



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:03 PM UTC

PDB ID : 2XMD / pdb_00002xmd
Title : G117H mutant of human butyrylcholinesterase in complex with echothiophate
Authors : Nachon, F.; Carletti, E.; Wandhammer, M.; Nicolet, Y.; Schopfer, L.M.; Masson, P.; Lockridge, O.
Deposited on : 2010-07-27
Resolution : 2.30 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

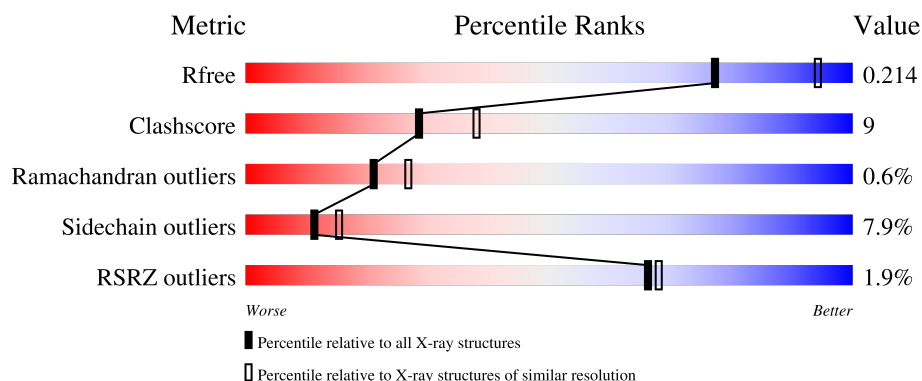
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	529	2% 78% 16% ..
2	B	3	67% 33%
2	C	3	67% 33%
3	D	3	100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4705 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.

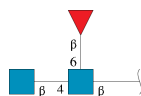
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	2	0
			4222	2724	711	772	15			

There are 5 discrepancies between the modelled and reference sequences:

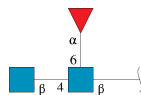
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	117	HIS	GLY	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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

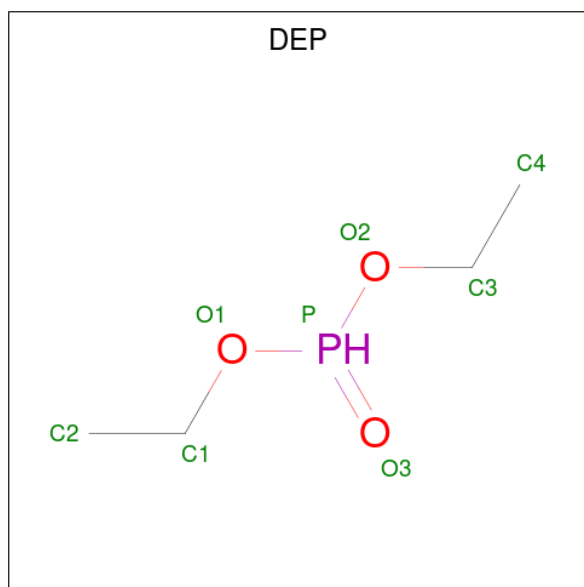


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

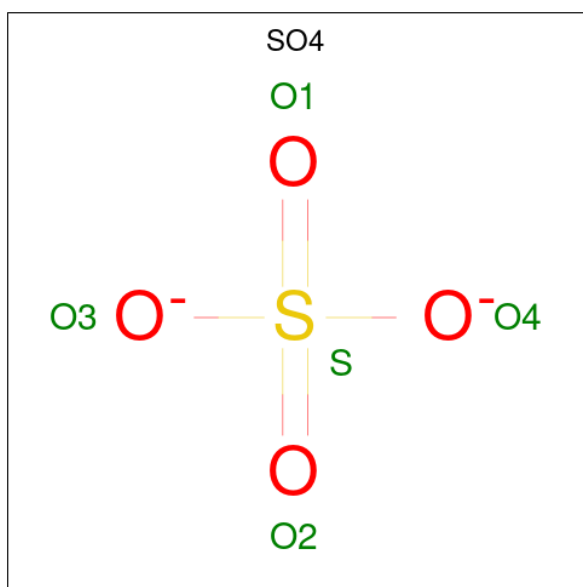
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	X	0	0
			21	21		

- Molecule 5 is DIETHYL PHOSPHONATE (CCD ID: DEP) (formula: $C_4H_{11}O_3P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			8	4	3	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Cl	0	0
			4	4		

- Molecule 8 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Br	0	0
			1	1		

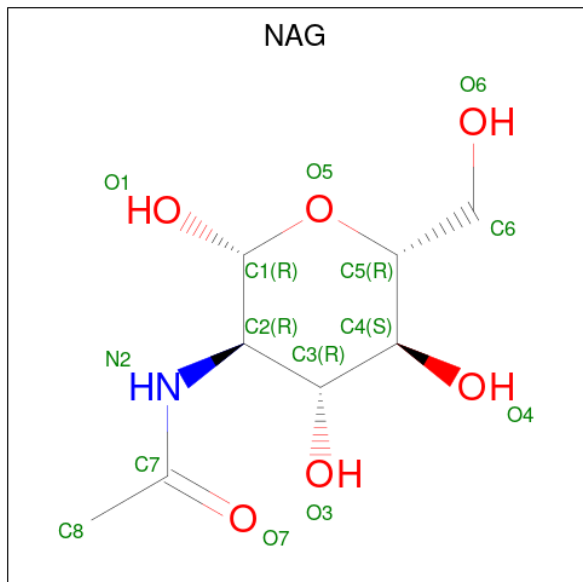
- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	Na	0	0
			2	2		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

