



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:44 AM UTC

PDB ID : 7U0N / pdb_00007u0n
Title : Crystal structure of chimeric omicron RBD (strain BA.1) complexed with human ACE2
Authors : Geng, Q.; Shi, K.; Ye, G.; Zhang, W.; Aihara, H.; Li, F.
Deposited on : 2022-02-18
Resolution : 2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

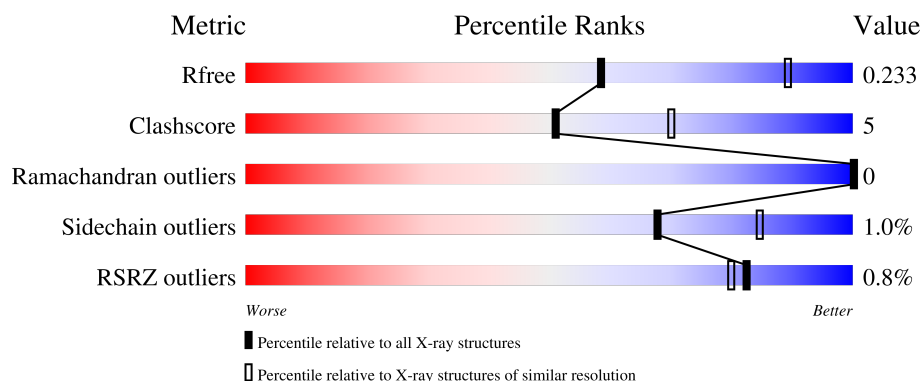
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

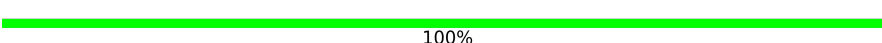
The reported resolution of this entry is 2.61 Å.

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



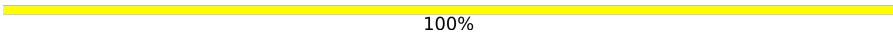
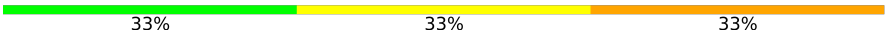
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 87% 12%
1	B	597	 83% 17%
2	E	217	 2% 75% 12% 13%
2	F	217	 2% 77% 10% 12%
3	C	3	 100%

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Mol	Chain	Length	Quality of chain
3	D	3	 67% 33%
3	G	3	 100%
3	I	3	 33% 33% 33%
3	J	3	 100%
4	K	2	 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
5	NAG	A	701	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13116 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.

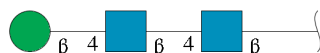
- Molecule 1 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	B	596	Total	C	N	O	S	0	1	0
			4871	3116	806	920	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	188	Total	C	N	O	S	0	0	0
			1500	966	247	278	9			
2	F	190	Total	C	N	O	S	0	0	0
			1515	975	250	281	9			

- 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.



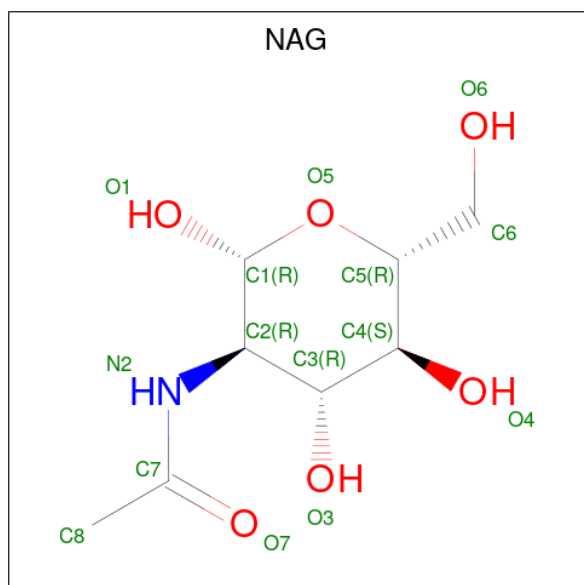
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 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
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

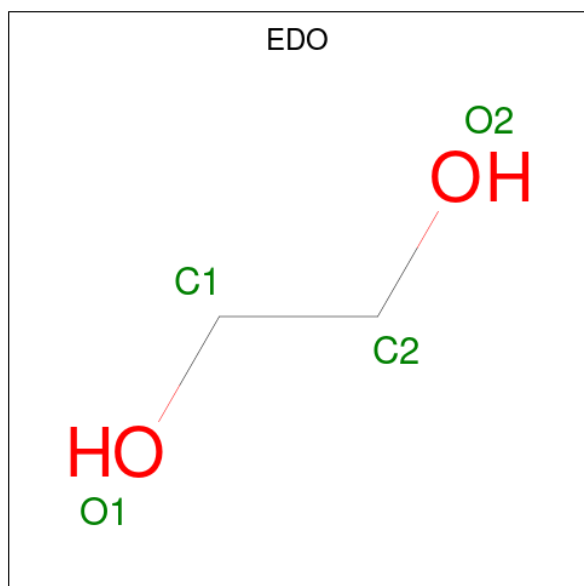
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	2	Total	Cl	0	0
			2	2		
7	B	2	Total	Cl	0	0
			2	2		
7	F	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

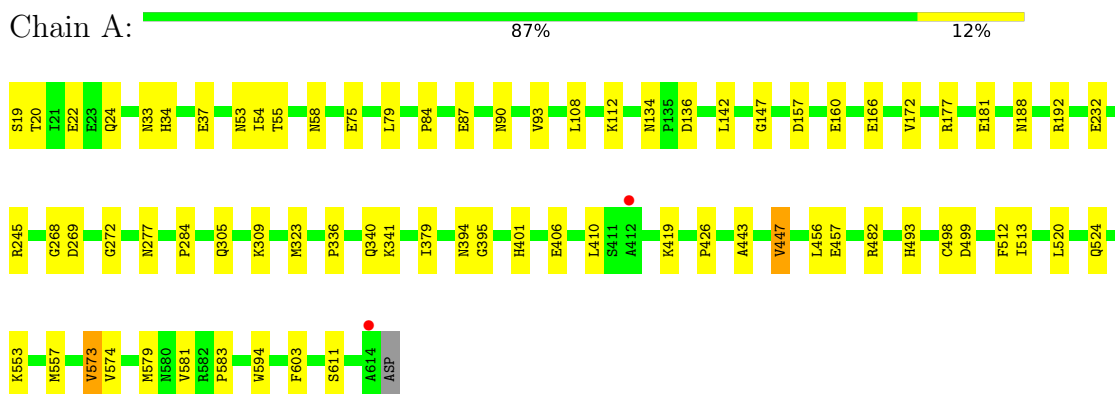
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	O	0	0
			4	4		
10	B	6	Total	O	0	0
			6	6		
10	E	2	Total	O	0	0
			2	2		
10	F	1	Total	O	0	0
			1	1		

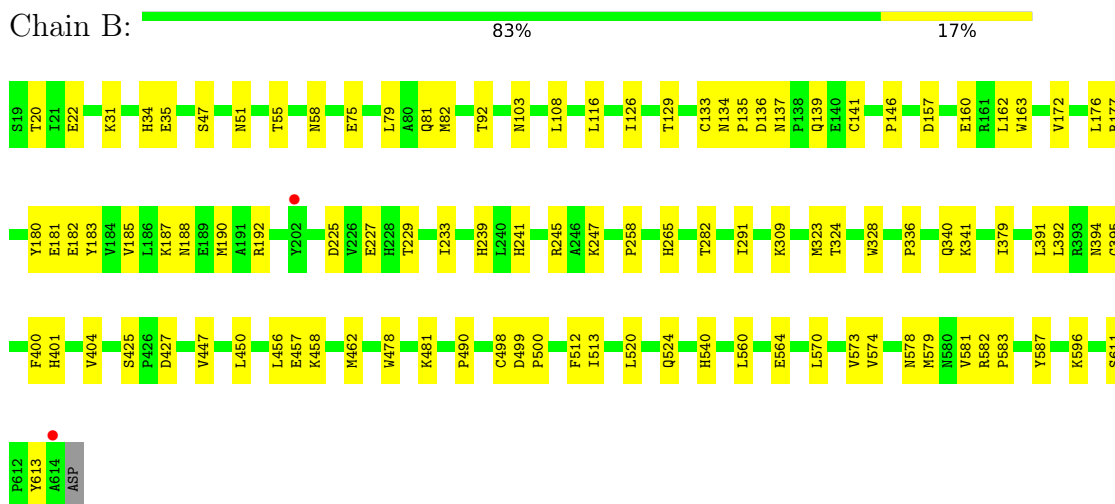
3 Residue-property plots

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.

