



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:58 PM UTC

PDB ID : 9U0G / pdb_00009u0g
Title : Crystal structure of the apo BRL2 ectodomain from Arabidopsis thaliana (monoclinic crystal form).
Authors : Caregnato, A.; Hothorn, M.
Deposited on : 2026-01-27
Resolution : 2.60 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

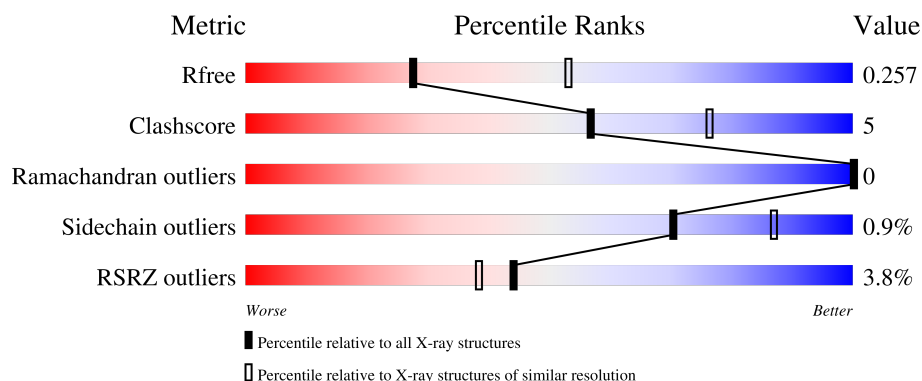
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	784	<div> <div>3%</div> <div>73%</div> <div>11%</div> <div>16%</div> </div>
1	B	784	<div> <div>4%</div> <div>74%</div> <div>9%</div> <div>17%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>
3	D	3	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	3	<div><div></div><div>33%</div><div>67%</div></div>
3	G	3	<div><div></div><div>100%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10366 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 Serine/threonine-protein kinase BRI1-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	0	0
			5045	3201	837	990	17			
1	B	654	Total	C	N	O	S	0	0	0
			5017	3184	832	984	17			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	734	ALA	-	expression tag	UNP Q9ZPS9
A	735	ALA	-	expression tag	UNP Q9ZPS9
A	736	ALA	-	expression tag	UNP Q9ZPS9
A	737	GLU	-	expression tag	UNP Q9ZPS9
A	738	ASN	-	expression tag	UNP Q9ZPS9
A	739	LEU	-	expression tag	UNP Q9ZPS9
A	740	TYR	-	expression tag	UNP Q9ZPS9
A	741	PHE	-	expression tag	UNP Q9ZPS9
A	742	GLN	-	expression tag	UNP Q9ZPS9
A	743	GLY	-	expression tag	UNP Q9ZPS9
A	744	SER	-	expression tag	UNP Q9ZPS9
A	745	ALA	-	expression tag	UNP Q9ZPS9
A	746	TRP	-	expression tag	UNP Q9ZPS9
A	747	SER	-	expression tag	UNP Q9ZPS9
A	748	HIS	-	expression tag	UNP Q9ZPS9
A	749	PRO	-	expression tag	UNP Q9ZPS9
A	750	GLN	-	expression tag	UNP Q9ZPS9
A	751	PHE	-	expression tag	UNP Q9ZPS9
A	752	GLU	-	expression tag	UNP Q9ZPS9
A	753	LYS	-	expression tag	UNP Q9ZPS9
A	754	GLY	-	expression tag	UNP Q9ZPS9
A	755	GLY	-	expression tag	UNP Q9ZPS9
A	756	GLY	-	expression tag	UNP Q9ZPS9
A	757	SER	-	expression tag	UNP Q9ZPS9
A	758	GLY	-	expression tag	UNP Q9ZPS9

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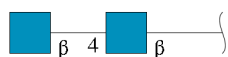
Chain	Residue	Modelled	Actual	Comment	Reference
A	759	GLY	-	expression tag	UNP Q9ZPS9
A	760	GLY	-	expression tag	UNP Q9ZPS9
A	761	SER	-	expression tag	UNP Q9ZPS9
A	762	GLY	-	expression tag	UNP Q9ZPS9
A	763	GLY	-	expression tag	UNP Q9ZPS9
A	764	SER	-	expression tag	UNP Q9ZPS9
A	765	ALA	-	expression tag	UNP Q9ZPS9
A	766	TRP	-	expression tag	UNP Q9ZPS9
A	767	SER	-	expression tag	UNP Q9ZPS9
A	768	HIS	-	expression tag	UNP Q9ZPS9
A	769	PRO	-	expression tag	UNP Q9ZPS9
A	770	GLN	-	expression tag	UNP Q9ZPS9
A	771	PHE	-	expression tag	UNP Q9ZPS9
A	772	GLU	-	expression tag	UNP Q9ZPS9
A	773	LYS	-	expression tag	UNP Q9ZPS9
A	774	GLY	-	expression tag	UNP Q9ZPS9
A	775	ALA	-	expression tag	UNP Q9ZPS9
A	776	HIS	-	expression tag	UNP Q9ZPS9
A	777	HIS	-	expression tag	UNP Q9ZPS9
A	778	HIS	-	expression tag	UNP Q9ZPS9
A	779	HIS	-	expression tag	UNP Q9ZPS9
A	780	HIS	-	expression tag	UNP Q9ZPS9
A	781	HIS	-	expression tag	UNP Q9ZPS9
A	782	HIS	-	expression tag	UNP Q9ZPS9
A	783	HIS	-	expression tag	UNP Q9ZPS9
A	784	HIS	-	expression tag	UNP Q9ZPS9
B	734	ALA	-	expression tag	UNP Q9ZPS9
B	735	ALA	-	expression tag	UNP Q9ZPS9
B	736	ALA	-	expression tag	UNP Q9ZPS9
B	737	GLU	-	expression tag	UNP Q9ZPS9
B	738	ASN	-	expression tag	UNP Q9ZPS9
B	739	LEU	-	expression tag	UNP Q9ZPS9
B	740	TYR	-	expression tag	UNP Q9ZPS9
B	741	PHE	-	expression tag	UNP Q9ZPS9
B	742	GLN	-	expression tag	UNP Q9ZPS9
B	743	GLY	-	expression tag	UNP Q9ZPS9
B	744	SER	-	expression tag	UNP Q9ZPS9
B	745	ALA	-	expression tag	UNP Q9ZPS9
B	746	TRP	-	expression tag	UNP Q9ZPS9
B	747	SER	-	expression tag	UNP Q9ZPS9
B	748	HIS	-	expression tag	UNP Q9ZPS9
B	749	PRO	-	expression tag	UNP Q9ZPS9