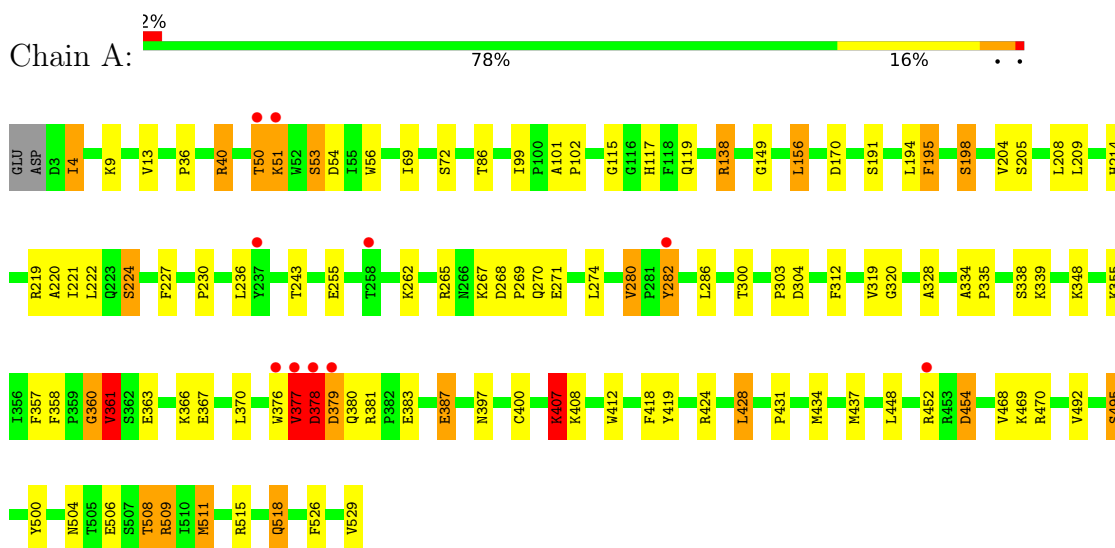
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	285	Total	O	0	0
			285	285		

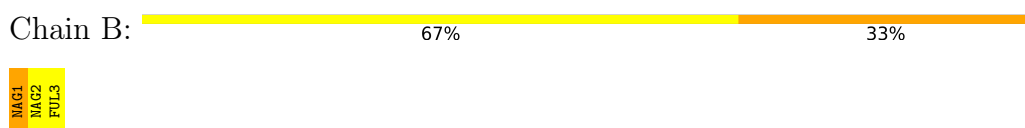
3 Residue-property plots

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.

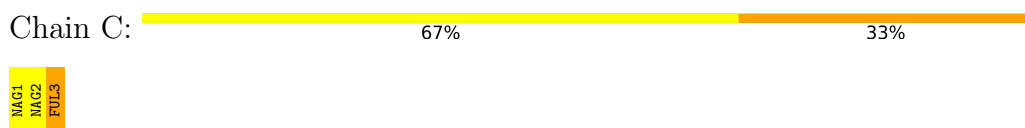
- Molecule 1: CHOLINESTERASE



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



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



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



MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.88Å 154.88Å 127.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.15 – 2.30 28.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (28.15-2.30) 95.9 (28.15-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.170 , 0.214 (Not available) , 0.214	Depositor DCC
R_{free} test set	1090 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	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	0.95	EDS
Total number of atoms	4705	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: UNX, DEP, SO4, FUC, NA, FUL, CL, BR, NAG, CA

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	10/4346 (0.2%)	1.22	21/5900 (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	1	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLY	C-O	6.34	1.29	1.23
1	A	36	PRO	CA-C	6.02	1.57	1.52
1	A	377	VAL	CA-CB	5.82	1.59	1.53
1	A	408	LYS	C-O	-5.75	1.17	1.24
1	A	515	ARG	CZ-NH1	5.68	1.40	1.32
1	A	194	LEU	C-O	5.61	1.30	1.23
1	A	86	THR	N-CA	5.42	1.52	1.45
1	A	400	CYS	CA-C	5.27	1.58	1.52
1	A	470	ARG	CA-C	5.21	1.59	1.52
1	A	230	PRO	CA-C	5.04	1.60	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	VAL	N-CA-C	8.35	126.70	109.34
1	A	358	PHE	CA-C-N	7.04	128.64	119.84
1	A	358	PHE	C-N-CA	7.04	128.64	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	CG-CD-NE	-5.82	99.19	112.00
1	A	53	SER	N-CA-C	-5.79	102.20	110.59
1	A	72	SER	CA-C-N	-5.71	116.24	123.15
1	A	72	SER	C-N-CA	-5.71	116.24	123.15
1	A	360	GLY	CA-C-N	5.64	132.12	121.97
1	A	360	GLY	C-N-CA	5.64	132.12	121.97
1	A	280	VAL	CA-C-N	-5.58	112.87	119.84
1	A	280	VAL	C-N-CA	-5.58	112.87	119.84
1	A	509	ARG	N-CA-C	5.43	118.44	109.85
1	A	526	PHE	N-CA-C	5.43	121.00	113.45
1	A	224	SER	CB-CA-C	-5.34	104.31	111.89
1	A	511	MET	N-CA-CB	-5.33	102.41	111.69
1	A	300	THR	N-CA-C	5.25	119.54	113.18
1	A	412	TRP	CA-C-N	-5.16	116.11	123.08
1	A	412	TRP	C-N-CA	-5.16	116.11	123.08
1	A	170	ASP	N-CA-C	-5.09	105.62	111.07
1	A	117	HIS	CB-CA-C	-5.07	103.41	111.48
1	A	407	LYS	CB-CG-CD	-5.04	99.72	111.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide
1	A	377	VAL	Peptide
1	A	378	ASP	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	4222	0	4115	72	0
2	B	38	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	38	0	34	1	0
3	D	38	0	34	0	0
4	A	21	0	0	2	0
5	A	8	0	10	1	0
6	A	5	0	0	0	0
7	A	4	0	0	0	0
8	A	1	0	0	0	0
9	A	2	0	0	0	0
10	A	1	0	0	0	1
11	A	42	0	39	1	0
12	A	285	0	0	10	0
All	All	4705	0	4266	76	1

