



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:03 AM UTC

PDB ID : 9D77 / pdb_00009d77
Title : Crystal form of Netrin-1 mimics nanotubes
Authors : Meier, M.; Krahn, N.J.; McDougall, M.D.; Rafiei, F.; Koch, M.; Stetefeld, J.
Deposited on : 2024-08-16
Resolution : 3.40 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

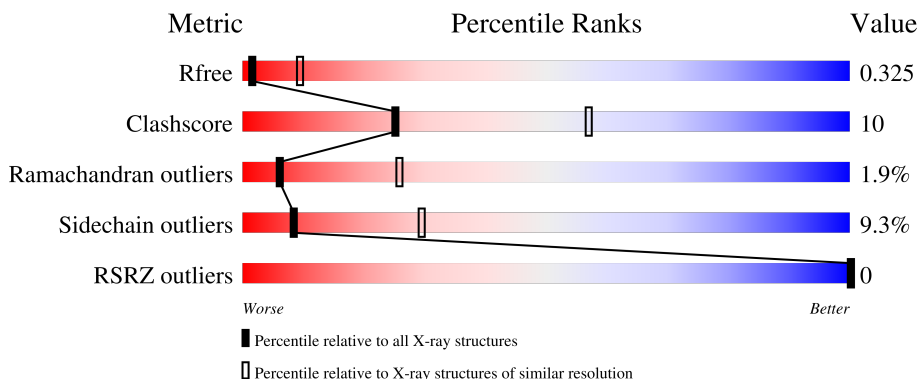
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

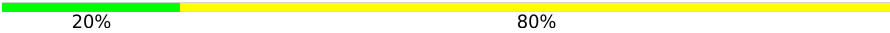
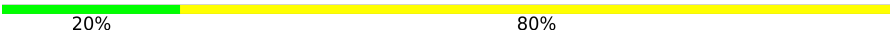
The reported resolution of this entry is 3.40 Å.

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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 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	443	 68% 22% • 6%
2	B	6	 50% 50%
3	C	5	 20% 80%
3	D	5	 20% 80%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3578 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.

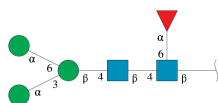
- Molecule 1 is a protein called Netrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3333	2041	629	625	38	0	6	0

There are 10 discrepancies between the modelled and reference sequences:

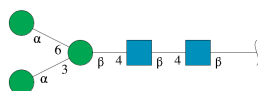
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	insertion	UNP Q90922
A	23	PRO	-	insertion	UNP Q90922
A	24	LEU	-	insertion	UNP Q90922
A	25	ALA	-	insertion	UNP Q90922
A	459	GLY	-	linker	UNP Q90922
A	460	SER	-	linker	UNP Q90922
A	461	LEU	-	expression tag	UNP Q90922
A	462	VAL	-	expression tag	UNP Q90922
A	463	PRO	-	expression tag	UNP Q90922
A	464	ARG	-	expression tag	UNP Q90922

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



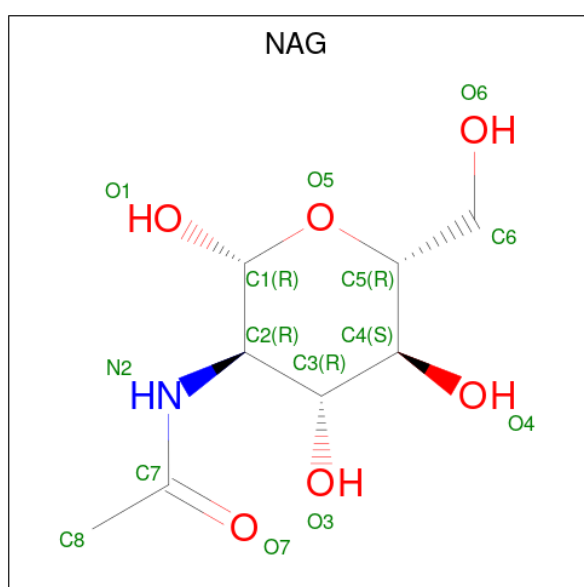
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	71	40	2	29	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 8 6 2	0	0
7	A	1	Total C O 8 6 2	0	0

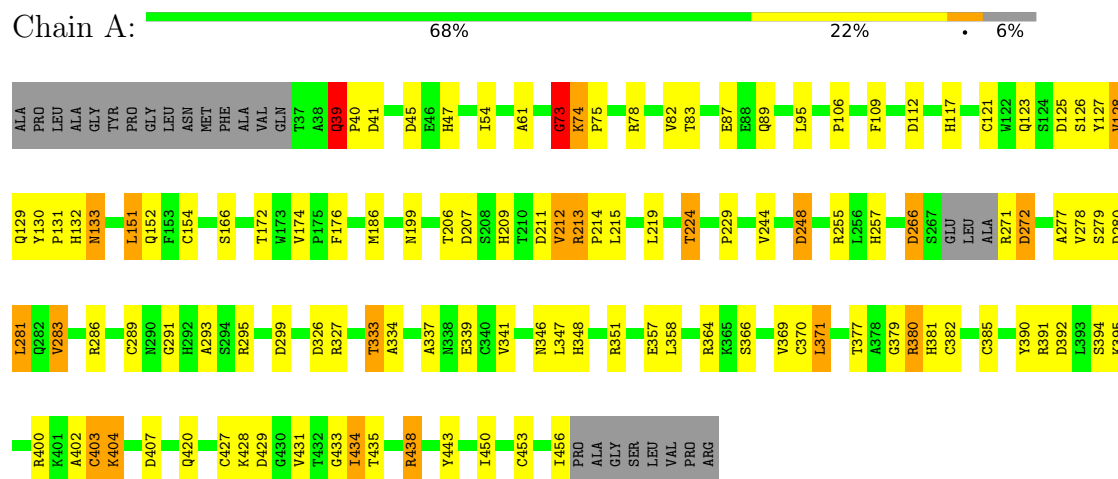
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	20	Total O 20 20	0	0

