



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:53 PM UTC

PDB ID : 3RGX / pdb_00003rgx
Title : Structural insight into brassinosteroid perception by BRI1
Authors : Chai, J.; Han, Z.; She, J.; Wang, J.; Cheng, W.; Wang, J.
Deposited on : 2011-04-11
Resolution : 2.47 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

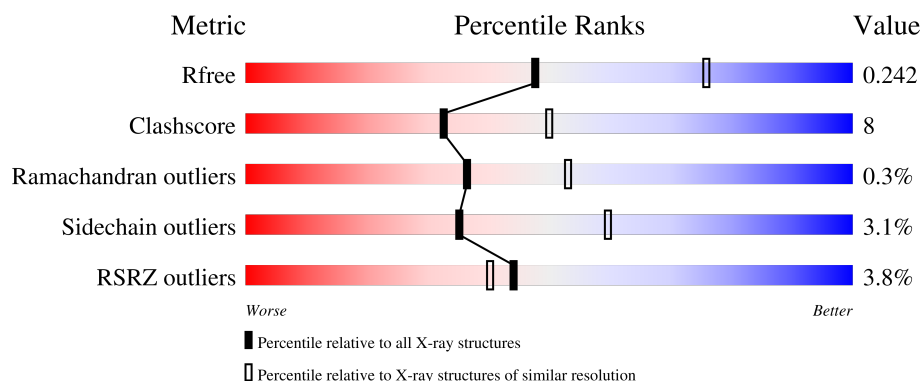
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	768	4% 79% 16% ••
2	B	3	100%
3	C	2	100%
3	E	2	50% 50%
3	F	2	100%

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Mol	Chain	Length	Quality of chain
4	D	4	25% 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	1	X	-	-	-
5	NAG	A	5101	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5890 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 Protein BRASSINOSTEROID INSENSITIVE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	734	5576	3526	921	1097	32	1	1	0

There are 6 discrepancies between the modelled and reference sequences:

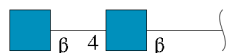
Chain	Residue	Modelled	Actual	Comment	Reference
A	785	HIS	-	expression tag	UNP O22476
A	786	HIS	-	expression tag	UNP O22476
A	787	HIS	-	expression tag	UNP O22476
A	788	HIS	-	expression tag	UNP O22476
A	789	HIS	-	expression tag	UNP O22476
A	790	HIS	-	expression tag	UNP O22476

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
			Total	C	N	O			
2	B	3	42	24	3	15	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.



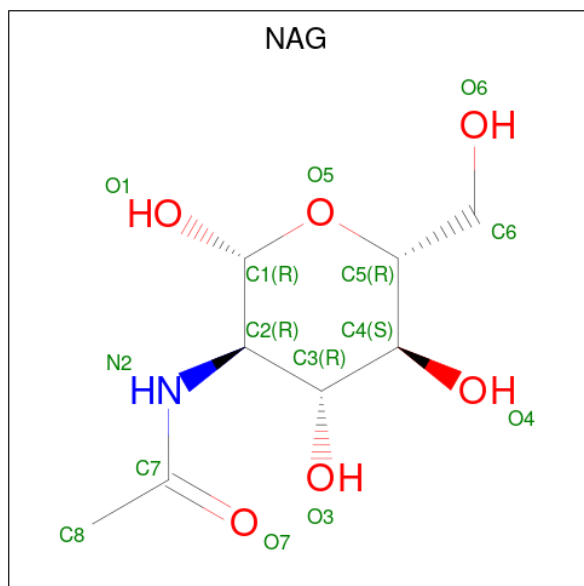
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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	4	Total	C	N	O	0	0	0
			56	32	4	20			

- 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		

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2

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

Chain D:  25% 75%

MAG1
MAG2
MAG3
MAG4

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.39Å 66.70Å 119.05Å 90.00° 120.98° 90.00°	Depositor
Resolution (Å)	48.01 – 2.47 48.01 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.01-2.47) 99.2 (48.01-2.47)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.199 , 0.246 0.194 , 0.242	Depositor DCC
R_{free} test set	2343 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5890	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: 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	0.41	0/5686	0.80	5/7714 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	ASN	CA-C-N	5.90	125.77	119.28
1	A	60	ASN	C-N-CA	5.90	125.77	119.28
1	A	187	GLY	N-CA-C	5.67	117.71	110.96
1	A	759	ASN	CA-C-N	5.52	126.74	119.84
1	A	759	ASN	C-N-CA	5.52	126.74	119.84

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	5576	0	5534	84	0
2	B	42	0	37	0	0
3	C	28	0	25	5	0
3	E	28	0	25	1	0
3	F	28	0	25	0	0
4	D	56	0	49	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	42	0	39	1	0
6	A	90	0	0	2	0
All	All	5890	0	5734	91	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 8.