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 (76) 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:99:ILE:HD11	12:A:2010:HOH:O	1.25	1.33
1:A:379:ASP:H	1:A:380:GLN:HA	1.00	1.16
1:A:379:ASP:N	1:A:380:GLN:HA	1.80	0.95
1:A:518:GLN:HE21	1:A:518:GLN:H	1.14	0.92
1:A:508:THR:OG1	12:A:2263:HOH:O	1.80	0.89
1:A:378:ASP:HB3	1:A:379:ASP:HA	1.62	0.81
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.64	0.80
1:A:379:ASP:H	1:A:380:GLN:CA	1.89	0.80
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.48	0.78
1:A:282:TYR:O	1:A:282:TYR:HD2	1.76	0.69
1:A:227:PHE:CD2	1:A:227:PHE:C	2.71	0.69
1:A:138:ARG:NE	12:A:2091:HOH:O	2.28	0.66
1:A:156:LEU:CD1	1:A:243:THR:HG21	2.26	0.66
1:A:4:ILE:H	1:A:4:ILE:HD12	1.62	0.64
1:A:370:LEU:C	1:A:370:LEU:HD23	2.25	0.61
4:A:1569:UNX:UNK	4:A:1570:UNX:UNK	1.45	0.61
1:A:500:TYR:CZ	1:A:511:MET:HB3	2.37	0.59
1:A:53:SER:O	1:A:54:ASP:CG	2.45	0.59
1:A:40:ARG:HE	1:A:40:ARG:H	1.49	0.59
1:A:518:GLN:H	1:A:518:GLN:NE2	1.94	0.59
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.38	0.58
1:A:101:ALA:HA	1:A:102:PRO:C	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TRP:C	1:A:56:TRP:CD1	2.82	0.58
1:A:4:ILE:HD12	1:A:4:ILE:N	2.18	0.57
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.43	0.55
1:A:407:LYS:HG3	1:A:495:SER:OG	2.07	0.54
5:A:1530:DEP:H31	12:A:2113:HOH:O	2.07	0.54
1:A:361:VAL:O	1:A:366:LYS:NZ	2.41	0.54
1:A:376:TRP:O	1:A:378:ASP:OD1	2.27	0.53
1:A:500:TYR:CE1	1:A:511:MET:HB3	2.44	0.53
1:A:319:VAL:O	1:A:418:PHE:HA	2.09	0.52
1:A:338:SER:HB2	2:B:1:NAG:H62	1.91	0.51
1:A:191:SER:HB2	2:C:3:FUL:H3	1.92	0.51
1:A:434:MET:HE2	1:A:437:MET:HE3	1.93	0.51
4:A:1540:UNX:UNK	4:A:1542:UNX:UNK	1.55	0.51
1:A:214[A]:HIS:HE1	12:A:2156:HOH:O	1.93	0.50
1:A:518:GLN:HE21	1:A:518:GLN:N	1.97	0.50
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.42	0.49
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.48	0.49
1:A:379:ASP:N	1:A:380:GLN:CA	2.62	0.48
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.67	0.48
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.97	0.48
1:A:407:LYS:HE2	1:A:407:LYS:HB2	1.23	0.48
1:A:452:ARG:C	1:A:454:ASP:H	2.23	0.47
1:A:328:ALA:HA	1:A:434:MET:CE	2.44	0.47
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.97	0.47
1:A:286:LEU:HD22	1:A:397:ASN:CG	2.40	0.46
1:A:268:ASP:O	1:A:269:PRO:C	2.57	0.45
1:A:495:SER:HB2	12:A:2199:HOH:O	2.14	0.45
1:A:267:LYS:HD2	1:A:271:GLU:OE2	2.17	0.45
1:A:50:THR:O	1:A:51:LYS:HB3	2.17	0.45
1:A:434:MET:HE2	1:A:437:MET:CE	2.47	0.44
1:A:265:ARG:NE	12:A:2134:HOH:O	2.28	0.44
1:A:383:GLU:O	1:A:387:GLU:HG2	2.17	0.44
1:A:265:ARG:NH2	12:A:2133:HOH:O	2.50	0.44
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.32	0.44
1:A:195:PHE:CB	1:A:221:ILE:HB	2.48	0.44
1:A:198:SER:HA	1:A:224:SER:O	2.18	0.44
1:A:119:GLN:OE1	1:A:149:GLY:HA2	2.17	0.44
1:A:379:ASP:OD1	1:A:381:ARG:HG3	2.18	0.44
1:A:282:TYR:O	1:A:282:TYR:CD2	2.63	0.43
1:A:267:LYS:HD3	1:A:267:LYS:HA	1.86	0.42
1:A:304:ASP:HB3	12:A:2017:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.50	0.42
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.55	0.41
11:A:1562:NAG:C8	12:A:2283:HOH:O	2.68	0.41
1:A:469:LYS:HA	1:A:469:LYS:HD3	1.94	0.41
1:A:508:THR:O	1:A:508:THR:HG22	2.20	0.41
1:A:40:ARG:H	1:A:40:ARG:NE	2.15	0.41
1:A:504:ASN:OD1	1:A:506:GLU:HG3	2.21	0.41
1:A:209:LEU:HD22	1:A:312:PHE:HB3	2.01	0.41
1:A:334:ALA:HB2	1:A:357:PHE:HE2	1.86	0.41
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.89	0.41
1:A:50:THR:O	1:A:51:LYS:CB	2.68	0.41
1:A:339:LYS:O	1:A:431:PRO:HG3	2.20	0.40
1:A:268:ASP:HB2	1:A:269:PRO:CD	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1537:CA:CA	10:A:1537:CA:CA[5_556]	1.55	0.65

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	527/529 (100%)	499 (95%)	25 (5%)	3 (1%)	21	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	361	VAL
1	A	379	ASP

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	455/455 (100%)	419 (92%)	36 (8%)	11	15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	13	VAL
1	A	40	ARG
1	A	50	THR
1	A	69	ILE
1	A	138	ARG
1	A	156	LEU
1	A	195	PHE
1	A	198	SER
1	A	236	LEU
1	A	255	GLU
1	A	262	LYS
1	A	270	GLN
1	A	274	LEU
1	A	280	VAL
1	A	282	TYR
1	A	348	LYS
1	A	355	LYS
1	A	361	VAL
1	A	363	GLU
1	A	367	GLU
1	A	377	VAL
1	A	378	ASP
1	A	387	GLU
1	A	407	LYS
1	A	428	LEU
1	A	448	LEU
1	A	454	ASP
1	A	468	VAL

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Mol	Chain	Res	Type
1	A	492	VAL
1	A	495	SER
1	A	508	THR
1	A	509	ARG
1	A	518	GLN
1	A	529	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	63	ASN
1	A	289	ASN
1	A	455	GLN
1	A	486	GLN
1	A	517	GLN
1	A	518	GLN

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	0.91	1 (7%)	17,19,21	2.46	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	2	2	14,14,15	0.71	0	17,19,21	1.80	3 (17%)
2	FUL	B	3	2	10,10,11	1.23	0	14,14,16	2.76	8 (57%)
2	NAG	C	1	1,2	14,14,15	1.00	0	17,19,21	2.11	6 (35%)
2	NAG	C	2	2	14,14,15	0.81	0	17,19,21	2.00	6 (35%)
2	FUL	C	3	2	10,10,11	1.15	1 (10%)	14,14,16	3.17	7 (50%)
3	NAG	D	1	1,3	14,14,15	0.80	0	17,19,21	2.85	6 (35%)
3	NAG	D	2	3	14,14,15	1.16	1 (7%)	17,19,21	1.18	2 (11%)
3	FUC	D	3	3	10,10,11	0.86	0	14,14,16	1.66	4 (28%)