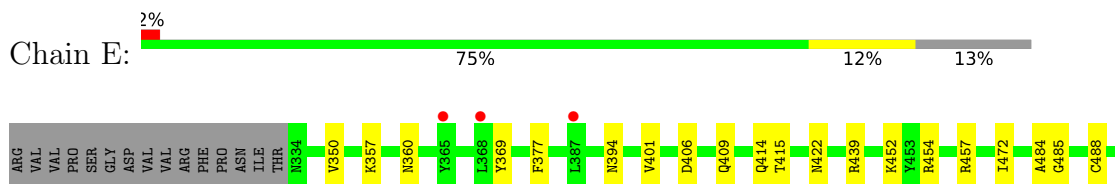
• Molecule 1: Angiotensin-converting enzyme 2

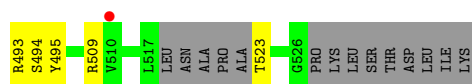


• Molecule 1: Angiotensin-converting enzyme 2

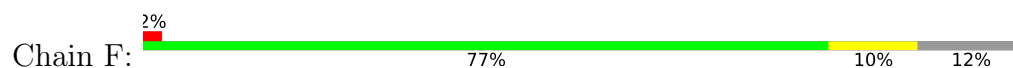


• Molecule 2: Spike protein S1





- Molecule 2: Spike protein S1



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



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



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



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



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





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

Chain K:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.13Å 120.18Å 113.33Å 90.00° 92.44° 90.00°	Depositor
Resolution (Å)	30.11 – 2.61 30.11 – 2.61	Depositor EDS
% Data completeness (in resolution range)	54.9 (30.11-2.61) 55.2 (30.11-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.188 , 0.235 0.188 , 0.233	Depositor DCC
R_{free} test set	1734 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	89.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13116	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: EDO, CL, BMA, MG, NAG, ZN

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	0.09	0/4999	0.27	0/6792
1	B	0.09	0/5008	0.29	0/6804
2	E	0.10	0/1542	0.38	0/2094
2	F	0.10	0/1558	0.40	0/2116
All	All	0.09	0/13107	0.31	0/17806

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	4633	43	0
1	B	4871	0	4638	58	0
2	E	1500	0	1424	15	0
2	F	1515	0	1442	16	0
3	C	39	0	34	0	0
3	D	39	0	34	1	0
3	G	39	0	34	1	0
3	I	39	0	34	1	0
3	J	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	28	0	25	0	0
5	A	56	0	52	8	0
5	B	28	0	26	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	F	1	0	0	1	0
8	B	12	0	18	1	0
9	B	1	0	0	0	0
10	A	4	0	0	0	0
10	B	6	0	0	0	0
10	E	2	0	0	0	0
10	F	1	0	0	2	0
All	All	13116	0	12454	133	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 5.

