



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:30 PM UTC

PDB ID : 3IB2 / pdb_00003ib2
Title : structure of the complex of C-terminal half (C-lobe) of bovine lactoferrin with
alpha-methyl-4-(2-methylpropyl) benzene acetic acid
Authors : Mir, R.; Vikram, G.; Kumar, R.P.; Sinha, M.; Singh, N.; Sharma, S.; Kaur,
P.; Singh, T.P.
Deposited on : 2009-07-15
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

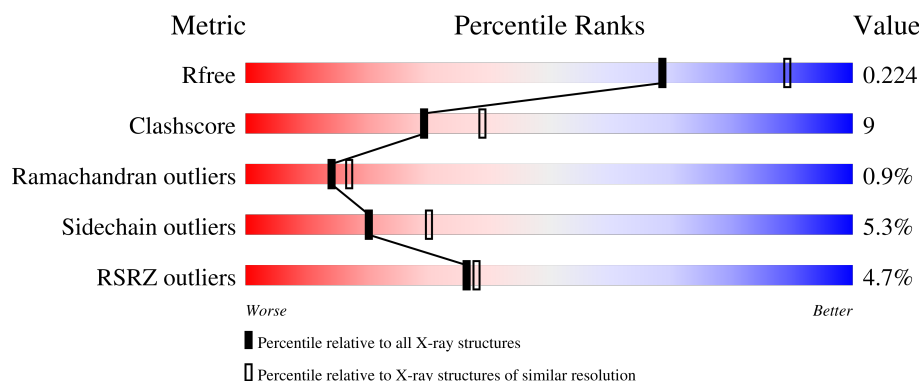
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	5% 80% 14% 5%
2	B	3	67% 33%
3	C	2	100%
3	D	2	50% 50%

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
2	MAN	B	3	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 2866 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
			2604	1622	454	507	21			

There are 2 discrepancies between the modelled and reference sequences:

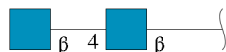
Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627

- Molecule 2 is an oligosaccharide called alpha-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	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



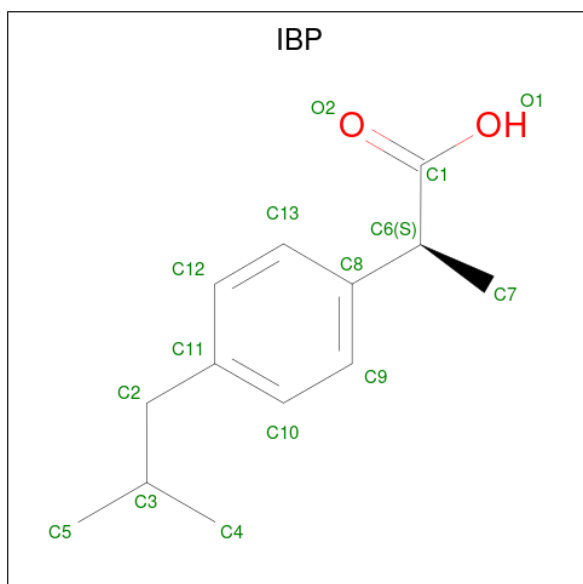
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

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

- Molecule 4 is IBUPROFEN (CCD ID: IBP) (formula: $C_{13}H_{18}O_2$).

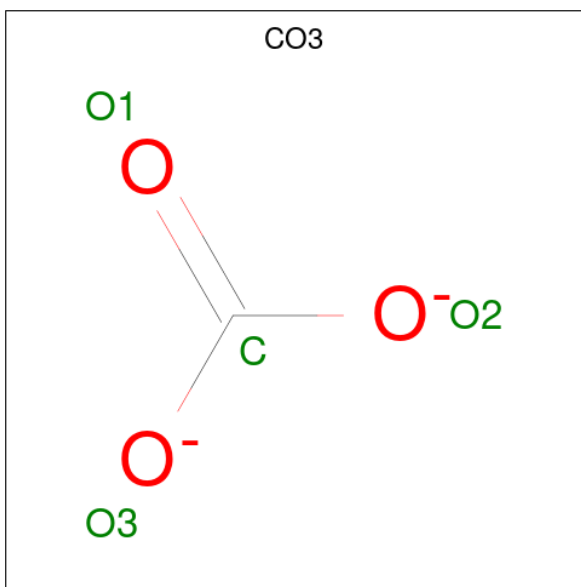


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			15	13	2		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 6 is CARBONATE ION (CCD ID: CO3) (formula: CO_3).

