



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 03:32 PM EDT

PDB ID : 8SPI  
Title : Crystal structure of chimeric omicron RBD (strain XBB.1.5) complexed with human ACE2  
Authors : Zhang, W.; Shi, K.; Aihara, H.; Li, F.  
Deposited on : 2023-05-03  
Resolution : 3.06 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

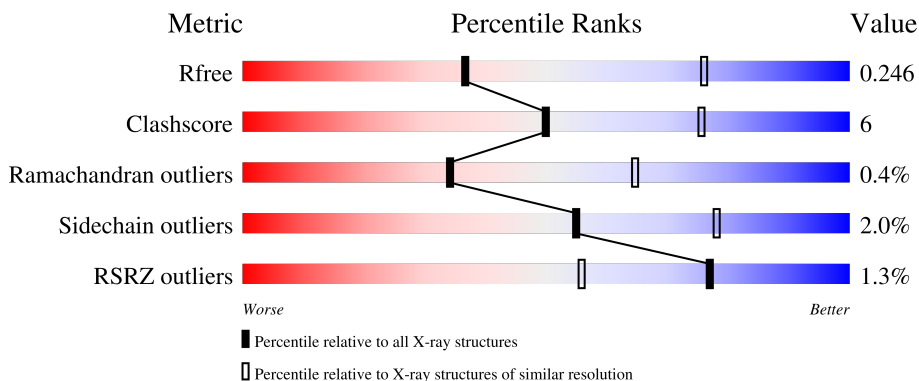
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 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.



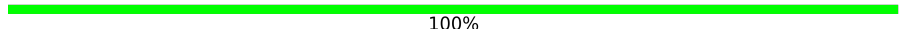
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	597	
1	B	597	
2	E	217	
2	F	217	
3	C	2	

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
3	I	2	 100%
3	M	2	 50% 50%
4	D	3	 100%
4	G	3	 100%
5	J	4	 50% 50%

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
3	NAG	C	2	-	-	-	X
8	NAG	B	705	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13107 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	596	4862	3111	805	917	29	0	0	0
1	B	596	4862	3111	805	917	29	0	0	0

- Molecule 2 is a protein called Spike protein S1.

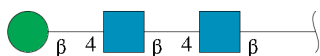
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	192	1514	974	251	280	9	0	0	0
2	F	194	1527	980	253	285	9	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



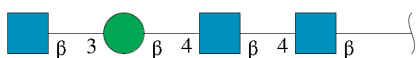
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	28	16	2	10	0	0	0
3	H	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0
3	M	2	28	16	2	10	0	0	0

- Molecule 4 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
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	4	Total	C	N	O	0	0	0
			53	30	3	20			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 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>).



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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

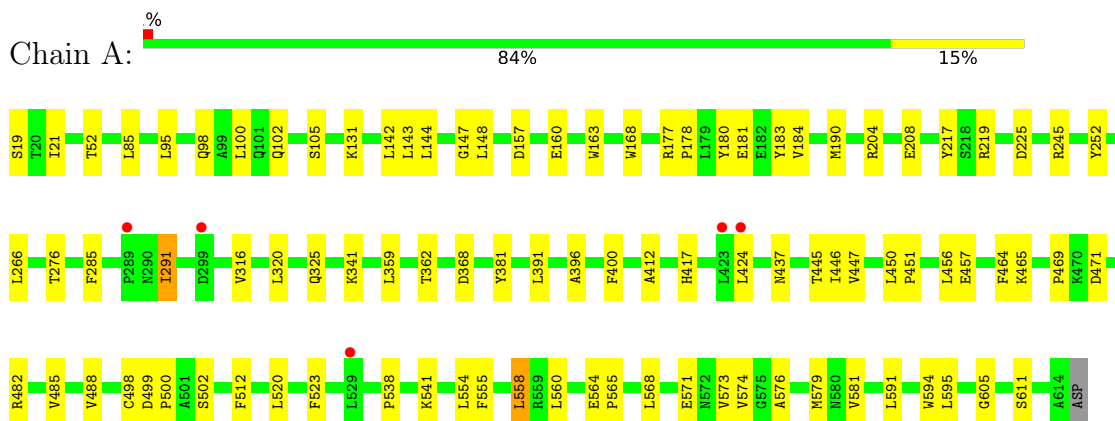
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O 1 1	0	0
10	B	1	Total O 1 1	0	0
10	E	1	Total O 1 1	0	0

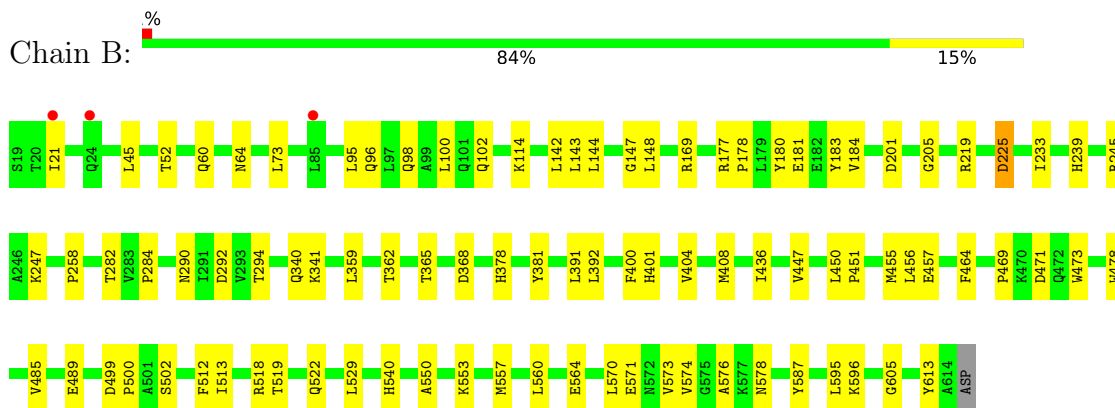
### 3 Residue-property plots [i](#)

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.

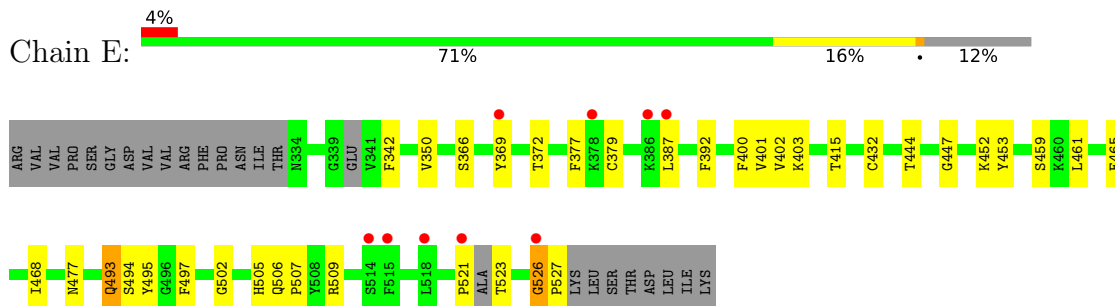
- Molecule 1: Angiotensin-converting enzyme 2



- Molecule 1: Angiotensin-converting enzyme 2



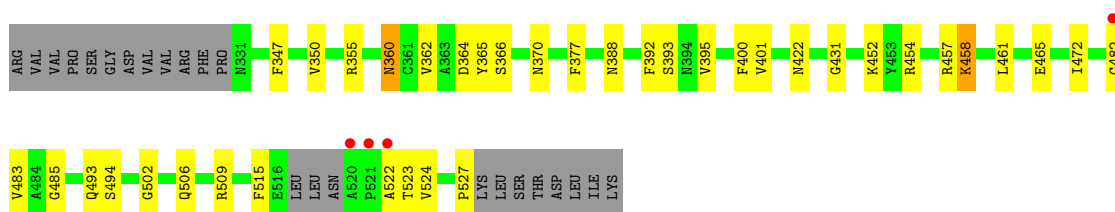
- Molecule 2: Spike protein S1





- Molecule 2: Spike protein S1

Chain F: 2% 72% 17% 11%



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

Chain C: 50% 50%



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

Chain H: 100%



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

Chain I: 100%



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

Chain M: 50% 50%



- Molecule 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%



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

Chain G:  100%

NAG1  
NAG2  
BMA3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

NAG1  
NAG2  
BMA3  
NAG4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.36Å 116.20Å 108.77Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	77.85 – 3.06 108.05 – 3.06	Depositor EDS
% Data completeness (in resolution range)	67.4 (77.85-3.06) 67.4 (108.05-3.06)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.190 , 0.243 0.193 , 0.246	Depositor DCC
$R_{free}$ test set	1276 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.4	Xtrriage
Anisotropy	0.097	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13107	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: BMA, ZN, EDO, CL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/4999	0.43	0/6792
1	B	0.24	0/4999	0.42	0/6792
2	E	0.30	0/1556	0.47	0/2115
2	F	0.28	0/1570	0.47	0/2136
All	All	0.25	0/13124	0.43	0/17835

