



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:09 AM BST

PDB ID : 5NMT
Title : Dimer structure of Sortilin ectodomain crystal form 1, 2.3A
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Deposited on : 2017-04-07
Resolution : 2.30 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

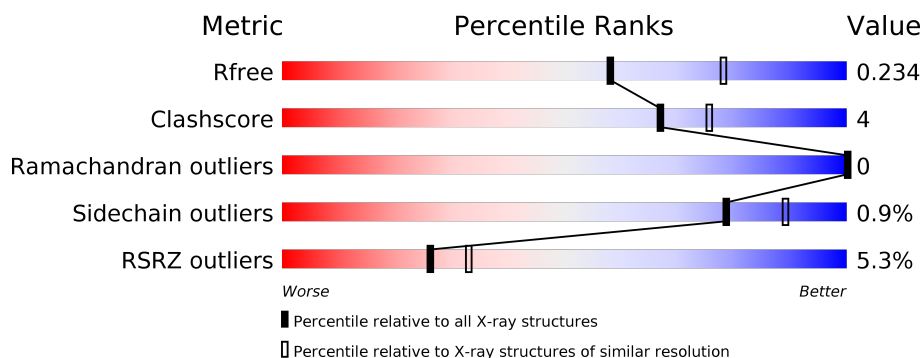
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	731	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	731	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>10%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
3	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
3	F	3	<div> <div>33%</div> <div>67%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10664 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	654	Total	C	N	O	S	0	0	0
			5146	3250	866	1001	29			
1	B	657	Total	C	N	O	S	0	1	0
			5167	3265	868	1004	30			

There are 18 discrepancies between the modelled and reference sequences:

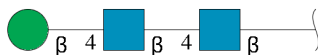
Chain	Residue	Modelled	Actual	Comment	Reference
A	723	ALA	-	expression tag	UNP Q6PHU5
A	724	ALA	-	expression tag	UNP Q6PHU5
A	725	ALA	-	expression tag	UNP Q6PHU5
A	726	HIS	-	expression tag	UNP Q6PHU5
A	727	HIS	-	expression tag	UNP Q6PHU5
A	728	HIS	-	expression tag	UNP Q6PHU5
A	729	HIS	-	expression tag	UNP Q6PHU5
A	730	HIS	-	expression tag	UNP Q6PHU5
A	731	HIS	-	expression tag	UNP Q6PHU5
B	723	ALA	-	expression tag	UNP Q6PHU5
B	724	ALA	-	expression tag	UNP Q6PHU5
B	725	ALA	-	expression tag	UNP Q6PHU5
B	726	HIS	-	expression tag	UNP Q6PHU5
B	727	HIS	-	expression tag	UNP Q6PHU5
B	728	HIS	-	expression tag	UNP Q6PHU5
B	729	HIS	-	expression tag	UNP Q6PHU5
B	730	HIS	-	expression tag	UNP Q6PHU5
B	731	HIS	-	expression tag	UNP Q6PHU5

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



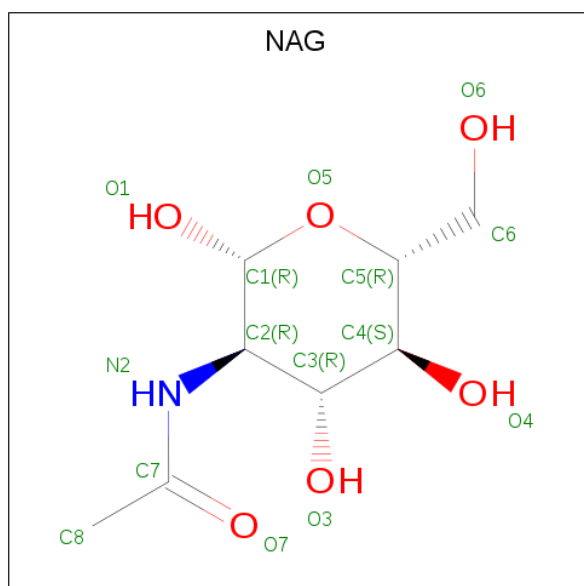
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	88	Total O 88 88	0	0
6	B	71	Total O 71 71	0	0

SER
ASN
ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS

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

Chain C:  100%

NAG1
NAG2

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

Chain E:  100%

NAG1
NAG2

- 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:  67% 33%

NAG1
NAG2
BNA3

- 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%

NAG1
NAG2
BNA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.02Å 131.13Å 154.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.64 – 2.30 69.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (69.64-2.30) 99.2 (69.64-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11 _2567: ???)	Depositor
R, R_{free}	0.205 , 0.234 0.205 , 0.234	Depositor DCC
R_{free} test set	2649 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.1	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	10664	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, CL

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	0.27	0/5265	0.47	0/7127
1	B	0.27	0/5292	0.48	0/7167
All	All	0.27	0/10557	0.47	0/14294