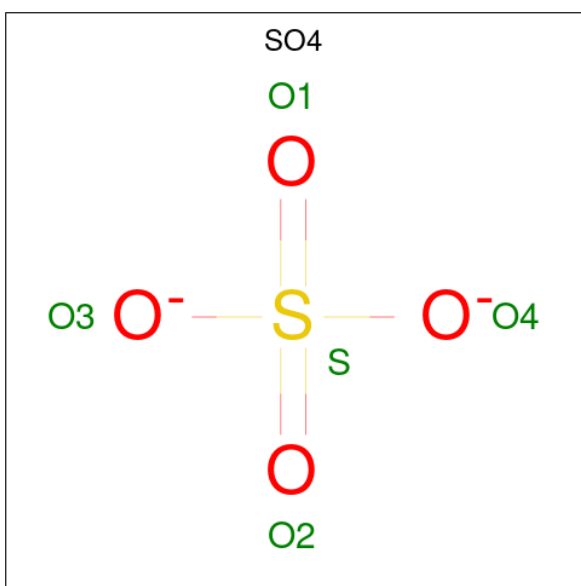


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

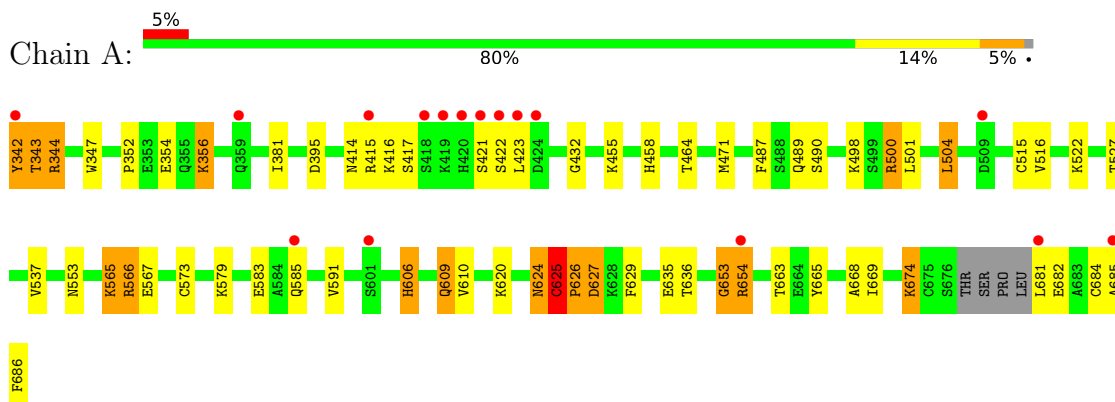
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	140	Total	O	0	0
			140	140		

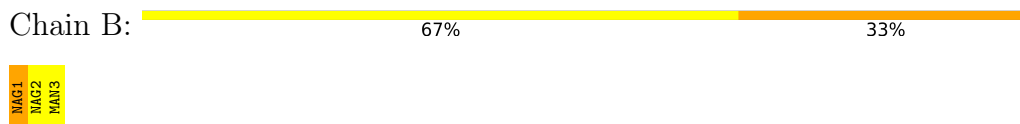
3 Residue-property plots [i](#)

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.

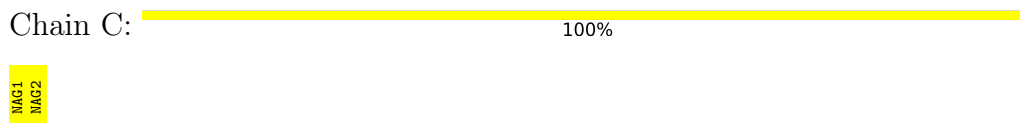
- Molecule 1: Lactotransferrin



- Molecule 2: alpha-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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.32Å 50.48Å 66.12Å 90.00° 107.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.29 20.00 – 2.29	Depositor EDS
% Data completeness (in resolution range)	87.3 (20.00-2.29) 87.3 (20.00-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.220 0.175 , 0.224	Depositor DCC
R_{free} test set	814 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2866	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, IBP, FE, MAN, CO3, NAG

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	1.28	11/2652 (0.4%)	1.29	14/3591 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	654	ARG	CD-NE	-7.11	1.36	1.46
1	A	566	ARG	C-N	6.00	1.41	1.33
1	A	395	ASP	CA-C	5.46	1.59	1.52
1	A	422	SER	N-CA	5.46	1.52	1.46
1	A	515	CYS	C-N	5.41	1.40	1.33
1	A	527	THR	CA-CB	5.41	1.61	1.53
1	A	624	ASN	CA-C	-5.20	1.45	1.52
1	A	606	HIS	ND1-CE1	5.11	1.37	1.32
1	A	352	PRO	C-N	-5.10	1.26	1.34
1	A	414	ASN	CG-ND2	-5.04	1.22	1.33
1	A	522	LYS	C-N	5.03	1.40	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	GLY	N-CA-C	-7.75	104.34	115.27
1	A	516	VAL	N-CA-CB	7.38	117.59	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	SER	N-CA-C	7.02	125.75	110.80
1	A	606	HIS	CB-CG-CD2	-6.89	122.24	131.20
1	A	627	ASP	N-CA-C	6.08	120.79	112.04
1	A	498	LYS	CG-CD-CE	6.00	125.11	111.30
1	A	354	GLU	N-CA-C	-5.96	104.72	112.23
1	A	516	VAL	CB-CA-C	-5.88	105.24	111.00
1	A	381	ILE	CB-CG1-CD1	5.85	126.09	113.80
1	A	464	THR	N-CA-C	5.67	117.15	110.97
1	A	606	HIS	CB-CG-ND1	5.30	130.65	122.70
1	A	620	LYS	N-CA-C	5.25	116.69	111.07
1	A	522	LYS	CG-CD-CE	5.04	122.89	111.30
1	A	347	TRP	N-CA-C	-5.02	102.09	110.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	TYR	Peptide
1	A	500	ARG	Sidechain
1	A	625	CYS	Peptide

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	2604	0	2519	46	0
2	B	39	0	34	2	0
3	C	28	0	25	0	0
3	D	28	0	25	1	0
4	A	15	0	17	1	0
5	A	1	0	0	0	0
6	A	4	0	0	0	0
7	A	2	0	0	0	0
8	A	5	0	0	0	0
9	A	140	0	0	0	0
All	All	2866	0	2620	46	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 9.