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	4862	0	4634	52	0
1	B	4862	0	4633	55	0
2	E	1514	0	1443	17	0
2	F	1527	0	1453	21	0
3	C	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
3	M	28	0	25	2	0
4	D	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	39	0	34	0	0
5	J	53	0	46	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
8	A	28	0	26	0	0
8	B	42	0	39	0	0
8	E	14	0	13	1	0
9	B	8	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
All	All	13107	0	12467	147	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 6.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:NH1	7:B:702:CL:CL	2.53	0.78
1:A:131:LYS:HG2	1:A:143:LEU:HB3	1.66	0.78
1:A:276:THR:HG1	1:A:445:THR:HG1	1.36	0.66
2:E:521:PRO:O	2:E:523:THR:N	2.29	0.66
2:F:393:SER:HA	2:F:522:ALA:HA	1.78	0.66
1:B:144:LEU:HA	1:B:148:LEU:HB2	1.79	0.64
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.79	0.64
1:B:245:ARG:NH2	1:B:605:GLY:O	2.24	0.63
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.32	0.63
1:B:245:ARG:NH1	1:B:258:PRO:O	2.33	0.61
1:A:245:ARG:NH2	1:A:605:GLY:O	2.34	0.61
1:A:19:SER:N	2:E:477:ASN:HD21	2.00	0.60
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.35	0.60
2:F:360:ASN:HA	2:F:523:THR:HB	1.83	0.59
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.67	0.59
1:B:52:THR:O	1:B:340:GLN:NE2	2.35	0.58
2:F:395:VAL:HG23	2:F:524:VAL:HG21	1.84	0.58
2:F:461:LEU:HD22	2:F:465:GLU:HB3	1.86	0.58
1:B:169:ARG:HH11	1:B:499:ASP:HB3	1.69	0.57
1:A:565:PRO:HD2	1:A:568:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HD13	1:B:564:GLU:HG3	1.86	0.56
3:M:2:NAG:H83	3:M:2:NAG:H3	1.89	0.55
1:B:290:ASN:HD21	1:B:292:ASP:HB3	1.71	0.54
1:B:553:LYS:NZ	1:B:573:VAL:O	2.37	0.54
1:B:205:GLY:HA2	1:B:219:ARG:HG2	1.90	0.54
1:A:571:GLU:HA	1:A:576:ALA:H	1.73	0.53
2:F:360:ASN:OD1	2:F:360:ASN:N	2.41	0.53
1:B:142:LEU:HD22	1:B:147:GLY:HA3	1.91	0.53
1:B:499:ASP:O	1:B:502:SER:OG	2.22	0.52
1:A:457:GLU:HG2	1:A:512:PHE:HB3	1.91	0.52
1:B:52:THR:HG22	1:B:359:LEU:HD13	1.93	0.51
3:I:1:NAG:H62	3:I:2:NAG:N2	2.25	0.51
2:E:461:LEU:HD22	2:E:465:GLU:HB3	1.92	0.50
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.93	0.50
1:B:571:GLU:HA	1:B:576:ALA:H	1.76	0.50
2:F:454:ARG:HD3	2:F:457:ARG:HD2	1.93	0.50
2:F:350:VAL:HA	2:F:400:PHE:HB2	1.93	0.49
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.94	0.49
1:B:225:ASP:OD2	1:B:578:ASN:ND2	2.42	0.49
1:B:60:GLN:O	1:B:64:ASN:ND2	2.41	0.49
1:B:180:TYR:HA	1:B:183:TYR:HB3	1.95	0.48
1:A:100:LEU:HG	1:A:391:LEU:HD21	1.95	0.48
2:E:452:LYS:HA	2:E:494:SER:HA	1.93	0.48
1:A:208:GLU:OE1	1:A:219:ARG:NH1	2.46	0.48
1:B:100:LEU:HG	1:B:391:LEU:HD21	1.94	0.48
1:A:144:LEU:HA	1:A:148:LEU:HB2	1.95	0.48
1:A:555:PHE:HA	1:A:558:LEU:HD22	1.96	0.47
1:A:591:LEU:O	1:A:595:LEU:HD23	2.14	0.47
1:B:450:LEU:HD21	1:B:519:THR:HG21	1.95	0.47
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.95	0.47
1:B:201:ASP:OD2	1:B:219:ARG:NH1	2.47	0.47
1:B:478:TRP:CD2	1:B:489:GLU:HB3	2.49	0.47
1:B:239:HIS:CE1	1:B:596:LYS:HG2	2.50	0.47
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.50	0.47
1:A:560:LEU:HD11	1:A:564:GLU:HG3	1.97	0.47
1:A:52:THR:HG22	1:A:359:LEU:HD13	1.97	0.47
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.96	0.46
1:A:594:TRP:HE3	1:A:595:LEU:HD22	1.81	0.46
1:B:169:ARG:NH1	1:B:499:ASP:HB3	2.29	0.46
1:A:451:PRO:HB2	1:A:485:VAL:HG13	1.98	0.46
1:B:96:GLN:HB3	1:B:391:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LYS:HB2	1:B:282:THR:HG22	1.98	0.46
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.98	0.45
1:A:217:TYR:OH	1:A:225:ASP:OD2	2.24	0.45
1:B:177:ARG:HB3	1:B:178:PRO:HD3	1.98	0.45
1:B:177:ARG:NH2	1:B:473:TRP:HB2	2.32	0.45
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.97	0.45
2:F:366:SER:O	2:F:370:ASN:HB2	2.15	0.45
1:B:294:THR:HG23	1:B:365:THR:HA	1.99	0.45
1:A:412:ALA:HA	1:A:417:HIS:CD2	2.52	0.45
1:B:529:LEU:HB3	1:B:550:ALA:HB1	1.99	0.45
1:B:143:LEU:HD23	1:B:143:LEU:H	1.82	0.45
1:A:538:PRO:HD2	1:A:541:LYS:HD3	1.98	0.44
2:E:379:CYS:HA	2:E:432:CYS:HA	1.98	0.44
1:A:291:ILE:HG23	1:A:424:LEU:HD22	2.00	0.44
1:A:362:THR:HG23	1:A:368:ASP:HB3	1.99	0.44
1:B:290:ASN:ND2	1:B:292:ASP:HB3	2.31	0.44
1:B:573:VAL:HG13	1:B:574:VAL:HG13	1.98	0.44
2:E:366:SER:HA	2:E:369:TYR:CE2	2.52	0.44
1:B:98:GLN:O	1:B:102:GLN:HG3	2.18	0.44
2:F:364:ASP:H	2:F:527:PRO:HD2	1.81	0.44
2:F:502:GLY:O	2:F:506:GLN:HG3	2.18	0.44
1:B:404:VAL:O	1:B:408:MET:HG2	2.18	0.44
2:F:452:LYS:HA	2:F:494:SER:HA	2.00	0.44
1:A:316:VAL:HA	1:A:320:LEU:O	2.18	0.44
2:F:458:LYS:HD2	2:F:458:LYS:H	1.82	0.44
1:A:177:ARG:HB3	1:A:178:PRO:HD3	1.99	0.43
1:A:252:TYR:CZ	1:A:266:LEU:HD22	2.53	0.43
1:A:396:ALA:HB3	1:A:400:PHE:CD1	2.53	0.43
1:B:184:VAL:HG22	1:B:464:PHE:HE1	1.83	0.43
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.53	0.43
2:E:392:PHE:O	2:E:523:THR:N	2.51	0.43
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.53	0.43
1:A:450:LEU:HB2	1:A:451:PRO:HD3	2.00	0.43
2:F:472:ILE:HG13	2:F:482:GLY:CA	2.49	0.43
2:E:444:THR:HG23	2:E:447:GLY:H	1.83	0.43
1:B:233:ILE:HD13	1:B:450:LEU:HD13	2.00	0.43
1:B:362:THR:HG23	1:B:368:ASP:HB3	2.01	0.43
1:A:285:PHE:O	1:A:437:ASN:ND2	2.48	0.43
1:A:204:ARG:HH22	1:A:465:LYS:NZ	2.17	0.42
1:A:482:ARG:HH21	1:A:611:SER:HB3	1.83	0.42
2:E:342:PHE:HB2	8:E:601:NAG:H82	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:O	1:A:102:GLN:HG3	2.20	0.42
1:A:554:LEU:HG	1:A:558:LEU:HD21	2.00	0.42
1:A:469:PRO:HB2	1:A:471:ASP:OD1	2.20	0.42
2:F:392:PHE:CD1	2:F:515:PHE:HB3	2.55	0.42
1:A:143:LEU:H	1:A:143:LEU:HD23	1.84	0.42
3:M:1:NAG:H61	3:M:2:NAG:O5	2.19	0.42
1:A:184:VAL:HG22	1:A:464:PHE:HE1	1.85	0.42
1:A:488:VAL:HG21	1:A:611:SER:HA	2.01	0.42
1:A:520:LEU:HD22	1:A:579:MET:HE2	2.01	0.42
1:B:378:HIS:CE1	1:B:401:HIS:HB3	2.54	0.42
2:E:403:LYS:HB2	2:E:495:TYR:CE1	2.55	0.42
1:B:284:PRO:HG2	1:B:436:ILE:HG22	2.01	0.42
1:B:595:LEU:HD23	1:B:595:LEU:HA	1.93	0.42
1:B:114:LYS:HD3	1:B:114:LYS:HA	1.83	0.42
1:B:451:PRO:HB2	1:B:485:VAL:HG13	2.02	0.42
2:F:350:VAL:HG22	2:F:422:ASN:HB3	2.01	0.42
1:A:499:ASP:N	1:A:500:PRO:HD2	2.35	0.41
2:E:526:GLY:N	2:E:527:PRO:HD3	2.35	0.41
2:F:362:VAL:HB	2:F:527:PRO:HG3	2.02	0.41
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.55	0.41
1:A:21:ILE:H	1:A:21:ILE:HD12	1.84	0.41
2:F:347:PHE:CD1	2:F:509:ARG:HD3	2.55	0.41
1:A:142:LEU:HD21	1:A:163:TRP:HH2	1.84	0.41
1:B:450:LEU:HB2	1:B:451:PRO:HD3	2.01	0.41
2:F:472:ILE:HG13	2:F:482:GLY:HA2	2.01	0.41
1:B:499:ASP:N	1:B:500:PRO:HD2	2.36	0.41
1:A:341:LYS:HA	1:A:341:LYS:HD2	1.79	0.41
1:A:499:ASP:O	1:A:502:SER:OG	2.25	0.41
1:A:142:LEU:HB2	1:A:147:GLY:HA3	2.03	0.41
1:B:469:PRO:HB2	1:B:471:ASP:OD1	2.20	0.41
2:E:502:GLY:O	2:E:506:GLN:HG3	2.20	0.41
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.92	0.41
1:B:96:GLN:HG2	1:B:392:LEU:HD13	2.03	0.41
1:B:455:MET:HE2	1:B:485:VAL:HG21	2.03	0.41
1:B:519:THR:O	1:B:522:GLN:HG2	2.20	0.41
2:E:453:TYR:CZ	2:E:493:GLN:HB3	2.56	0.41
2:F:431:GLY:HA2	2:F:515:PHE:CE2	2.56	0.41
1:A:105:SER:HA	1:A:190:MET:HG3	2.02	0.41
2:E:403:LYS:HD2	2:E:505:HIS:ND1	2.36	0.40
1:B:400:PHE:O	1:B:404:VAL:HG23	2.22	0.40
2:E:350:VAL:HA	2:E:400:PHE:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD12	1:A:147:GLY:C	2.42	0.40
1:B:570:LEU:O	1:B:574:VAL:HG22	2.21	0.40
2:E:497:PHE:CD2	2:E:507:PRO:HB3	2.56	0.40
2:F:365:TYR:HD2	2:F:388:ASN:HA	1.87	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	594/597 (100%)	575 (97%)	18 (3%)	1 (0%)	47 77
1	B	594/597 (100%)	574 (97%)	19 (3%)	1 (0%)	47 77
2	E	186/217 (86%)	164 (88%)	20 (11%)	2 (1%)	14 42
2	F	190/217 (88%)	170 (90%)	18 (10%)	2 (1%)	14 42
All	All	1564/1628 (96%)	1483 (95%)	75 (5%)	6 (0%)	34 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	613	TYR
2	F	485	GLY
2	E	459	SER
1	A	291	ILE
2	E	526	GLY
2	F	483	VAL

