



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 05:45 AM EDT

PDB ID : 2XYB  
Title : CRYSTAL STRUCTURE OF A FULLY FUNCTIONAL LACCASE FROM  
THE LIGNINOLYTIC FUNGUS PYCNOPORUS CINNABARINUS  
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Deposited on : 2010-11-17  
Resolution : 1.75 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

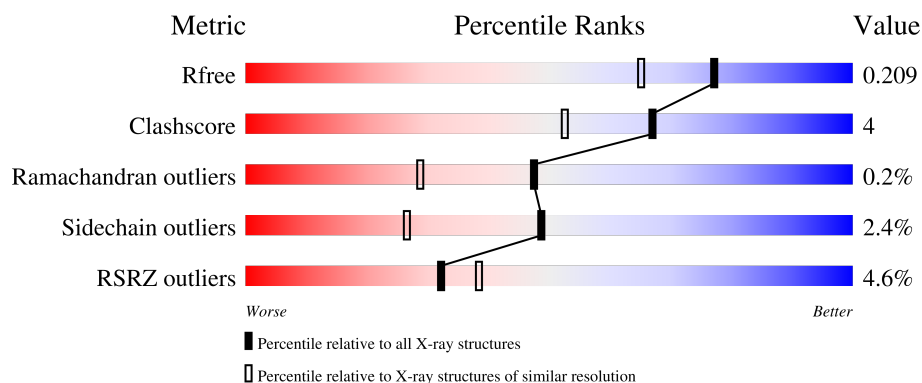
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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  $\geq 3$ , 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	497	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
2	B	4	<div> <div>50%</div> <div>50%</div> </div>
3	C	2	<div> <div>100%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
4	E	3	<div> <div>33%</div> <div>67%</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
7	NAG	A	514	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 4791 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 LACCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	8	0
			3859	2465	648	734	12			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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	B	4	Total	C	N	O	0	0	0
			50	28	2	20			

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

- Molecule 4 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.

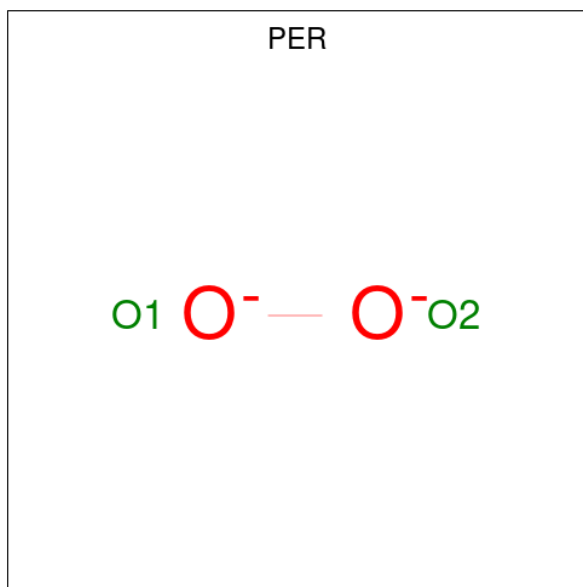


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cu	0	0
			4	4		

- Molecule 6 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



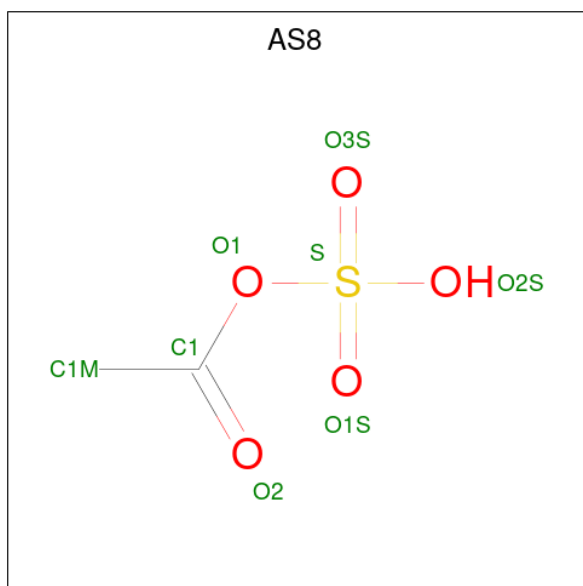
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			2	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 8 is ACETYSULFATE (three-letter code: AS8) (formula:  $C_2H_4O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	S	0	0
			8	2	5	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	Zn	0	0
			8	8		

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	Na	0	0
			1	1		

- Molecule 14 is water.

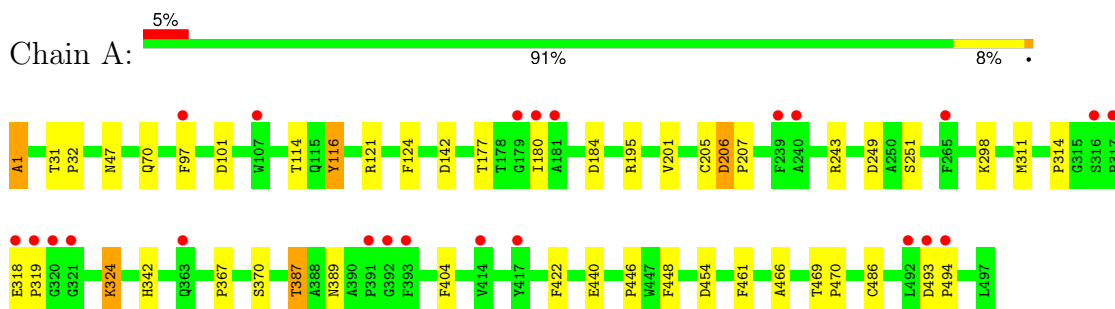
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	712	Total	O	0	0
			712	712		