All (133) 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:53:ASN:ND2	5:A:701:NAG:C1	1.72	1.49
5:A:701:NAG:O3	5:A:701:NAG:H82	1.24	1.31
5:A:701:NAG:O3	5:A:701:NAG:C8	2.03	1.05
1:A:53:ASN:ND2	5:A:701:NAG:C2	2.21	1.04
1:A:53:ASN:CG	5:A:701:NAG:C1	2.54	0.78
1:A:53:ASN:ND2	5:A:701:NAG:H2	1.99	0.77
2:E:485:GLY:H	2:E:488:CYS:HB2	1.50	0.77
2:F:385:THR:O	2:F:388:ASN:ND2	2.24	0.71
2:E:369:TYR:HA	2:E:377:PHE:HE2	1.56	0.70
1:B:177:ARG:HD3	1:B:498:CYS:HB2	1.73	0.70
1:B:177:ARG:NH1	1:B:181:GLU:OE2	2.26	0.67
1:A:245:ARG:NH2	1:A:603:PHE:O	2.28	0.66
2:F:493:ARG:NH1	10:F:701:HOH:O	2.31	0.64
1:B:146:PRO:HD2	8:B:707:EDO:H12	1.79	0.63
1:A:55:THR:OG1	1:A:58:ASN:ND2	2.26	0.63
2:F:364:ASP:HA	2:F:527:PRO:HD3	1.81	0.62
1:A:177:ARG:HD3	1:A:498:CYS:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.83	0.61
1:B:126:ILE:HD11	1:B:176:LEU:HG	1.81	0.61
1:B:55:THR:OG1	1:B:58:ASN:ND2	2.31	0.60
1:B:75:GLU:O	1:B:79:LEU:HD13	2.02	0.59
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.85	0.58
1:A:90:ASN:HB3	1:A:93:VAL:HG22	1.85	0.58
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.85	0.57
2:E:415:THR:HG21	3:D:3:BMA:H4	1.87	0.56
1:B:126:ILE:HA	1:B:129:THR:HG22	1.87	0.56
1:A:166:GLU:OE1	1:A:493:HIS:NE2	2.31	0.55
2:F:401:VAL:HG22	2:F:509:ARG:HG2	1.87	0.55
1:A:336:PRO:HB2	1:A:340:GLN:HB3	1.89	0.54
1:B:324:THR:HB	7:F:602:CL:CL	2.45	0.54
1:B:245:ARG:NH1	1:B:258:PRO:O	2.40	0.53
1:A:34:HIS:CE1	2:E:493:ARG:HB3	2.44	0.53
1:A:142:LEU:HB3	1:A:147:GLY:HA3	1.91	0.52
2:E:452:LYS:HA	2:E:494:SER:HA	1.90	0.52
1:B:135:PRO:HD3	1:B:163:TRP:HE1	1.74	0.52
1:B:34:HIS:CE1	2:F:493:ARG:HB3	2.44	0.52
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.91	0.52
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.92	0.51
1:A:53:ASN:ND2	5:A:701:NAG:O5	2.38	0.51
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.91	0.51
1:B:134:ASN:HD21	1:B:136:ASP:HB2	1.75	0.51
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.93	0.51
2:F:367:VAL:C	2:F:369:TYR:H	2.19	0.51
1:A:406:GLU:O	1:A:410:LEU:HD13	2.11	0.50
1:A:419:LYS:HE3	1:A:426:PRO:HA	1.94	0.50
1:B:425:SER:OG	1:B:427:ASP:OD1	2.24	0.50
1:A:75:GLU:O	1:A:79:LEU:HD13	2.12	0.50
1:A:134:ASN:HD21	1:A:136:ASP:HB2	1.76	0.49
1:A:323:MET:HE1	1:A:379:ILE:HG21	1.94	0.49
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.93	0.49
2:F:393:SER:O	2:F:523:THR:OG1	2.26	0.49
1:A:53:ASN:HD22	5:A:701:NAG:H2	1.75	0.49
1:B:239:HIS:CE1	1:B:596:LYS:HG2	2.48	0.49
1:B:336:PRO:HB2	1:B:340:GLN:HB3	1.95	0.48
2:E:350:VAL:HG22	2:E:422:ASN:HB3	1.95	0.48
1:A:54:ILE:HD12	1:A:341:LYS:HG2	1.94	0.48
1:B:108:LEU:HD11	1:B:190:MET:HB2	1.96	0.48
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.95	0.47
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.95	0.47
1:B:400:PHE:HZ	1:B:570:LEU:HB2	1.79	0.47
2:E:409:GLN:HA	2:E:414:GLN:HG3	1.95	0.47
1:B:81:GLN:NE2	1:B:103:ASN:OD1	2.33	0.47
1:A:336:PRO:HG2	1:A:340:GLN:O	2.14	0.47
2:E:454:ARG:HD3	2:E:457:ARG:HB2	1.97	0.47
1:A:268:GLY:O	1:A:277:ASN:ND2	2.34	0.46
2:E:357:LYS:HE3	2:E:394:ASN:HD22	1.79	0.46
1:A:177:ARG:NH1	1:A:181:GLU:OE2	2.48	0.46
1:B:20:THR:HG22	1:B:22:GLU:H	1.80	0.46
1:B:225:ASP:O	1:B:229:THR:HG22	2.15	0.46
1:B:229:THR:OG1	1:B:581:VAL:HB	2.15	0.46
1:B:31:LYS:HD2	2:F:493:ARG:HH12	1.81	0.46
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.97	0.46
1:B:79:LEU:HA	1:B:82:MET:HE2	1.98	0.45
1:B:188:ASN:HB3	1:B:192:ARG:HE	1.81	0.45
3:I:1:NAG:HO6	3:I:2:NAG:HN2	1.59	0.45
1:A:443:ALA:HA	1:A:447:VAL:HG13	1.97	0.45
1:B:134:ASN:ND2	1:B:136:ASP:HB2	2.31	0.45
1:B:478:TRP:HA	1:B:481:LYS:HB2	1.99	0.45
1:A:482:ARG:HH21	1:A:611:SER:HB3	1.81	0.45
1:B:227:GLU:OE2	1:B:458:LYS:HE2	2.17	0.45
1:B:116:LEU:HD11	1:B:187:LYS:HE2	1.98	0.45
1:B:582:ARG:HB3	1:B:583:PRO:HD3	1.98	0.45
2:E:493:ARG:HD3	2:E:493:ARG:HA	1.82	0.45
2:F:452:LYS:HG2	2:F:494:SER:HB3	1.99	0.44
1:B:611:SER:C	1:B:613:TYR:H	2.26	0.44
1:B:247:LYS:HB2	1:B:282:THR:HG22	2.00	0.44
1:A:394:ASN:OD1	1:A:395:GLY:N	2.51	0.44
1:A:20:THR:HG22	1:A:22:GLU:H	1.82	0.43
1:B:578:ASN:OD1	1:B:579:MET:N	2.50	0.43
2:F:490:PHE:CE2	2:F:492:LEU:HB2	2.54	0.43
1:A:269:ASP:OD1	1:A:272:GLY:N	2.51	0.43
1:B:241:HIS:CE1	1:B:245:ARG:HH21	2.37	0.43
1:B:133:CYS:HA	1:B:141:CYS:HA	2.01	0.43
1:B:92:THR:HG23	1:B:392:LEU:HD21	2.01	0.43
1:B:180:TYR:HA	1:B:183:TYR:HB3	2.00	0.42
1:A:493:HIS:ND1	1:A:499:ASP:OD2	2.51	0.42
1:B:265:HIS:CE1	1:B:490:PRO:HB3	2.54	0.42
1:A:108:LEU:HD23	1:A:112:LYS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:HB3	1:A:192:ARG:HE	1.84	0.42
2:F:440:ASN:OD1	2:F:440:ASN:N	2.50	0.42
1:B:35:GLU:HB2	10:F:701:HOH:O	2.19	0.42
1:B:394:ASN:OD1	1:B:395:GLY:N	2.51	0.42
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.55	0.42
1:A:305:GLN:O	1:A:309:LYS:HB2	2.19	0.42
1:B:309:LYS:HD2	1:B:328:TRP:CH2	2.55	0.42
1:A:553:LYS:HE2	1:A:573:VAL:O	2.20	0.42
2:F:365:TYR:HD2	2:F:388:ASN:HA	1.84	0.42
1:A:284:PRO:HB3	1:A:594:TRP:CH2	2.55	0.41
2:E:472:ILE:HD12	2:E:484:ALA:HB2	2.02	0.41
2:F:367:VAL:O	2:F:368:LEU:HB2	2.19	0.41
3:G:1:NAG:O6	3:G:2:NAG:N2	2.44	0.41
1:B:560:LEU:HD13	1:B:564:GLU:HG3	2.01	0.41
1:A:33:ASN:O	1:A:37:GLU:HB2	2.20	0.41
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.55	0.41
1:B:47:SER:O	1:B:51:ASN:ND2	2.40	0.41
1:B:291:ILE:H	1:B:291:ILE:HG13	1.68	0.41
1:A:84:PRO:HG2	1:A:87:GLU:HB2	2.02	0.41
1:B:391:LEU:H	1:B:391:LEU:HD12	1.86	0.41
2:E:360:ASN:HA	2:E:523:THR:HB	2.03	0.41
2:F:496:SER:O	2:F:498:ARG:HG3	2.21	0.41
1:B:182:GLU:HA	1:B:185:VAL:HG12	2.03	0.41
2:F:379:CYS:HA	2:F:432:CYS:HA	2.03	0.41
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.56	0.40
2:E:369:TYR:HA	2:E:377:PHE:CE2	2.46	0.40
1:B:137:ASN:OD1	1:B:139:GLN:HG2	2.21	0.40
1:B:229:THR:OG1	1:B:520:LEU:HD21	2.21	0.40
1:B:499:ASP:N	1:B:500:PRO:HD2	2.36	0.40
2:E:406:ASP:OD2	2:E:495:TYR:OH	2.32	0.40
2:F:452:LYS:HG2	2:F:494:SER:HA	2.03	0.40
1:A:19:SER:HB2	1:A:24:GLN:HE21	1.86	0.40
1:B:400:PHE:O	1:B:404:VAL:HG23	2.22	0.40
1:B:458:LYS:NZ	1:B:462:MET:HE3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	595/597 (100%)	575 (97%)	20 (3%)	0	100	100
2	E	184/217 (85%)	172 (94%)	12 (6%)	0	100	100
2	F	186/217 (86%)	170 (91%)	16 (9%)	0	100	100
All	All	1559/1628 (96%)	1491 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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%)	520 (99%)	6 (1%)	65	83
1	B	527/527 (100%)	520 (99%)	7 (1%)	61	81
2	E	164/190 (86%)	163 (99%)	1 (1%)	78	90
2	F	166/190 (87%)	166 (100%)	0	100	100
All	All	1383/1434 (96%)	1369 (99%)	14 (1%)	68	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	VAL
1	A	401	HIS

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Mol	Chain	Res	Type
1	A	447	VAL
1	A	557	MET
1	A	573	VAL
1	A	574	VAL
1	B	162	LEU
1	B	172	VAL
1	B	341	LYS
1	B	401	HIS
1	B	447	VAL
1	B	573	VAL
1	B	574	VAL
2	E	439	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	34	HIS
1	A	64	ASN
1	A	239	HIS
1	A	340	GLN
1	A	345	HIS
1	A	599	ASN
1	B	24	GLN
1	B	34	HIS
1	B	58	ASN
1	B	96	GLN
1	B	175	GLN
1	B	194	ASN
1	B	340	GLN
1	B	345	HIS
1	B	522	GLN
1	B	535	HIS
2	E	394	ASN
2	F	388	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 ⓘ

