



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:39 PM BST

PDB ID : 5NFG  
Title : Structure of recombinant cardosin B from *Cynara cardunculus*  
Authors : Pereira, P.J.B.; Figueiredo, A.C.; Manso, J.A.; Almeida, C.M.; Simoes, I.  
Deposited on : 2017-03-14  
Resolution : 2.38 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.

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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 : 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

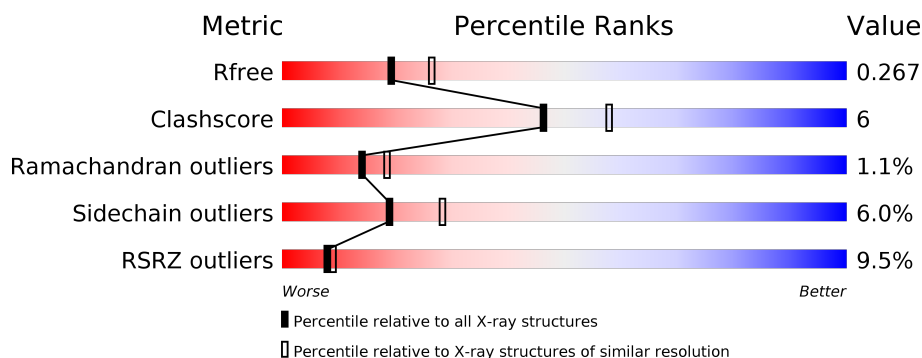
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\geq 3$ , 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	383	<div> <div>8%</div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	B	383	<div> <div>9%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>
2	C	6	<div> <div>33%</div> <div>67%</div> </div>
2	E	6	<div> <div>33%</div> <div>67%</div> </div>
3	D	4	<div> <div>100%</div> </div>
3	F	4	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5400 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.

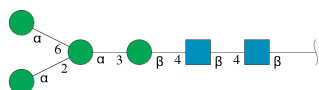
- Molecule 1 is a protein called Procardosin-B,Procardosin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	1	0
			2530	1606	403	509	12			
1	B	328	Total	C	N	O	S	0	0	0
			2485	1581	397	495	12			

There are 10 discrepancies between the modelled and reference sequences:

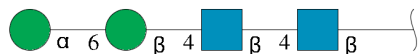
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9XFX4
A	45	ARG	SER	conflict	UNP Q9XFX4
A	292	GLY	-	linker	UNP Q9XFX4
A	293	GLY	-	linker	UNP Q9XFX4
A	294	GLY	-	linker	UNP Q9XFX4
B	1	MET	-	initiating methionine	UNP Q9XFX4
B	45	ARG	SER	conflict	UNP Q9XFX4
B	292	GLY	-	linker	UNP Q9XFX4
B	293	GLY	-	linker	UNP Q9XFX4
B	294	GLY	-	linker	UNP Q9XFX4

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-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	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 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
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

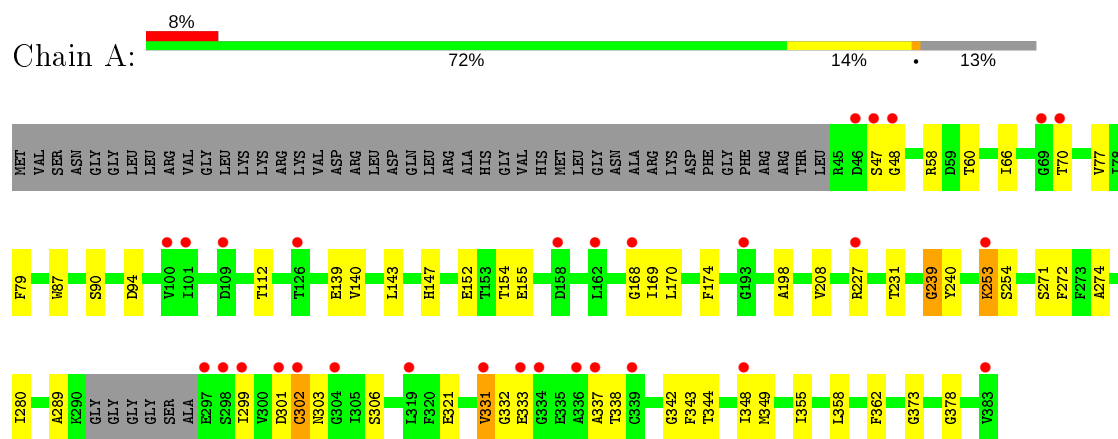
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	74	Total	O	0	0
			74	74		

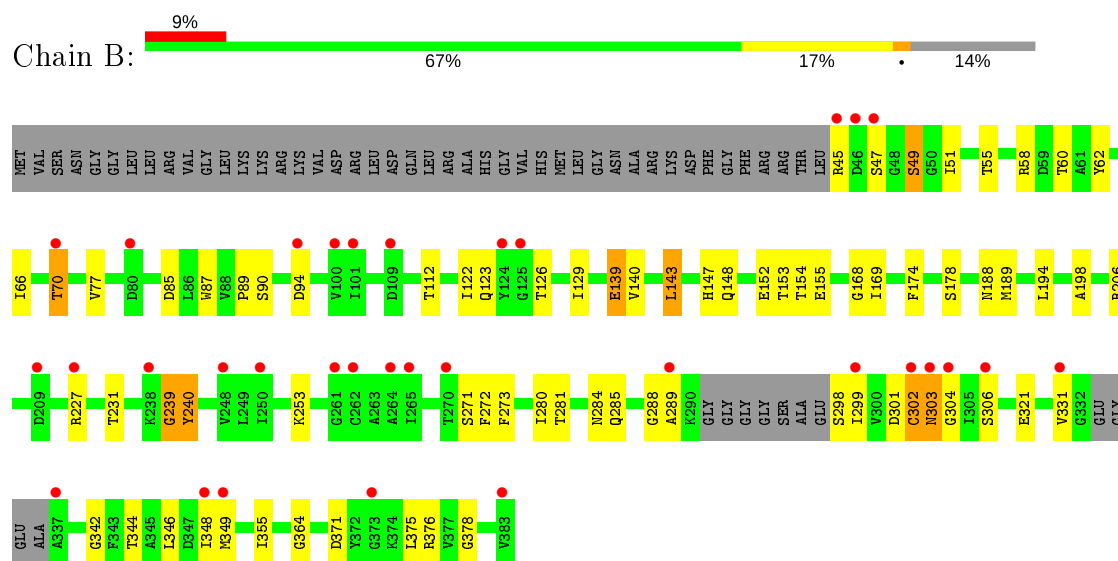
### 3 Residue-property plots [i](#)

