



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 01:58 PM EDT

PDB ID : 5I81
Title : aSMase with zinc
Authors : Zhou, Y.F.; Wei, R.R.
Deposited on : 2016-02-18
Resolution : 2.25 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

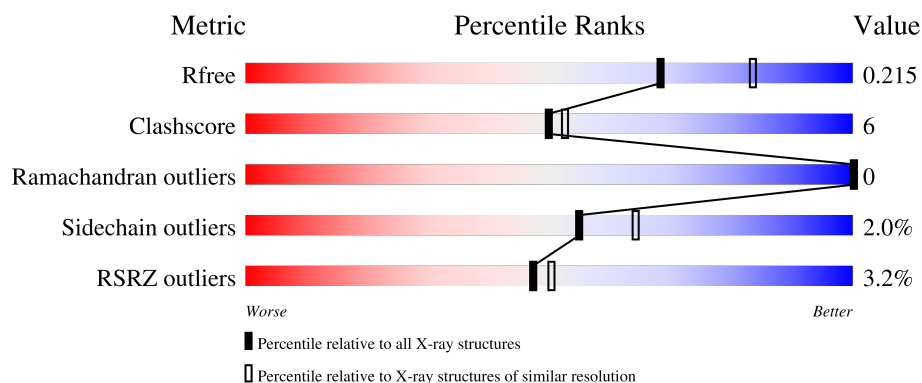
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	583	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>• 9%</div> </div> </div>
2	B	2	<div> <div>100%</div> </div>
3	C	3	<div> <div>67%</div> <div>33%</div> </div>
4	D	2	<div> <div>100%</div> </div>

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	BMA	C	3	-	-	-	X
4	MAN	D	1	-	-	-	X
5	NAG	A	701	-	-	-	X
5	NAG	A	712	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4588 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 Sphingomyelin phosphodiesterase.

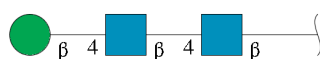
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	1	0
			4171	2690	720	738	23			

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



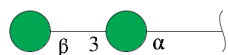
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



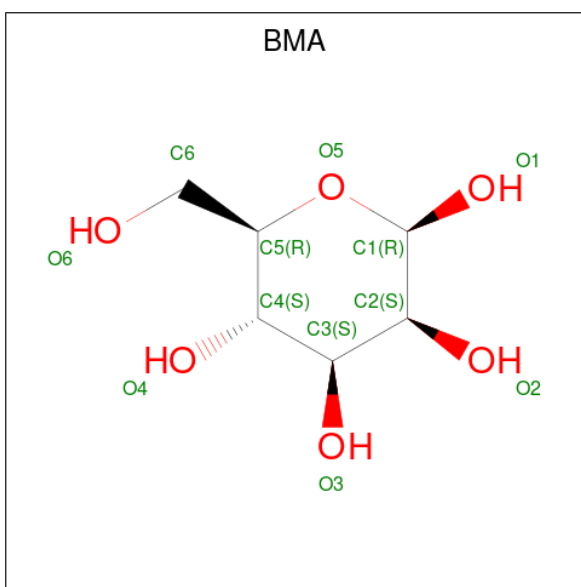
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