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

5.5 Carbohydrates ⓘ

17 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	0.28	0	17,19,21	0.51	0
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	0.59	0
3	BMA	C	3	3	11,11,12	0.62	0	15,15,17	0.71	0
3	NAG	D	1	1,3	14,14,15	0.38	0	17,19,21	0.61	0
3	NAG	D	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	BMA	D	3	3	11,11,12	0.56	0	15,15,17	0.64	0
3	NAG	G	1	1,3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.46	0
3	BMA	G	3	3	11,11,12	0.73	0	15,15,17	1.10	1 (6%)
3	NAG	I	1	1,3	14,14,15	0.33	0	17,19,21	0.68	1 (5%)
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.45	0
3	BMA	I	3	3	11,11,12	0.65	0	15,15,17	0.76	0
3	NAG	J	1	1,3	14,14,15	0.35	0	17,19,21	0.53	0
3	NAG	J	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	BMA	J	3	3	11,11,12	0.58	0	15,15,17	0.68	0
4	NAG	K	1	1,4	14,14,15	0.43	0	17,19,21	0.67	1 (5%)
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.44	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	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-O5-C5	2.34	115.32	112.19
4	K	1	NAG	C1-O5-C5	2.21	115.15	112.19
3	I	1	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

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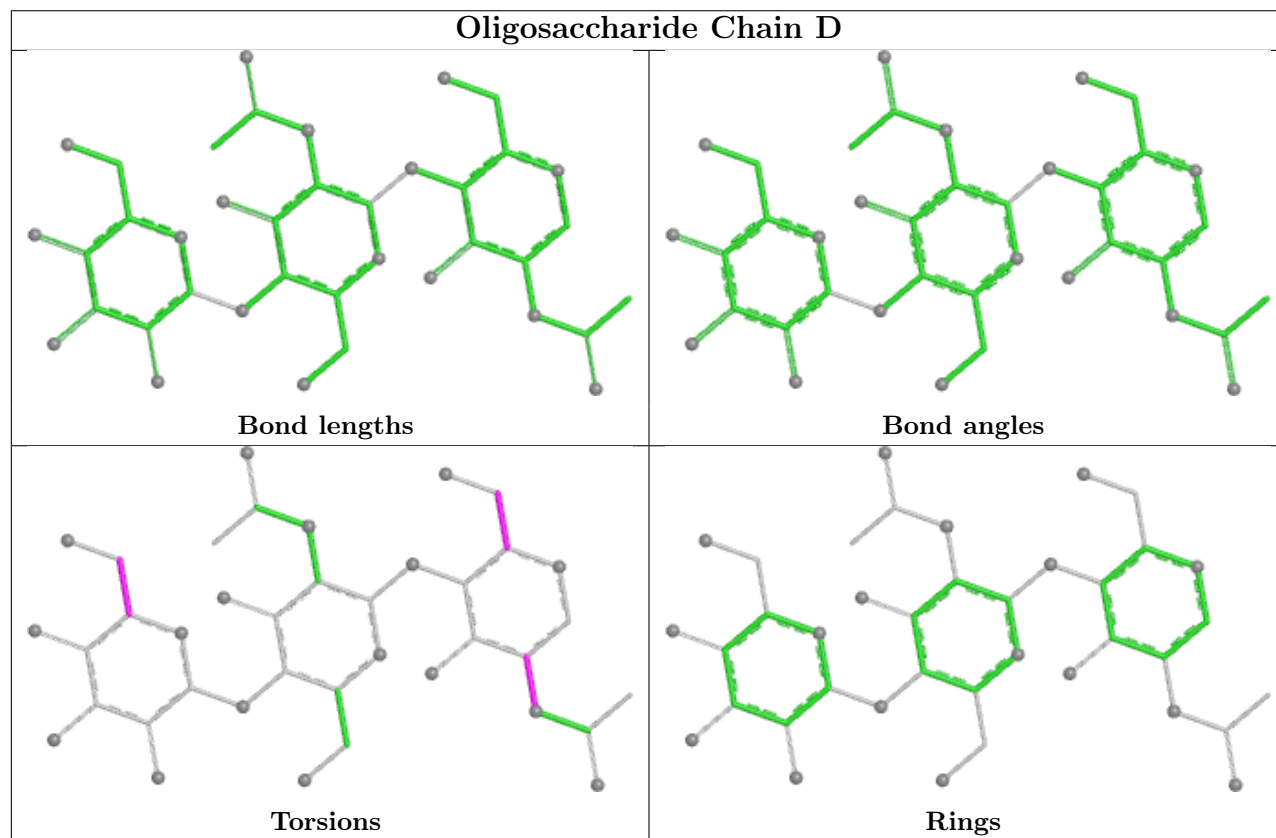
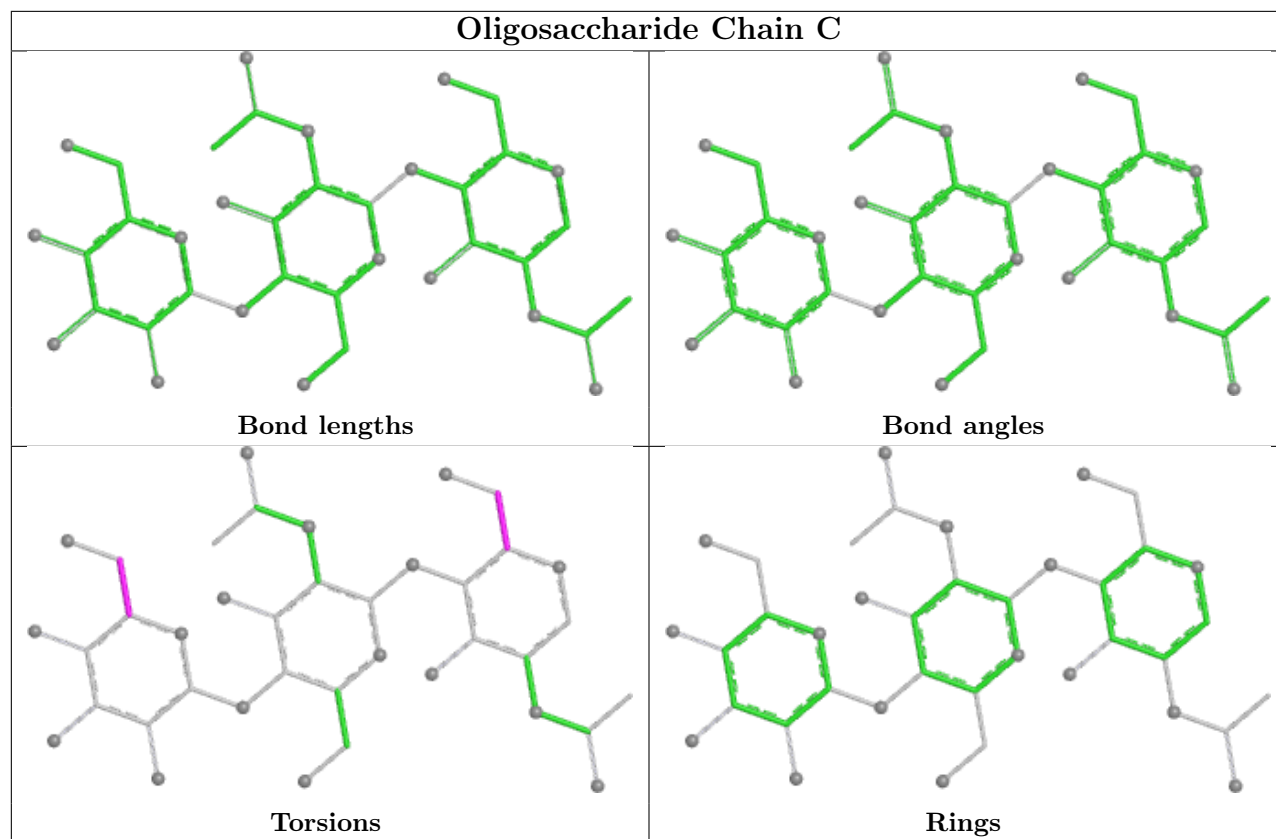
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6

