



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:13 AM UTC

PDB ID : 7UFK / pdb_00007ufk
Title : Crystal structure of chimeric omicron RBD (strain BA.2) complexed with human ACE2
Authors : Zhang, W.; Shi, K.; Geng, Q.; Ye, G.; Aihara, H.; Li, F.
Deposited on : 2022-03-22
Resolution : 2.38 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

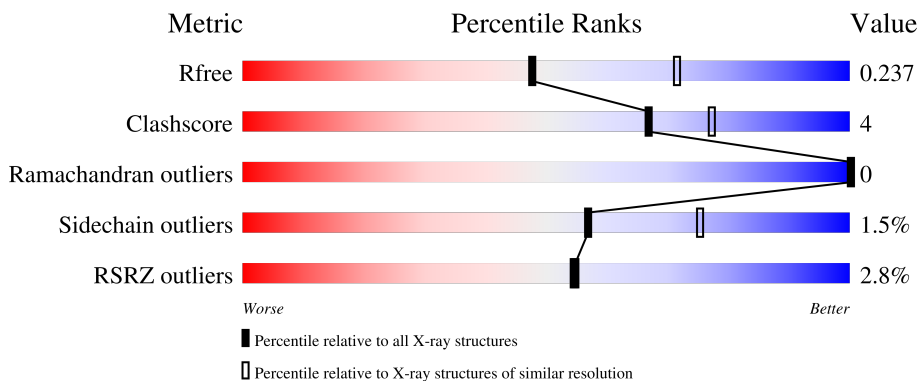
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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.



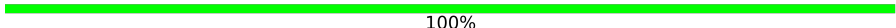

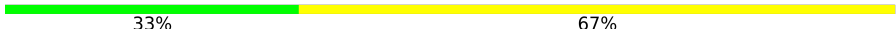

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 ≥ 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	 3% 88% 12%
1	B	597	 2% 88% 11%
2	E	217	 3% 77% 10% 13%
2	F	217	 6% 76% 11% 13%
3	C	2	 100%

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Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	K	2	 100%
4	D	3	 100%
4	G	3	 33% 67%
5	J	4	 75% 25%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 13092 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	188	1504	968	249	277	10	0	1	0
2	F	188	1501	966	249	277	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	I	2	28	16	2	10	0	0	0
3	K	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 alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is ZINC ION (CCD ID: 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 (CCD ID: 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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	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	E	1	14	8	1	5	0	0
8	F	1	14	8	1	5	0	0

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
9	A	1	1	1	0	0

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

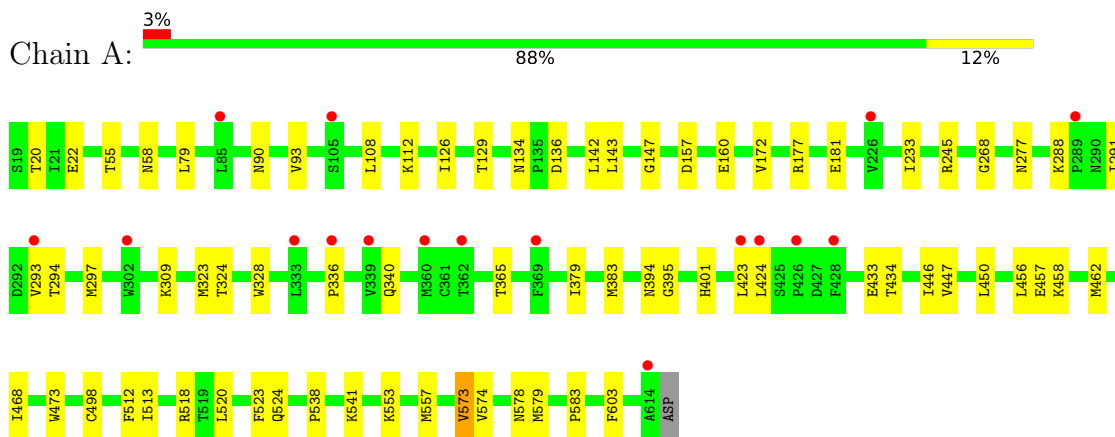
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total O 8 8	0	0
11	B	11	Total O 11 11	0	0
11	E	2	Total O 2 2	0	0
11	F	1	Total O 1 1	0	0

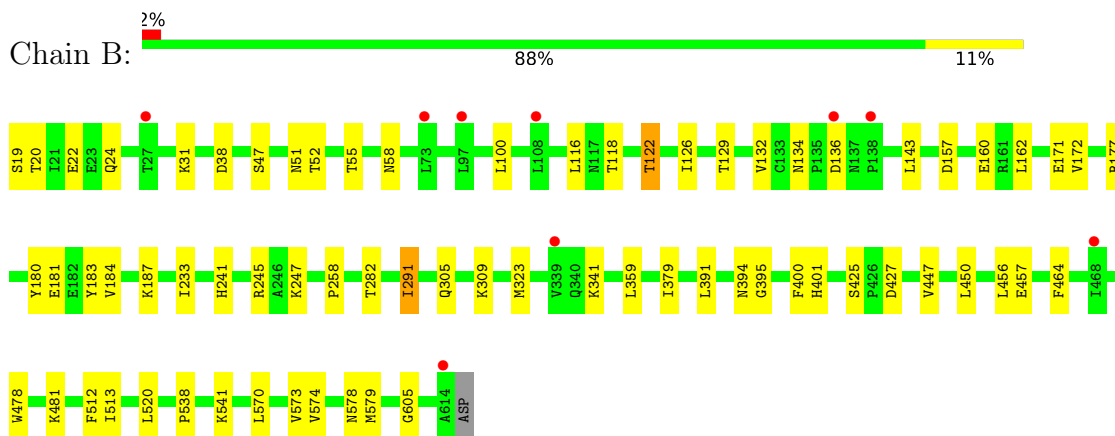
3 Residue-property plots [i](#)

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.

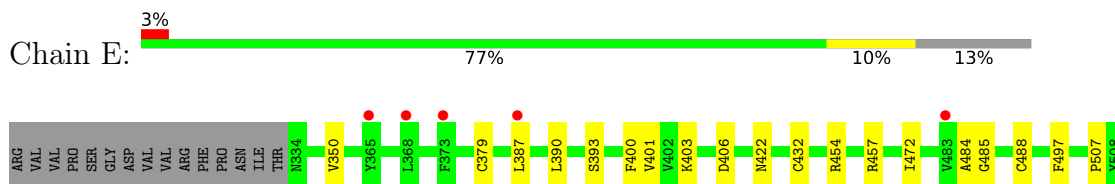
- Molecule 1: Angiotensin-converting enzyme 2

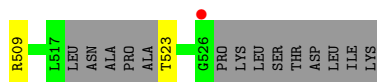


- Molecule 1: Angiotensin-converting enzyme 2

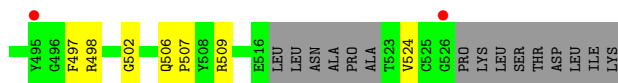
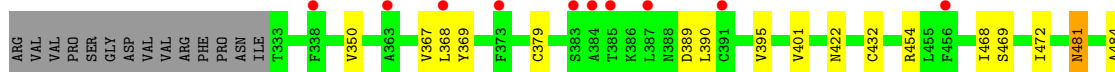
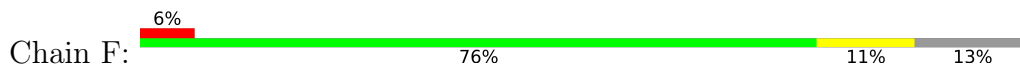