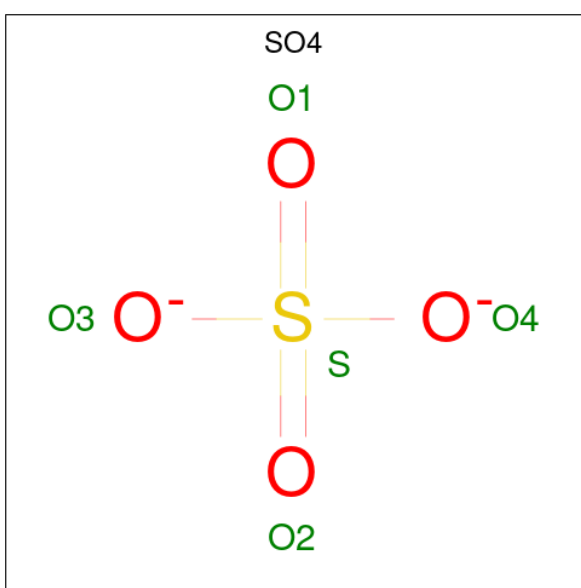


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

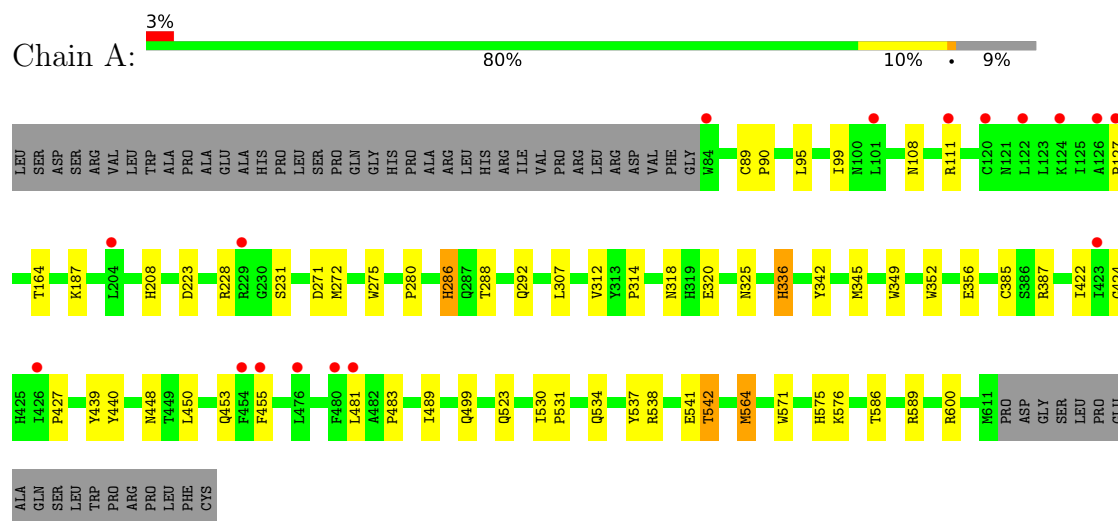
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	176	Total	O	0	0
			176	176		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

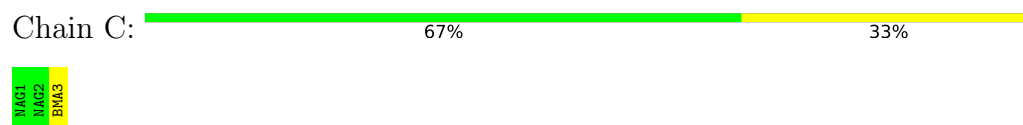
- Molecule 1: Sphingomyelin phosphodiesterase



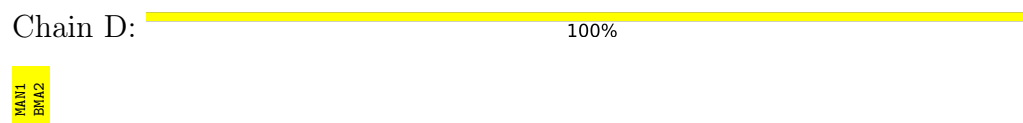
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.63Å 132.63Å 189.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.81 – 2.25 49.12 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.81-2.25) 99.7 (49.12-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.24Å)	Xtriage
Refinement program	PHENIX (dev_2229: ???)	Depositor
R, R_{free}	0.184 , 0.205 0.201 , 0.215	Depositor DCC
R_{free} test set	2326 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4588	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: ZN, MAN, BMA, NAG, SO4

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	0.60	0/4318	0.68	1/5919 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	307	LEU	CA-CB-CG	-6.54	100.26	115.30

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	4171	0	4033	44	0
2	B	28	0	24	0	0
3	C	39	0	33	0	0
4	D	22	0	19	0	0
5	A	84	0	76	5	0
6	A	11	0	10	0	0
7	A	2	0	0	0	0
8	A	55	0	0	2	0
9	A	176	0	0	8	0
All	All	4588	0	4195	50	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 6.