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: Procardosin-B,Procardosin-B



#### • Molecule 1: Procardosin-B,Procardosin-B



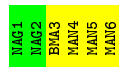
#### • Molecule 2: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



- Molecule 3: 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

Chain D:



- Molecule 3: 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

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.58 Å 143.13 Å 64.71 Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	61.58 – 2.38 61.58 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.9 (61.58-2.38) 99.0 (61.58-2.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.37 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.222 , 0.270 0.222 , 0.267	Depositor DCC
$R_{free}$ test set	1807 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.6	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5119e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.46	0/2590	0.62	0/3518
1	B	0.45	0/2544	0.62	0/3455
All	All	0.46	0/5134	0.62	0/6973

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	2530	0	2370	28	0
1	B	2485	0	2338	39	0
2	C	72	0	61	0	0
2	E	72	0	61	0	0
3	D	50	0	43	1	0
3	F	50	0	43	2	0
4	A	67	0	0	1	0
4	B	74	0	0	0	0
All	All	5400	0	4916	64	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 (64) 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:B:90:SER:HB2	1:B:152:GLU:HB3	1.61	0.81
1:A:332:GLY:HA3	1:A:337:ALA:HA	1.70	0.73
1:A:90:SER:HB2	1:A:152:GLU:HB3	1.70	0.73
1:A:174:PHE:HB2	1:A:239:GLY:HA2	1.71	0.72
1:B:174:PHE:HB2	1:B:239:GLY:HA2	1.75	0.69
1:A:289:ALA:HB1	1:A:299:ILE:HG23	1.76	0.67
1:B:301:ASP:O	1:B:302:CYS:HB2	1.97	0.65
1:A:301:ASP:O	1:A:302:CYS:HB2	1.96	0.64
1:B:289:ALA:HB2	1:B:299:ILE:HG23	1.80	0.64
1:A:112:THR:O	4:A:501:HOH:O	2.13	0.64
1:A:87:TRP:CZ2	1:A:169:ILE:HD13	2.38	0.58
1:A:331:VAL:HG12	1:A:338:THR:HB	1.86	0.57
1:A:253:LYS:HE3	1:A:254:SER:H	1.70	0.57
1:A:154:THR:HG22	1:A:155:GLU:HG3	1.87	0.56
1:B:273:PHE:O	1:B:344:THR:HG22	2.08	0.54
1:B:49:SER:HB3	1:B:51:ILE:HG12	1.90	0.54
1:B:122:ILE:HD12	1:B:129:ILE:HD11	1.90	0.54
1:B:198:ALA:HB2	3:D:2:NAG:H83	1.92	0.52
1:B:87:TRP:CZ2	1:B:169:ILE:HD13	2.44	0.52
1:A:198:ALA:HB2	3:F:2:NAG:H83	1.91	0.51
1:B:281:THR:O	1:B:285:GLN:HG3	2.10	0.51
1:B:189:MET:HA	1:B:194:LEU:HD12	1.93	0.50
1:B:302:CYS:O	1:B:304:GLY:N	2.44	0.50
1:B:206:ARG:HD3	1:B:364:GLY:HA3	1.93	0.49
1:A:231:THR:O	1:A:378:GLY:HA2	2.12	0.49
1:B:298:SER:O	1:B:299:ILE:HG13	2.12	0.49
1:B:148:GLN:OE1	1:B:188:ASN:ND2	2.39	0.48
1:A:168:GLY:C	1:A:169:ILE:HD12	2.33	0.48
1:B:346:LEU:HD21	1:B:348:ILE:HD11	1.96	0.48
1:A:174:PHE:HB2	1:A:239:GLY:CA	2.43	0.47
1:A:348:ILE:HB	1:A:355:ILE:HG22	1.96	0.46
1:B:70:THR:HG23	1:B:112:THR:OG1	2.16	0.46
1:B:174:PHE:HB2	1:B:239:GLY:CA	2.45	0.46
1:B:154:THR:HG22	1:B:155:GLU:HG3	1.98	0.45
1:B:231:THR:O	1:B:378:GLY:HA2	2.17	0.45
1:B:280:ILE:HG22	1:B:284:ASN:ND2	2.32	0.44
1:A:348:ILE:HB	1:A:355:ILE:CG2	2.47	0.44
1:A:272:PHE:HB3	1:A:342:GLY:O	2.18	0.44
1:B:66:ILE:HG22	1:B:140:VAL:HG13	1.99	0.44
1:A:280:ILE:HD12	1:A:343:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:HB2	1:B:47:SER:HB2	1.99	0.44
1:B:371:ASP:HB3	1:B:376:ARG:HG3	2.00	0.44
1:B:371:ASP:HB3	1:B:376:ARG:CG	2.48	0.44
1:B:58:ARG:O	1:B:60:THR:HG23	2.18	0.43
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.85	0.43
1:A:58:ARG:HA	1:A:208:VAL:HG21	2.01	0.43
1:A:79:PHE:CE2	1:A:170:LEU:HD13	2.54	0.42
1:B:139:GLU:HA	1:B:143:LEU:O	2.19	0.42
1:B:289:ALA:CB	1:B:299:ILE:HG23	2.46	0.42
1:B:284:ASN:O	1:B:288:GLY:HA2	2.19	0.42
1:A:373:GLY:O	3:F:4:MAN:O3	2.38	0.42
1:A:358:LEU:HD23	1:A:362:PHE:CD2	2.54	0.42
1:B:168:GLY:C	1:B:169:ILE:HD12	2.40	0.41
1:B:89:PRO:HA	1:B:153:THR:OG1	2.19	0.41
1:A:227:ARG:HD3	1:B:47:SER:OG	2.21	0.41
1:B:272:PHE:HB3	1:B:342:GLY:O	2.20	0.41
1:B:348:ILE:HB	1:B:355:ILE:HB	2.03	0.41
1:A:58:ARG:O	1:A:60:THR:HG23	2.20	0.41
1:A:66:ILE:HG22	1:A:140:VAL:HG13	2.02	0.41
1:A:48:GLY:N	1:B:227:ARG:HB2	2.36	0.40
1:B:240:TYR:CD1	1:B:240:TYR:N	2.87	0.40
1:B:85:ASP:OD1	1:B:178:SER:OG	2.30	0.40
1:B:55:THR:O	1:B:62:TYR:HA	2.21	0.40
1:A:274:ALA:HA	1:A:344:THR:O	2.21	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	330/383 (86%)	315 (96%)	11 (3%)	4 (1%)	13 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	322/383 (84%)	309 (96%)	10 (3%)	3 (1%)	17	23
All	All	652/766 (85%)	624 (96%)	21 (3%)	7 (1%)	14	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	ASN
1	A	302	CYS
1	B	302	CYS
1	A	333	GLU
1	B	239	GLY
1	A	239	GLY
1	A	303	ASN

