



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:33 AM UTC

PDB ID : 1BLF / pdb_00001blf
Title : STRUCTURE OF DIFERRIC BOVINE LACTOFERRIN AT 2.8
ANGSTROMS RESOLUTION
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Deposited on : 1997-08-20
Resolution : 2.80 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

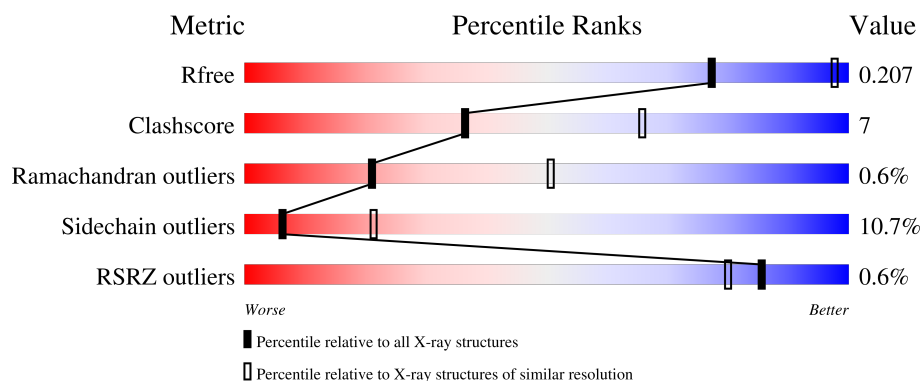
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	689	71% 25% . .
2	B	3	67% 33%
3	C	6	67% 33%

2 Entry composition [i](#)

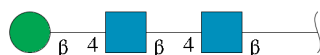
There are 7 unique types of molecules in this entry. The entry contains 5495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LACTOFERRIN.

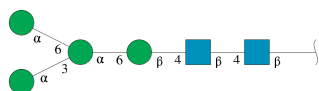
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	0	0
			5310	3338	937	997	38			

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

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

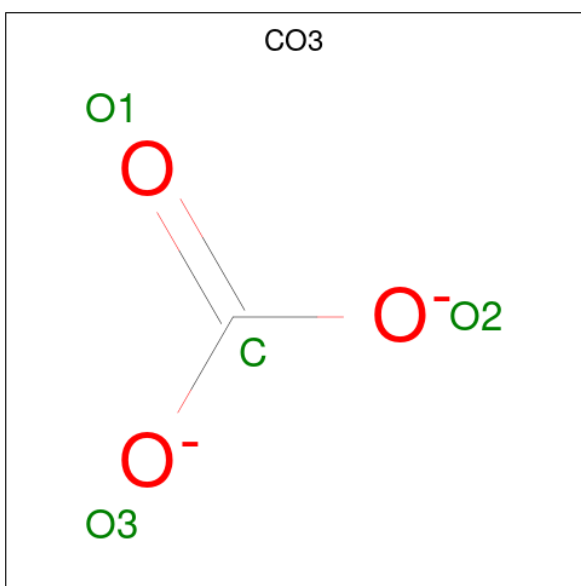


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Fe	0	0
			2	2		

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



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

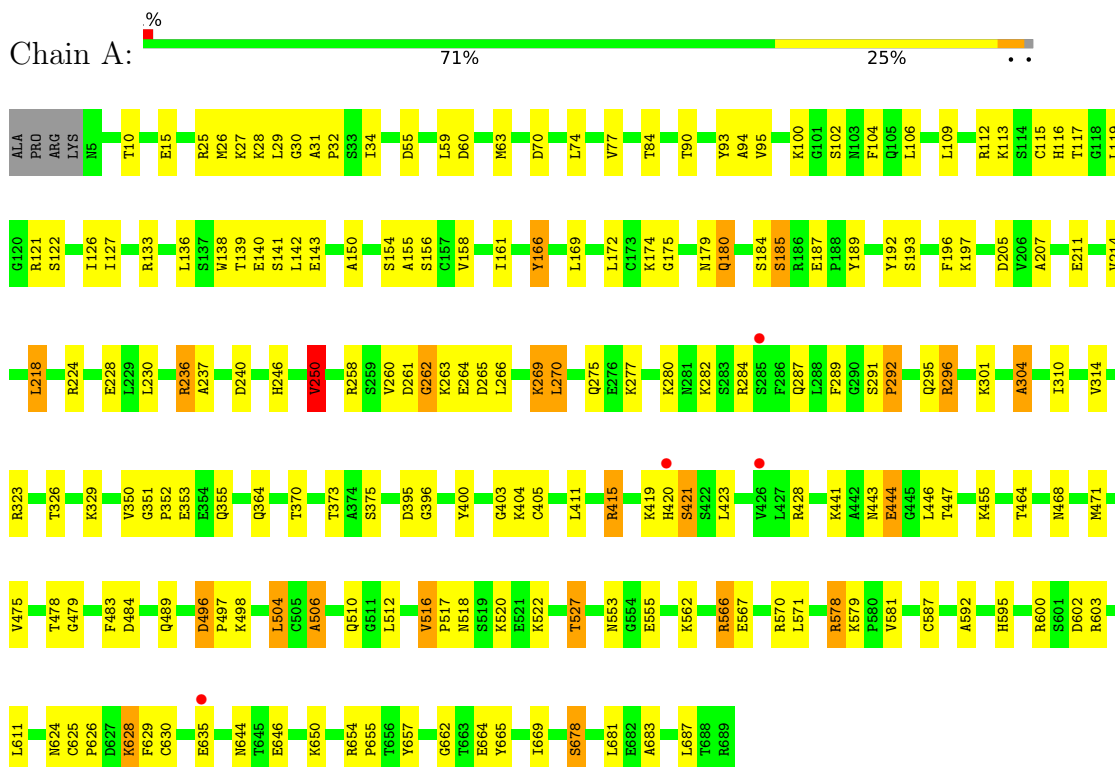
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	50	Total	O	0	0
			50	50		