All (91) 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:583:GLN:C	1:A:585:GLY:HA3	1.95	0.90
1:A:590:ASN:CG	1:A:591:PHE:H	1.93	0.77
1:A:290:LEU:HG	1:A:314:ALA:HB2	1.69	0.74
1:A:584:SER:N	1:A:585:GLY:HA3	2.02	0.73
1:A:207:ILE:HD11	1:A:229:VAL:HG12	1.72	0.72
1:A:336:PHE:HB3	1:A:364:MET:HE2	1.72	0.72
1:A:770:CYS:O	1:A:772:PRO:HD3	1.89	0.72
1:A:382:PRO:O	1:A:407:LEU:HD11	1.91	0.70
1:A:180:LEU:HB2	1:A:207:ILE:HG22	1.75	0.68
1:A:362:LEU:HD11	1:A:384:SER:HB2	1.77	0.66
1:A:276:ILE:HD11	1:A:298:LEU:HD22	1.79	0.64
1:A:336:PHE:HB3	1:A:364:MET:CE	2.29	0.62
1:A:577:PRO:O	1:A:580:MET:HG2	1.99	0.62
1:A:551:ASN:HD21	3:E:1:NAG:H82	1.63	0.62
1:A:583:GLN:O	1:A:585:GLY:HA3	1.99	0.62
1:A:290:LEU:HD21	1:A:311:LEU:HA	1.82	0.61
1:A:590:ASN:ND2	1:A:591:PHE:H	1.99	0.61
1:A:34:ARG:O	1:A:38:GLN:HG3	2.02	0.60
1:A:603:ASP:OD1	1:A:605:MET:HB2	2.02	0.59
1:A:586:LYS:HA	1:A:652:ASN:O	2.03	0.58
1:A:677:MET:HE3	1:A:680:LEU:HD22	1.85	0.58
1:A:116:SER:O	1:A:118:PHE:HD1	1.87	0.56
1:A:424:GLN:HB3	1:A:446:HIS:CD2	2.42	0.55
5:A:5101:NAG:H61	6:A:842:HOH:O	2.06	0.55
1:A:88:PHE:CD1	1:A:115:VAL:HA	2.41	0.55
1:A:702:ARG:O	1:A:727:MET:HG3	2.07	0.55
1:A:625:GLN:O	1:A:628:ARG:HB2	2.08	0.54
3:C:2:NAG:O7	3:C:2:NAG:H3	2.07	0.53
1:A:597:TYR:CG	1:A:615:LEU:HD11	2.44	0.52
1:A:162:PHE:CE2	1:A:166:VAL:HG12	2.43	0.52
1:A:509:SER:HB3	1:A:531:TRP:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LEU:HB2	1:A:736:ASN:OD1	2.11	0.51
1:A:590:ASN:CG	1:A:591:PHE:N	2.61	0.51
1:A:155:VAL:CG2	1:A:180:LEU:HD23	2.41	0.50
1:A:449:PHE:HE1	1:A:472:TRP:CZ2	2.30	0.50
1:A:681:PHE:CD1	1:A:682:ILE:HG13	2.46	0.50
1:A:630:SER:O	4:D:3:NAG:H61	2.11	0.49
1:A:36:ILE:O	1:A:40:ILE:HG12	2.13	0.49
1:A:767:LEU:HB3	1:A:768:PRO:HD2	1.94	0.48
1:A:409:ASN:O	1:A:410:LEU:C	2.57	0.48
1:A:335:PHE:C	1:A:335:PHE:CD1	2.91	0.48
1:A:409:ASN:O	1:A:412:GLN:HB2	2.13	0.48
1:A:589:ALA:HA	1:A:650:PHE:HB2	1.95	0.48
3:C:1:NAG:O4	3:C:2:NAG:H61	2.13	0.48
4:D:2:NAG:O4	4:D:3:NAG:H4	2.14	0.47
1:A:648:PRO:HD2	1:A:657:MET:HE1	1.95	0.47
1:A:515:ASN:HA	1:A:538:LEU:HA	1.95	0.47
1:A:681:PHE:CE1	1:A:682:ILE:HG13	2.50	0.47
3:C:1:NAG:H61	3:C:2:NAG:H2	1.97	0.47
1:A:584:SER:N	1:A:585:GLY:CA	2.74	0.47
4:D:3:NAG:H3	4:D:4:NAG:O5	2.16	0.46
1:A:637:ILE:O	1:A:637:ILE:HG23	2.14	0.46
1:A:769:ARG:HH11	1:A:769:ARG:HG2	1.81	0.46
1:A:295:TYR:CZ	3:C:1:NAG:H82	2.50	0.46
1:A:449:PHE:HE1	1:A:472:TRP:CH2	2.35	0.45
1:A:280:GLN:HE21	1:A:280:GLN:HB2	1.61	0.45
6:A:840:HOH:O	4:D:1:NAG:H81	2.16	0.45
1:A:472:TRP:HB2	1:A:496:ASP:O	2.17	0.44
1:A:383:GLU:O	1:A:386:THR:HG23	2.17	0.44
1:A:650:PHE:CD1	1:A:654:GLY:HA3	2.52	0.44
1:A:333:PRO:HA	1:A:334:PRO:HD2	1.78	0.44
1:A:655:SER:HB3	1:A:679:TYR:HB2	2.00	0.44
1:A:68:THR:HB	1:A:76:SER:HB3	2.00	0.44
1:A:207:ILE:CD1	1:A:229:VAL:HA	2.48	0.44
1:A:411:CYS:HB3	1:A:416:ASN:ND2	2.33	0.44
1:A:767:LEU:HB3	1:A:768:PRO:CD	2.48	0.43
1:A:590:ASN:O	1:A:591:PHE:HB2	2.18	0.43
1:A:42:PHE:HB2	1:A:94:SER:HB3	1.99	0.43
1:A:415:LYS:C	1:A:415:LYS:HD3	2.43	0.43
1:A:162:PHE:CZ	1:A:166:VAL:HG12	2.54	0.43
1:A:51:LEU:HD23	1:A:51:LEU:HA	1.81	0.42
1:A:704:LEU:HD21	1:A:707:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:TYR:CE2	3:C:1:NAG:H82	2.54	0.42
1:A:358:MET:HE3	1:A:362:LEU:HG	2.01	0.42
1:A:769:ARG:HH11	1:A:769:ARG:CG	2.32	0.42
1:A:442:LEU:HD12	1:A:442:LEU:HA	1.76	0.42
1:A:577:PRO:HG2	1:A:580:MET:HB3	2.02	0.42
1:A:765:TYR:CD1	1:A:766:PRO:HA	2.55	0.42
1:A:45:VAL:O	1:A:45:VAL:HG12	2.20	0.42
1:A:505:PRO:HG2	1:A:508:LEU:HG	2.01	0.42
1:A:439:CYS:HB2	1:A:442:LEU:HD22	2.03	0.41
1:A:358:MET:CG	1:A:382:PRO:HG2	2.50	0.41
1:A:32:LEU:O	1:A:36:ILE:HG22	2.21	0.41
1:A:116:SER:O	1:A:118:PHE:CD1	2.71	0.41
1:A:284:PRO:HA	1:A:304:THR:O	2.21	0.41
1:A:299:ALA:HA	1:A:324:SER:O	2.21	0.41
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.89	0.40
1:A:459:SER:C	1:A:461:GLY:N	2.79	0.40
1:A:46:LEU:HA	1:A:47:PRO:HD3	1.94	0.40
1:A:211:LYS:HD3	1:A:211:LYS:HA	1.93	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	729/768 (95%)	667 (92%)	60 (8%)	2 (0%)	36 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	LYS
1	A	760	PRO

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	652/677 (96%)	632 (97%)	20 (3%)	35 60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	115	VAL
1	A	126	SER
1	A	166	VAL
1	A	186	SER
1	A	207	ILE
1	A	391	SER
1	A	415	LYS
1	A	416	ASN
1	A	417	THR
1	A	440	SER
1	A	492	THR
1	A	608	GLU
1	A	627	ASN
1	A	628	ARG
1	A	637	ILE
1	A	640	ARG
1	A	727	MET
1	A	731	ILE
1	A	771	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	50	ASN
1	A	85	ASN
1	A	204	HIS
1	A	248	GLN