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: Netrin-1



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



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



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



MAG1	MAG2	BMA3	MAN4	MAN5
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4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	189.26Å 189.26Å 45.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.77 – 3.40 35.77 – 3.40	Depositor EDS
% Data completeness (in resolution range)	68.7 (35.77-3.40) 68.9 (35.77-3.40)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.39Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.297 , 0.335 0.290 , 0.325	Depositor DCC
R_{free} test set	743 reflections (5.57%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	1.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.123 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3578	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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: MPD, CA, NAG, BMA, MAN, FUC, CL

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	0.59	0/3413	1.21	16/4616 (0.3%)

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	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	45	ASP	CA-CB-CG	7.50	120.09	112.60
1	A	95	LEU	N-CA-CB	-6.85	99.97	110.65
1	A	248	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	404	LYS	CB-CG-CD	5.93	124.95	111.30
1	A	257	HIS	CA-CB-CG	5.90	119.70	113.80
1	A	89	GLN	N-CA-CB	-5.88	103.35	110.53
1	A	407	ASP	CA-CB-CG	5.58	118.17	112.60
1	A	73	GLY	CA-C-N	5.48	128.87	121.20
1	A	73	GLY	C-N-CA	5.48	128.87	121.20
1	A	117	HIS	CA-CB-CG	5.47	119.27	113.80
1	A	41	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	39	GLN	CB-CA-C	5.21	120.44	110.17
1	A	112	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	176	PHE	N-CA-CB	-5.14	101.81	110.49
1	A	47	HIS	CA-CB-CG	5.09	118.89	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	LEU	Peptide
1	A	255	ARG	Sidechain
1	A	271	ARG	Peptide
1	A	351[A]	ARG	Sidechain
1	A	73	GLY	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	3333	0	3148	67	0
2	B	71	0	61	0	0
3	C	61	0	52	0	0
3	D	61	0	52	0	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
6	A	1	0	0	1	0
7	A	16	0	28	2	0
8	A	20	0	0	17	0
All	All	3578	0	3354	67	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 10.

