C37-N2-C22

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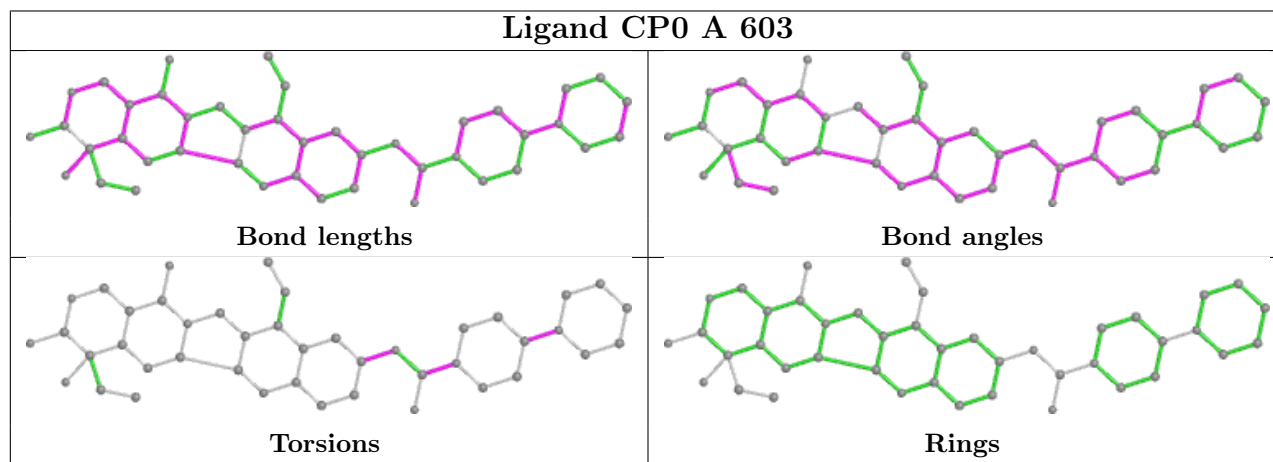
Mol	Chain	Res	Type	Atoms
6	A	603	CP0	O2-C37-N2-C26
5	A	602	NAG	O5-C5-C6-O6
6	A	603	CP0	C9-C10-O2-C37
5	A	602	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
6	A	603	CP0	C36-C24-N3-C29

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	NAG	2	0
6	A	603	CP0	4	0
5	A	601	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	533/543 (98%)	-0.53	4 (0%) 86 84	19, 36, 59, 81	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	ALA	4.2
1	A	535	THR	3.6
1	A	4	SER	2.9
1	A	57	VAL	2.6