### 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	269/305 (88%)	255 (95%)	14 (5%)	23	35
1	B	265/305 (87%)	247 (93%)	18 (7%)	16	23
All	All	534/610 (88%)	502 (94%)	32 (6%)	19	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	70	THR
1	A	77	VAL
1	A	94	ASP
1	A	139	GLU
1	A	143	LEU
1	A	147	HIS
1	A	240	TYR
1	A	253	LYS

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Mol	Chain	Res	Type
1	A	271	SER
1	A	306	SER
1	A	321	GLU
1	A	331	VAL
1	A	349	MET
1	B	45	ARG
1	B	49	SER
1	B	70	THR
1	B	77	VAL
1	B	94	ASP
1	B	123	GLN
1	B	126	THR
1	B	139	GLU
1	B	143	LEU
1	B	147	HIS
1	B	240	TYR
1	B	253	LYS
1	B	271	SER
1	B	303	ASN
1	B	306	SER
1	B	321	GLU
1	B	331	VAL
1	B	349	MET

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 ⓘ

20 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	0.46	0	17,19,21	0.68	0
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.47	0
2	BMA	C	3	2	11,11,12	1.32	2 (18%)	15,15,17	1.07	3 (20%)
2	MAN	C	4	2	11,11,12	1.31	2 (18%)	15,15,17	1.59	3 (20%)
2	MAN	C	5	2	11,11,12	1.30	2 (18%)	15,15,17	1.12	2 (13%)
2	MAN	C	6	2	11,11,12	0.98	1 (9%)	15,15,17	1.29	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.27	0	17,19,21	1.05	1 (5%)
3	NAG	D	2	3	14,14,15	0.46	0	17,19,21	0.58	0
3	BMA	D	3	3	11,11,12	0.64	0	15,15,17	1.57	5 (33%)
3	MAN	D	4	3	11,11,12	0.74	0	15,15,17	0.87	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.41	0	17,19,21	0.63	0
2	NAG	E	2	2	14,14,15	0.39	0	17,19,21	0.43	0
2	BMA	E	3	2	11,11,12	1.66	4 (36%)	15,15,17	1.52	3 (20%)
2	MAN	E	4	2	11,11,12	1.06	1 (9%)	15,15,17	1.67	4 (26%)
2	MAN	E	5	2	11,11,12	0.97	1 (9%)	15,15,17	1.13	2 (13%)
2	MAN	E	6	2	11,11,12	0.98	1 (9%)	15,15,17	1.22	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.39	0	17,19,21	1.11	1 (5%)
3	NAG	F	2	3	14,14,15	0.55	0	17,19,21	0.64	0
3	BMA	F	3	3	11,11,12	1.08	1 (9%)	15,15,17	1.52	4 (26%)
3	MAN	F	4	3	11,11,12	0.93	0	15,15,17	0.86	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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	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
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	BMA	O5-C1	-2.86	1.39	1.43
2	C	4	MAN	C4-C5	2.86	1.59	1.53
2	C	3	BMA	O5-C1	-2.79	1.39	1.43
2	E	3	BMA	C2-C3	-2.69	1.48	1.52
2	C	4	MAN	O5-C5	2.62	1.48	1.43
3	F	3	BMA	C1-C2	2.58	1.58	1.52
2	C	5	MAN	O5-C5	2.55	1.48	1.43
2	E	6	MAN	O5-C5	2.50	1.48	1.43
2	E	3	BMA	C1-C2	2.49	1.57	1.52
2	E	4	MAN	C4-C5	2.39	1.58	1.53
2	C	3	BMA	C4-C5	2.38	1.58	1.53
2	C	5	MAN	C2-C3	2.32	1.55	1.52
2	E	5	MAN	C2-C3	2.30	1.55	1.52
2	C	6	MAN	O5-C5	2.26	1.48	1.43
2	E	3	BMA	C4-C5	2.01	1.57	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	4.10	117.75	112.19
3	F	1	NAG	C1-O5-C5	4.05	117.67	112.19
2	E	3	BMA	O2-C2-C3	-3.90	102.33	110.14
2	C	4	MAN	C1-O5-C5	3.80	117.34	112.19
3	D	1	NAG	C1-O5-C5	3.79	117.33	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6	MAN	O2-C2-C3	-3.43	103.27	110.14
2	E	6	MAN	O2-C2-C3	-3.01	104.10	110.14
2	E	4	MAN	O2-C2-C3	-2.96	104.21	110.14
3	D	3	BMA	O5-C1-C2	2.93	115.30	110.77
2	C	4	MAN	C1-C2-C3	-2.91	106.09	109.67
3	F	3	BMA	O5-C1-C2	2.91	115.26	110.77
2	E	5	MAN	C1-O5-C5	2.65	115.79	112.19
2	E	3	BMA	C3-C4-C5	2.64	114.95	110.24
3	D	3	BMA	C1-O5-C5	2.53	115.62	112.19
3	F	3	BMA	C1-O5-C5	2.48	115.56	112.19
2	E	4	MAN	O3-C3-C2	2.48	114.75	109.99
2	C	4	MAN	O2-C2-C3	-2.44	105.25	110.14
2	C	3	BMA	C1-O5-C5	2.37	115.41	112.19
2	C	3	BMA	O2-C2-C3	-2.36	105.41	110.14
3	D	3	BMA	C1-C2-C3	2.30	112.49	109.67
2	C	5	MAN	C1-O5-C5	2.29	115.29	112.19
3	D	3	BMA	O2-C2-C3	-2.27	105.58	110.14
3	D	3	BMA	C3-C4-C5	-2.18	106.35	110.24
2	E	4	MAN	C1-C2-C3	-2.15	107.02	109.67
2	C	5	MAN	O2-C2-C1	2.13	113.51	109.15
3	D	4	MAN	O2-C2-C3	-2.13	105.88	110.14
3	F	3	BMA	C3-C4-C5	-2.12	106.45	110.24
2	E	5	MAN	C1-C2-C3	-2.11	107.07	109.67
2	E	3	BMA	C1-O5-C5	2.08	115.01	112.19
3	F	3	BMA	C1-C2-C3	2.05	112.18	109.67
2	C	3	BMA	C3-C4-C5	2.02	113.84	110.24
3	D	4	MAN	C1-O5-C5	2.02	114.92	112.19
2	C	6	MAN	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	MAN	O5-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	6	MAN	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6