All (67) 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:172:THR:O	8:A:601:HOH:O	1.92	0.88
1:A:213[B]:ARG:HD2	1:A:214:PRO:HA	1.55	0.88
1:A:212[A]:VAL:HG23	1:A:213[A]:ARG:HD3	1.56	0.85
1:A:427:CYS:O	7:A:505:MPD:O4	1.93	0.83
1:A:166:SER:OG	8:A:601:HOH:O	1.98	0.79
1:A:402:ALA:O	1:A:403:CYS:SG	2.42	0.78
1:A:280:ASP:O	8:A:602:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG12	8:A:603:HOH:O	1.86	0.76
1:A:126:SER:C	8:A:603:HOH:O	2.31	0.73
1:A:125:ASP:O	8:A:603:HOH:O	2.12	0.68
1:A:129:GLN:O	1:A:132:HIS:N	2.27	0.68
1:A:357:GLU:HB2	7:A:504:MPD:H12	1.79	0.65
1:A:392:ASP:OD2	1:A:394:SER:OG	2.15	0.64
1:A:337:ALA:O	8:A:604:HOH:O	2.15	0.64
1:A:326:ASP:OD2	1:A:366:SER:OG	2.13	0.61
1:A:272:ASP:OD1	1:A:272:ASP:N	2.34	0.61
1:A:166:SER:HA	8:A:601:HOH:O	2.03	0.58
1:A:348:HIS:CD2	1:A:377:THR:HG21	2.39	0.57
1:A:364:ARG:HH21	1:A:364:ARG:CG	2.19	0.55
1:A:39:GLN:HB3	1:A:40:PRO:HD3	1.89	0.55
1:A:379:GLY:O	1:A:381:HIS:N	2.39	0.55
1:A:54:ILE:HD13	1:A:291:GLY:HA2	1.87	0.55
1:A:74:LYS:H	1:A:74:LYS:HD2	1.72	0.55
1:A:385:CYS:O	1:A:420:GLN:NE2	2.40	0.54
1:A:123:GLN:HG2	1:A:277:ALA:HB2	1.88	0.54
1:A:61:ALA:HB2	1:A:283:VAL:HG12	1.90	0.54
1:A:133:ASN:OD1	1:A:133:ASN:N	2.40	0.53
1:A:39:GLN:CB	1:A:40:PRO:CD	2.87	0.53
1:A:211:ASP:OD1	1:A:213[A]:ARG:NH1	2.41	0.53
1:A:152:GLN:N	8:A:602:HOH:O	2.20	0.51
1:A:74:LYS:H	1:A:74:LYS:CD	2.22	0.51
1:A:127:TYR:N	8:A:603:HOH:O	2.43	0.50
1:A:400[B]:ARG:NH1	6:A:503:CL:CL	2.82	0.49
1:A:121:CYS:SG	1:A:279:SER:HB3	2.53	0.49
1:A:206:THR:O	1:A:206:THR:HG23	2.12	0.48
1:A:128:VAL:CG1	8:A:603:HOH:O	2.55	0.48
1:A:390:TYR:HA	1:A:420:GLN:O	2.13	0.48
1:A:129:GLN:HG3	1:A:130:TYR:N	2.29	0.48
1:A:400[A]:ARG:NH2	8:A:610:HOH:O	2.46	0.48
1:A:370:CYS:SG	1:A:381:HIS:HA	2.54	0.47
1:A:214:PRO:HD2	8:A:608:HOH:O	2.14	0.47
1:A:370:CYS:O	1:A:371:LEU:HD13	2.14	0.47
1:A:54:ILE:HG21	1:A:286:ARG:HD3	1.96	0.46
1:A:434:ILE:HD12	1:A:434:ILE:H	1.81	0.46
1:A:279:SER:O	1:A:280:ASP:HB2	2.16	0.45
1:A:74:LYS:HA	1:A:75:PRO:HA	1.80	0.45
1:A:391:ARG:NH2	1:A:395:LYS:O	2.46	0.45
1:A:358:LEU:HD23	1:A:380:ARG:NH1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:CYS:CB	1:A:293:ALA:HB3	2.47	0.44
1:A:402:ALA:O	1:A:403:CYS:CB	2.64	0.44
1:A:199:ASN:HD22	1:A:199:ASN:HA	1.73	0.43
1:A:433:GLY:HA2	1:A:438:ARG:HH11	1.83	0.43
1:A:379:GLY:O	1:A:382:CYS:N	2.51	0.43
1:A:337:ALA:HB1	8:A:604:HOH:O	2.17	0.43
1:A:54:ILE:CG2	1:A:286:ARG:HD3	2.49	0.43
1:A:224:THR:HB	1:A:244:VAL:HG12	2.01	0.42
1:A:443:TYR:HB3	1:A:453:CYS:HB3	2.01	0.42
1:A:427:CYS:HB3	1:A:431:VAL:HB	2.01	0.42
1:A:106:PRO:HD2	1:A:109:PHE:CE2	2.55	0.41
1:A:333:THR:OG1	1:A:334:ALA:N	2.54	0.41
1:A:151:LEU:HA	8:A:602:HOH:O	2.21	0.41
1:A:166:SER:CA	8:A:601:HOH:O	2.65	0.41
1:A:130:TYR:HA	1:A:131:PRO:C	2.46	0.41
1:A:346:ASN:O	1:A:347:LEU:HB2	2.21	0.41
1:A:78:ARG:NH1	1:A:266:ASP:OD2	2.54	0.40
1:A:281:LEU:HA	8:A:602:HOH:O	2.21	0.40
1:A:213[A]:ARG:CD	1:A:213[A]:ARG:H	2.33	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	419/443 (95%)	378 (90%)	33 (8%)	8 (2%)	6 26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	380	ARG

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Mol	Chain	Res	Type
1	A	403	CYS
1	A	429	ASP
1	A	266	ASP
1	A	327	ARG
1	A	229	PRO
1	A	73	GLY

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	373/385 (97%)	336 (90%)	37 (10%)	7 26

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	82	VAL
1	A	83	THR
1	A	87	GLU
1	A	128	VAL
1	A	133	ASN
1	A	151	LEU
1	A	154	CYS
1	A	174	VAL
1	A	186	MET
1	A	207	ASP
1	A	209	HIS
1	A	212[A]	VAL
1	A	212[B]	VAL
1	A	213[A]	ARG
1	A	213[B]	ARG
1	A	215	LEU
1	A	224	THR
1	A	248	ASP
1	A	272	ASP

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Mol	Chain	Res	Type
1	A	278	VAL
1	A	281	LEU
1	A	283	VAL
1	A	295[A]	ARG
1	A	295[B]	ARG
1	A	333	THR
1	A	339	GLU
1	A	341	VAL
1	A	369	VAL
1	A	371	LEU
1	A	404	LYS
1	A	428	LYS
1	A	434	ILE
1	A	435	THR
1	A	438	ARG
1	A	450	ILE
1	A	456	ILE

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

Mol	Chain	Res	Type
1	A	177	GLN
1	A	198	GLN
1	A	199	ASN
1	A	236	ASN
1	A	282	GLN
1	A	292	HIS
1	A	338	ASN
1	A	346	ASN
1	A	372	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 ⓘ

16 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	0.56	0	17,19,21	1.98	5 (29%)
2	NAG	B	2	2	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
2	BMA	B	3	2	11,11,12	0.59	0	15,15,17	0.63	0
2	MAN	B	4	2	11,11,12	0.63	0	15,15,17	1.06	0
2	MAN	B	5	2	11,11,12	0.80	0	15,15,17	0.94	0
2	FUC	B	6	2	10,10,11	0.78	0	14,14,16	1.58	1 (7%)
3	NAG	C	1	1,3	14,14,15	0.88	0	17,19,21	2.54	6 (35%)
3	NAG	C	2	3	14,14,15	1.35	2 (14%)	17,19,21	2.87	8 (47%)
3	BMA	C	3	3	11,11,12	0.52	0	15,15,17	0.86	1 (6%)
3	MAN	C	4	3	11,11,12	0.61	0	15,15,17	0.99	0
3	MAN	C	5	3	11,11,12	0.69	0	15,15,17	0.99	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.52	0	17,19,21	1.77	3 (17%)
3	NAG	D	2	3	14,14,15	0.34	0	17,19,21	1.37	2 (11%)
3	BMA	D	3	3	11,11,12	0.65	0	15,15,17	0.96	1 (6%)
3	MAN	D	4	3	11,11,12	0.64	0	15,15,17	0.80	0
3	MAN	D	5	3	11,11,12	0.60	0	15,15,17	1.19	2 (13%)

