



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2021 – 06:08 PM JST

PDB ID : 7EV0  
Title : Crystal structure of pepsin cleaved C-terminal half of lactoferrin at 2.7Å resolution  
Authors : Singh, J.; Ahmad, M.I.; Maurya, A.; Sharma, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2021-05-19  
Resolution : 2.70 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:

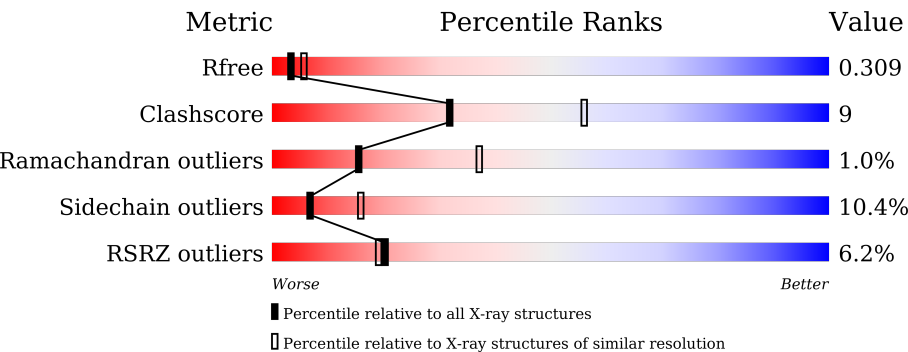
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.70 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.



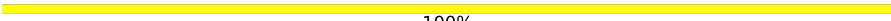
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	348	<div><div>5%</div><div><div></div><div>68%</div><div>29%</div><div>.</div></div></div>
1	P	348	<div><div>7%</div><div><div></div><div>76%</div><div>22%</div><div>.</div></div></div>
2	E	2	<div><div></div><div>100%</div></div>
2	Z	2	<div><div></div><div>100%</div></div>
3	B	3	<div><div></div><div><div>67%</div><div>33%</div></div></div>
4	C	4	<div><div><div>25%</div><div>75%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	D	4	 100%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5620 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 Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2657	1655	465	516	21			
1	P	348	Total	C	N	O	S	0	0	0
			2657	1655	465	516	21			

- 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	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 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	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

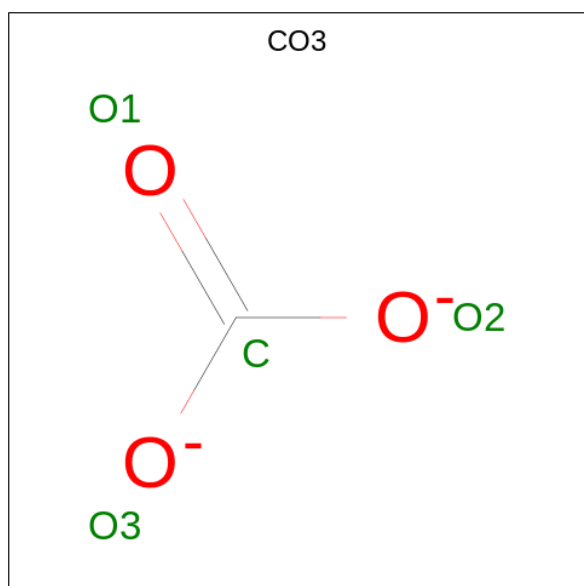


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

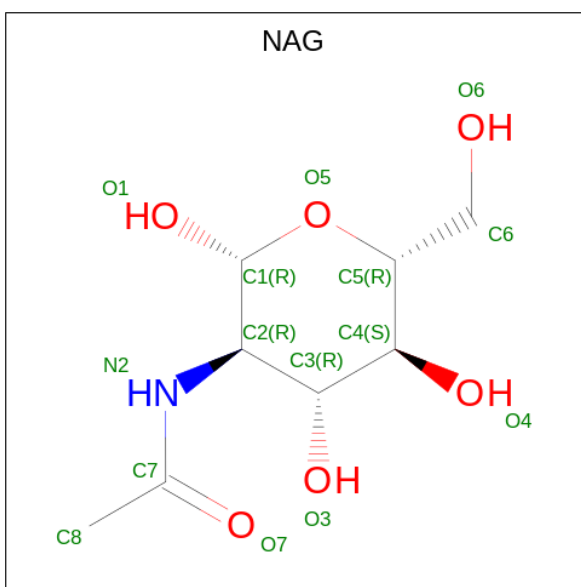
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		
5	P	1	Total	Fe	0	0
			1	1		

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		
6	P	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

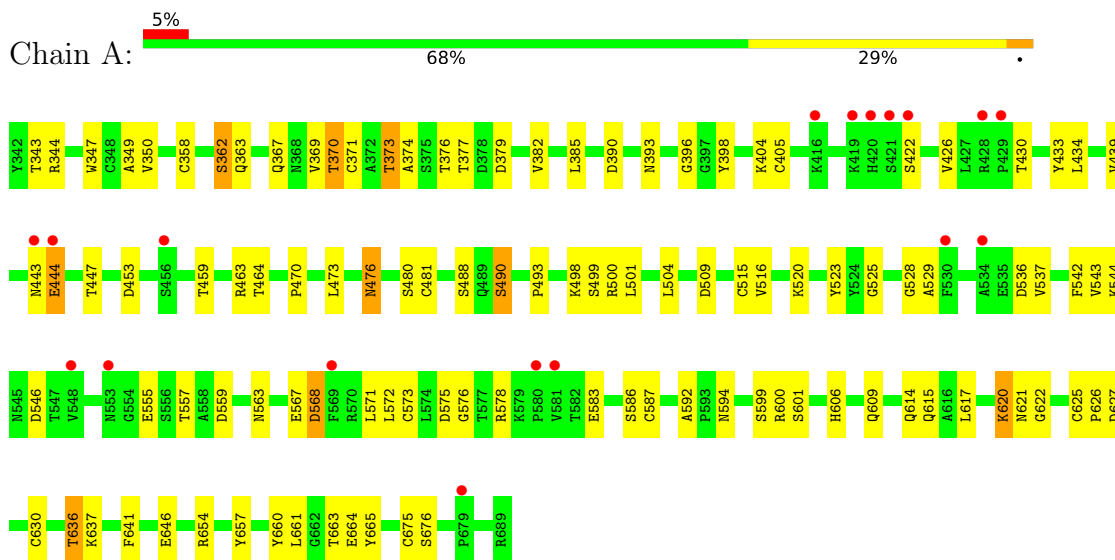
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	43	Total	O	0	0
			43	43		
8	P	44	Total	O	0	0
			44	44		