### 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.

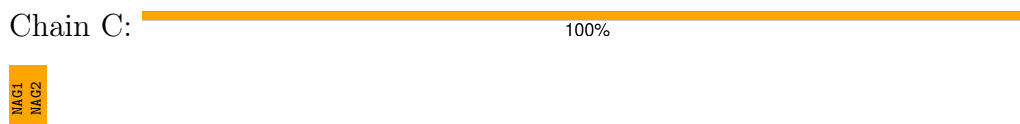
- Molecule 1: LACCASE



- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.30Å 62.90Å 91.42Å 90.00° 126.70° 90.00°	Depositor
Resolution (Å)	72.55 – 1.75 45.67 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.55-1.75) 99.6 (45.67-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.164 , 0.208 0.165 , 0.209	Depositor DCC
$R_{free}$ test set	3365 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CU, MAN, ACT, NA, PER, AS8, GOL, ZN, 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	0.88	2/4008 (0.0%)	0.83	4/5504 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	CYS	CB-SG	5.50	1.91	1.82
1	A	1	ALA	N-CA	5.22	1.56	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ALA	N-CA-C	7.09	130.15	111.00
1	A	121	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	121	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	201	VAL	CB-CA-C	-5.07	101.77	111.40

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	3859	0	3669	26	1
2	B	50	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	1	0
3	D	28	0	25	1	0
4	E	39	0	34	2	0
5	A	4	0	0	0	0
6	A	2	0	0	0	0
7	A	14	0	13	0	0
8	A	8	0	4	0	0
9	A	4	0	3	0	0
10	A	10	0	0	0	0
11	A	24	0	32	2	0
12	A	8	0	0	0	0
13	A	1	0	0	0	0
14	A	712	0	0	8	0
All	All	4791	0	3848	31	1

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 (31) 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:493:ASP:OD1	1:A:494:PRO:HD2	1.78	0.84
1:A:440[B]:GLU:OE2	14:A:601:HOH:O	1.98	0.81
4:E:2:NAG:O3	4:E:3:BMA:H2	1.86	0.76
1:A:311[B]:MET:HE2	14:A:1217:HOH:O	1.94	0.67
1:A:101:ASP:HB3	14:A:1083:HOH:O	1.98	0.63
1:A:311[B]:MET:HE3	14:A:916:HOH:O	2.02	0.60
1:A:367:PRO:HG2	1:A:370:SER:HB2	1.83	0.59
3:C:1:NAG:H61	3:C:2:NAG:C1	2.34	0.57
1:A:324[B]:LYS:CE	14:A:1040:HOH:O	2.53	0.57
3:D:1:NAG:O4	3:D:2:NAG:H83	2.05	0.56
1:A:1:ALA:N	1:A:142:ASP:OD2	2.39	0.55
1:A:31:THR:HA	1:A:32:PRO:C	2.26	0.55
1:A:249:ASP:O	11:A:524:GOL:H32	2.09	0.53
1:A:342:HIS:CE1	14:A:624:HOH:O	2.63	0.51
1:A:469:THR:N	1:A:470:PRO:CD	2.75	0.49
1:A:324[B]:LYS:HE3	14:A:1040:HOH:O	2.13	0.49
1:A:387:THR:OG1	1:A:389:ASN:HB2	2.12	0.48
1:A:446:PRO:HA	1:A:466:ALA:HA	1.94	0.48
1:A:101:ASP:OD1	1:A:101:ASP:N	2.47	0.47
1:A:318:GLU:O	1:A:319:PRO:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:BMA:H61	2:B:4:MAN:O2	2.15	0.46
1:A:206:ASP:HB3	1:A:207:PRO:CD	2.46	0.45
1:A:251:SER:OG	11:A:524:GOL:O2	2.36	0.44
1:A:404:PHE:O	1:A:422:PHE:HA	2.18	0.43
1:A:114:THR:HA	1:A:454:ASP:OD2	2.18	0.42
1:A:70:GLN:HE22	1:A:97:PHE:CB	2.33	0.41
1:A:116:TYR:CE1	1:A:205[B]:CYS:SG	3.13	0.41
1:A:47:ASN:ND2	14:A:626:HOH:O	2.53	0.41
1:A:314:PRO:HG3	1:A:440[A]:GLU:HG2	2.02	0.41
4:E:2:NAG:H4	4:E:3:BMA:O2	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:OD2	1:A:195[A]:ARG:NH2[4_545]	2.06	0.14

## 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	503/497 (101%)	492 (98%)	10 (2%)	1 (0%)	47 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASP

### 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	428/420 (102%)	417 (97%)	11 (3%)	46 23

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

Mol	Chain	Res	Type
1	A	116	TYR
1	A	124	PHE
1	A	177	THR
1	A	180	ILE
1	A	243	ARG
1	A	298	LYS
1	A	324[A]	LYS
1	A	324[B]	LYS
1	A	387	THR
1	A	448	PHE
1	A	461	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	70	GLN
1	A	71	GLN
1	A	252	GLN
1	A	336	ASN
1	A	360	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 ⓘ