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

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

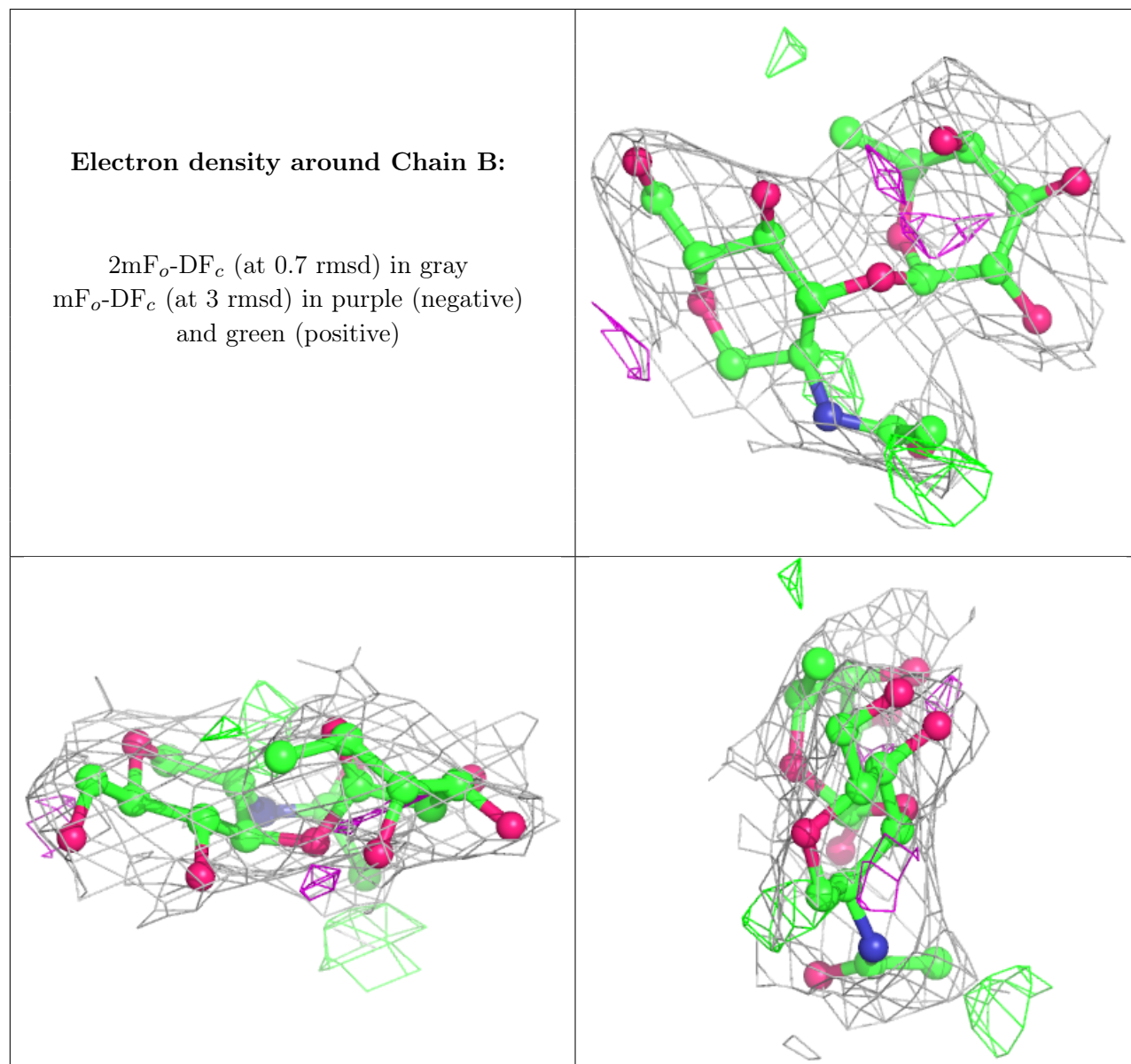
### 6.3 Carbohydrates [i](#)

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
4	NAG	D	1	14/15	0.73	0.54	103,105,107,108	0
4	MAN	D	2	11/12	0.73	0.34	97,99,102,104	0
3	NAG	C	1	14/15	0.79	0.34	87,91,95,96	0
2	NAG	B	1	14/15	0.82	0.29	73,78,81,83	0
2	FUL	B	2	10/11	0.85	0.41	85,87,88,88	0
3	FUC	C	2	10/11	0.87	0.34	94,95,95,95	0

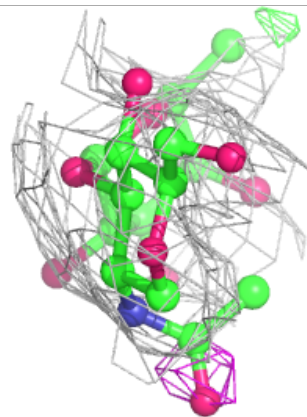
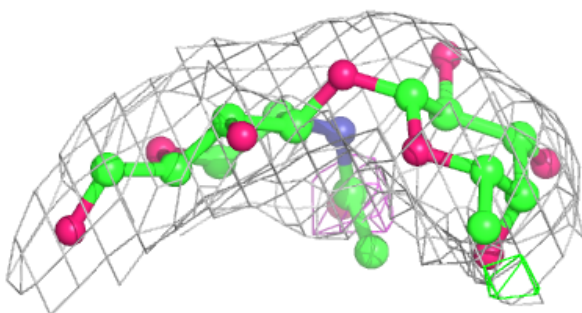
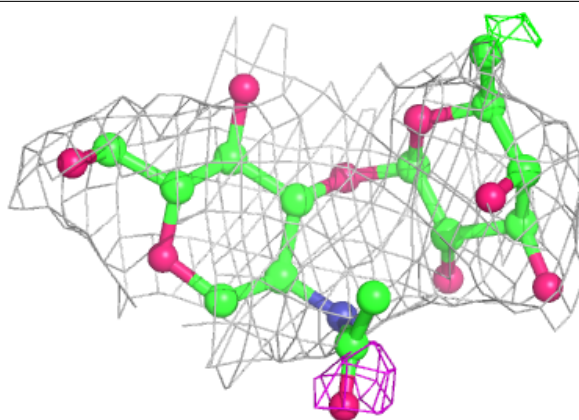
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

