



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 07:26 AM BST

PDB ID : 5ZNN
Title : Crystal structure of ligand-free form of the Vps10 ectodomain of Sortilin
Authors : Yabe-Wada, T.; Unno, M.
Deposited on : 2018-04-10
Resolution : 2.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

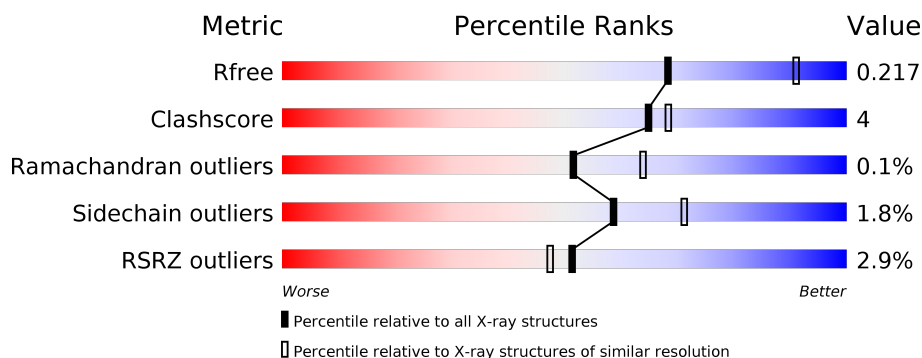
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on 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	679	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	679	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>.</div> </div> </div>
2	C	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
2	E	3	<div> <div>100%</div> </div>
2	F	3	<div> <div>100%</div> </div>
2	G	3	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10780 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 Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	6	0
			5019	3179	831	976	33			
1	B	649	Total	C	N	O	S	0	7	0
			5080	3220	836	992	32			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	745	ILE	-	expression tag	UNP Q6PHU5
A	746	GLU	-	expression tag	UNP Q6PHU5
A	747	GLY	-	expression tag	UNP Q6PHU5
A	748	ARG	-	expression tag	UNP Q6PHU5
A	749	HIS	-	expression tag	UNP Q6PHU5
A	750	HIS	-	expression tag	UNP Q6PHU5
A	751	HIS	-	expression tag	UNP Q6PHU5
A	752	HIS	-	expression tag	UNP Q6PHU5
A	753	HIS	-	expression tag	UNP Q6PHU5
A	754	HIS	-	expression tag	UNP Q6PHU5
B	745	ILE	-	expression tag	UNP Q6PHU5
B	746	GLU	-	expression tag	UNP Q6PHU5
B	747	GLY	-	expression tag	UNP Q6PHU5
B	748	ARG	-	expression tag	UNP Q6PHU5
B	749	HIS	-	expression tag	UNP Q6PHU5
B	750	HIS	-	expression tag	UNP Q6PHU5
B	751	HIS	-	expression tag	UNP Q6PHU5
B	752	HIS	-	expression tag	UNP Q6PHU5
B	753	HIS	-	expression tag	UNP Q6PHU5
B	754	HIS	-	expression tag	UNP Q6PHU5

- Molecule 2 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.



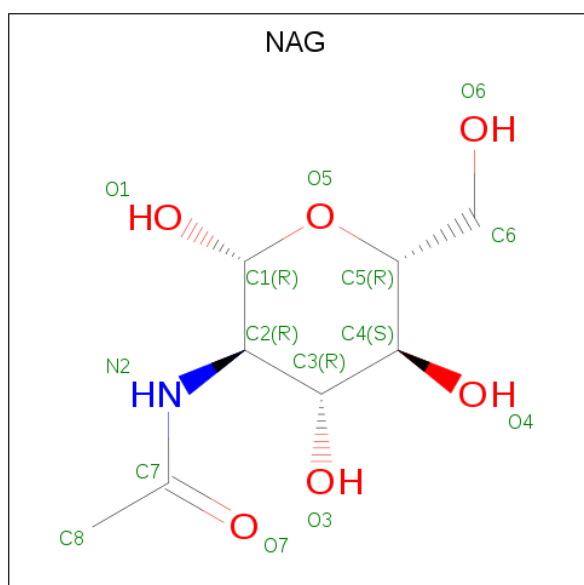
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

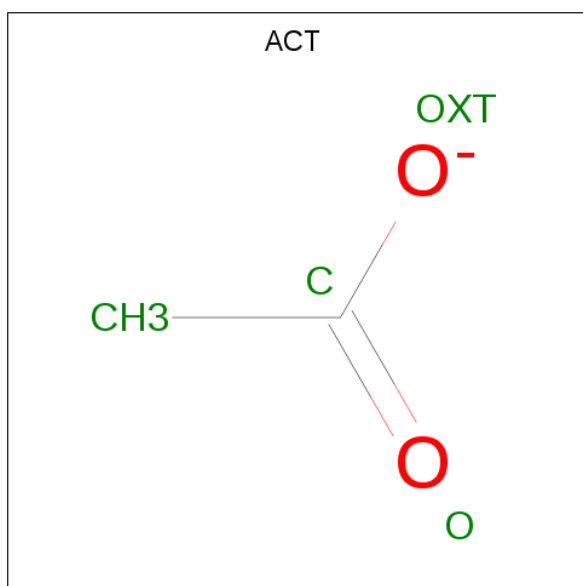


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	3	Total	Na	0	0
			3	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	190	Total 190	O 190	0	0
7	B	244	Total 244	O 244	0	0



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

Chain E:  100%



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

Chain F:  100%



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

Chain G:  67% 33%



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

Chain D:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.26Å 138.50Å 146.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.61 – 2.45 44.04 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.61-2.45) 99.5 (44.04-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.180 , 0.217 0.180 , 0.217	Depositor DCC
R_{free} test set	2950 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.9	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	0.95	EDS
Total number of atoms	10780	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: NA, BMA, NAG, ACT

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	0.26	0/5155	0.46	0/7001
1	B	0.26	0/5225	0.48	0/7090
All	All	0.26	0/10380	0.47	0/14091