All (46) 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:342:TYR:N	1:A:606:HIS:HE1	1.45	1.15
1:A:342:TYR:N	1:A:606:HIS:CE1	2.20	1.09
1:A:471:MET:HE1	1:A:487:PHE:HE2	1.19	1.03
1:A:343:THR:HA	1:A:606:HIS:NE2	1.83	0.93
1:A:668:ALA:HB1	2:B:1:NAG:H83	1.51	0.88
1:A:343:THR:HG23	1:A:343:THR:O	1.77	0.85
1:A:342:TYR:HB2	1:A:606:HIS:CE1	2.12	0.84
1:A:635:GLU:O	1:A:636:THR:HG22	1.80	0.82
1:A:342:TYR:CA	1:A:606:HIS:CE1	2.62	0.82
1:A:625:CYS:O	1:A:627:ASP:N	2.15	0.80
1:A:471:MET:HE1	1:A:487:PHE:CE2	2.12	0.77
1:A:573:CYS:SG	1:A:579:LYS:HD2	2.28	0.74
1:A:489:GLN:HB3	1:A:504:LEU:HD13	1.72	0.70
1:A:668:ALA:CB	2:B:1:NAG:H83	2.20	0.70
1:A:342:TYR:CB	1:A:606:HIS:CE1	2.74	0.70
1:A:342:TYR:HB2	1:A:606:HIS:ND1	2.10	0.67
1:A:343:THR:HA	1:A:606:HIS:CE1	2.30	0.66
1:A:565:LYS:HD3	1:A:567:GLU:H	1.62	0.64
1:A:565:LYS:CD	1:A:567:GLU:H	2.14	0.60
1:A:504:LEU:HG	1:A:537:VAL:HG12	1.84	0.59
1:A:624:ASN:O	1:A:625:CYS:O	2.19	0.59
1:A:342:TYR:C	1:A:606:HIS:NE2	2.61	0.59
1:A:490:SER:HB2	1:A:501:LEU:HA	1.84	0.59
1:A:343:THR:O	1:A:343:THR:CG2	2.49	0.58
1:A:342:TYR:C	1:A:606:HIS:CE1	2.83	0.57
1:A:458:HIS:HE1	1:A:471:MET:HE3	1.72	0.54
1:A:625:CYS:HA	1:A:629:PHE:O	2.07	0.53
1:A:674:LYS:HD3	1:A:681:LEU:HD21	1.89	0.53
1:A:553:ASN:HD21	1:A:565:LYS:HE2	1.74	0.51
1:A:565:LYS:HD3	1:A:566:ARG:N	2.26	0.50
1:A:565:LYS:HD3	1:A:565:LYS:C	2.37	0.49
1:A:585:GLN:HG2	3:D:1:NAG:H81	1.95	0.47
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.51	0.46
1:A:455:LYS:HB3	1:A:504:LEU:HD21	1.98	0.45
1:A:625:CYS:HB3	1:A:626:PRO:HD3	1.99	0.44
1:A:565:LYS:HD2	1:A:567:GLU:HB2	1.98	0.43
1:A:684:CYS:C	1:A:686:PHE:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLN:HB3	1:A:504:LEU:CD1	2.46	0.43
1:A:432:GLY:CA	4:A:3960:IBP:H51	2.49	0.42
1:A:653:GLY:O	1:A:654:ARG:C	2.61	0.42
1:A:490:SER:C	1:A:504:LEU:HB2	2.44	0.42
1:A:344:ARG:HE	1:A:344:ARG:HB2	1.73	0.42
1:A:356:LYS:HE3	1:A:356:LYS:HB2	1.89	0.41
1:A:682:GLU:O	1:A:682:GLU:HG3	2.21	0.41
1:A:565:LYS:HD3	1:A:567:GLU:N	2.31	0.40
1:A:609:GLN:HG2	1:A:610:VAL:N	2.36	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%)	307 (91%)	27 (8%)	3 (1%)	14 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	625	CYS
1	A	685	ALA
1	A	626	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/286 (99%)	267 (95%)	15 (5%)	20	30

All (15) 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	415	ARG
1	A	416	LYS
1	A	417	SER
1	A	423	LEU
1	A	500	ARG
1	A	504	LEU
1	A	565	LYS
1	A	583	GLU
1	A	591	VAL
1	A	609	GLN
1	A	663	THR
1	A	674	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	606	HIS
1	A	621	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