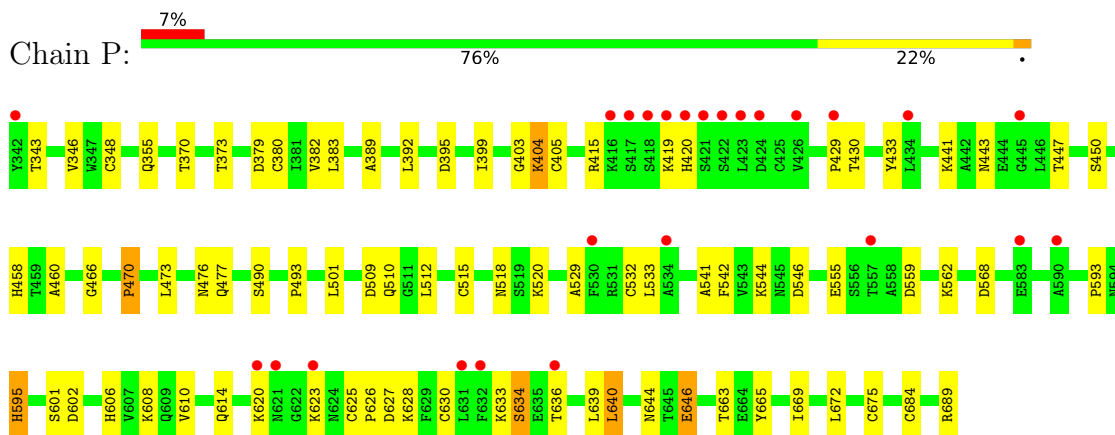
### 3 Residue-property plots

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: Lactotransferrin



- Molecule 1: Lactotransferrin



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



MAG1  
MAG2

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

Chain E:  100%MAG1  
MAG2

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

Chain B:  67%  33%MAG1  
MAG2  
BMA3

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

Chain C:  25%  75%MAG1  
MAG2  
BMA3  
MAN4

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

Chain D:  100%MAG1  
MAG2  
BMA3  
MAN4



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.51Å 81.76Å 111.79Å 90.00° 130.32° 90.00°	Depositor
Resolution (Å)	67.11 – 2.70 67.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (67.11-2.70) 97.6 (67.03-2.70)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.241 , 0.314 0.245 , 0.309	Depositor DCC
$R_{free}$ test set	1430 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: BMA, CO3, NAG, FE, 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	0.72	1/2707 (0.0%)	0.83	0/3669
1	P	0.70	0/2707	0.82	0/3669
All	All	0.71	1/5414 (0.0%)	0.82	0/7338

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	GLU	CD-OE2	6.78	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	490	SER	Peptide

### 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2657	0	2581	58	1
1	P	2657	0	2581	42	0
2	E	28	0	25	0	0
2	Z	28	0	25	0	0
3	B	39	0	34	1	0
4	C	50	0	43	0	0
4	D	50	0	43	0	0
5	A	1	0	0	0	0
5	P	1	0	0	0	0
6	A	4	0	0	1	0
6	P	4	0	0	0	0
7	A	14	0	13	0	0
8	A	43	0	0	5	0
8	P	44	0	0	11	0
All	All	5620	0	5345	97	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 9.

All (97) 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:P:684:CYS:HB3	8:P:805:HOH:O	1.80	0.79
1:A:390:ASP:O	1:A:599:SER:OG	2.04	0.71
1:P:593:PRO:O	8:P:801:HOH:O	2.10	0.69
1:A:363:GLN:HG2	1:P:476:ASN:OD1	1.94	0.68
1:A:470:PRO:HB3	1:A:542:PHE:CD1	2.29	0.67
1:P:466:GLY:HA2	1:P:542:PHE:O	1.94	0.67
1:P:399:ILE:O	8:P:802:HOH:O	2.12	0.66
1:P:684:CYS:CB	8:P:805:HOH:O	2.42	0.65
1:P:473:LEU:O	1:P:476:ASN:O	2.16	0.63
1:P:404:LYS:C	8:P:805:HOH:O	2.36	0.63
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.34	0.62
1:A:379:ASP:O	1:A:382:VAL:HB	2.03	0.59
1:P:405:CYS:N	8:P:805:HOH:O	2.35	0.59
1:A:367:GLN:NE2	1:P:476:ASN:HB2	2.18	0.58
1:P:529:ALA:O	1:P:532:CYS:HB3	2.04	0.57
1:P:346:VAL:HB	1:P:389:ALA:HA	1.87	0.56
1:A:594:ASN:O	1:A:660:TYR:OH	2.17	0.56
1:P:405:CYS:HA	8:P:805:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:THR:O	1:A:606:HIS:NE2	2.39	0.55
1:A:367:GLN:NE2	8:A:804:HOH:O	2.38	0.55
1:A:439:VAL:HG11	1:A:572:LEU:HD11	1.88	0.55
1:A:490:SER:HB2	1:A:501:LEU:HA	1.88	0.55
1:P:379:ASP:O	1:P:382:VAL:HB	2.07	0.55
1:A:362:SER:HA	1:A:369:VAL:O	2.08	0.54
1:P:395:ASP:HA	1:P:595:HIS:CD2	2.43	0.54
1:P:510:GLN:HB2	1:P:512:LEU:HG	1.90	0.54
1:A:571:LEU:O	1:A:587:CYS:SG	2.67	0.53
1:A:453:ASP:O	1:A:488:SER:HB3	2.09	0.53
1:A:459:THR:HA	1:A:525:GLY:O	2.09	0.52
1:P:405:CYS:CA	8:P:805:HOH:O	2.56	0.52
1:P:634:SER:HB3	1:P:639:LEU:HB2	1.90	0.52
1:A:473:LEU:HA	1:A:476:ASN:HB2	1.92	0.52
1:P:355:GLN:NE2	1:P:373:THR:OG1	2.43	0.51
1:P:665:TYR:CZ	1:P:669:ILE:HD11	2.45	0.51
1:A:620:LYS:HD3	1:A:646:GLU:HA	1.92	0.51
1:P:447:THR:N	1:P:450:SER:OG	2.44	0.51
1:A:614:GLN:NE2	3:B:1:NAG:O7	2.44	0.51
1:P:399:ILE:O	1:P:403:GLY:N	2.37	0.50
1:P:470:PRO:HB3	1:P:542:PHE:CE1	2.47	0.50
1:P:490:SER:HB2	1:P:501:LEU:HA	1.94	0.49
1:A:358:CYS:C	1:A:371:CYS:SG	2.91	0.49
1:A:434:LEU:O	1:A:544:LYS:HA	2.12	0.49
1:A:350:VAL:HG13	1:A:376:THR:C	2.33	0.49
1:A:379:ASP:OD2	8:A:801:HOH:O	2.20	0.48
1:A:385:LEU:HD21	1:A:405:CYS:O	2.14	0.48
1:A:382:VAL:O	1:A:385:LEU:HB2	2.14	0.47
1:P:630:CYS:HB2	8:P:839:HOH:O	2.14	0.47
1:A:404:LYS:NZ	1:A:657:TYR:OH	2.44	0.47
1:A:374:ALA:HB1	1:A:379:ASP:HB2	1.97	0.47
1:A:664:GLU:N	1:A:664:GLU:OE2	2.47	0.47
1:A:641:PHE:C	8:A:811:HOH:O	2.54	0.47
1:A:439:VAL:HG21	1:A:572:LEU:HD21	1.98	0.46
1:A:463:ARG:NH2	6:A:702:CO3:O1	2.39	0.46
1:A:470:PRO:HB3	1:A:542:PHE:CE1	2.49	0.46
1:A:493:PRO:HA	1:A:515:CYS:SG	2.56	0.46
1:A:523:TYR:HA	1:A:528:GLY:CA	2.45	0.46
1:A:349:ALA:O	1:A:373:THR:HA	2.16	0.46
1:A:367:GLN:NE2	8:A:808:HOH:O	2.49	0.46
1:A:600:ARG:HG3	8:A:823:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:470:PRO:HB3	1:P:542:PHE:CD1	2.50	0.46
1:P:343:THR:O	1:P:606:HIS:NE2	2.45	0.46
1:P:348:CYS:SG	1:P:383:LEU:HD12	2.55	0.46
1:A:393:ASN:HD22	1:A:641:PHE:HA	1.81	0.45
1:P:620:LYS:HE3	1:P:646:GLU:HG2	1.98	0.45
1:P:458:HIS:N	8:P:810:HOH:O	2.50	0.44
1:A:426:VAL:HG22	1:A:615:GLN:HE22	1.83	0.44
1:A:396:GLY:CA	1:A:661:LEU:HD21	2.48	0.44
1:A:367:GLN:HE22	1:P:476:ASN:HB2	1.81	0.44
1:P:518:ASN:OD1	1:P:520:LYS:HB2	2.18	0.44
1:A:377:THR:HG21	1:A:398:TYR:CG	2.53	0.44
1:A:636:THR:OG1	1:A:637:LYS:N	2.50	0.44
1:A:439:VAL:CG1	1:A:572:LEU:HD11	2.48	0.43
1:A:433:TYR:CZ	1:A:592:ALA:CB	3.01	0.43
1:A:347:TRP:N	1:A:370:THR:O	2.47	0.43
1:P:380:CYS:HB3	1:P:392:LEU:HD13	1.99	0.43
1:P:433:TYR:CD2	1:P:544:LYS:HD3	2.53	0.43
1:A:529:ALA:HB3	1:A:543:VAL:CG1	2.49	0.43
1:A:622:GLY:HA3	1:A:625:CYS:HB3	2.00	0.43
1:P:460:ALA:HA	1:P:493:PRO:HD2	2.00	0.43
1:P:625:CYS:HA	1:P:626:PRO:HA	1.82	0.43
1:P:395:ASP:N	8:P:803:HOH:O	2.15	0.42
1:A:626:PRO:HA	1:A:630:CYS:SG	2.59	0.42
1:A:523:TYR:HA	1:A:528:GLY:HA3	2.02	0.42
1:A:568:ASP:OD1	1:A:568:ASP:N	2.52	0.42
1:A:481:CYS:HB3	1:A:675:CYS:HB3	1.96	0.41
1:P:493:PRO:HA	1:P:515:CYS:SG	2.60	0.41
1:P:533:LEU:HB2	1:P:541:ALA:HB2	2.02	0.41
1:P:610:VAL:O	1:P:614:GLN:HG2	2.19	0.41
1:A:575:ASP:OD1	1:A:576:GLY:N	2.53	0.41
1:A:516:VAL:O	1:A:516:VAL:CG1	2.68	0.41
1:P:420:HIS:HE1	1:P:429:PRO:HD2	1.85	0.41
1:A:443:ASN:O	1:A:578:ARG:NH2	2.54	0.41
1:P:672:LEU:O	1:P:675:CYS:HB2	2.20	0.41
1:A:464:THR:HG23	1:A:665:TYR:CZ	2.56	0.40
1:A:433:TYR:CZ	1:A:592:ALA:HB3	2.56	0.40
1:A:516:VAL:O	1:A:516:VAL:HG13	2.20	0.40
1:A:660:TYR:O	1:A:660:TYR:CG	2.74	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:444:GLU:OE2	1:A:621:ASN:OD1[4_546]	2.14	0.06