- Molecule 2: Spike protein S1





- Molecule 2: Spike protein S1



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



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



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



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



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



MAC1
MAC2
BMA3

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

Chain J:  75% 25%

MAC1
MAC2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.40Å 117.86Å 113.02Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	29.01 – 2.38 29.01 – 2.38	Depositor EDS
% Data completeness (in resolution range)	51.4 (29.01-2.38) 48.7 (29.01-2.38)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.40Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.192 , 0.235 0.194 , 0.237	Depositor DCC
R_{free} test set	2116 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtrriage
Anisotropy	0.035	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for -h,-l,-k 0.000 for -h,l,k 0.027 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13092	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, ZN, BMA, EDO, NA, NAG, 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	0.07	0/4999	0.18	0/6792
1	B	0.07	0/4999	0.19	0/6792
2	E	0.06	0/1546	0.21	0/2099
2	F	0.07	0/1543	0.23	0/2094
All	All	0.07	0/13087	0.20	0/17777

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	4632	35	0
1	B	4862	0	4633	34	0
2	E	1504	0	1422	11	0
2	F	1501	0	1427	15	0
3	C	28	0	25	0	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
4	D	39	0	34	0	0
4	G	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	50	0	43	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	0	0
8	A	56	0	52	0	0
8	B	28	0	26	0	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
9	A	1	0	0	0	0
10	B	12	0	18	0	0
11	A	8	0	0	0	0
11	B	11	0	0	0	0
11	E	2	0	0	0	0
11	F	1	0	0	0	0
All	All	13092	0	12422	94	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 4.

All (94) 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:245:ARG:NH2	1:A:603:PHE:O	2.29	0.66
1:B:55:THR:OG1	1:B:58:ASN:ND2	2.28	0.64
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.80	0.63
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.33	0.62
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.83	0.60
1:A:142:LEU:HB3	1:A:147:GLY:HA3	1.82	0.60
2:F:367:VAL:HG13	2:F:368:LEU:HD13	1.85	0.59
1:A:268:GLY:O	1:A:277:ASN:ND2	2.31	0.59
2:E:485:GLY:H	2:E:488:CYS:HB2	1.68	0.58
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.87	0.57
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.87	0.56
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.40	0.55
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.90	0.54
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.90	0.54
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.90	0.53
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.91	0.53
1:B:245:ARG:NH1	1:B:258:PRO:O	2.41	0.53
1:B:126:ILE:HA	1:B:129:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.92	0.52
2:E:393:SER:O	2:E:523:THR:OG1	2.23	0.52
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.91	0.52
1:B:19:SER:HB2	1:B:24:GLN:HE21	1.74	0.51
1:A:294:THR:HG23	1:A:365:THR:HA	1.93	0.50
1:B:425:SER:OG	1:B:427:ASP:OD1	2.22	0.50
1:A:293:VAL:HB	1:A:423:LEU:HB3	1.93	0.50
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.94	0.50
2:F:454:ARG:NH2	2:F:469:SER:O	2.43	0.50
1:B:132:VAL:HG12	1:B:171:GLU:HG3	1.95	0.48
2:E:454:ARG:HD3	2:E:457:ARG:HB2	1.95	0.48
2:F:367:VAL:C	2:F:369:TYR:H	2.21	0.48
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.95	0.48
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.95	0.48
1:B:241:HIS:CE1	1:B:245:ARG:HH21	2.31	0.48
1:A:394:ASN:OD1	1:A:395:GLY:N	2.47	0.48
1:A:108:LEU:HD23	1:A:112:LYS:HB3	1.95	0.47
1:B:100:LEU:HG	1:B:391:LEU:HD21	1.96	0.47
1:B:143:LEU:HD23	1:B:143:LEU:H	1.80	0.47
1:B:400:PHE:HZ	1:B:570:LEU:HB2	1.80	0.47
2:F:472:ILE:HD12	2:F:484:ALA:HB2	1.96	0.47
1:B:118:THR:O	1:B:122:THR:OG1	2.33	0.46
1:A:143:LEU:H	1:A:143:LEU:HD23	1.80	0.46
1:A:291:ILE:HG23	1:A:424:LEU:HD21	1.96	0.46
1:B:245:ARG:NH2	1:B:605:GLY:O	2.31	0.46
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.81	0.46
2:F:395:VAL:HG23	2:F:524:VAL:HG21	1.98	0.46
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.97	0.45
1:A:324:THR:HG23	1:A:383:MET:HE2	1.99	0.45
1:B:291:ILE:H	1:B:291:ILE:HG13	1.64	0.45
1:B:394:ASN:OD1	1:B:395:GLY:N	2.49	0.45
2:E:472:ILE:HD12	2:E:484:ALA:HB2	1.99	0.45
1:B:305:GLN:O	1:B:309:LYS:HB2	2.16	0.45
2:E:350:VAL:HA	2:E:400:PHE:HB2	1.99	0.44
1:B:52:THR:HG22	1:B:359:LEU:HD13	1.99	0.44
1:B:538:PRO:HD2	1:B:541:LYS:HD3	2.00	0.44
1:B:578:ASN:OD1	1:B:579:MET:N	2.49	0.44
2:F:389:ASP:OD1	2:F:389:ASP:N	2.47	0.44
2:E:379:CYS:HA	2:E:432:CYS:HA	1.99	0.43
1:A:55:THR:HG1	1:A:58:ASN:HD22	1.59	0.43
1:A:288:LYS:HE3	1:A:433:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:HG22	1:B:22:GLU:H	1.83	0.43
1:B:247:LYS:HB2	1:B:282:THR:HG22	2.00	0.43
1:A:538:PRO:HD2	1:A:541:LYS:HD3	2.01	0.43
2:F:481:ASN:OD1	2:F:481:ASN:N	2.52	0.43
1:B:47:SER:O	1:B:51:ASN:ND2	2.46	0.43
1:A:20:THR:HG22	1:A:22:GLU:H	1.83	0.43
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.54	0.43
2:F:379:CYS:HA	2:F:432:CYS:HA	2.01	0.42
1:B:184:VAL:HG22	1:B:464:PHE:HE1	1.84	0.42
1:A:323:MET:HE1	1:A:379:ILE:HG21	2.01	0.42
1:A:553:LYS:HE2	1:A:573:VAL:O	2.20	0.42
1:A:309:LYS:HD2	1:A:328:TRP:CH2	2.54	0.42
1:B:478:TRP:HA	1:B:481:LYS:HB2	2.02	0.42
2:E:350:VAL:HG22	2:E:422:ASN:HB3	2.02	0.42
2:F:497:PHE:CD2	2:F:507:PRO:HB3	2.55	0.42
1:B:180:TYR:HA	1:B:183:TYR:HB3	2.01	0.42
1:A:336:PRO:HG2	1:A:340:GLN:O	2.20	0.42
1:B:134:ASN:HD21	1:B:136:ASP:HB2	1.85	0.42
1:A:126:ILE:HA	1:A:129:THR:HG22	2.01	0.42
2:E:497:PHE:CD2	2:E:507:PRO:HB3	2.55	0.41
1:A:134:ASN:HD21	1:A:136:ASP:HB2	1.83	0.41
2:E:403:LYS:HG2	2:E:406:ASP:CG	2.45	0.41
1:A:336:PRO:HB2	1:A:340:GLN:HB3	2.03	0.41
1:B:38:ASP:OD1	2:F:498:ARG:NH2	2.53	0.41
2:E:387:LEU:HA	2:E:390:LEU:HD12	2.03	0.41
2:F:367:VAL:O	2:F:368:LEU:HB2	2.19	0.41
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.86	0.41
2:F:350:VAL:HG22	2:F:422:ASN:HB3	2.02	0.41
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.55	0.41
1:A:458:LYS:NZ	1:A:462:MET:HE3	2.36	0.41
1:A:288:LYS:HD3	1:A:434:THR:HG23	2.03	0.40
1:A:578:ASN:OD1	1:A:579:MET:N	2.51	0.40
1:B:116:LEU:HD11	1:B:187:LYS:HE2	2.01	0.40
2:F:502:GLY:O	2:F:506:GLN:HG3	2.22	0.40
2:F:390:LEU:HD23	2:F:390:LEU:HA	1.96	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%)	574 (97%)	20 (3%)	0	100	100
1	B	594/597 (100%)	574 (97%)	20 (3%)	0	100	100
2	E	185/217 (85%)	173 (94%)	12 (6%)	0	100	100
2	F	184/217 (85%)	171 (93%)	13 (7%)	0	100	100
All	All	1557/1628 (96%)	1492 (96%)	65 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	517 (98%)	9 (2%)	53	72
1	B	526/527 (100%)	516 (98%)	10 (2%)	50	69
2	E	163/189 (86%)	163 (100%)	0	100	100
2	F	163/189 (86%)	161 (99%)	2 (1%)	63	79
All	All	1378/1432 (96%)	1357 (98%)	21 (2%)	57	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	172	VAL