All (50) 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)
5:A:713:NAG:O4	5:A:714:NAG:C1	1.64	1.43
5:A:711:NAG:O4	5:A:712:NAG:C1	1.64	1.42
5:A:711:NAG:O7	9:A:801:HOH:O	1.62	1.13
8:A:717:SO4:O1	9:A:802:HOH:O	1.85	0.94
1:A:286[A]:HIS:O	1:A:286[A]:HIS:ND1	2.12	0.82
5:A:711:NAG:C4	5:A:712:NAG:C1	2.60	0.80
1:A:292:GLN:NE2	9:A:805:HOH:O	2.25	0.69
1:A:537:TYR:HB2	1:A:542:THR:HG21	1.73	0.69
1:A:489:ILE:N	8:A:725:SO4:O1	2.24	0.67
1:A:538:ARG:NH1	1:A:541:GLU:OE1	2.27	0.67
1:A:318:ASN:HD22	1:A:325:ASN:HD21	1.46	0.64
1:A:127:PRO:HG2	1:A:223:ASP:OD1	1.97	0.63
1:A:342:TYR:HA	1:A:345:MET:HE2	1.81	0.63
1:A:108:ASN:ND2	1:A:111:ARG:HH21	2.00	0.60
1:A:95:LEU:O	1:A:99:ILE:HG12	2.03	0.58
1:A:534:GLN:NE2	9:A:803:HOH:O	2.15	0.58
1:A:318:ASN:HB2	1:A:325:ASN:HD22	1.70	0.56
1:A:538:ARG:O	1:A:542:THR:HG23	2.06	0.55
1:A:187:LYS:H	1:A:448:ASN:HD21	1.53	0.55
1:A:571:TRP:O	1:A:575:HIS:HD2	1.90	0.54
1:A:271:ASP:HB3	1:A:272:MET:CE	2.40	0.52
1:A:422:ILE:HG13	1:A:450:LEU:HD21	1.93	0.51
1:A:275:TRP:O	1:A:314:PRO:HA	2.11	0.51
1:A:318:ASN:HB2	1:A:325:ASN:ND2	2.26	0.51
1:A:356:GLU:HB2	9:A:885:HOH:O	2.10	0.51
1:A:440:TYR:CD1	1:A:600:ARG:HB2	2.47	0.48
1:A:586:THR:HA	1:A:589:ARG:NH1	2.27	0.48
1:A:208:HIS:HD2	1:A:280:PRO:O	1.95	0.48
1:A:427:PRO:HG3	1:A:481:LEU:HD13	1.95	0.48
1:A:483:PRO:HB2	1:A:576:LYS:HD3	1.96	0.48
1:A:314:PRO:HG2	1:A:349:TRP:CD2	2.48	0.48
1:A:271:ASP:O	1:A:272:MET:HG3	2.13	0.47
1:A:424:GLY:O	1:A:455:PHE:HA	2.15	0.46
1:A:312:VAL:HB	1:A:352:TRP:CD2	2.52	0.45
5:A:713:NAG:C4	5:A:714:NAG:C1	2.82	0.45
1:A:89:CYS:HB3	1:A:90:PRO:HD3	2.00	0.44
1:A:356:GLU:CB	9:A:885:HOH:O	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:HB3	1:A:272:MET:HE2	1.99	0.44
1:A:288:THR:O	1:A:292:GLN:HG2	2.18	0.44
1:A:564:MET:HE2	1:A:589:ARG:HD3	1.99	0.43
1:A:312:VAL:HB	1:A:352:TRP:CE2	2.54	0.43
1:A:336:HIS:CD2	1:A:336:HIS:H	2.36	0.43
1:A:228:ARG:HG2	1:A:231:SER:OG	2.19	0.43
1:A:455:PHE:HB2	1:A:481:LEU:HD22	2.00	0.43
1:A:575:HIS:HE1	9:A:968:HOH:O	2.02	0.42
1:A:208:HIS:CD2	1:A:280:PRO:O	2.72	0.42
1:A:530:ILE:HG13	1:A:531:PRO:HD2	2.02	0.42
1:A:387:ARG:HG3	9:A:857:HOH:O	2.20	0.42
1:A:439:TYR:OH	1:A:453:GLN:NE2	2.53	0.41
1:A:318:ASN:HD22	1:A:325:ASN:ND2	2.14	0.41

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	527/583 (90%)	506 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	449/495 (91%)	439 (98%)	10 (2%)	52 61

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

Mol	Chain	Res	Type
1	A	164	THR
1	A	286[A]	HIS
1	A	286[B]	HIS
1	A	320	GLU
1	A	336	HIS
1	A	385	CYS
1	A	499	GLN
1	A	523	GLN
1	A	542	THR
1	A	564	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	208	HIS
1	A	287	GLN
1	A	292	GLN
1	A	319	HIS
1	A	325	ASN
1	A	336	HIS
1	A	448	ASN
1	A	453	GLN
1	A	499	GLN
1	A	523	GLN
1	A	555	ASN
1	A	575	HIS

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 ⓘ

7 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	2,1	14,14,15	0.42	0	17,19,21	0.80	1 (5%)
2	NAG	B	2	2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
3	NAG	C	1	3,1	14,14,15	0.39	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.25	0	17,19,21	0.54	0
3	BMA	C	3	3	11,11,12	0.65	0	15,15,17	1.43	2 (13%)
4	MAN	D	1	4	11,11,12	0.55	0	15,15,17	1.98	5 (33%)
4	BMA	D	2	4	11,11,12	0.79	1 (9%)	15,15,17	1.44	2 (13%)

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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
4	MAN	D	1	4	-	1/2/19/22	0/1/1/1
4	BMA	D	2	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	BMA	O5-C1	-2.14	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	MAN	O3-C3-C2	4.37	118.36	109.99
4	D	2	BMA	C1-O5-C5	-4.27	106.41	112.19
4	D	1	MAN	C3-C4-C5	3.66	116.76	110.24
4	D	1	MAN	C1-O5-C5	2.94	116.18	112.19
3	C	3	BMA	C1-C2-C3	2.87	113.19	109.67
2	B	1	NAG	C1-O5-C5	2.63	115.75	112.19
3	C	3	BMA	O5-C1-C2	-2.41	107.05	110.77
4	D	1	MAN	O2-C2-C1	-2.18	104.70	109.15
4	D	1	MAN	O3-C3-C4	-2.06	105.58	110.35
2	B	2	NAG	C1-O5-C5	2.04	114.96	112.19
4	D	2	BMA	C1-C2-C3	-2.02	107.18	109.67

There are no chirality outliers.