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	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	FUL	C	3	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	3.45	1.57	1.52
2	C	3	FUL	O5-C1	-2.50	1.39	1.43
2	B	1	NAG	O5-C1	-2.27	1.39	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUL	C1-C2-C3	-6.88	99.63	109.64
2	C	3	FUL	C1-C2-C3	-6.71	99.87	109.64
3	D	1	NAG	C2-N2-C7	6.19	131.19	122.90
3	D	1	NAG	C8-C7-N2	6.04	126.14	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	FUL	C1-O5-C5	-5.83	99.20	112.97
2	C	2	NAG	C1-O5-C5	5.80	119.95	112.19
2	B	1	NAG	C1-C2-N2	-5.45	101.84	110.43
2	C	3	FUL	C3-C4-C5	4.92	117.28	109.81
2	C	1	NAG	C1-C2-N2	4.77	117.94	110.43
2	B	1	NAG	C2-N2-C7	4.37	128.76	122.90
3	D	1	NAG	C1-O5-C5	4.30	117.95	112.19
2	B	2	NAG	C4-C3-C2	4.07	116.98	111.02
2	B	3	FUL	C1-O5-C5	-3.83	103.93	112.97
3	D	1	NAG	O5-C1-C2	-3.76	105.47	111.29
2	B	1	NAG	C3-C4-C5	-3.75	103.43	110.23
2	B	2	NAG	C2-N2-C7	3.57	127.68	122.90
2	C	1	NAG	O5-C5-C6	3.28	114.04	107.66
3	D	1	NAG	O7-C7-N2	-3.27	116.21	121.98
2	C	3	FUL	C2-C3-C4	-3.18	105.27	110.86
2	B	2	NAG	C1-C2-N2	3.15	115.40	110.43
2	B	3	FUL	C3-C4-C5	3.11	114.55	109.81
2	B	3	FUL	O2-C2-C3	3.08	116.54	110.15
2	B	1	NAG	O6-C6-C5	2.95	121.38	111.33
2	C	3	FUL	O3-C3-C2	2.87	115.92	110.05
2	C	1	NAG	C6-C5-C4	2.78	119.84	113.02
3	D	3	FUC	O3-C3-C4	2.77	116.91	110.38
2	B	1	NAG	C6-C5-C4	2.77	119.82	113.02
2	C	3	FUL	O4-C4-C5	-2.75	103.66	109.74
2	B	3	FUL	O5-C1-C2	-2.65	104.47	110.79
3	D	3	FUC	C6-C5-C4	2.65	117.92	113.08
3	D	3	FUC	O4-C4-C5	2.64	115.55	109.74
3	D	1	NAG	O7-C7-C8	-2.48	117.63	122.05
2	C	1	NAG	C1-O5-C5	-2.41	108.96	112.19
2	C	2	NAG	C4-C3-C2	-2.40	107.50	111.02
2	B	3	FUL	O5-C5-C6	2.38	112.56	107.40
2	B	3	FUL	C2-C3-C4	2.38	115.04	110.86
2	C	3	FUL	O2-C2-C3	2.32	114.95	110.15
3	D	3	FUC	O5-C5-C4	2.32	113.72	109.55
2	C	2	NAG	C1-C2-N2	-2.31	106.79	110.43
2	B	3	FUL	C6-C5-C4	2.30	117.28	113.08
2	B	1	NAG	C8-C7-N2	2.24	119.84	116.12
2	C	1	NAG	C8-C7-N2	2.20	119.77	116.12
2	C	2	NAG	C2-N2-C7	-2.14	120.03	122.90
3	D	2	NAG	O4-C4-C3	2.13	115.39	110.38
3	D	2	NAG	O5-C5-C6	2.11	111.76	107.66
2	C	2	NAG	C6-C5-C4	2.11	118.19	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O7-C7-C8	-2.10	118.32	122.05
2	C	1	NAG	O3-C3-C4	2.06	115.24	110.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

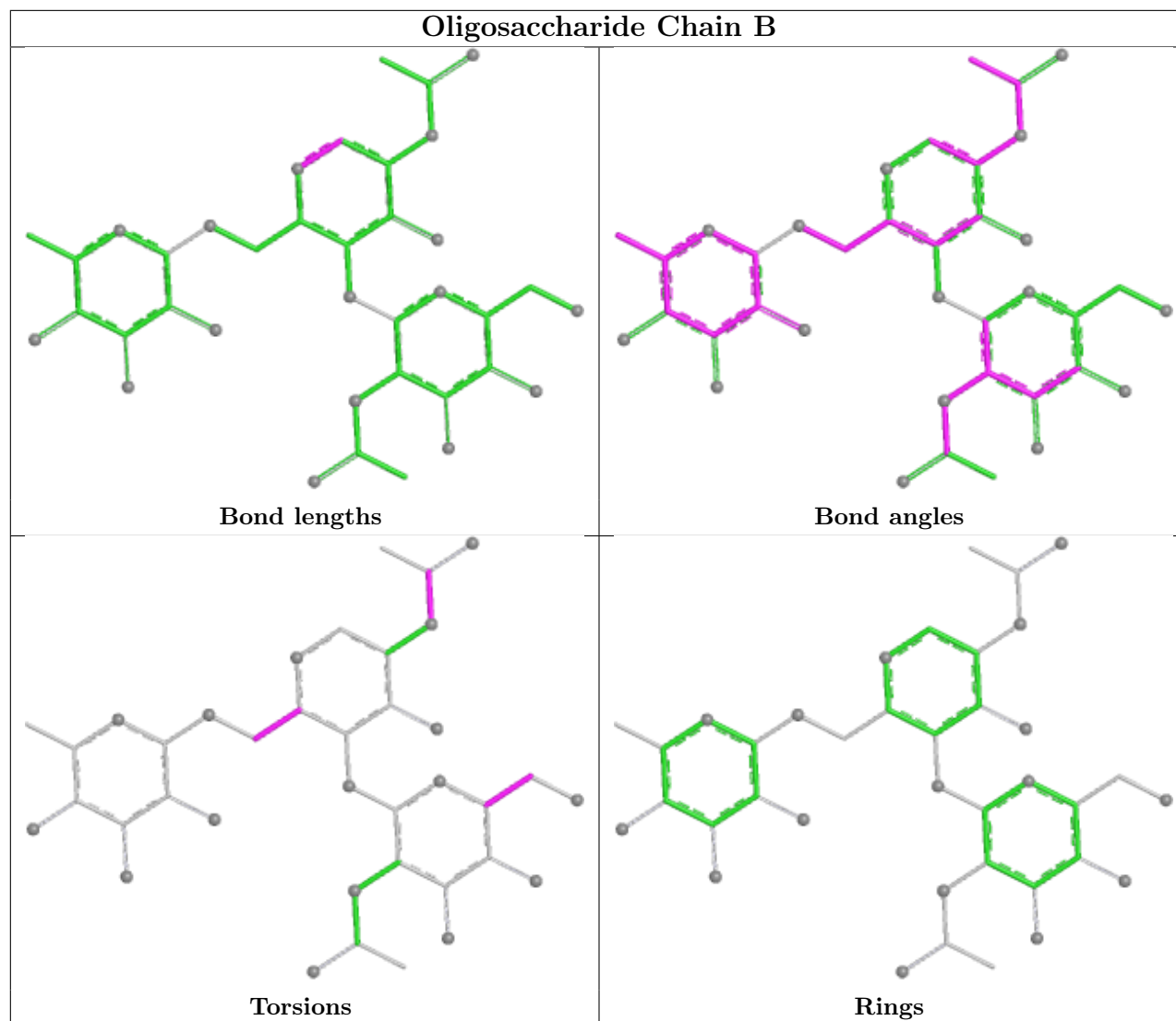
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
2	B	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6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

