



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:50 AM BST

PDB ID : 2PX1
Title : crystal structure of the complex of bovine lactoferrin C-lobe with Ribose at 2.5 Å resolution
Authors : Mir, R.; Vikram, G.; Sinha, M.; Sharma, S.; Kaur, P.; Singh, T.P.
Deposited on : 2007-05-14
Resolution : 2.50 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

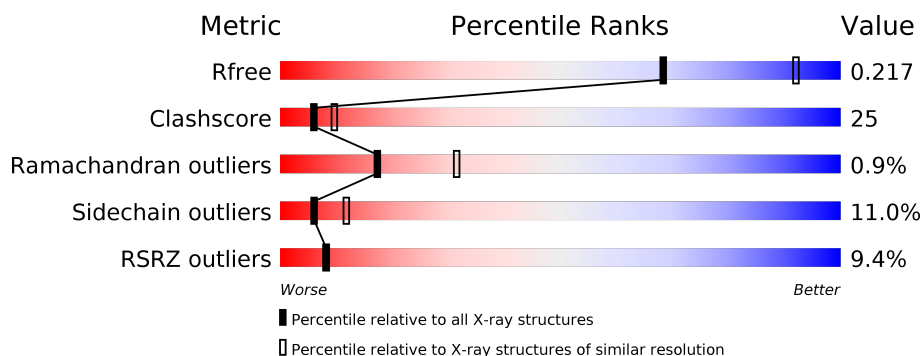
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	345	<div> <div>9%</div> <div>66%</div> <div>27%</div> <div>6%</div> </div>
2	B	2	<div>100%</div>
3	C	4	<div>75%</div> <div>25%</div>
4	D	3	<div>100%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	2	-	-	-	X
3	BMA	C	4	-	-	-	X
4	NDG	D	2	-	-	X	-
4	BMA	D	3	-	-	X	X
5	RIP	A	694	-	-	-	X
5	RIP	A	695	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 2919 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 Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2605	1622	454	508	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627

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



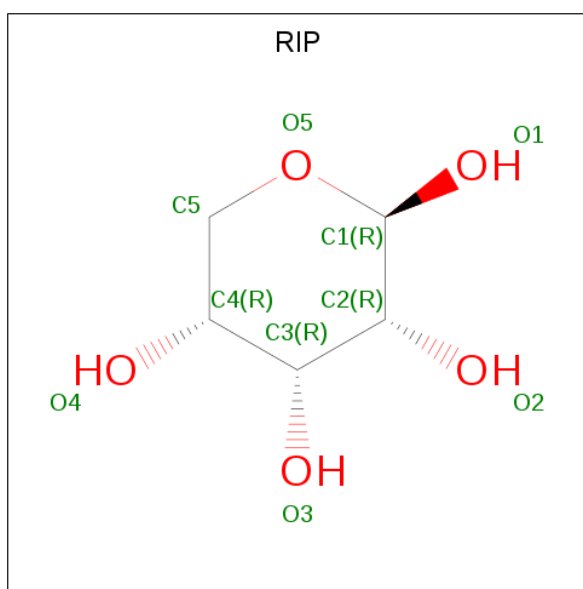
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



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

- Molecule 5 is beta-D-ribose (three-letter code: RIP) (formula: C₅H₁₀O₅).

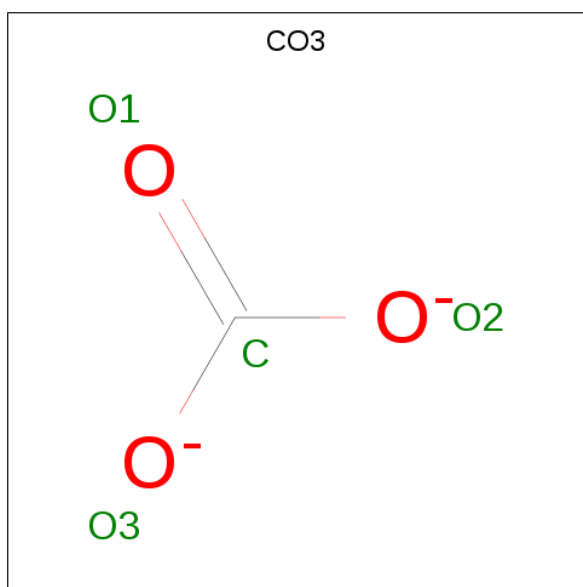


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	5	5		
5	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Fe	0	0
			1	1		

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).