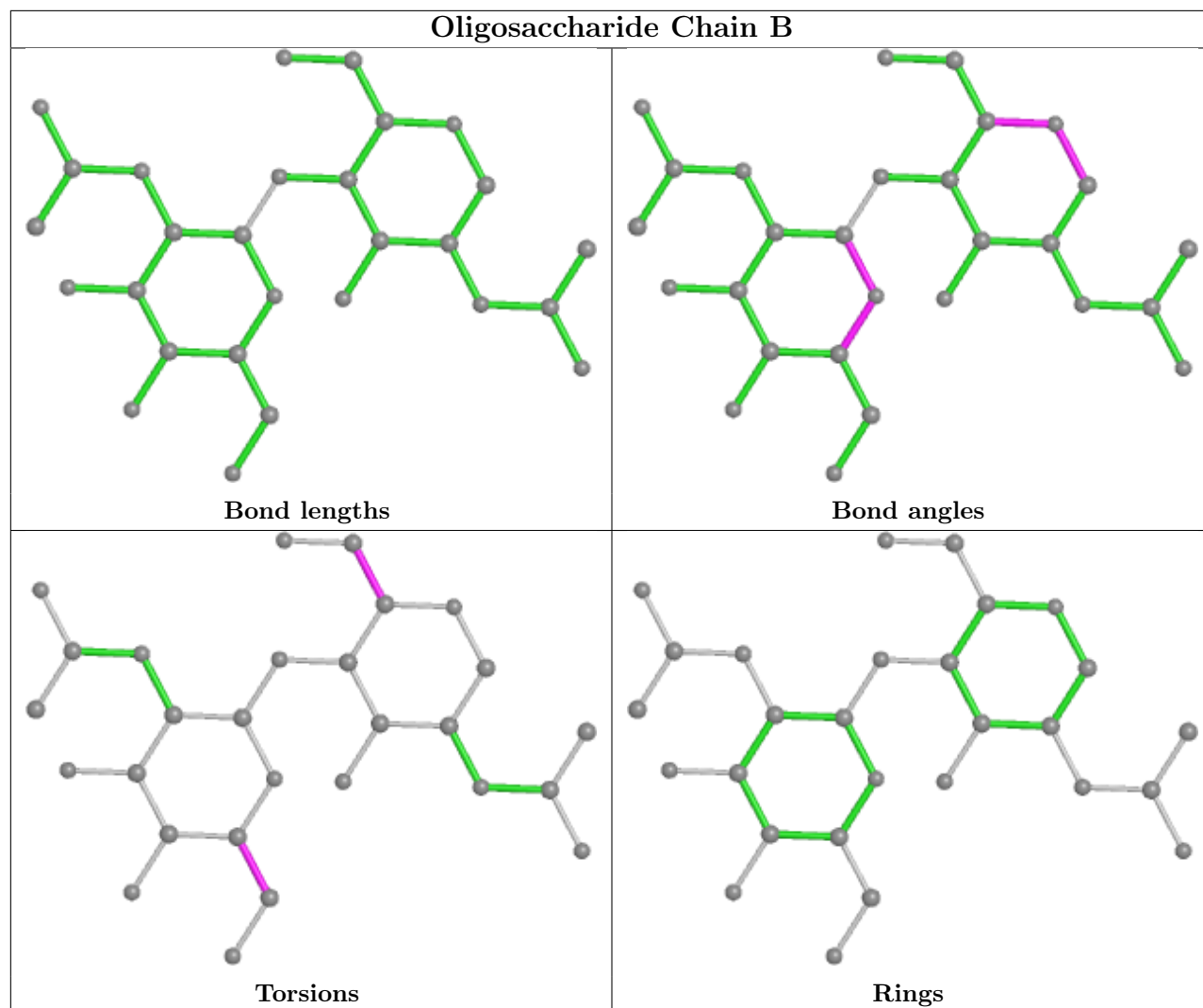
All (9) torsion outliers are listed below:

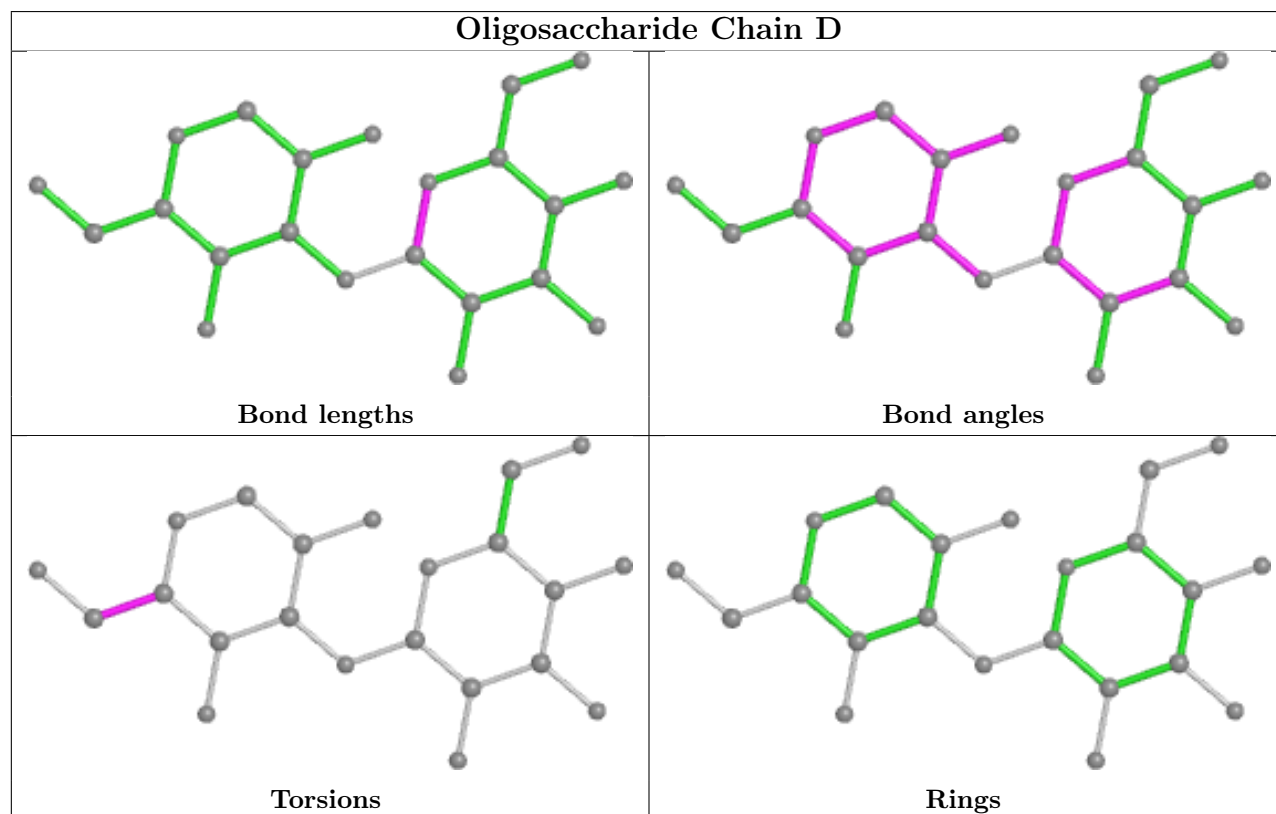
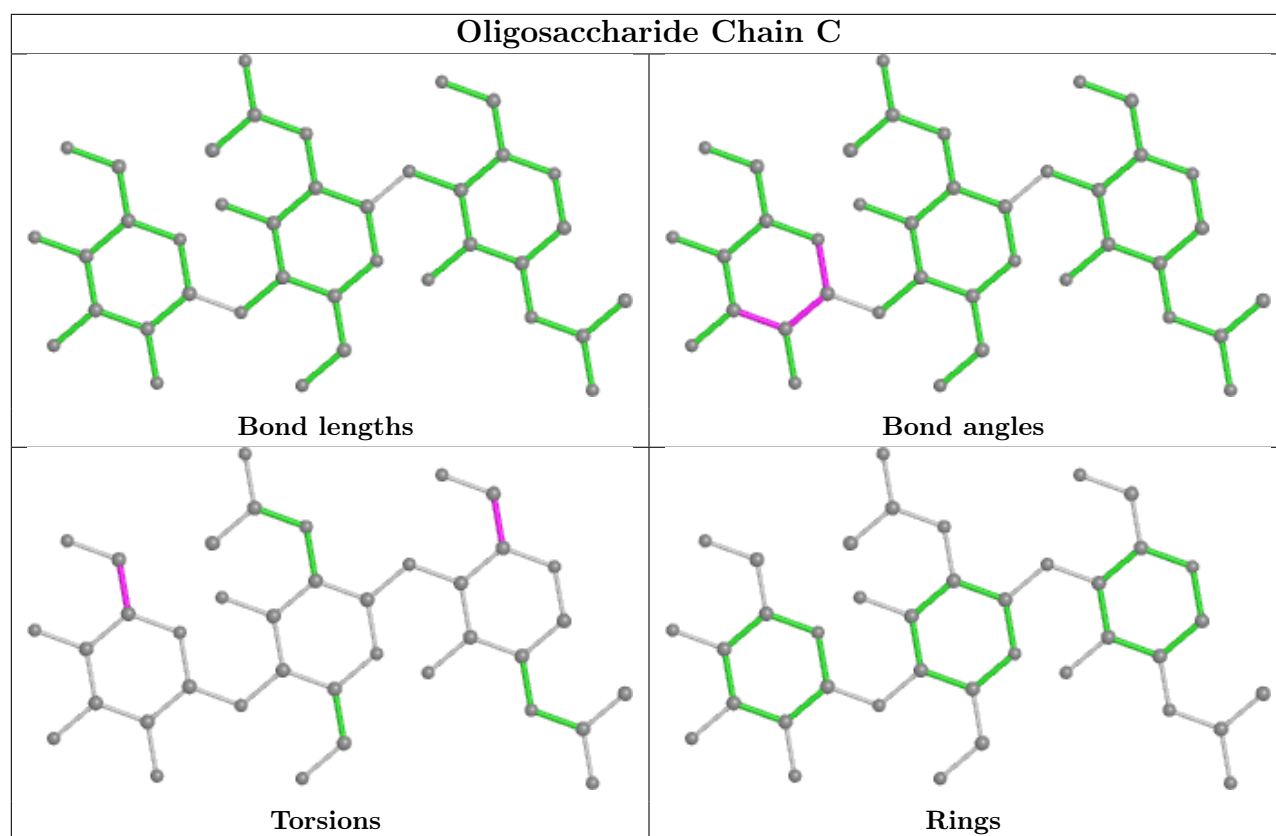
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	1	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	727	-	4,4,4	0.19	0	6,6,6	0.21	0
8	SO4	A	717	-	4,4,4	0.25	0	6,6,6	0.45	0
5	NAG	A	713	1	14,14,15	0.53	0	17,19,21	0.80	1 (5%)
5	NAG	A	701	1	14,14,15	0.19	0	17,19,21	0.51	0
5	NAG	A	702	-	14,14,15	0.61	0	17,19,21	0.47	0
8	SO4	A	718	-	4,4,4	0.05	0	6,6,6	0.33	0
8	SO4	A	725	-	4,4,4	0.17	0	6,6,6	0.66	0
8	SO4	A	722	-	4,4,4	0.09	0	6,6,6	0.20	0
5	NAG	A	712	-	14,14,15	0.89	1 (7%)	17,19,21	0.80	0
8	SO4	A	720	-	4,4,4	0.16	0	6,6,6	0.37	0
8	SO4	A	726	-	4,4,4	0.22	0	6,6,6	0.16	0
8	SO4	A	724	-	4,4,4	0.13	0	6,6,6	0.70	0
6	BMA	A	705	-	11,11,12	1.67	4 (36%)	15,15,17	1.27	2 (13%)
8	SO4	A	719	-	4,4,4	0.15	0	6,6,6	0.41	0
5	NAG	A	711	1	14,14,15	0.43	0	17,19,21	0.51	0
8	SO4	A	721	-	4,4,4	0.20	0	6,6,6	0.38	0
8	SO4	A	723	-	4,4,4	0.18	0	6,6,6	0.51	0
5	NAG	A	714	-	14,14,15	0.36	0	17,19,21	0.52	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
5	NAG	A	713	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	702	-	-	2/6/23/26	0/1/1/1
5	NAG	A	712	-	-	4/6/23/26	0/1/1/1
6	BMA	A	705	-	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	711	1	-	2/6/23/26	0/1/1/1