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Mol	Chain	Res	Type
1	A	249	HIS
1	A	280	GLN
1	A	294	GLN
1	A	412	GLN
1	A	413	ASN
1	A	416	ASN
1	A	419	GLN
1	A	446	HIS
1	A	551	ASN
1	A	610	HIS
1	A	687	HIS
1	A	705	ASN
1	A	735	ASN
1	A	737	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 ⓘ

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	B	1	1,2	14,14,15	0.63	0	17,19,21	0.86	1 (5%)
2	NAG	B	2	2	14,14,15	0.61	0	17,19,21	1.64	3 (17%)
2	NAG	B	3	2	14,14,15	0.44	0	17,19,21	1.18	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.56	0	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	1.40	2 (11%)
4	NAG	D	1	4,1	14,14,15	0.69	0	17,19,21	1.46	2 (11%)
4	NAG	D	2	4	14,14,15	0.57	0	17,19,21	1.19	2 (11%)
4	NAG	D	3	4	14,14,15	0.49	0	17,19,21	1.20	2 (11%)
4	NAG	D	4	4	14,14,15	0.46	0	17,19,21	0.66	0
3	NAG	E	1	1,3	14,14,15	0.42	0	17,19,21	0.91	1 (5%)
3	NAG	E	2	3	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.41	0	17,19,21	1.12	2 (11%)
3	NAG	F	2	3	14,14,15	0.47	0	17,19,21	1.15	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	NAG	B	3	2	-	4/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	3	4	-	4/6/23/26	0/1/1/1
4	NAG	D	4	4	-	3/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C1-O5-C5	4.83	118.66	112.19
2	B	3	NAG	C1-O5-C5	4.37	118.05	112.19
2	B	2	NAG	C1-O5-C5	4.36	118.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C1-O5-C5	3.34	116.66	112.19
3	C	1	NAG	C1-O5-C5	3.21	116.49	112.19
3	C	2	NAG	C2-N2-C7	3.03	126.96	122.90
4	D	2	NAG	O4-C4-C3	2.85	117.09	110.38
3	C	2	NAG	C3-C4-C5	2.81	115.32	110.23
3	F	1	NAG	C1-O5-C5	2.66	115.75	112.19
3	F	2	NAG	C1-C2-N2	2.62	114.56	110.43
3	F	1	NAG	C2-N2-C7	-2.53	119.51	122.90
4	D	3	NAG	C1-O5-C5	2.53	115.58	112.19
4	D	2	NAG	C1-O5-C5	2.46	115.48	112.19
2	B	2	NAG	O5-C5-C4	2.40	116.67	110.83
3	E	1	NAG	C2-N2-C7	-2.34	119.77	122.90
4	D	1	NAG	C3-C4-C5	-2.26	106.14	110.23
3	F	2	NAG	C4-C3-C2	-2.25	107.72	111.02
2	B	1	NAG	C1-O5-C5	2.18	115.11	112.19
4	D	3	NAG	O5-C1-C2	-2.08	108.07	111.29
2	B	2	NAG	C4-C3-C2	-2.08	107.98	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	1	NAG	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	3	NAG	C3-C2-N2-C7
2	B	3	NAG	C8-C7-N2-C2
2	B	3	NAG	O7-C7-N2-C2
3	C	2	NAG	C3-C2-N2-C7
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	NAG	C8-C7-N2-C2
4	D	3	NAG	O7-C7-N2-C2
4	D	4	NAG	C8-C7-N2-C2
4	D	4	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2

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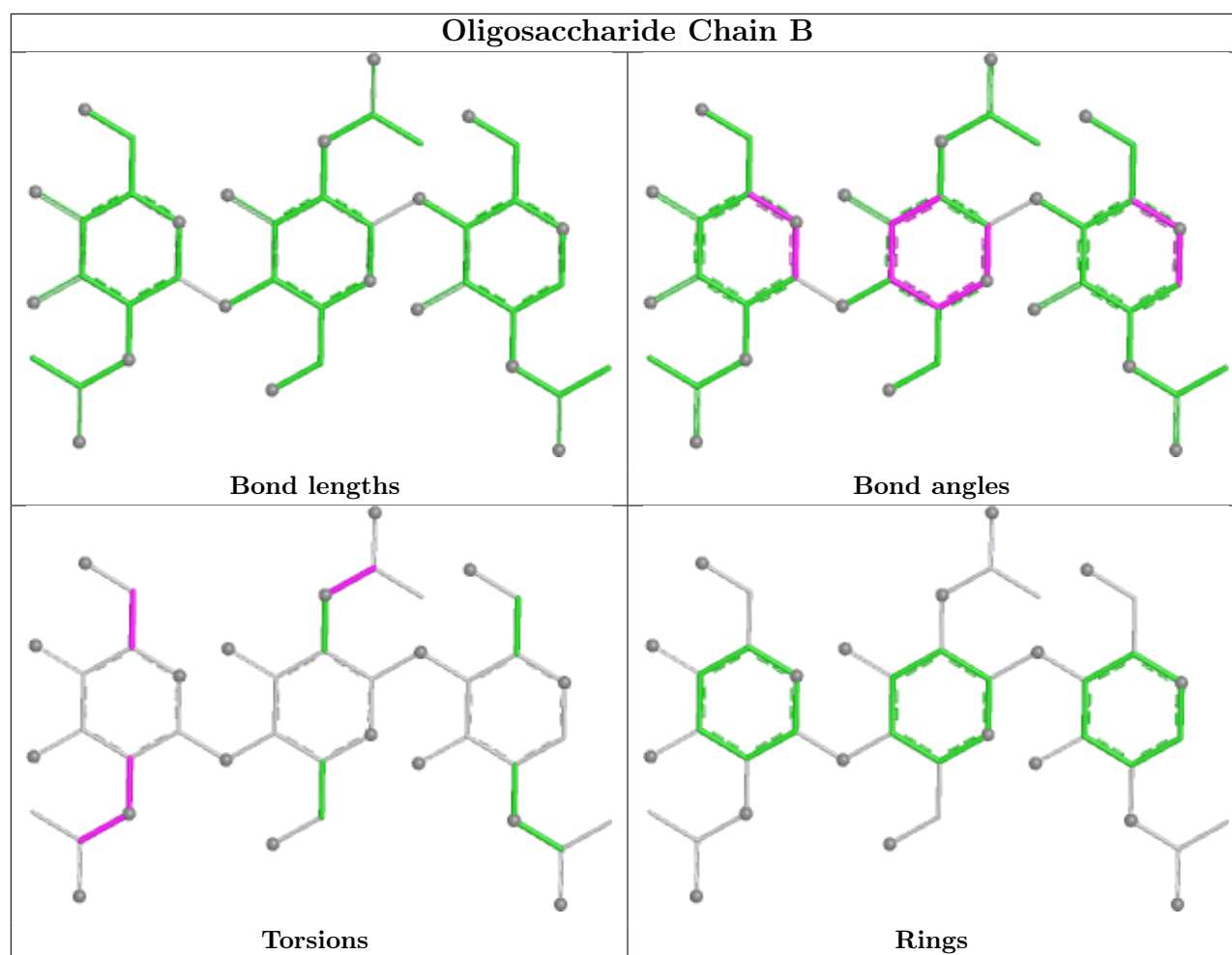
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
4	D	3	NAG	C4-C5-C6-O6
3	C	2	NAG	O7-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	D	3	NAG	O5-C5-C6-O6
2	B	3	NAG	O5-C5-C6-O6
3	F	1	NAG	O7-C7-N2-C2
4	D	4	NAG	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2