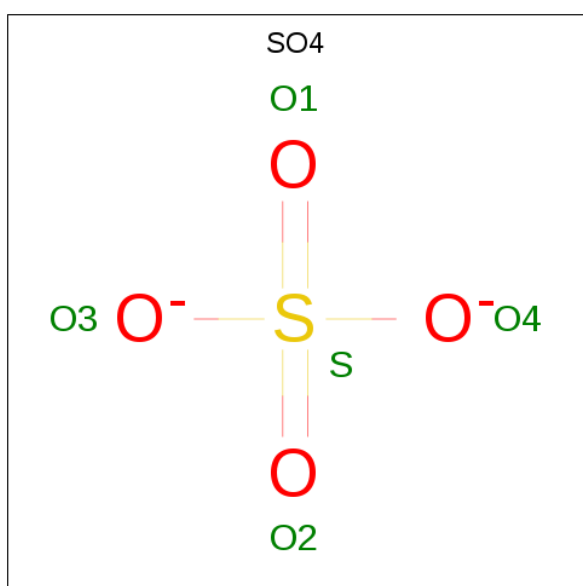


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

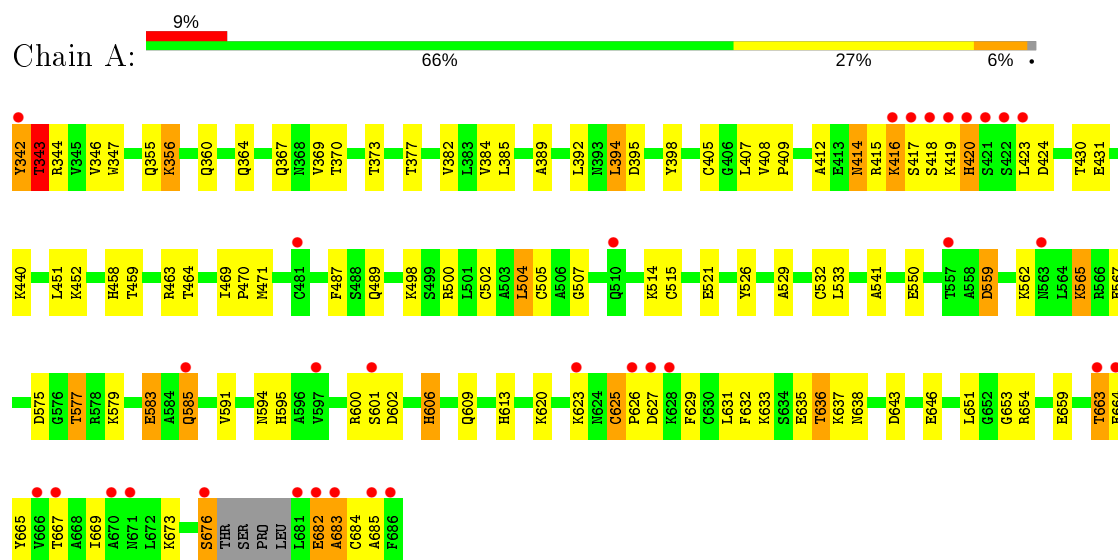
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	165	Total	O	0	0
			165	165		

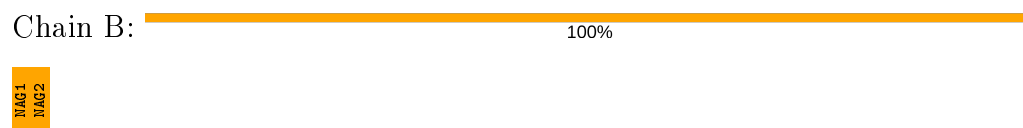
3 Residue-property plots

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.

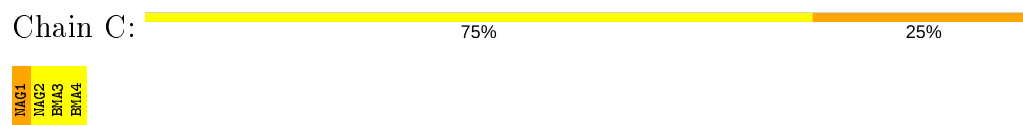
• Molecule 1: Lactotransferrin



• 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)-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-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MA01
MD02
BM03

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.91Å 49.63Å 64.70Å 90.00° 105.88° 90.00°	Depositor
Resolution (Å)	19.96 – 2.50 29.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.96-2.50) 99.4 (29.39-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.228 0.200 , 0.217	Depositor DCC
R_{free} test set	656 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	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	0.94	EDS
Total number of atoms	2919	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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: CO3, BMA, NAG, ZN, RIP, NDG, SO4, FE

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	0.53	0/2653	0.84	3/3591 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	343	THR	N-CA-C	8.95	135.17	111.00
1	A	342	TYR	CA-CB-CG	7.05	126.79	113.40
1	A	394	LEU	CA-CB-CG	5.54	128.04	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	2605	0	2519	117	0
2	B	28	0	25	2	0
3	C	50	0	43	2	0
4	D	39	0	33	13	0
5	A	20	0	20	3	0
6	A	1	0	0	0	0
7	A	4	0	0	1	0
8	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	5	0	0	0	0
10	A	165	0	0	56	0
All	All	2919	0	2640	134	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 25.