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

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C2-N2	3.13	1.51	1.46
3	C	2	NAG	C4-C3	2.02	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	-6.19	101.94	111.02
3	C	2	NAG	C2-N2-C7	5.65	130.47	122.90
3	C	2	NAG	C1-O5-C5	5.41	119.44	112.19
2	B	1	NAG	C1-C2-N2	5.41	118.96	110.43
3	C	1	NAG	C1-C2-N2	4.75	117.92	110.43
3	C	2	NAG	O4-C4-C5	4.70	120.91	109.32
2	B	6	FUC	O5-C1-C2	-4.19	100.79	110.79
3	C	1	NAG	O3-C3-C2	3.89	117.48	109.40
3	D	1	NAG	C4-C3-C2	-3.83	105.41	111.02
3	D	2	NAG	C1-O5-C5	3.68	117.12	112.19
3	D	1	NAG	C1-C2-N2	3.54	116.02	110.43
3	C	2	NAG	O7-C7-C8	-3.29	116.20	122.05
3	C	2	NAG	C1-C2-N2	3.28	115.60	110.43
3	D	1	NAG	C2-N2-C7	3.27	127.28	122.90
3	C	2	NAG	C6-C5-C4	3.21	120.91	113.02
2	B	1	NAG	C4-C3-C2	-3.16	106.39	111.02
2	B	2	NAG	C2-N2-C7	3.14	127.10	122.90
3	C	1	NAG	O5-C1-C2	-3.04	106.59	111.29
2	B	1	NAG	O5-C1-C2	-2.84	106.90	111.29
3	C	1	NAG	O7-C7-N2	2.84	126.99	121.98
3	C	1	NAG	O7-C7-C8	-2.70	117.25	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-C2-C3	2.63	113.48	109.64
3	C	2	NAG	O7-C7-N2	2.62	126.61	121.98
2	B	1	NAG	O5-C5-C6	-2.57	102.66	107.66
3	D	3	BMA	C3-C4-C5	2.46	114.70	110.23
3	D	2	NAG	C2-N2-C7	2.46	126.20	122.90
3	D	5	MAN	O5-C1-C2	-2.34	105.20	110.79
3	C	2	NAG	O5-C5-C6	-2.33	103.13	107.66
3	D	5	MAN	C6-C5-C4	-2.27	107.45	113.02
3	C	5	MAN	O5-C5-C6	2.14	111.82	107.66
2	B	1	NAG	O7-C7-C8	-2.13	118.27	122.05

There are no chirality outliers.

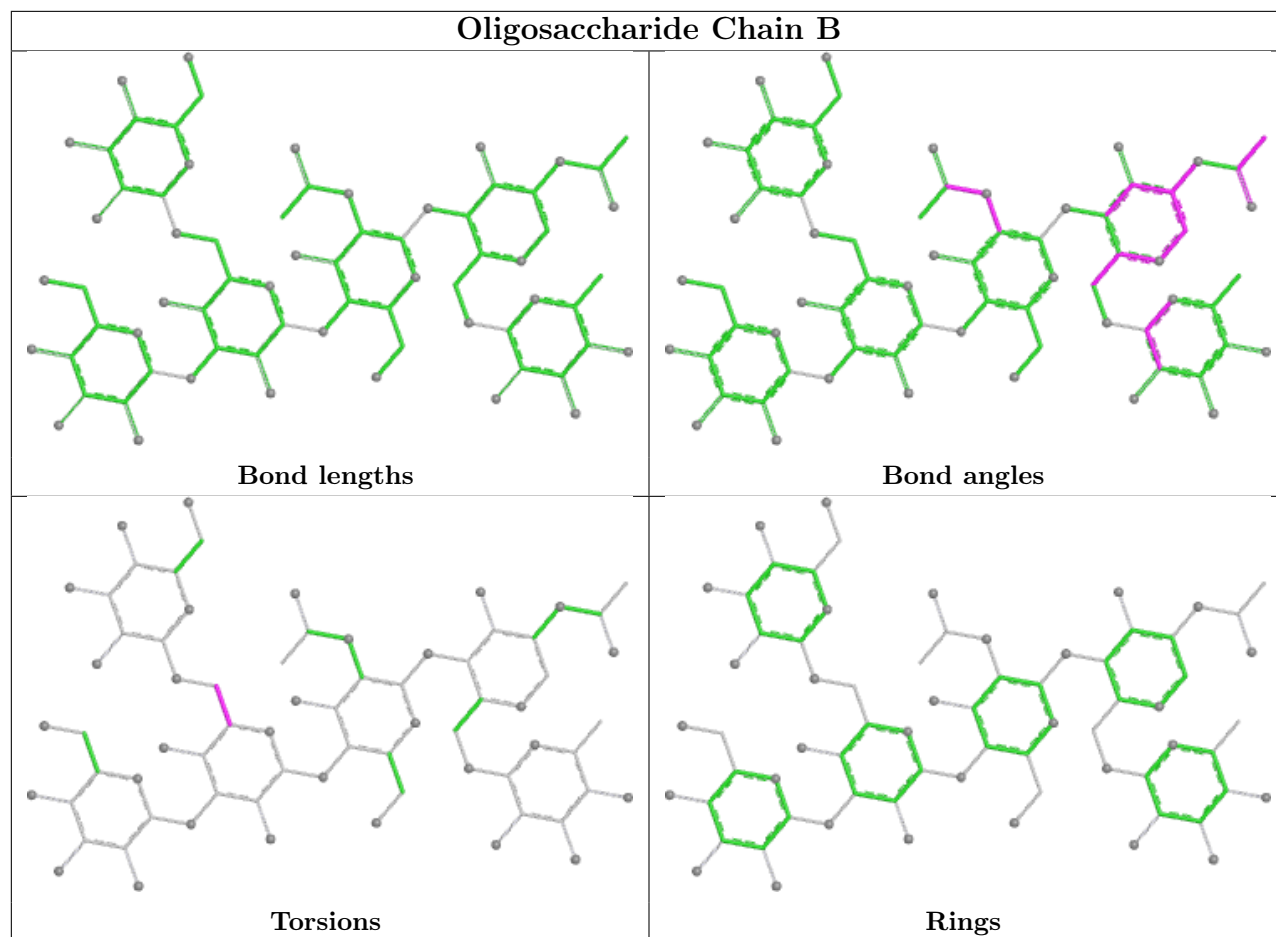
All (13) torsion outliers are listed below:

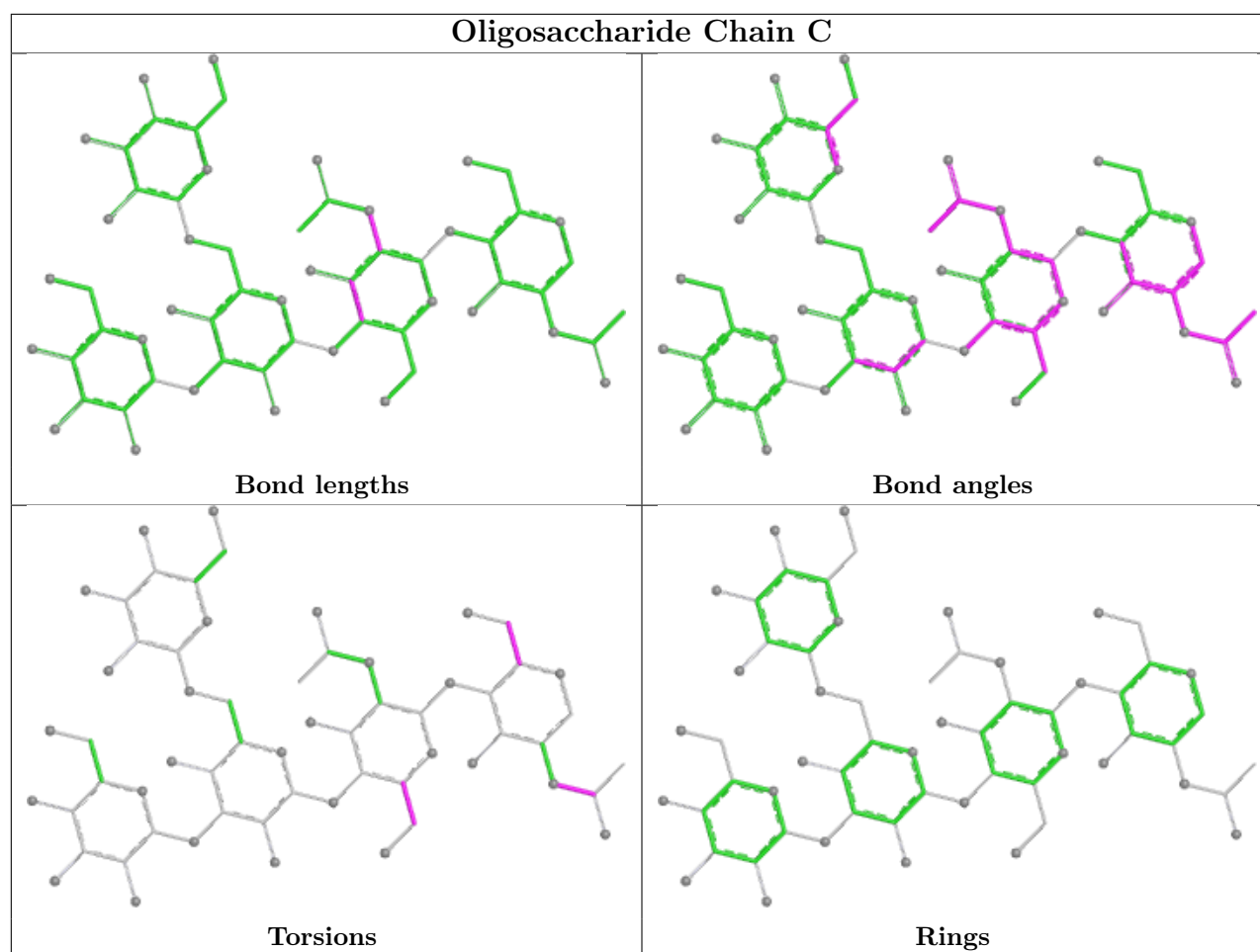
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C1-C2-N2-C7
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	D	4	MAN	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C3-C2-N2-C7
2	B	3	BMA	C4-C5-C6-O6