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Mol	Chain	Res	Type
1	A	297	MET
1	A	401	HIS
1	A	447	VAL
1	A	518	ARG
1	A	557	MET
1	A	573	VAL
1	A	574	VAL
1	B	31	LYS
1	B	122	THR
1	B	162	LEU
1	B	172	VAL
1	B	291	ILE
1	B	341	LYS
1	B	401	HIS
1	B	447	VAL
1	B	573	VAL
1	B	574	VAL
2	F	468	ILE
2	F	481	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	239	HIS
1	A	345	HIS
1	A	417	HIS
1	A	599	ASN
1	B	24	GLN
1	B	58	ASN
1	B	96	GLN
1	B	175	GLN
1	B	345	HIS
2	F	370	ASN
2	F	460	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1	1,3	14,14,15	0.39	0	17,19,21	0.63	0
3	NAG	C	2	3	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	D	1	1,4	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	BMA	D	3	4	11,11,12	0.59	0	15,15,17	0.72	0
4	NAG	G	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	G	2	4	14,14,15	0.17	0	17,19,21	0.74	1 (5%)
4	BMA	G	3	4	11,11,12	0.55	0	15,15,17	0.82	0
3	NAG	I	1	1,3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.42	0
5	NAG	J	1	1,5	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	J	2	5	14,14,15	0.22	0	17,19,21	0.39	0
5	BMA	J	3	5	11,11,12	0.58	0	15,15,17	0.84	0
5	MAN	J	4	5	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
3	NAG	K	1	1,3	14,14,15	0.28	0	17,19,21	0.49	0
3	NAG	K	2	3	14,14,15	0.25	0	17,19,21	0.43	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,4	-	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	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	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	MAN	J	4	5	-	1/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	-3.21	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4	MAN	C1-O5-C5	2.42	115.42	112.19
4	G	2	NAG	C1-O5-C5	2.24	115.19	112.19
4	G	1	NAG	C3-C4-C5	2.22	114.25	110.23
5	J	4	MAN	O2-C2-C3	-2.08	105.85	110.15

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

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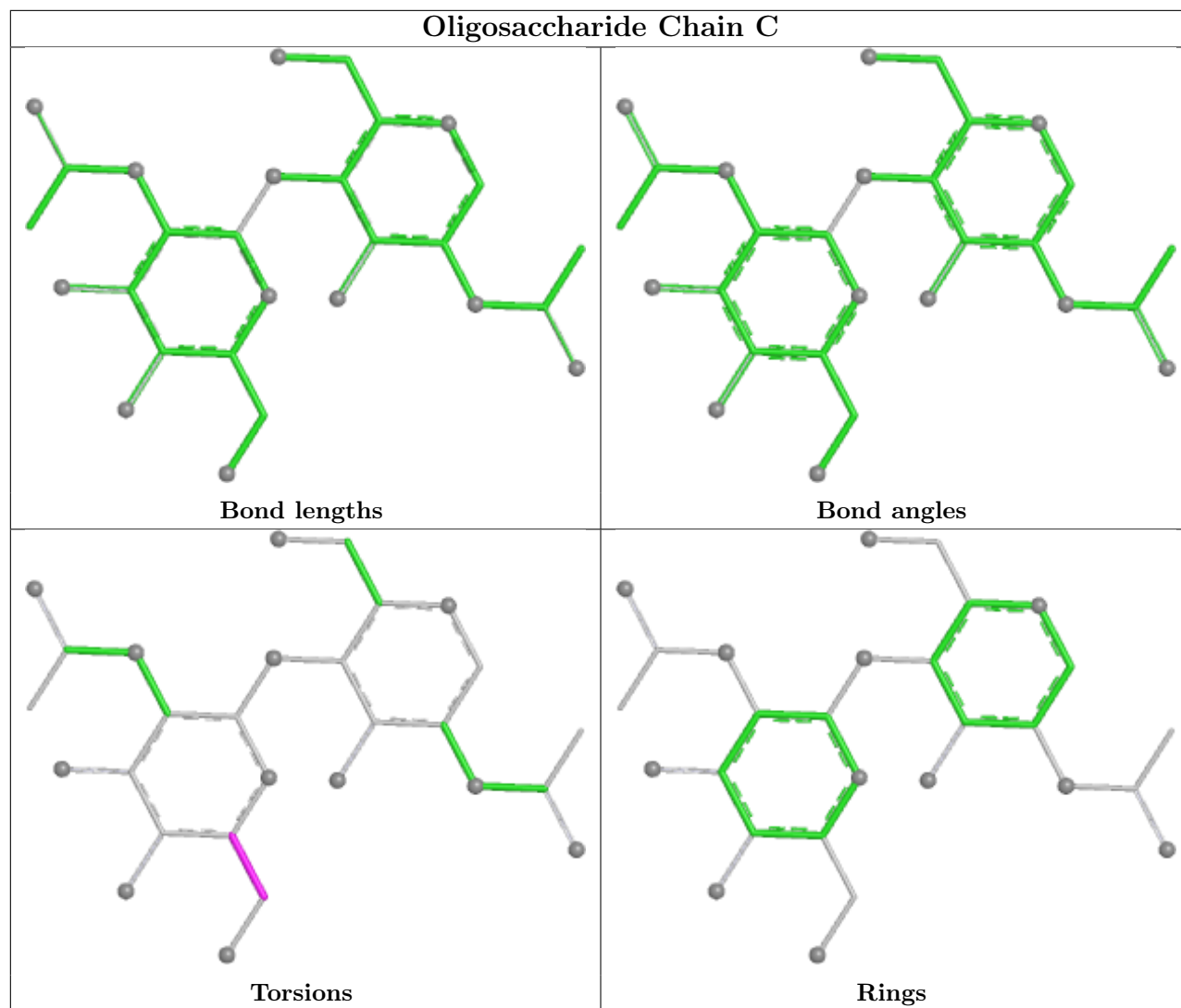
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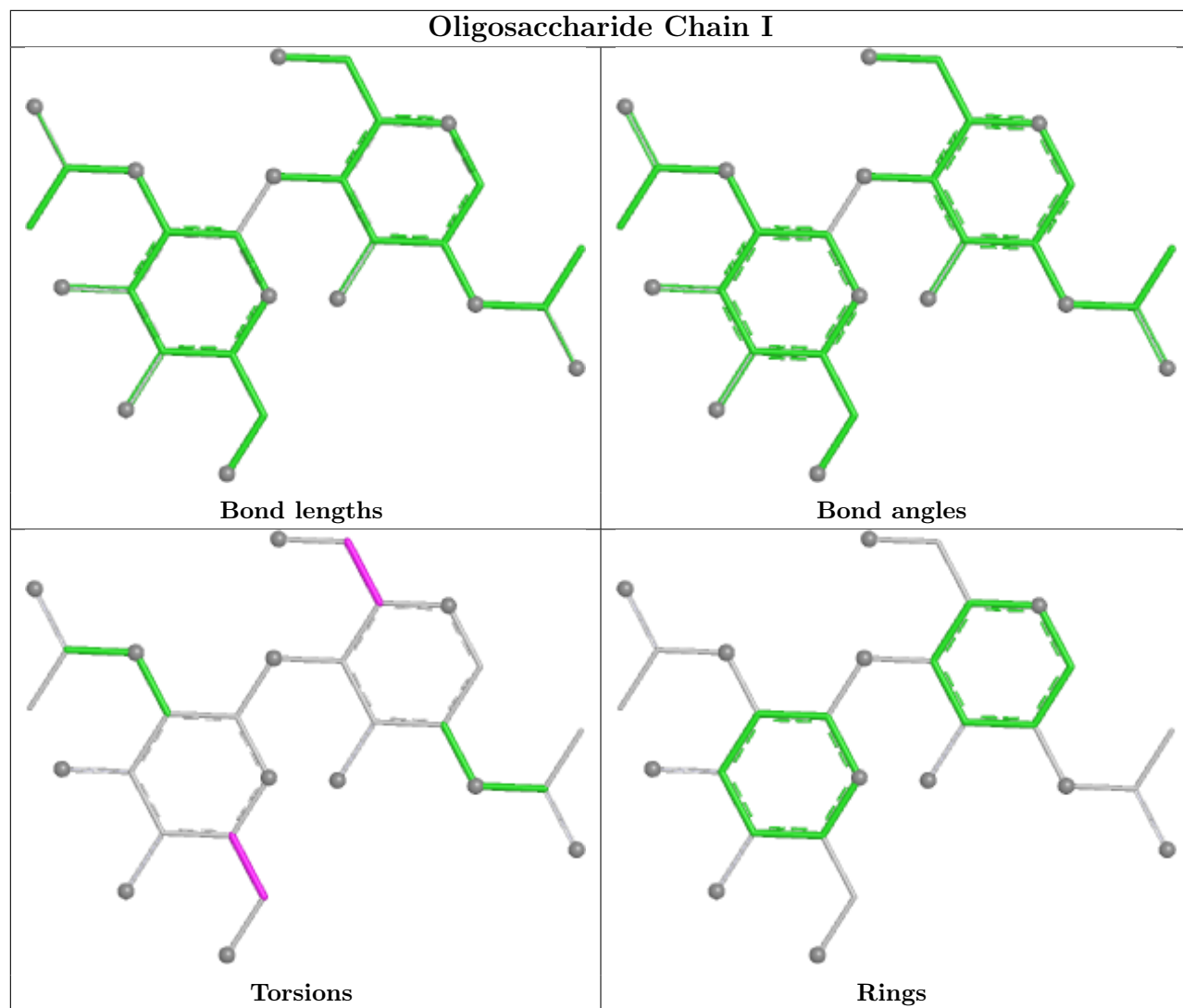
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	J	4	MAN	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6