5	NAG	A	714	-	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	BMA	C4-C3	2.94	1.59	1.52
5	A	712	NAG	O5-C1	-2.75	1.39	1.43
6	A	705	BMA	O5-C5	2.67	1.48	1.43
6	A	705	BMA	C2-C3	2.35	1.56	1.52
6	A	705	BMA	C4-C5	2.08	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	705	BMA	C1-O5-C5	2.90	116.12	112.19
6	A	705	BMA	C3-C4-C5	2.21	114.19	110.24
5	A	713	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	712	NAG	C1-C2-N2-C7
5	A	713	NAG	C4-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	A	713	NAG	O5-C5-C6-O6
5	A	712	NAG	C4-C5-C6-O6
5	A	702	NAG	O5-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6
5	A	712	NAG	O5-C5-C6-O6
5	A	712	NAG	C3-C2-N2-C7
5	A	711	NAG	C4-C5-C6-O6
6	A	705	BMA	C4-C5-C6-O6
5	A	711	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	717	SO4	1	0
5	A	713	NAG	2	0
8	A	725	SO4	1	0
5	A	712	NAG	2	0
5	A	711	NAG	3	0
5	A	714	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	528/583 (90%)	0.04	17 (3%)	47 50	35, 55, 84, 111	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	TRP	4.6
1	A	122	LEU	3.5
1	A	481	LEU	3.0
1	A	454	PHE	2.8
1	A	126	ALA	2.5
1	A	423	ILE	2.5
1	A	120	CYS	2.4
1	A	111	ARG	2.4
1	A	455	PHE	2.4
1	A	127	PRO	2.3
1	A	426	ILE	2.3
1	A	204	LEU	2.3
1	A	124	LYS	2.2
1	A	229	ARG	2.2
1	A	480	PHE	2.0
1	A	101	LEU	2.0
1	A	476	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.