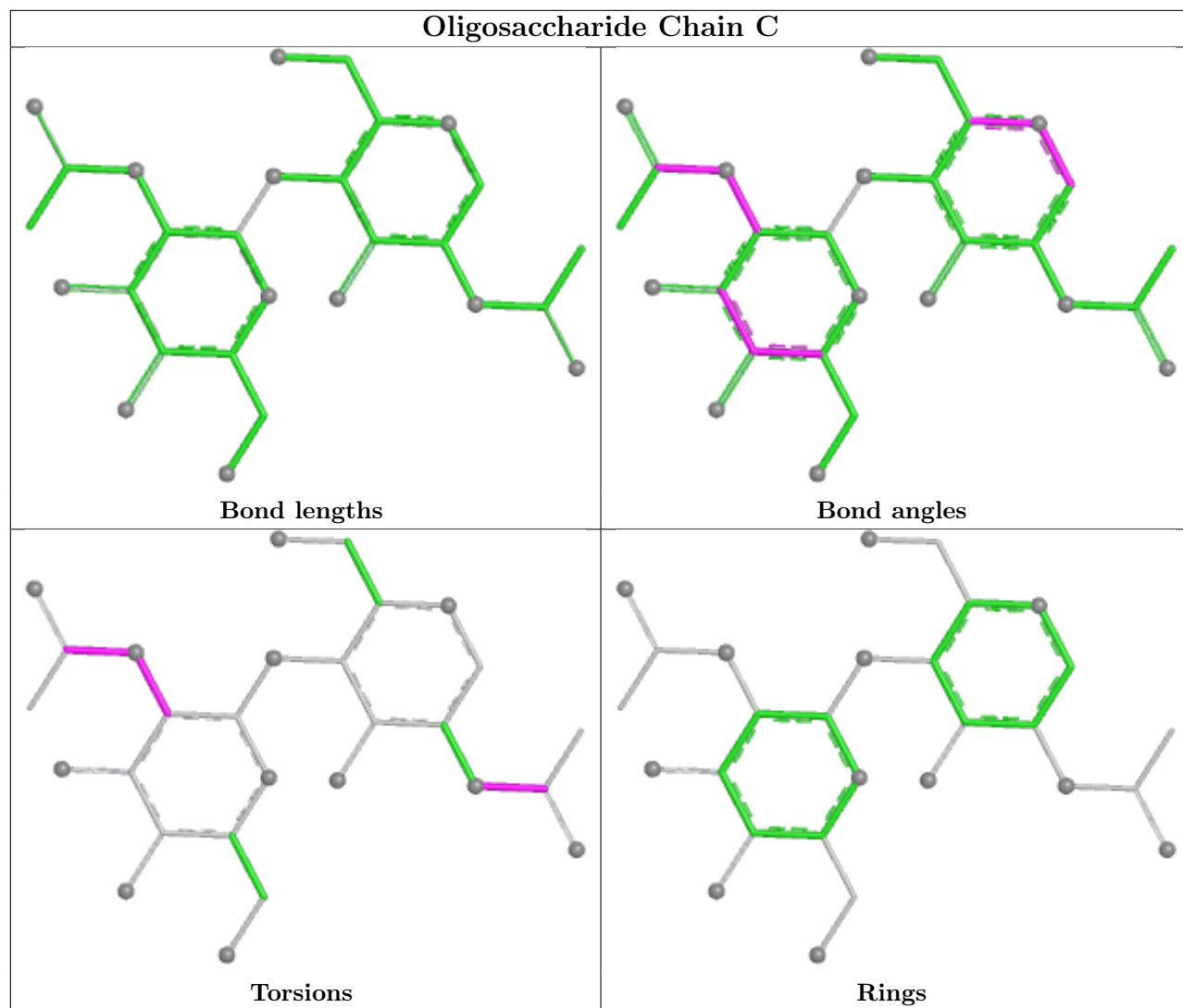
There are no ring outliers.