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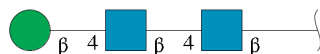
Chain	Residue	Modelled	Actual	Comment	Reference
B	750	GLN	-	expression tag	UNP Q9ZPS9
B	751	PHE	-	expression tag	UNP Q9ZPS9
B	752	GLU	-	expression tag	UNP Q9ZPS9
B	753	LYS	-	expression tag	UNP Q9ZPS9
B	754	GLY	-	expression tag	UNP Q9ZPS9
B	755	GLY	-	expression tag	UNP Q9ZPS9
B	756	GLY	-	expression tag	UNP Q9ZPS9
B	757	SER	-	expression tag	UNP Q9ZPS9
B	758	GLY	-	expression tag	UNP Q9ZPS9
B	759	GLY	-	expression tag	UNP Q9ZPS9
B	760	GLY	-	expression tag	UNP Q9ZPS9
B	761	SER	-	expression tag	UNP Q9ZPS9
B	762	GLY	-	expression tag	UNP Q9ZPS9
B	763	GLY	-	expression tag	UNP Q9ZPS9
B	764	SER	-	expression tag	UNP Q9ZPS9
B	765	ALA	-	expression tag	UNP Q9ZPS9
B	766	TRP	-	expression tag	UNP Q9ZPS9
B	767	SER	-	expression tag	UNP Q9ZPS9
B	768	HIS	-	expression tag	UNP Q9ZPS9
B	769	PRO	-	expression tag	UNP Q9ZPS9
B	770	GLN	-	expression tag	UNP Q9ZPS9
B	771	PHE	-	expression tag	UNP Q9ZPS9
B	772	GLU	-	expression tag	UNP Q9ZPS9
B	773	LYS	-	expression tag	UNP Q9ZPS9
B	774	GLY	-	expression tag	UNP Q9ZPS9
B	775	ALA	-	expression tag	UNP Q9ZPS9
B	776	HIS	-	expression tag	UNP Q9ZPS9
B	777	HIS	-	expression tag	UNP Q9ZPS9
B	778	HIS	-	expression tag	UNP Q9ZPS9
B	779	HIS	-	expression tag	UNP Q9ZPS9
B	780	HIS	-	expression tag	UNP Q9ZPS9
B	781	HIS	-	expression tag	UNP Q9ZPS9
B	782	HIS	-	expression tag	UNP Q9ZPS9
B	783	HIS	-	expression tag	UNP Q9ZPS9
B	784	HIS	-	expression tag	UNP Q9ZPS9

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



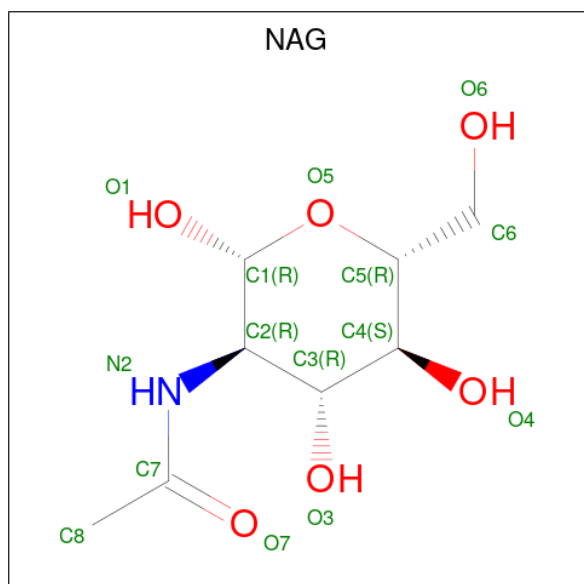
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

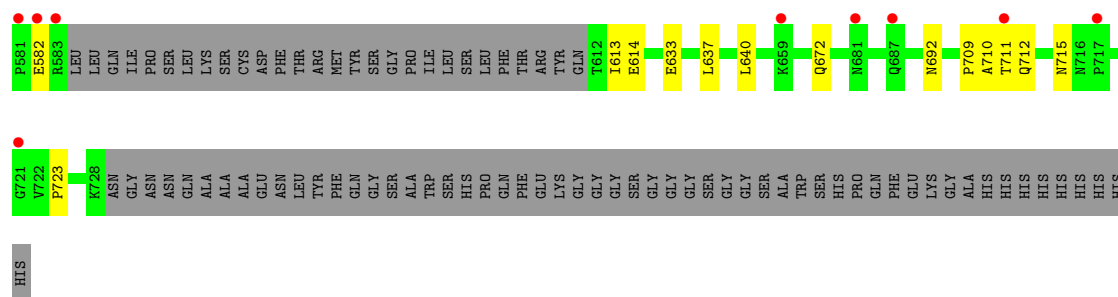
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	26	Total	O	0	0
			26	26		



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

Chain C: 100%

MAG1
MAG2

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

Chain E: 50% 50%

MAG1
MAG2

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

Chain D: 33% 67%

MAG1
MAG2
BMA3

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

Chain F: 33% 67%

MAG1
MAG2
BMA3

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

Chain G: 100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.90Å 211.61Å 67.17Å 90.00° 112.61° 90.00°	Depositor
Resolution (Å)	63.91 – 2.60 63.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (63.91-2.60) 91.0 (63.91-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.231 , 0.259 0.231 , 0.257	Depositor DCC
R_{free} test set	2993 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10366	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.09	0/5144	0.26	0/7001
1	B	0.08	0/5114	0.25	0/6958
All	All	0.08	0/10258	0.26	0/13959

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

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	5045	0	5035	53	0
1	B	5017	0	5006	47	0
2	C	28	0	25	0	0
2	E	28	0	25	1	0
3	D	39	0	34	0	0
3	F	39	0	34	0	0
3	G	39	0	34	2	0
4	A	42	0	39	0	0
4	B	42	0	39	1	0
5	A	21	0	0	0	0
5	B	26	0	0	0	0
All	All	10366	0	10271	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 5.