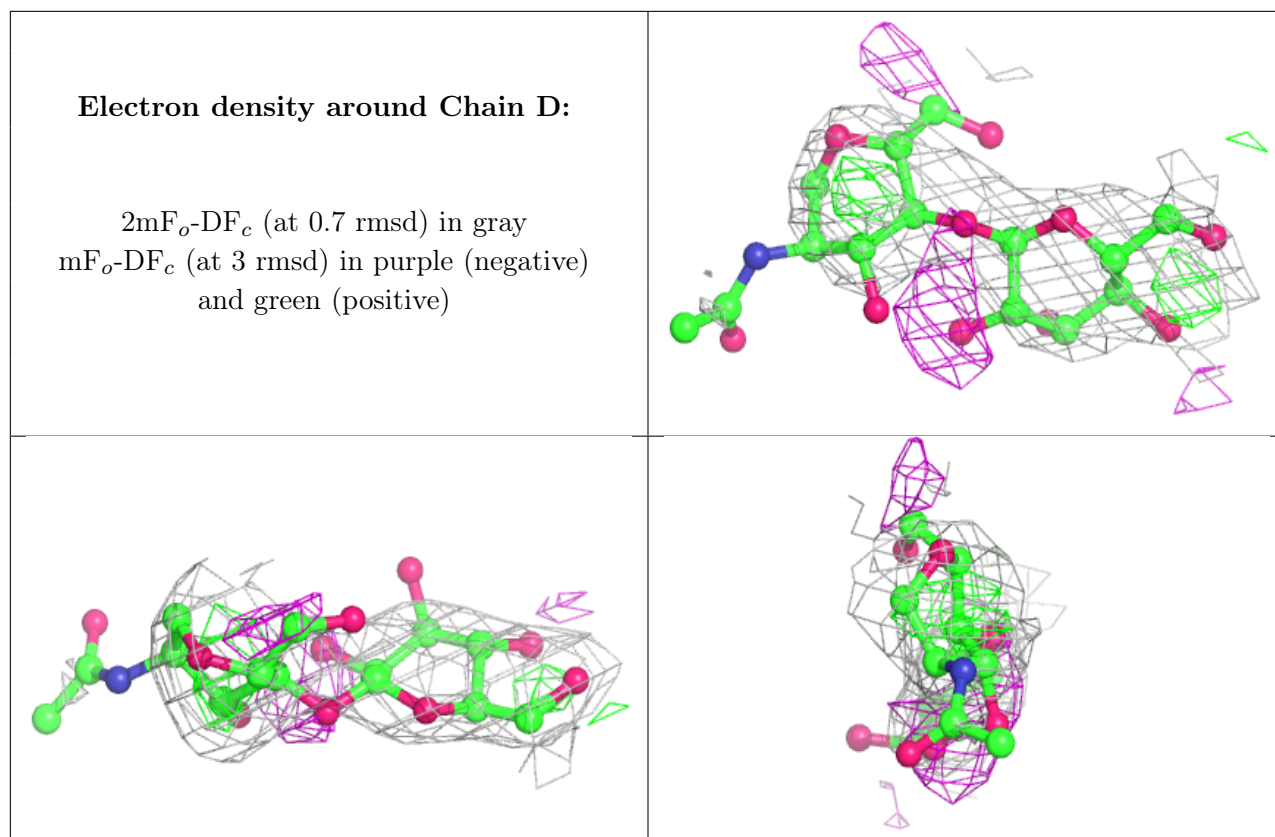
charide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)