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	5146	0	4922	35	0
1	B	5167	0	4951	47	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	39	0	34	1	0
3	F	39	0	34	1	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	2	0	0	0	0
6	A	88	0	0	0	0
6	B	71	0	0	0	0
All	All	10664	0	10043	81	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 (81) 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:258:ASP:OD2	1:A:262:THR:OG1	2.13	0.63
1:B:305:SER:HB3	1:B:351:ILE:HD12	1.83	0.60
1:B:607:GLU:HG3	1:B:630:PRO:HB3	1.84	0.59
1:B:95:THR:HB	1:B:110:LYS:H	1.68	0.57
1:B:258:ASP:OD2	1:B:262:THR:OG1	2.16	0.57
1:B:598:LYS:NZ	1:B:639:ASP:OD2	2.38	0.56
1:B:495:LEU:HD12	1:B:500:ILE:HB	1.88	0.55
1:B:642:CYS:SG	1:B:648:ARG:HG3	2.47	0.55
1:B:304:TRP:CD1	1:B:712:LEU:HD11	2.41	0.55
1:B:407:LEU:HD11	1:B:482:TRP:HE1	1.71	0.55
1:A:431:ALA:O	1:A:435:ILE:HG12	2.07	0.54
1:B:256:THR:HG21	1:B:260:GLY:H	1.72	0.54
1:A:103:ILE:HD12	1:B:392:ILE:HB	1.89	0.53
1:A:584:TYR:CZ	1:A:622:ARG:HD3	2.44	0.53
1:B:256:THR:HG22	1:B:258:ASP:H	1.74	0.52
1:B:140:ALA:HB3	1:B:150:ILE:HB	1.92	0.52
1:A:451:ALA:HB1	1:A:454:ILE:HD12	1.92	0.51
1:A:670:LEU:HD23	1:A:671:TYR:HD2	1.76	0.51
1:A:304:TRP:CD1	1:A:712:LEU:HD11	2.46	0.51
1:A:305:SER:HB3	1:A:351:ILE:HD12	1.92	0.51
1:A:314:GLN:HG3	1:A:315:GLU:HG3	1.93	0.51
1:B:431:ALA:O	1:B:435:ILE:HG12	2.11	0.51
1:A:502:VAL:HG13	1:A:514:ILE:HG23	1.92	0.50
1:A:642:CYS:SG	1:A:648:ARG:HG3	2.51	0.50
1:A:346:SER:HB3	1:A:353:TYR:CE2	2.46	0.50
1:A:510:PRO:HB2	1:A:533:PRO:HB2	1.94	0.49
1:A:461:VAL:HG12	1:A:462:GLY:H	1.78	0.48
1:B:472:VAL:HB	1:B:486:LEU:HB2	1.96	0.48
1:A:620:ASN:OD1	1:A:622:ARG:HG2	2.13	0.48
1:B:256:THR:HG23	1:B:262:THR:O	2.14	0.47
1:B:284:VAL:HG21	1:B:712:LEU:HD23	1.96	0.47
1:A:326:ASP:O	1:A:348:ASP:HA	2.13	0.47
1:B:608:GLN:HB3	1:B:626:VAL:HB	1.97	0.47
1:B:451:ALA:HB1	1:B:454:ILE:HD12	1.96	0.47
1:B:326:ASP:O	1:B:348:ASP:HA	2.15	0.46
1:B:424:GLU:C	1:B:426:SER:H	2.19	0.46
1:A:472:VAL:HB	1:A:486:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:N	1:B:287:ASP:OD1	2.49	0.46
1:A:140:ALA:HB3	1:A:150:ILE:HB	1.98	0.46
1:B:256:THR:HG21	1:B:260:GLY:N	2.30	0.46
1:B:634:PRO:HA	1:B:691:GLN:O	2.15	0.46
1:A:640:PHE:CZ	1:A:696:PRO:HD2	2.51	0.46
1:B:198:LEU:HD23	1:B:228:TRP:CE2	2.51	0.46
1:B:239:HIS:NE2	1:B:242:GLY:O	2.44	0.46
1:A:674:GLU:HG3	1:A:705:LYS:HB3	1.98	0.45
1:A:454:ILE:HD11	1:A:520:GLU:HG2	1.97	0.45
1:B:502:VAL:HG13	1:B:514:ILE:HG23	1.98	0.45
1:B:55:ARG:HA	1:B:55:ARG:NE	2.32	0.45
1:B:90:VAL:HA	1:B:114:SER:O	2.17	0.45
1:B:414:LYS:HD2	1:B:461:VAL:HG21	1.98	0.45
1:A:598:LYS:NZ	1:A:639:ASP:OD2	2.50	0.44
1:B:572:LYS:HB3	1:B:572:LYS:HE2	1.79	0.44
1:A:284:VAL:HG21	1:A:712:LEU:HD23	1.99	0.44
1:B:510:PRO:HB2	1:B:533:PRO:HB2	2.00	0.44
1:B:291:THR:HG22	1:B:315:GLU:HG3	2.00	0.43
1:B:346:SER:HB3	1:B:353:TYR:CE2	2.53	0.43
1:B:538:GLY:HA3	1:B:553:TRP:CZ2	2.54	0.43
1:A:377:LEU:HA	1:A:377:LEU:HD12	1.89	0.43
1:A:90:VAL:HA	1:A:114:SER:O	2.18	0.43
1:A:99:VAL:HB	1:A:134:ARG:NH1	2.33	0.43
1:B:66:ASN:HB3	1:B:570:ASP:HB3	2.00	0.43
1:B:380:VAL:HA	1:B:397:THR:O	2.18	0.42
1:A:271:TYR:CG	1:A:292:ARG:HD3	2.54	0.42
1:B:370:ASP:HA	1:B:431:ALA:HB3	2.01	0.42
1:A:304:TRP:CG	1:A:712:LEU:HD11	2.54	0.42
1:B:206:LEU:HB2	1:B:223:VAL:HG21	2.01	0.42
1:B:538:GLY:HA3	1:B:553:TRP:CH2	2.54	0.42
1:A:117:TYR:HB2	3:D:1:NAG:H61	2.01	0.41
1:A:261:LYS:HD3	1:A:261:LYS:HA	1.86	0.41
1:B:261:LYS:HD3	1:B:261:LYS:HA	1.92	0.41
1:A:256:THR:HG23	1:A:262:THR:O	2.21	0.41
1:A:461:VAL:HG12	1:A:462:GLY:N	2.36	0.41
1:A:501:ILE:O	1:A:516:PHE:HA	2.21	0.41
1:B:117:TYR:HB2	3:F:1:NAG:H61	2.02	0.41
1:B:425:CYS:H	1:B:461:VAL:HG13	1.84	0.41
1:B:305:SER:HB2	1:B:671:TYR:CE1	2.55	0.41
1:A:321:LEU:HD11	1:A:331:HIS:HB2	2.02	0.40
1:B:640:PHE:CZ	1:B:696:PRO:HD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:CD1	1:B:500:ILE:HB	2.50	0.40
1:B:495:LEU:HB2	1:B:547:SER:OG	2.21	0.40
1:A:380:VAL:HG11	1:A:478:GLY: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	644/731 (88%)	621 (96%)	23 (4%)	0	100	100
1	B	652/731 (89%)	628 (96%)	24 (4%)	0	100	100
All	All	1296/1462 (89%)	1249 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/626 (91%)	568 (100%)	3 (0%)	88	95
1	B	574/626 (92%)	567 (99%)	7 (1%)	71	84
All	All	1145/1252 (92%)	1135 (99%)	10 (1%)	78	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	LEU
1	A	597	TYR
1	A	605	TYR
1	B	52	ASP
1	B	53	CYS
1	B	56	LEU
1	B	287	ASP
1	B	337	ASP
1	B	415	CYS
1	B	597	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