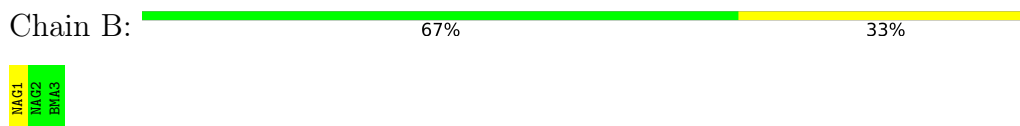
3 Residue-property plots [i](#)

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: LACTOFERRIN



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



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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



MA1	MA2	MA3	MA4	MA5	MA6
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	138.86Å 87.01Å 73.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.80) 97.0 (30.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.81Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.217 , 0.280 0.203 , 0.207	Depositor DCC
R_{free} test set	2154 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5495	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: BMA, NAG, CO3, FE, 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	0.84	1/5422 (0.0%)	1.43	55/7335 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	571	LEU	CA-C	-5.75	1.45	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	654	ARG	CA-C-N	-19.98	94.87	119.84
1	A	654	ARG	C-N-CA	-19.98	94.87	119.84
1	A	351	GLY	CA-C-N	11.77	131.21	118.97
1	A	351	GLY	C-N-CA	11.77	131.21	118.97
1	A	310	ILE	CA-C-N	11.08	131.17	119.76
1	A	310	ILE	C-N-CA	11.08	131.17	119.76
1	A	678	SER	CA-C-N	10.55	130.76	119.05
1	A	678	SER	C-N-CA	10.55	130.76	119.05
1	A	291	SER	CA-C-N	9.67	130.34	120.38
1	A	291	SER	C-N-CA	9.67	130.34	120.38
1	A	166	TYR	CA-C-N	9.54	129.78	119.28
1	A	166	TYR	C-N-CA	9.54	129.78	119.28
1	A	496	ASP	CA-C-N	8.76	128.91	119.28
1	A	496	ASP	C-N-CA	8.76	128.91	119.28
1	A	510	GLN	N-CA-C	-7.57	103.88	113.72
1	A	428	ARG	CA-C-N	7.50	127.42	119.85
1	A	428	ARG	C-N-CA	7.50	127.42	119.85
1	A	187	GLU	N-CA-C	-7.44	100.42	109.72
1	A	553	ASN	N-CA-C	7.37	121.56	111.54
1	A	262	GLY	N-CA-C	7.15	123.14	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	LEU	CA-C-N	6.97	126.79	119.05
1	A	218	LEU	C-N-CA	6.97	126.79	119.05
1	A	60	ASP	N-CA-C	-6.59	99.85	110.32
1	A	506	ALA	N-CA-C	6.59	121.61	112.45
1	A	292	PRO	N-CA-C	6.46	118.59	110.70
1	A	314	VAL	CB-CA-C	-6.41	103.58	111.08
1	A	405	CYS	N-CA-C	-6.16	104.94	112.88
1	A	396	GLY	N-CA-C	6.12	121.41	113.27
1	A	250	VAL	CA-C-N	6.06	125.82	119.76
1	A	250	VAL	C-N-CA	6.06	125.82	119.76
1	A	185	SER	CA-C-N	5.68	128.17	120.38
1	A	185	SER	C-N-CA	5.68	128.17	120.38
1	A	139	THR	CA-C-N	5.66	128.65	120.38
1	A	139	THR	C-N-CA	5.66	128.65	120.38
1	A	662	GLY	CA-C-N	5.64	129.28	120.82
1	A	662	GLY	C-N-CA	5.64	129.28	120.82
1	A	478	THR	N-CA-C	-5.64	104.62	112.45
1	A	421	SER	N-CA-C	-5.60	107.70	114.75
1	A	136	LEU	N-CA-C	5.56	117.34	111.28
1	A	420	HIS	N-CA-C	5.54	118.32	110.50
1	A	468	ASN	N-CA-C	5.40	117.87	111.33
1	A	304	ALA	N-CA-C	-5.29	101.08	109.96
1	A	237	ALA	N-CA-C	5.28	112.77	108.07
1	A	70	ASP	N-CA-C	-5.26	103.41	109.93
1	A	421	SER	CA-C-O	5.25	124.45	118.47
1	A	600	ARG	CA-C-N	5.20	127.50	120.38
1	A	600	ARG	C-N-CA	5.20	127.50	120.38
1	A	187	GLU	CA-C-N	5.18	124.87	119.64
1	A	187	GLU	C-N-CA	5.18	124.87	119.64
1	A	479	GLY	N-CA-C	-5.16	105.98	114.76
1	A	184	SER	CA-C-N	5.12	128.88	120.63
1	A	184	SER	C-N-CA	5.12	128.88	120.63
1	A	326	THR	CA-C-N	5.08	127.09	120.28
1	A	326	THR	C-N-CA	5.08	127.09	120.28
1	A	133	ARG	N-CA-C	5.06	121.00	109.81