### 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	346/348 (99%)	313 (90%)	32 (9%)	1 (0%)	41	66
1	P	346/348 (99%)	292 (84%)	48 (14%)	6 (2%)	9	23
All	All	692/696 (99%)	605 (87%)	80 (12%)	7 (1%)	15	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	636	THR
1	P	477	GLN
1	P	595	HIS
1	P	419	LYS
1	P	636	THR
1	P	640	LEU
1	P	470	PRO

#### 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	289/289 (100%)	254 (88%)	35 (12%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	289/289 (100%)	264 (91%)	25 (9%)	10	23
All	All	578/578 (100%)	518 (90%)	60 (10%)	7	16

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	A	362	SER
1	A	370	THR
1	A	373	THR
1	A	422	SER
1	A	430	THR
1	A	447	THR
1	A	476	ASN
1	A	480	SER
1	A	498	LYS
1	A	499	SER
1	A	500	ARG
1	A	504	LEU
1	A	509	ASP
1	A	520	LYS
1	A	536	ASP
1	A	537	VAL
1	A	546	ASP
1	A	555	GLU
1	A	557	THR
1	A	559	ASP
1	A	563	ASN
1	A	567	GLU
1	A	568	ASP
1	A	573	CYS
1	A	583	GLU
1	A	586	SER
1	A	601	SER
1	A	609	GLN
1	A	617	LEU
1	A	620	LYS
1	A	627	ASP
1	A	654	ARG
1	A	663	THR
1	A	676	SER
1	P	370	THR

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Mol	Chain	Res	Type
1	P	404	LYS
1	P	415	ARG
1	P	430	THR
1	P	441	LYS
1	P	443	ASN
1	P	509	ASP
1	P	546	ASP
1	P	555	GLU
1	P	559	ASP
1	P	562	LYS
1	P	568	ASP
1	P	601	SER
1	P	602	ASP
1	P	608	LYS
1	P	623	LYS
1	P	627	ASP
1	P	628	LYS
1	P	633	LYS
1	P	634	SER
1	P	640	LEU
1	P	644	ASN
1	P	646	GLU
1	P	663	THR
1	P	689	ARG

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	355	GLN
1	A	367	GLN
1	A	468	ASN
1	P	355	GLN
1	P	468	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 ⓘ