### 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	526/527 (100%)	519 (99%)	7 (1%)	69 86
1	B	526/527 (100%)	517 (98%)	9 (2%)	60 82
2	E	165/189 (87%)	158 (96%)	7 (4%)	30 60
2	F	166/189 (88%)	161 (97%)	5 (3%)	41 69
All	All	1383/1432 (97%)	1355 (98%)	28 (2%)	55 78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	95	LEU
1	A	325	GLN
1	A	381	TYR
1	A	447	VAL
1	A	558	LEU
1	A	581	VAL
1	B	21	ILE
1	B	45	LEU
1	B	95	LEU
1	B	225	ASP
1	B	341	LYS
1	B	381	TYR
1	B	447	VAL
1	B	518	ARG
1	B	557	MET
2	E	372	THR
2	E	377	PHE
2	E	387	LEU
2	E	402	VAL
2	E	415	THR
2	E	468	ILE
2	E	493	GLN
2	F	355	ARG
2	F	360	ASN
2	F	377	PHE
2	F	458	LYS
2	F	493	GLN

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

Mol	Chain	Res	Type
1	B	472	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](#)

18 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	C	1	3,1	14,14,15	0.44	0	17,19,21	0.74	1 (5%)
3	NAG	C	2	3	14,14,15	0.35	0	17,19,21	0.40	0
4	NAG	D	1	4,1	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	D	2	4	14,14,15	0.25	0	17,19,21	0.43	0
4	BMA	D	3	4	11,11,12	0.66	0	15,15,17	0.75	0
4	NAG	G	1	4,1	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	G	2	4	14,14,15	0.20	0	17,19,21	0.49	0
4	BMA	G	3	4	11,11,12	0.64	0	15,15,17	0.75	0
3	NAG	H	1	3,1	14,14,15	0.35	0	17,19,21	1.08	2 (11%)
3	NAG	H	2	3	14,14,15	0.46	0	17,19,21	0.82	1 (5%)
3	NAG	I	1	3,1	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	I	2	3	14,14,15	0.34	0	17,19,21	0.54	0
5	NAG	J	1	1,5	14,14,15	0.33	0	17,19,21	0.47	0
5	NAG	J	2	5	14,14,15	0.23	0	17,19,21	0.41	0
5	BMA	J	3	5	11,11,12	1.13	1 (9%)	15,15,17	1.52	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	J	4	5	14,14,15	0.84	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	M	1	3,2	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.58	0	17,19,21	1.29	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	C	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	NAG	J	4	5	-	4/6/23/26	0/1/1/1
3	NAG	M	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	NAG	O5-C1	2.50	1.47	1.43
5	J	3	BMA	C2-C3	2.36	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	3	BMA	C1-C2-C3	4.39	115.06	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	C2-N2-C7	4.31	129.03	122.90
5	J	4	NAG	C1-O5-C5	3.21	116.54	112.19
3	H	1	NAG	O4-C4-C5	2.88	116.45	109.30
3	H	2	NAG	C1-O5-C5	2.79	115.97	112.19
3	H	1	NAG	C1-O5-C5	2.61	115.73	112.19
3	C	1	NAG	C1-O5-C5	2.25	115.23	112.19
3	M	2	NAG	C1-C2-N2	2.04	113.97	110.49

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	J	4	NAG	C8-C7-N2-C2
5	J	4	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
5	J	4	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6

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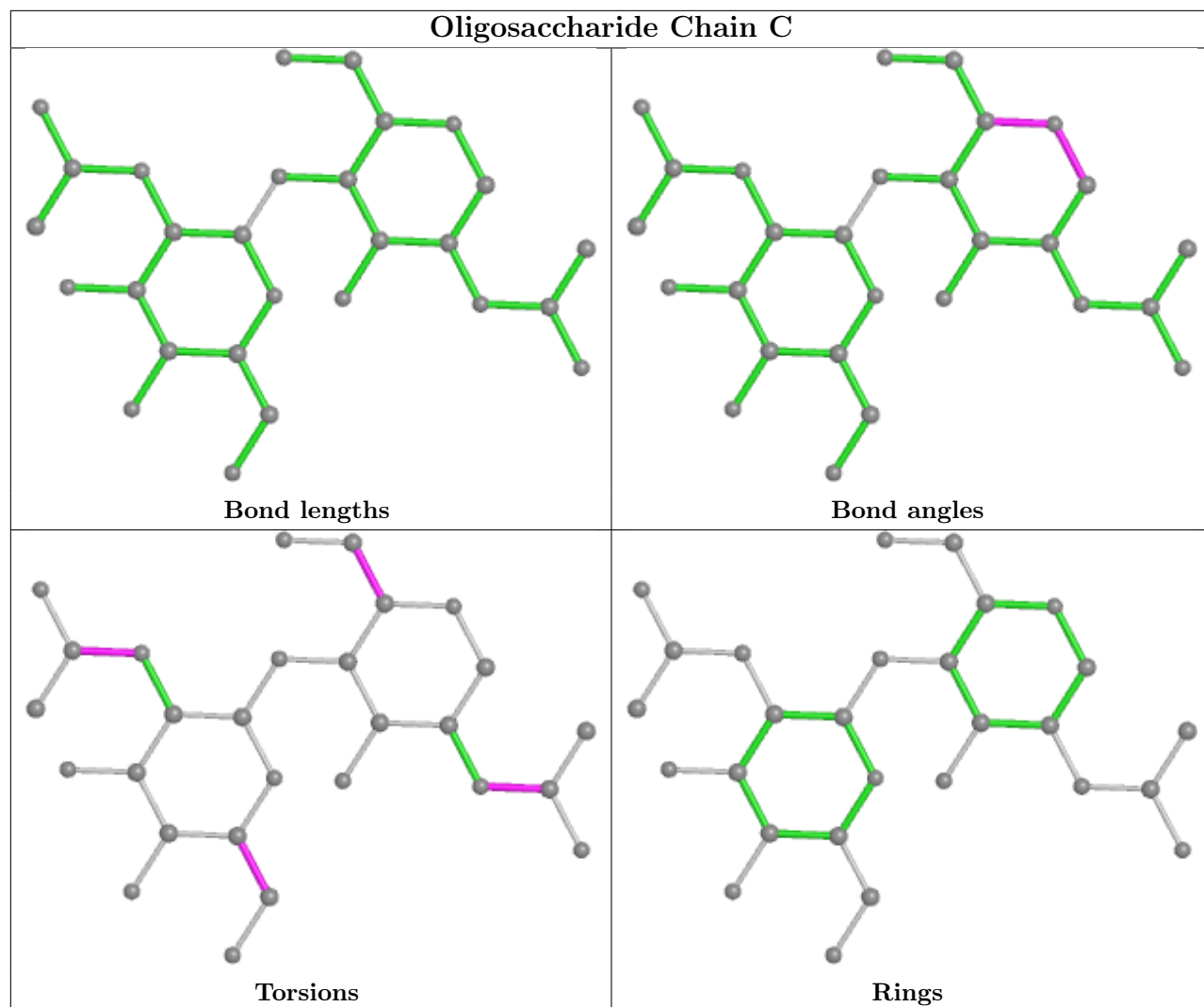
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
5	J	4	NAG	O5-C5-C6-O6
3	H	2	NAG	C3-C2-N2-C7
3	H	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C3-C2-N2-C7