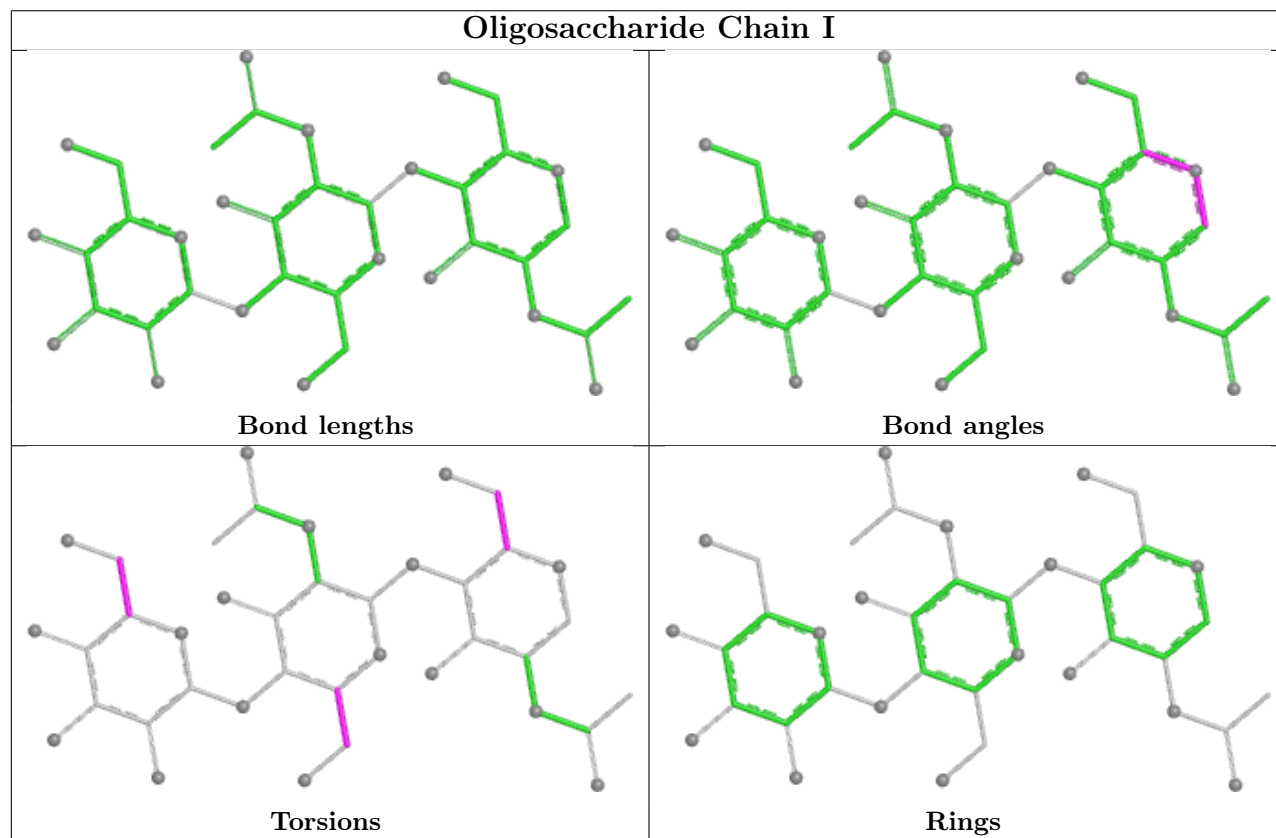
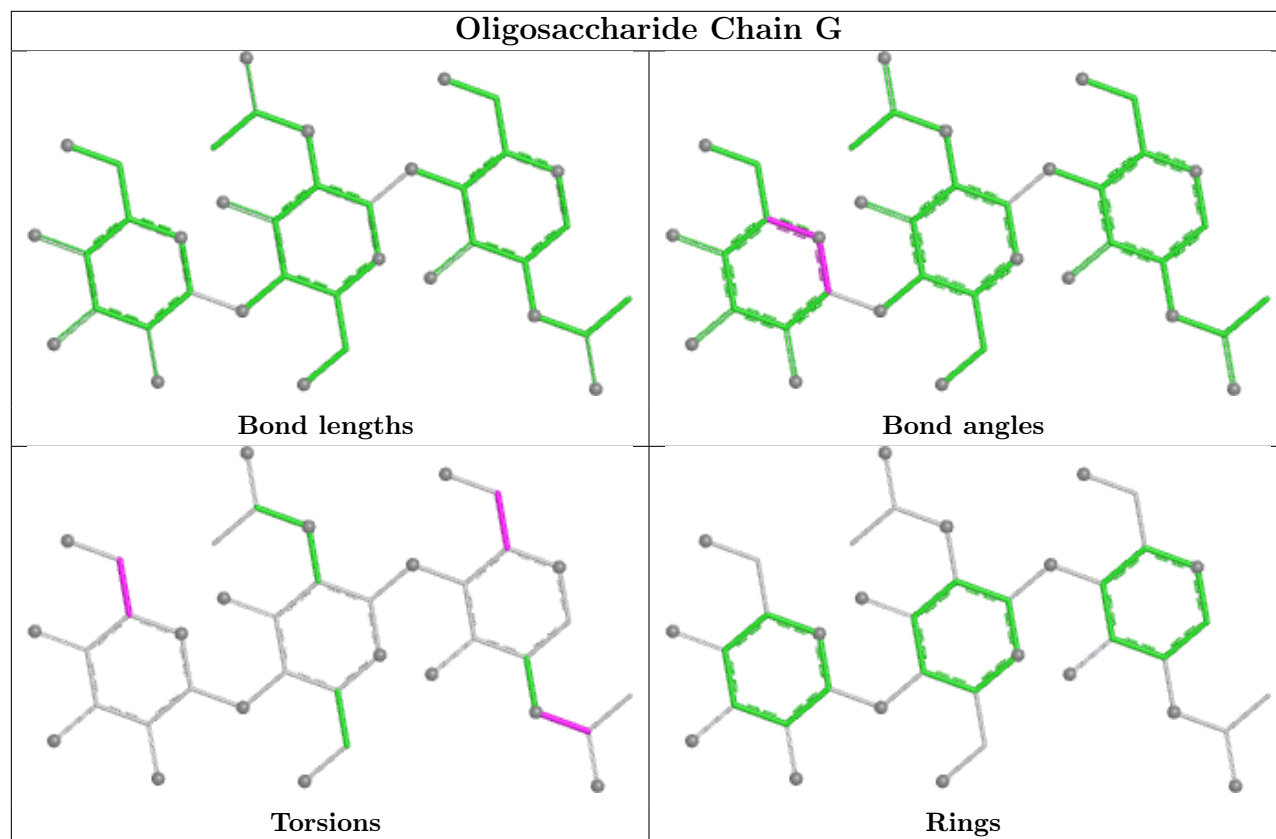
There are no ring outliers.