All (134) 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:369:VAL:HG13	10:A:1107:HOH:O	1.41	1.21
10:A:1137:HOH:O	4:D:3:BMA:H62	1.43	1.16
1:A:514:LYS:HE3	10:A:1110:HOH:O	1.44	1.15
1:A:419:LYS:HB3	10:A:1105:HOH:O	1.62	0.99
1:A:585:GLN:CD	1:A:585:GLN:H	1.63	0.98
1:A:458:HIS:HB3	10:A:1052:HOH:O	1.70	0.90
1:A:343:THR:HA	1:A:606:HIS:HE1	1.38	0.88
1:A:458:HIS:HE1	1:A:471:MET:HE3	1.40	0.87
1:A:458:HIS:CE1	1:A:471:MET:HE3	2.09	0.85
1:A:654:ARG:HD3	10:A:1145:HOH:O	1.76	0.85
4:D:2:NDG:O3	4:D:3:BMA:O2	1.76	0.80
1:A:424:ASP:HA	10:A:1048:HOH:O	1.80	0.80
1:A:458:HIS:HE1	1:A:471:MET:CE	1.94	0.80
1:A:423:LEU:HB2	10:A:1096:HOH:O	1.82	0.78
1:A:343:THR:HA	1:A:606:HIS:CE1	2.19	0.78
10:A:1153:HOH:O	2:B:1:NAG:O7	2.01	0.77
1:A:638:ASN:HD22	1:A:643:ASP:H	1.32	0.77
10:A:1050:HOH:O	4:D:3:BMA:O2	2.02	0.76
1:A:585:GLN:H	1:A:585:GLN:NE2	1.83	0.76
1:A:416:LYS:HB2	10:A:1146:HOH:O	1.85	0.76
1:A:676:SER:HB3	10:A:1165:HOH:O	1.86	0.75
1:A:638:ASN:ND2	1:A:643:ASP:H	1.83	0.75
1:A:620:LYS:HD2	1:A:646:GLU:HG3	1.68	0.75
1:A:416:LYS:HE2	10:A:1050:HOH:O	1.87	0.74
10:A:1138:HOH:O	4:D:2:NDG:C6	2.36	0.74
1:A:514:LYS:HB2	10:A:1056:HOH:O	1.87	0.74
10:A:1112:HOH:O	4:D:3:BMA:H3	1.88	0.73
1:A:343:THR:CA	1:A:606:HIS:HE1	2.02	0.72
1:A:585:GLN:HG2	10:A:1155:HOH:O	1.88	0.71
1:A:575:ASP:OD1	1:A:577:THR:HB	1.90	0.71
1:A:659:GLU:HG3	10:A:1163:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1138:HOH:O	4:D:2:NDG:C5	2.39	0.71
1:A:635:GLU:O	1:A:636:THR:HG22	1.92	0.69
1:A:600:ARG:HD2	10:A:1091:HOH:O	1.93	0.69
10:A:1138:HOH:O	4:D:2:NDG:H6C2	1.91	0.69
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.76	0.68
1:A:685:ALA:HB1	10:A:1141:HOH:O	1.93	0.67
1:A:585:GLN:NE2	4:D:1:NAG:H81	2.10	0.67
1:A:347:TRP:HB2	10:A:1107:HOH:O	1.94	0.67
1:A:565:LYS:HD3	1:A:567:GLU:H	1.61	0.66
1:A:458:HIS:CE1	1:A:471:MET:CE	2.76	0.65
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.26	0.65
1:A:431:GLU:HG2	10:A:1154:HOH:O	1.96	0.65
1:A:559:ASP:HB3	10:A:1121:HOH:O	1.97	0.64
1:A:342:TYR:HB2	1:A:606:HIS:CE1	2.32	0.64
5:A:694:RIP:C5	10:A:1059:HOH:O	2.47	0.62
1:A:355:GLN:HG3	1:A:373:THR:OG1	1.99	0.62
1:A:342:TYR:HB2	1:A:606:HIS:NE2	2.14	0.62
1:A:653:GLY:O	1:A:654:ARG:C	2.37	0.62
1:A:382:VAL:HG23	10:A:1089:HOH:O	2.01	0.61
1:A:416:LYS:HD2	4:D:3:BMA:H2	1.81	0.61
10:A:1150:HOH:O	2:B:2:NAG:H4	2.00	0.60
1:A:342:TYR:CB	1:A:606:HIS:CE1	2.85	0.59
5:A:694:RIP:H51	10:A:1059:HOH:O	2.01	0.59
1:A:414:ASN:HD21	1:A:430:THR:HA	1.67	0.59
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.38	0.59
1:A:343:THR:HG23	10:A:1079:HOH:O	2.02	0.58
1:A:635:GLU:HG3	10:A:1161:HOH:O	2.04	0.57
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.39	0.57
1:A:385:LEU:HD23	1:A:407:LEU:HD21	1.85	0.56
10:A:1050:HOH:O	4:D:2:NDG:H3	2.05	0.56
1:A:625:CYS:HA	1:A:629:PHE:O	2.04	0.56
1:A:585:GLN:CD	1:A:585:GLN:N	2.42	0.56
10:A:1050:HOH:O	4:D:2:NDG:C3	2.52	0.56
10:A:1049:HOH:O	3:C:1:NAG:C8	2.53	0.56
1:A:663:THR:O	1:A:667:THR:HG23	2.06	0.55
1:A:342:TYR:HD2	1:A:606:HIS:CG	2.24	0.55
1:A:418:SER:HB3	10:A:1137:HOH:O	2.05	0.55
1:A:415:ARG:HD3	10:A:1106:HOH:O	2.05	0.55
1:A:405:CYS:HA	1:A:684:CYS:HB2	1.88	0.54
1:A:369:VAL:CG1	10:A:1107:HOH:O	2.23	0.53
1:A:625:CYS:HB3	1:A:626:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:LYS:HD3	10:A:1102:HOH:O	2.09	0.53
1:A:417:SER:HB2	10:A:1095:HOH:O	2.09	0.53
1:A:682:GLU:O	1:A:683:ALA:HB2	2.09	0.53
1:A:471:MET:CE	1:A:487:PHE:HE2	2.23	0.52
1:A:430:THR:HB	1:A:594:ASN:ND2	2.25	0.51
1:A:471:MET:HE2	1:A:487:PHE:HE2	1.76	0.51
1:A:669:ILE:O	1:A:673:LYS:HG3	2.11	0.51
1:A:625:CYS:CB	1:A:626:PRO:HD3	2.40	0.50
1:A:676:SER:CB	10:A:1165:HOH:O	2.52	0.50
1:A:342:TYR:HB3	1:A:606:HIS:ND1	2.26	0.50
1:A:502:CYS:O	1:A:514:LYS:NZ	2.44	0.50
1:A:342:TYR:C	1:A:606:HIS:CE1	2.85	0.50
1:A:585:GLN:NE2	1:A:585:GLN:N	2.56	0.50
1:A:377:THR:HG21	1:A:398:TYR:CD2	2.47	0.49
1:A:416:LYS:HD2	4:D:3:BMA:C2	2.42	0.49
1:A:682:GLU:HG3	10:A:1151:HOH:O	2.12	0.49
1:A:382:VAL:CG2	10:A:1089:HOH:O	2.58	0.49
1:A:550:GLU:HG2	10:A:1128:HOH:O	2.11	0.49
1:A:343:THR:N	1:A:606:HIS:CE1	2.81	0.49
1:A:416:LYS:CE	10:A:1050:HOH:O	2.56	0.48
1:A:392:LEU:HD11	1:A:394:LEU:HD21	1.93	0.48
1:A:632:PHE:O	1:A:643:ASP:HA	2.14	0.47
1:A:579:LYS:HD3	1:A:583:GLU:HG2	1.97	0.47
1:A:585:GLN:CG	10:A:1155:HOH:O	2.57	0.47
1:A:673:LYS:HE2	10:A:1053:HOH:O	2.15	0.47
5:A:694:RIP:O5	10:A:1059:HOH:O	2.20	0.47
1:A:609:GLN:HG2	1:A:613:HIS:CE1	2.50	0.47
1:A:625:CYS:O	1:A:626:PRO:C	2.53	0.46
1:A:505:CYS:HB3	1:A:521:GLU:OE1	2.14	0.46
1:A:625:CYS:CB	1:A:626:PRO:CD	2.94	0.46
1:A:342:TYR:CD2	1:A:606:HIS:CD2	3.04	0.46
1:A:419:LYS:O	1:A:420:HIS:HB2	2.16	0.46
1:A:343:THR:N	1:A:606:HIS:HE1	2.14	0.45
1:A:342:TYR:HD2	1:A:606:HIS:HB2	1.82	0.45
1:A:638:ASN:HD22	1:A:643:ASP:N	2.07	0.45
1:A:635:GLU:N	10:A:1073:HOH:O	2.50	0.45
1:A:609:GLN:NE2	10:A:1034:HOH:O	2.26	0.44
1:A:412:ALA:HB2	1:A:651:LEU:HD21	2.00	0.44
1:A:533:LEU:HB2	1:A:541:ALA:HB2	2.00	0.44
4:D:2:NDG:C3	4:D:3:BMA:O2	2.63	0.44
1:A:356:LYS:O	1:A:360:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:HB3	1:A:606:HIS:CE1	2.53	0.43
1:A:384:VAL:HA	1:A:389:ALA:O	2.18	0.43
1:A:646:GLU:HB2	10:A:1146:HOH:O	2.18	0.43
1:A:342:TYR:HB3	1:A:606:HIS:CG	2.53	0.43
1:A:562:LYS:NZ	10:A:1121:HOH:O	2.49	0.43
1:A:342:TYR:OH	10:A:1159:HOH:O	2.21	0.42
1:A:463:ARG:NH2	7:A:201:CO3:O1	2.49	0.42
1:A:364:GLN:HG3	1:A:629:PHE:HB2	2.01	0.42
10:A:1049:HOH:O	3:C:1:NAG:H82	2.19	0.42
1:A:507:GLY:CA	1:A:514:LYS:HA	2.49	0.42
1:A:464:THR:O	1:A:469:ILE:HG12	2.20	0.42
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.55	0.41
1:A:408:VAL:HA	1:A:409:PRO:HD3	1.88	0.41
1:A:489:GLN:HB3	1:A:504:LEU:HD13	2.03	0.41
1:A:417:SER:HB2	1:A:431:GLU:OE1	2.20	0.41
1:A:431:GLU:CG	10:A:1154:HOH:O	2.63	0.41
1:A:585:GLN:CD	10:A:1155:HOH:O	2.60	0.41
1:A:469:ILE:N	1:A:470:PRO:HD2	2.36	0.40
1:A:637:LYS:HG2	10:A:1147:HOH:O	2.21	0.40
1:A:459:THR:HG22	1:A:526:TYR:HA	2.04	0.40
1:A:529:ALA:O	1:A:532:CYS:HB3	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	337/345 (98%)	308 (91%)	26 (8%)	3 (1%)	17	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	CYS
1	A	343	THR
1	A	683	ALA

