



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:26 PM UTC

PDB ID : 3GXN / pdb_00003gxn
Title : Crystal structure of apo alpha-galactosidase A at pH 4.5
Authors : Lieberman, R.L.
Deposited on : 2009-04-02
Resolution : 3.01 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

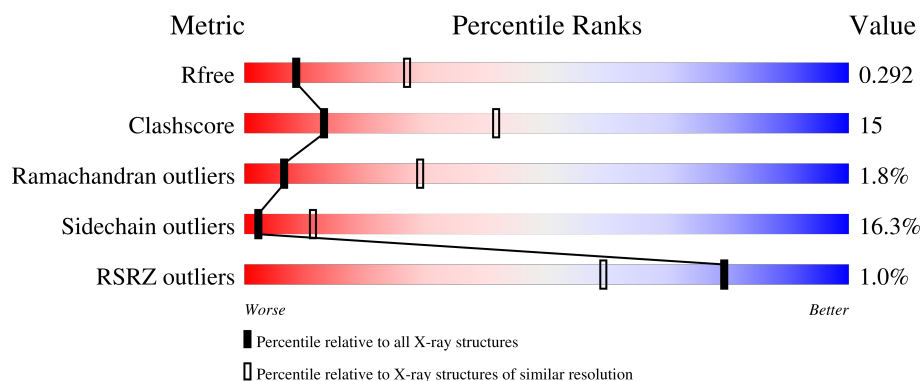
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	398	% 60% 30% 7% ..
1	B	398	% 60% 30% 7% ..
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6305 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 Alpha-galactosidase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			
1	B	390	Total	C	N	O	S	0	0	0
			3122	1988	534	574	26			