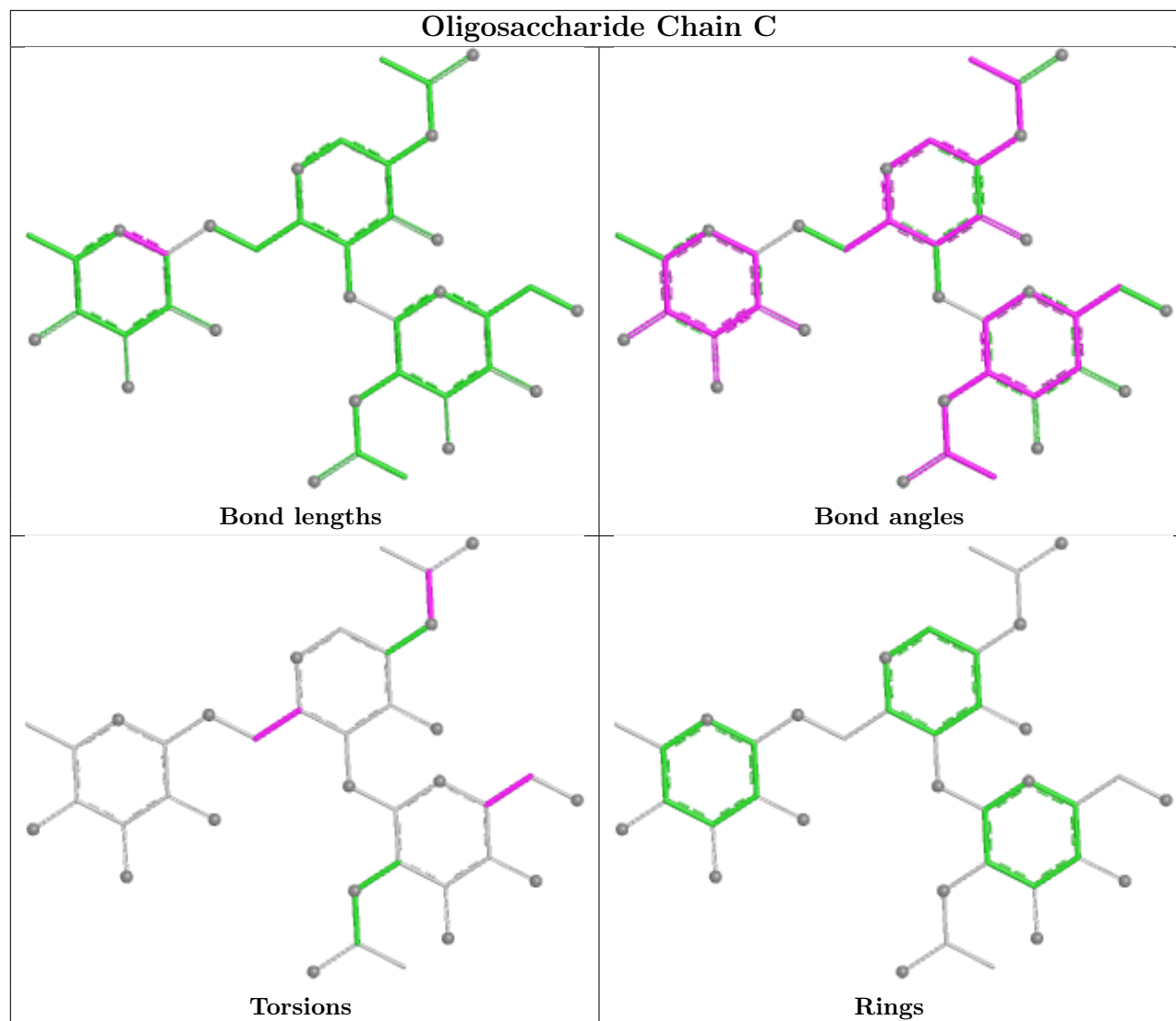
There are no ring outliers.