7 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.69	0	17,19,21	1.37	3 (17%)
2	NAG	B	2	2	14,14,15	0.82	0	17,19,21	1.83	3 (17%)
2	MAN	B	3	2	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
3	NAG	C	1	1,3	14,14,15	0.74	0	17,19,21	2.25	6 (35%)
3	NAG	C	2	3	14,14,15	0.83	1 (7%)	17,19,21	2.14	6 (35%)
3	NAG	D	1	1,3	14,14,15	0.95	1 (7%)	17,19,21	1.86	4 (23%)
3	NAG	D	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.87	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.45	1.55	1.52
3	D	1	NAG	O5-C1	-2.33	1.39	1.43
3	D	2	NAG	C1-C2	2.24	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	5.60	130.41	122.90
2	B	2	NAG	C4-C3-C2	5.25	118.72	111.02
3	C	1	NAG	C1-O5-C5	5.08	119.00	112.19
3	D	2	NAG	C2-N2-C7	4.75	129.27	122.90
3	D	1	NAG	C1-O5-C5	4.51	118.23	112.19
3	C	2	NAG	C1-C2-N2	4.25	117.14	110.43
3	C	1	NAG	C2-N2-C7	3.90	128.12	122.90
3	D	2	NAG	C1-O5-C5	3.70	117.14	112.19
2	B	1	NAG	C2-N2-C7	-3.36	118.39	122.90
3	D	1	NAG	O5-C1-C2	-3.24	106.28	111.29
3	C	1	NAG	C4-C3-C2	3.23	115.75	111.02
3	C	1	NAG	C3-C4-C5	3.19	116.01	110.23
2	B	2	NAG	C2-N2-C7	3.13	127.09	122.90
3	D	1	NAG	C2-N2-C7	-2.93	118.97	122.90
3	C	1	NAG	O7-C7-N2	2.90	127.10	121.98
3	D	2	NAG	O5-C1-C2	2.73	115.51	111.29
2	B	1	NAG	C1-O5-C5	2.59	115.66	112.19
3	C	2	NAG	C3-C4-C5	-2.36	105.94	110.23
2	B	3	MAN	C3-C4-C5	2.28	114.37	110.23
3	C	2	NAG	O5-C5-C4	-2.28	105.28	110.83
3	C	2	NAG	O5-C5-C6	2.19	111.93	107.66
3	C	1	NAG	O7-C7-C8	-2.18	118.17	122.05
3	D	2	NAG	O7-C7-C8	-2.13	118.26	122.05
2	B	2	NAG	O3-C3-C2	-2.11	105.02	109.40
2	B	1	NAG	C4-C3-C2	2.08	114.06	111.02
3	D	1	NAG	O4-C4-C3	-2.06	105.52	110.38
3	C	2	NAG	O4-C4-C5	2.05	114.37	109.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3	MAN	C1

All (11) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

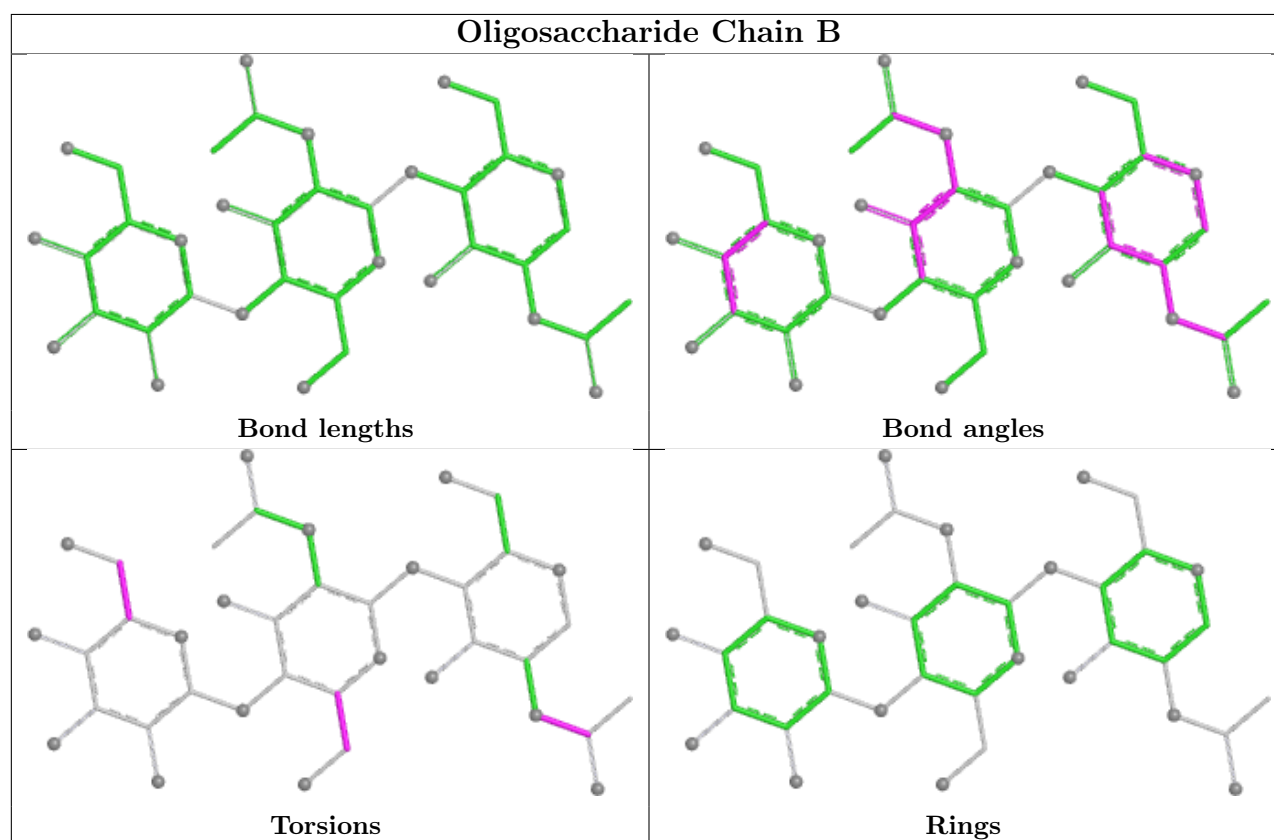
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2