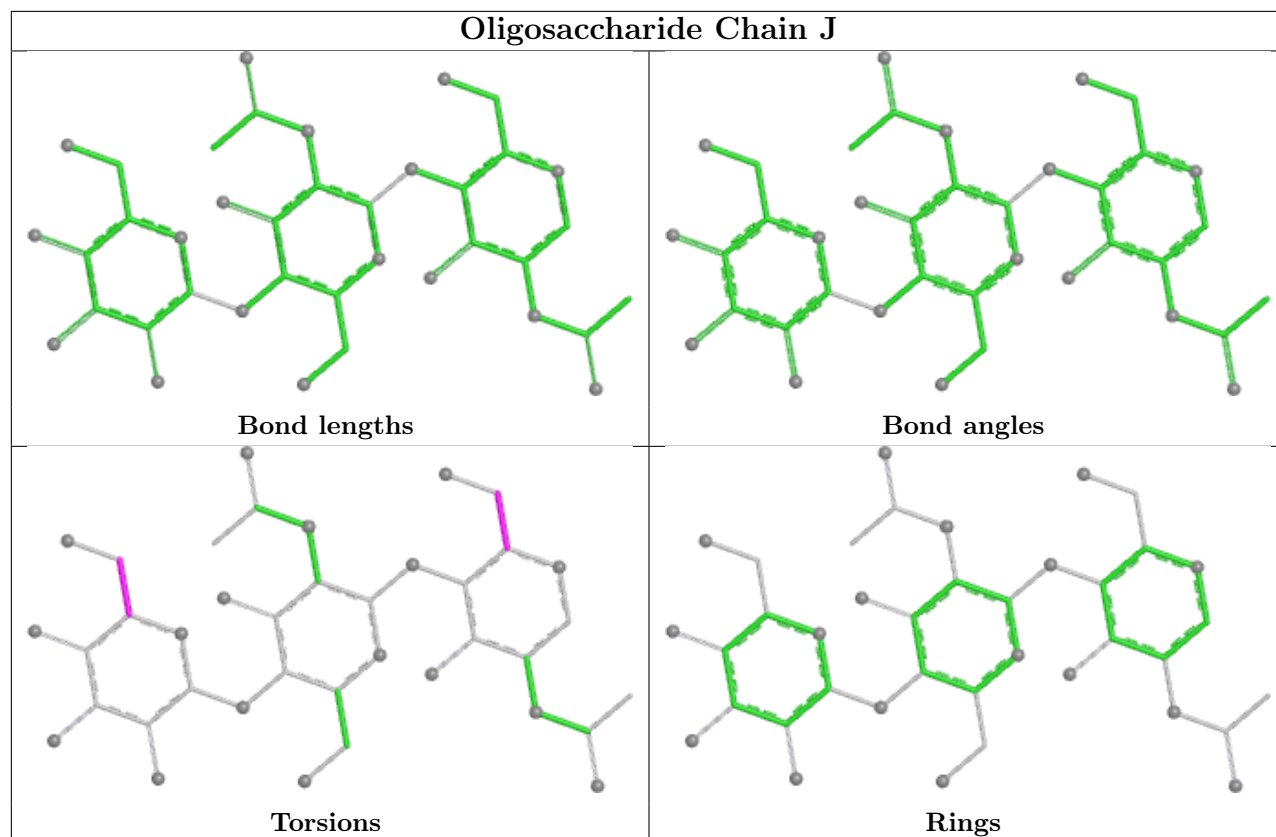
5 monomers are involved in 3 short contacts:

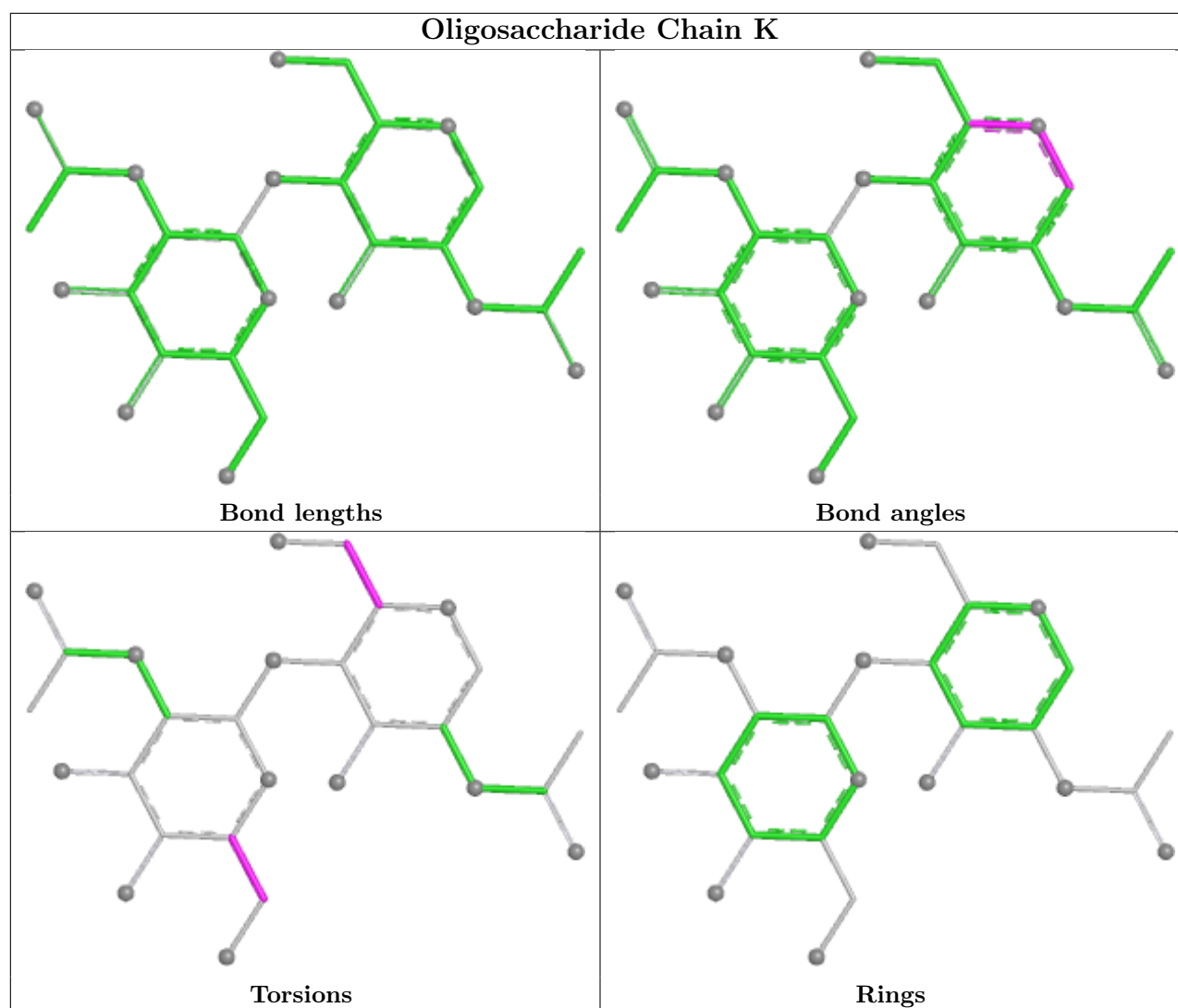
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	I	1	NAG	1	0
3	I	2	NAG	1	0
3	D	3	BMA	1	0
3	G	1	NAG	1	0