15 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$
3	NAG	B	1	3,1	14,14,15	0.66	0	17,19,21	2.57	6 (35%)
3	NAG	B	2	3	14,14,15	0.52	0	17,19,21	2.25	3 (17%)
3	BMA	B	3	3	11,11,12	0.60	0	15,15,17	1.74	3 (20%)
4	NAG	C	1	1,4	14,14,15	0.46	0	17,19,21	1.82	3 (17%)
4	NAG	C	2	4	14,14,15	0.58	0	17,19,21	1.09	0
4	BMA	C	3	4	11,11,12	0.71	0	15,15,17	2.83	6 (40%)
4	MAN	C	4	4	11,11,12	0.60	0	15,15,17	2.17	2 (13%)
4	NAG	D	1	1,4	14,14,15	0.29	0	17,19,21	2.32	3 (17%)
4	NAG	D	2	4	14,14,15	0.55	0	17,19,21	2.37	4 (23%)
4	BMA	D	3	4	11,11,12	0.55	0	15,15,17	2.09	6 (40%)
4	MAN	D	4	4	11,11,12	0.63	0	15,15,17	2.29	4 (26%)
2	NAG	E	1	1,2	14,14,15	0.54	0	17,19,21	1.54	2 (11%)
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	1.40	3 (17%)
2	NAG	Z	1	1,2	14,14,15	0.54	0	17,19,21	1.21	3 (17%)
2	NAG	Z	2	2	14,14,15	0.44	0	17,19,21	1.15	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1
3	BMA	B	3	3	-	2/2/19/22	0/1/1/1
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Z	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C1-O5-C5	8.09	123.16	112.19
3	B	2	NAG	C1-O5-C5	7.87	122.85	112.19
4	D	2	NAG	C1-O5-C5	7.70	122.62	112.19
4	D	4	MAN	C1-O5-C5	7.39	122.20	112.19
4	C	3	BMA	C1-O5-C5	7.21	121.96	112.19
3	B	1	NAG	O5-C5-C6	-6.31	97.31	107.20
4	C	4	MAN	C1-O5-C5	6.07	120.42	112.19
4	C	1	NAG	C1-O5-C5	5.86	120.12	112.19
4	C	3	BMA	C1-C2-C3	5.32	116.21	109.67
4	C	4	MAN	C1-C2-C3	4.80	115.57	109.67
3	B	1	NAG	C1-O5-C5	4.74	118.61	112.19
4	D	3	BMA	C1-C2-C3	4.72	115.47	109.67
3	B	3	BMA	C1-C2-C3	4.56	115.28	109.67
2	E	2	NAG	O5-C5-C6	3.85	113.24	107.20
2	E	1	NAG	C3-C4-C5	3.75	116.92	110.24
3	B	1	NAG	O4-C4-C3	-3.70	101.79	110.35
3	B	1	NAG	O4-C4-C5	3.53	118.05	109.30
3	B	3	BMA	C1-O5-C5	3.32	116.69	112.19
4	D	3	BMA	O5-C5-C6	2.98	111.88	107.20
4	D	3	BMA	C1-O5-C5	2.97	116.21	112.19
2	E	1	NAG	C4-C3-C2	2.95	115.33	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	O5-C5-C4	2.94	117.99	110.83
4	C	3	BMA	O5-C1-C2	2.83	115.13	110.77
2	Z	1	NAG	O5-C5-C6	2.80	111.60	107.20
4	D	2	NAG	O4-C4-C3	-2.78	103.93	110.35
3	B	3	BMA	O5-C1-C2	2.74	115.00	110.77
4	C	3	BMA	C3-C4-C5	-2.69	105.44	110.24
4	C	3	BMA	O2-C2-C3	-2.69	104.76	110.14
3	B	1	NAG	C4-C3-C2	2.67	114.94	111.02
4	D	4	MAN	C2-C3-C4	2.58	115.35	110.89
4	D	2	NAG	O4-C4-C5	2.55	115.62	109.30
4	D	3	BMA	C3-C4-C5	-2.54	105.70	110.24
4	C	3	BMA	O4-C4-C5	2.50	115.50	109.30
4	C	1	NAG	O5-C1-C2	-2.48	107.37	111.29
4	C	1	NAG	C3-C4-C5	2.47	114.64	110.24
3	B	2	NAG	C3-C4-C5	2.46	114.63	110.24
4	D	2	NAG	O5-C5-C6	-2.43	103.39	107.20
2	Z	2	NAG	O5-C1-C2	2.43	115.13	111.29
4	D	3	BMA	O4-C4-C5	2.42	115.30	109.30
2	E	2	NAG	C4-C3-C2	2.37	114.49	111.02
4	D	1	NAG	C3-C4-C5	2.36	114.44	110.24
4	D	4	MAN	C1-C2-C3	2.34	112.54	109.67
3	B	1	NAG	O5-C5-C4	2.22	116.22	110.83
2	Z	2	NAG	C4-C3-C2	2.19	114.22	111.02
3	B	2	NAG	O5-C1-C2	2.14	114.66	111.29
2	Z	1	NAG	O5-C1-C2	-2.12	107.93	111.29
2	E	2	NAG	C1-O5-C5	2.11	115.05	112.19
4	D	4	MAN	C3-C4-C5	2.09	113.96	110.24
2	Z	1	NAG	O4-C4-C3	-2.01	105.70	110.35
4	D	3	BMA	O5-C5-C4	-2.00	105.95	110.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
2	Z	2	NAG	C4-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	C	3	BMA	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6

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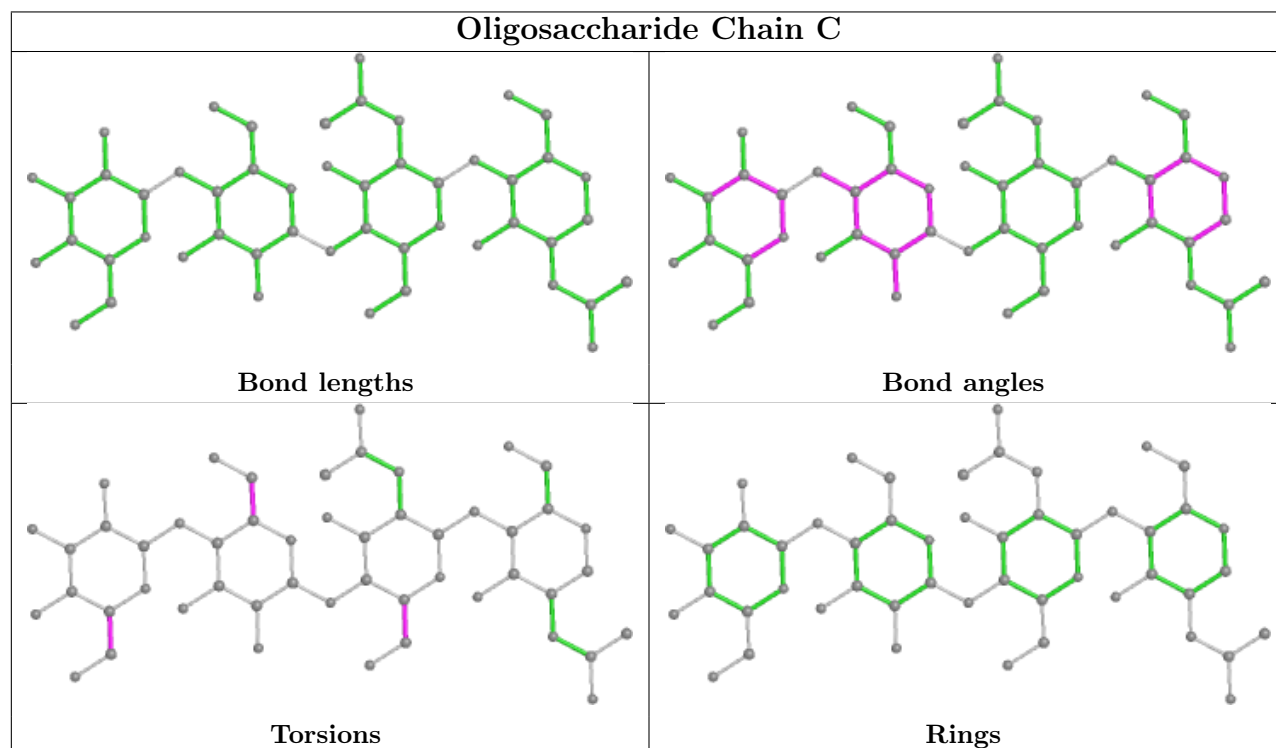
Mol	Chain	Res	Type	Atoms
4	C	4	MAN	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
2	Z	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
3	B	3	BMA	C4-C5-C6-O6
3	B	3	BMA	O5-C5-C6-O6