11 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	0.79	0	17,19,21	1.66	4 (23%)
2	NAG	B	2	2	14,14,15	1.08	0	17,19,21	1.90	6 (35%)
2	BMA	B	3	2	11,11,12	0.59	0	15,15,17	1.95	4 (26%)
2	MAN	B	4	2	11,11,12	0.56	0	15,15,17	1.96	5 (33%)
3	NAG	C	1	3,1	14,14,15	0.74	0	17,19,21	1.62	3 (17%)
3	NAG	C	2	3	14,14,15	0.46	0	17,19,21	1.64	4 (23%)
3	NAG	D	1	3,1	14,14,15	0.72	0	17,19,21	1.00	0
3	NAG	D	2	3	14,14,15	0.42	0	17,19,21	1.96	6 (35%)
4	NAG	E	1	4,1	14,14,15	0.90	1 (7%)	17,19,21	1.49	2 (11%)
4	NAG	E	2	4	14,14,15	0.62	0	17,19,21	1.68	3 (17%)
4	BMA	E	3	4	11,11,12	0.56	0	15,15,17	0.99	1 (6%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	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	E	1	NAG	C1-C2	2.72	1.56	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	C1-O5-C5	5.12	119.04	112.19
2	B	4	MAN	C2-C3-C4	-4.42	103.08	110.86
3	D	2	NAG	C2-N2-C7	-3.97	117.58	122.90
3	D	2	NAG	C1-O5-C5	3.92	117.44	112.19
3	C	1	NAG	O5-C1-C2	3.81	117.19	111.29
4	E	2	NAG	C4-C3-C2	3.66	116.38	111.02
3	C	2	NAG	C1-O5-C5	3.61	117.02	112.19
3	D	2	NAG	C3-C4-C5	3.50	116.58	110.23
2	B	2	NAG	O7-C7-N2	3.46	128.10	121.98
2	B	2	NAG	O4-C4-C5	-3.36	101.04	109.32
2	B	4	MAN	C1-C2-C3	-3.32	104.82	109.64
2	B	1	NAG	O4-C4-C5	-3.31	101.18	109.32
3	C	1	NAG	C3-C4-C5	-3.29	104.26	110.23
2	B	3	BMA	C2-C3-C4	-3.24	105.17	110.86
3	C	2	NAG	O5-C1-C2	3.18	116.21	111.29
4	E	1	NAG	C2-N2-C7	-3.14	118.69	122.90
4	E	2	NAG	C1-O5-C5	-3.05	108.10	112.19
2	B	1	NAG	O7-C7-C8	-2.99	116.72	122.05
3	C	1	NAG	O5-C5-C6	2.92	113.34	107.66
2	B	2	NAG	C8-C7-N2	-2.78	111.51	116.12
4	E	1	NAG	C1-C2-N2	2.67	114.65	110.43
2	B	2	NAG	C4-C3-C2	-2.67	107.10	111.02
2	B	4	MAN	O5-C5-C4	-2.63	104.42	110.83
2	B	4	MAN	C1-O5-C5	-2.57	108.74	112.19
3	C	2	NAG	C2-N2-C7	-2.50	119.55	122.90
4	E	2	NAG	O4-C4-C5	-2.42	103.37	109.32
3	D	2	NAG	C6-C5-C4	-2.37	107.21	113.02
4	E	3	BMA	C1-O5-C5	2.30	115.26	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	BMA	O5-C5-C4	2.29	116.39	110.83
2	B	1	NAG	C8-C7-N2	2.25	119.85	116.12
2	B	2	NAG	C1-O5-C5	-2.22	109.21	112.19
3	D	2	NAG	O5-C1-C2	-2.22	107.86	111.29
2	B	2	NAG	O5-C5-C4	-2.17	105.55	110.83
2	B	3	BMA	C3-C4-C5	2.14	114.11	110.23
3	C	2	NAG	O5-C5-C4	-2.13	105.64	110.83
2	B	1	NAG	C1-O5-C5	2.11	115.01	112.19
2	B	4	MAN	O5-C5-C6	2.07	111.69	107.66
3	D	2	NAG	O5-C5-C4	2.06	115.83	110.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	BMA	O5-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C1-C2-N2-C7