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	5310	0	5216	77	0
2	B	39	0	34	0	0
3	C	72	0	61	0	0
4	A	14	0	13	0	0
5	A	2	0	0	0	0
6	A	8	0	0	1	0
7	A	50	0	0	3	0
All	All	5495	0	5324	77	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 7.

All (77) 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:113:LYS:HB3	1:A:172:LEU:HD11	1.65	0.77
1:A:218:LEU:HB2	1:A:224:ARG:HG3	1.68	0.74
1:A:471:MET:HE3	1:A:483:PHE:HB2	1.70	0.73
1:A:353:GLU:N	7:A:725:HOH:O	2.24	0.70
1:A:624:ASN:HB3	1:A:628:LYS:HB2	1.73	0.69
1:A:32:PRO:HD3	1:A:269:LYS:HE2	1.75	0.69
1:A:579:LYS:HD2	1:A:587:CYS:HB2	1.76	0.68
1:A:258:ARG:HB2	1:A:262:GLY:HA2	1.79	0.65
1:A:506:ALA:HB3	1:A:522:LYS:HB3	1.79	0.64
1:A:150:ALA:HA	1:A:169:LEU:HD21	1.80	0.62
1:A:352:PRO:HG3	1:A:520:LYS:HD2	1.81	0.61
1:A:59:LEU:HB3	1:A:63:MET:HB2	1.83	0.60
1:A:32:PRO:HG2	1:A:270:LEU:HB2	1.84	0.60
1:A:455:LYS:HD2	1:A:504:LEU:HD21	1.85	0.57
1:A:122:SER:HB3	1:A:250:VAL:HG11	1.87	0.56
1:A:95:VAL:HG12	1:A:246:HIS:HA	1.87	0.55
1:A:292:PRO:HB2	1:A:295:GLN:HG3	1.88	0.55
1:A:175:GLY:HA3	1:A:180:GLN:HA	1.88	0.55
1:A:115:CYS:HB2	1:A:207:ALA:HA	1.88	0.54
1:A:527:THR:HB	7:A:711:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:HB2	1:A:169:LEU:HD11	1.92	0.52
1:A:350:VAL:HG12	1:A:518:ASN:HB3	1.93	0.50
1:A:138:TRP:CE2	1:A:140:GLU:HG3	2.47	0.50
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.48	0.48
1:A:411:LEU:HD23	1:A:650:LYS:HA	1.94	0.48
1:A:441:LYS:HG3	1:A:570:ARG:CZ	2.44	0.47
1:A:74:LEU:HD23	1:A:258:ARG:HA	1.96	0.47
1:A:116:HIS:CD2	1:A:158:VAL:HG22	2.50	0.47
1:A:196:PHE:HZ	1:A:218:LEU:HD11	1.80	0.47
1:A:196:PHE:CE1	1:A:214:VAL:HG23	2.50	0.47
1:A:258:ARG:NH1	1:A:261:ASP:O	2.48	0.47
1:A:566:ARG:HG3	1:A:581:VAL:HG21	1.97	0.47
1:A:269:LYS:HE2	1:A:269:LYS:HB3	1.83	0.46
1:A:102:SER:HB2	1:A:236:ARG:HH12	1.80	0.46
1:A:106:LEU:HD13	1:A:230:LEU:HB3	1.98	0.45
1:A:93:TYR:HB2	1:A:211:GLU:HB3	1.98	0.45
1:A:29:LEU:HD13	1:A:277:LYS:HG2	1.98	0.45
1:A:263:LYS:HB3	1:A:266:LEU:HD12	1.99	0.45
1:A:289:PHE:CD1	1:A:304:ALA:HB3	2.52	0.45
1:A:498:LYS:HD3	1:A:498:LYS:HA	1.56	0.44
1:A:104:PHE:HB3	1:A:112:ARG:NH2	2.33	0.44
1:A:100:LYS:HG2	1:A:228:GLU:HG3	1.99	0.44