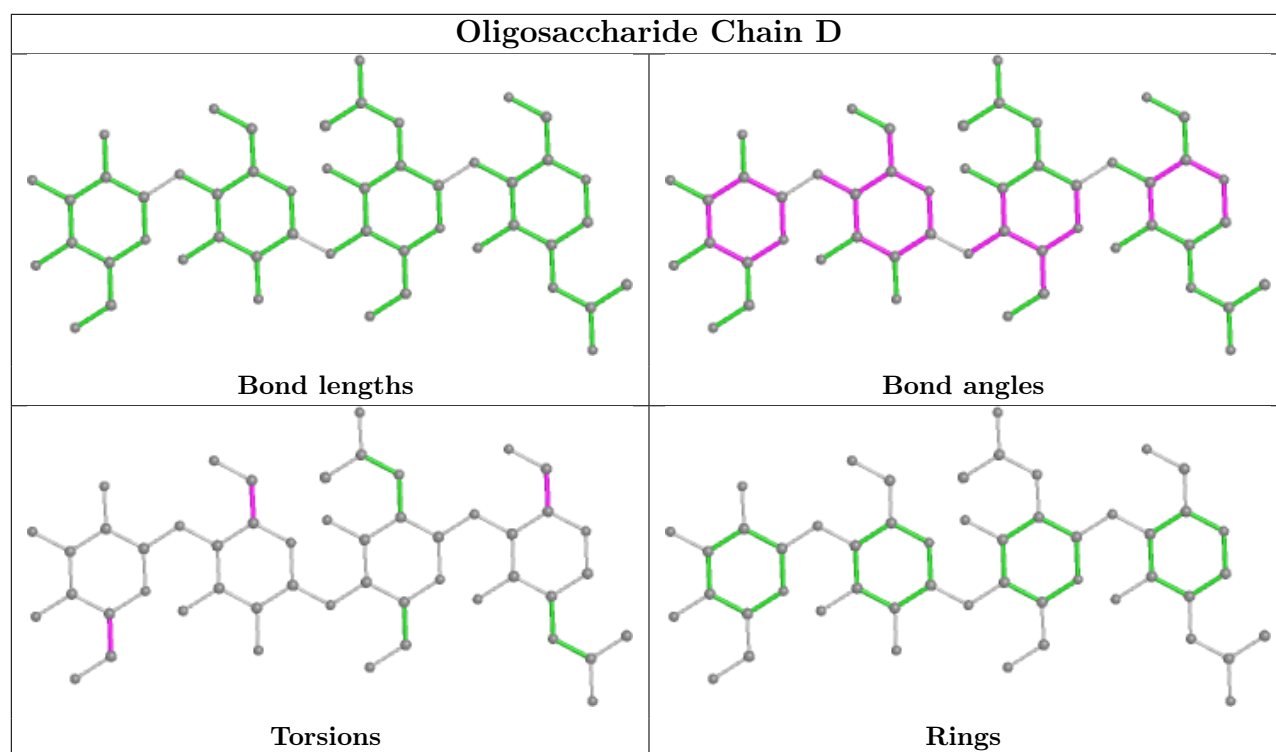
There are no ring outliers.

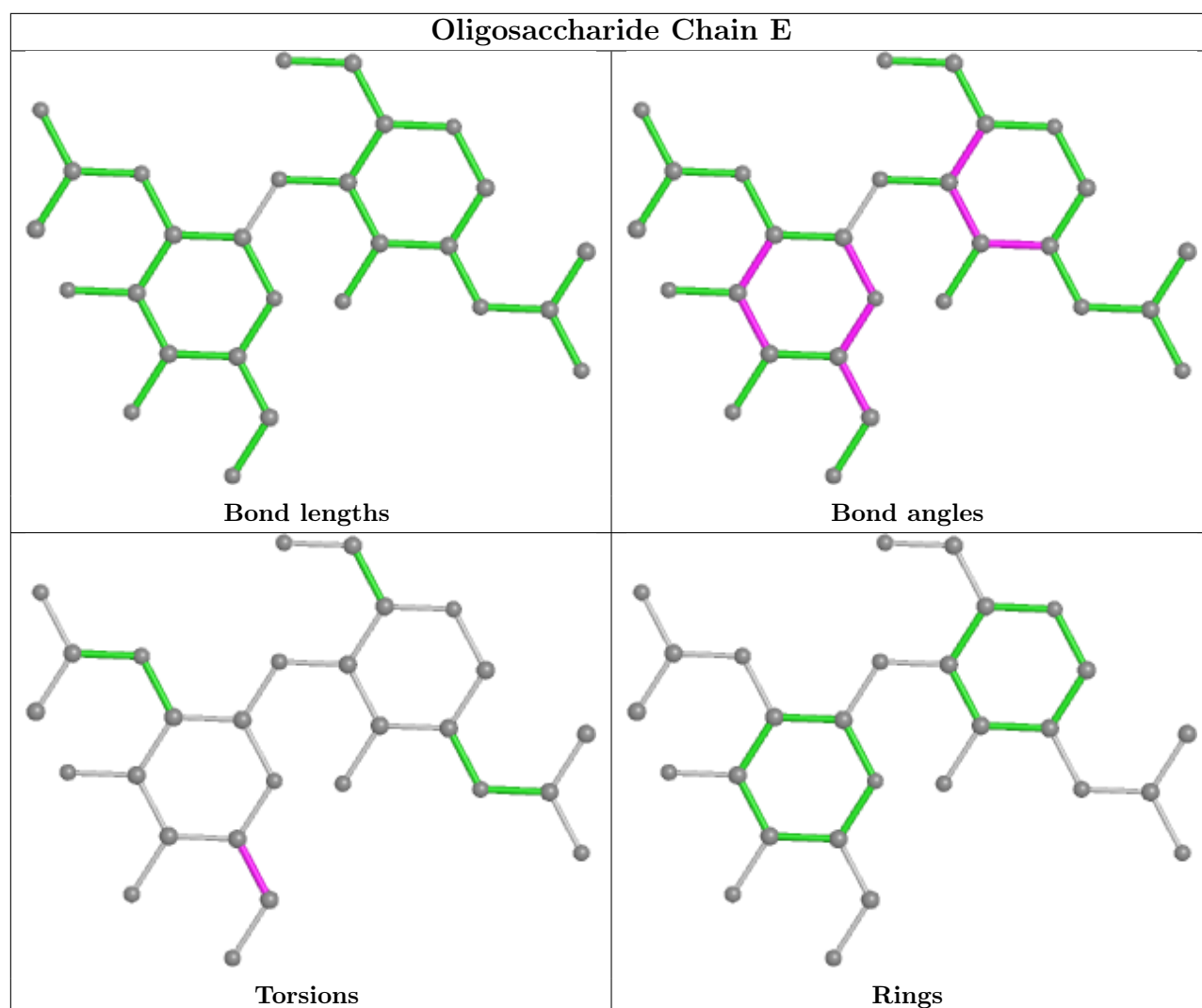
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	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](#)