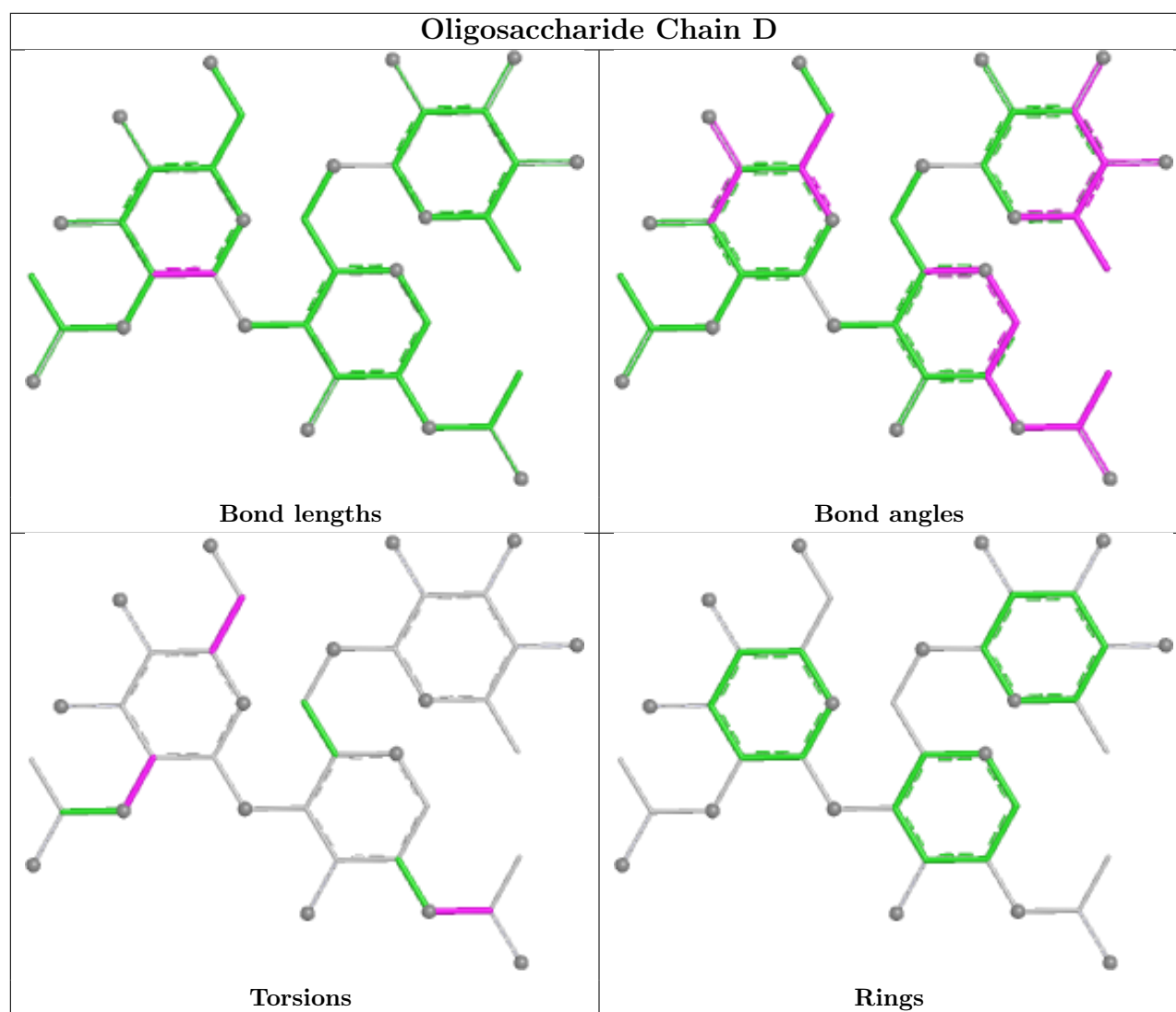
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FUL	1	0
2	B	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 34 ligands modelled in this entry, 21 are unknown and 8 are monoatomic - leaving 5 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	DEP	A	1530	1	4,7,7	0.83	0	2,7,7	1.14	0
11	NAG	A	1562	1	14,14,15	0.59	0	17,19,21	2.53	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1531	-	4,4,4	0.12	0	6,6,6	0.66	0
11	NAG	A	1561	1	14,14,15	0.90	0	17,19,21	1.62	5 (29%)
11	NAG	A	1560	1	14,14,15	0.93	0	17,19,21	1.97	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
5	DEP	A	1530	1	-	0/2/6/6	-
11	NAG	A	1561	1	-	1/6/23/26	0/1/1/1
11	NAG	A	1562	1	-	4/6/23/26	0/1/1/1
11	NAG	A	1560	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1562	NAG	C1-O5-C5	7.96	122.86	112.19
11	A	1560	NAG	O5-C5-C6	5.11	117.60	107.66
11	A	1562	NAG	O5-C1-C2	-4.37	104.53	111.29
11	A	1560	NAG	O5-C1-C2	-3.61	105.70	111.29
11	A	1561	NAG	O5-C1-C2	-3.03	106.61	111.29
11	A	1561	NAG	C4-C3-C2	2.86	115.21	111.02
11	A	1561	NAG	C1-O5-C5	2.58	115.64	112.19
11	A	1560	NAG	C8-C7-N2	2.55	120.35	116.12
11	A	1560	NAG	C1-O5-C5	2.40	115.41	112.19
11	A	1562	NAG	C1-C2-N2	2.39	114.20	110.43
11	A	1561	NAG	O7-C7-C8	-2.39	117.81	122.05
11	A	1562	NAG	C2-N2-C7	2.37	126.08	122.90
11	A	1561	NAG	O5-C5-C4	-2.15	105.59	110.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1562	NAG	C1-C2-N2-C7
11	A	1562	NAG	C3-C2-N2-C7
11	A	1560	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	A	1560	NAG	C4-C5-C6-O6
11	A	1562	NAG	O5-C5-C6-O6
11	A	1562	NAG	C4-C5-C6-O6
11	A	1560	NAG	C8-C7-N2-C2
11	A	1560	NAG	O7-C7-N2-C2
11	A	1561	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1530	DEP	1	0
11	A	1562	NAG	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	527/529 (99%)	-0.32	10 (1%) 66 68	14, 37, 68, 95	5 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	4.4
1	A	237	TYR	3.5
1	A	379	ASP	3.2
1	A	50	THR	3.0
1	A	258	THR	2.7
1	A	282	TYR	2.6
1	A	376	TRP	2.2
1	A	51	LYS	2.1
1	A	378	ASP	2.0
1	A	452	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.