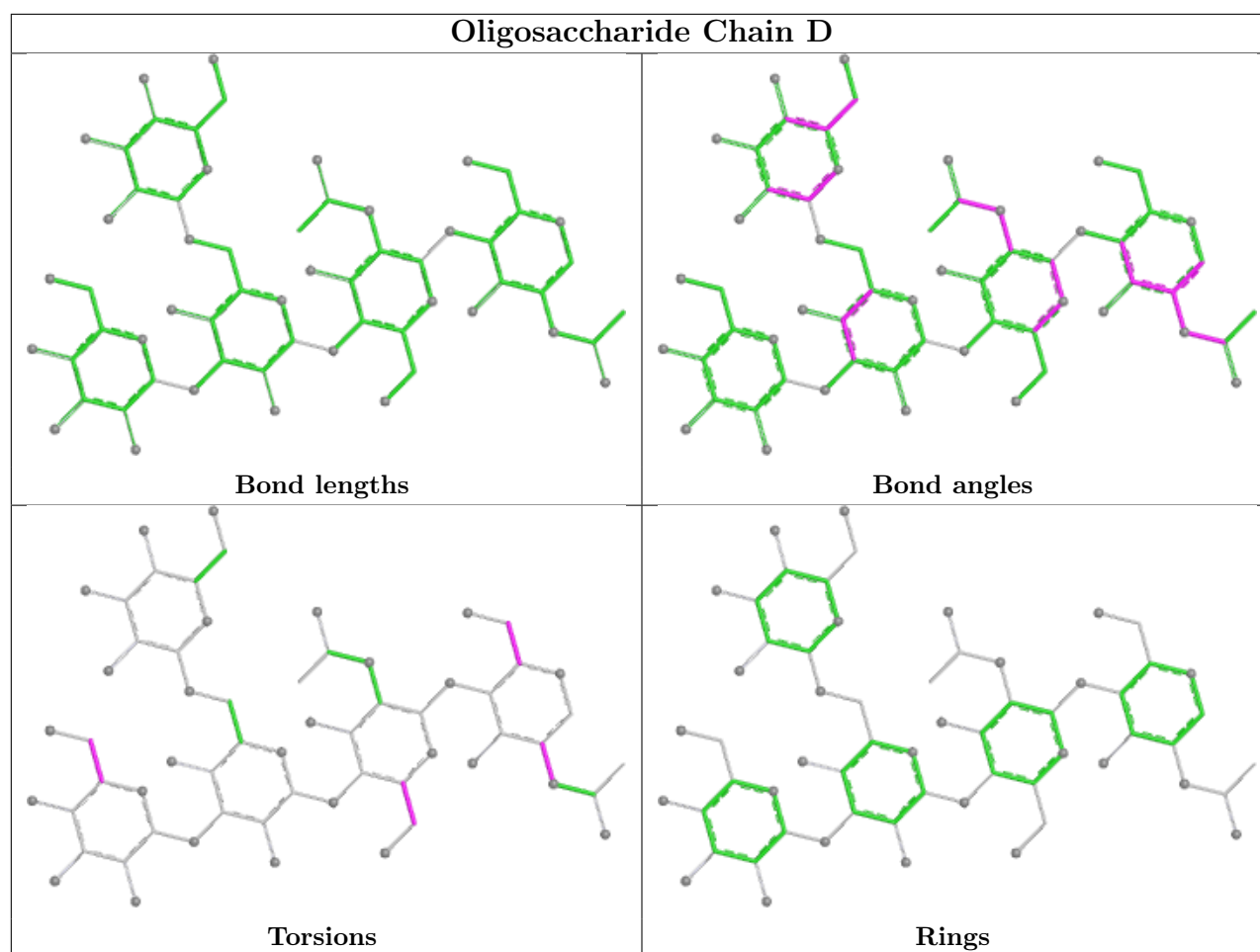
There are no ring outliers.

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	$\# Z > 2$
7	MPD	A	504	-	7,7,7	0.14	0	9,10,10	0.39	0
7	MPD	A	505	-	7,7,7	0.16	0	9,10,10	0.52	0
4	NAG	A	501	1	14,14,15	1.02	1 (7%)	17,19,21	1.80	3 (17%)

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
7	MPD	A	504	-	-	2/5/5/5	-
7	MPD	A	505	-	-	0/5/5/5	-
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	C1-C2	2.55	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C2-N2-C7	4.83	129.37	122.90
4	A	501	NAG	C1-O5-C5	2.91	116.09	112.19
4	A	501	NAG	C1-C2-N2	2.19	113.88	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	504	MPD	C2-C3-C4-O4
7	A	504	MPD	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	504	MPD	1	0
7	A	505	MPD	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	417/443 (94%)	-1.21	0 100 100	33, 81, 141, 181	6 (1%)

There are no RSRZ outliers to report.

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.