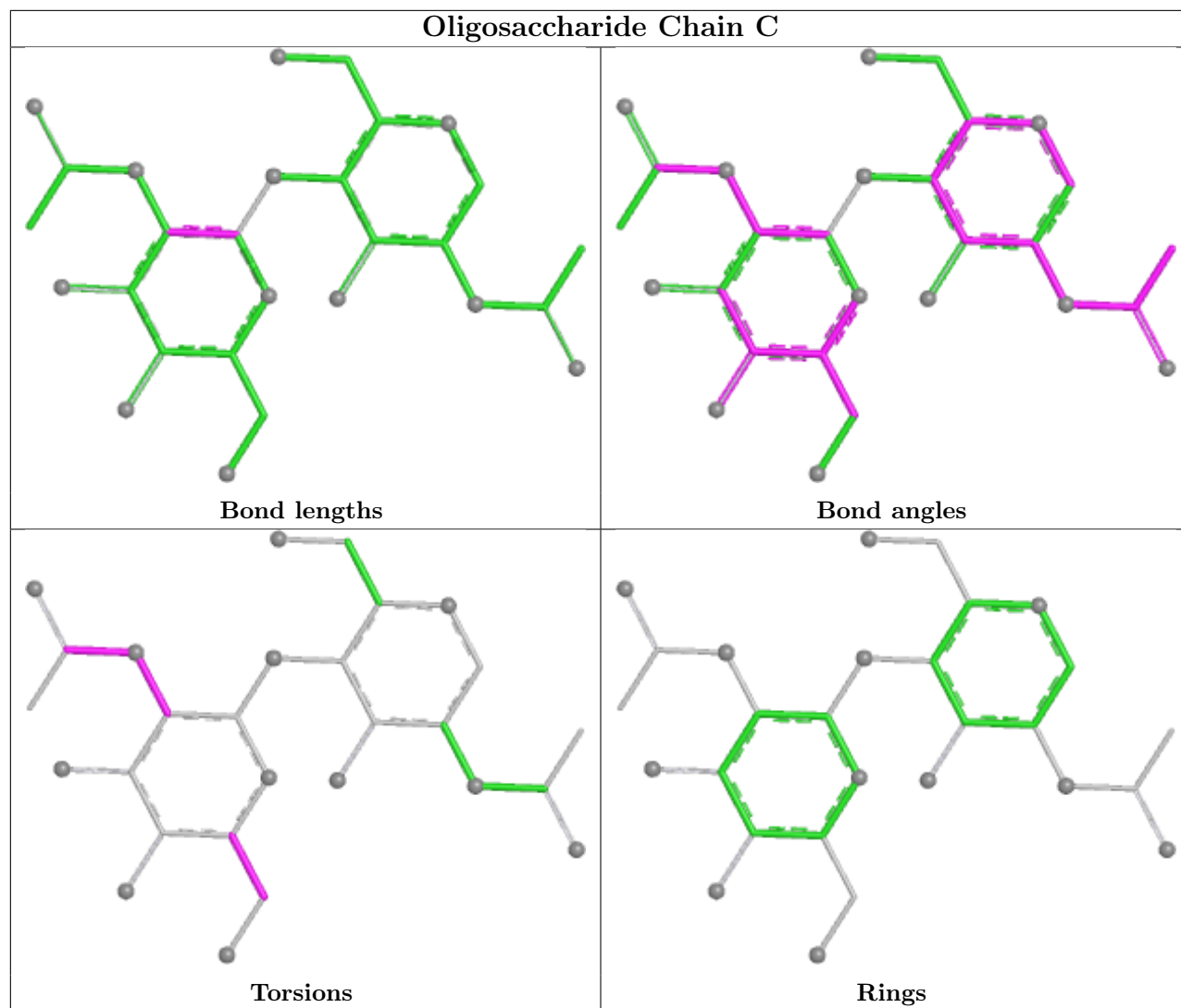
There are no ring outliers.