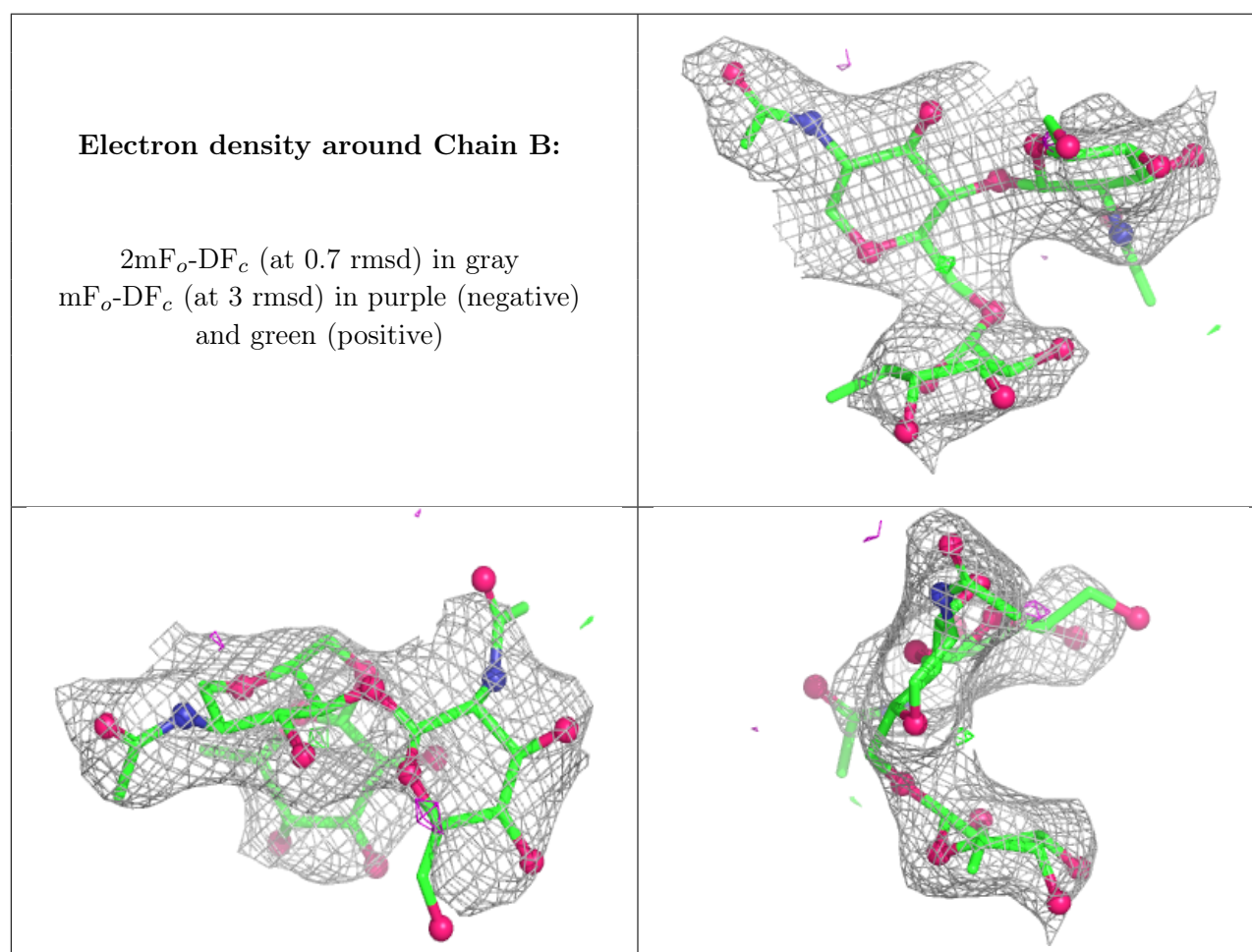
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.72	0.14	81,86,88,88	0
2	FUL	B	3	10/11	0.74	0.15	71,73,75,76	0

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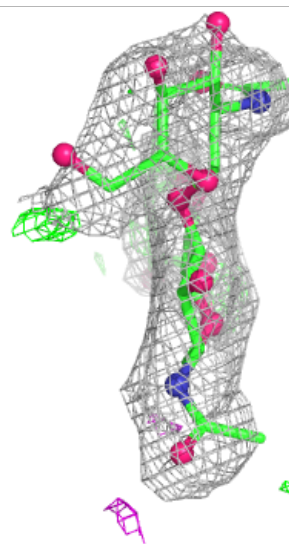
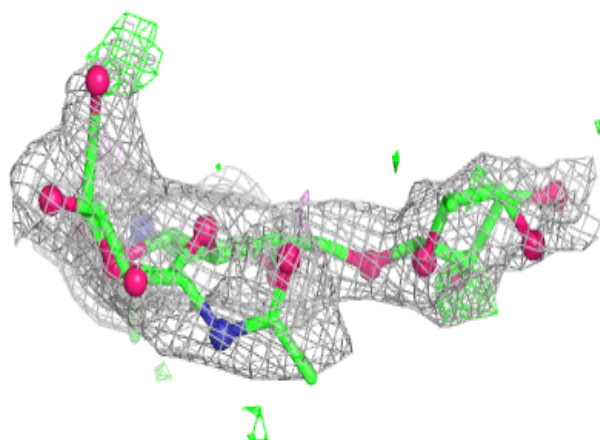
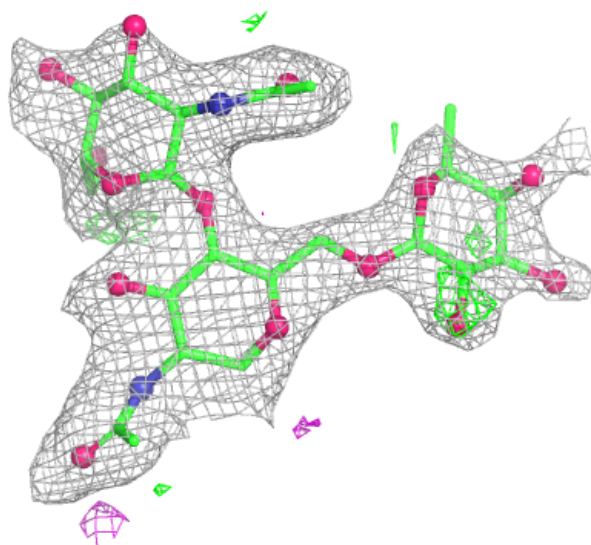
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	2	14/15	0.76	0.13	64,68,71,71	0
2	NAG	B	2	14/15	0.79	0.14	74,83,87,88	0
3	NAG	D	1	14/15	0.83	0.12	49,61,71,76	0
2	FUL	C	3	10/11	0.83	0.23	31,34,40,41	10
3	FUC	D	3	10/11	0.87	0.10	56,61,64,66	0
2	NAG	C	1	14/15	0.88	0.10	48,60,65,72	0
2	NAG	B	1	14/15	0.93	0.09	42,51,65,68	0