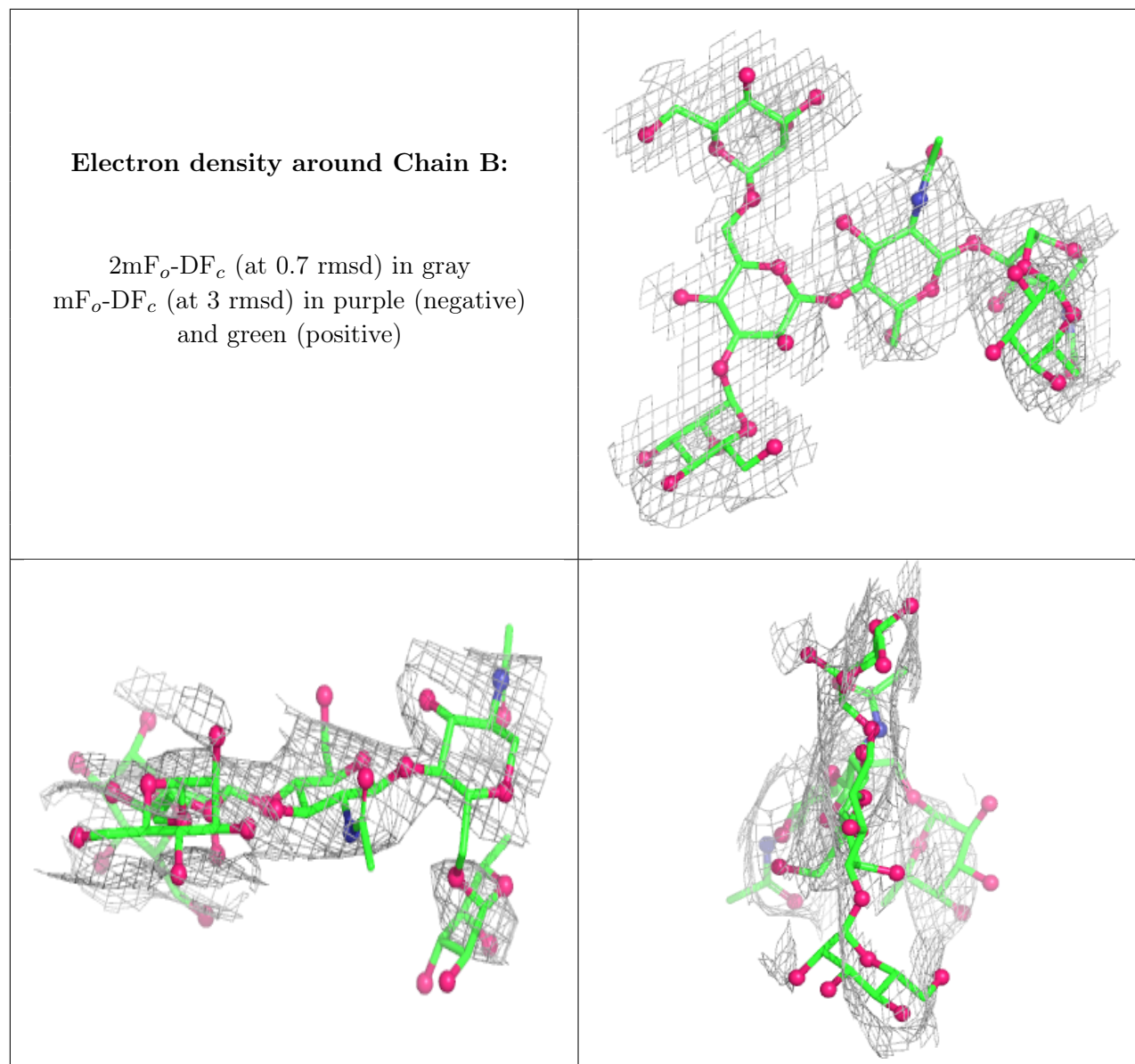
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	4	11/12	0.96	0.06	167,174,183,189	0
3	BMA	D	3	11/12	0.96	0.06	160,162,167,169	0
3	MAN	D	4	11/12	0.96	0.07	164,171,180,182	0
3	NAG	D	2	14/15	0.97	0.05	154,160,162,163	0
2	NAG	B	2	14/15	0.98	0.07	116,120,131,134	0
2	FUC	B	6	10/11	0.98	0.10	129,131,135,136	0
3	NAG	D	1	14/15	0.98	0.06	142,150,154,155	0
3	MAN	D	5	11/12	0.98	0.05	165,169,172,173	0
3	BMA	C	3	11/12	0.99	0.04	112,120,133,138	0
3	MAN	C	4	11/12	0.99	0.06	113,124,130,131	0
3	MAN	C	5	11/12	0.99	0.04	140,144,152,156	0
2	NAG	B	1	14/15	0.99	0.05	102,104,113,119	0
2	MAN	B	5	11/12	0.99	0.06	139,145,152,154	0
2	BMA	B	3	11/12	0.99	0.04	139,144,151,160	0