1:A:446:LEU:HA	1:A:446:LEU:HD12	1.45	0.44
1:A:100:LYS:HD3	1:A:228:GLU:HG3	1.99	0.44
1:A:193:SER:HB2	1:A:296:ARG:HG3	1.98	0.44
1:A:113:LYS:HG2	1:A:155:ALA:HB3	2.00	0.43
1:A:10:THR:HA	7:A:737:HOH:O	2.18	0.43
1:A:464:THR:HG21	1:A:592:ALA:HB1	2.00	0.43
1:A:364:GLN:HG3	1:A:629:PHE:HB2	1.99	0.43
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.84	0.43
1:A:444:GLU:H	1:A:444:GLU:HG2	1.50	0.43
1:A:126:ILE:HG22	1:A:127:ILE:HD13	2.01	0.43
1:A:193:SER:CB	1:A:296:ARG:HG3	2.49	0.43
1:A:29:LEU:HA	1:A:29:LEU:HD23	1.78	0.42
1:A:109:LEU:HA	1:A:112:ARG:HG3	1.99	0.42
1:A:116:HIS:HB2	1:A:158:VAL:HA	1.99	0.42
1:A:400:TYR:CZ	1:A:404:LYS:HD2	2.54	0.42
1:A:489:GLN:HB3	1:A:504:LEU:HD13	2.01	0.42
1:A:603:ARG:HA	1:A:603:ARG:HD2	1.82	0.42
1:A:189:TYR:HE1	1:A:197:LYS:HD3	1.84	0.42
1:A:516:VAL:HA	1:A:517:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:OD1	1:A:258:ARG:NH2	2.53	0.42
1:A:626:PRO:HA	1:A:630:CYS:SG	2.59	0.42
1:A:665:TYR:CZ	1:A:669:ILE:HD11	2.55	0.42
1:A:683:ALA:O	1:A:687:LEU:HG	2.19	0.42
1:A:625:CYS:HA	1:A:626:PRO:HA	1.61	0.42
1:A:415:ARG:HA	1:A:646:GLU:H	1.85	0.41
1:A:403:GLY:HA3	1:A:657:TYR:CG	2.55	0.41
1:A:611:LEU:HA	1:A:611:LEU:HD23	1.64	0.41
1:A:166:TYR:HB3	1:A:169:LEU:HD12	2.02	0.41
1:A:443:ASN:O	1:A:578:ARG:NH2	2.54	0.41
1:A:117:THR:HG22	1:A:192:TYR:HA	2.03	0.41
1:A:94:ALA:HB3	1:A:127:ILE:HG21	2.02	0.41
1:A:562:LYS:HB3	1:A:562:LYS:HE3	1.89	0.41
1:A:678:SER:HB3	1:A:681:LEU:HB2	2.02	0.41
1:A:496:ASP:HA	1:A:497:PRO:HD3	1.72	0.41
1:A:121:ARG:HB3	6:A:702:CO3:O3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	683/689 (99%)	637 (93%)	42 (6%)	4 (1%)	21 51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	655	PRO
1	A	30	GLY
1	A	31	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	570/573 (100%)	509 (89%)	61 (11%)	6 21

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	25	ARG
1	A	26	MET
1	A	28	LYS
1	A	34	ILE
1	A	77	VAL
1	A	84	THR
1	A	90	THR
1	A	141	SER
1	A	142	LEU
1	A	143	GLU
1	A	154	SER
1	A	156	SER
1	A	161	ILE
1	A	174	LYS
1	A	179	ASN
1	A	180	GLN
1	A	185	SER
1	A	205	ASP
1	A	236	ARG
1	A	240	ASP
1	A	250	VAL
1	A	260	VAL
1	A	264	GLU
1	A	265	ASP
1	A	269	LYS
1	A	270	LEU
1	A	275	GLN
1	A	280	LYS
1	A	282	LYS