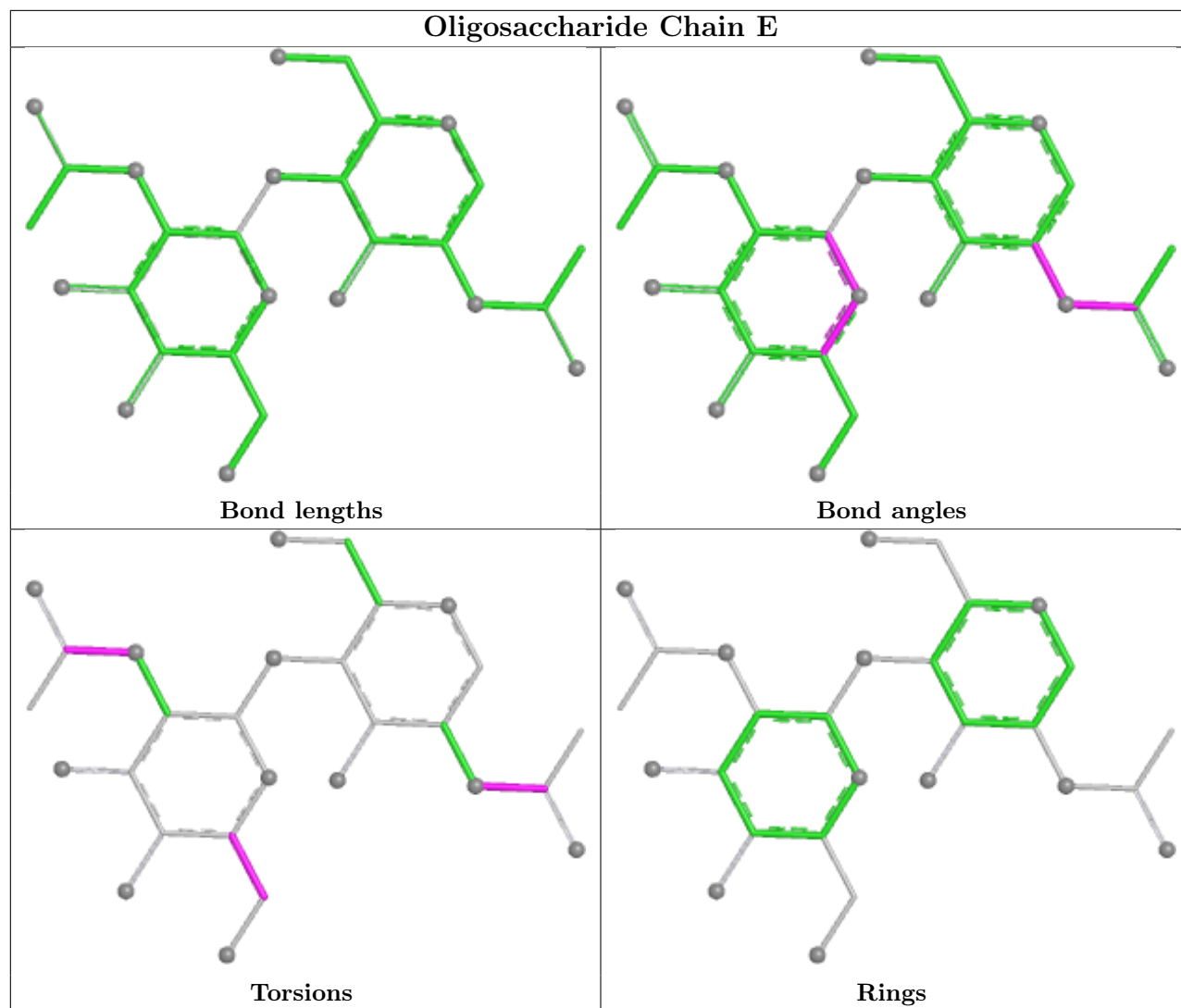
7 monomers are involved in 10 short contacts:

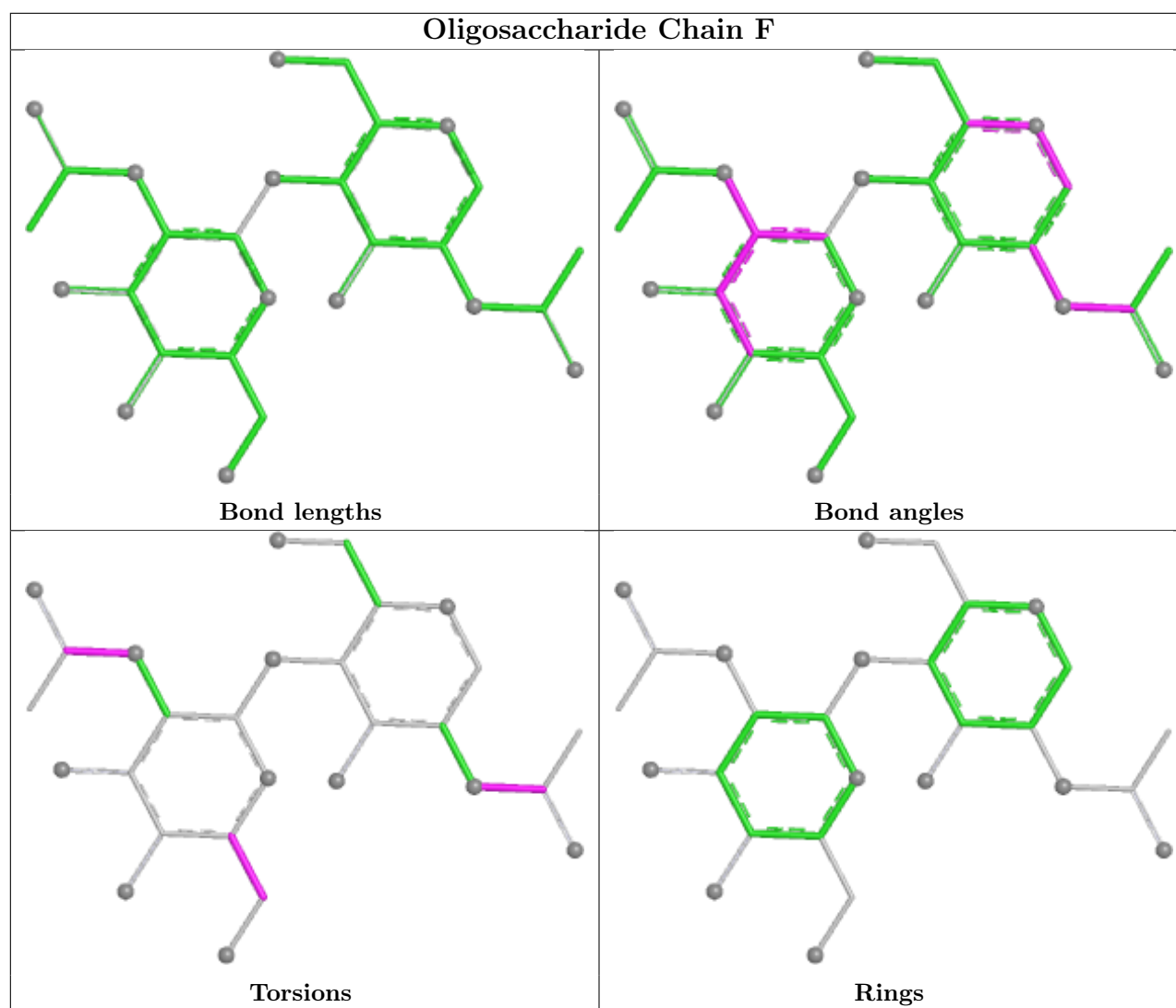
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
3	C	1	NAG	4	0
4	D	4	NAG	1	0
4	D	2	NAG	1	0
3	C	2	NAG	3	0
3	E	1	NAG	1	0
4	D	3	NAG	3	0