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	87	LEU	Peptide

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	5019	0	4722	42	0
1	B	5080	0	4813	43	0
2	C	39	0	33	1	0
2	E	39	0	34	0	0
2	F	39	0	34	0	0
2	G	39	0	34	1	0
3	D	28	0	25	2	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	12	0	9	1	0
6	B	4	0	3	1	0
7	A	190	0	0	2	0
7	B	244	0	0	0	0
All	All	10780	0	9746	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (82) 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:129:GLN:H	1:B:499:MET:HE1	1.49	0.77
1:B:270:HIS:NE2	1:B:275:CYS:SG	2.58	0.76
1:A:412:TYR:OH	3:D:1:NAG:O7	2.03	0.75
1:A:725:MET:HG2	1:A:727:PRO:HD3	1.72	0.71
1:A:336:SER:HB2	1:A:382:ILE:HD12	1.74	0.69
1:A:368:ASP:OD1	1:A:393:TYR:OH	2.08	0.69
1:B:452:ASN:ND2	1:B:453:LYS:O	2.26	0.68
1:A:165:ARG:HH12	1:A:185:GLU:HG3	1.63	0.62
1:A:358[A]:MET:HE1	1:A:672:LEU:HD21	1.82	0.62
1:B:689:GLN:HB2	1:B:692:LEU:HD22	1.79	0.62
1:B:545:ILE:HD11	1:B:583:ILE:HD11	1.82	0.62
1:A:358[A]:MET:SD	1:A:431:GLN:NE2	2.73	0.61
1:A:545:ILE:HD12	1:A:583:ILE:HD11	1.82	0.61
1:A:545:ILE:HG22	1:A:558:TYR:HB3	1.81	0.60
1:A:96:ASN:ND2	7:A:903:HOH:O	2.34	0.59
1:B:681:GLU:HB3	2:G:1:NAG:H82	1.85	0.57
1:A:274:SER:HB2	1:B:368:ASP:HB2	1.85	0.57
1:B:691:GLU:HG2	1:B:692:LEU:HD13	1.86	0.57
1:B:418:SER:OG	1:B:420:ASP:OD1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229[A]:LEU:HD21	1:A:265:ILE:HD13	1.89	0.55
1:B:641:LEU:HB2	1:B:655:TYR:HD1	1.72	0.55
1:A:535:ILE:HD11	1:A:545:ILE:HG13	1.89	0.55
1:A:377:SER:HB3	1:A:384:TYR:CE2	2.43	0.54
1:B:588:GLU:HG2	1:B:590:PHE:O	2.08	0.53
1:A:106:LEU:HB2	1:A:595:TRP:CD1	2.44	0.52
1:A:229[A]:LEU:HD22	1:A:237:LEU:HD11	1.91	0.52
1:A:181:ILE:HD13	1:A:218:MET:HE1	1.91	0.52
1:B:336:SER:HB3	1:B:382:ILE:HD12	1.90	0.52
1:A:533:VAL:HG21	1:A:581:ILE:HD13	1.93	0.51
1:B:641:LEU:HB2	1:B:655:TYR:CD1	2.45	0.50
1:B:503:VAL:HB	1:B:517:LEU:HB2	1.94	0.50
1:A:526:LEU:HG	1:A:531:ILE:HB	1.93	0.50
1:A:477:LEU:HB3	1:A:487:ILE:HG23	1.93	0.49
1:B:251:HIS:CE1	1:B:269:THR:HG21	2.48	0.49
1:B:477:LEU:HB3	1:B:487[A]:ILE:HG23	1.95	0.48
1:B:223:GLN:HG3	1:B:262:ASN:H	1.77	0.48
1:B:121:VAL:HA	1:B:145:SER:O	2.13	0.48
1:A:121:VAL:HA	1:A:145:SER:O	2.13	0.48
1:B:459:HIS:CE1	6:B:813:ACT:H1	2.49	0.48
1:A:689:GLN:NE2	7:A:911:HOH:O	2.45	0.48
1:A:605:ILE:HD13	1:A:605:ILE:HA	1.73	0.47
1:A:629:LYS:NZ	1:A:667:SER:OG	2.42	0.47
1:B:453:LYS:C	1:B:455:GLU:H	2.18	0.47
1:A:438:LEU:HD11	1:A:513:TRP:HE1	1.81	0.46
1:A:358[B]:MET:HE2	1:A:358[B]:MET:HB3	1.81	0.46
1:A:579[B]:MET:HG3	2:C:1:NAG:H81	1.97	0.46
1:B:377:SER:HB2	1:B:384:TYR:CE2	2.50	0.46
1:A:673:CYS:SG	1:A:679:ARG:HG3	2.55	0.46
1:A:482:ALA:HB1	1:A:485:ILE:HD12	1.98	0.46
1:B:181:ILE:HD13	1:B:218:MET:HE1	1.96	0.46
1:A:229[A]:LEU:HD23	1:A:239:VAL:HG12	1.98	0.45
1:B:223:GLN:HG3	1:B:262:ASN:N	2.31	0.45
1:B:324:ARG:HD2	1:B:337:MET:SD	2.57	0.45
1:A:237:LEU:HB2	1:A:254:VAL:HG21	1.99	0.44
1:A:719:ASP:OD1	1:A:721:CYS:HB2	2.18	0.44
1:B:541:PRO:HB2	1:B:564:PRO:HB2	1.98	0.44
1:A:443:ASN:ND2	1:A:443:ASN:O	2.50	0.44
1:B:673:CYS:SG	1:B:679:ARG:HG3	2.58	0.44
1:A:418:SER:OG	1:A:420:ASP:OD1	2.31	0.43
1:B:242:ASN:ND2	1:B:245:GLU:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:VAL:HG21	1:B:581[A]:ILE:HD13	2.00	0.43
1:B:719:ASP:OD1	1:B:721:CYS:HB2	2.18	0.43
1:A:503:VAL:HB	1:A:517:LEU:HB2	2.01	0.43
1:B:482:ALA:HB1	1:B:485:ILE:HD12	2.00	0.43
1:B:241:LYS:HG2	1:B:290:LEU:HD13	2.01	0.42
1:A:701:LEU:HB3	1:A:706:GLU:HG3	2.00	0.42
1:A:665:PRO:HA	1:A:722:GLN:O	2.20	0.42
1:B:197:ARG:HD2	1:B:243:PHE:O	2.20	0.42
1:B:720:LYS:HD3	1:B:720:LYS:HA	1.82	0.42
6:A:813:ACT:H1	1:B:131:PRO:HD2	2.01	0.42
1:B:545:ILE:HG13	1:B:560:PHE:CD2	2.55	0.41
1:B:371:PHE:CD1	1:B:390:ARG:HA	2.55	0.41
1:B:569:GLY:HA3	1:B:584:TRP:CH2	2.56	0.41
1:A:353:ALA:HB1	3:D:1:NAG:H83	2.03	0.41
1:A:165:ARG:NH1	1:A:185:GLU:HG3	2.33	0.41
1:B:411:VAL:HA	1:B:428:THR:O	2.20	0.41
1:B:660:GLN:N	1:B:660:GLN:HE21	2.19	0.41
1:B:94:LEU:HG	1:B:605:ILE:HD11	2.03	0.41
1:B:629:LYS:HD3	1:B:629:LYS:HA	1.91	0.41
1:B:526:LEU:HB2	1:B:531:ILE:HB	2.04	0.40
1:A:423:ILE:HB	1:B:134:ILE:HD12	2.03	0.40
1:A:411:VAL:HA	1:A:428:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	642/679 (95%)	618 (96%)	24 (4%)	0	100	100
1	B	649/679 (96%)	625 (96%)	23 (4%)	1 (0%)	47	57
All	All	1291/1358 (95%)	1243 (96%)	47 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	652	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	549/589 (93%)	541 (98%)	8 (2%)	65	76
1	B	560/589 (95%)	547 (98%)	13 (2%)	50	63
All	All	1109/1178 (94%)	1088 (98%)	21 (2%)	59	69