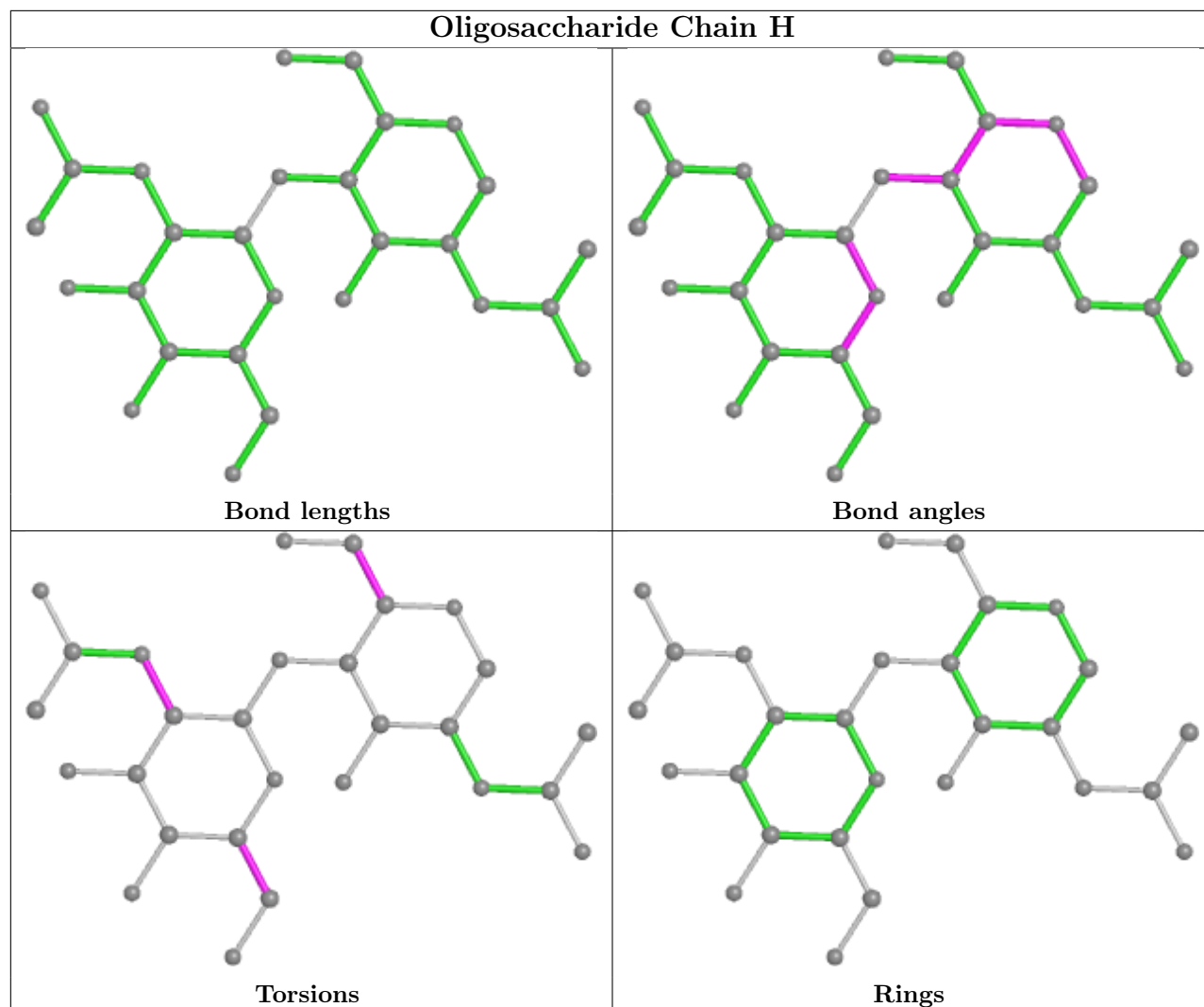
There are no ring outliers.

4 monomers are involved in 3 short contacts:

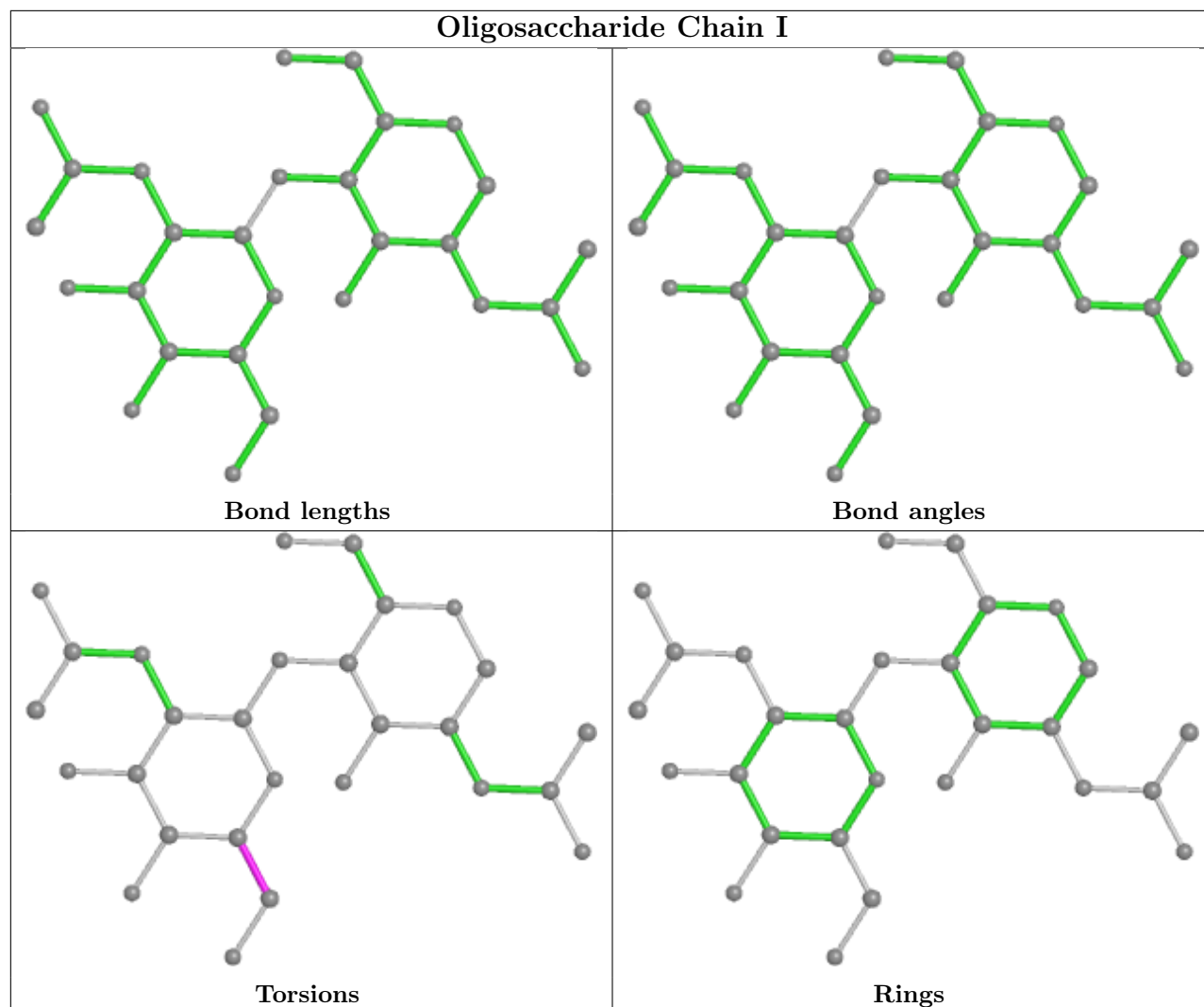
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
3	M	2	NAG	2	0
3	I	2	NAG	1	0
3	I	1	NAG	1	0