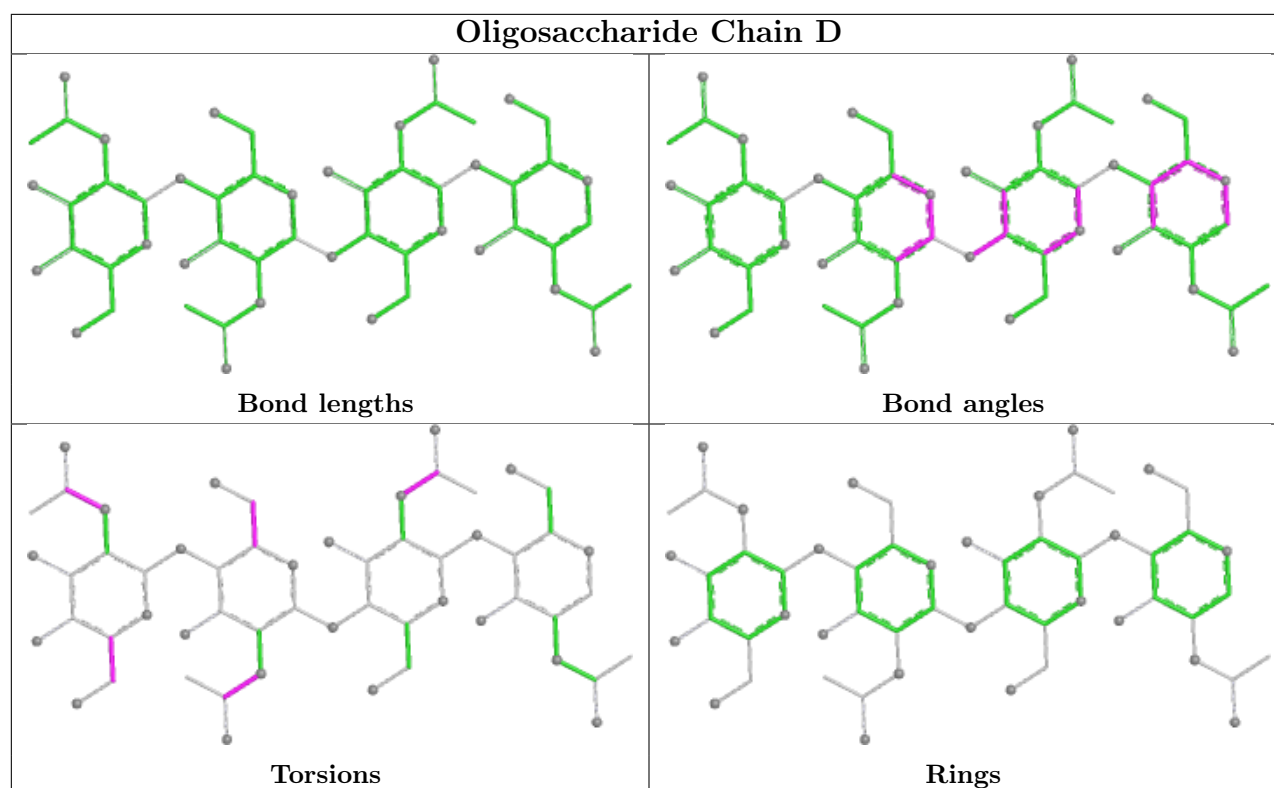
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
5	NAG	A	3511	1	14,14,15	0.44	0	17,19,21	0.84	1 (5%)
5	NAG	A	5101	1	14,14,15	0.61	0	17,19,21	0.98	2 (11%)
5	NAG	A	1121	1	14,14,15	0.47	0	17,19,21	0.97	1 (5%)

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
5	NAG	A	3511	1	-	0/6/23/26	0/1/1/1
5	NAG	A	5101	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	1121	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1121	NAG	C1-O5-C5	2.71	115.81	112.19
5	A	5101	NAG	C2-N2-C7	-2.56	119.47	122.90
5	A	5101	NAG	C4-C3-C2	2.15	114.16	111.02
5	A	3511	NAG	C1-O5-C5	2.12	115.03	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	5101	NAG	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5101	NAG	C8-C7-N2-C2
5	A	5101	NAG	O7-C7-N2-C2
5	A	5101	NAG	O5-C5-C6-O6
5	A	1121	NAG	O5-C5-C6-O6
5	A	1121	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5101	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	734/768 (95%)	0.16	28 (3%) 44 40	21, 60, 99, 136	2 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	772	PRO	4.4
1	A	584	SER	3.8
1	A	31	SER	3.2
1	A	166	VAL	3.2
1	A	591	PHE	3.1
1	A	640	ARG	3.1
1	A	638	THR	3.1
1	A	606	LYS	3.0
1	A	413	ASN	3.0
1	A	165	LYS	2.9
1	A	602	ASN	2.6
1	A	93	SER	2.6
1	A	416	ASN	2.5
1	A	415	LYS	2.4
1	A	655	SER	2.3
1	A	583	GLN	2.3
1	A	618	PHE	2.3
1	A	555	GLU	2.3
1	A	641	VAL	2.2
1	A	586	LYS	2.2
1	A	45	VAL	2.2
1	A	411	CYS	2.1
1	A	651	ASP	2.1
1	A	587	ILE	2.1
1	A	603	ASP	2.1
1	A	771	ASP	2.1
1	A	639	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	414	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](#)