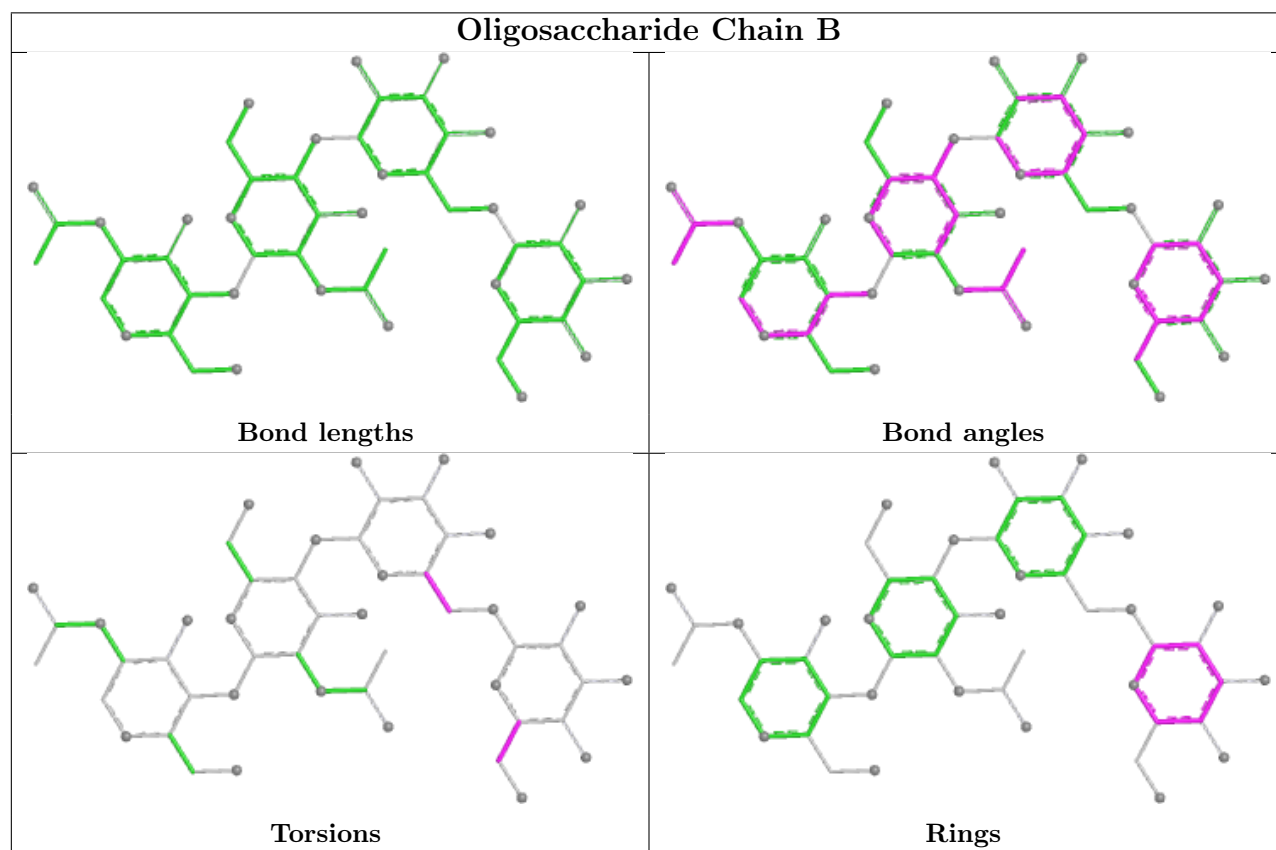
All (1) ring outliers are listed below:

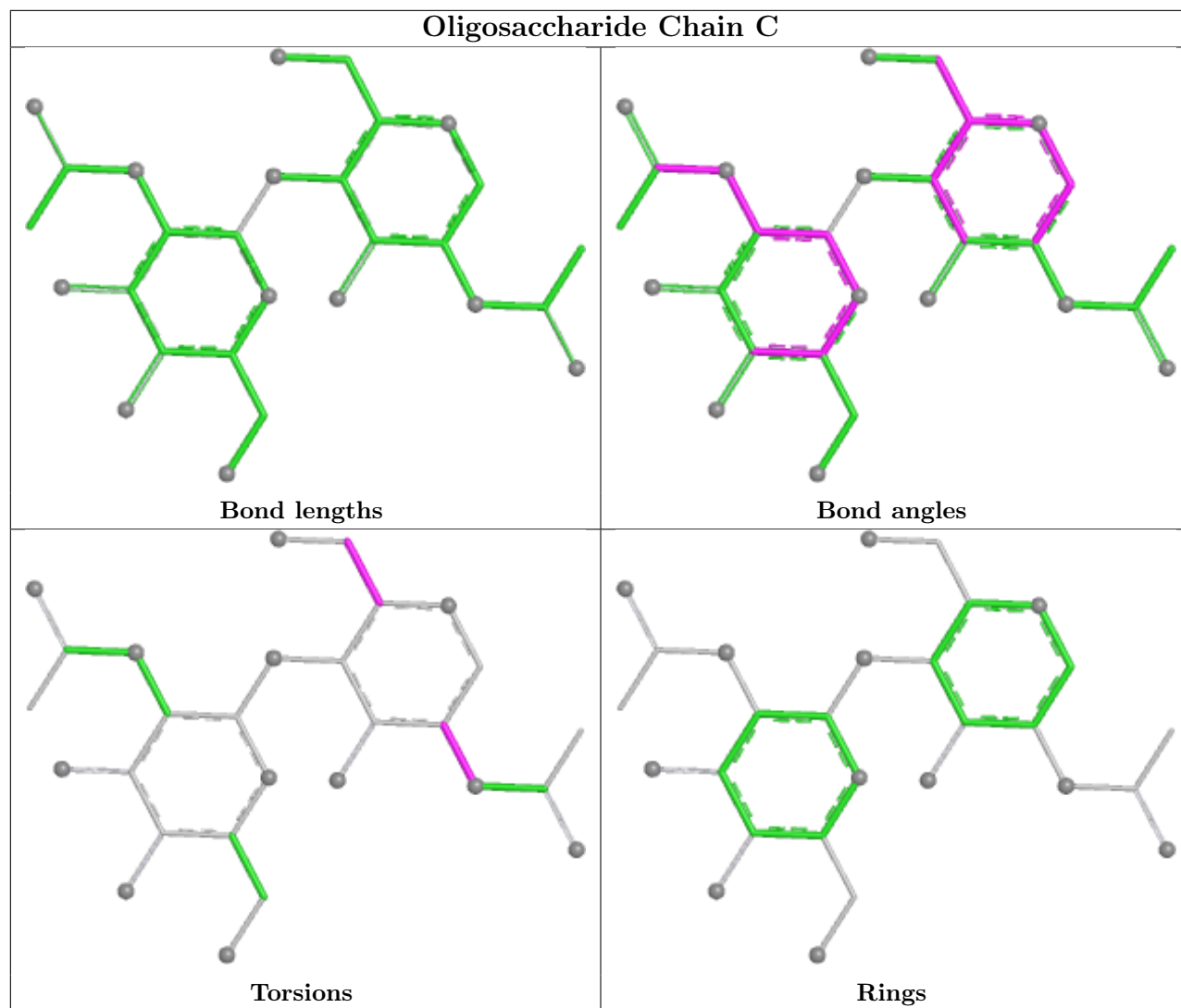
Mol	Chain	Res	Type	Atoms
2	B	4	MAN	C1-C2-C3-C4-C5-O5