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:194:SER:HA	1:A:221:SER:HB2	1.70	0.74
1:A:710:ALA:HB2	1:A:723:PRO:HB2	1.72	0.72
1:B:538:ARG:HD2	1:B:541:ARG:HH12	1.54	0.71
1:B:225:ILE:HD12	1:B:247:SER:HB2	1.73	0.70
1:B:292:VAL:HG12	1:B:315:GLY:HA3	1.75	0.68
1:B:538:ARG:NH2	1:B:633:GLU:OE1	2.26	0.66
1:A:711:THR:HG23	1:A:712:GLN:HE21	1.63	0.63
1:B:711:THR:HG23	1:B:712:GLN:HE21	1.65	0.60
1:A:127:LEU:HD21	1:A:150:LYS:HE2	1.84	0.59
1:A:637:LEU:HD21	1:A:640:LEU:HD13	1.84	0.59
1:A:551:LEU:HD13	1:A:575:GLU:HG3	1.84	0.59
1:A:292:VAL:HG12	1:A:315:GLY:HA3	1.85	0.58
1:A:225:ILE:HD12	1:A:247:SER:HB2	1.85	0.57
1:A:656:GLY:HA3	1:A:678:SER:HB2	1.86	0.57
1:A:672:GLN:HE21	1:B:91:SER:HB2	1.70	0.56
1:B:159:LEU:HB3	1:B:164:PHE:HE2	1.70	0.56
1:B:538:ARG:HB3	1:B:541:ARG:HH22	1.71	0.56
1:B:637:LEU:HD21	1:B:640:LEU:HD13	1.86	0.56
1:A:496:ARG:HG2	1:B:546:LYS:HE3	1.87	0.55
1:A:388:THR:HG22	1:A:410:TYR:HB2	1.89	0.55
1:B:74:THR:HB	1:B:82:GLU:HB2	1.90	0.54
1:A:458:GLN:HE21	1:A:482:ARG:HH12	1.56	0.53
1:B:194:SER:HA	1:B:221:SER:HB2	1.90	0.53
1:A:165:THR:HG22	1:A:188:ASN:HD22	1.73	0.53
1:B:171:ASP:HA	1:B:174:LEU:HG	1.90	0.53
1:B:127:LEU:HD21	1:B:150:LYS:HE2	1.91	0.52
1:A:159:LEU:HB3	1:A:164:PHE:HE2	1.74	0.52
1:A:140:ILE:HA	1:A:163:ASN:HB3	1.92	0.51
1:B:709:PRO:HG2	1:B:712:GLN:HG2	1.93	0.51
1:B:484:THR:HG22	1:B:506:ASN:HB3	1.92	0.51
1:B:165:THR:HG22	1:B:188:ASN:HD22	1.76	0.51
1:B:140:ILE:HA	1:B:163:ASN:HB3	1.93	0.51
1:A:575:GLU:OE2	1:A:577:SER:HB2	2.12	0.49
1:A:193:ILE:HG13	1:A:216:ILE:HG21	1.95	0.49
1:B:388:THR:HG22	1:B:410:TYR:HB2	1.95	0.49
1:A:538:ARG:HE	1:A:630:GLU:HG2	1.78	0.49
1:A:171:ASP:HA	1:A:174:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HD13	1:B:582:GLU:OE2	2.14	0.48
1:B:190:THR:HG21	4:B:802:NAG:H62	1.96	0.48
1:A:576:PHE:HA	1:A:579:ILE:HD12	1.96	0.48
1:A:176:SER:HB3	1:A:179:LEU:HB3	1.95	0.47
1:B:329:GLN:OE1	1:B:353:ARG:NH1	2.47	0.47
1:A:91:SER:HB2	1:B:672:GLN:HE21	1.79	0.47
1:A:614:GLU:HG2	1:A:636:ALA:HB1	1.97	0.47
1:A:692:ASN:ND2	1:A:715:ASN:HD22	2.13	0.47
1:A:662:GLY:HA2	1:A:685:LEU:HA	1.96	0.46
1:B:490:ASP:O	1:B:493:ILE:HG12	2.16	0.46
1:B:223:SER:HA	2:E:1:NAG:H82	1.97	0.46
1:B:47:LYS:HD2	1:B:61:TRP:HB2	1.98	0.46
1:A:408:LEU:HD12	1:B:579:ILE:HD13	1.98	0.46
1:A:76:LEU:HB3	1:A:81:THR:HG21	1.96	0.45
1:B:556:THR:HB	1:B:577:SER:HA	1.98	0.45
1:B:614:GLU:HA	1:B:637:LEU:HA	1.98	0.45
1:A:579:ILE:HD13	1:B:408:LEU:HD12	1.99	0.45
1:A:52:ASP:HB3	1:A:91:SER:HB3	1.99	0.45
1:B:288:ASN:HA	3:G:1:NAG:H81	1.98	0.45
1:B:692:ASN:ND2	1:B:715:ASN:HD22	2.15	0.45
1:A:632:GLY:HA3	1:A:654:THR:HB	2.00	0.44
1:A:164:PHE:HB2	1:A:187:ASN:HB3	1.98	0.44
1:B:323:ARG:HH11	1:B:345:SER:HB3	1.82	0.44
1:A:401:LEU:HD13	1:A:404:ILE:HD11	1.99	0.44
1:A:490:ASP:O	1:A:493:ILE:HG12	2.18	0.44
1:B:43:LEU:HD12	1:B:67:PRO:HB3	1.98	0.44
1:B:538:ARG:HH11	1:B:541:ARG:NH1	2.16	0.44
1:B:176:SER:HB3	1:B:179:LEU:HB3	2.00	0.43
1:A:106:SER:HA	1:A:129:LEU:HA	2.00	0.43
1:A:265:THR:HG22	1:A:288:ASN:HB2	1.99	0.43
1:A:141:GLY:O	1:A:164:PHE:HA	2.18	0.43
1:A:614:GLU:HA	1:A:637:LEU:HA	2.01	0.42
1:A:43:LEU:HD12	1:A:67:PRO:HB3	2.01	0.42
1:A:521:LEU:HB3	1:A:540:GLY:HA2	2.00	0.42
1:A:51:GLN:HG2	1:A:92:GLY:HA2	2.01	0.42
1:A:254:LEU:HD21	1:A:257:LEU:HB2	2.02	0.42
1:B:710:ALA:HB2	1:B:723:PRO:HB2	2.01	0.42
1:A:115:PHE:HB2	1:A:137:SER:O	2.20	0.42
1:B:79:ARG:NH2	1:B:103:ASP:OD1	2.52	0.41
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.91	0.41
1:A:694:GLU:OE1	1:A:717:PRO:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:VAL:O	1:B:572:GLY:N	2.54	0.41
1:A:371:CYS:HB2	1:A:394:ALA:O	2.21	0.41
1:A:484:THR:HG22	1:A:506:ASN:HB3	2.02	0.41
1:B:576:PHE:HA	1:B:579:ILE:HD12	2.02	0.41
1:A:129:LEU:HA	1:A:129:LEU:HD12	1.92	0.41
1:A:431:TRP:CE3	1:A:432:TYR:HB2	2.56	0.41
1:B:288:ASN:HD22	3:G:1:NAG:C8	2.34	0.41
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.94	0.41
1:A:74:THR:HB	1:A:82:GLU:HB2	2.03	0.41
1:B:106:SER:HA	1:B:129:LEU:HA	2.02	0.41
1:A:698:PRO:HB3	1:A:727:CYS:SG	2.60	0.41
1:B:141:GLY:O	1:B:164:PHE:HA	2.21	0.40
1:B:522:VAL:HA	1:B:613:ILE:HA	2.03	0.40
1:B:164:PHE:HB2	1:B:187:ASN:HB3	2.02	0.40
1:B:318:PRO:O	1:B:321:ILE:HG12	2.20	0.40
1:B:265:THR:HG22	1:B:288:ASN:HB2	2.03	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	653/784 (83%)	601 (92%)	52 (8%)	0	100	100
1	B	646/784 (82%)	599 (93%)	47 (7%)	0	100	100
All	All	1299/1568 (83%)	1200 (92%)	99 (8%)	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	591/697 (85%)	588 (100%)	3 (0%)	81	92
1	B	588/697 (84%)	580 (99%)	8 (1%)	59	81
All	All	1179/1394 (85%)	1168 (99%)	11 (1%)	70	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	ARG
1	A	382	LEU
1	A	576	PHE
1	B	263	ARG
1	B	382	LEU
1	B	546	LYS
1	B	551	LEU
1	B	552	LEU
1	B	560	VAL
1	B	576	PHE
1	B	580	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	HIS
1	A	335	ASN
1	A	423	GLN
1	A	427	GLN
1	A	434	ASN
1	A	458	GLN
1	A	472	ASN
1	A	674	GLN
1	A	692	ASN
1	A	712	GLN
1	B	261	HIS

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Mol	Chain	Res	Type
1	B	310	ASN
1	B	335	ASN
1	B	423	GLN
1	B	427	GLN
1	B	434	ASN
1	B	458	GLN
1	B	660	ASN
1	B	674	GLN
1	B	692	ASN
1	B	712	GLN

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 ⓘ

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.72	0	17,19,21	1.29	3 (17%)
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	1.24	2 (11%)
3	NAG	D	1	3,1	14,14,15	0.71	0	17,19,21	1.05	2 (11%)
3	NAG	D	2	3	14,14,15	0.69	0	17,19,21	0.82	0
3	BMA	D	3	3	11,11,12	0.80	0	15,15,17	2.42	6 (40%)
2	NAG	E	1	2,1	14,14,15	0.73	0	17,19,21	1.16	1 (5%)
2	NAG	E	2	2	14,14,15	0.71	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	3,1	14,14,15	0.71	0	17,19,21	0.99	2 (11%)
3	NAG	F	2	3	14,14,15	0.70	0	17,19,21	0.83	0
3	BMA	F	3	3	11,11,12	0.80	0	15,15,17	2.41	6 (40%)
3	NAG	G	1	3,1	14,14,15	0.70	0	17,19,21	0.96	0
3	NAG	G	2	3	14,14,15	0.72	0	17,19,21	1.20	1 (5%)
3	BMA	G	3	3	11,11,12	0.85	0	15,15,17	2.11	3 (20%)