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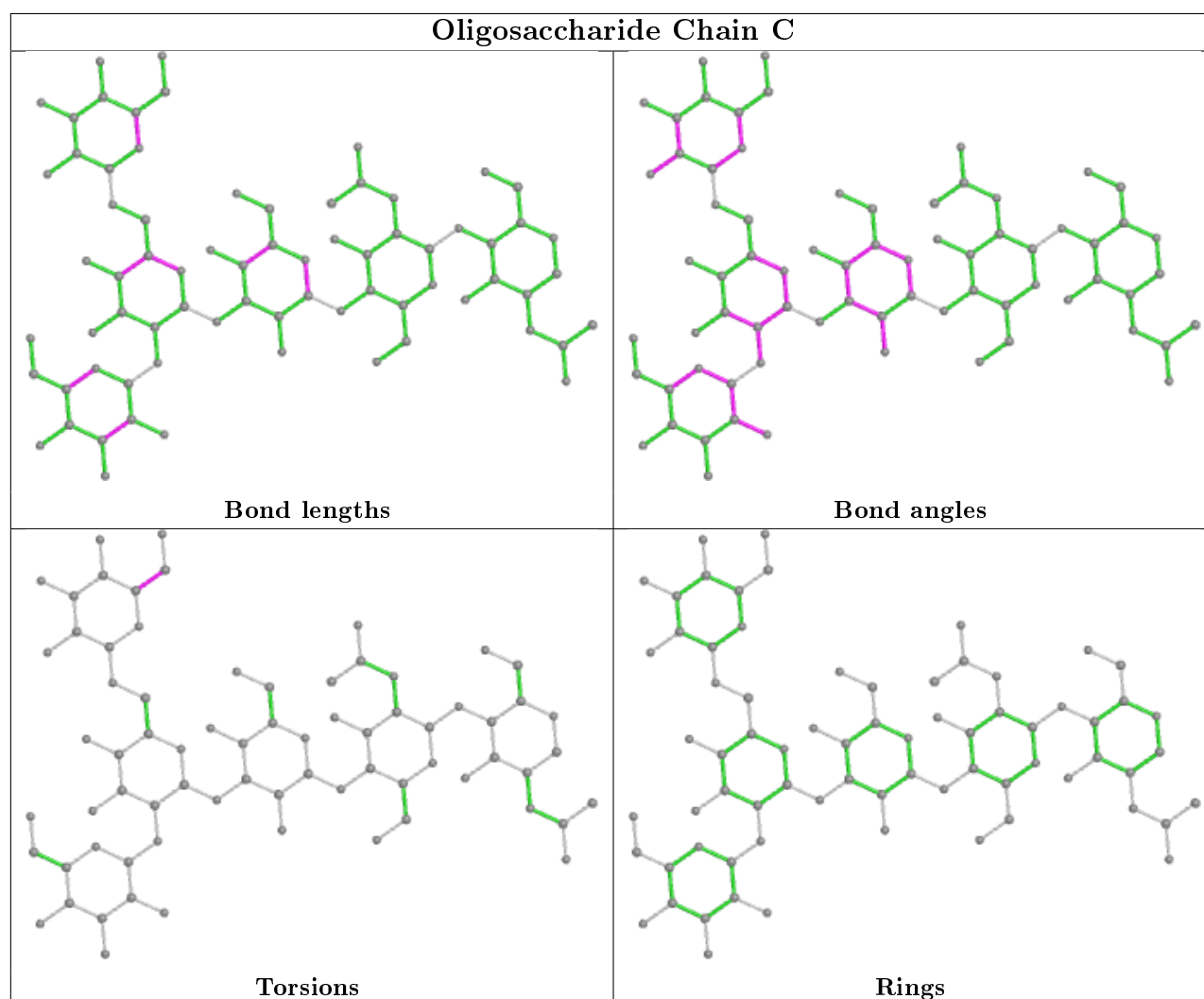
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