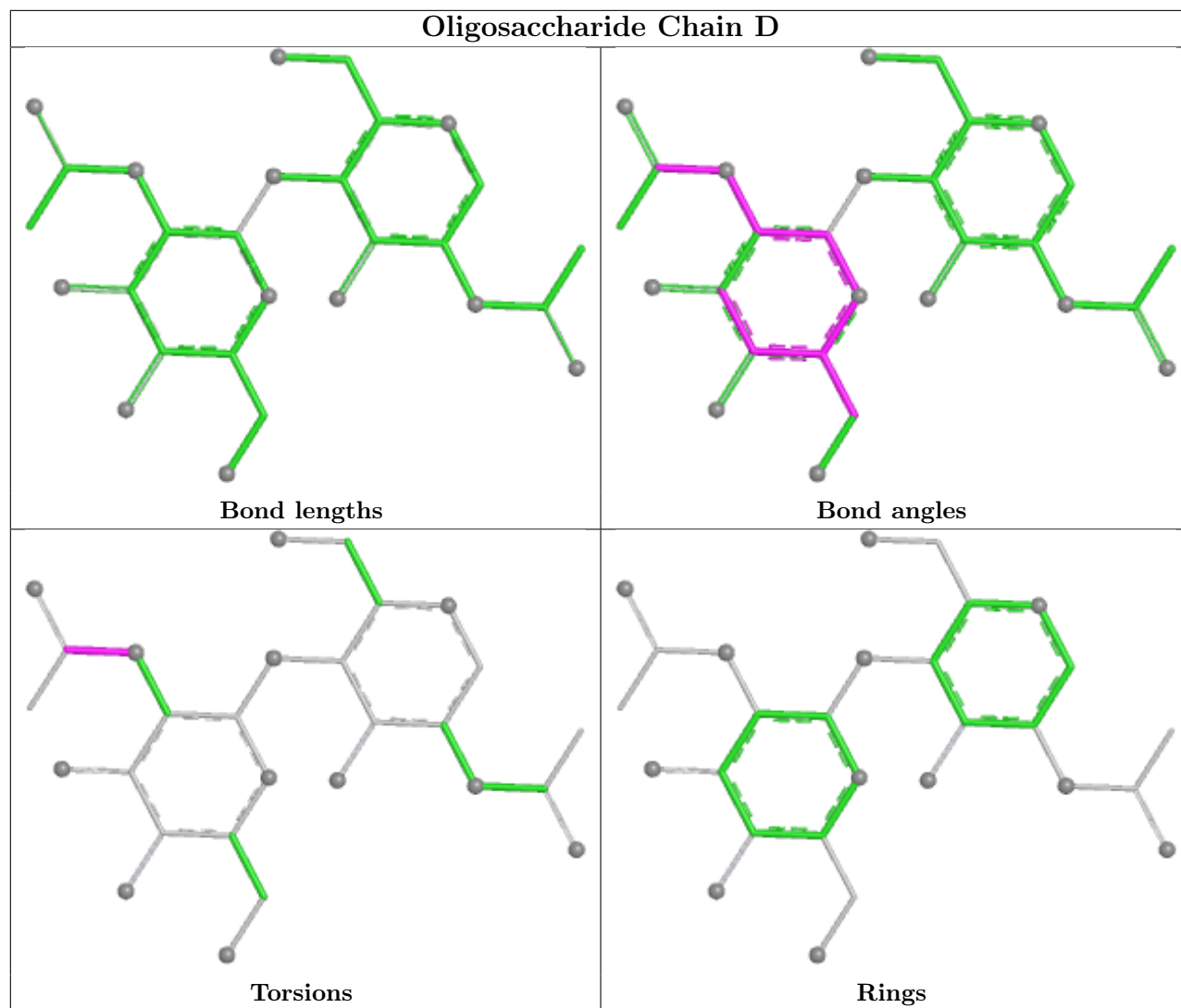
8 monomers are involved in 5 short contacts:

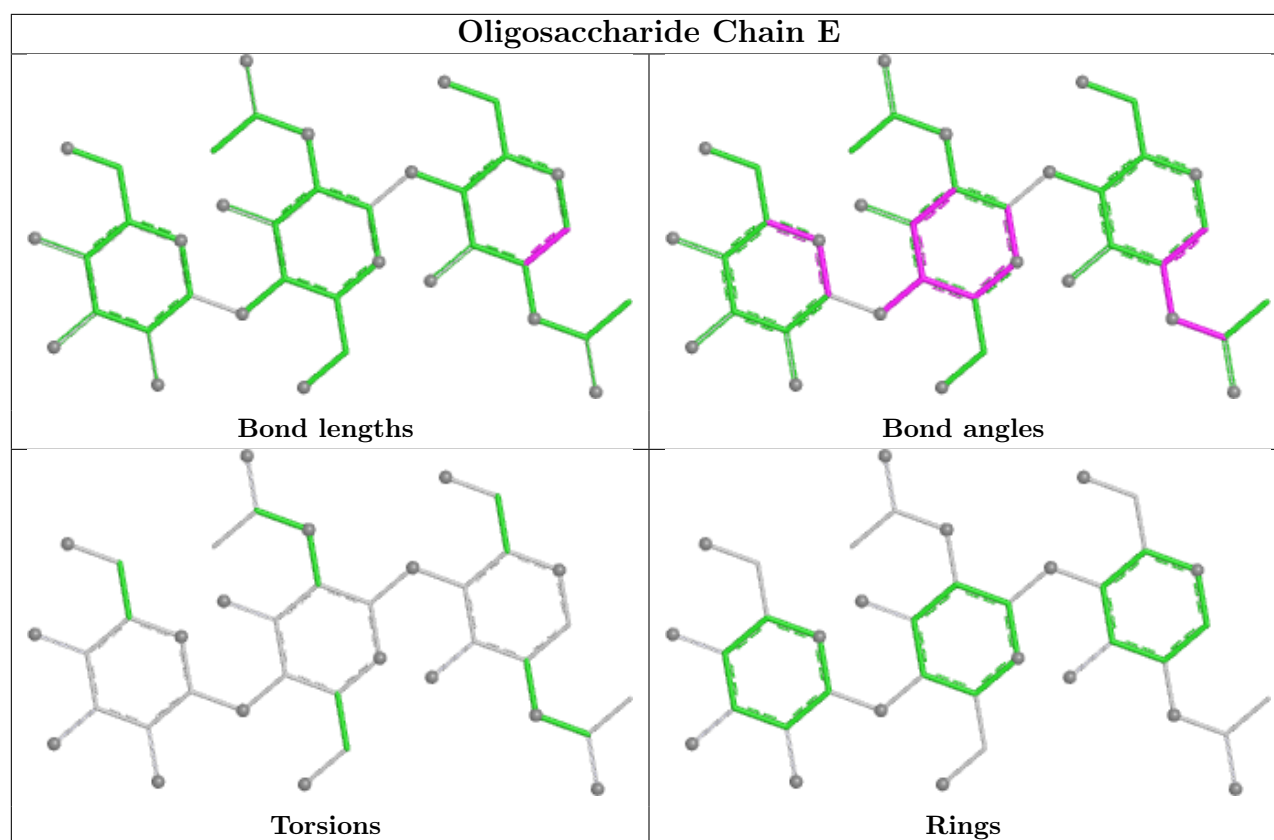
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	MAN	1	0
3	C	2	NAG	1	0
3	D	2	NAG	1	0
3	D	1	NAG	1	0
3	C	1	NAG	1	0
4	E	2	NAG	2	0
2	B	3	BMA	1	0
4	E	3	BMA	2	0

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 23 ligands modelled in this entry, 13 are monoatomic - leaving 10 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	$\# Z  > 2$
11	GOL	A	525	-	5,5,5	0.34	0	5,5,5	0.33	0
8	AS8	A	518	-	6,7,7	0.84	0	6,10,10	2.90	4 (66%)
11	GOL	A	524	-	5,5,5	0.43	0	5,5,5	0.40	0
9	ACT	A	519	12	3,3,3	0.95	0	3,3,3	2.19	2 (66%)
11	GOL	A	523	-	5,5,5	0.44	0	5,5,5	0.46	0
11	GOL	A	522	-	5,5,5	0.41	0	5,5,5	1.02	0
10	SO4	A	520	-	4,4,4	0.39	0	6,6,6	0.24	0
7	NAG	A	514	1	14,14,15	0.80	1 (7%)	17,19,21	1.67	4 (23%)
10	SO4	A	521	12	4,4,4	0.31	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PER	A	505	5	0,1,1	-	-	-		

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
11	GOL	A	525	-	-	0/4/4/4	-
8	AS8	A	518	-	-	0/0/5/5	-
11	GOL	A	523	-	-	0/4/4/4	-
11	GOL	A	522	-	-	2/4/4/4	-
11	GOL	A	524	-	-	2/4/4/4	-
7	NAG	A	514	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	514	NAG	C1-C2	2.10	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	518	AS8	O1-S-O1S	3.87	119.37	107.56
8	A	518	AS8	O1-S-O3S	3.77	119.05	107.56
7	A	514	NAG	O5-C1-C2	3.67	116.97	111.29
7	A	514	NAG	C4-C3-C2	3.39	115.99	111.02
8	A	518	AS8	O2S-S-O1S	-3.18	97.41	108.56
9	A	519	ACT	OXT-C-O	-3.08	110.59	122.03
8	A	518	AS8	O2S-S-O3S	-2.75	98.94	108.56
7	A	514	NAG	C2-N2-C7	2.73	126.56	122.90
7	A	514	NAG	C1-O5-C5	2.55	115.60	112.19
9	A	519	ACT	OXT-C-CH3	2.08	123.79	115.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	522	GOL	C1-C2-C3-O3
11	A	524	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	A	522	GOL	O2-C2-C3-O3
11	A	524	GOL	O1-C1-C2-O2
7	A	514	NAG	C4-C5-C6-O6
7	A	514	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	524	GOL	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	497/497 (100%)	0.02	23 (4%)	32 38	18, 27, 41, 71	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	ILE	10.8
1	A	316	SER	4.5
1	A	181	ALA	4.3
1	A	414	VAL	3.7
1	A	494	PRO	3.1
1	A	363	GLN	3.0
1	A	318	GLU	2.7
1	A	493	ASP	2.6
1	A	317	PRO	2.5
1	A	392	GLY	2.5
1	A	240	ALA	2.4
1	A	320	GLY	2.4
1	A	417	TYR	2.4
1	A	107	TRP	2.4
1	A	391	PRO	2.2
1	A	265	PHE	2.2
1	A	97	PHE	2.1
1	A	239	PHE	2.1
1	A	321	GLY	2.1
1	A	492	LEU	2.1
1	A	319	PRO	2.0
1	A	393	PHE	2.0
1	A	179	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