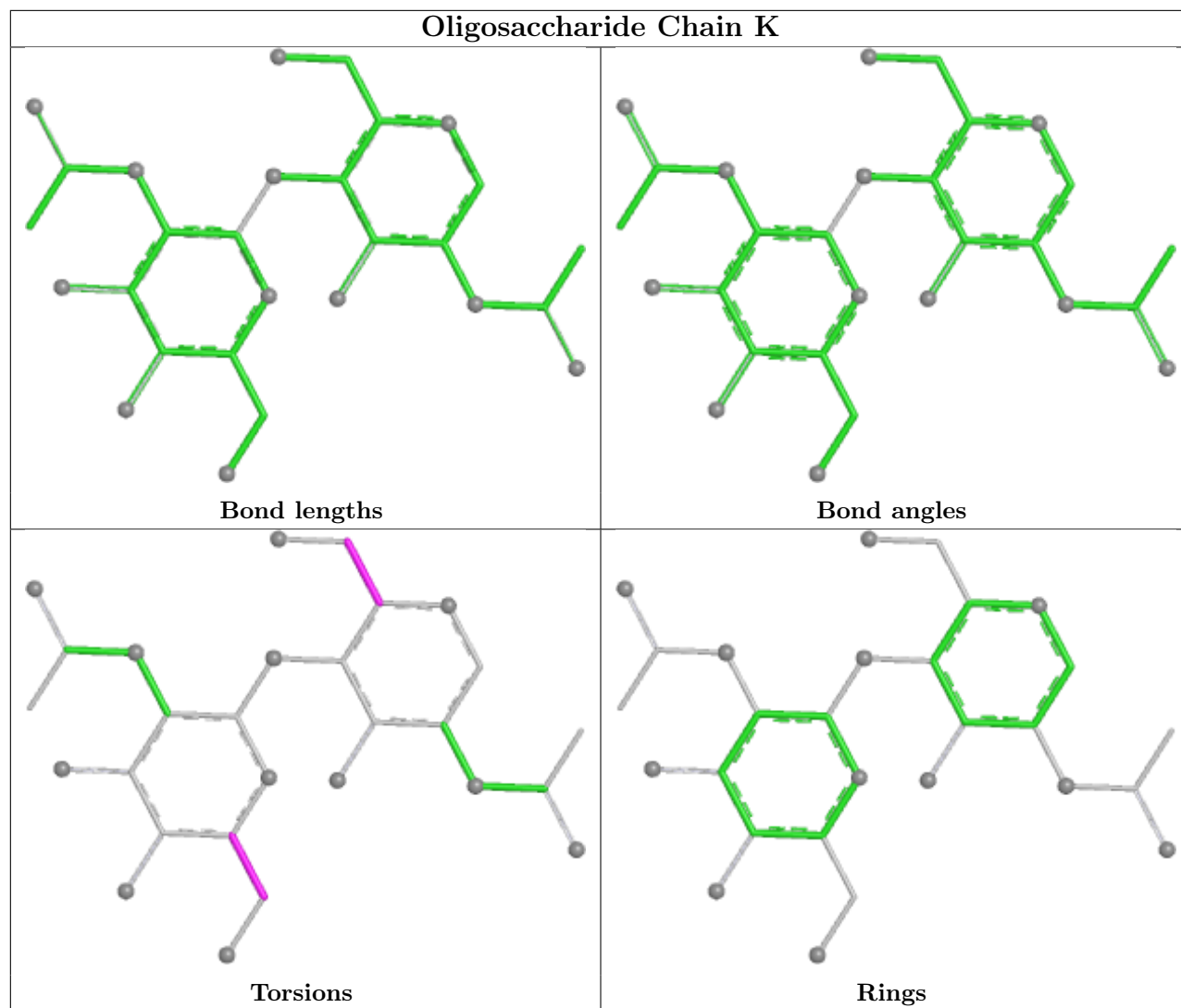
There are no ring outliers.