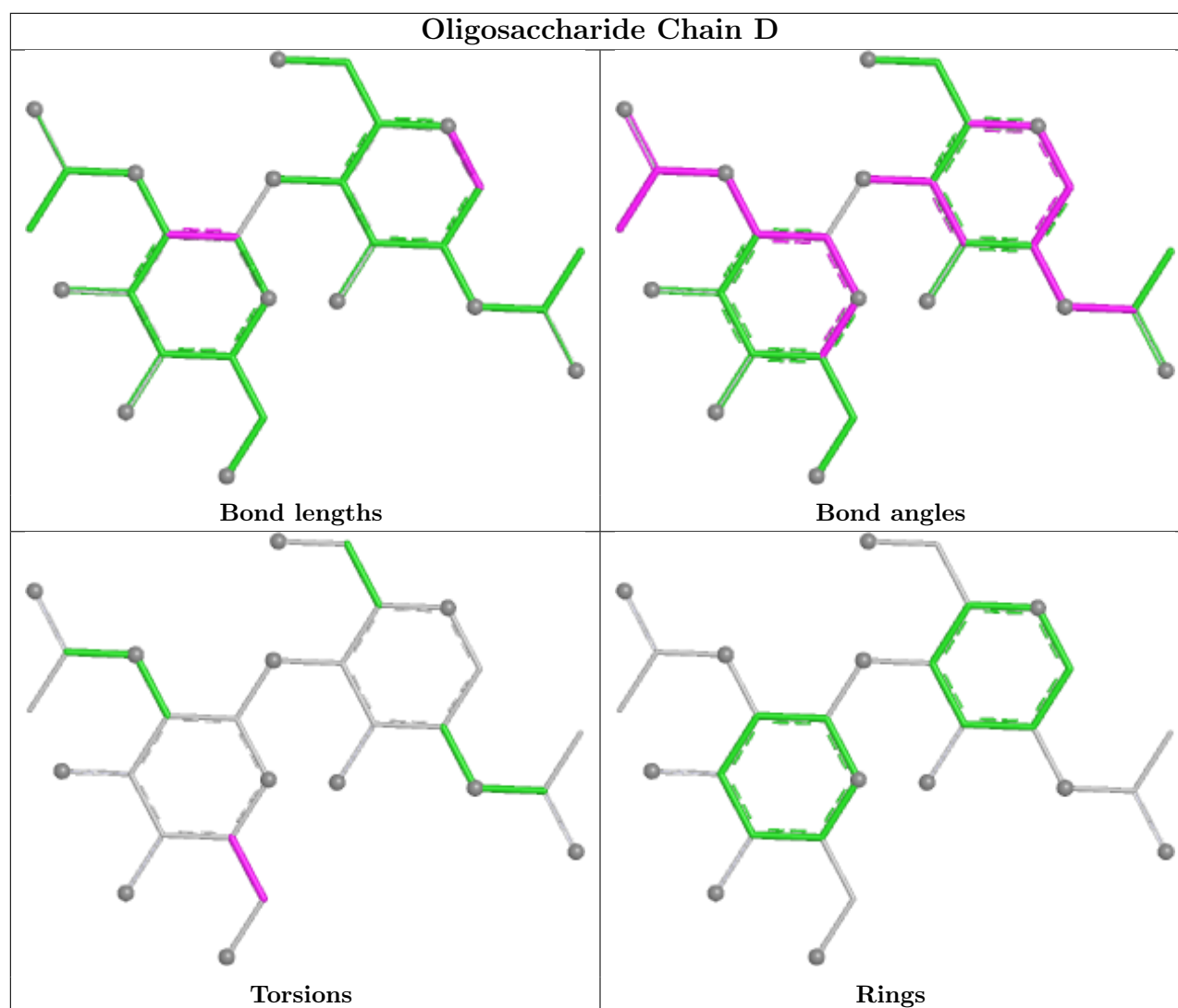
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	2	0
3	D	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	A	5	-	4,4,4	0.15	0	6,6,6	0.39	0
6	CO3	A	691	5	3,3,3	0.96	0	2,3,3	0.72	0
4	IBP	A	3960	-	15,15,15	0.97	0	20,20,20	3.74	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IBP	A	3960	-	-	6/12/12/12	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3960	IBP	C11-C2-C3	16.04	160.06	114.49
4	A	3960	IBP	C8-C6-C1	-3.66	98.29	108.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3960	IBP	C11-C2-C3-C5
4	A	3960	IBP	C11-C2-C3-C4
4	A	3960	IBP	C10-C11-C2-C3
4	A	3960	IBP	C12-C11-C2-C3
4	A	3960	IBP	O1-C1-C6-C8
4	A	3960	IBP	O2-C1-C6-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3960	IBP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	341/345 (98%)	-0.15	16 (4%)	36 38	10, 27, 53, 86	5 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	ASP	4.5
1	A	359	GLN	4.3
1	A	342	TYR	4.0
1	A	601	SER	3.9
1	A	422	SER	3.9
1	A	585	GLN	3.7
1	A	509	ASP	3.1
1	A	419	LYS	3.1
1	A	685	ALA	2.5
1	A	421	SER	2.4
1	A	420	HIS	2.3
1	A	418	SER	2.2
1	A	415	ARG	2.1
1	A	681	LEU	2.1
1	A	423	LEU	2.1
1	A	654	ARG	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.