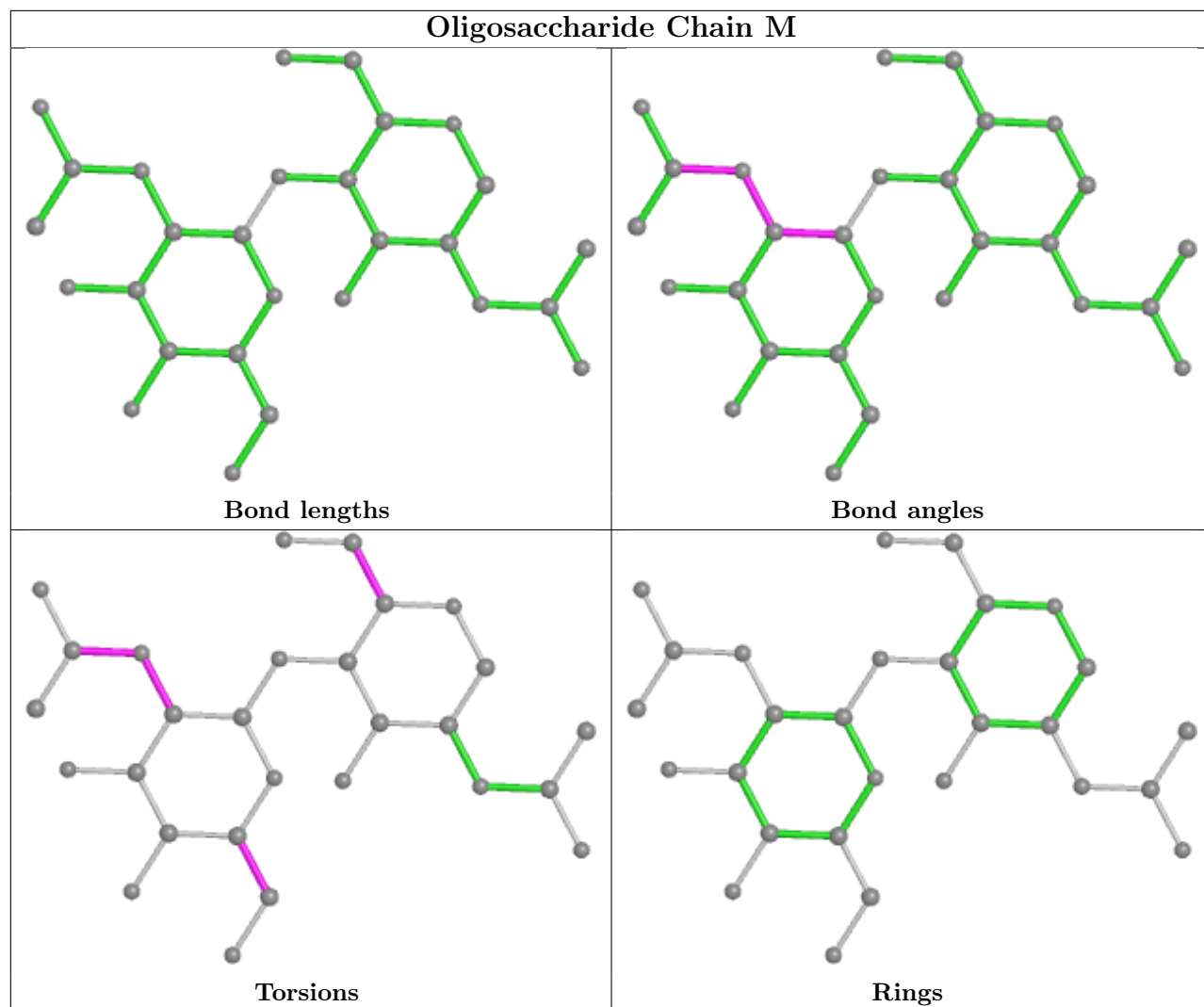
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

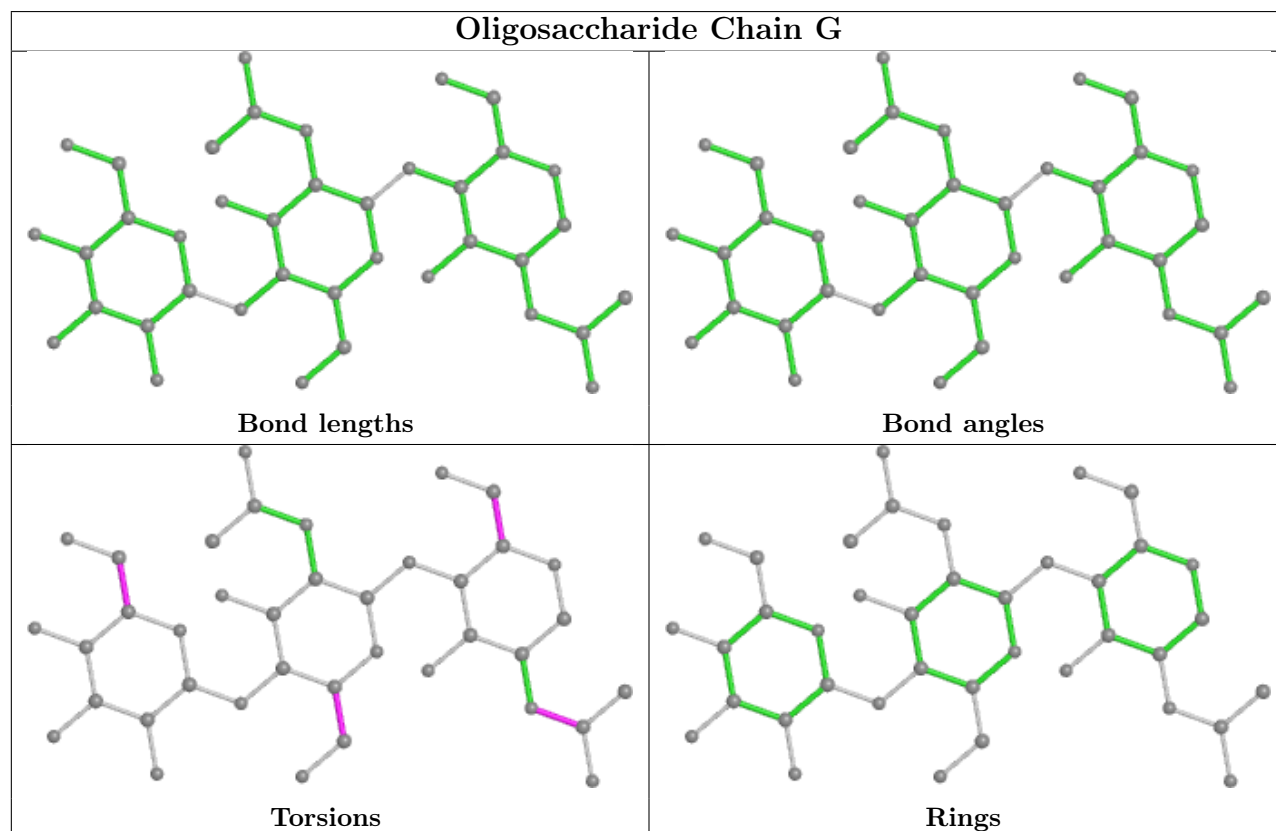
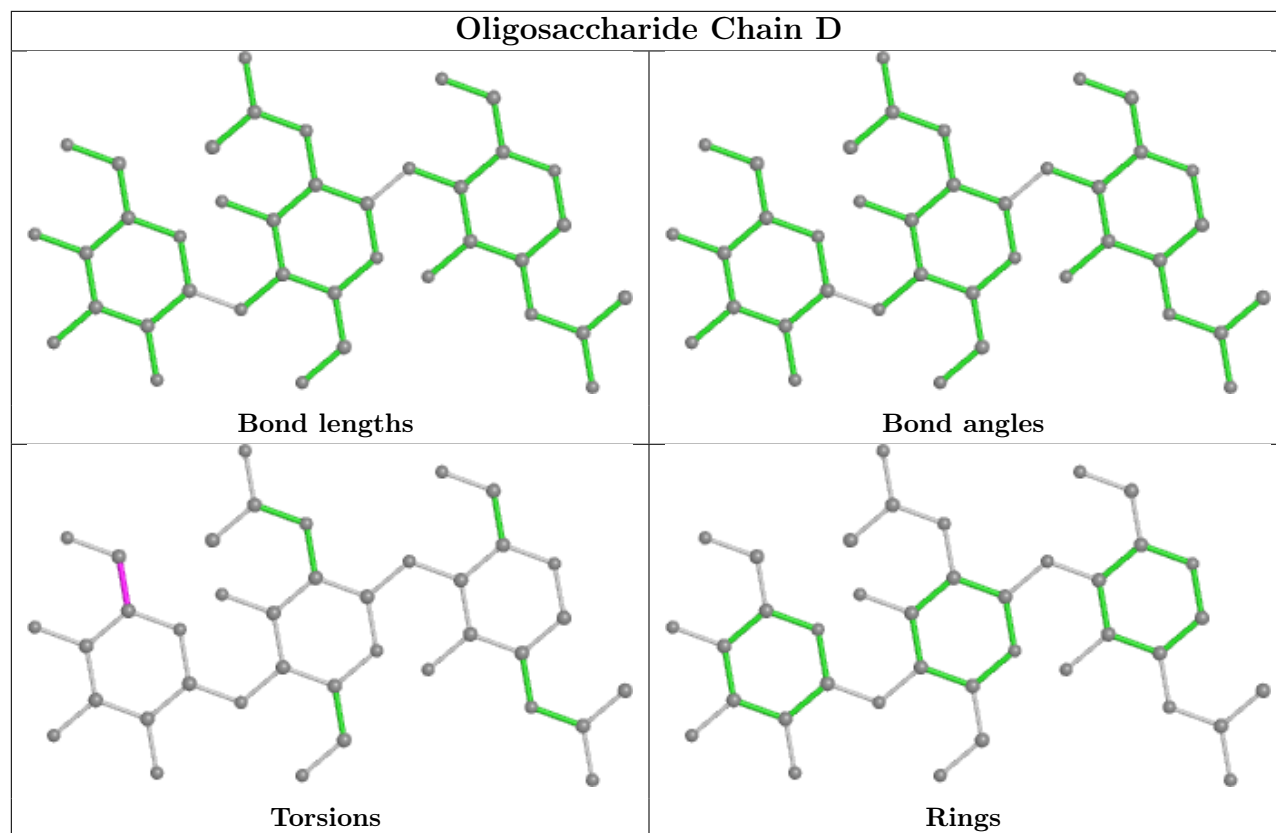