10 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	0.28	0	17,19,21	0.73	0
2	NAG	C	2	2	14,14,15	0.27	0	17,19,21	0.70	0
3	NAG	D	1	1,3	14,14,15	0.35	0	17,19,21	0.88	1 (5%)
3	NAG	D	2	3	14,14,15	0.36	0	17,19,21	1.45	3 (17%)
3	BMA	D	3	3	11,11,12	0.33	0	15,15,17	0.81	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	0.34	0	17,19,21	1.23	3 (17%)
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.86	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.33	0	17,19,21	0.76	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
3	BMA	F	3	3	11,11,12	0.32	0	15,15,17	0.79	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	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
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O4-C4-C3	3.52	118.48	110.35
3	D	2	NAG	O4-C4-C5	-2.77	102.42	109.30
2	E	1	NAG	O4-C4-C3	-2.58	104.39	110.35
3	D	3	BMA	O5-C1-C2	-2.49	106.93	110.77
2	E	2	NAG	C4-C3-C2	-2.21	107.78	111.02
2	E	1	NAG	C6-C5-C4	-2.20	107.85	113.00
3	F	2	NAG	O4-C4-C5	-2.17	103.92	109.30
3	D	1	NAG	O5-C5-C6	2.11	110.51	107.20
3	D	2	NAG	O5-C5-C6	2.09	110.47	107.20
2	E	1	NAG	C2-N2-C7	-2.07	119.95	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