Of 5 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
6	CO3	P	702	5	0,3,3	0.00	-	0,3,3	0.00	-
6	CO3	A	702	5	0,3,3	0.00	-	0,3,3	0.00	-
7	NAG	A	703	1	14,14,15	1.51	1 (7%)	17,19,21	1.19	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	703	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	703	NAG	C1-C2	2.52	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	703	NAG	C2-N2-C7	-2.57	119.24	122.90
7	A	703	NAG	C3-C4-C5	2.16	114.09	110.24

There are no chirality outliers.

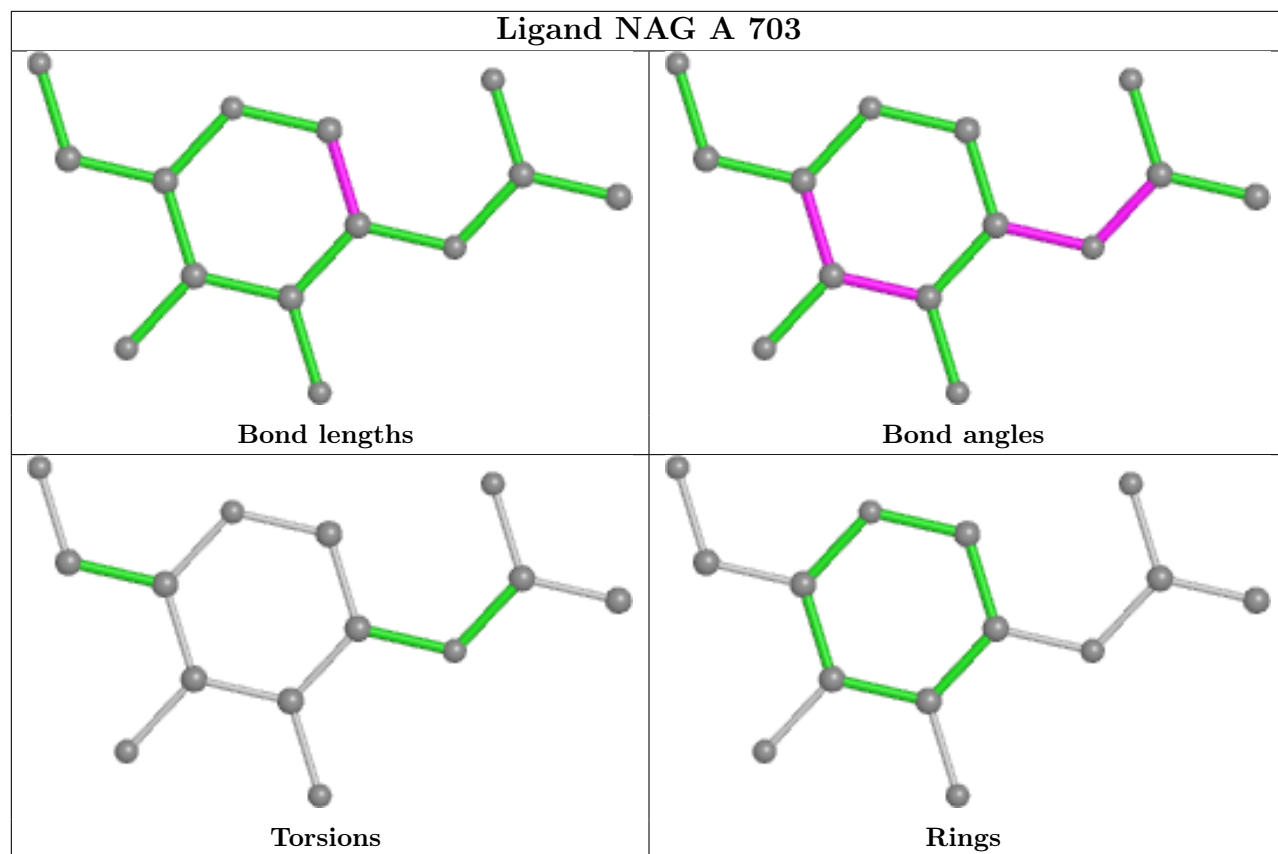
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	CO3	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 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

### 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	348/348 (100%)	0.54	18 (5%) 27 25	43, 79, 119, 158	0
1	P	348/348 (100%)	0.62	25 (7%) 15 13	48, 90, 132, 166	0
All	All	696/696 (100%)	0.58	43 (6%) 20 19	43, 84, 128, 166	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	429	PRO	7.1
1	A	421	SER	6.5
1	P	419	LYS	5.9
1	A	420	HIS	5.0
1	P	434	LEU	4.9
1	A	422	SER	4.1
1	P	620	LYS	4.1
1	P	421	SER	4.1
1	P	417	SER	4.1
1	P	534	ALA	4.0
1	A	443	ASN	3.8
1	P	621	ASN	3.8
1	A	534	ALA	3.7
1	A	444	GLU	3.6
1	P	530	PHE	3.5
1	P	423	LEU	3.4
1	P	420	HIS	3.3
1	P	418	SER	3.3
1	A	569	PHE	3.3
1	P	631	LEU	3.2
1	A	429	PRO	3.2
1	P	623	LYS	3.1
1	P	416	LYS	3.0
1	A	419	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	P	557	THR	2.9
1	P	590	ALA	2.9
1	A	428	ARG	2.9
1	P	583	GLU	2.8
1	A	456	SER	2.8
1	A	581	VAL	2.6
1	P	445	GLY	2.6
1	A	553	ASN	2.5
1	P	342	TYR	2.5
1	P	422	SER	2.3
1	A	679	PRO	2.3
1	P	636	THR	2.2
1	P	424	ASP	2.2
1	P	426	VAL	2.2
1	A	580	PRO	2.1
1	A	548	VAL	2.0
1	A	416	LYS	2.0
1	P	632	PHE	2.0
1	A	530	PHE	2.0