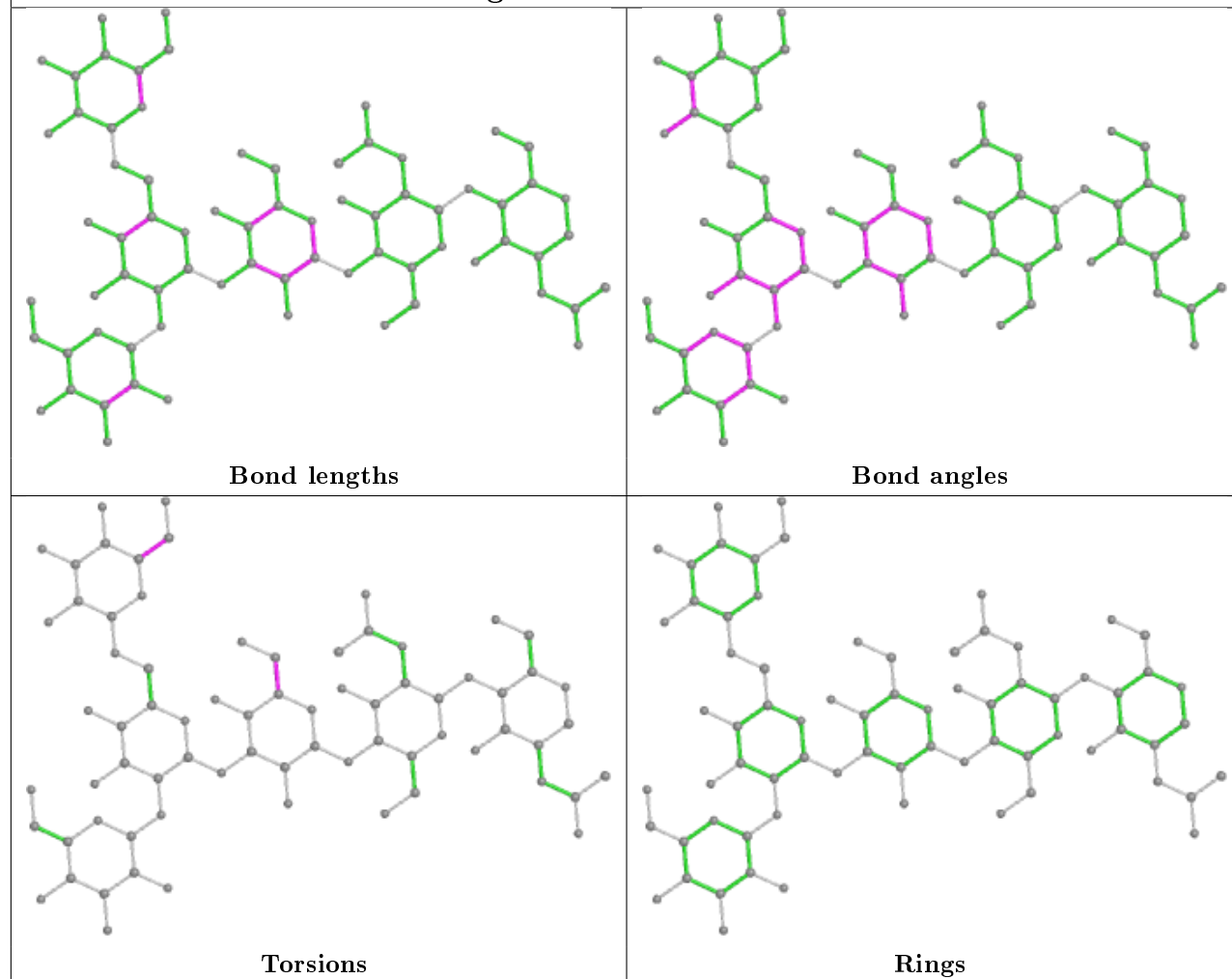
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	MAN	1	0
3	F	2	NAG	1	0
3	D	2	NAG	1	0