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Mol	Chain	Res	Type
1	A	284	ARG
1	A	287	GLN
1	A	296	ARG
1	A	301	LYS
1	A	323	ARG
1	A	329	LYS
1	A	355	GLN
1	A	370	THR
1	A	373	THR
1	A	375	SER
1	A	415	ARG
1	A	419	LYS
1	A	421	SER
1	A	423	LEU
1	A	444	GLU
1	A	447	THR
1	A	475	VAL
1	A	484	ASP
1	A	504	LEU
1	A	512	LEU
1	A	516	VAL
1	A	527	THR
1	A	555	GLU
1	A	566	ARG
1	A	567	GLU
1	A	578	ARG
1	A	602	ASP
1	A	628	LYS
1	A	635	GLU
1	A	644	ASN
1	A	664	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	146	GLN
1	A	179	ASN
1	A	249	GLN
1	A	330	ASN
1	A	468	ASN
1	A	489	GLN

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Mol	Chain	Res	Type
1	A	551	ASN
1	A	614	GLN
1	A	642	ASN
1	A	644	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 ⓘ

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	0.57	0	17,19,21	0.85	1 (5%)
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	0.68	0
2	BMA	B	3	2	11,11,12	0.42	0	15,15,17	0.65	0
3	NAG	C	1	1,3	14,14,15	0.61	0	17,19,21	0.88	1 (5%)
3	NAG	C	2	3	14,14,15	0.57	0	17,19,21	0.62	1 (5%)
3	BMA	C	3	3	11,11,12	0.53	0	15,15,17	0.78	0
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	0.82	0
3	MAN	C	5	3	11,11,12	0.44	0	15,15,17	0.72	0
3	MAN	C	6	3	11,11,12	0.40	0	15,15,17	0.77	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	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	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	2.74	115.85	112.19
2	B	1	NAG	C1-O5-C5	2.43	115.44	112.19
3	C	2	NAG	O5-C5-C6	2.00	111.56	107.66

There are no chirality outliers.

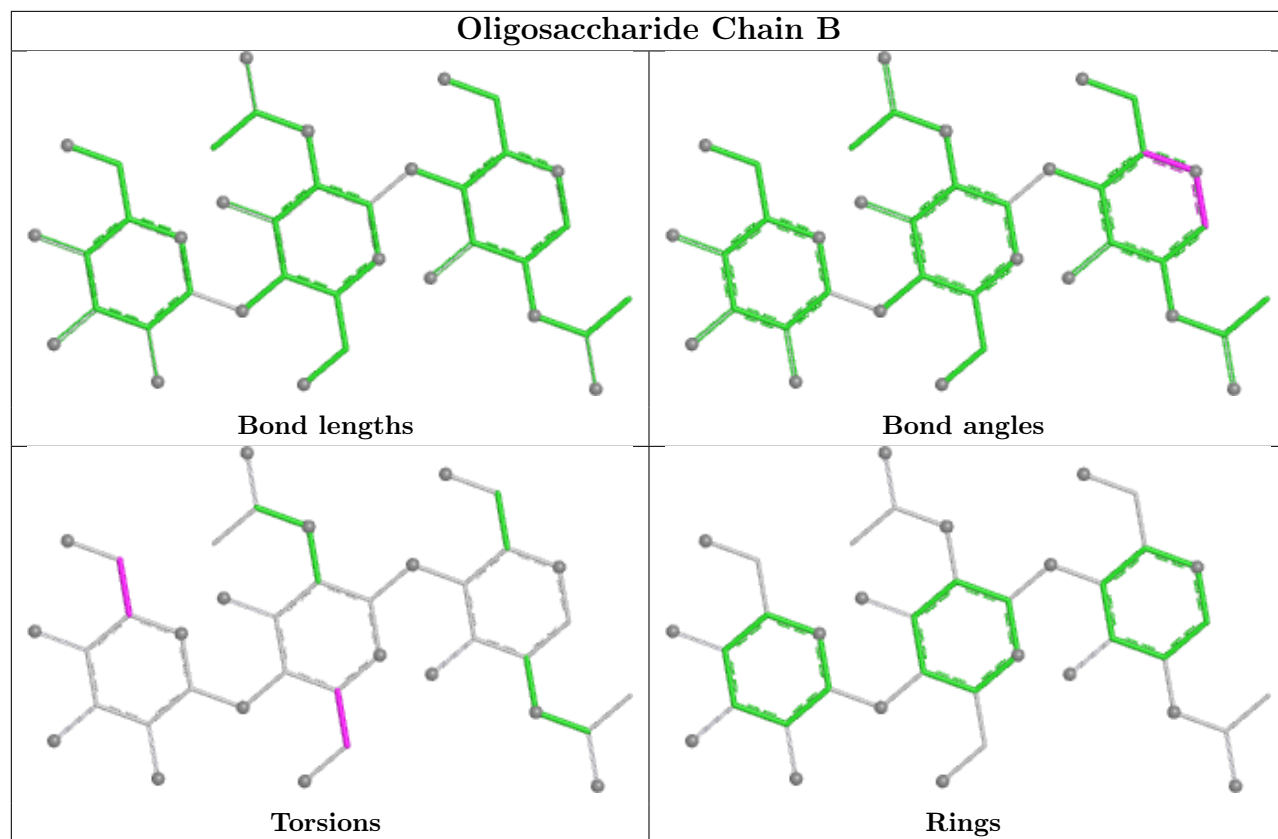
All (8) torsion outliers are listed below:

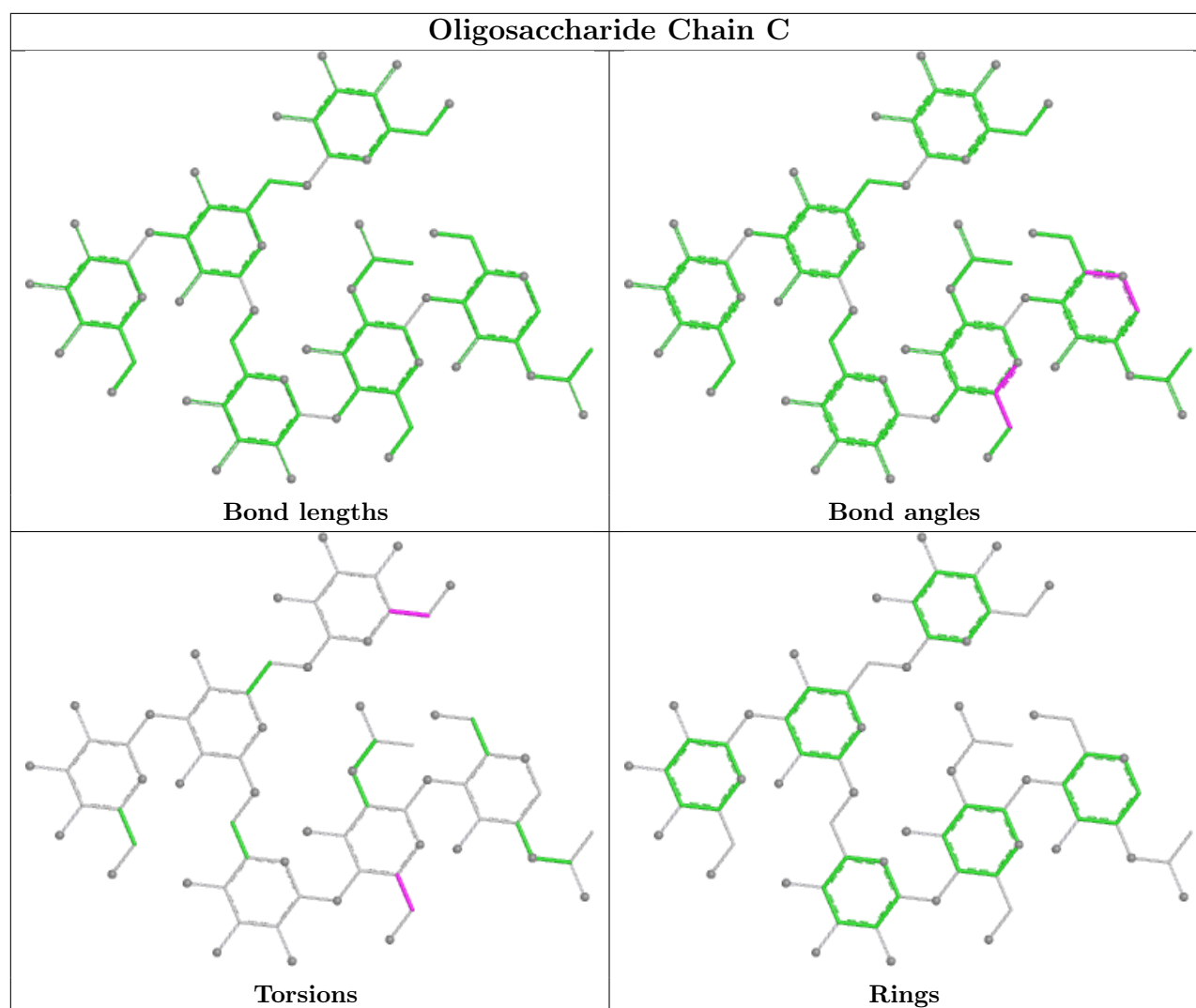
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 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	$\# Z > 2$
6	CO3	A	702	5	3,3,3	0.84	0	2,3,3	0.21	0
4	NAG	A	690(A)	1	14,14,15	0.50	0	17,19,21	1.01	2 (11%)
6	CO3	A	703	5	3,3,3	0.97	0	2,3,3	0.33	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
4	NAG	A	690(A)	1	-	0/6/23/26	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	690(A)	NAG	C1-C2-N2	2.33	114.10	110.43
4	A	690(A)	NAG	C4-C3-C2	-2.05	108.01	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	CO3	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	685/689 (99%)	0.09	4 (0%) 85 80	40, 69, 104, 119	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	SER	2.3
1	A	635	GLU	2.2
1	A	420	HIS	2.1
1	A	426	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.