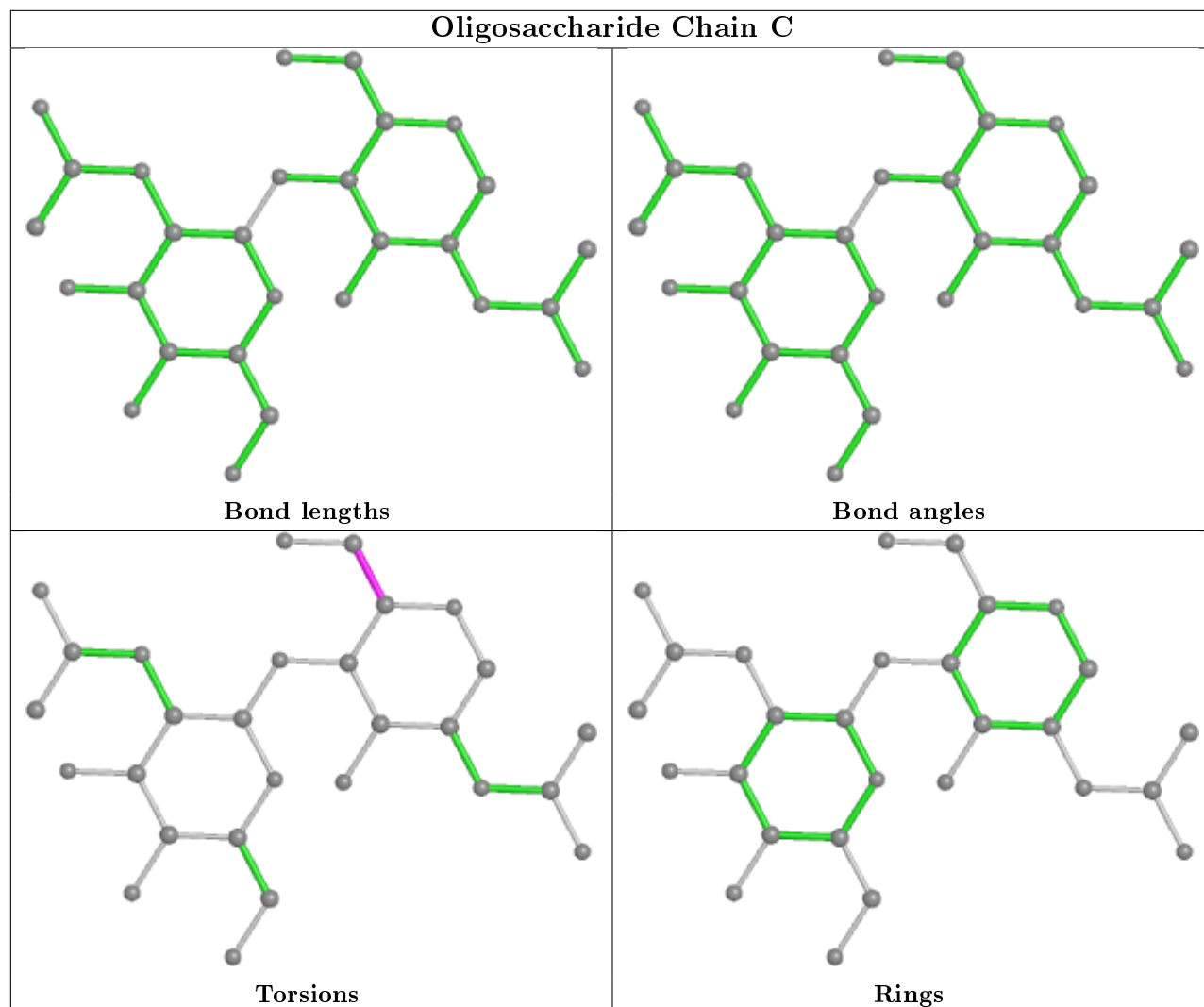
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

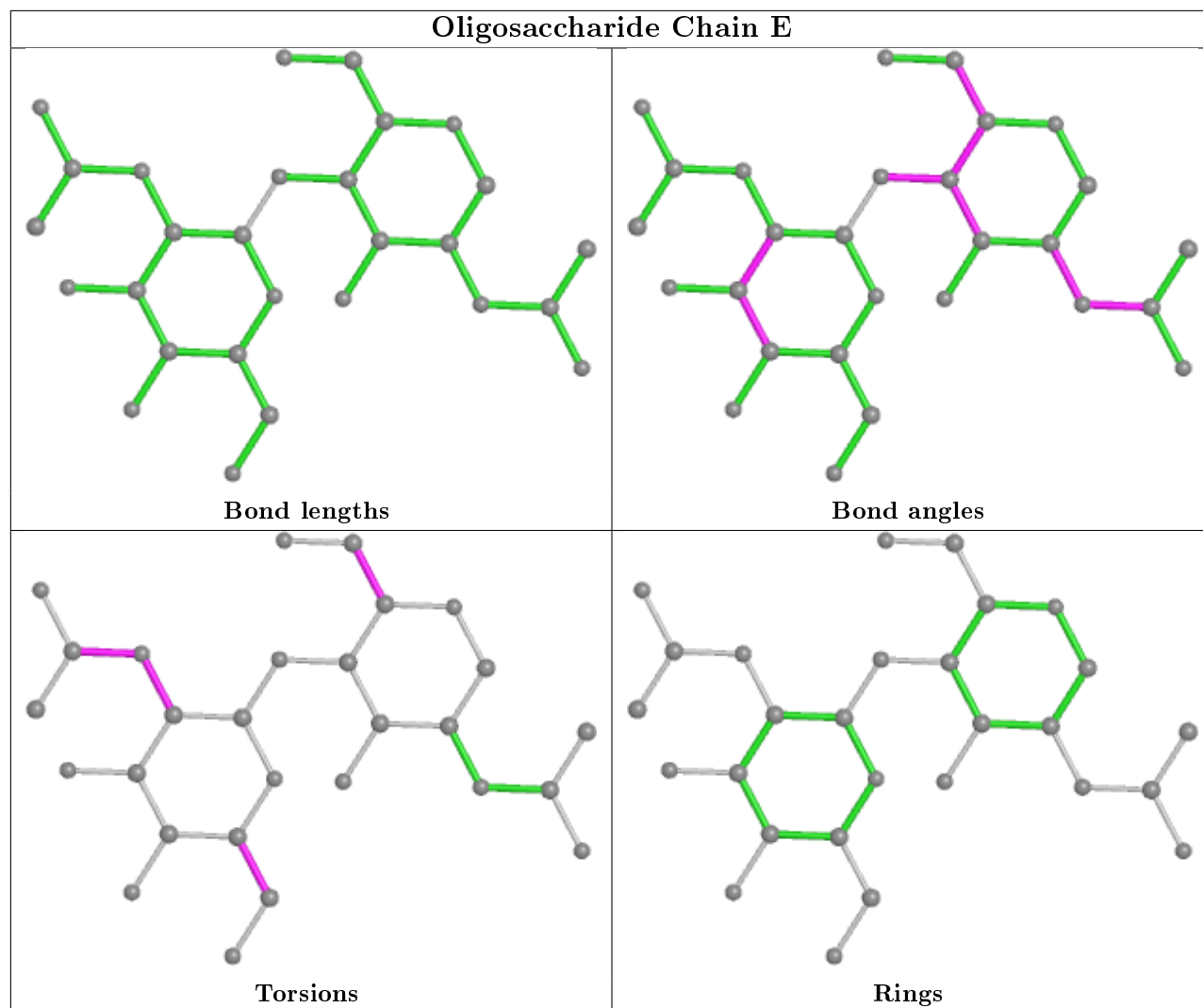
There are no ring outliers.