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 19 ligands modelled in this entry, 8 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	EDO	B	707	-	3,3,3	0.43	0	2,2,2	0.34	0
8	EDO	B	705	-	3,3,3	0.42	0	2,2,2	0.38	0
5	NAG	A	701	-	14,14,15	0.32	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	701	1	14,14,15	0.42	0	17,19,21	0.53	0
5	NAG	A	706	1	14,14,15	0.36	0	17,19,21	0.61	1 (5%)
8	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.35	0
5	NAG	A	705	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	B	706	1	14,14,15	0.44	0	17,19,21	0.62	1 (5%)
5	NAG	F	601	2	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	A	704	1	14,14,15	0.25	0	17,19,21	0.46	0
5	NAG	E	601	2	14,14,15	0.33	0	17,19,21	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	EDO	B	707	-	-	1/1/1/1	-
8	EDO	B	705	-	-	0/1/1/1	-
5	NAG	A	701	-	-	5/6/23/26	0/1/1/1
5	NAG	B	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
8	EDO	B	704	-	-	0/1/1/1	-
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	B	706	1	-	2/6/23/26	0/1/1/1
5	NAG	F	601	2	-	0/6/23/26	0/1/1/1
5	NAG	A	704	1	-	2/6/23/26	0/1/1/1
5	NAG	E	601	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	NAG	C1-O5-C5	2.07	114.96	112.19
5	B	706	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	704	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	701	NAG	O5-C5-C6-O6
5	A	704	NAG	O5-C5-C6-O6
5	A	705	NAG	O5-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	A	701	NAG	C8-C7-N2-C2
5	A	701	NAG	O7-C7-N2-C2
5	A	705	NAG	C4-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	B	701	NAG	C4-C5-C6-O6
5	A	701	NAG	C3-C2-N2-C7
5	B	701	NAG	O5-C5-C6-O6
5	B	706	NAG	O5-C5-C6-O6
5	B	706	NAG	C4-C5-C6-O6
8	B	707	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	707	EDO	1	0
5	A	701	NAG	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.25	2 (0%) 90 88	52, 87, 132, 179	0
1	B	596/597 (99%)	-0.30	2 (0%) 90 88	32, 82, 141, 217	1 (0%)
2	E	188/217 (86%)	-0.17	4 (2%) 63 59	58, 87, 165, 205	0
2	F	190/217 (87%)	0.05	5 (2%) 57 52	70, 112, 170, 202	0
All	All	1570/1628 (96%)	-0.22	13 (0%) 82 80	32, 88, 149, 217	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	456	PHE	4.9
1	B	202	TYR	3.6
1	A	614	ALA	3.5
2	F	495	TYR	3.3
2	F	368	LEU	3.1
2	E	365	TYR	2.5
2	E	368	LEU	2.4
2	E	510	VAL	2.4
2	F	395	VAL	2.4
2	E	387	LEU	2.3
2	F	350	VAL	2.2
1	B	614	ALA	2.1
1	A	412	ALA	2.1

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

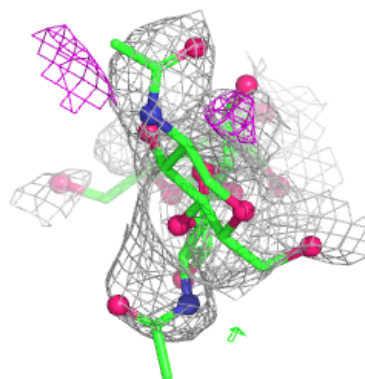
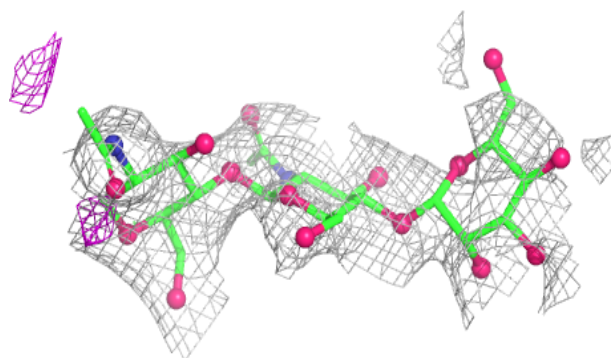
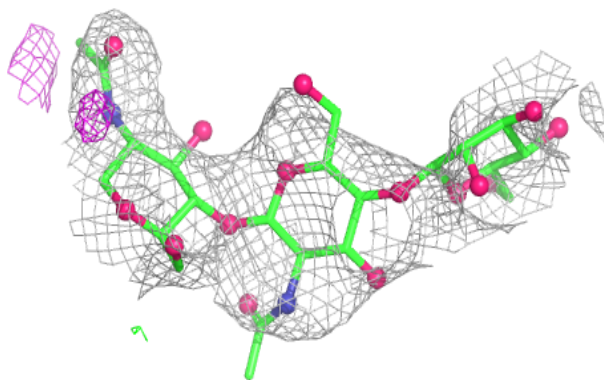
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	-	-	89,122,142,151	0
3	NAG	C	2	14/15	-	-	136,153,161,169	0
3	BMA	C	3	11/12	-	-	130,165,172,178	0
3	NAG	D	1	14/15	-	-	85,99,111,113	0
3	NAG	D	2	14/15	-	-	110,120,127,129	0
3	BMA	D	3	11/12	-	-	97,126,137,140	0
3	BMA	G	3	11/12	0.52	0.11	107,128,137,143	0
3	NAG	J	2	14/15	0.79	0.08	72,80,89,96	0
3	BMA	I	3	11/12	0.82	0.06	124,138,149,150	0
3	NAG	G	1	14/15	0.82	0.08	94,99,109,124	0
3	NAG	J	1	14/15	0.85	0.07	60,79,92,98	0
3	NAG	G	2	14/15	0.87	0.07	99,116,120,126	0
3	NAG	I	1	14/15	0.91	0.07	104,110,123,128	0
3	NAG	I	2	14/15	0.92	0.06	107,139,148,151	0
3	BMA	J	3	11/12	-	-	87,103,108,111	0
4	NAG	K	1	14/15	-	-	79,107,129,132	0
4	NAG	K	2	14/15	-	-	104,135,148,151	0

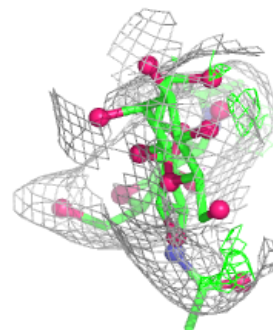
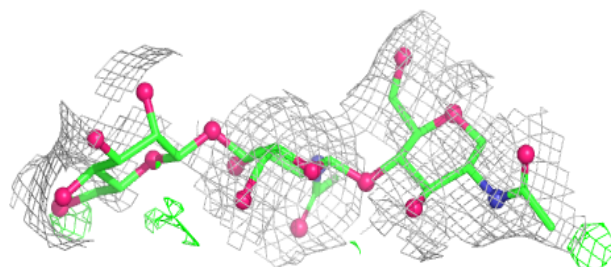
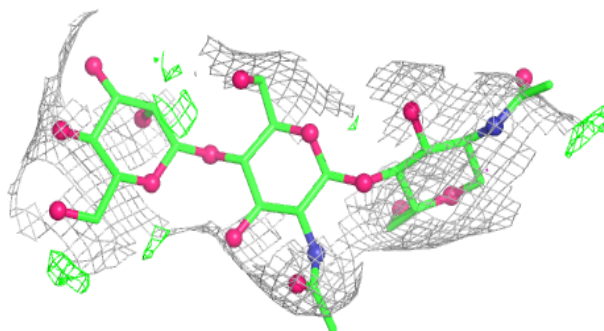
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