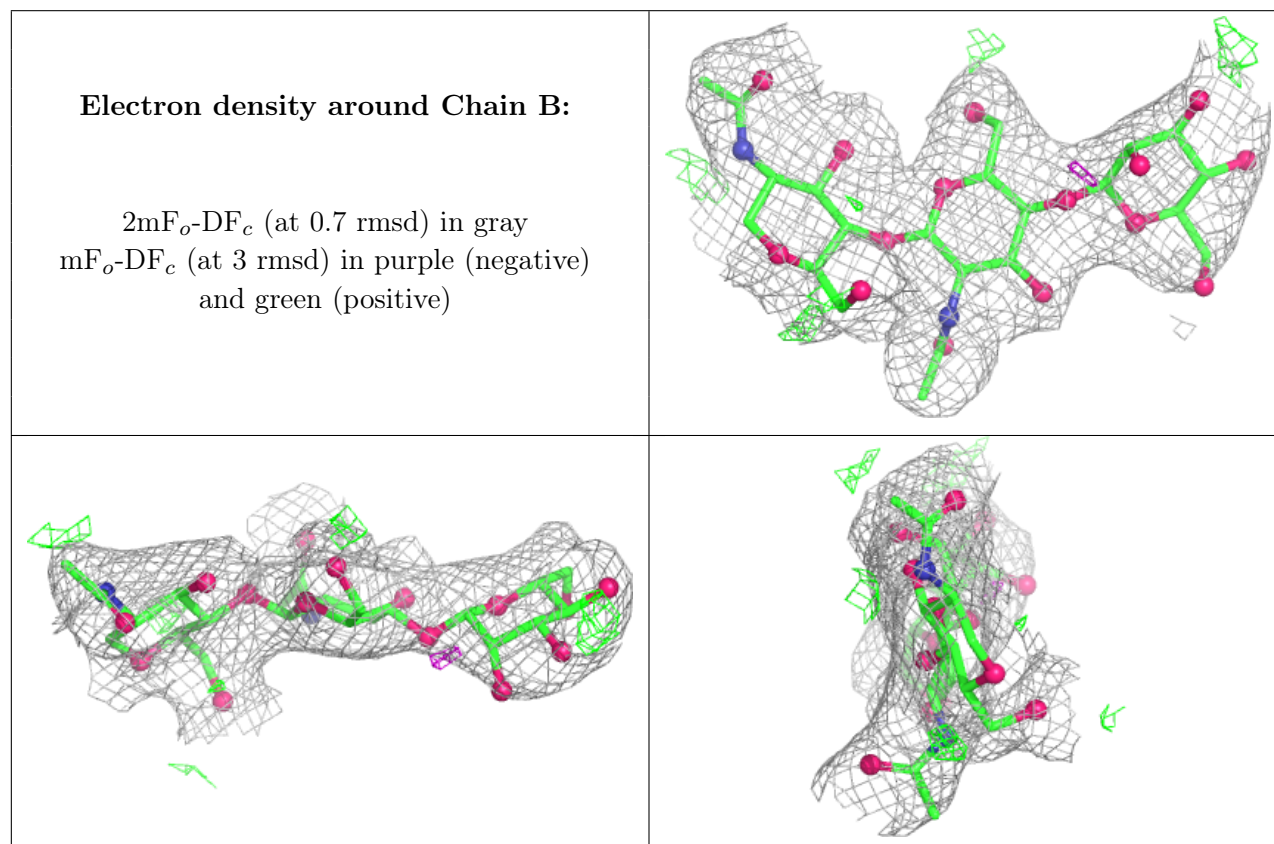
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	B	3	11/12	0.73	0.11	86,92,98,103	0
3	BMA	C	3	11/12	0.79	0.10	62,66,70,73	0
3	MAN	C	6	11/12	0.81	0.11	87,90,96,101	0
2	NAG	B	2	14/15	0.85	0.10	72,77,82,86	0
3	MAN	C	4	11/12	0.89	0.13	69,71,78,84	0
2	NAG	B	1	14/15	0.90	0.09	63,69,77,78	0
3	MAN	C	5	11/12	0.91	0.11	70,73,78,83	0
3	NAG	C	2	14/15	0.92	0.09	53,58,66,68	0