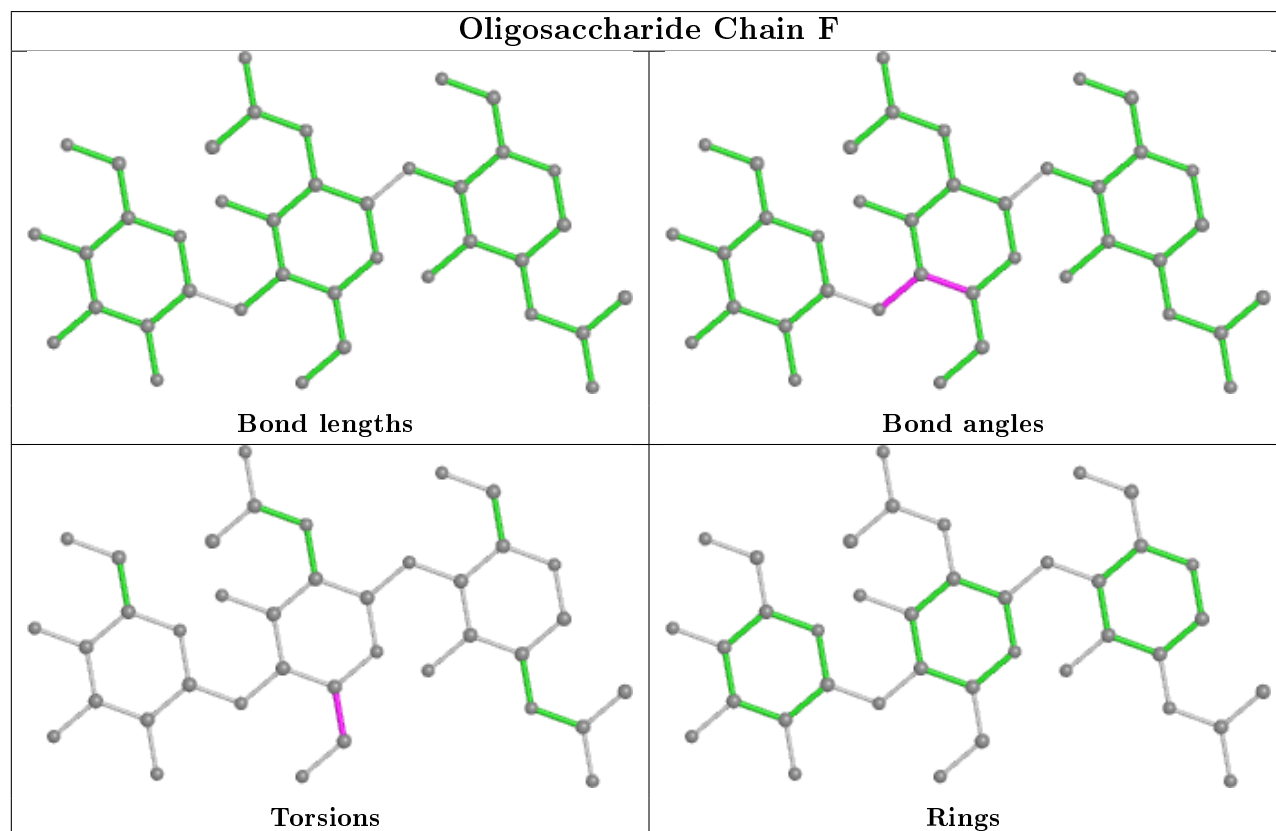
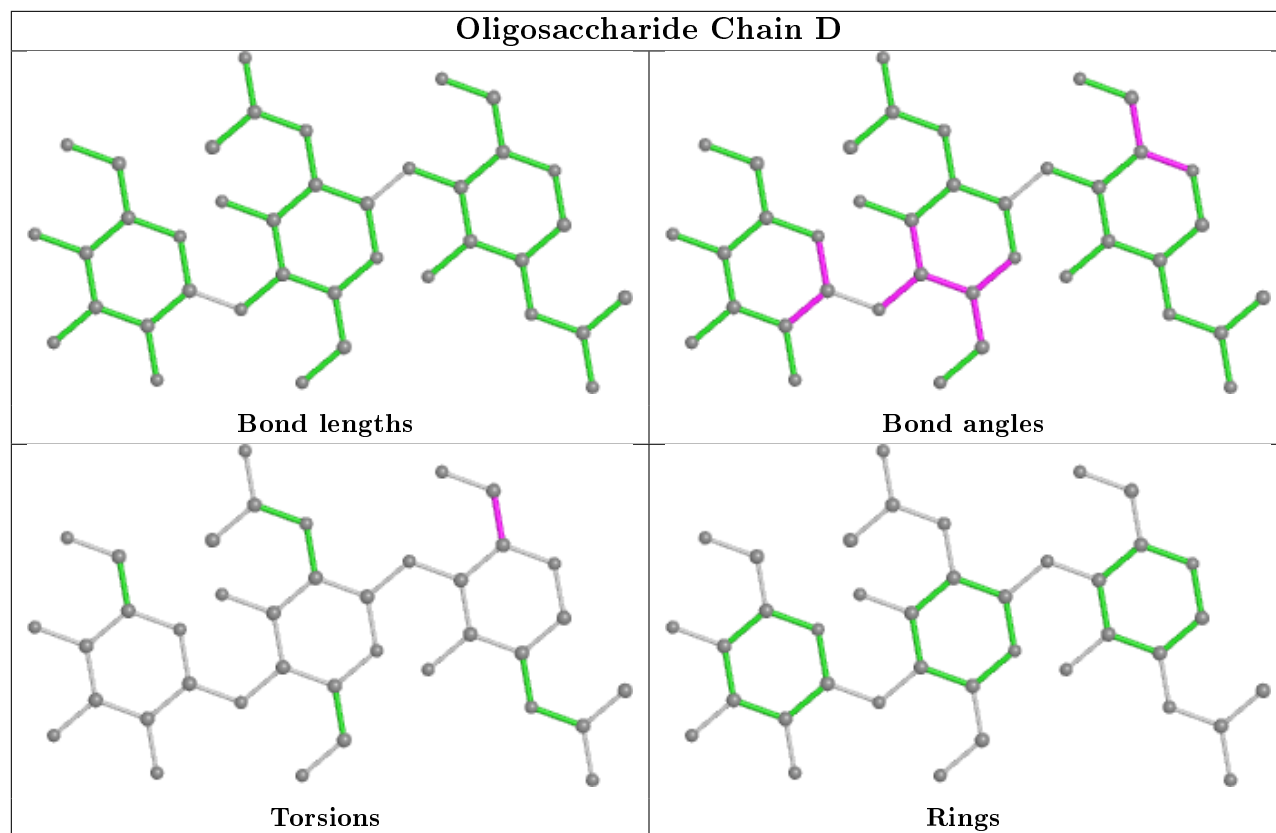
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	D	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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
4	NAG	A	807	1	14,14,15	0.29	0	17,19,21	0.70	0
4	NAG	B	801	1	14,14,15	0.29	0	17,19,21	0.71	0
4	NAG	A	801	1	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	B	807	1	14,14,15	0.26	0	17,19,21	0.70	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	B	801	1	-	0/6/23/26	0/1/1/1
4	NAG	A	801	1	-	6/6/23/26	0/1/1/1
4	NAG	B	807	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	A	801	NAG	C1-C2-N2-C7
4	A	801	NAG	O5-C5-C6-O6
4	B	807	NAG	C1-C2-N2-C7
4	A	801	NAG	C3-C2-N2-C7
4	A	801	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	807	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	654/731 (89%)	0.36	34 (5%)	27 34	34, 59, 102, 141	0
1	B	657/731 (89%)	0.37	36 (5%)	25 31	36, 60, 105, 134	0
All	All	1311/1462 (89%)	0.37	70 (5%)	26 33	34, 59, 104, 141	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	THR	8.4
1	B	56	LEU	8.4
1	A	241	ASN	6.4
1	B	627	ALA	6.2
1	A	312	VAL	5.8
1	A	627	ALA	5.6
1	B	708	THR	4.6
1	B	287	ASP	4.3
1	B	313	GLY	4.3
1	B	711	PHE	4.2
1	B	55	ARG	4.2
1	A	414	LYS	4.2
1	B	416	ASP	4.1
1	A	290	THR	4.1
1	B	312	VAL	4.0
1	A	415	CYS	3.9
1	A	289	ASP	3.8
1	A	288	LYS	3.6
1	B	626	VAL	3.6
1	A	160	ARG	3.5
1	B	628	LYS	3.3
1	A	706	LYS	3.3
1	B	420	LYS	3.3
1	B	289	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	712	LEU	3.2
1	B	160	ARG	3.1
1	A	196	TYR	3.0
1	A	625	VAL	3.0
1	B	713	ASN	2.9
1	A	514	ILE	2.8
1	B	514	ILE	2.8
1	B	561	THR	2.8
1	A	311	SER	2.7
1	A	222	ALA	2.7
1	B	261	LYS	2.7
1	B	241	ASN	2.6
1	B	314	GLN	2.6
1	B	705	LYS	2.6
1	A	221	LYS	2.6
1	B	315	GLU	2.6
1	A	58	ASP	2.6
1	A	416	ASP	2.6
1	B	707	CYS	2.6
1	B	704	LYS	2.5
1	B	581	GLU	2.4
1	A	605	TYR	2.4
1	A	286	ALA	2.4
1	A	238	THR	2.4
1	A	240	VAL	2.4
1	A	314	GLN	2.4
1	A	287	ASP	2.3
1	B	53	CYS	2.3
1	A	704	LYS	2.3
1	B	52	ASP	2.2
1	A	315	GLU	2.2
1	B	461	VAL	2.2
1	A	705	LYS	2.1
1	A	223	VAL	2.1
1	A	200	LEU	2.1
1	A	203	GLU	2.1
1	A	425	CYS	2.1
1	B	414	LYS	2.1
1	A	263	PHE	2.1
1	B	286	ALA	2.1
1	B	558	SER	2.1
1	B	709	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	GLU	2.0
1	B	221	LYS	2.0
1	B	318	TYR	2.0
1	A	259	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