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

Mol	Chain	Res	Type
1	A	274	SER
1	A	369	THR
1	A	395	THR
1	A	396	THR
1	A	419	GLU
1	A	470	LEU
1	A	494	ASP
1	A	499	MET
1	B	87	LEU
1	B	185[A]	GLU
1	B	185[B]	GLU
1	B	346	GLU
1	B	380	ARG
1	B	472	VAL
1	B	591	ILE
1	B	612	GLU
1	B	630	ASP
1	B	650	GLN
1	B	660	GLN
1	B	692	LEU
1	B	715	LYS

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

Mol	Chain	Res	Type
1	B	639	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 ⓘ

14 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	1,2	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	1.88	3 (17%)
2	BMA	C	3	2	11,11,12	0.61	0	15,15,17	0.75	0
3	NAG	D	1	1,3	14,14,15	0.44	0	17,19,21	1.53	2 (11%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	0.64	0
2	NAG	E	1	1,2	14,14,15	0.53	0	17,19,21	0.77	0
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.66	0
2	BMA	E	3	2	11,11,12	0.67	0	15,15,17	0.69	0
2	NAG	F	1	1,2	14,14,15	0.51	0	17,19,21	0.98	0
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	0.59	0
2	BMA	F	3	2	11,11,12	0.64	0	15,15,17	0.53	0
2	NAG	G	1	1,2	14,14,15	0.46	0	17,19,21	1.03	1 (5%)
2	NAG	G	2	2	14,14,15	0.50	0	17,19,21	0.70	0
2	BMA	G	3	2	11,11,12	0.65	0	15,15,17	0.82	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
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	4.35	129.10	122.90
2	C	2	NAG	C1-O5-C5	3.96	117.56	112.19
3	D	1	NAG	C1-O5-C5	3.58	117.05	112.19
3	D	1	NAG	C4-C3-C2	-3.52	105.86	111.02
2	C	2	NAG	C4-C3-C2	-3.14	106.42	111.02
2	G	1	NAG	C1-O5-C5	2.73	115.89	112.19
2	C	1	NAG	C1-O5-C5	2.23	115.21	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C3-C2-N2-C7
2	G	3	BMA	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

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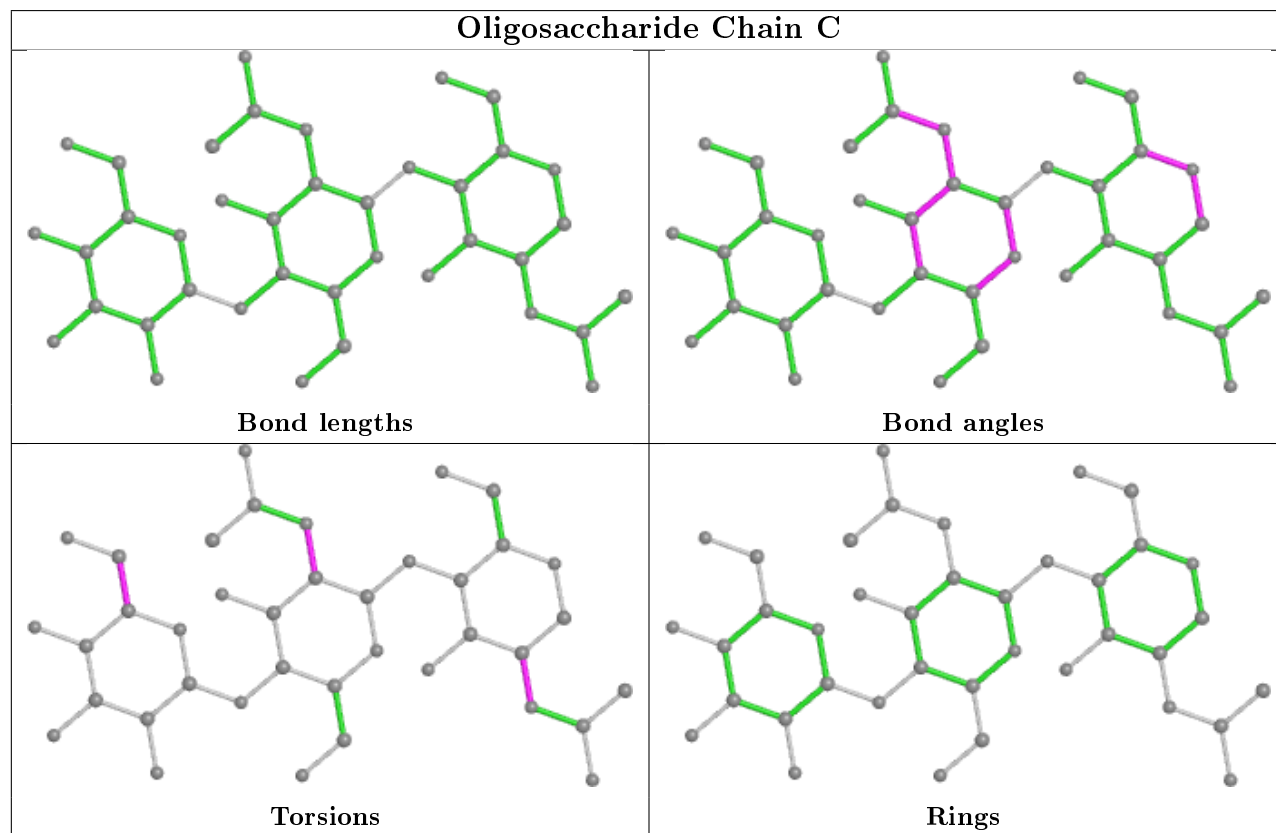
Mol	Chain	Res	Type	Atoms
2	C	3	BMA	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7
3	D	1	NAG	C3-C2-N2-C7
2	F	1	NAG	C1-C2-N2-C7