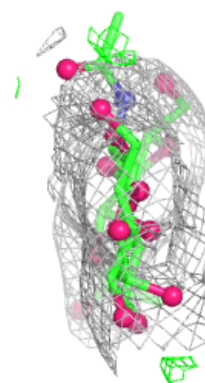
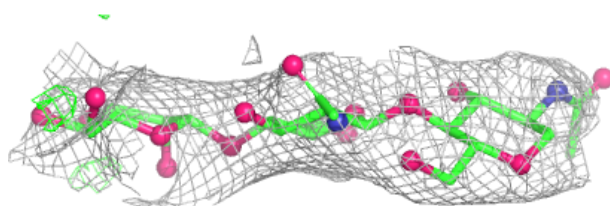
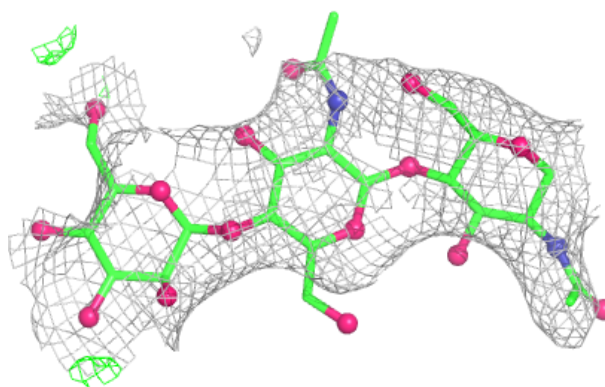
**Electron density around Chain D:**

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

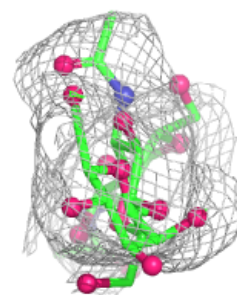
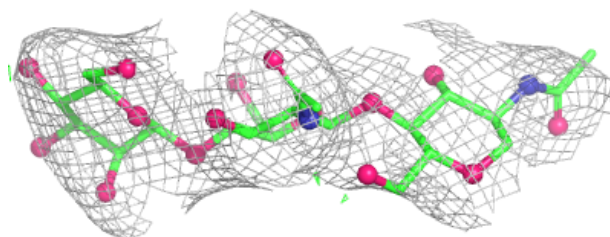
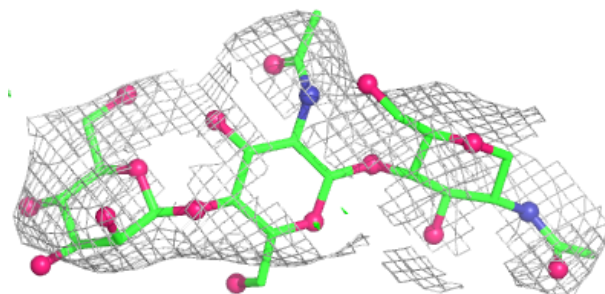


Electron density around Chain G:

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

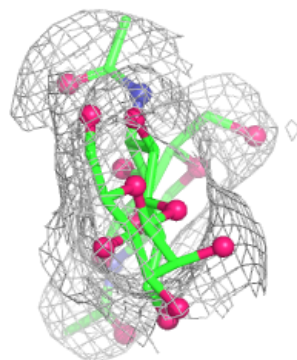
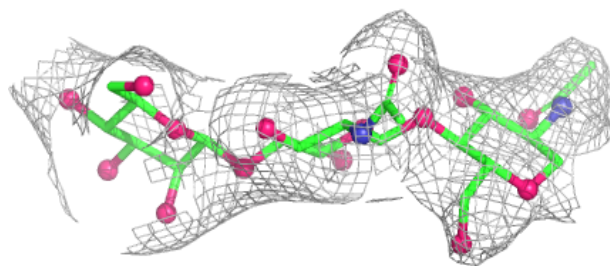
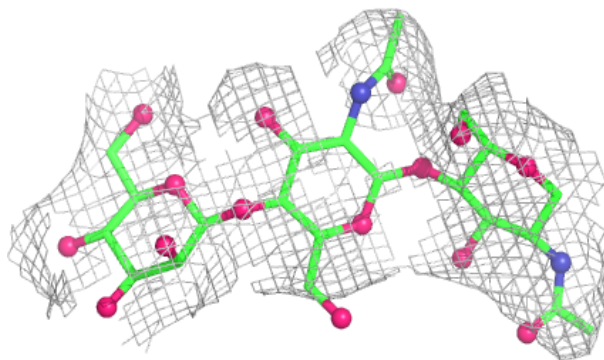
**Electron density around Chain I:**

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

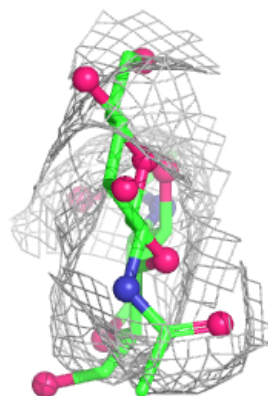
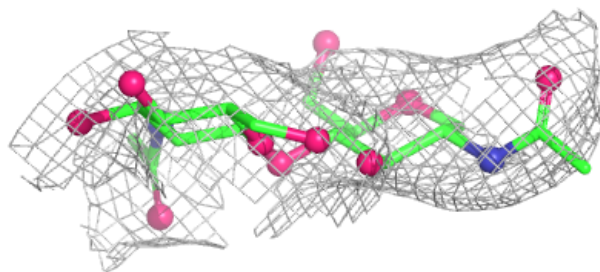
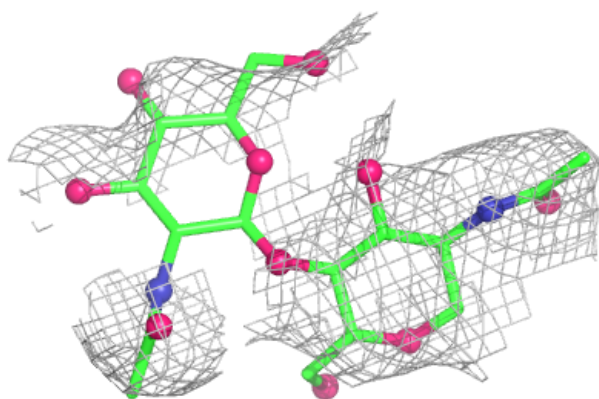


Electron density around Chain J:

$2mF_o-DF_c$ (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)



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
5	NAG	B	701	14/15	0.69	0.10	120,133,142,146	0
5	NAG	F	601	14/15	0.74	0.08	118,139,148,151	0
5	NAG	A	701	14/15	0.76	0.09	96,113,130,134	0
5	NAG	A	704	14/15	0.76	0.08	105,126,130,131	0
5	NAG	B	706	14/15	0.77	0.08	83,121,124,124	0
5	NAG	A	706	14/15	0.78	0.07	95,118,127,138	0
5	NAG	A	705	14/15	0.78	0.09	99,118,141,148	0
5	NAG	E	601	14/15	0.80	0.09	105,119,139,144	0
7	CL	A	707	1/1	0.82	0.17	109,109,109,109	0
8	EDO	B	705	4/4	0.82	0.12	71,84,84,85	0
7	CL	B	703	1/1	0.83	0.17	101,101,101,101	0
8	EDO	B	707	4/4	0.88	0.06	85,86,87,90	0
7	CL	F	602	1/1	0.91	0.09	76,76,76,76	0
8	EDO	B	704	4/4	0.91	0.10	67,70,83,85	0
9	MG	B	709	1/1	0.93	0.19	78,78,78,78	0
7	CL	A	703	1/1	0.95	0.09	63,63,63,63	0
7	CL	B	708	1/1	0.96	0.04	88,88,88,88	0
6	ZN	B	702	1/1	0.96	0.05	87,87,87,87	0
6	ZN	A	702	1/1	0.98	0.05	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.