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	282/286 (99%)	251 (89%)	31 (11%)	6 12

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	THR
1	A	344	ARG
1	A	356	LYS
1	A	367	GLN
1	A	414	ASN
1	A	416	LYS
1	A	420	HIS
1	A	440	LYS
1	A	451	LEU
1	A	498	LYS
1	A	500	ARG
1	A	504	LEU
1	A	515	CYS
1	A	559	ASP
1	A	565	LYS
1	A	577	THR
1	A	583	GLU
1	A	585	GLN
1	A	591	VAL
1	A	601	SER
1	A	602	ASP
1	A	606	HIS
1	A	623	LYS
1	A	627	ASP

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Mol	Chain	Res	Type
1	A	631	LEU
1	A	633	LYS
1	A	636	THR
1	A	663	THR
1	A	664	GLU
1	A	676	SER
1	A	682	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	GLN
1	A	359	GLN
1	A	393	ASN
1	A	414	ASN
1	A	449	ASN
1	A	606	HIS
1	A	609	GLN
1	A	613	HIS
1	A	638	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

9 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	0.55	0	17,19,21	1.45	1 (5%)
2	NAG	B	2	2	14,14,15	0.60	0	17,19,21	1.13	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.86	0	17,19,21	2.07	4 (23%)
3	NAG	C	2	3	14,14,15	0.84	1 (7%)	17,19,21	1.50	4 (23%)
3	BMA	C	3	3	11,11,12	1.39	2 (18%)	15,15,17	0.74	0
3	BMA	C	4	3	11,11,12	1.05	1 (9%)	15,15,17	1.45	3 (20%)
4	NAG	D	1	1,4	14,14,15	0.91	1 (7%)	17,19,21	1.88	4 (23%)
4	NDG	D	2	4	14,14,15	0.81	0	17,19,21	2.42	5 (29%)
4	BMA	D	3	4	11,11,12	1.13	1 (9%)	15,15,17	2.36	4 (26%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C4-C5	3.40	1.60	1.53
3	C	4	BMA	O5-C5	2.60	1.48	1.43
4	D	1	NAG	C4-C5	2.46	1.58	1.53
3	C	3	BMA	O5-C5	2.11	1.47	1.43
4	D	3	BMA	C2-C3	2.10	1.55	1.52
3	C	2	NAG	C4-C5	2.08	1.57	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-C2-C3	7.37	118.72	109.67
4	D	2	NDG	O5-C1-C2	6.73	121.92	111.29
3	C	1	NAG	C4-C3-C2	-5.65	102.74	111.02
4	D	2	NDG	C1-O5-C5	5.19	119.22	112.19
2	B	1	NAG	C4-C3-C2	4.71	117.92	111.02
3	C	1	NAG	C2-N2-C7	4.49	129.30	122.90
4	D	1	NAG	C1-C2-N2	4.06	117.43	110.49
4	D	1	NAG	O5-C1-C2	-3.54	105.69	111.29
3	C	4	BMA	C1-C2-C3	-3.27	105.64	109.67
2	B	2	NAG	C4-C3-C2	3.14	115.62	111.02
3	C	4	BMA	C6-C5-C4	-3.11	105.73	113.00
3	C	1	NAG	C1-C2-N2	2.81	115.28	110.49
3	C	2	NAG	C6-C5-C4	-2.80	106.45	113.00
3	C	2	NAG	C1-O5-C5	2.65	115.78	112.19
4	D	2	NDG	C6-C5-C4	-2.64	106.81	113.00
4	D	3	BMA	O5-C5-C6	2.63	111.33	107.20
4	D	1	NAG	C8-C7-N2	2.54	120.41	116.10
4	D	2	NDG	O3-C3-C2	-2.49	104.32	109.47
4	D	3	BMA	C2-C3-C4	2.48	115.19	110.89
4	D	2	NDG	C4-C3-C2	2.31	114.40	111.02
3	C	2	NAG	C2-N2-C7	-2.28	119.66	122.90
3	C	1	NAG	O7-C7-N2	2.27	126.12	121.95
4	D	1	NAG	C3-C4-C5	2.25	114.25	110.24
3	C	4	BMA	O5-C5-C6	2.24	110.71	107.20
4	D	3	BMA	O5-C1-C2	2.20	114.16	110.77
3	C	2	NAG	C3-C4-C5	2.11	114.00	110.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