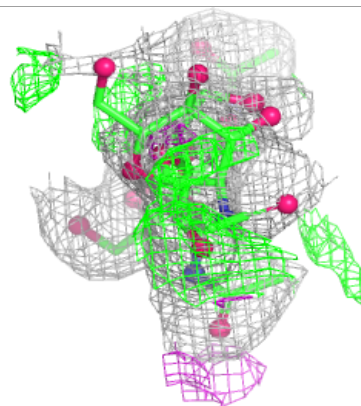
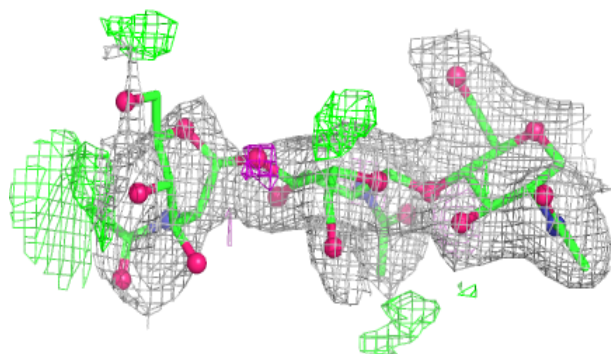
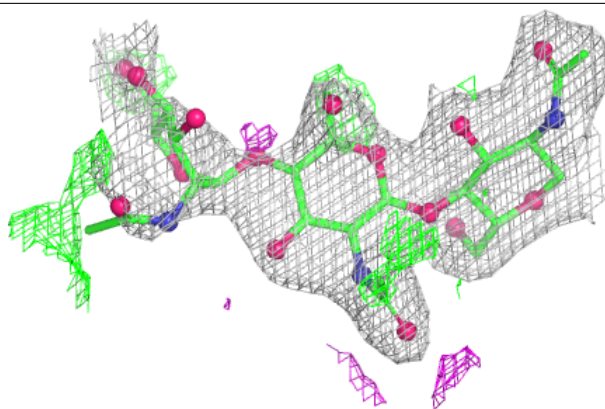
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	F	2	14/15	0.39	0.22	121,128,129,129	0
2	NAG	B	3	14/15	0.43	0.22	114,122,127,128	0
3	NAG	C	2	14/15	0.52	0.21	73,88,100,102	0
4	NAG	D	3	14/15	0.56	0.24	109,119,124,130	0
4	NAG	D	4	14/15	0.61	0.20	129,137,142,142	0
3	NAG	E	2	14/15	0.64	0.23	114,117,121,121	0
3	NAG	E	1	14/15	0.75	0.18	83,90,103,109	0
3	NAG	F	1	14/15	0.78	0.17	75,91,101,112	0
2	NAG	B	2	14/15	0.86	0.15	59,68,86,102	0
4	NAG	D	2	14/15	0.91	0.11	64,70,81,94	0
3	NAG	C	1	14/15	0.93	0.10	38,52,59,68	0
4	NAG	D	1	14/15	0.96	0.08	40,50,55,58	0
2	NAG	B	1	14/15	0.98	0.06	34,40,48,50	0

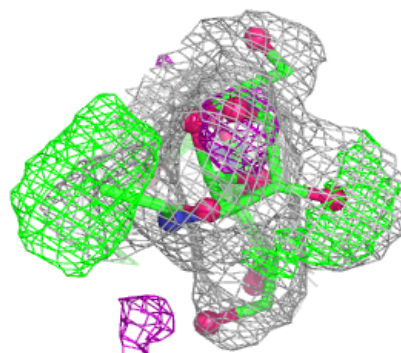
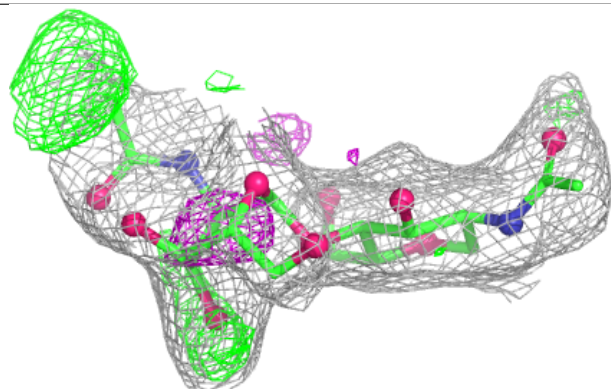
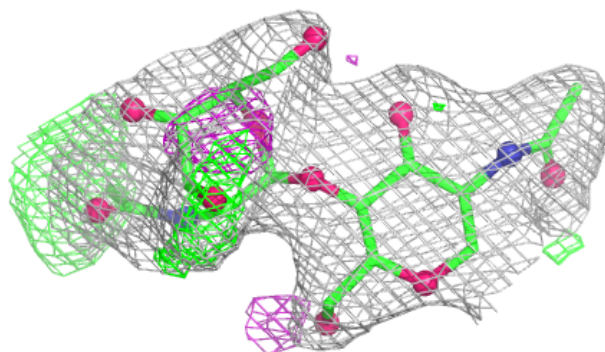
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

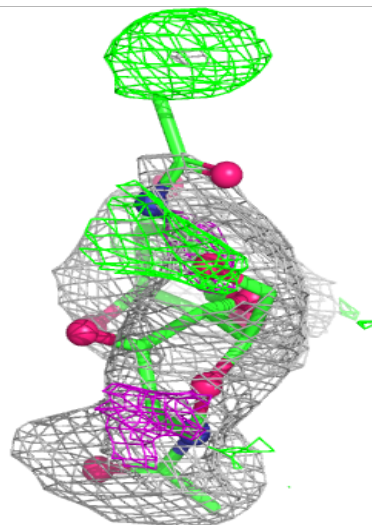
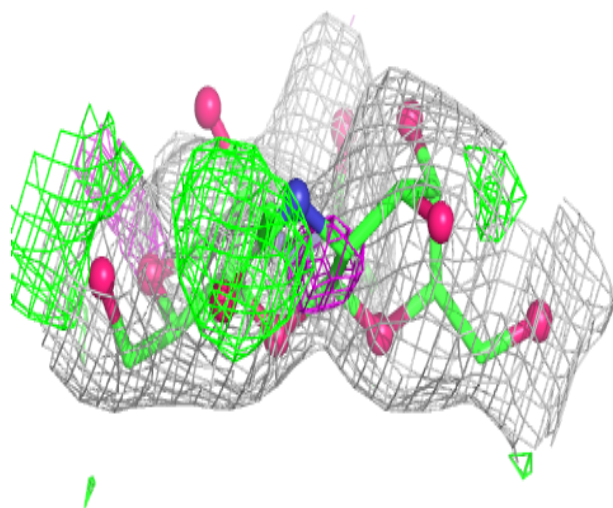
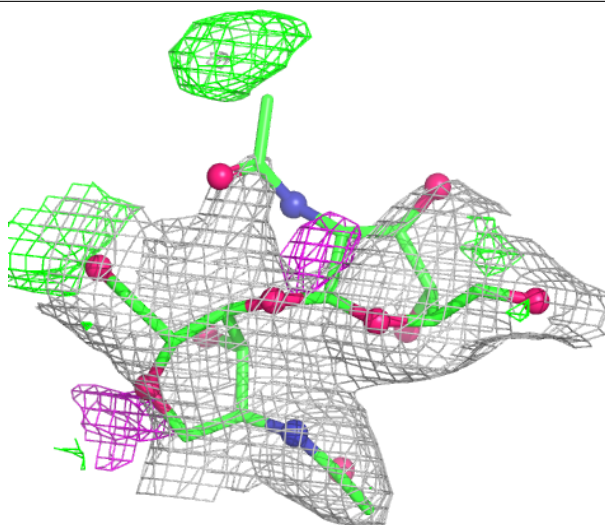
**Electron density around Chain C:**