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

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

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-O5-C5	7.00	121.56	112.19
3	F	3	BMA	C1-O5-C5	6.96	121.51	112.19
3	G	3	BMA	C1-O5-C5	6.08	120.33	112.19
3	D	3	BMA	C3-C4-C5	3.61	116.77	110.23
3	F	3	BMA	C3-C4-C5	3.61	116.77	110.23
3	G	2	NAG	C2-N2-C7	3.20	127.19	122.90
2	E	2	NAG	C2-N2-C7	3.17	127.14	122.90
2	C	2	NAG	C2-N2-C7	2.99	126.91	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	C2-C3-C4	2.71	115.63	110.86
3	D	3	BMA	C2-C3-C4	2.70	115.62	110.86
3	G	3	BMA	C3-C4-C5	2.67	115.08	110.23
2	C	1	NAG	C1-O5-C5	2.56	115.62	112.19
3	D	1	NAG	C1-O5-C5	2.52	115.57	112.19
3	G	3	BMA	C2-C3-C4	2.49	115.24	110.86
2	E	1	NAG	C1-O5-C5	2.47	115.49	112.19
2	C	2	NAG	C1-O5-C5	2.39	115.39	112.19
2	E	2	NAG	C1-O5-C5	2.37	115.37	112.19
3	F	1	NAG	C2-N2-C7	2.31	126.00	122.90
3	D	1	NAG	C2-N2-C7	2.21	125.86	122.90
3	D	3	BMA	O4-C4-C3	-2.16	105.27	110.38
3	D	3	BMA	O5-C5-C4	2.16	116.09	110.83
3	F	3	BMA	O5-C5-C4	2.16	116.07	110.83
3	F	3	BMA	O4-C4-C3	-2.15	105.30	110.38
3	F	1	NAG	C1-O5-C5	2.14	115.05	112.19
3	F	3	BMA	O3-C3-C2	-2.13	105.70	110.05
2	C	1	NAG	C1-C2-N2	2.09	113.72	110.43
3	D	3	BMA	O3-C3-C2	-2.05	105.88	110.05
2	C	1	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

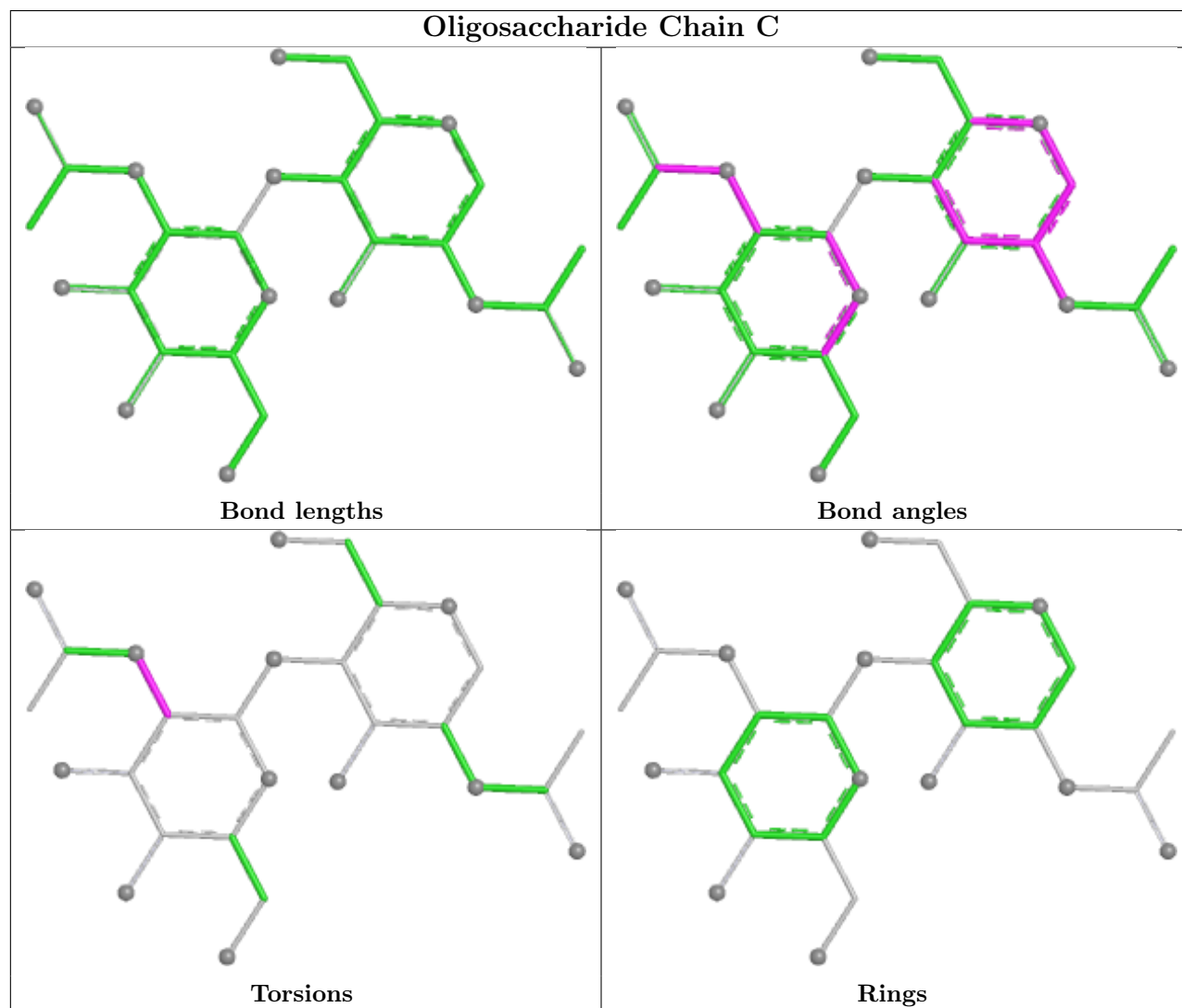
Mol	Chain	Res	Type	Atoms
3	G	3	BMA	O5-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	G	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7