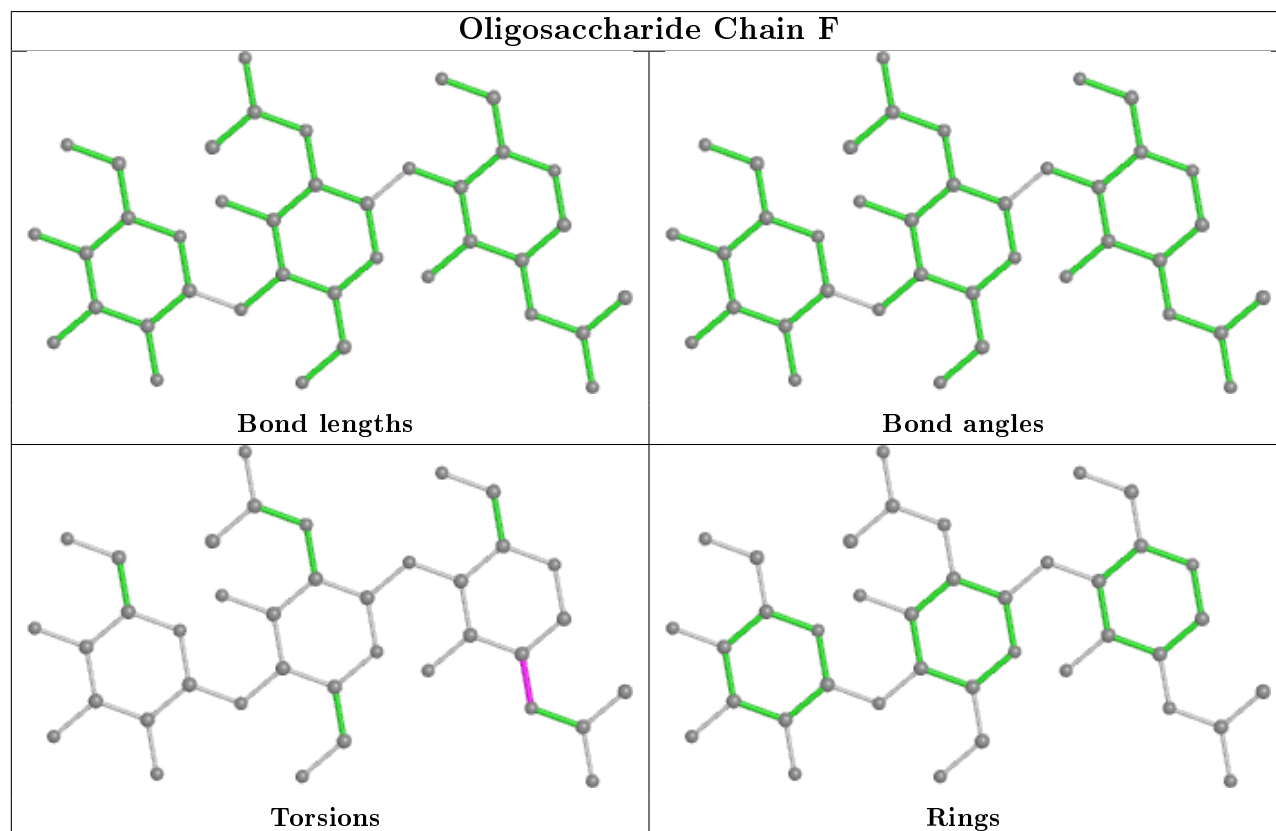
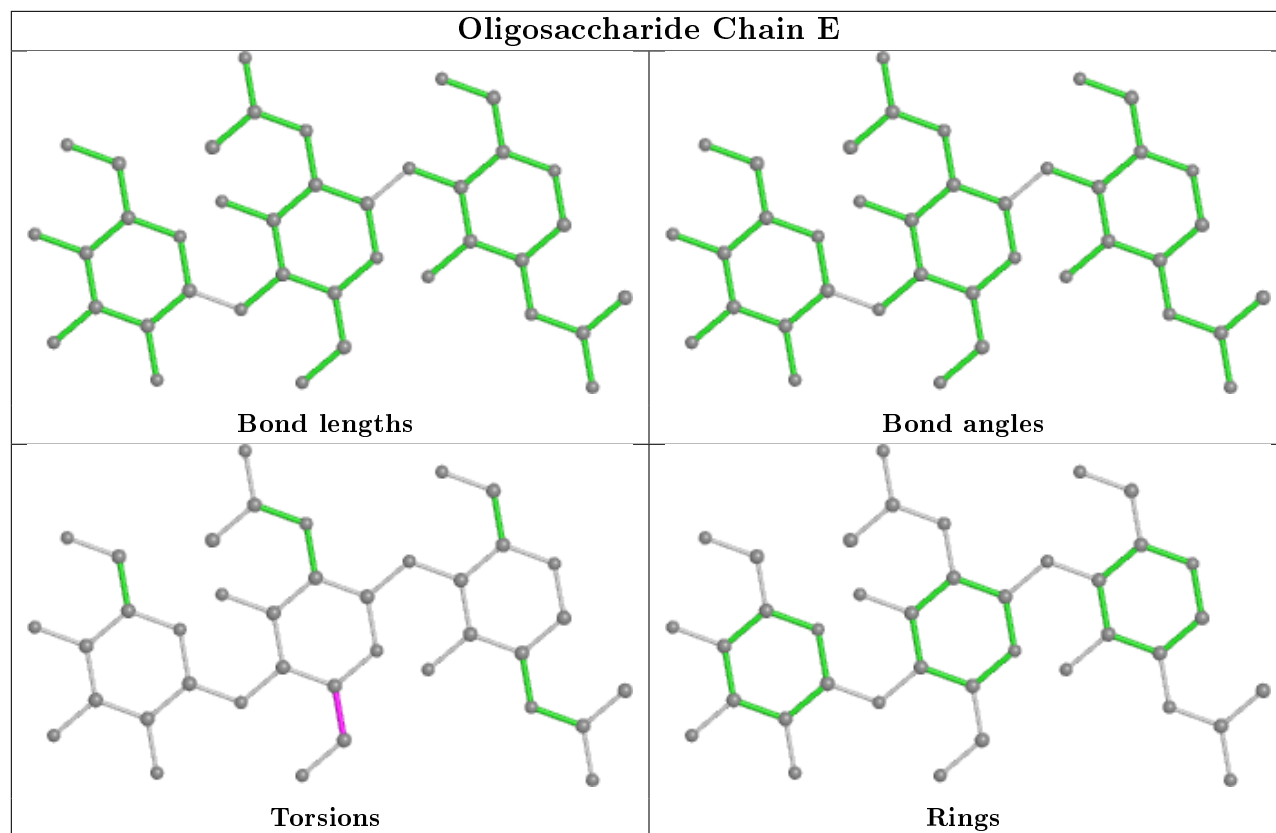
There are no ring outliers.