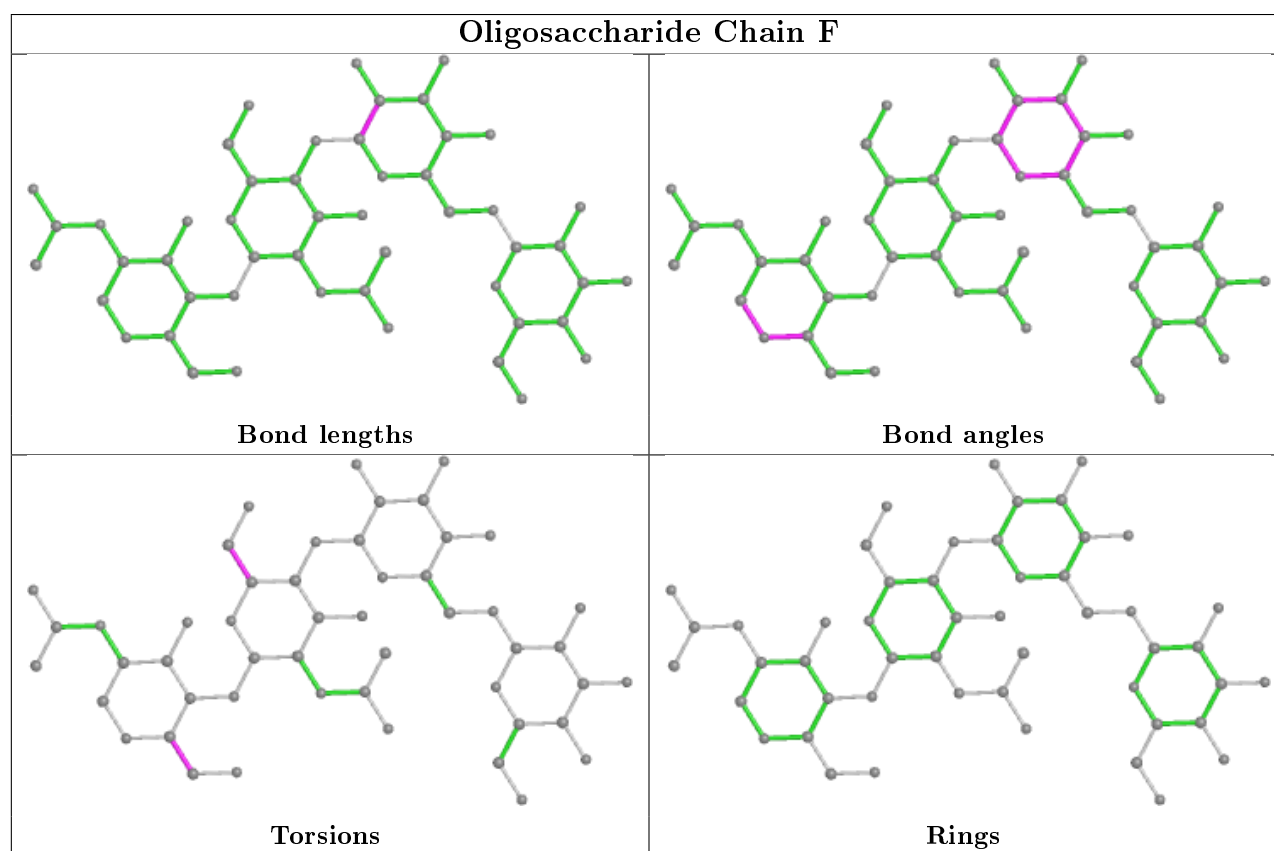
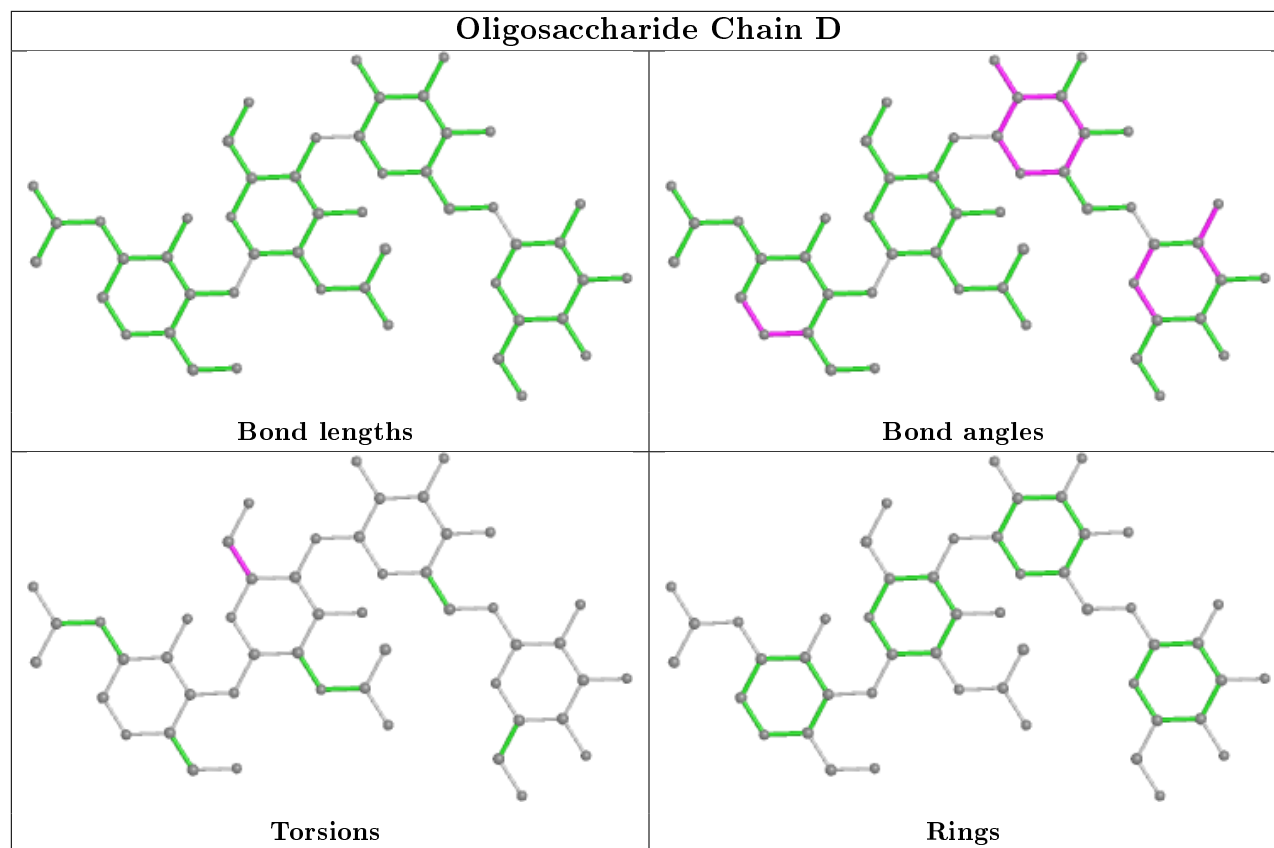
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## Oligosaccharide Chain E





## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.







## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	333/383 (86%)	1.00	30 (9%)  	20, 44, 89, 130	0
1	B	328/383 (85%)	1.02	33 (10%)  	20, 46, 86, 126	0
All	All	661/766 (86%)	1.01	63 (9%)  	20, 44, 86, 130	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	ASP	8.2
1	A	331	VAL	6.4
1	A	126	THR	5.6
1	B	303	ASN	5.5
1	B	331	VAL	5.0
1	A	299	ILE	4.8
1	A	297	GLU	4.8
1	B	302	CYS	4.3
1	A	46	ASP	4.2
1	B	101	ILE	4.0
1	A	304	GLY	3.8
1	A	336	ALA	3.6
1	A	333	GLU	3.6
1	B	209	ASP	3.4
1	B	109	ASP	3.1
1	A	298	SER	3.1
1	A	47	SER	3.0
1	A	70	THR	3.0
1	B	299	ILE	2.9
1	B	349	MET	2.9
1	A	162	LEU	2.9
1	B	94	ASP	2.8
1	B	264	ALA	2.7
1	B	70	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	47	SER	2.7
1	A	253	LYS	2.7
1	A	339	CYS	2.6
1	B	250	ILE	2.6
1	A	101	ILE	2.6
1	A	383	VAL	2.5
1	B	265	ILE	2.5
1	A	301	ASP	2.5
1	B	306	SER	2.4
1	B	337	ALA	2.4
1	A	158	ASP	2.4
1	B	383	VAL	2.4
1	B	270	THR	2.4
1	B	125	GLY	2.3
1	B	304	GLY	2.3
1	B	373	GLY	2.3
1	A	302	CYS	2.3
1	B	261	GLY	2.3
1	A	227	ARG	2.3
1	B	45	ARG	2.3
1	A	334	GLY	2.2
1	B	289	ALA	2.2
1	B	124	TYR	2.2
1	A	100	VAL	2.2
1	A	319	LEU	2.2
1	A	109	ASP	2.2
1	A	337	ALA	2.2
1	B	100	VAL	2.1
1	B	262	CYS	2.1
1	B	248	VAL	2.1
1	A	69	GLY	2.1
1	B	238	LYS	2.1
1	B	348	ILE	2.1
1	A	168	GLY	2.1
1	B	80	ASP	2.0
1	A	348	ILE	2.0
1	A	48	GLY	2.0
1	A	193	GLY	2.0
1	B	227	ARG	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 ⓘ

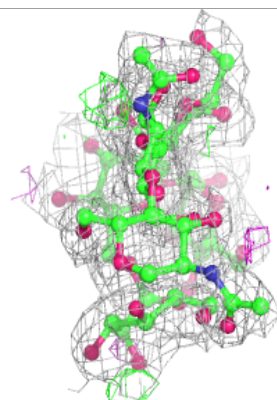
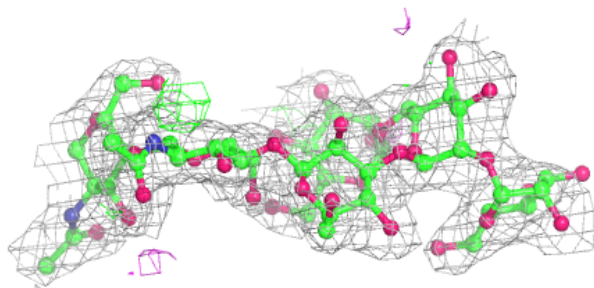
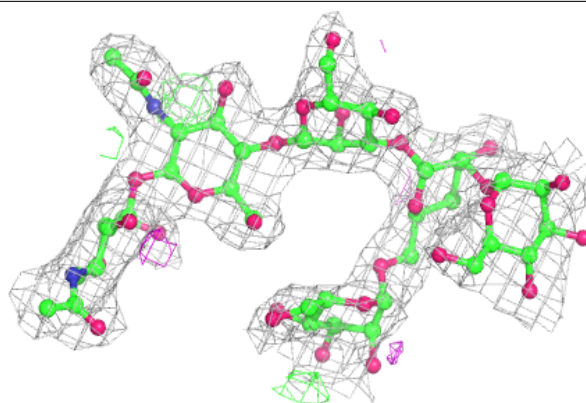
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MAN	F	4	11/12	0.51	0.40	81,95,106,107	0
3	MAN	D	4	11/12	0.59	0.37	81,91,100,101	0
2	MAN	E	5	11/12	0.70	0.31	75,81,84,85	0
2	MAN	E	6	11/12	0.72	0.27	73,76,83,90	0
3	BMA	F	3	11/12	0.74	0.32	80,87,93,101	0
3	BMA	D	3	11/12	0.79	0.32	91,99,103,104	0
2	MAN	C	6	11/12	0.81	0.26	50,63,75,78	0
2	MAN	C	5	11/12	0.83	0.24	67,74,77,79	0
2	BMA	E	3	11/12	0.86	0.20	34,56,66,68	0
2	MAN	E	4	11/12	0.87	0.18	33,58,69,75	0
2	BMA	C	3	11/12	0.87	0.19	33,47,56,63	0
3	NAG	D	2	14/15	0.87	0.20	26,50,68,82	0
3	NAG	F	2	14/15	0.88	0.22	48,55,73,80	0
2	NAG	C	2	14/15	0.89	0.18	25,43,52,58	0
2	NAG	E	2	14/15	0.90	0.19	27,42,60,66	0
2	MAN	C	4	11/12	0.92	0.16	39,49,58,59	0
3	NAG	D	1	14/15	0.93	0.15	24,39,50,56	0
2	NAG	E	1	14/15	0.94	0.16	28,40,51,62	0
3	NAG	F	1	14/15	0.95	0.17	21,36,50,55	0
2	NAG	C	1	14/15	0.96	0.15	31,39,51,56	0