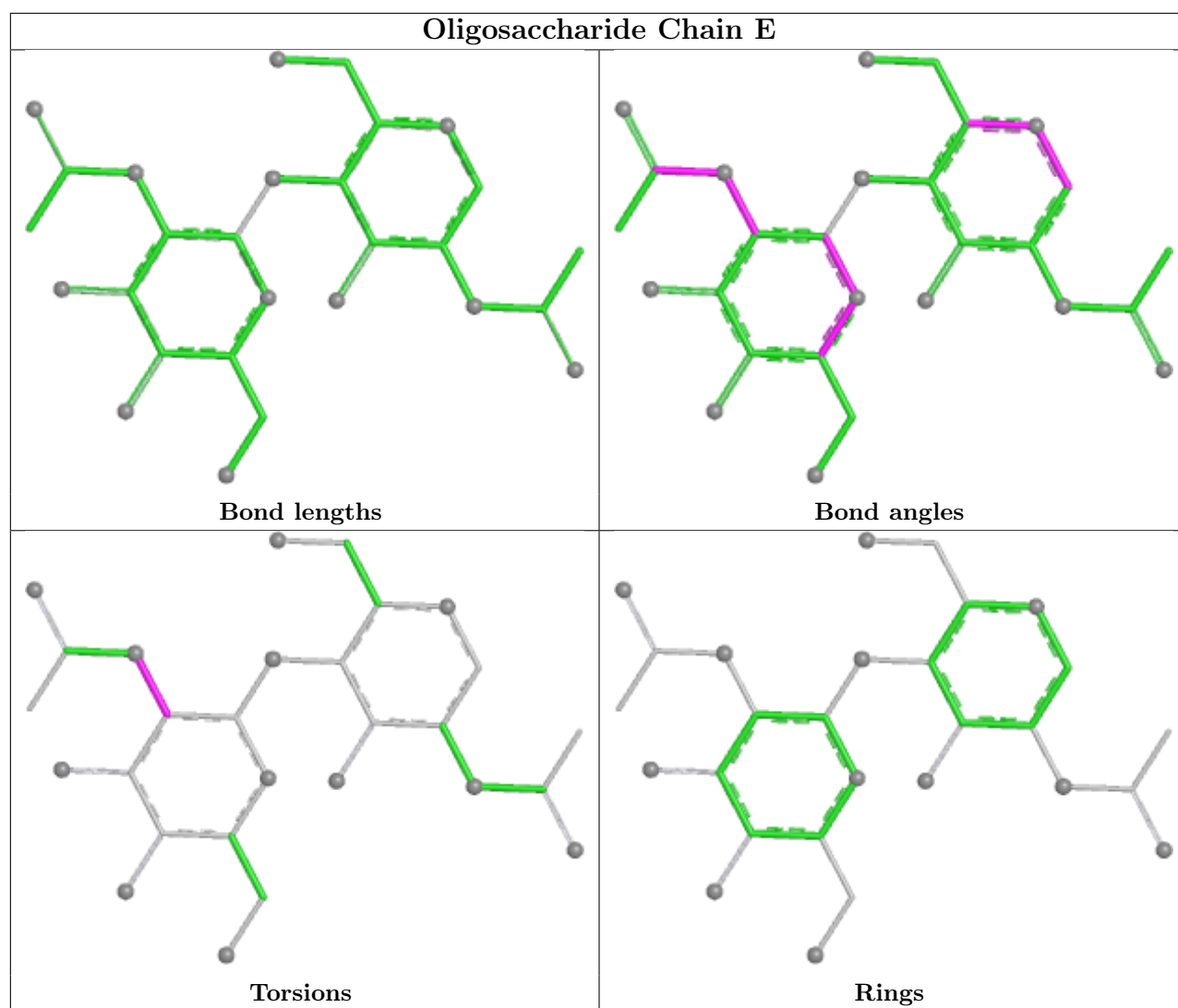
There are no ring outliers.

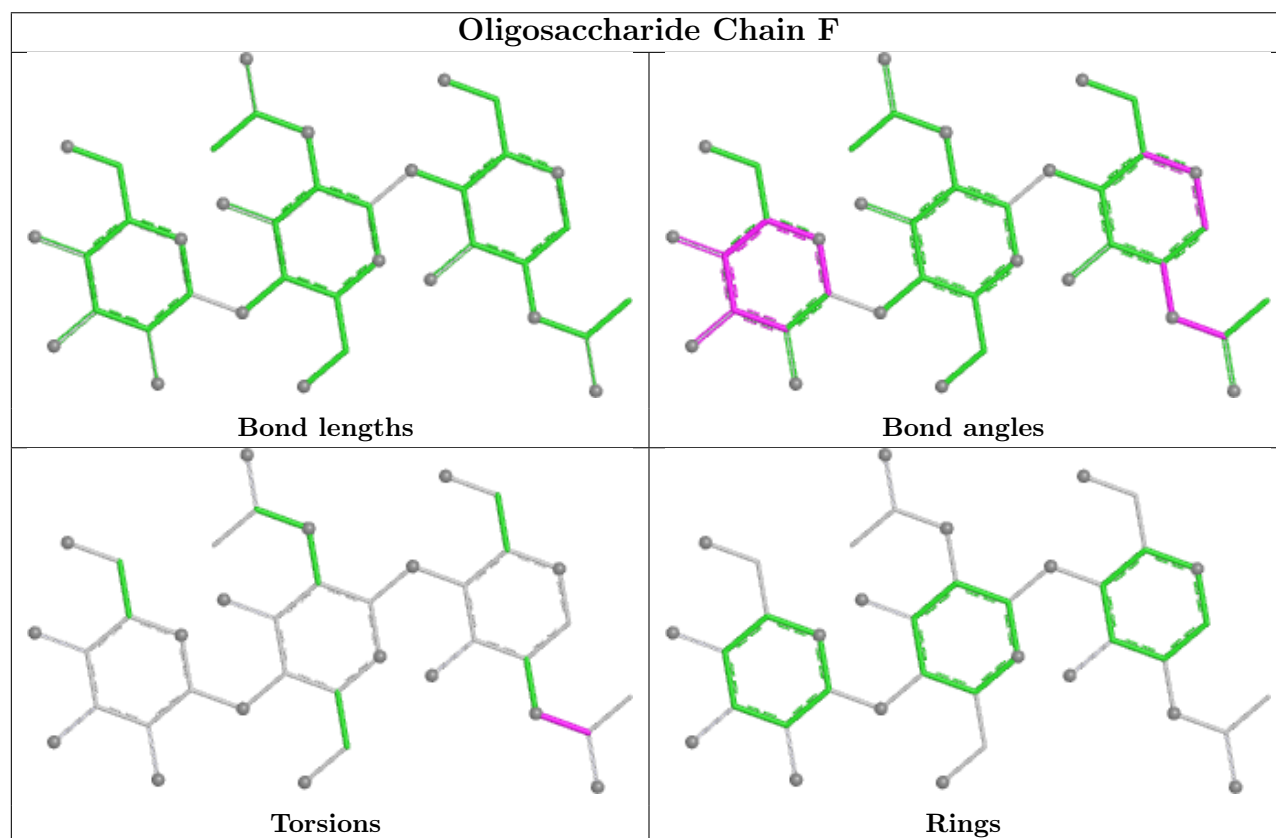
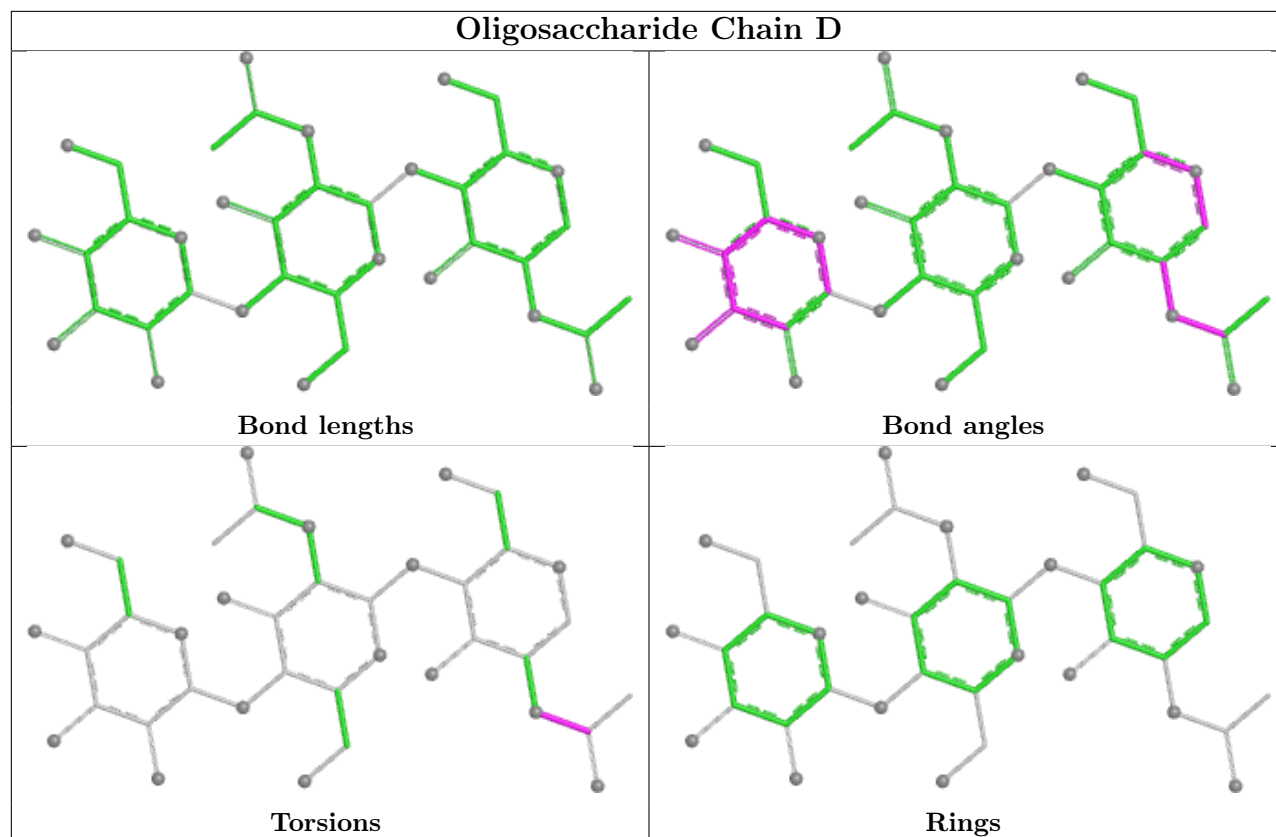
2 monomers are involved in 3 short contacts:

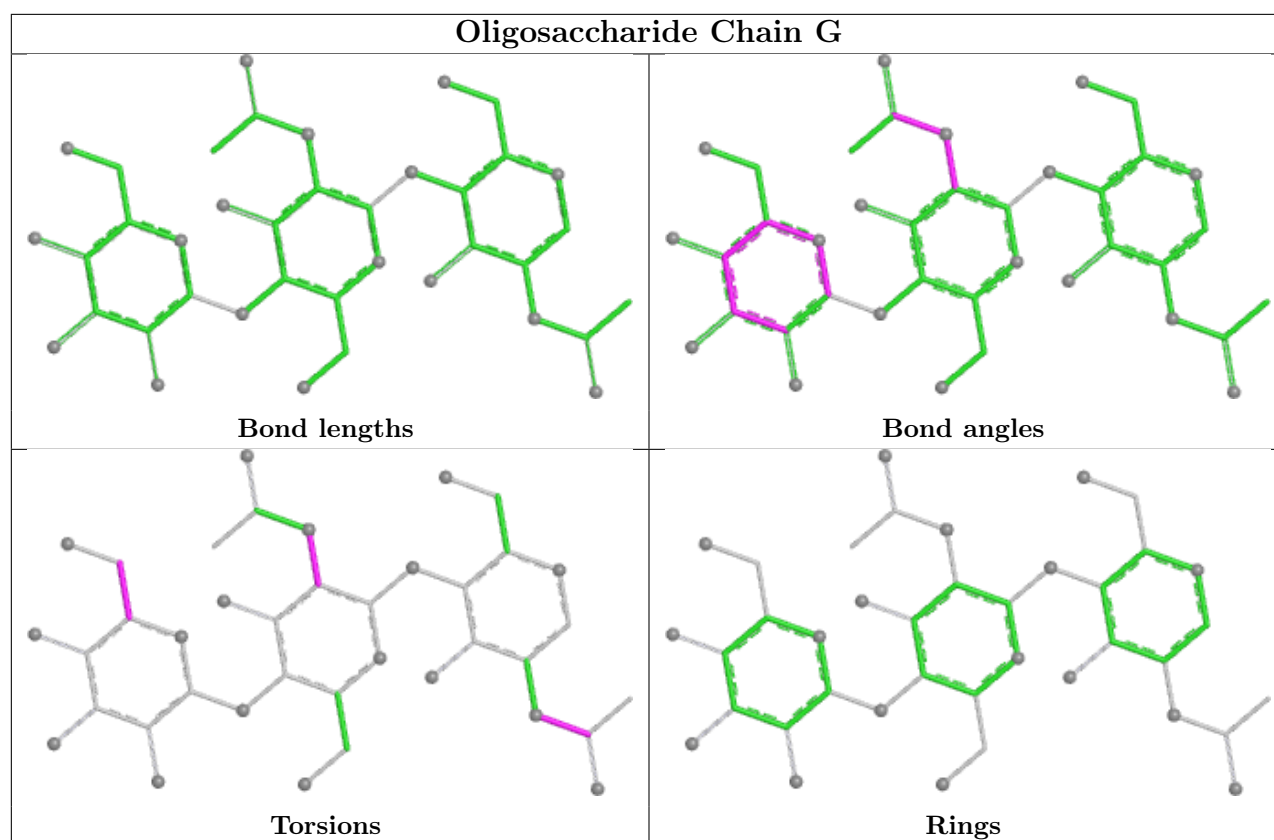
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	2	0
2	E	1	NAG	1	0

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](#)

6 ligands 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	$\# Z > 2$
4	NAG	A	801	1	14,14,15	0.71	0	17,19,21	0.88	0
4	NAG	B	802	1	14,14,15	0.71	0	17,19,21	1.25	1 (5%)
4	NAG	B	803	1	14,14,15	0.71	0	17,19,21	0.84	0
4	NAG	A	802	1	14,14,15	0.71	0	17,19,21	1.25	1 (5%)
4	NAG	B	801	1	14,14,15	0.69	0	17,19,21	0.84	0
4	NAG	A	803	1	14,14,15	0.71	0	17,19,21	0.83	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
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	NAG	B	803	1	-	0/6/23/26	0/1/1/1
4	NAG	A	802	1	-	0/6/23/26	0/1/1/1
4	NAG	B	801	1	-	0/6/23/26	0/1/1/1
4	NAG	A	803	1	-	0/6/23/26	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(°)
4	B	802	NAG	C1-O5-C5	3.88	117.38	112.19
4	A	802	NAG	C1-O5-C5	3.84	117.34	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	NAG	1	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

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, 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	659/784 (84%)	0.37	22 (3%)	49 43	52, 74, 124, 180	0
1	B	654/784 (83%)	0.45	28 (4%)	40 34	56, 80, 120, 172	0
All	All	1313/1568 (83%)	0.41	50 (3%)	44 38	52, 77, 121, 180	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	570	VAL	4.6
1	A	578	GLY	4.3
1	B	582	GLU	4.1
1	B	578	GLY	3.5
1	B	576	PHE	3.5
1	A	581	PRO	3.4
1	B	193	ILE	3.3
1	A	728	LYS	3.3
1	B	581	PRO	3.2
1	A	543	PRO	3.2
1	A	547	ALA	3.1
1	B	572	GLY	3.1
1	A	576	PHE	3.1
1	B	561	ARG	3.0
1	A	580	ARG	3.0
1	A	577	SER	2.8
1	A	561	ARG	2.8
1	B	717	PRO	2.7
1	B	33	GLN	2.7
1	A	583	ARG	2.7
1	B	547	ALA	2.7
1	A	542	GLN	2.7
1	B	72	GLY	2.4
1	B	711	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	556	THR	2.4
1	B	555	ASN	2.4
1	A	91	SER	2.3
1	B	119	SER	2.3
1	B	577	SER	2.3
1	B	687	GLN	2.3
1	B	721	GLY	2.2
1	A	679	PHE	2.2
1	B	579	ILE	2.2
1	B	541	ARG	2.2
1	B	151	TYR	2.2
1	A	722	VAL	2.2
1	B	681	ASN	2.1
1	A	687	GLN	2.1
1	B	583	ARG	2.1
1	B	659	LYS	2.1
1	B	55	ASN	2.1
1	A	193	ILE	2.1
1	B	557	MET	2.1
1	A	349	CYS	2.1
1	A	443	ILE	2.1
1	A	688	ILE	2.1
1	B	560	VAL	2.1
1	A	239	ASN	2.0
1	B	359	SER	2.0
1	B	488	PRO	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.