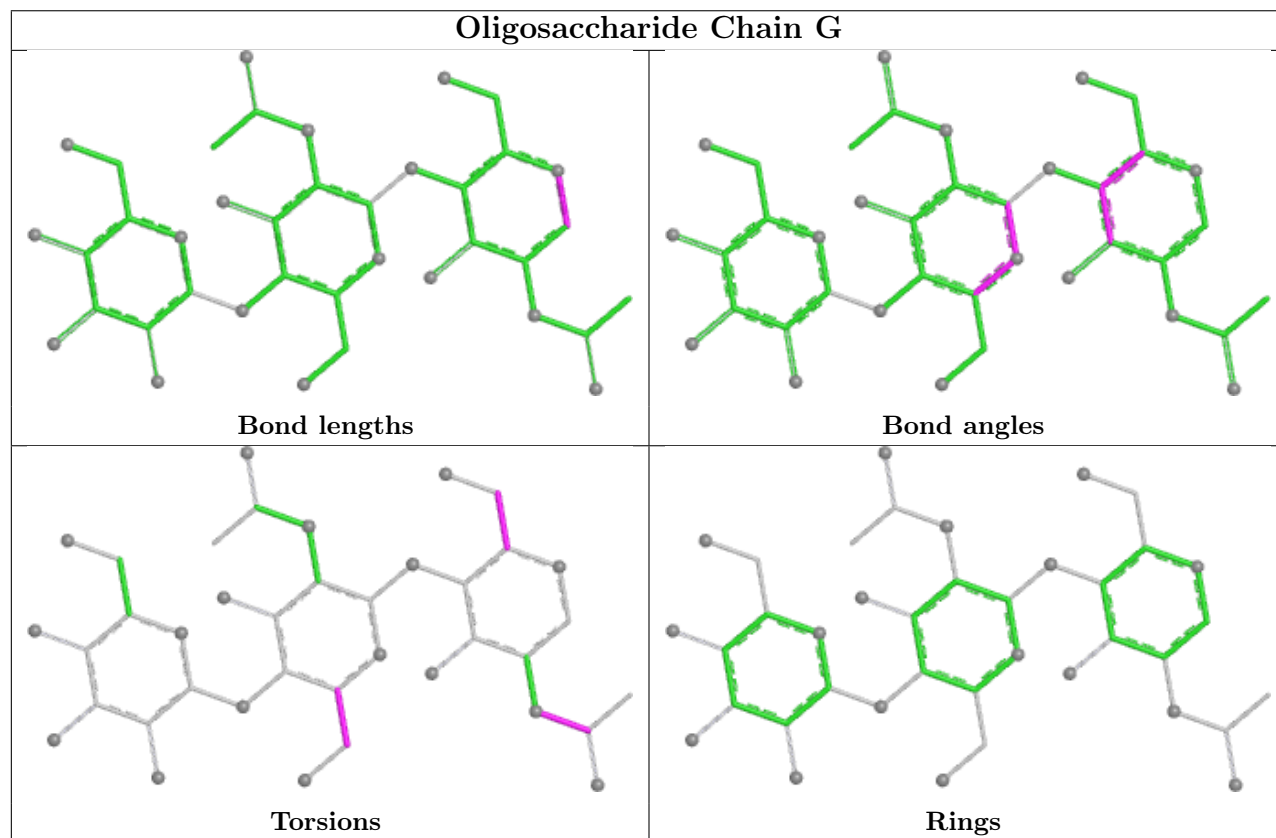
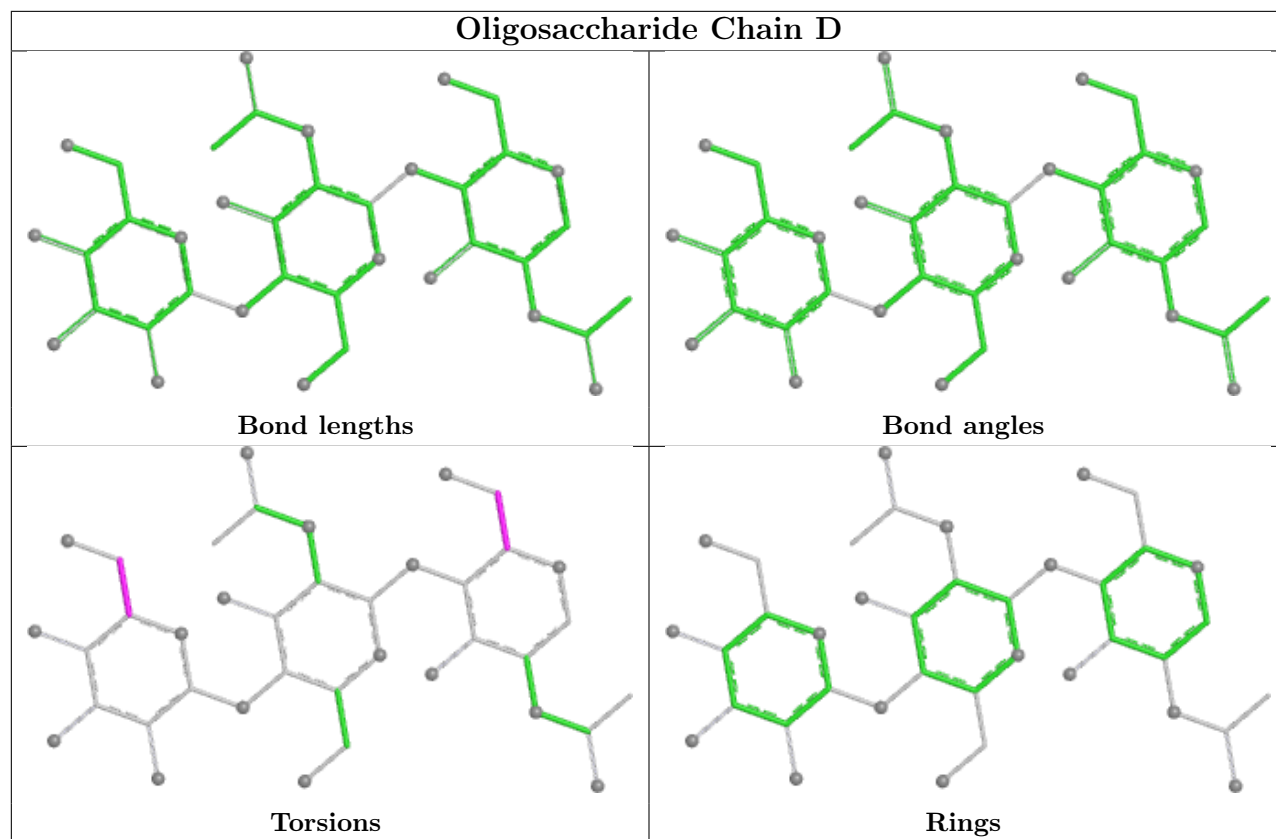
No monomer is involved in short contacts.