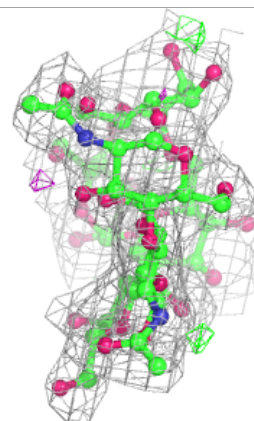
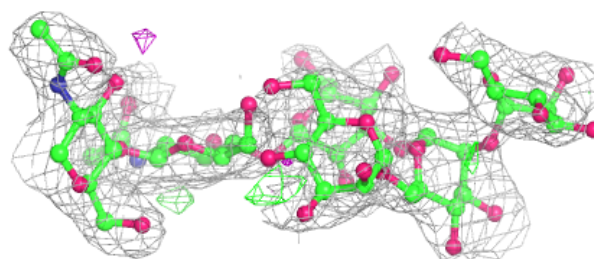
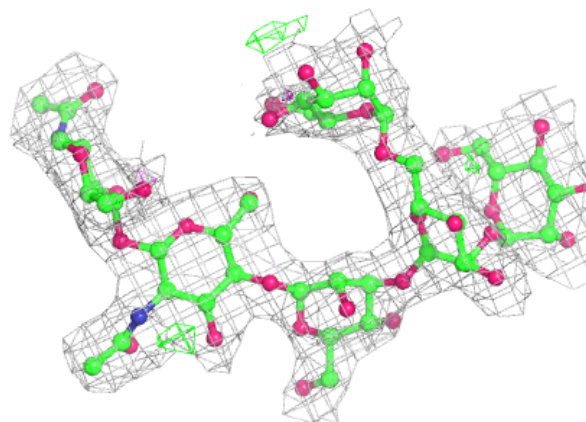
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

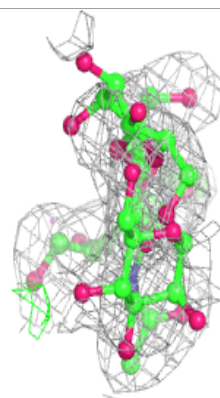
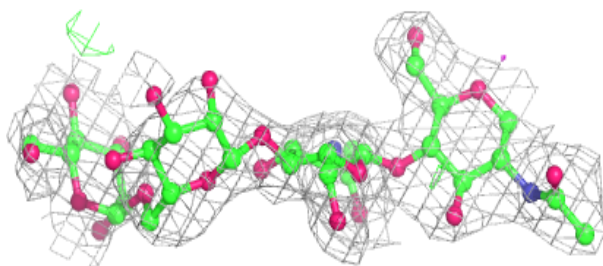
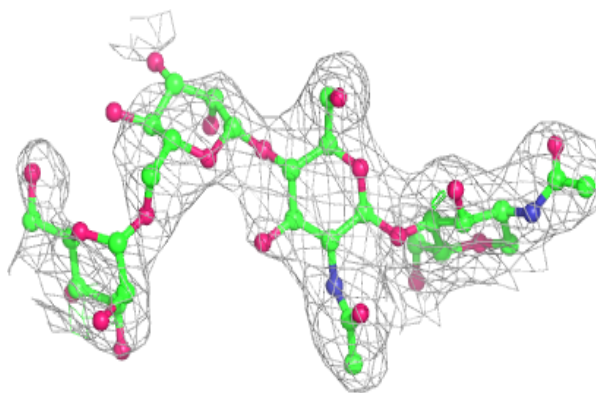
**Electron density around Chain E:**

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

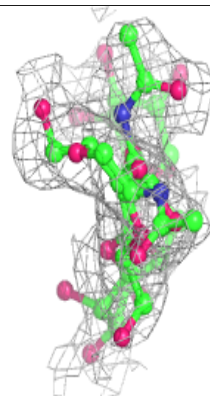
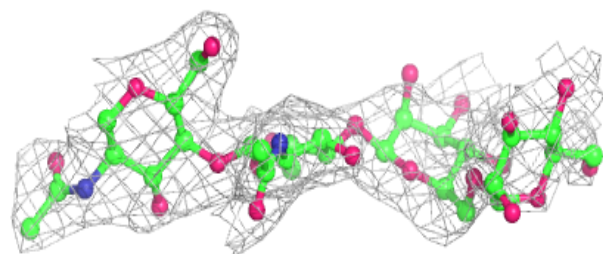
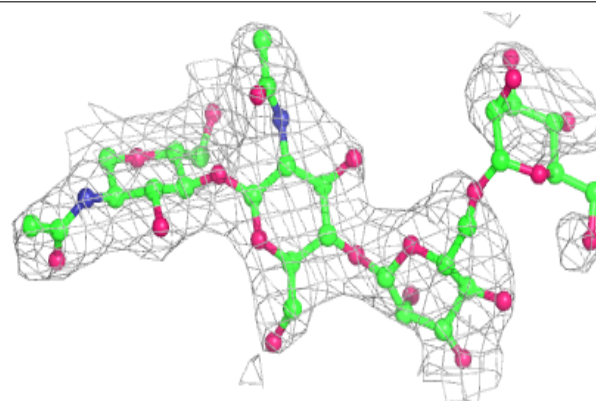


**Electron density around Chain D:**

$2mF_o-DF_c$  (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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.