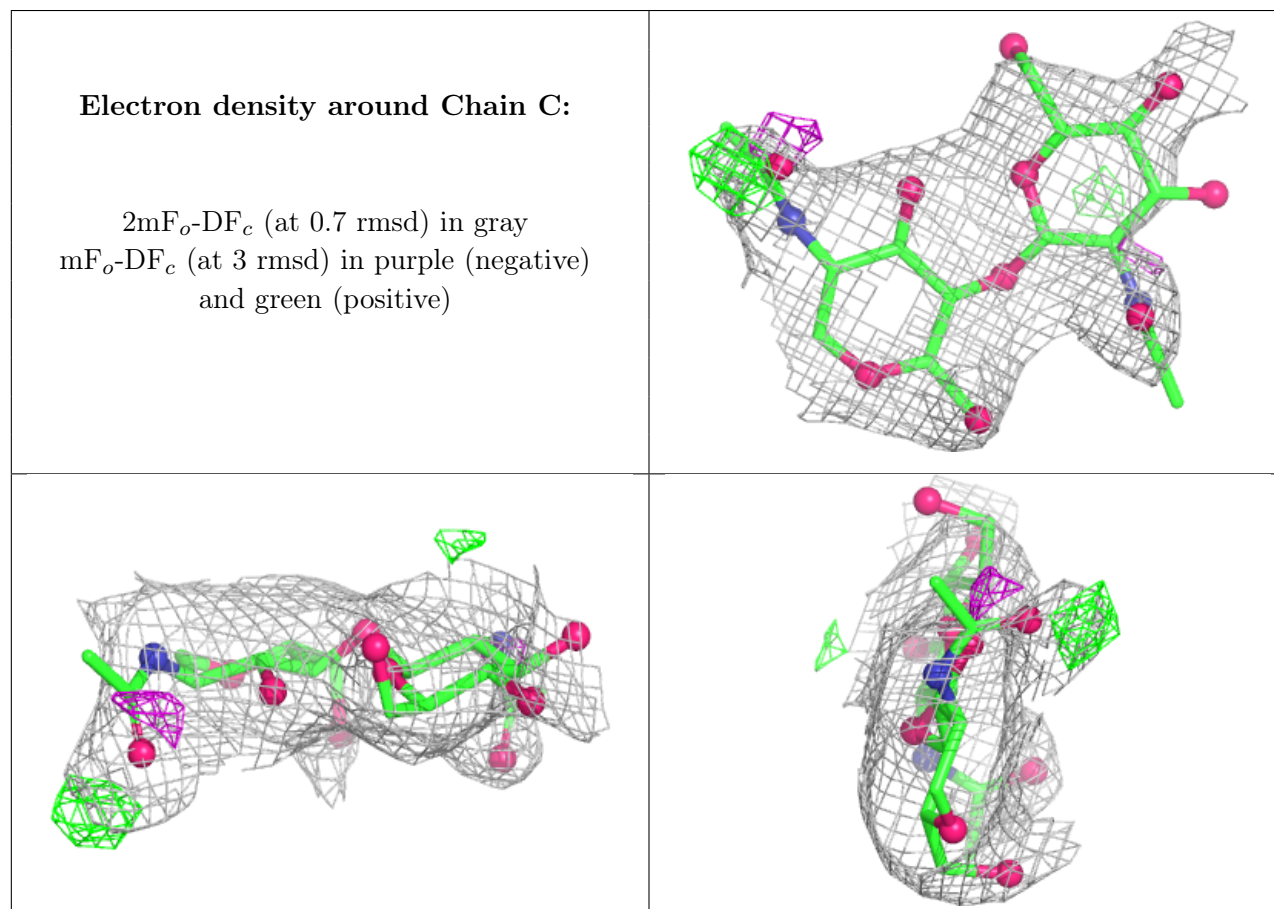
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	G	3	11/12	0.06	0.18	134,138,140,140	0
3	BMA	D	3	11/12	0.29	0.15	114,123,129,132	0

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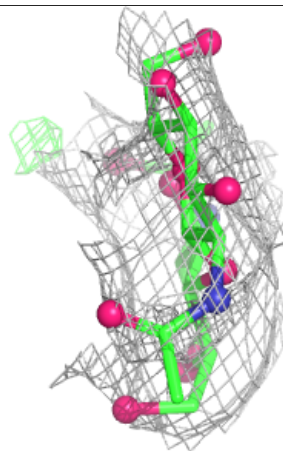
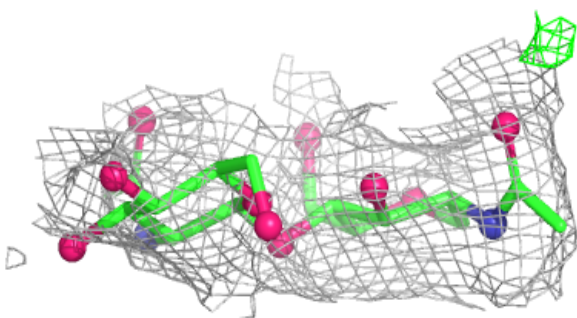
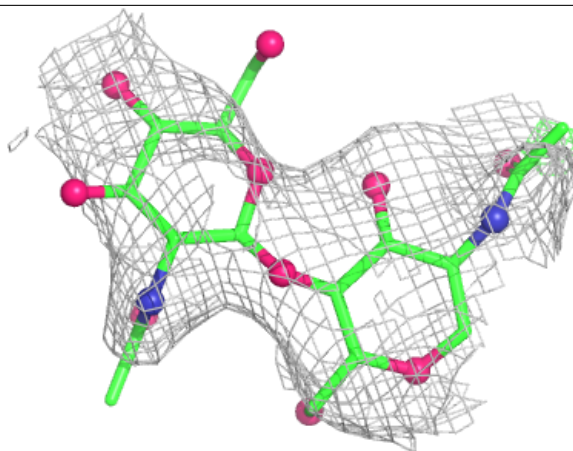
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	E	2	14/15	0.42	0.17	127,136,140,140	0
3	BMA	F	3	11/12	0.53	0.13	112,119,124,126	0
2	NAG	C	2	14/15	0.56	0.16	116,124,132,136	0
3	NAG	G	2	14/15	0.67	0.17	105,115,126,131	0
3	NAG	G	1	14/15	0.68	0.15	88,98,110,113	0
2	NAG	C	1	14/15	0.75	0.14	89,99,112,116	0
2	NAG	E	1	14/15	0.76	0.13	106,114,119,127	0
3	NAG	F	2	14/15	0.81	0.11	61,91,108,113	0
3	NAG	F	1	14/15	0.88	0.10	58,64,79,81	0
3	NAG	D	2	14/15	0.88	0.09	64,87,100,106	0
3	NAG	D	1	14/15	0.88	0.11	53,59,73,74	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.