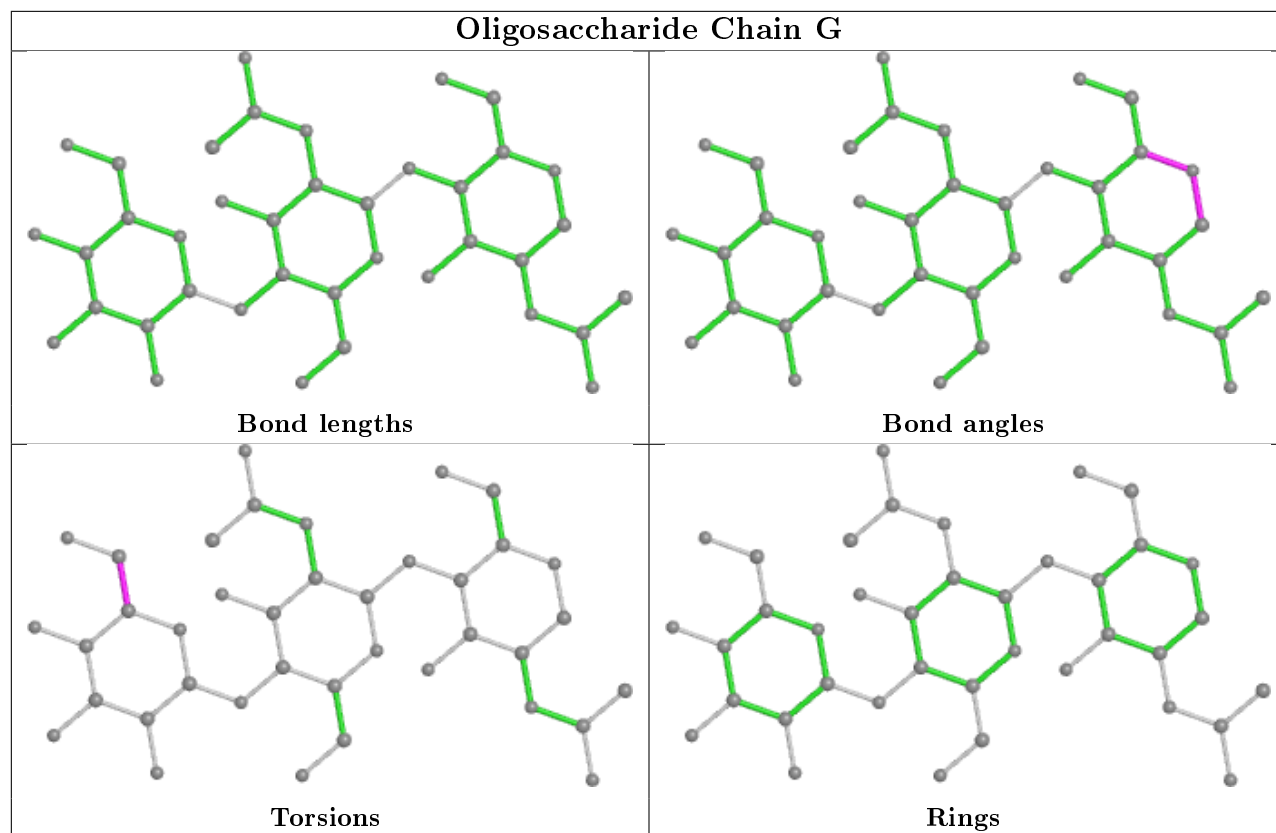
3 monomers are involved in 4 short contacts:

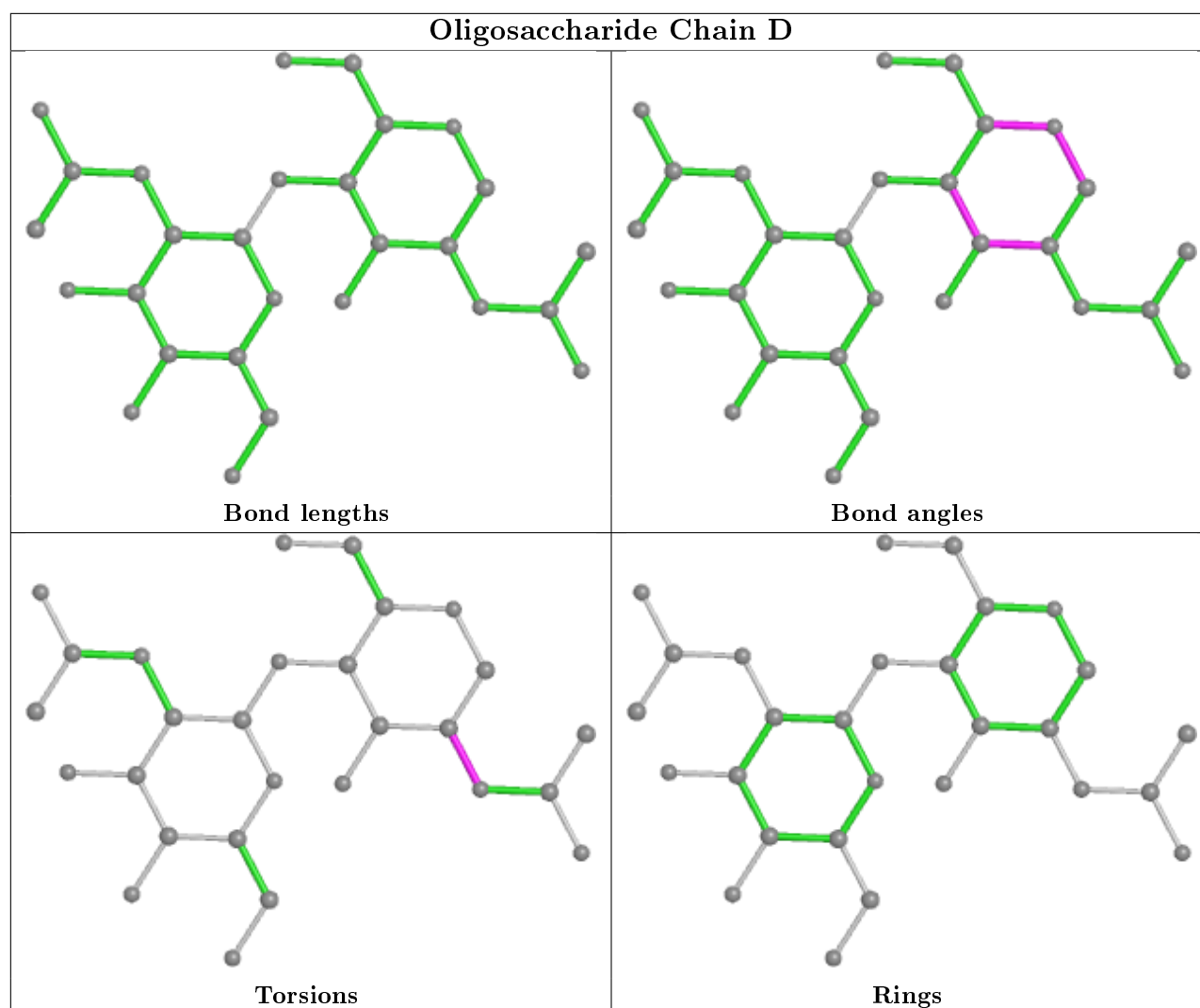
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	C	1	NAG	1	0
3	D	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\# Z > 2$
6	ACT	B	813	-	1,3,3	5.19	1 (100%)	0,3,3	0.00	-
4	NAG	A	807	1	14,14,15	0.53	0	17,19,21	0.82	0
6	ACT	A	813	-	1,3,3	6.56	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	A	811	-	1,3,3	6.46	1 (100%)	0,3,3	0.00	-
4	NAG	A	806	1	14,14,15	0.46	0	17,19,21	0.87	1 (5%)
6	ACT	A	812	-	1,3,3	6.55	1 (100%)	0,3,3	0.00	-
4	NAG	B	807	1	14,14,15	0.60	0	17,19,21	0.81	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	807	1	-	0/6/23/26	0/1/1/1
4	NAG	A	806	1	-	2/6/23/26	0/1/1/1
4	NAG	B	807	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	813	ACT	CH3-C	6.56	1.57	1.48
6	A	812	ACT	CH3-C	6.55	1.57	1.48
6	A	811	ACT	CH3-C	6.46	1.57	1.48
6	B	813	ACT	CH3-C	5.19	1.55	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	806	NAG	C1-O5-C5	2.64	115.78	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	807	NAG	C4-C5-C6-O6
4	B	807	NAG	O5-C5-C6-O6
4	A	806	NAG	C4-C5-C6-O6
4	A	806	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	813	ACT	1	0
6	A	813	ACT	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	644/679 (94%)	-0.07	11 (1%)	70 66	33, 52, 107, 176	0
1	B	649/679 (95%)	0.05	27 (4%)	36 33	24, 48, 105, 181	0
All	All	1293/1358 (95%)	-0.01	38 (2%)	51 47	24, 50, 108, 181	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	15.0
1	B	86	ARG	6.7
1	B	271	VAL	6.0
1	B	366	PRO	5.8
1	B	660	GLN	4.9
1	B	653	ARG	4.8
1	A	738	CYS	4.6
1	B	652	GLY	4.5
1	A	368	ASP	4.3
1	A	271	VAL	4.3
1	B	279	LEU	4.3
1	B	367	GLY	3.9
1	B	627	ASP	3.9
1	B	273	GLY	3.8
1	B	661	PRO	3.8
1	B	87	LEU	3.7
1	B	590	PHE	3.6
1	B	655	TYR	3.5
1	A	658	ALA	3.4
1	A	700	CYS	3.2
1	B	589	SER	3.2
1	A	86	ARG	3.2
1	A	367	GLY	3.1
1	A	660	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	636	TYR	3.0
1	B	272	ASN	3.0
1	B	324	ARG	2.9
1	A	88	PRO	2.8
1	B	656	VAL	2.7
1	B	345	GLN	2.6
1	B	454	ASN	2.4
1	B	704	LYS	2.4
1	B	322	THR	2.4
1	B	277	ALA	2.4
1	B	85	GLY	2.2
1	B	612	GLU	2.2
1	B	628	TYR	2.1
1	A	349	TYR	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 [i](#)