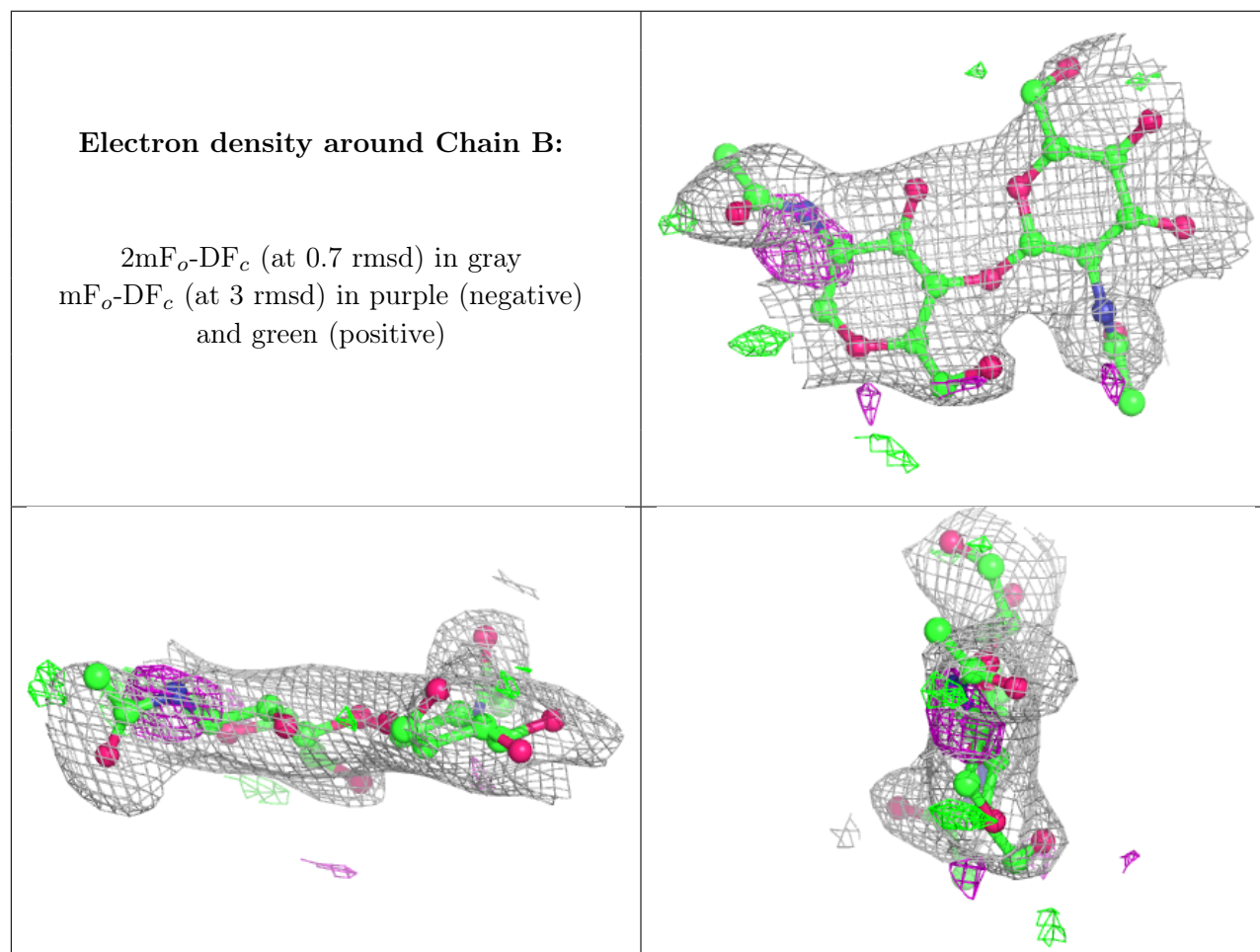
6.3 Carbohydrates [i](#)