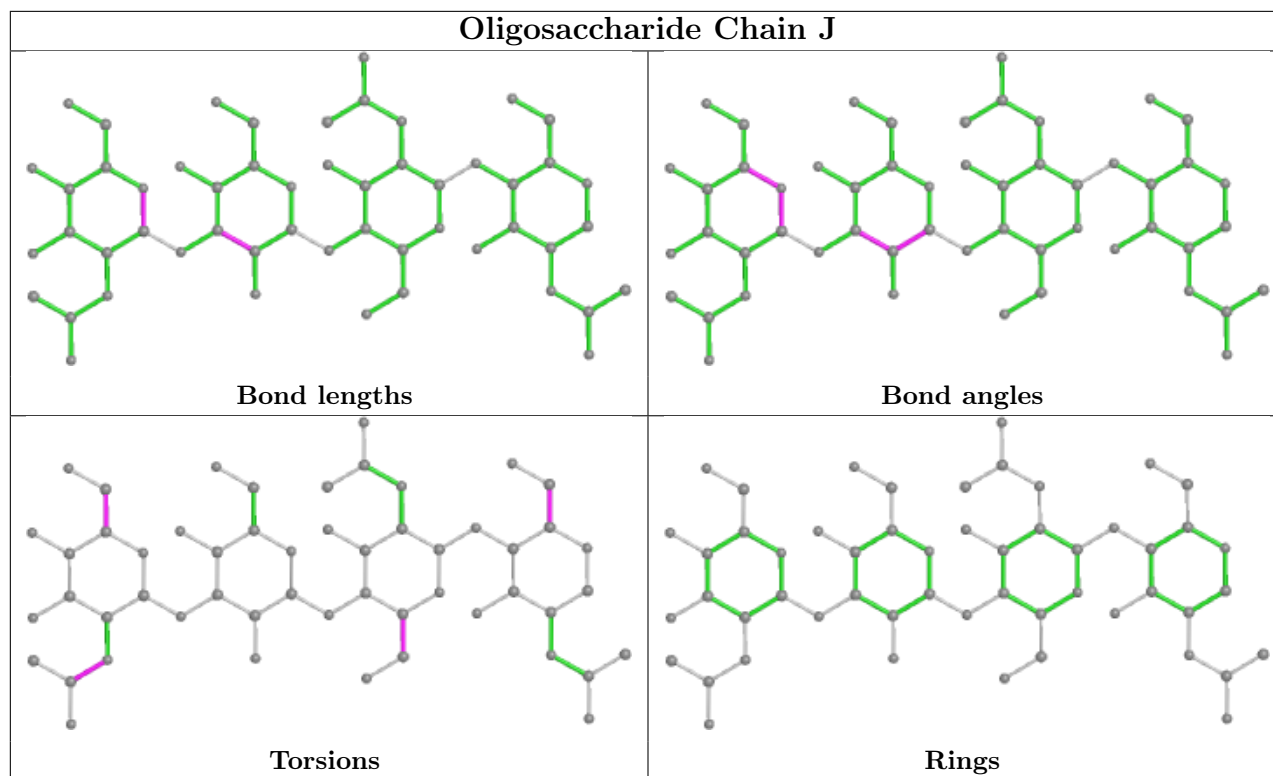












## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z  > 2$
8	NAG	A	704	1	14,14,15	0.26	0	17,19,21	0.48	0
9	EDO	B	703	-	3,3,3	0.46	0	2,2,2	0.34	0
8	NAG	E	601	2	14,14,15	0.25	0	17,19,21	0.42	0
9	EDO	B	704	-	3,3,3	0.46	0	2,2,2	0.32	0
8	NAG	B	707	1	14,14,15	0.29	0	17,19,21	0.47	0
8	NAG	B	706	1	14,14,15	0.36	0	17,19,21	0.49	0
8	NAG	A	703	1	14,14,15	0.31	0	17,19,21	0.47	0
8	NAG	B	705	1	14,14,15	0.23	0	17,19,21	0.47	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
8	NAG	A	704	1	-	1/6/23/26	0/1/1/1
9	EDO	B	703	-	-	0/1/1/1	-
8	NAG	E	601	2	-	2/6/23/26	0/1/1/1
9	EDO	B	704	-	-	0/1/1/1	-
8	NAG	B	707	1	-	2/6/23/26	0/1/1/1
8	NAG	B	706	1	-	2/6/23/26	0/1/1/1
8	NAG	A	703	1	-	2/6/23/26	0/1/1/1
8	NAG	B	705	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	705	NAG	O5-C5-C6-O6
8	E	601	NAG	O5-C5-C6-O6
8	B	706	NAG	O5-C5-C6-O6
8	A	703	NAG	O5-C5-C6-O6
8	B	706	NAG	C4-C5-C6-O6
8	B	705	NAG	C4-C5-C6-O6
8	E	601	NAG	C4-C5-C6-O6
8	B	707	NAG	O5-C5-C6-O6
8	A	703	NAG	C4-C5-C6-O6
8	B	707	NAG	C4-C5-C6-O6
8	A	704	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	601	NAG	1	0

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	596/597 (99%)	-0.13	5 (0%) 86 70	44, 80, 122, 173	0
1	B	596/597 (99%)	-0.14	3 (0%) 91 79	33, 67, 113, 173	0
2	E	192/217 (88%)	0.19	9 (4%) 31 14	44, 73, 138, 192	0
2	F	194/217 (89%)	-0.01	4 (2%) 63 39	53, 89, 138, 204	0
All	All	1578/1628 (96%)	-0.08	21 (1%) 77 56	33, 75, 127, 204	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	521	PRO	9.2
2	E	387	LEU	3.7
1	B	21	ILE	3.5
2	E	369	TYR	3.4
2	E	386	LYS	3.4
1	B	85	LEU	3.2
1	A	299	ASP	3.2
1	A	289	PRO	2.9
2	F	520	ALA	2.6
2	F	482	GLY	2.5
2	E	378	LYS	2.5
2	E	521	PRO	2.5
2	E	526	GLY	2.4
1	B	24	GLN	2.2
2	F	522	ALA	2.2
2	E	515	PHE	2.2
1	A	423	LEU	2.1
2	E	514	SER	2.1
1	A	424	LEU	2.1
1	A	529	LEU	2.1
2	E	518	LEU	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.

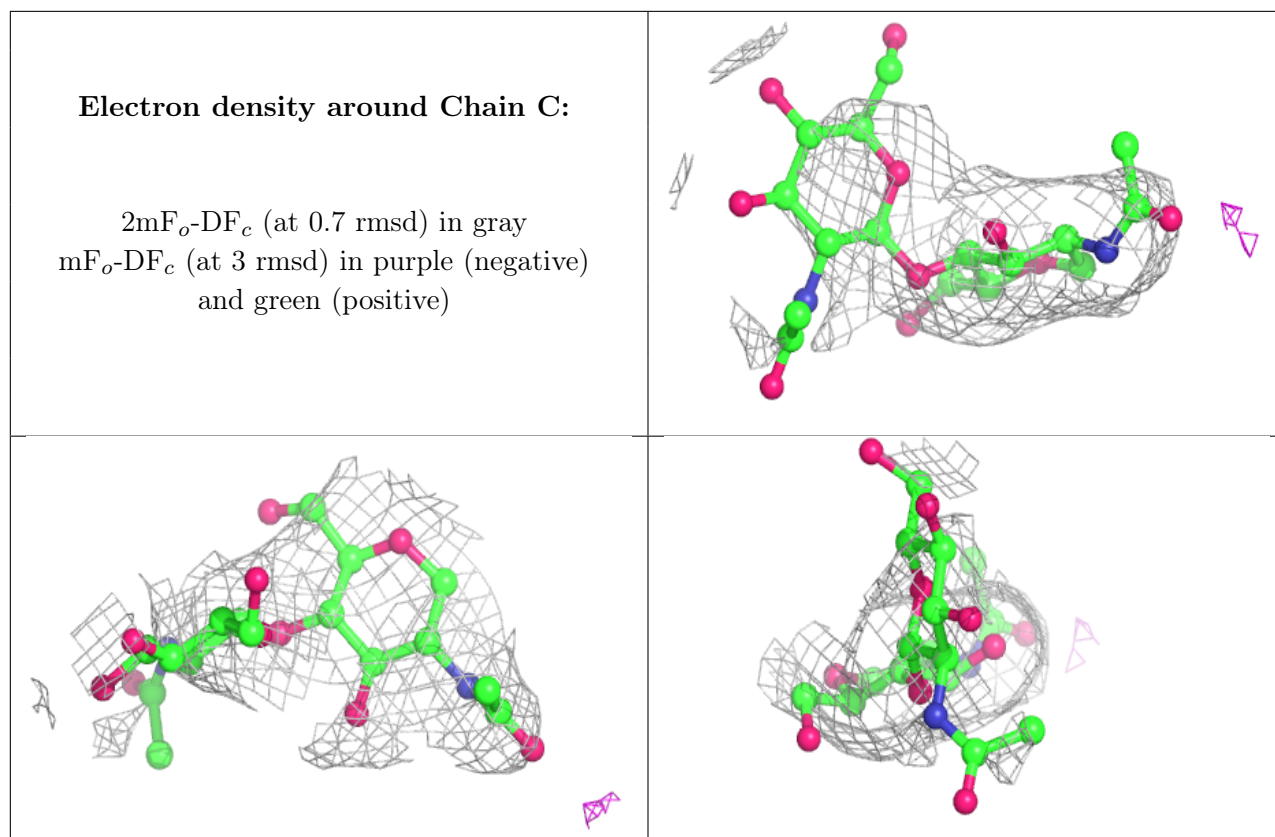
## 6.3 Carbohydrates [i](#)