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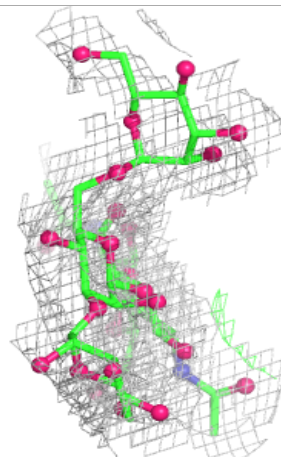
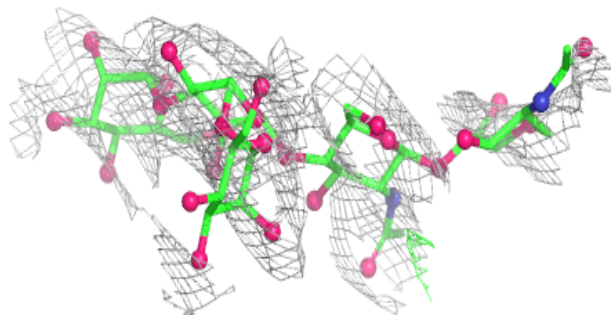
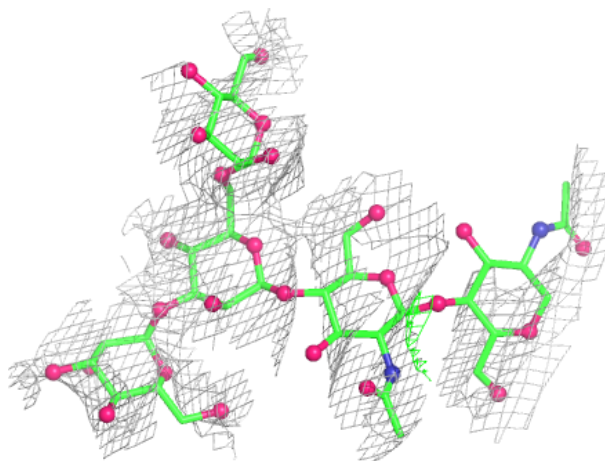
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	1	14/15	0.99	0.07	88,92,104,107	0
3	NAG	C	2	14/15	0.99	0.06	88,95,102,105	0

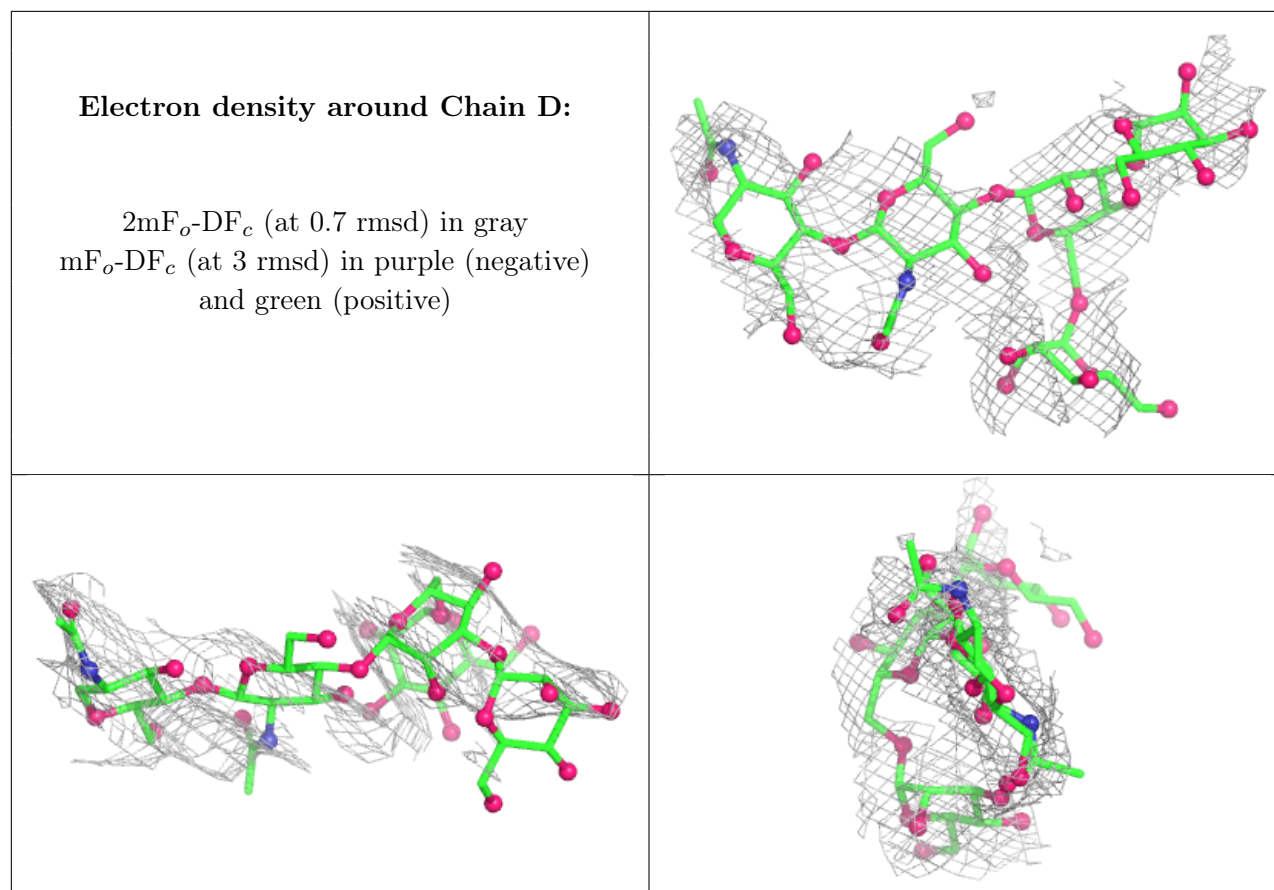
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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	NAG	A	501	14/15	0.96	0.08	134,156,178,181	0
7	MPD	A	504	8/8	0.98	0.07	96,117,129,156	0
6	CL	A	503	1/1	1.00	0.02	70,70,70,70	0
5	CA	A	502	1/1	1.00	0.02	11,11,11,11	0
7	MPD	A	505	8/8	1.00	0.03	52,58,63,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.