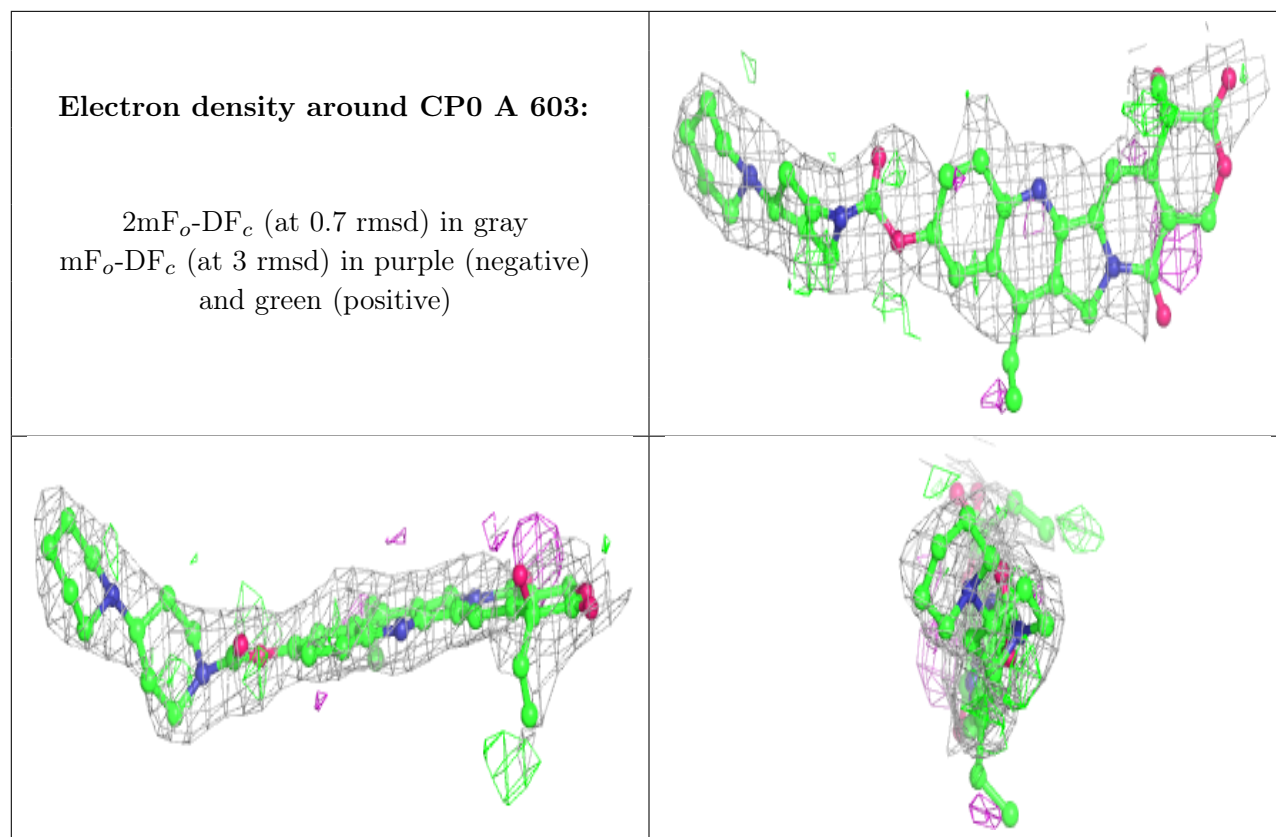


## 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
6	CP0	A	603	43/43	0.80	0.26	44,76,89,91	0
5	NAG	A	601	14/15	0.81	0.34	113,114,114,114	0
5	NAG	A	602	14/15	0.90	0.20	62,64,67,67	0
7	IOD	A	604	1/1	0.93	0.06	66,66,66,66	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.