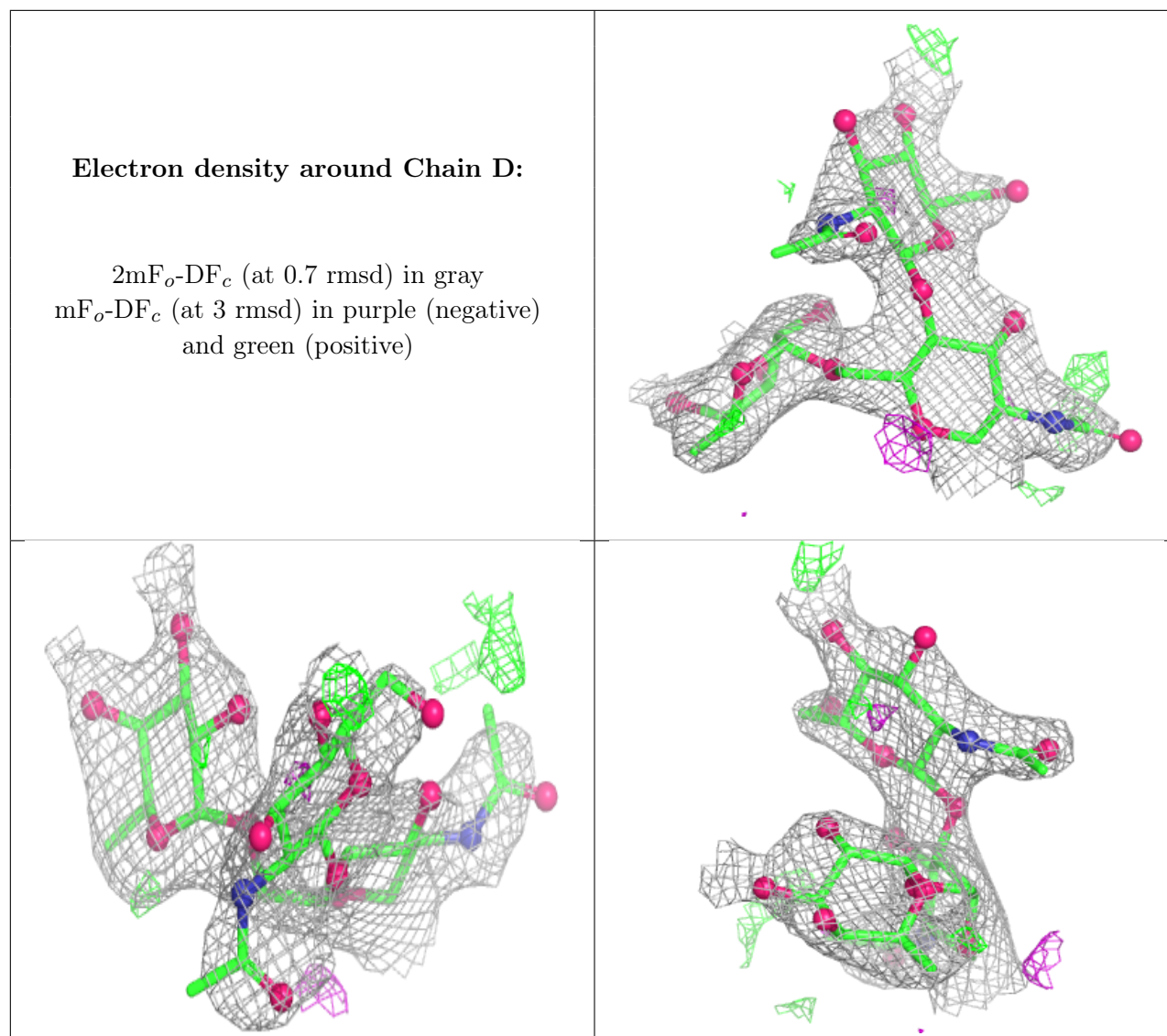
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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(Å ²)	Q<0.9
11	NAG	A	1560	14/15	0.58	0.15	64,75,77,77	0
9	NA	A	1567	1/1	0.73	0.29	66,66,66,66	0
11	NAG	A	1561	14/15	0.74	0.15	55,65,73,74	0
11	NAG	A	1562	14/15	0.74	0.20	61,66,76,77	9
4	UNX	A	1543	1/1	0.81	0.09	29,29,29,29	0
4	UNX	A	1547	1/1	0.82	0.20	33,33,33,33	0
4	UNX	A	1541	1/1	0.85	0.14	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	UNX	A	1549	1/1	0.85	0.11	32,32,32,32	0
4	UNX	A	1548	1/1	0.89	0.09	16,16,16,16	0
4	UNX	A	1538	1/1	0.89	0.07	14,14,14,14	0
4	UNX	A	1571	1/1	0.89	0.12	37,37,37,37	0
7	CL	A	1566	1/1	0.89	0.13	74,74,74,74	0
4	UNX	A	1544	1/1	0.90	0.11	26,26,26,26	0
4	UNX	A	1551	1/1	0.90	0.14	43,43,43,43	0
4	UNX	A	1553	1/1	0.92	0.08	36,36,36,36	0
4	UNX	A	1572	1/1	0.93	0.06	29,29,29,29	0
9	NA	A	1536	1/1	0.93	0.32	52,52,52,52	0
4	UNX	A	1550	1/1	0.94	0.04	22,22,22,22	0
4	UNX	A	1569	1/1	0.94	0.07	37,37,37,37	0
4	UNX	A	1546	1/1	0.94	0.14	26,26,26,26	0
4	UNX	A	1552	1/1	0.94	0.08	37,37,37,37	0
7	CL	A	1532	1/1	0.94	0.20	64,64,64,64	0
7	CL	A	1534	1/1	0.94	0.19	62,62,62,62	0
4	UNX	A	1542	1/1	0.95	0.05	21,21,21,21	0
4	UNX	A	1545	1/1	0.95	0.13	18,18,18,18	0
4	UNX	A	1568	1/1	0.95	0.08	8,8,8,8	0
6	SO4	A	1531	5/5	0.95	0.10	38,44,47,48	5
7	CL	A	1533	1/1	0.98	0.05	37,37,37,37	0
4	UNX	A	1539	1/1	0.98	0.11	17,17,17,17	0
4	UNX	A	1570	1/1	0.98	0.13	2,2,2,2	0
4	UNX	A	1540	1/1	0.98	0.03	21,21,21,21	0
5	DEP	A	1530	8/8	0.99	0.04	26,29,31,34	0
8	BR	A	1535	1/1	0.99	0.09	42,42,42,42	0
10	CA	A	1537	1/1	0.99	0.06	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.