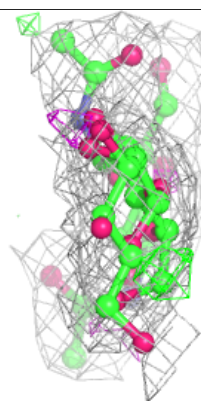
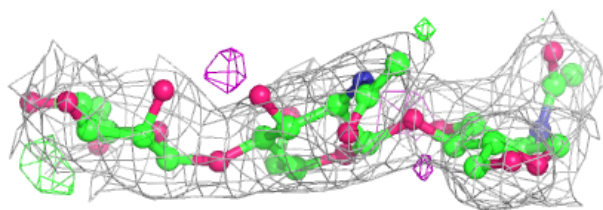
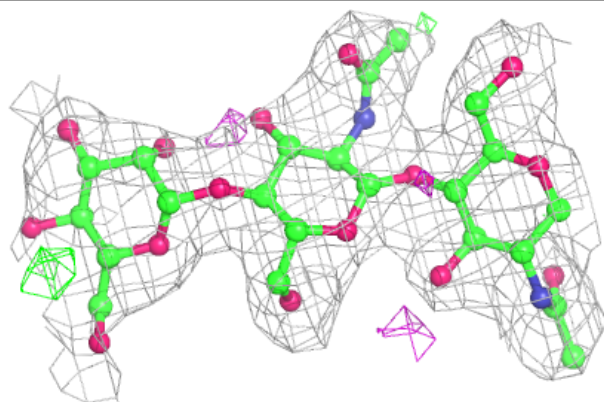
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	G	3	11/12	0.50	0.40	130,136,139,141	0
2	BMA	E	3	11/12	0.61	0.21	111,115,116,116	0
2	BMA	F	3	11/12	0.65	0.23	88,99,101,102	0
2	NAG	G	2	14/15	0.71	0.36	117,128,135,138	0
2	BMA	C	3	11/12	0.76	0.21	105,112,117,121	0
2	NAG	G	1	14/15	0.86	0.29	82,101,109,110	0
2	NAG	E	2	14/15	0.86	0.18	75,89,103,110	0
2	NAG	F	2	14/15	0.90	0.11	54,61,76,94	0
3	NAG	D	1	14/15	0.91	0.15	40,49,56,63	0
2	NAG	C	2	14/15	0.91	0.18	60,68,81,93	0
3	NAG	D	2	14/15	0.93	0.10	60,66,76,78	0
2	NAG	C	1	14/15	0.95	0.14	40,48,60,68	0
2	NAG	F	1	14/15	0.96	0.10	26,39,48,51	0
2	NAG	E	1	14/15	0.97	0.15	31,43,47,57	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.

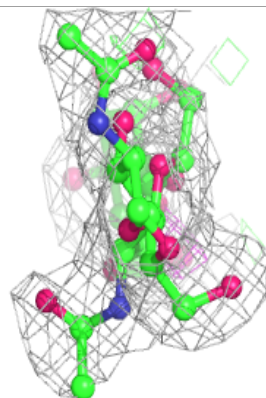
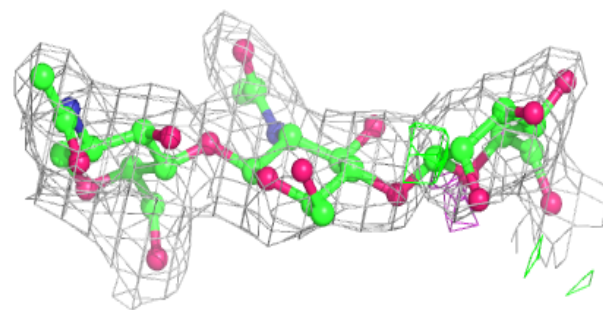
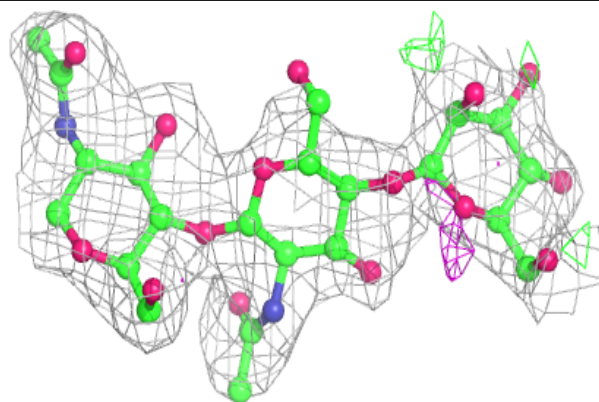
Electron density around Chain C:

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



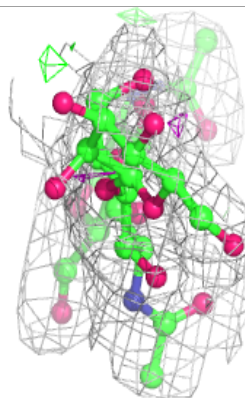
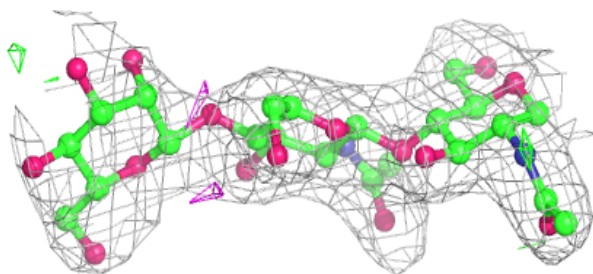
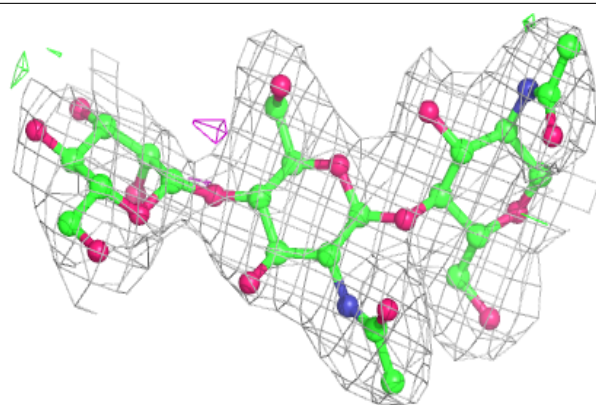
Electron density around Chain E:

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

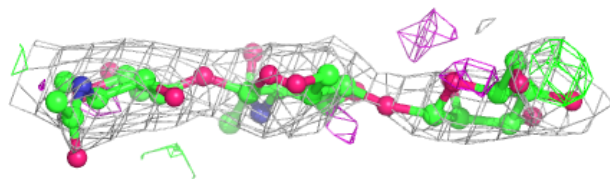
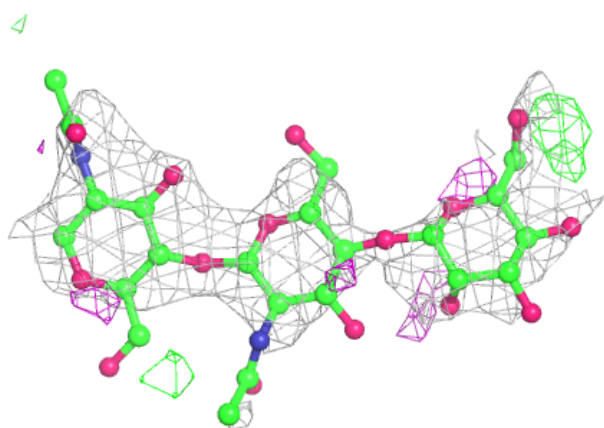


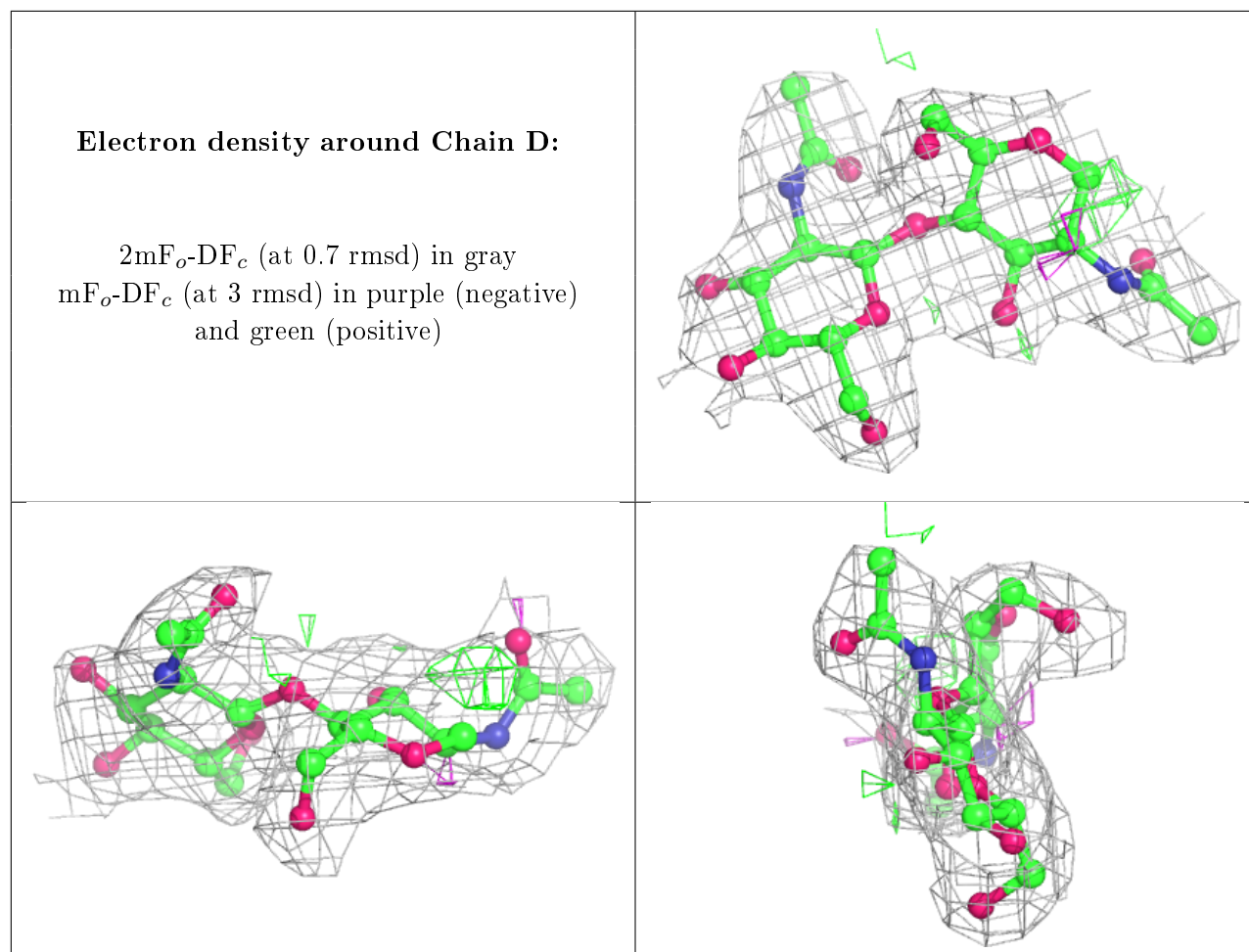
Electron density around Chain F:

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

**Electron density around Chain G:**

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





6.4 Ligands ⓘ

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
4	NAG	B	807	14/15	0.71	0.18	69,85,94,96	0
4	NAG	A	807	14/15	0.78	0.25	73,87,94,97	0
4	NAG	A	806	14/15	0.81	0.14	46,63,70,72	0
5	NA	A	809	1/1	0.85	0.59	88,88,88,88	0
6	ACT	A	812	4/4	0.86	0.11	85,88,90,91	0
5	NA	B	811	1/1	0.87	0.24	73,73,73,73	0
5	NA	A	810	1/1	0.88	0.54	88,88,88,88	0
5	NA	B	812	1/1	0.89	0.27	65,65,65,65	0
6	ACT	B	813	4/4	0.90	0.21	52,59,59,65	0
6	ACT	A	811	4/4	0.90	0.19	82,89,91,91	0
5	NA	A	808	1/1	0.94	0.69	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ACT	A	813	4/4	0.95	0.23	67,70,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.