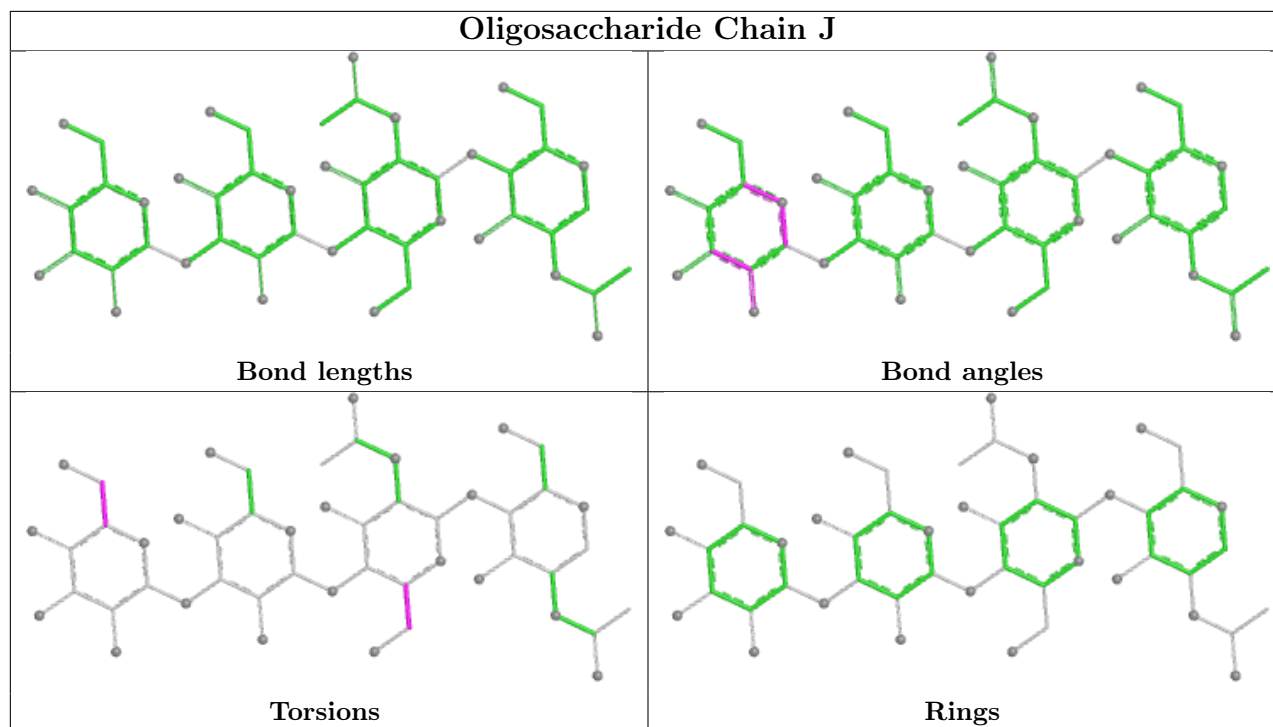
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	706	1	14,14,15	0.24	0	17,19,21	0.47	0
8	NAG	A	703	1	14,14,15	0.25	0	17,19,21	0.45	0
10	EDO	B	703	-	3,3,3	0.43	0	2,2,2	0.38	0
10	EDO	B	707	-	3,3,3	0.43	0	2,2,2	0.38	0
8	NAG	B	705	1	14,14,15	0.25	0	17,19,21	0.49	0
8	NAG	A	705	1	14,14,15	0.20	0	17,19,21	0.47	0
8	NAG	B	706	1	14,14,15	0.25	0	17,19,21	0.45	0
8	NAG	E	601	2	14,14,15	0.28	0	17,19,21	0.42	0
8	NAG	F	601	2	14,14,15	0.23	0	17,19,21	0.46	0
8	NAG	A	704	1	14,14,15	0.23	0	17,19,21	0.43	0
10	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.39	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	706	1	-	0/6/23/26	0/1/1/1
8	NAG	A	703	1	-	1/6/23/26	0/1/1/1
10	EDO	B	703	-	-	0/1/1/1	-
10	EDO	B	707	-	-	0/1/1/1	-
8	NAG	B	705	1	-	0/6/23/26	0/1/1/1
8	NAG	A	705	1	-	2/6/23/26	0/1/1/1
8	NAG	B	706	1	-	1/6/23/26	0/1/1/1
8	NAG	E	601	2	-	1/6/23/26	0/1/1/1
8	NAG	F	601	2	-	2/6/23/26	0/1/1/1
8	NAG	A	704	1	-	2/6/23/26	0/1/1/1
10	EDO	B	704	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 95th 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 ²)	Q<0.9
1	A	596/597 (99%)	0.28	17 (2%) 53 53	40, 72, 122, 164	0
1	B	596/597 (99%)	0.21	9 (1%) 72 71	33, 70, 122, 192	0
2	E	188/217 (86%)	0.26	6 (3%) 50 50	42, 68, 132, 177	1 (0%)
2	F	188/217 (86%)	0.55	12 (6%) 25 24	54, 88, 145, 167	0
All	All	1568/1628 (96%)	0.28	44 (2%) 55 54	33, 72, 127, 192	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	614	ALA	5.2
2	F	456	PHE	4.4
1	A	424	LEU	4.0
2	F	368	LEU	3.5
2	E	365	TYR	3.3
2	F	526	GLY	3.3
1	A	85	LEU	3.3
2	F	387	LEU	3.1
1	A	333	LEU	3.0
1	A	362	THR	2.9
1	A	289	PRO	2.8
2	F	373	PHE	2.8
1	A	369	PHE	2.7
2	E	526	GLY	2.7
1	B	339	VAL	2.7
2	E	387	LEU	2.7
1	A	293	VAL	2.6
2	E	373	PHE	2.5
2	F	385	THR	2.5
1	B	614	ALA	2.5
2	F	338	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	138	PRO	2.5
1	A	360	MET	2.5
1	A	105	SER	2.4
2	F	384	ALA	2.4
1	B	27	THR	2.3
1	A	339	VAL	2.3
1	A	423	LEU	2.3
2	F	363	ALA	2.3
2	F	391	CYS	2.2
1	A	302	TRP	2.2
2	F	495	TYR	2.2
2	E	368	LEU	2.2
1	A	226	VAL	2.2
1	A	336	PRO	2.2
2	F	383	SER	2.2
1	B	108	LEU	2.1
1	A	426	PRO	2.1
2	E	483	VAL	2.1
1	B	136	ASP	2.1
1	B	468	ILE	2.1
1	A	428	PHE	2.1
1	B	97	LEU	2.0
1	B	73	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, 95th 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.