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
3	NAG	C	2	14/15	0.58	0.44	129,147,154,157	0
5	NAG	J	4	14/15	0.64	0.34	103,126,132,143	0
4	BMA	G	3	11/12	0.69	0.21	97,125,136,137	0
4	BMA	D	3	11/12	0.69	0.24	91,107,119,122	0
3	NAG	I	2	14/15	0.72	0.29	111,128,135,135	0
3	NAG	H	2	14/15	0.72	0.28	104,132,142,152	0
5	BMA	J	3	11/12	0.79	0.15	85,100,105,113	0
3	NAG	M	2	14/15	0.80	0.22	101,127,135,136	0
4	NAG	G	2	14/15	0.85	0.27	109,123,137,148	0
3	NAG	M	1	14/15	0.85	0.23	88,116,130,135	0
3	NAG	I	1	14/15	0.86	0.22	108,118,130,130	0
4	NAG	D	1	14/15	0.90	0.22	87,97,100,100	0
3	NAG	C	1	14/15	0.90	0.17	94,106,131,133	0
5	NAG	J	2	14/15	0.91	0.17	59,81,92,93	0
3	NAG	H	1	14/15	0.91	0.16	73,90,109,118	0
4	NAG	G	1	14/15	0.91	0.22	97,117,124,124	0
5	NAG	J	1	14/15	0.93	0.17	41,63,72,74	0
4	NAG	D	2	14/15	0.93	0.22	86,102,108,114	0

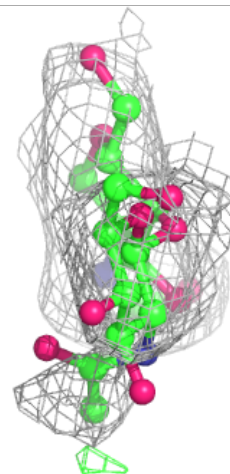
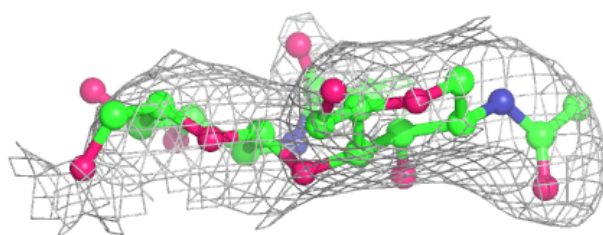
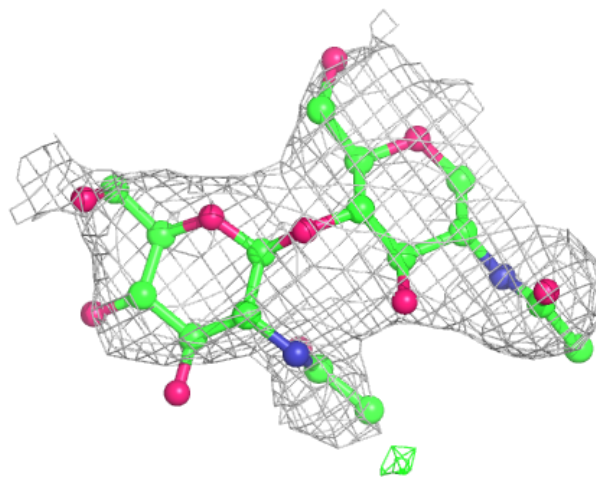
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

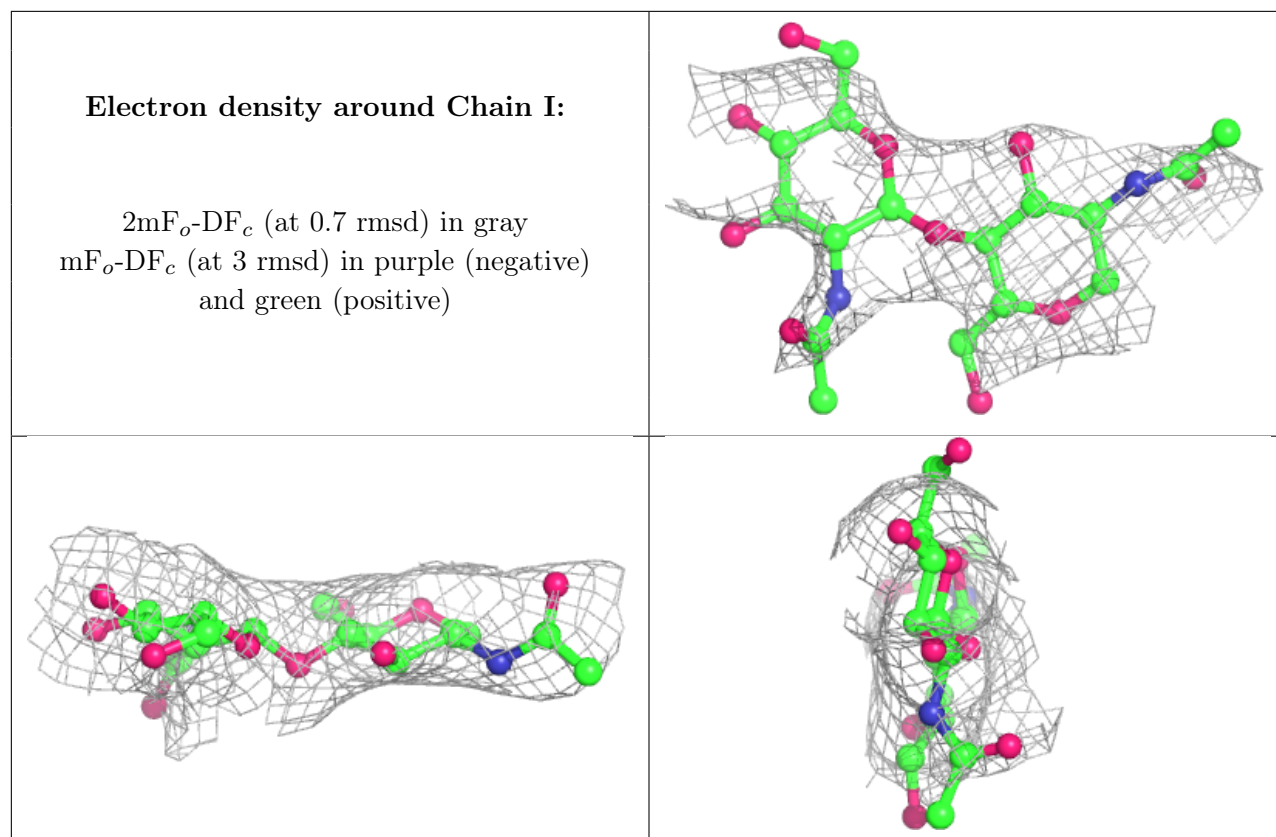




**Electron density around Chain H:**

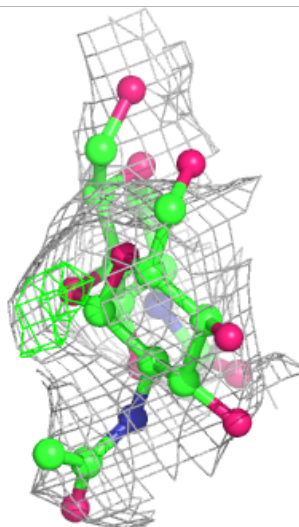
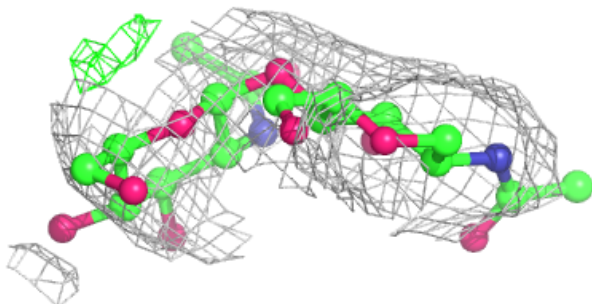
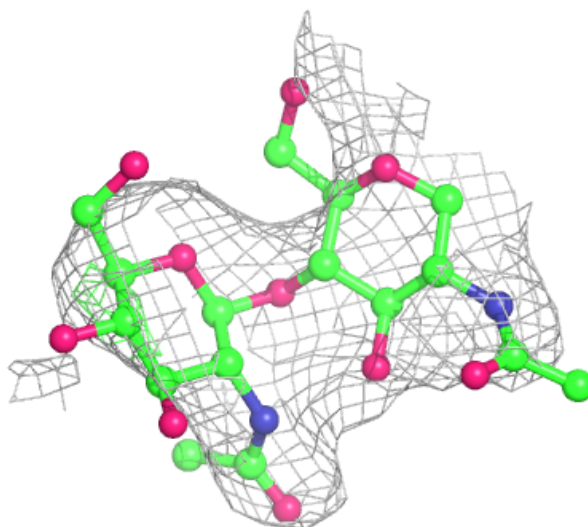
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