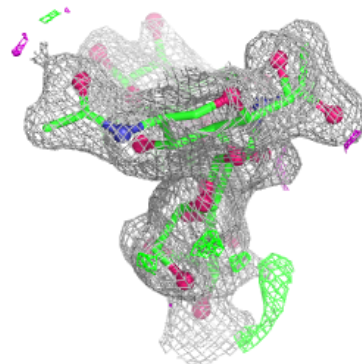
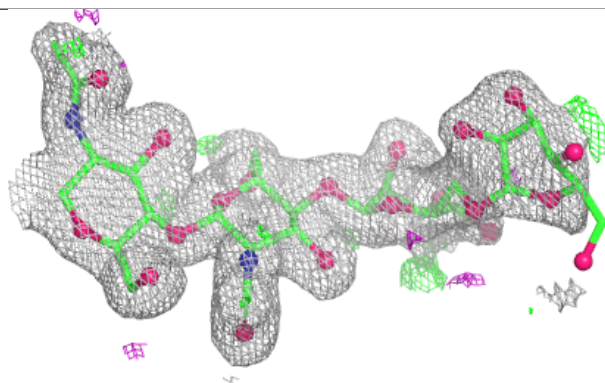
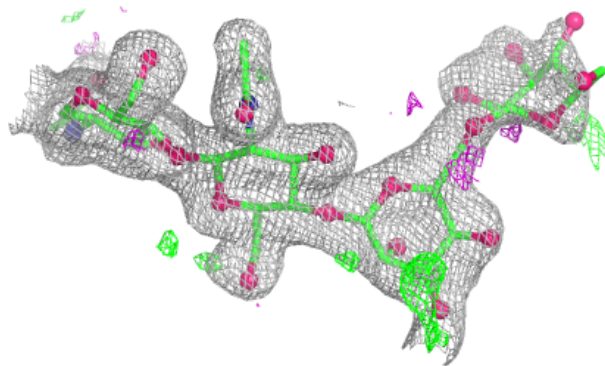
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	2	14/15	0.70	0.32	68,74,75,75	0
4	BMA	E	3	11/12	0.74	0.32	73,77,79,80	0
2	MAN	B	4	11/12	0.77	0.38	83,85,88,89	0
2	BMA	B	3	11/12	0.79	0.26	54,64,71,78	0
3	NAG	C	2	14/15	0.79	0.30	57,72,75,78	0
4	NAG	E	2	14/15	0.87	0.25	40,51,57,67	0
3	NAG	C	1	14/15	0.91	0.17	43,49,55,64	0
3	NAG	D	1	14/15	0.92	0.08	46,54,57,60	0
4	NAG	E	1	14/15	0.92	0.08	30,38,43,44	0
2	NAG	B	2	14/15	0.95	0.14	24,30,41,45	0
2	NAG	B	1	14/15	0.96	0.09	22,28,37,37	0

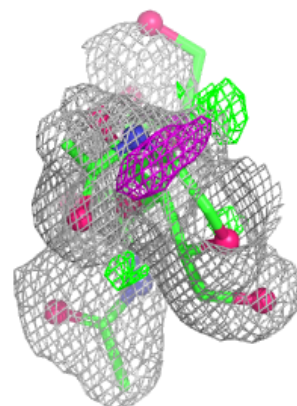
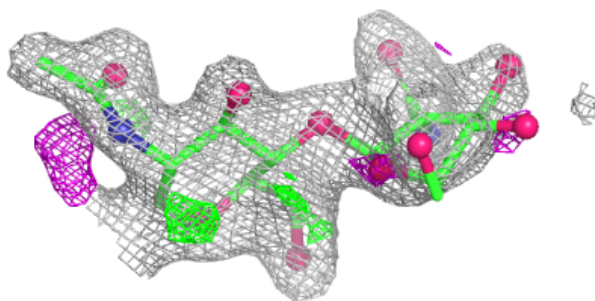
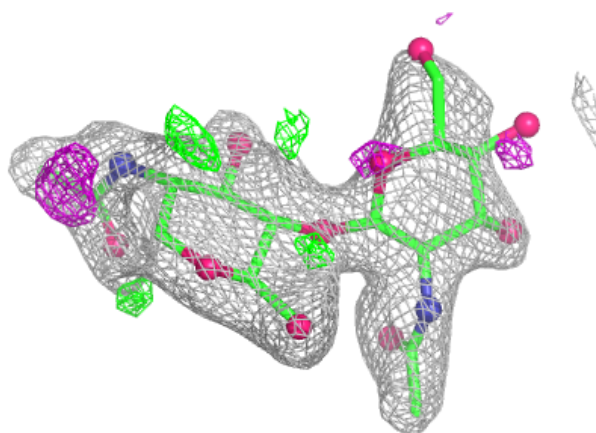
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