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



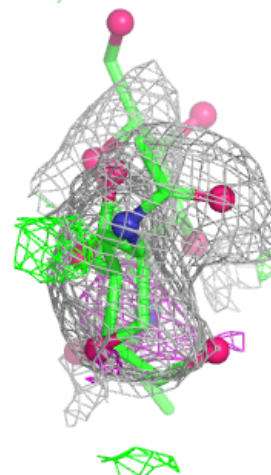
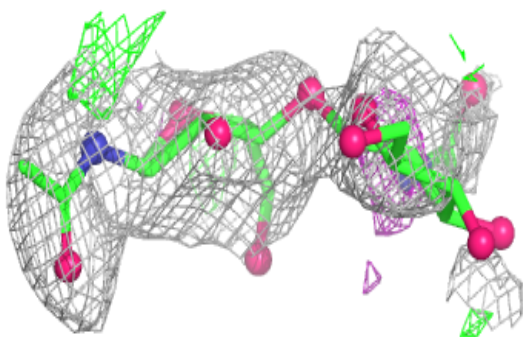
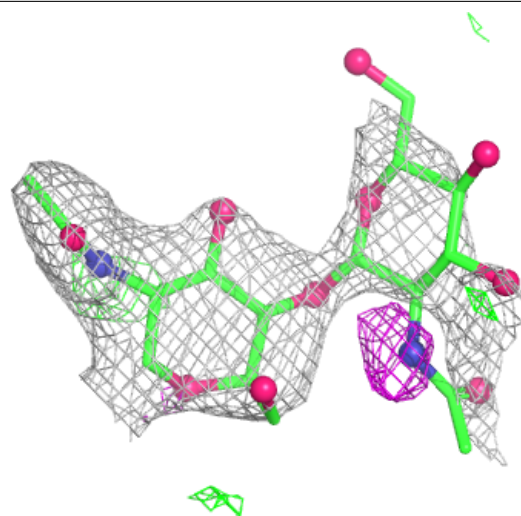
Electron density around Chain E:

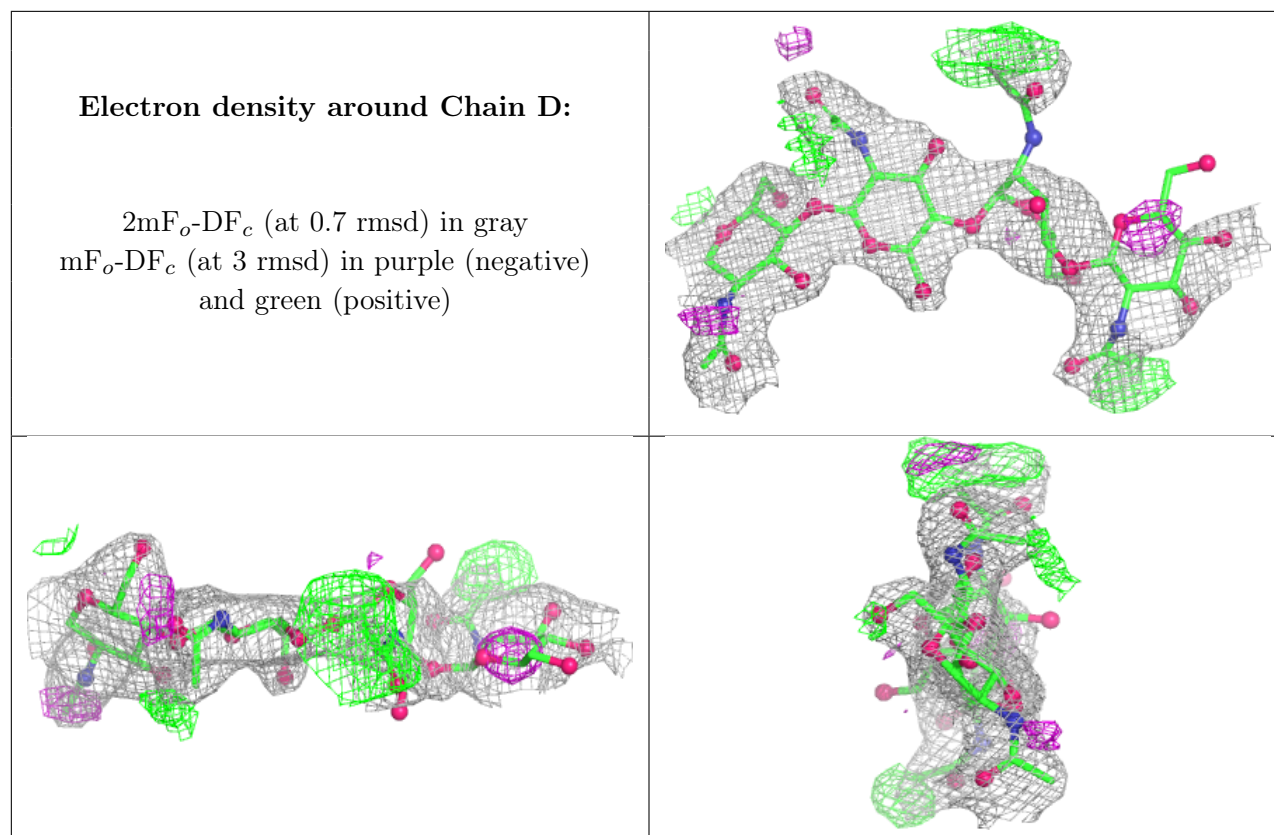
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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($\text{\AA}^2$)	Q<0.9
5	NAG	A	3511	14/15	0.65	0.15	80,87,89,90	0
5	NAG	A	5101	14/15	0.75	0.16	89,98,102,103	0
5	NAG	A	1121	14/15	0.78	0.17	82,89,97,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.