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.

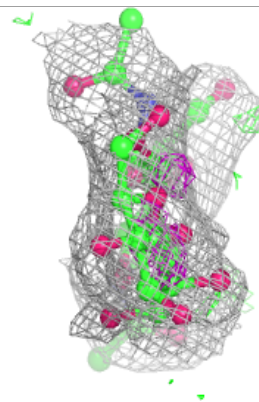
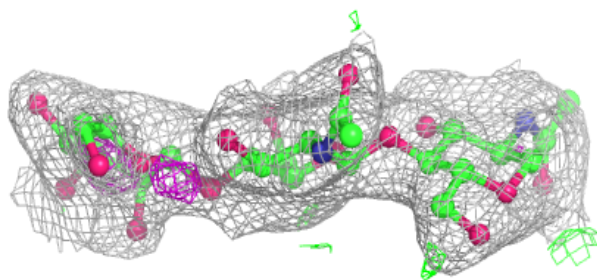
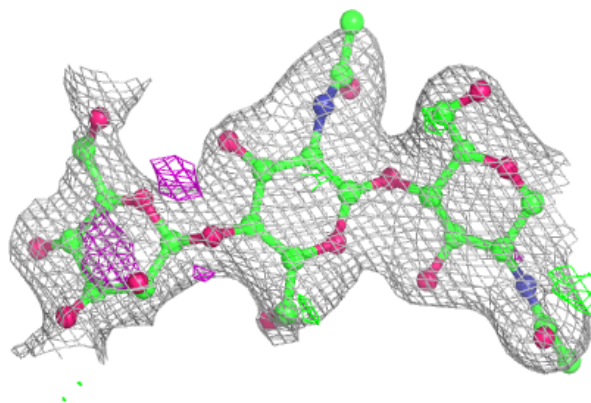
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	1	11/12	0.66	0.42	100,105,108,111	0
3	BMA	C	3	11/12	0.77	0.44	108,110,111,111	0
4	BMA	D	2	11/12	0.80	0.35	93,96,99,99	0
3	NAG	C	2	14/15	0.84	0.31	82,90,99,104	0
2	NAG	B	1	14/15	0.85	0.25	64,77,86,86	0
2	NAG	B	2	14/15	0.88	0.25	83,89,102,104	0
3	NAG	C	1	14/15	0.92	0.17	62,75,80,83	0

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

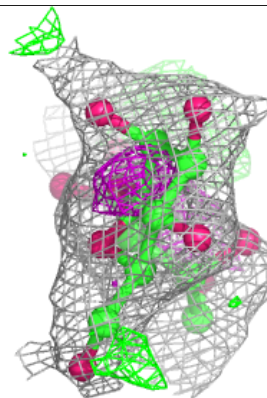
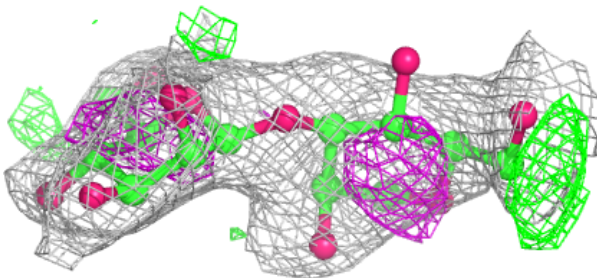
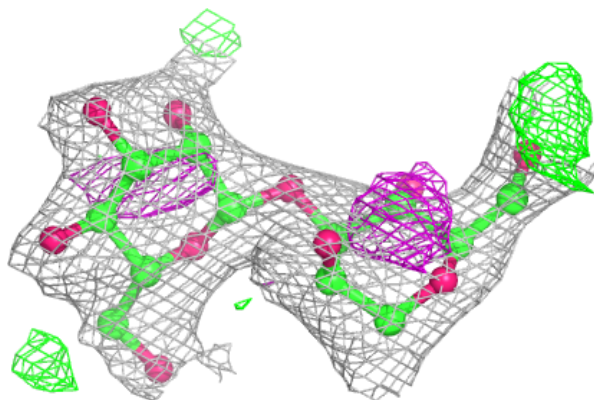


Electron density around Chain C:

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

**Electron density around Chain D:**

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



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
5	NAG	A	701	14/15	0.50	0.44	88,92,93,94	14
6	BMA	A	705	11/12	0.62	0.28	110,114,118,120	0
8	SO4	A	726	5/5	0.74	0.38	102,103,104,105	1
8	SO4	A	725	5/5	0.75	0.32	84,85,87,91	5
5	NAG	A	712	14/15	0.77	0.42	99,107,112,113	0
5	NAG	A	702	14/15	0.82	0.30	78,88,97,98	0
8	SO4	A	727	5/5	0.83	0.36	98,98,100,103	1
8	SO4	A	724	5/5	0.85	0.17	91,94,97,100	1
5	NAG	A	714	14/15	0.86	0.25	92,107,113,116	0
8	SO4	A	723	5/5	0.86	0.26	87,87,88,89	1
8	SO4	A	722	5/5	0.87	0.39	91,93,94,96	1
5	NAG	A	711	14/15	0.91	0.23	58,73,80,90	0
8	SO4	A	719	5/5	0.91	0.23	101,101,104,105	1
8	SO4	A	718	5/5	0.92	0.18	90,90,90,90	5
5	NAG	A	713	14/15	0.93	0.12	49,59,69,73	0
8	SO4	A	717	5/5	0.93	0.21	79,79,80,85	1
8	SO4	A	721	5/5	0.94	0.26	95,96,97,98	1
8	SO4	A	720	5/5	0.96	0.12	74,76,78,78	4
7	ZN	A	715	1/1	0.99	0.16	65,65,65,65	0
7	ZN	A	716	1/1	1.00	0.12	66,66,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.