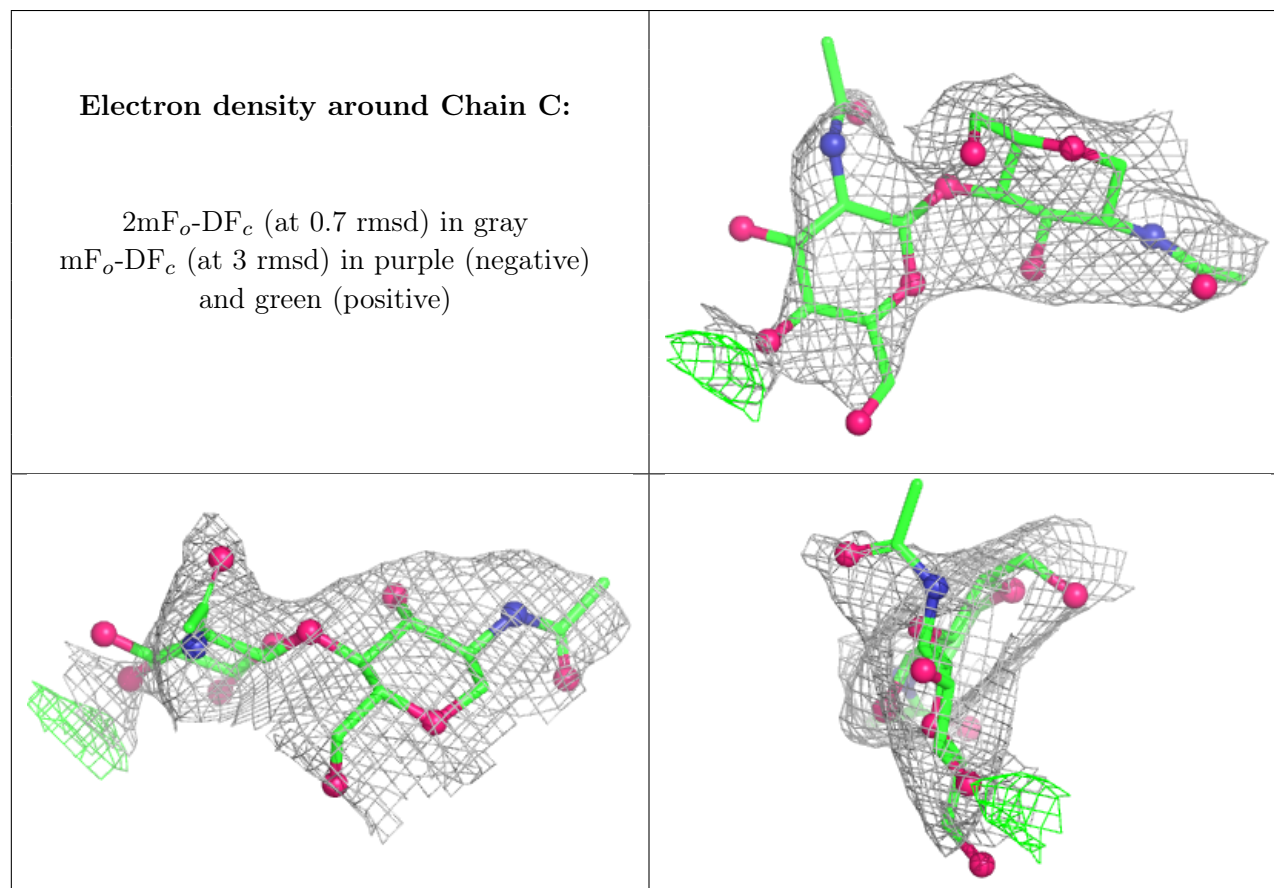
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	80,92,102,117	0
3	NAG	C	2	14/15	-	-	100,116,124,134	0
4	BMA	G	3	11/12	0.49	0.15	125,142,161,161	0
5	NAG	J	2	14/15	0.57	0.12	53,66,86,94	0
3	NAG	K	1	14/15	-	-	59,100,121,123	0

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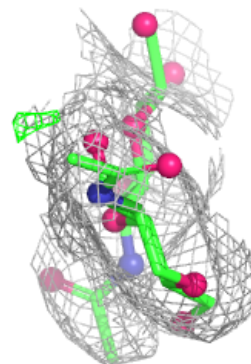
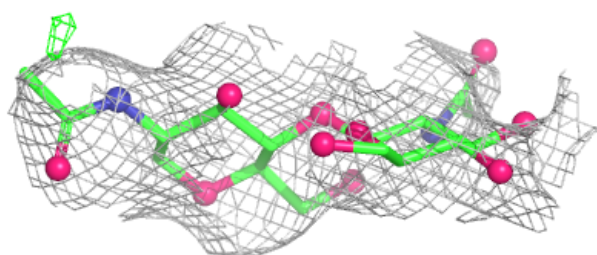
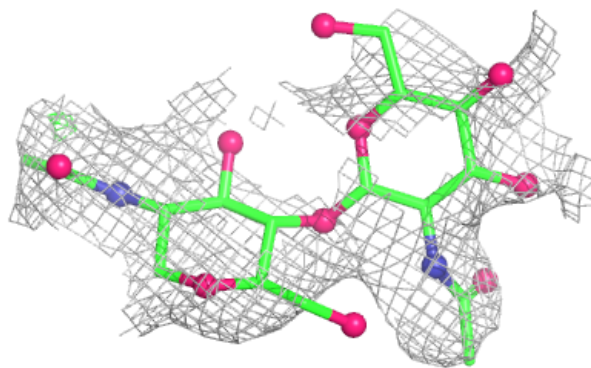
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	K	2	14/15	-	-	95,131,141,143	0
4	NAG	D	1	14/15	-	-	72,82,96,98	0
4	NAG	D	2	14/15	-	-	95,122,146,149	0
4	BMA	D	3	11/12	-	-	102,128,136,137	0
4	NAG	G	1	14/15	0.76	0.17	111,121,151,155	0
4	NAG	G	2	14/15	0.80	0.12	106,122,136,138	0
5	NAG	J	1	14/15	0.82	0.09	42,54,77,80	0
3	NAG	I	2	14/15	0.89	0.09	84,129,143,145	0
3	NAG	I	1	14/15	0.92	0.08	92,103,127,133	0
5	BMA	J	3	11/12	-	-	83,101,104,111	0
5	MAN	J	4	11/12	-	-	91,104,116,130	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.

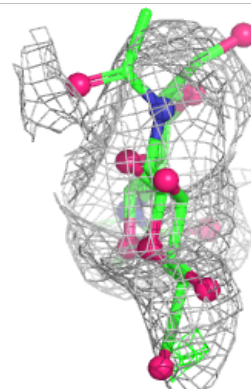
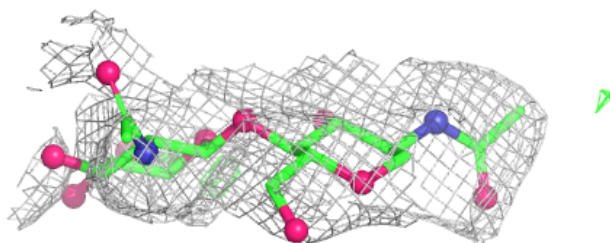
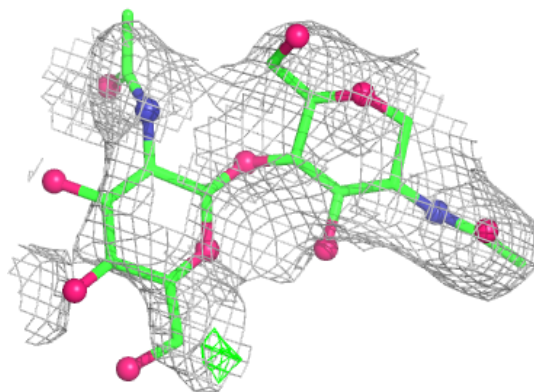


Electron density around Chain I:

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

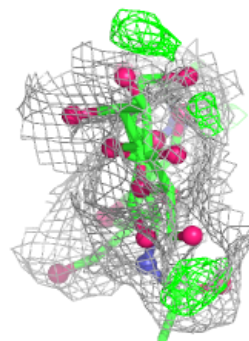
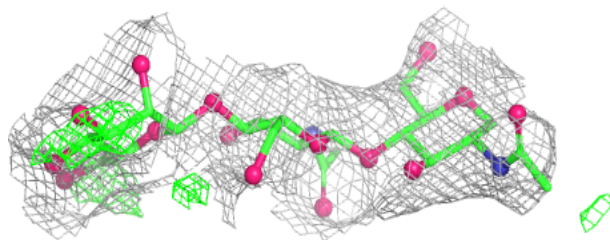
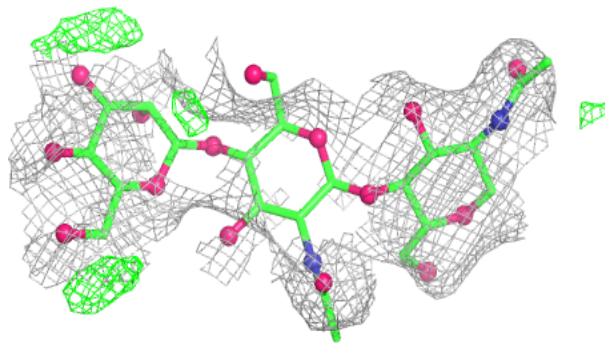
**Electron density around Chain K:**

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

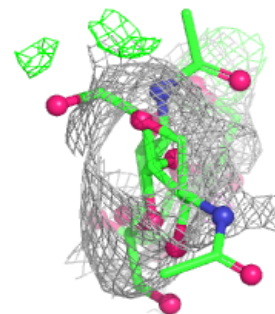
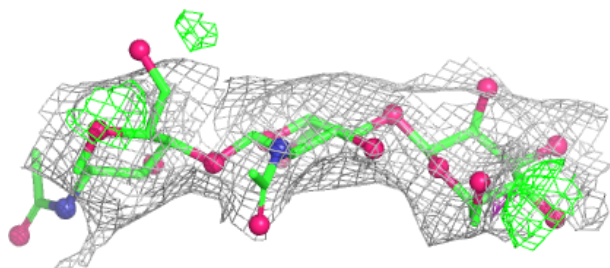
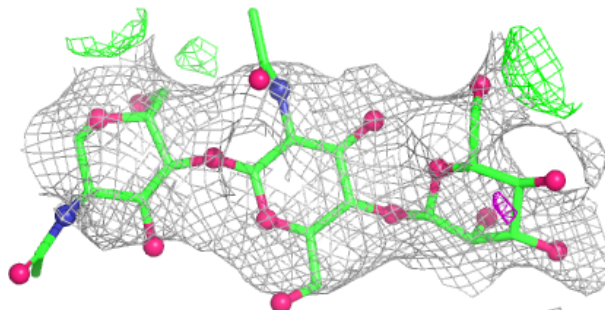


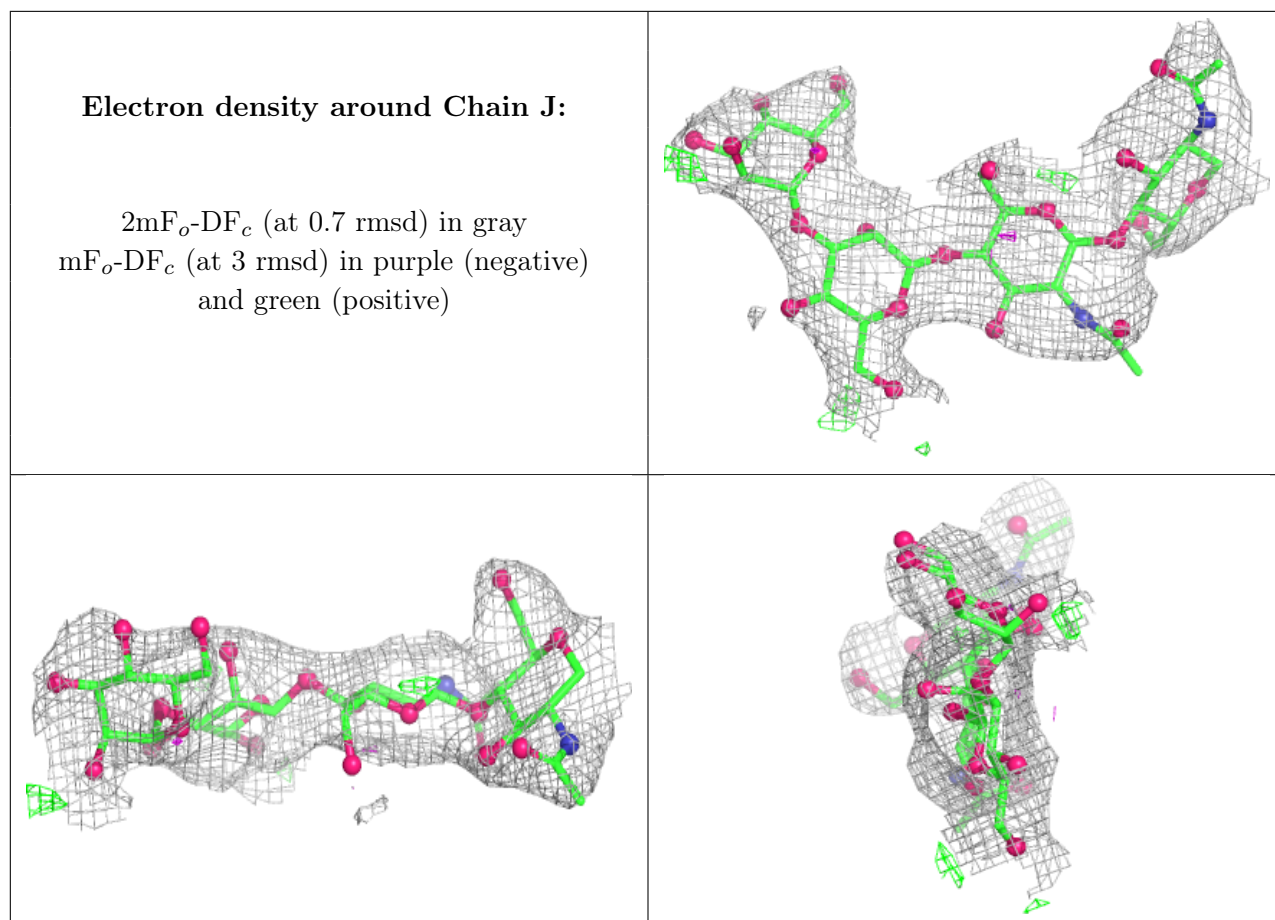
Electron density around Chain D:

$2mF_o-DF_c$ (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, 95th 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 ²)	Q<0.9
8	NAG	A	704	14/15	0.60	0.13	88,132,150,151	0
8	NAG	B	706	14/15	0.63	0.12	72,110,119,119	0
8	NAG	A	703	14/15	0.66	0.13	72,113,120,125	0
8	NAG	A	706	14/15	0.76	0.10	78,105,122,132	0
8	NAG	B	705	14/15	0.77	0.10	53,102,123,123	0
8	NAG	A	705	14/15	0.77	0.14	83,95,117,122	0
9	NA	A	707	1/1	0.78	0.17	70,70,70,70	0
8	NAG	F	601	14/15	0.80	0.12	92,107,131,136	0
8	NAG	E	601	14/15	0.81	0.10	82,106,126,132	0
7	CL	B	702	1/1	0.87	0.10	72,72,72,72	0
10	EDO	B	704	4/4	0.87	0.10	52,66,74,74	0
10	EDO	B	707	4/4	0.89	0.09	54,57,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	B	703	4/4	0.93	0.10	56,57,59,73	0
7	CL	A	702	1/1	0.94	0.08	70,70,70,70	0
6	ZN	B	701	1/1	0.96	0.04	65,65,65,65	0
6	ZN	A	701	1/1	0.98	0.05	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.