## 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.

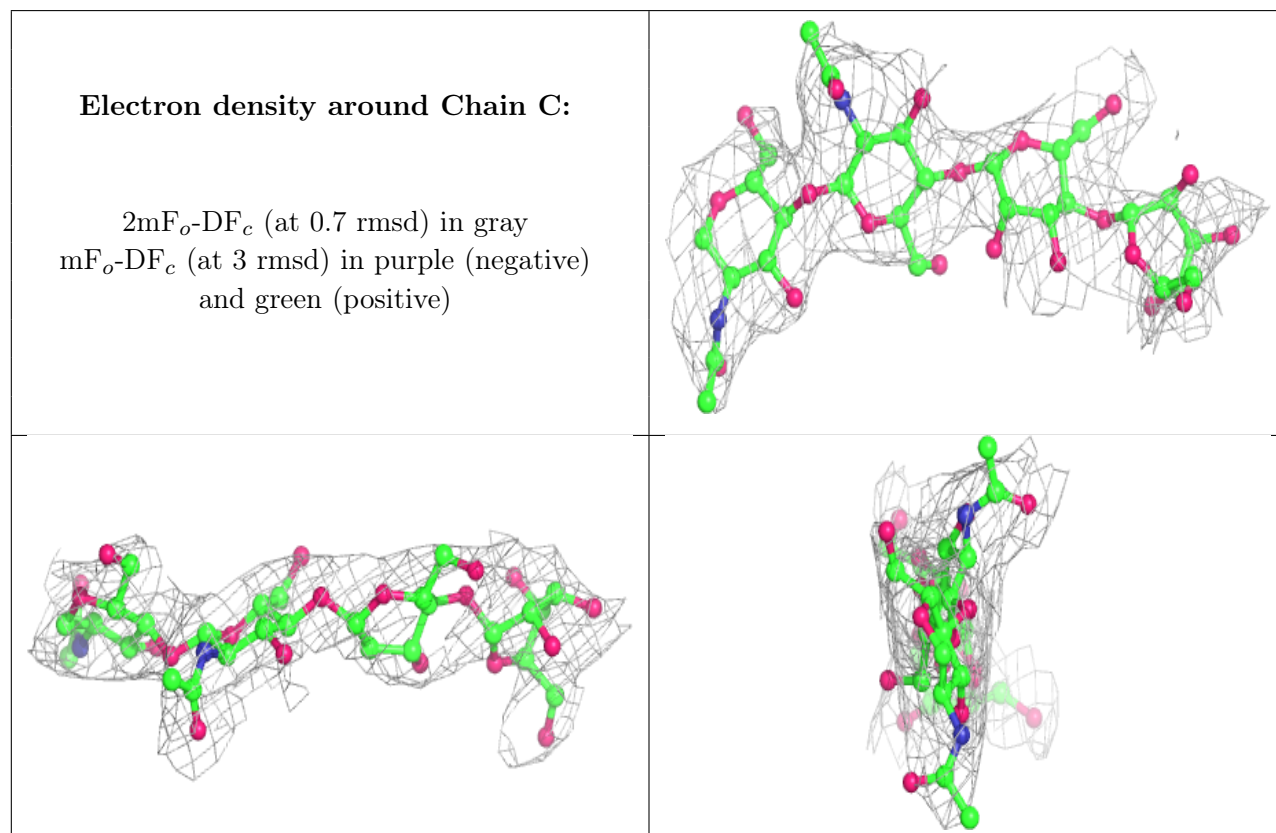
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MAN	C	4	11/12	0.58	0.29	133,167,183,184	0
4	MAN	D	4	11/12	0.68	0.24	130,162,177,178	0
4	BMA	C	3	11/12	0.71	0.20	133,158,171,173	0
4	BMA	D	3	11/12	0.77	0.33	167,171,182,182	0
2	NAG	Z	2	14/15	0.82	0.15	146,168,194,200	0
2	NAG	Z	1	14/15	0.83	0.25	97,110,134,145	0
2	NAG	E	2	14/15	0.84	0.28	127,149,165,170	0
4	NAG	C	2	14/15	0.84	0.23	122,136,146,157	0
3	BMA	B	3	11/12	0.86	0.14	105,121,127,132	0

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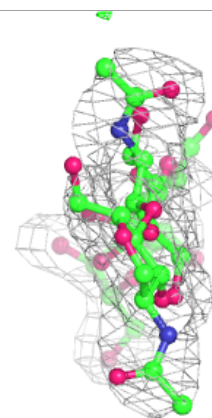
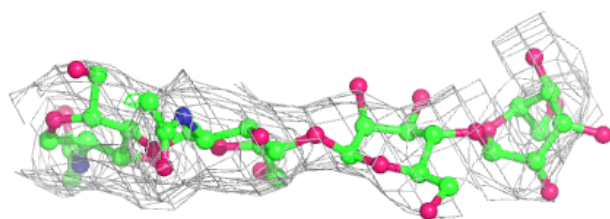
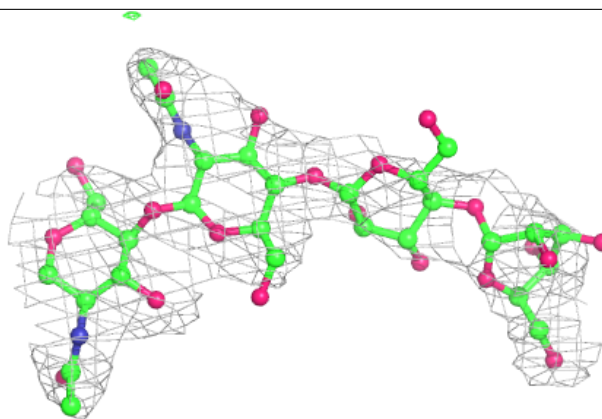
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	D	2	14/15	0.89	0.14	106,120,135,148	0
3	NAG	B	2	14/15	0.90	0.13	103,114,130,132	0
2	NAG	E	1	14/15	0.91	0.20	125,145,171,177	0
4	NAG	C	1	14/15	0.91	0.21	100,109,117,130	0
3	NAG	B	1	14/15	0.93	0.16	62,80,89,93	0
4	NAG	D	1	14/15	0.94	0.16	90,98,110,113	0