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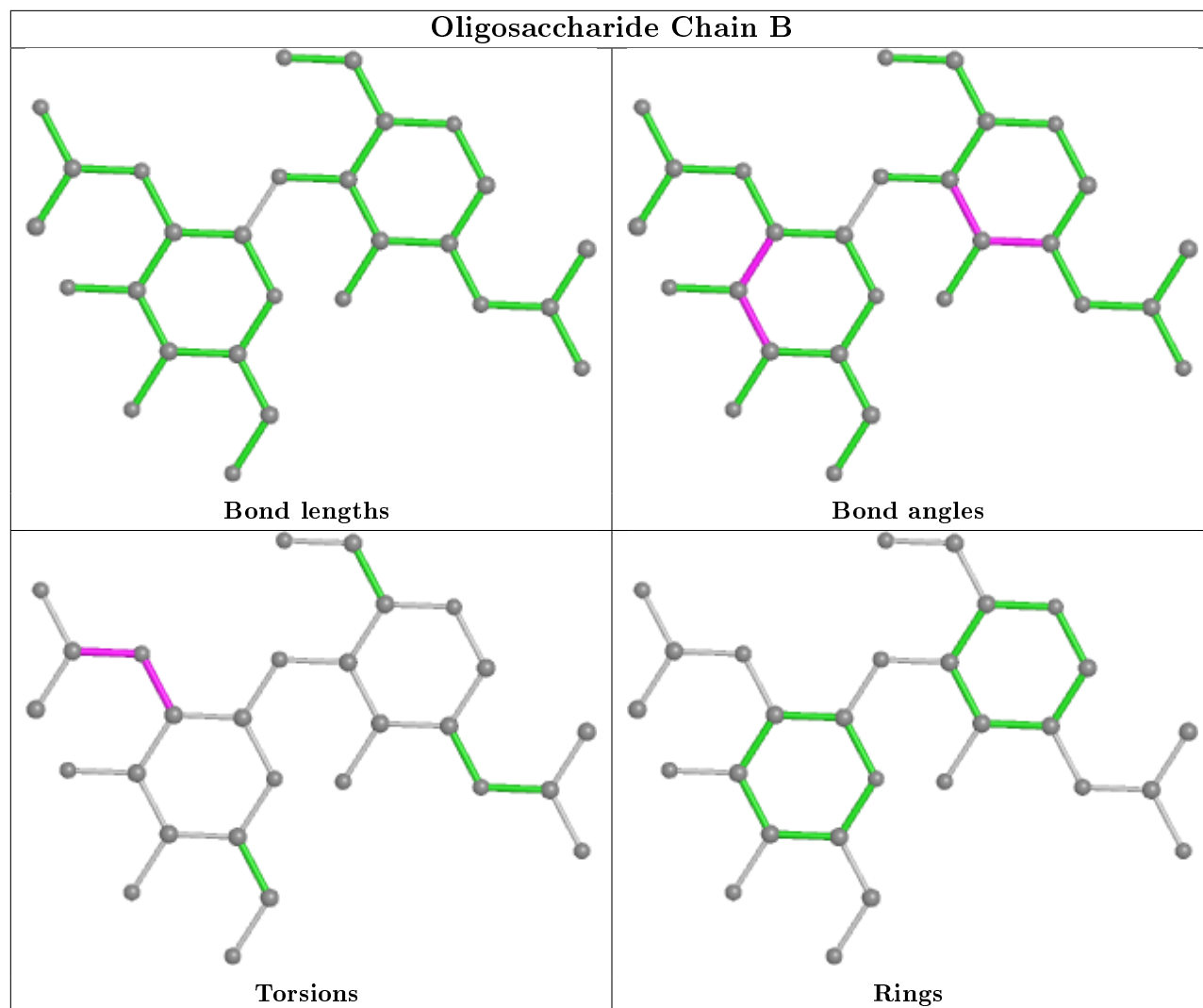
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
3	C	3	BMA	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
3	C	4	BMA	O5-C5-C6-O6
3	C	1	NAG	C3-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2

There are no ring outliers.