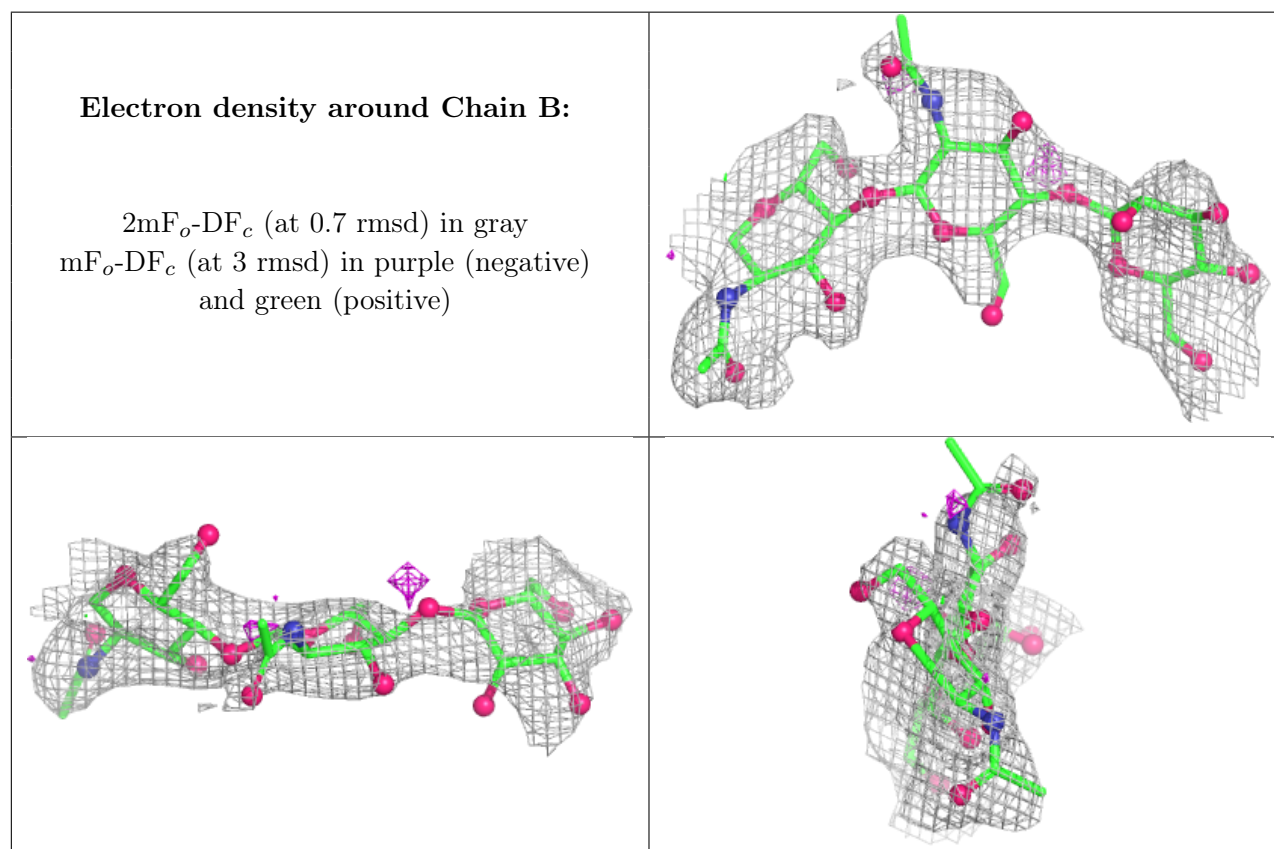
6.3 Carbohydrates [i](#)

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.

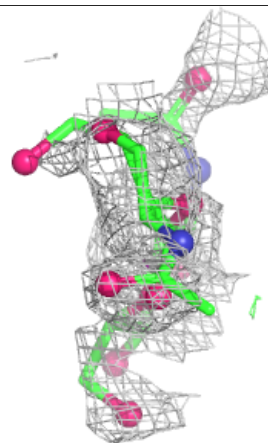
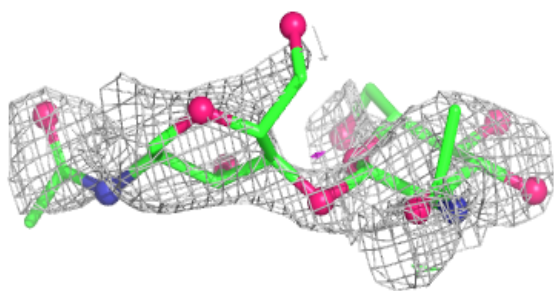
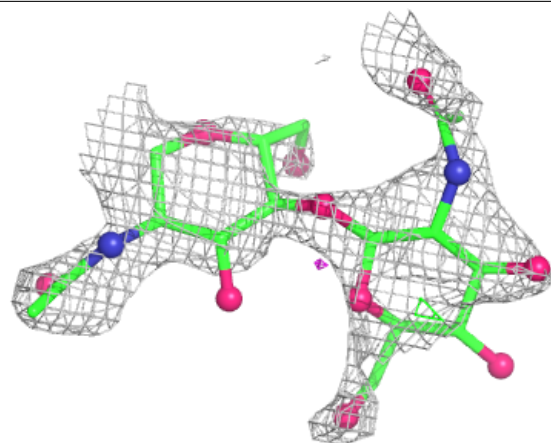
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	2	14/15	0.54	0.15	94,97,99,101	0
2	MAN	B	3	11/12	0.60	0.13	85,86,88,88	0
3	NAG	C	1	14/15	0.73	0.14	66,73,80,87	0
2	NAG	B	2	14/15	0.81	0.15	70,75,78,82	0
2	NAG	B	1	14/15	0.86	0.11	47,55,60,64	0
3	NAG	D	2	14/15	0.86	0.10	55,58,64,67	0
3	NAG	D	1	14/15	0.93	0.07	31,36,42,50	0