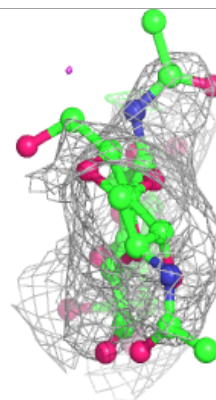
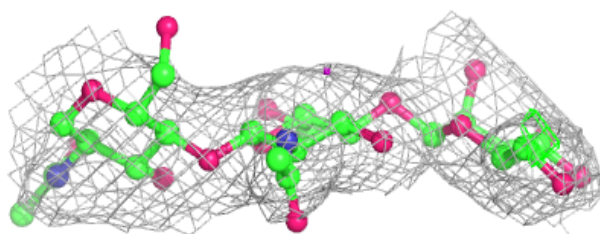
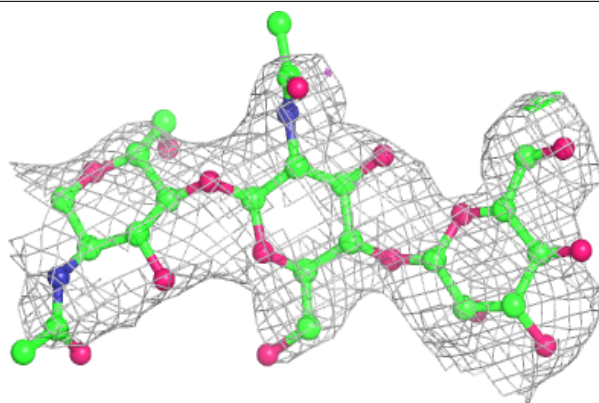
**Electron density around Chain M:**

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

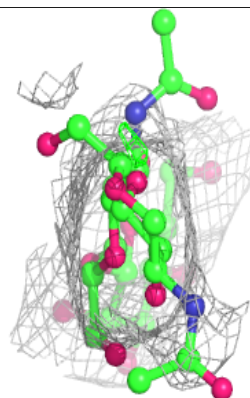
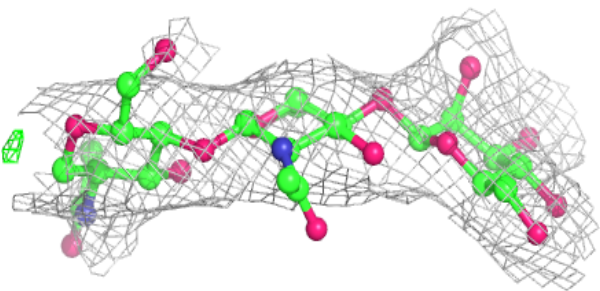
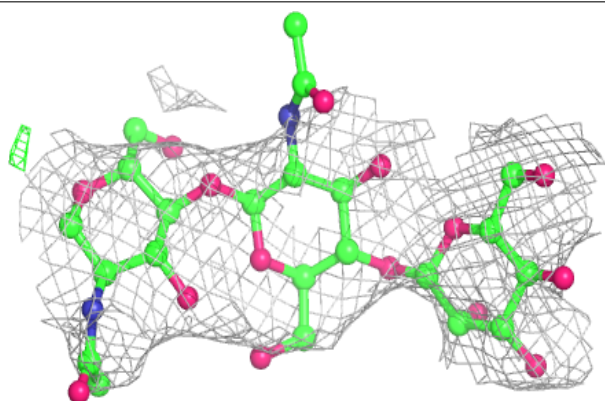


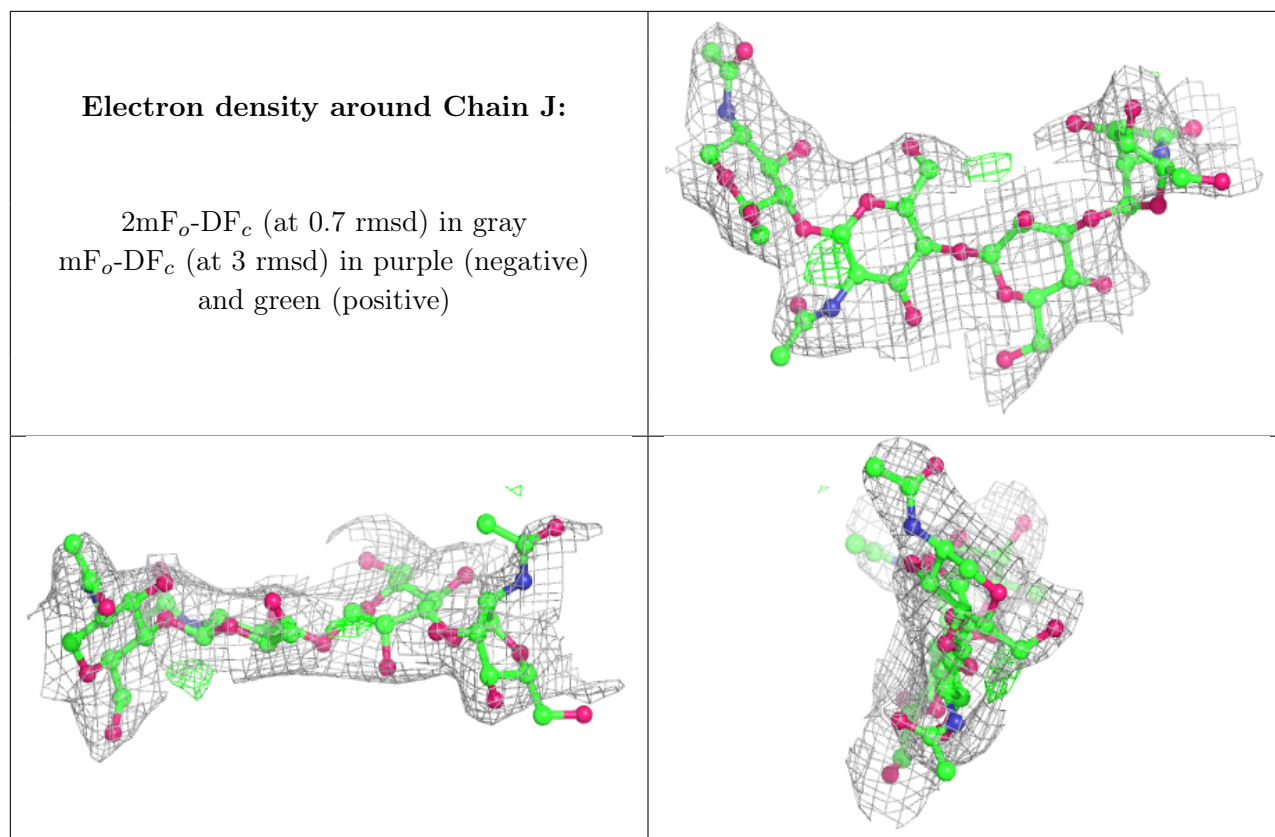
**Electron density around Chain D:**

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

**Electron density around Chain G:**

$2mF_o-DF_c$  (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
8	NAG	A	704	14/15	0.72	0.24	97,122,129,129	0
8	NAG	B	705	14/15	0.73	0.42	83,109,124,127	0
8	NAG	B	706	14/15	0.73	0.24	103,118,132,135	0
8	NAG	E	601	14/15	0.73	0.36	93,116,119,122	0
8	NAG	B	707	14/15	0.77	0.29	69,88,101,107	0
8	NAG	A	703	14/15	0.82	0.18	78,90,97,99	0
9	EDO	B	704	4/4	0.85	0.17	43,54,61,63	0
9	EDO	B	703	4/4	0.91	0.29	43,49,55,63	0
6	ZN	B	701	1/1	0.93	0.11	92,92,92,92	0
7	CL	A	702	1/1	0.94	0.24	104,104,104,104	0
6	ZN	A	701	1/1	0.95	0.11	111,111,111,111	0
7	CL	B	702	1/1	0.96	0.24	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.