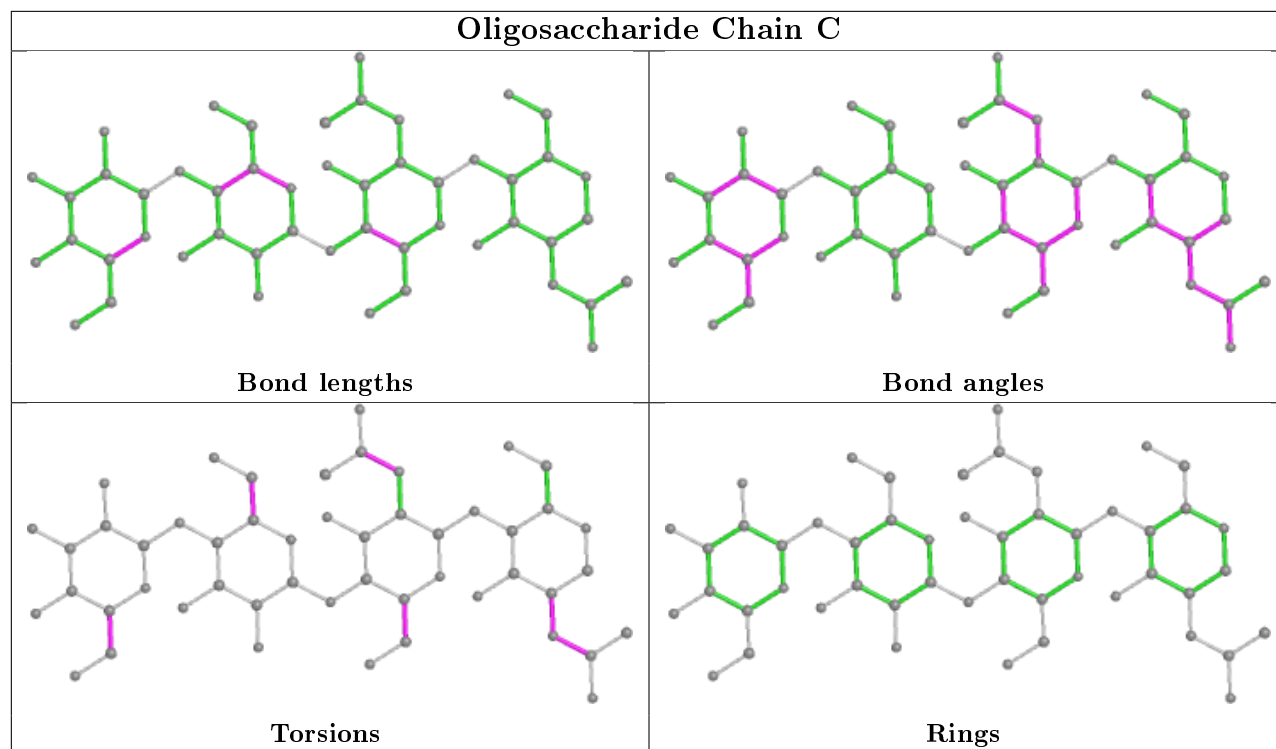
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	1	0
4	D	3	BMA	7	0
4	D	2	NDG	7	0
3	C	1	NAG	2	0
4	D	1	NAG	1	0