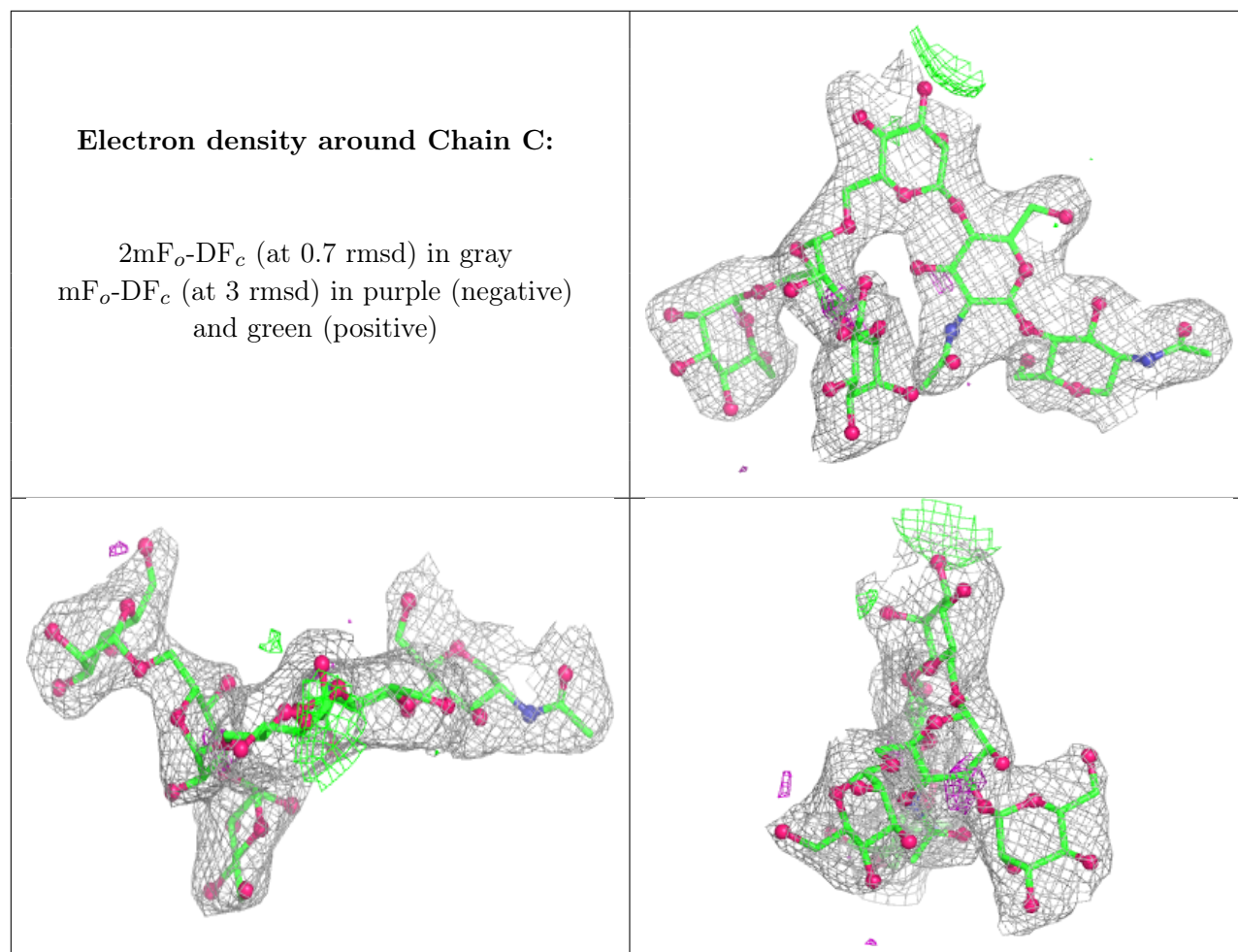
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	0.96	0.07	44,50,57,59	0

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.





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	NAG	A	690(A)	14/15	0.78	0.13	87,92,100,102	0
6	CO3	A	702	4/4	0.97	0.10	38,41,41,41	0
5	FE	A	700	1/1	0.99	0.03	61,61,61,61	0
6	CO3	A	703	4/4	0.99	0.06	30,33,33,33	0
5	FE	A	701	1/1	1.00	0.02	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.