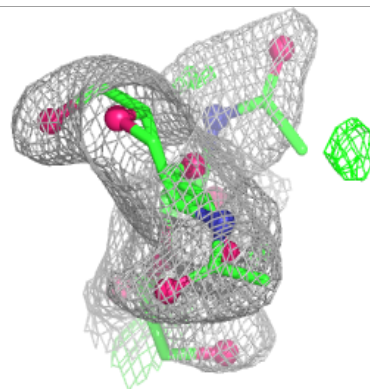
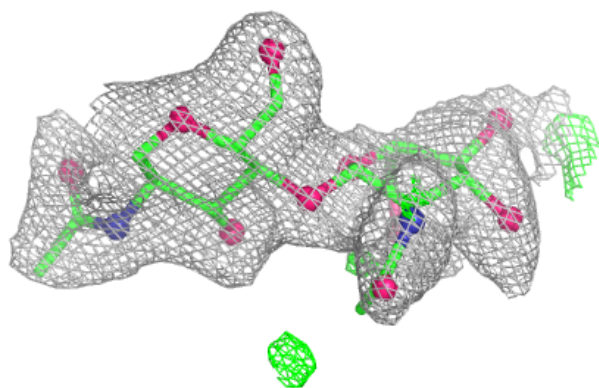
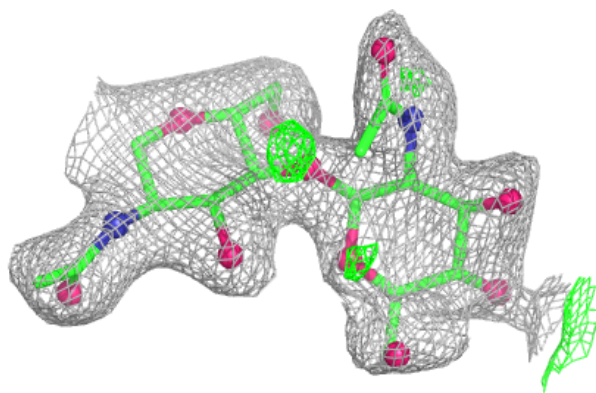
**Electron density around Chain C:**

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

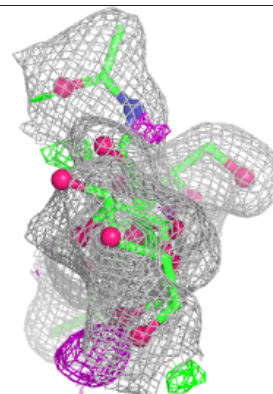
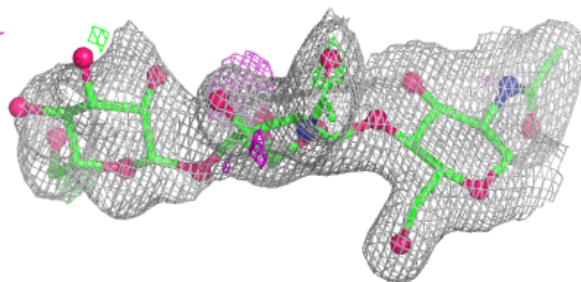
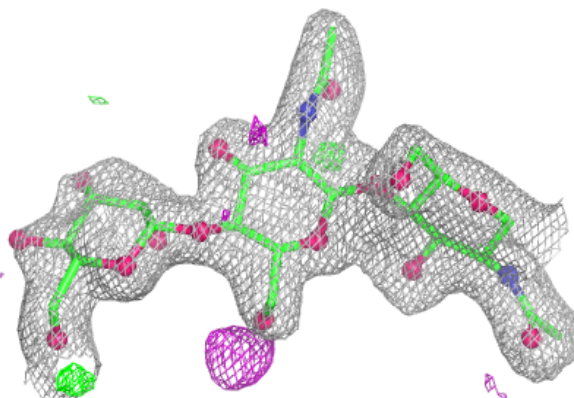


**Electron density around Chain D:**

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

**Electron density around Chain E:**

$2mF_o-DF_c$  (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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	NAG	A	514	14/15	0.70	0.41	69,78,79,79	0
13	NA	A	534	1/1	0.84	0.22	43,43,43,43	0
10	SO4	A	520	5/5	0.86	0.17	56,62,67,68	0
11	GOL	A	525	6/6	0.88	0.22	30,41,45,45	0
12	ZN	A	533	1/1	0.89	0.21	84,84,84,84	0
11	GOL	A	524	6/6	0.91	0.16	47,53,55,55	0
12	ZN	A	532	1/1	0.92	0.08	63,63,63,63	0
11	GOL	A	522	6/6	0.93	0.12	30,41,46,46	0
12	ZN	A	527	1/1	0.94	0.04	38,38,38,38	0
12	ZN	A	529	1/1	0.95	0.11	61,61,61,61	0
9	ACT	A	519	4/4	0.95	0.09	27,33,34,35	0
10	SO4	A	521	5/5	0.96	0.13	63,70,72,73	0
8	AS8	A	518	8/8	0.97	0.17	26,35,42,47	0
11	GOL	A	523	6/6	0.97	0.08	32,34,35,35	0
12	ZN	A	531	1/1	0.97	0.12	54,54,54,54	0
12	ZN	A	528	1/1	0.98	0.03	42,42,42,42	0
12	ZN	A	530	1/1	0.98	0.08	53,53,53,53	0
5	CU	A	501	1/1	0.99	0.06	29,29,29,29	0
12	ZN	A	526	1/1	0.99	0.03	33,33,33,33	0
5	CU	A	502	1/1	0.99	0.06	29,29,29,29	0
5	CU	A	504	1/1	0.99	0.02	35,35,35,35	0
6	PER	A	505	2/2	0.99	0.09	27,27,27,30	0
5	CU	A	503	1/1	1.00	0.08	25,25,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.