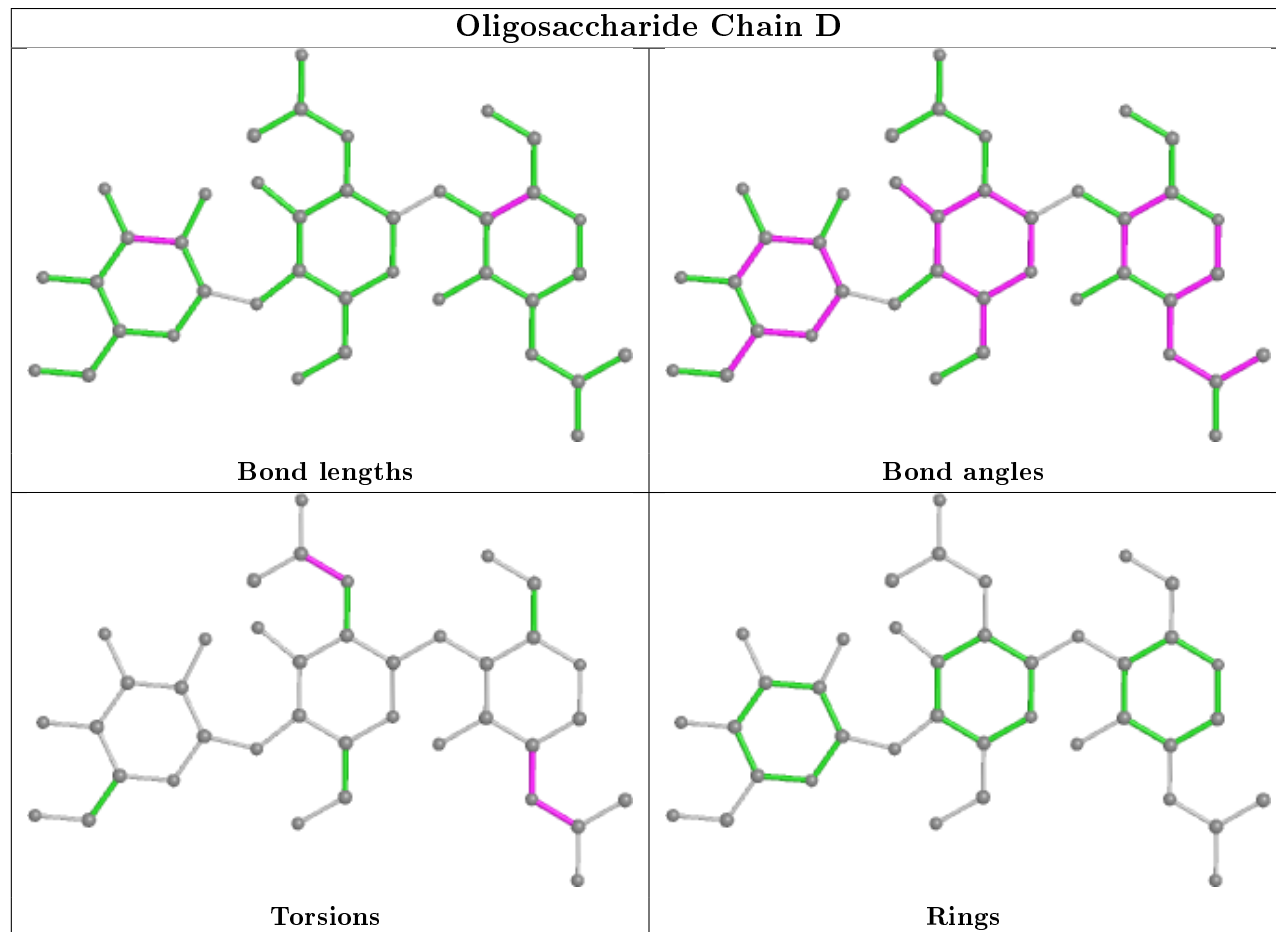
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 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
5	RIP	A	695	-	10,10,10	1.23	1 (10%)	14,14,14	1.46	3 (21%)
7	CO3	A	201	6	0,3,3	0.00	-	0,3,3	0.00	-
5	RIP	A	694	-	10,10,10	1.44	1 (10%)	14,14,14	1.71	3 (21%)
9	SO4	A	1002	-	4,4,4	0.30	0	6,6,6	0.16	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	RIP	A	695	-	-	-	0/1/1/1
5	RIP	A	694	-	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	694	RIP	C4-C3	3.47	1.57	1.52
5	A	695	RIP	O3-C3	-2.21	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	694	RIP	O5-C5-C4	3.32	115.90	110.77
5	A	694	RIP	C5-C4-C3	3.02	113.37	109.67
5	A	694	RIP	C5-O5-C1	2.69	117.24	112.71
5	A	695	RIP	C5-O5-C1	-2.29	108.86	112.71
5	A	695	RIP	O3-C3-C2	2.23	115.50	110.35
5	A	695	RIP	C5-C4-C3	2.18	112.34	109.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	201	CO3	1	0
5	A	694	RIP	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	341/345 (98%)	0.49	32 (9%) 8 8	21, 41, 65, 88	7 (2%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	SER	9.6
1	A	422	SER	8.8
1	A	418	SER	7.2
1	A	601	SER	6.4
1	A	420	HIS	6.3
1	A	423	LEU	5.3
1	A	683	ALA	5.1
1	A	682	GLU	4.6
1	A	685	ALA	4.4
1	A	666	VAL	4.4
1	A	419	LYS	3.9
1	A	681	LEU	3.3
1	A	416	LYS	3.2
1	A	481	CYS	3.2
1	A	667	THR	3.1
1	A	663	THR	3.0
1	A	342	TYR	2.8
1	A	670	ALA	2.8
1	A	417	SER	2.7
1	A	664	GLU	2.7
1	A	671	ASN	2.5
1	A	686	PHE	2.5
1	A	628	LYS	2.5
1	A	557	THR	2.4
1	A	563	ASN	2.4
1	A	623	LYS	2.4
1	A	676	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	627	ASP	2.3
1	A	585	GLN	2.3
1	A	510	GLN	2.2
1	A	626	PRO	2.1
1	A	597	VAL	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](#)

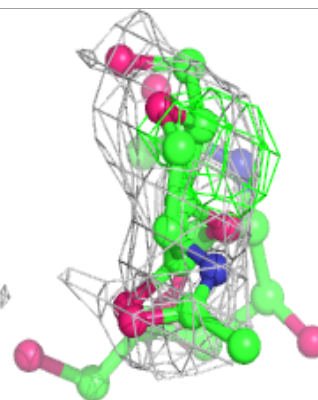
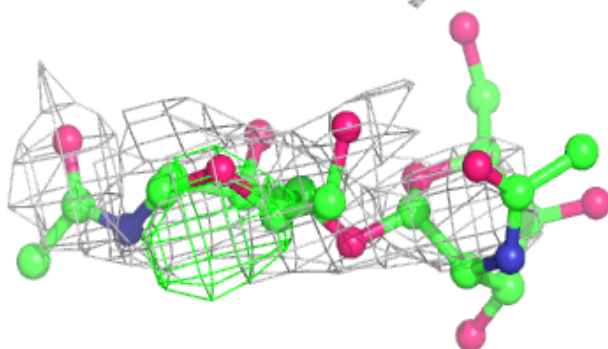
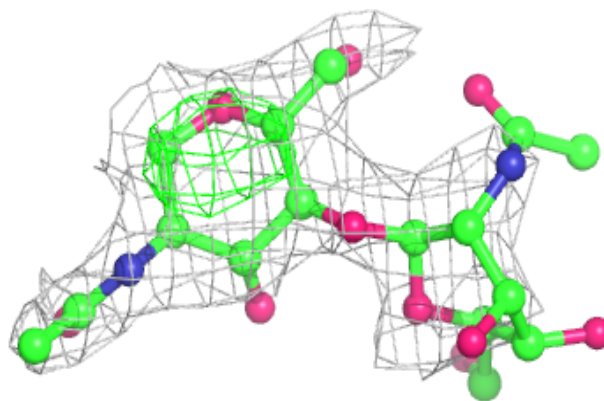
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	C	4	11/12	0.51	0.54	66,67,68,69	11
2	NAG	B	2	14/15	0.56	0.63	59,61,63,63	14
4	NDG	D	2	14/15	0.63	0.31	55,57,60,63	14
3	BMA	C	3	11/12	0.73	0.22	58,60,61,64	11
4	BMA	D	3	11/12	0.75	0.46	66,68,69,70	11
2	NAG	B	1	14/15	0.79	0.21	48,51,53,56	14
3	NAG	C	2	14/15	0.83	0.21	49,50,52,55	14
3	NAG	C	1	14/15	0.86	0.26	39,42,44,46	14
4	NAG	D	1	14/15	0.88	0.37	40,42,46,51	14