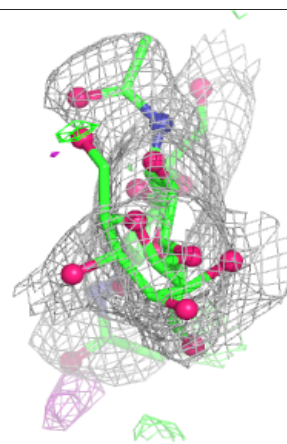
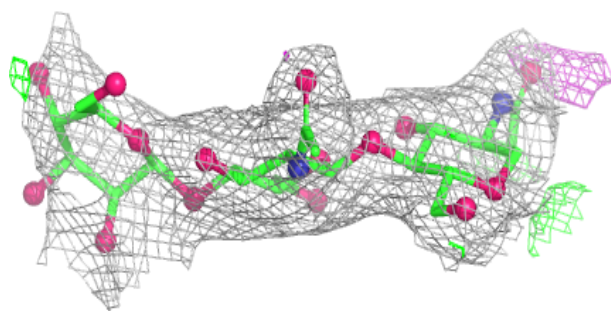
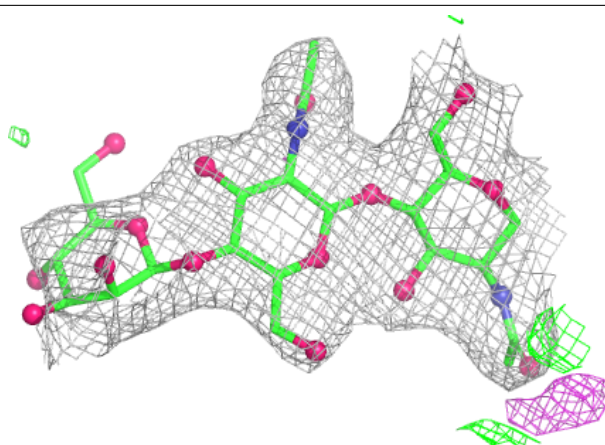
Electron density around Chain E:

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



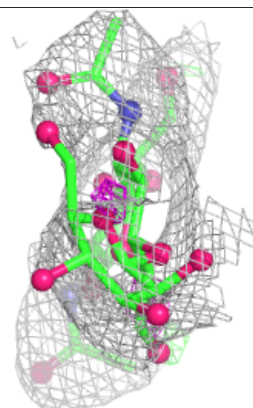
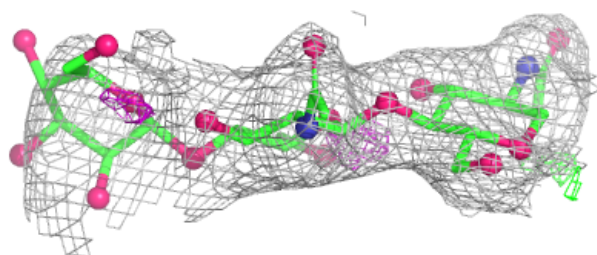
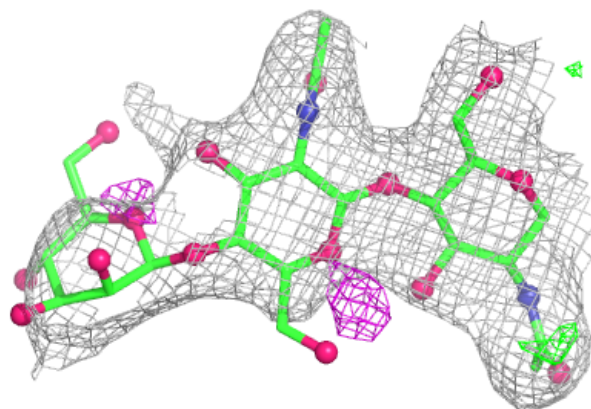
Electron density around Chain D:

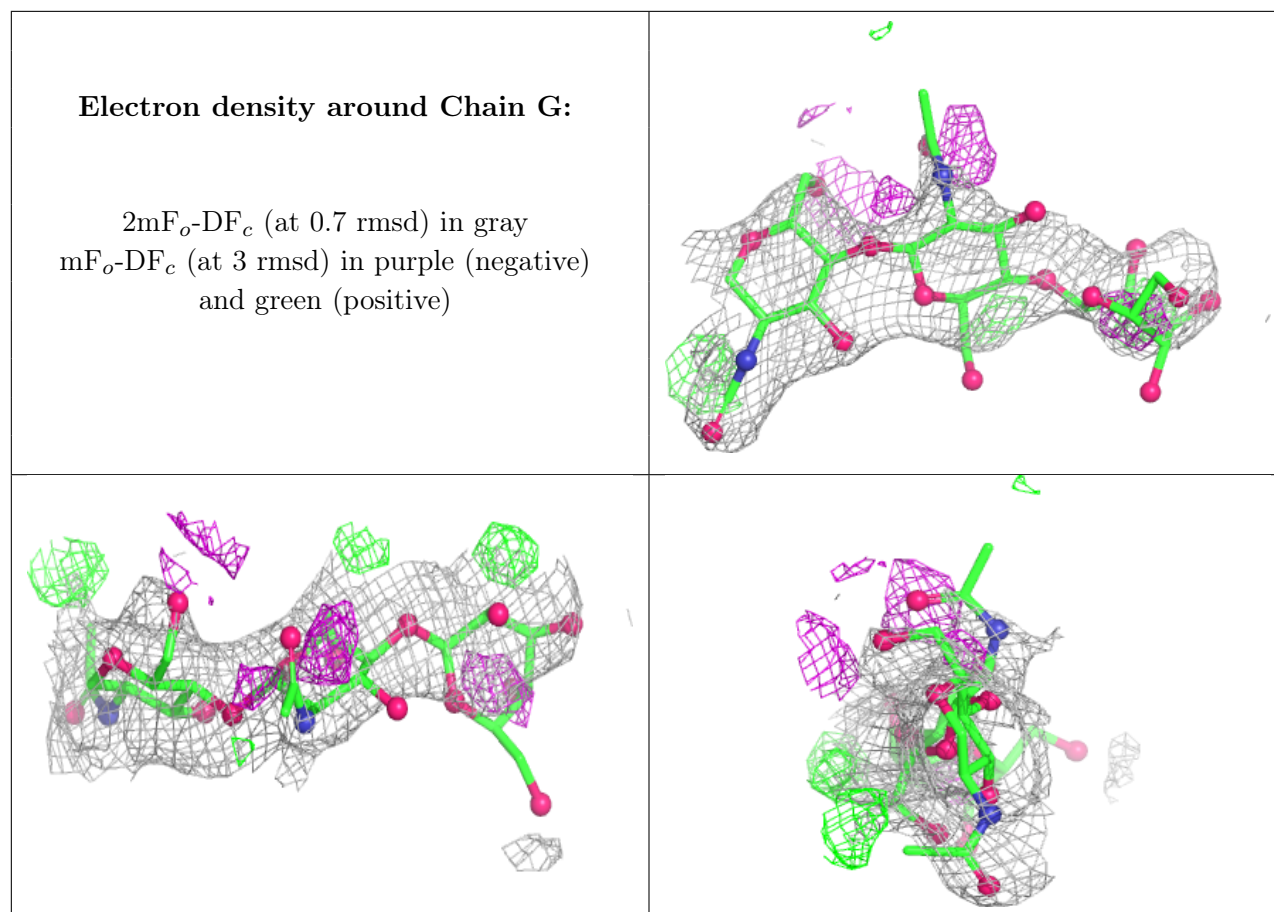
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
4	NAG	B	803	14/15	0.58	0.16	108,118,123,123	0
4	NAG	B	802	14/15	0.60	0.18	108,113,120,128	0
4	NAG	A	803	14/15	0.66	0.13	82,97,103,109	0
4	NAG	B	801	14/15	0.69	0.14	100,105,111,113	0
4	NAG	A	801	14/15	0.70	0.14	92,96,105,105	0
4	NAG	A	802	14/15	0.70	0.16	102,108,120,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.