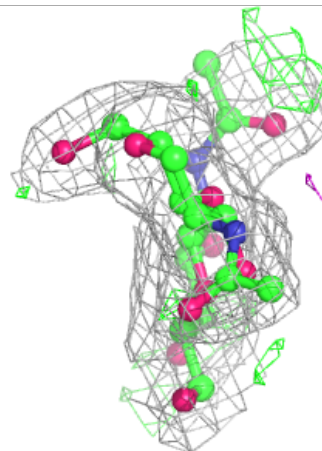
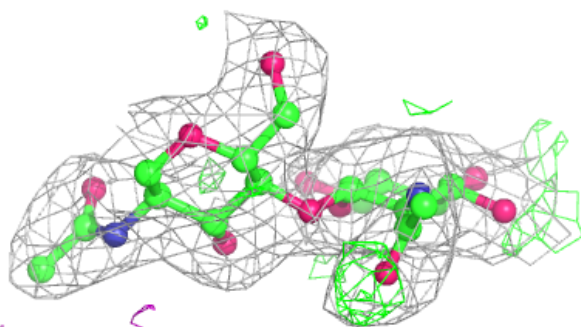
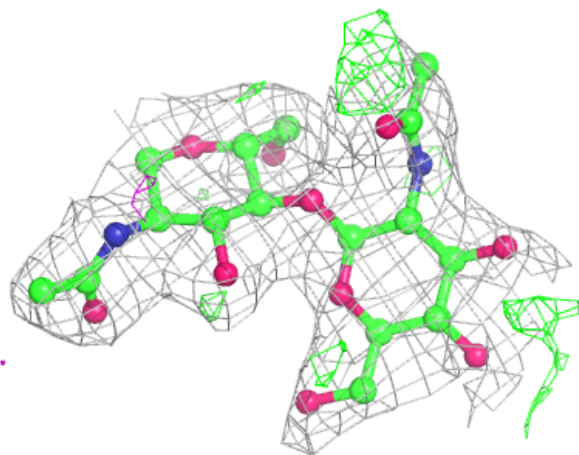
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	F	3	11/12	0.65	0.22	120,125,128,131	0
3	BMA	D	3	11/12	0.81	0.23	102,110,112,114	0
2	NAG	C	2	14/15	0.85	0.15	77,85,97,98	0
2	NAG	E	2	14/15	0.86	0.20	68,78,85,94	0
3	NAG	F	2	14/15	0.87	0.15	90,97,107,116	0
3	NAG	D	2	14/15	0.89	0.17	67,80,87,95	0
3	NAG	D	1	14/15	0.92	0.14	49,55,63,68	0
3	NAG	F	1	14/15	0.93	0.12	61,73,77,83	0
2	NAG	E	1	14/15	0.94	0.16	44,49,61,67	0
2	NAG	C	1	14/15	0.94	0.12	46,53,58,66	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.