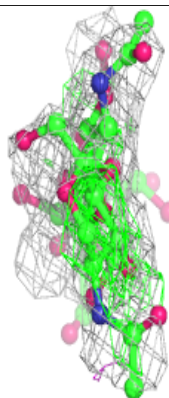
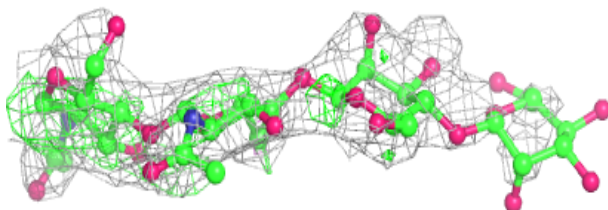
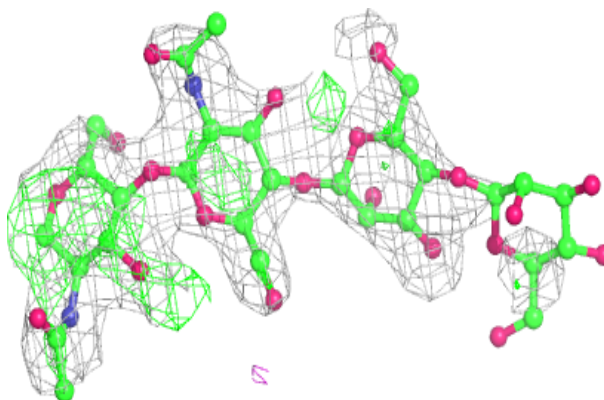
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

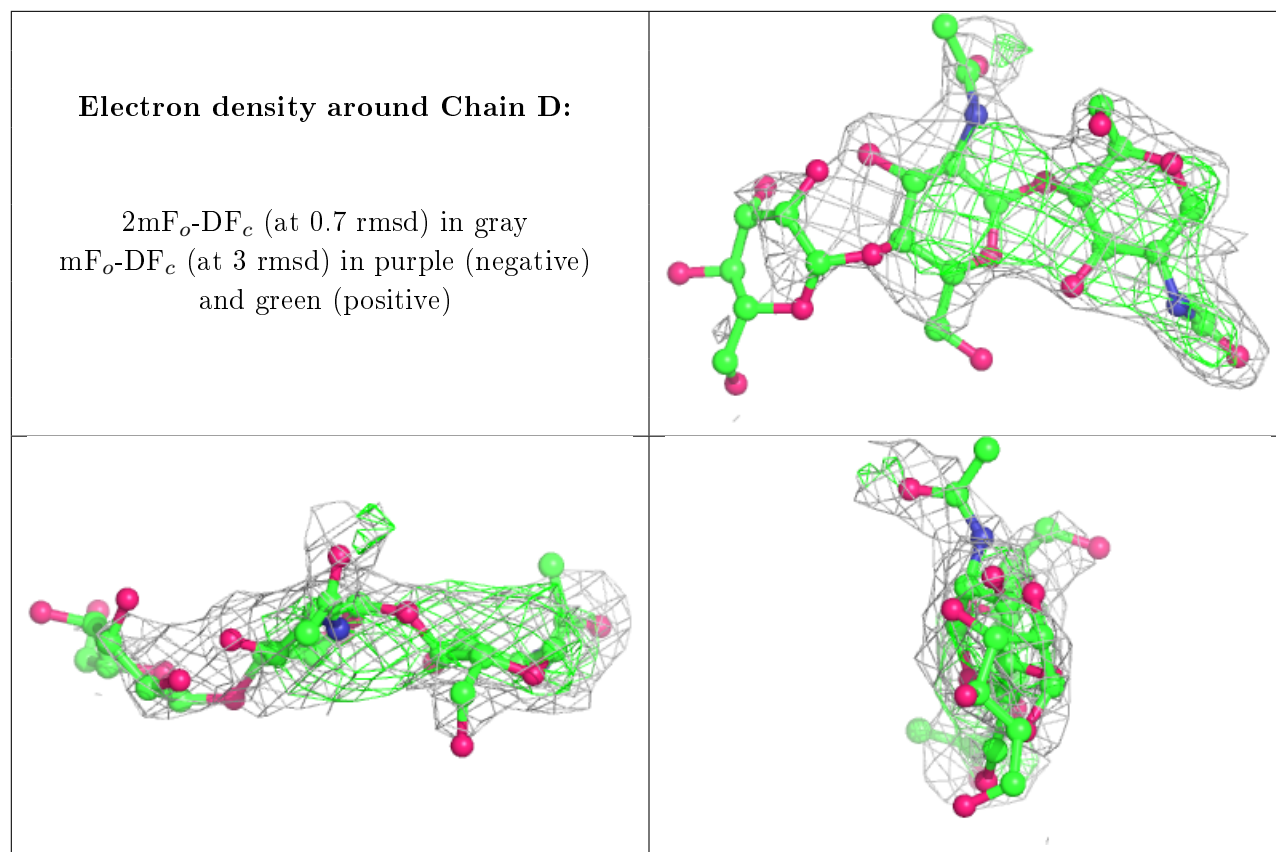
Electron density around Chain B:

$2mF_o-DF_c$ (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)





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
5	RIP	A	694	10/10	0.43	0.52	59,59,60,60	10
5	RIP	A	695	10/10	0.70	0.59	56,57,57,57	10
9	SO4	A	1002	5/5	0.95	0.20	30,30,31,31	5
8	ZN	A	302	1/1	0.98	0.10	46,46,46,46	0
6	FE	A	1001	1/1	0.99	0.14	32,32,32,32	0
7	CO3	A	201	4/4	0.99	0.27	28,29,29,30	0
8	ZN	A	301	1/1	0.99	0.10	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.