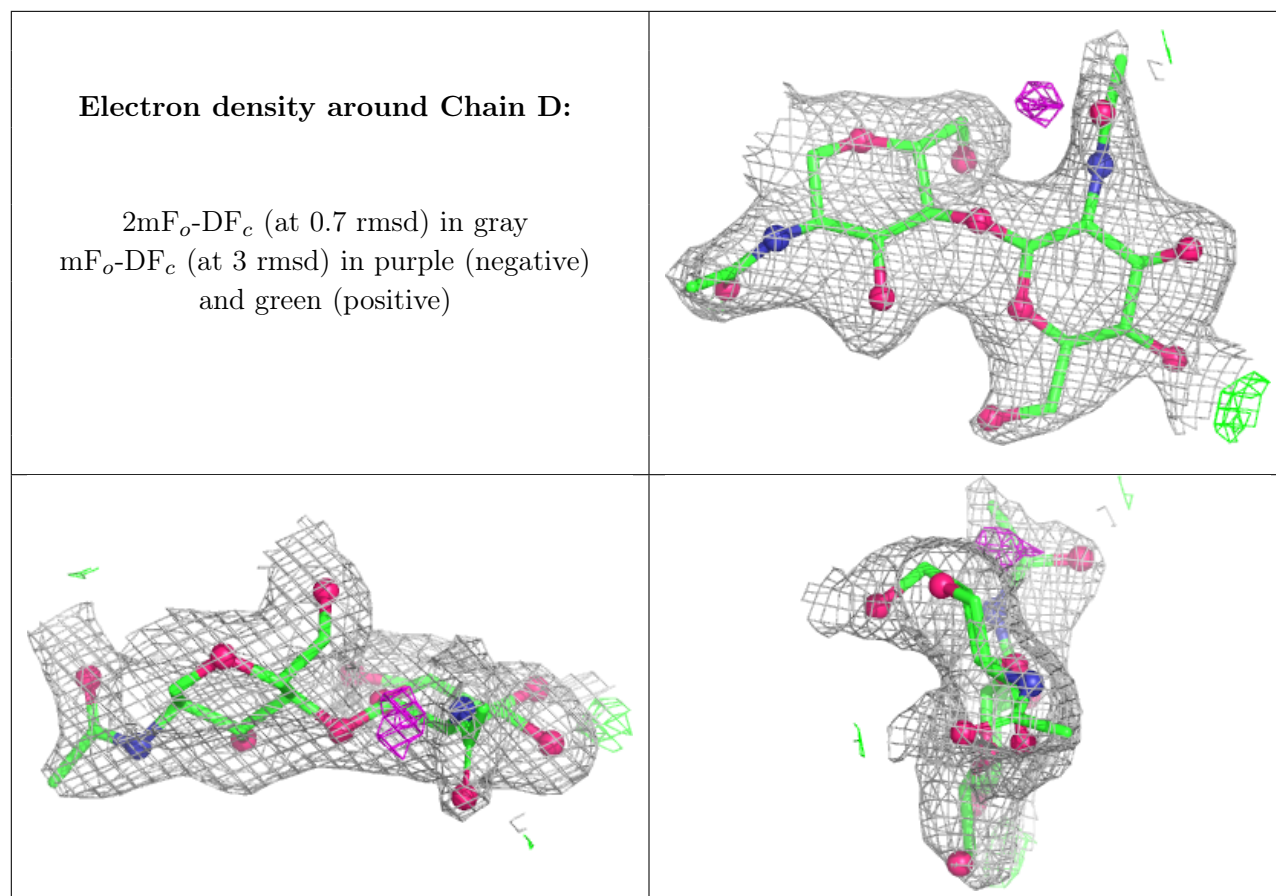
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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)





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($\text{\AA}^2$)	Q<0.9
4	IBP	A	3960	15/15	0.75	0.28	66,67,69,69	15
6	CO3	A	691	4/4	0.89	0.10	10,13,14,15	0
8	SO4	A	5	5/5	0.91	0.11	30,31,31,34	5
7	ZN	A	692	1/1	0.97	0.10	37,37,37,37	0
7	ZN	A	4	1/1	0.99	0.04	37,37,37,37	0
5	FE	A	1001	1/1	0.99	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.