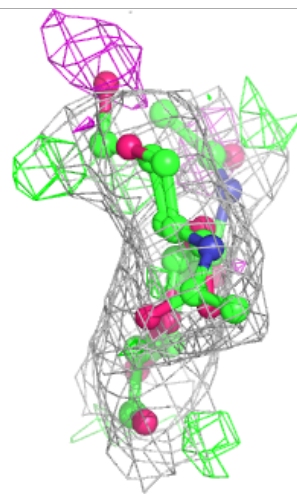
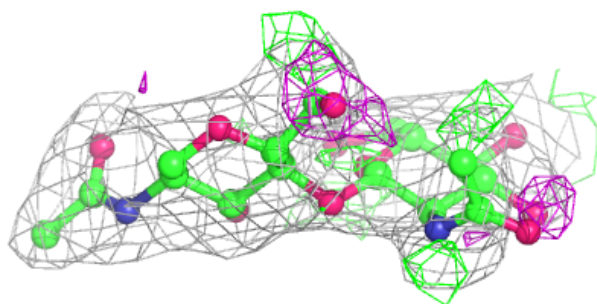
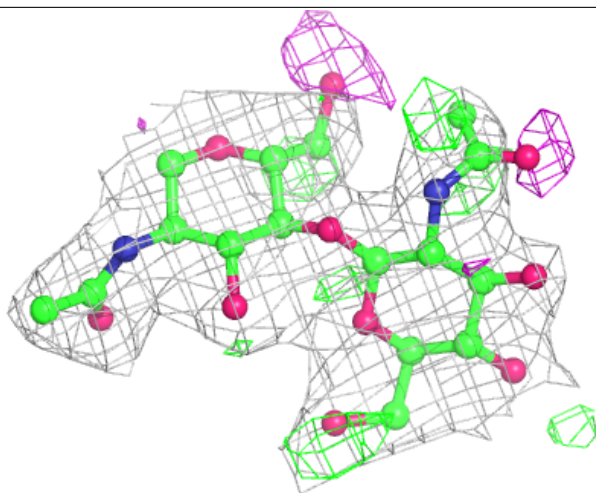
Electron density around Chain C:

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



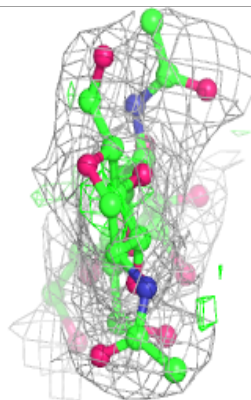
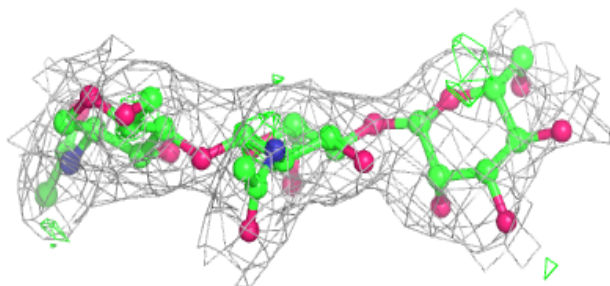
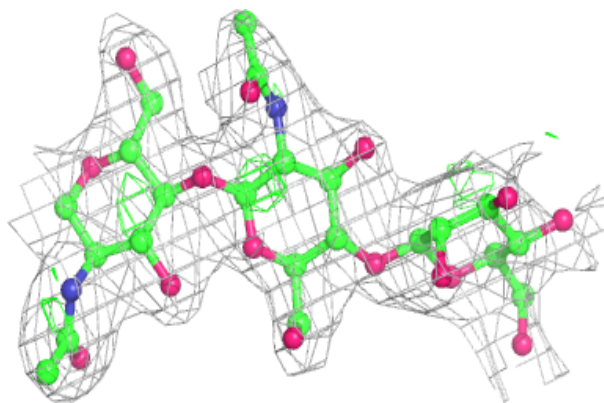
Electron density around Chain E:

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

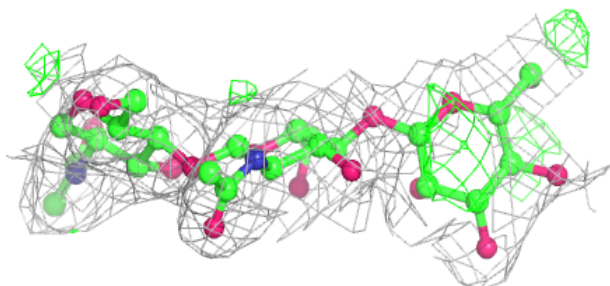
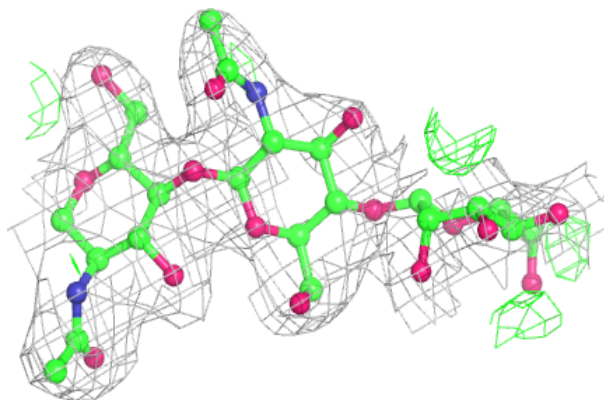


Electron density around Chain D:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
4	NAG	A	801	14/15	0.76	0.28	100,109,117,118	0
5	CL	A	808	1/1	0.78	0.17	76,76,76,76	0
4	NAG	B	807	14/15	0.86	0.18	90,99,106,112	0
4	NAG	B	801	14/15	0.88	0.20	95,100,103,105	0
4	NAG	A	807	14/15	0.90	0.13	88,96,98,101	0
5	CL	A	809	1/1	0.94	0.13	79,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.