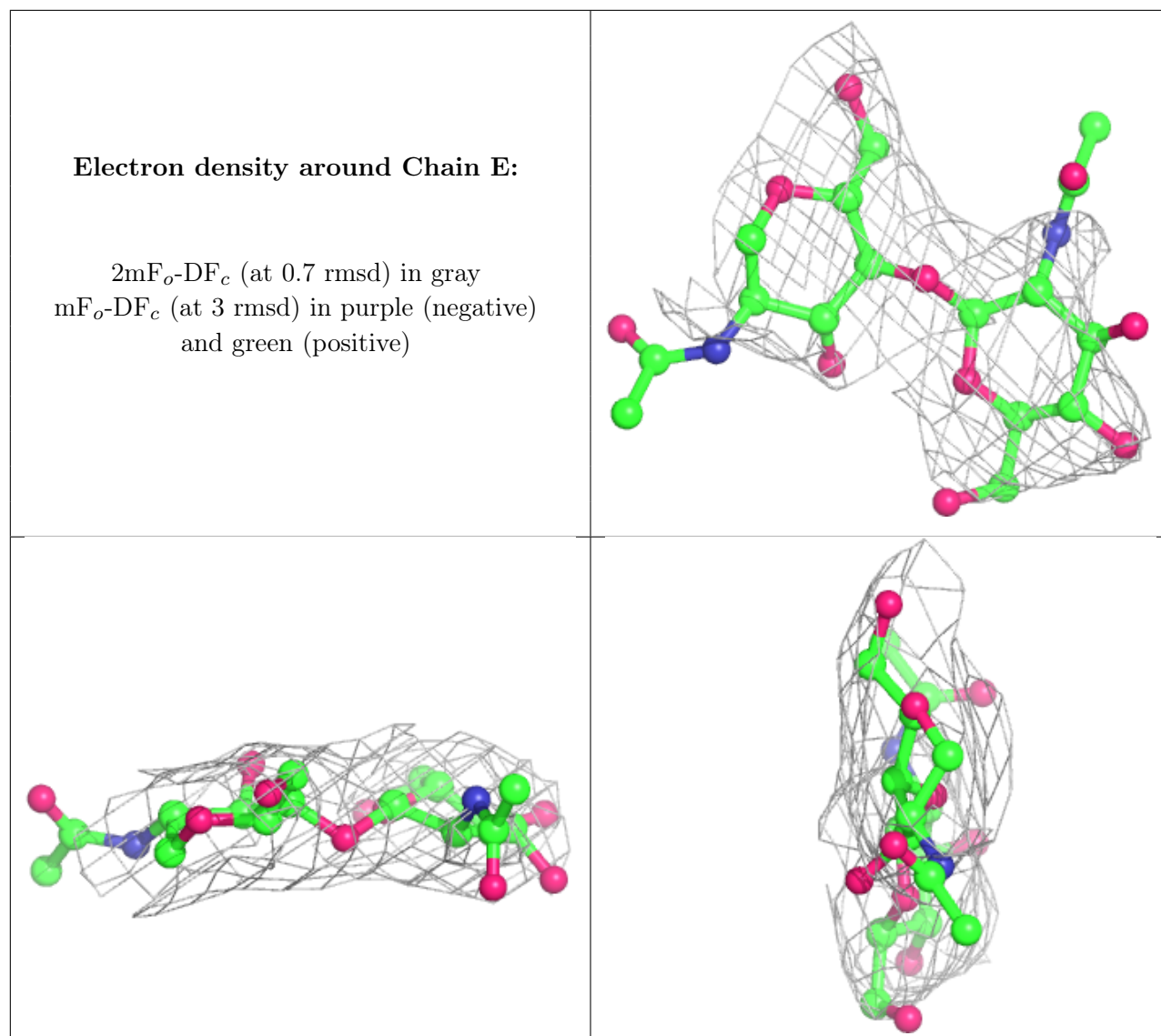
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain D:**

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





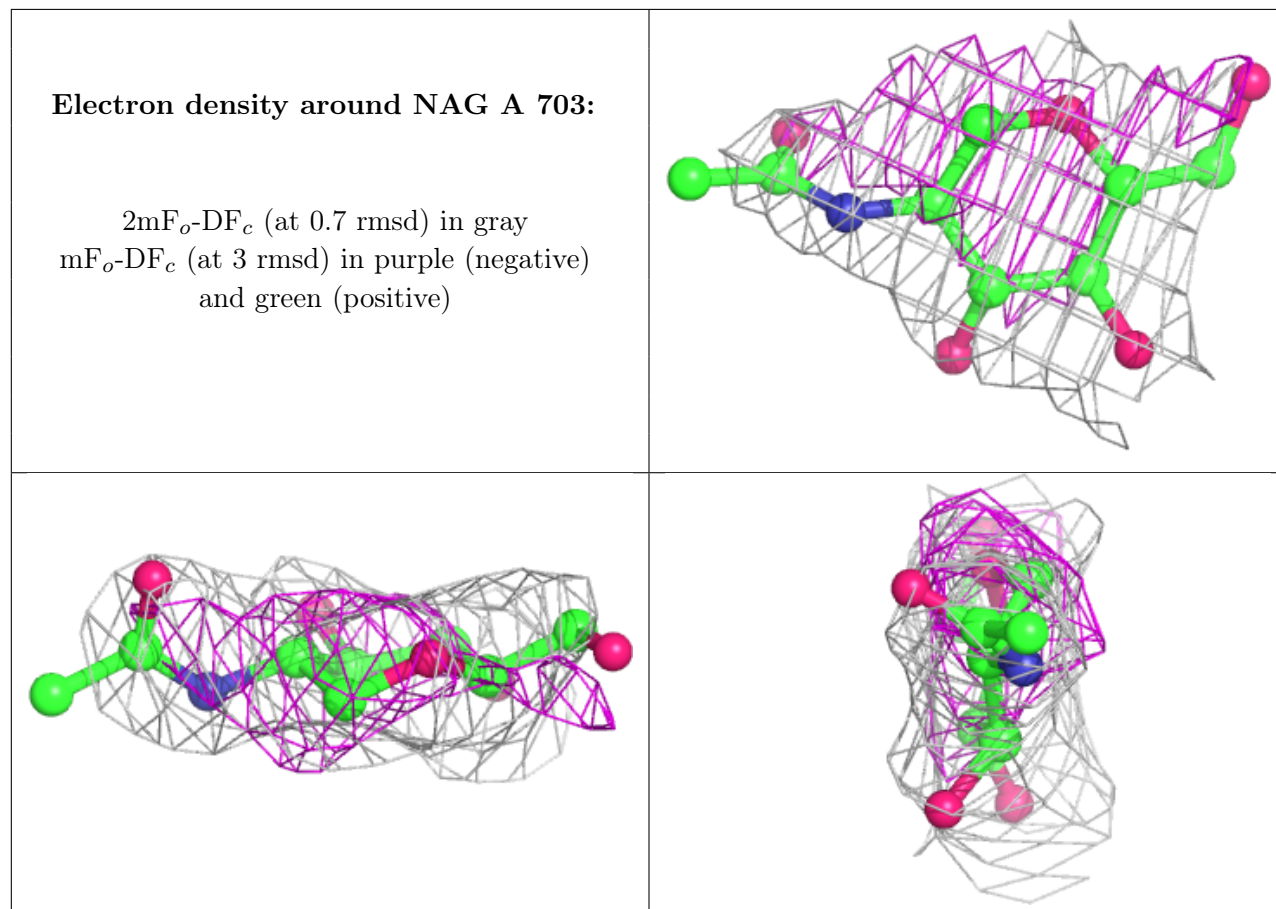
## 6.4 Ligands [i](#)

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
7	NAG	A	703	14/15	0.87	0.39	66,70,77,79	0
6	CO3	A	702	4/4	0.96	0.12	50,55,60,61	0
6	CO3	P	702	4/4	0.98	0.10	53,56,56,62	0
5	FE	P	701	1/1	0.99	0.10	70,70,70,70	0
5	FE	A	701	1/1	0.99	0.09	64,64,64,64	0

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.