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



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

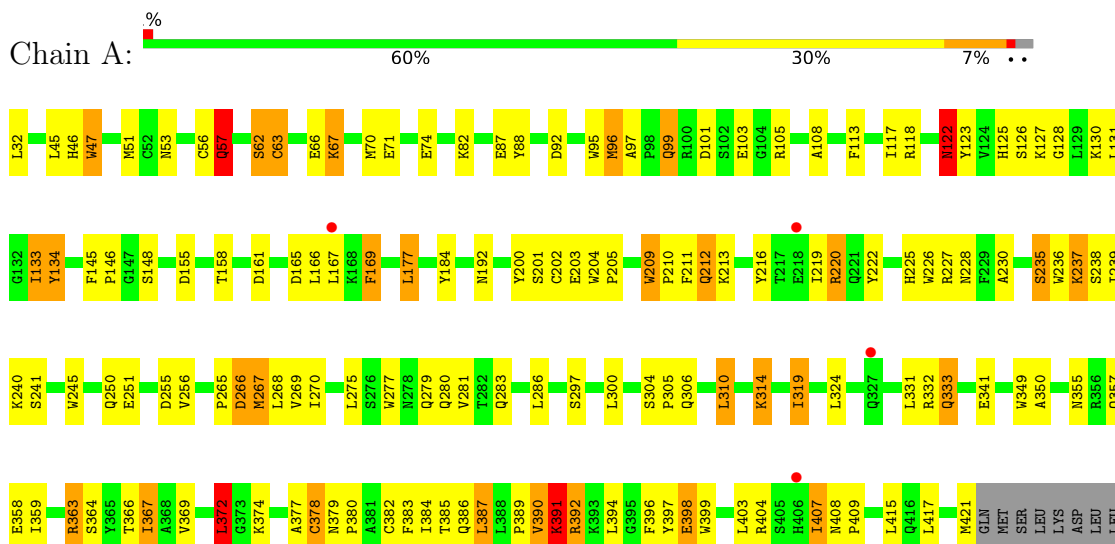


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

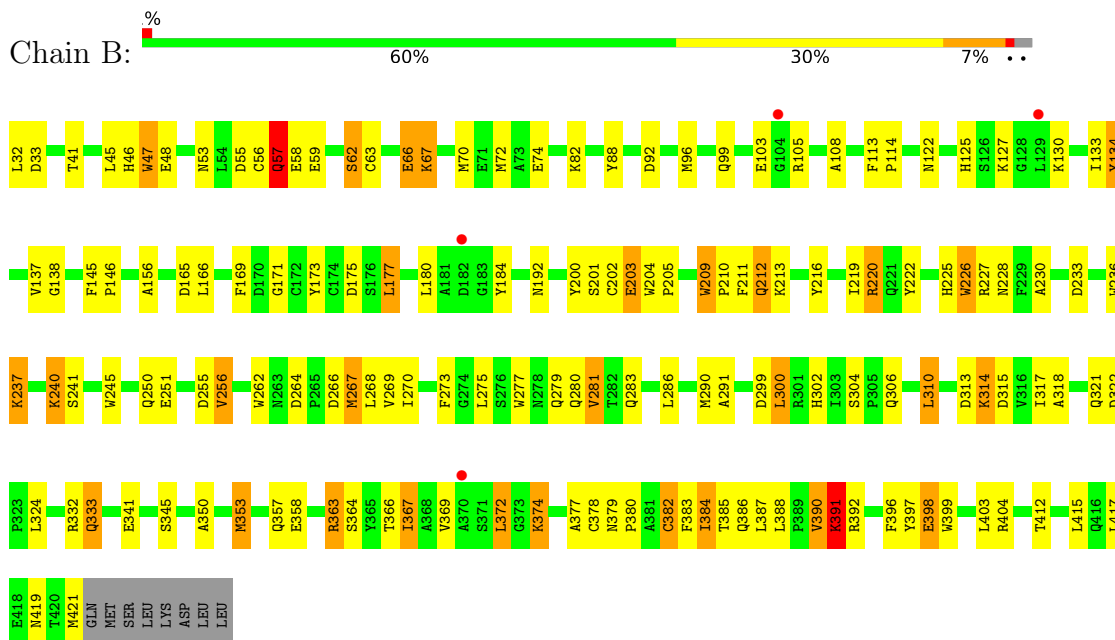
3 Residue-property plots

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: Alpha-galactosidase A



• Molecule 1: Alpha-galactosidase A



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

Chain C:  50% 50%

MAG1
MAG2

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

Chain D:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.38Å 90.38Å 217.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.66 – 3.01 44.66 – 3.01	Depositor EDS
% Data completeness (in resolution range)	88.1 (44.66-3.01) 88.3 (44.66-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.301 0.229 , 0.292	Depositor DCC
R_{free} test set	971 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 122.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: NAG, SO4

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	1.04	2/3209 (0.1%)	1.22	17/4358 (0.4%)
1	B	0.99	1/3209 (0.0%)	1.19	10/4358 (0.2%)
All	All	1.01	3/6418 (0.0%)	1.21	27/8716 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	ILE	CA-C	5.77	1.59	1.52
1	B	302	HIS	CA-C	-5.61	1.46	1.53
1	A	407	ILE	CA-CB	5.27	1.61	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	VAL	N-CA-C	13.29	122.12	111.62
1	A	47	TRP	N-CA-C	7.64	120.34	111.02
1	A	304	SER	CA-C-N	-6.80	112.77	119.64
1	A	304	SER	C-N-CA	-6.80	112.77	119.64
1	B	156	ALA	N-CA-C	-6.62	103.98	111.07
1	B	304	SER	CA-C-N	-6.57	113.01	119.64
1	B	304	SER	C-N-CA	-6.57	113.01	119.64
1	A	101	ASP	CA-C-N	6.44	128.91	120.28
1	A	101	ASP	C-N-CA	6.44	128.91	120.28
1	B	47	TRP	N-CA-C	6.34	121.76	111.37
1	A	394	LEU	N-CA-C	-6.33	100.55	110.36
1	B	226	TRP	N-CA-C	5.78	118.06	108.99
1	A	131	LEU	N-CA-C	5.74	117.87	108.52
1	B	419	ASN	N-CA-C	5.59	119.35	109.96
1	B	281	VAL	N-CA-CB	5.53	118.07	110.54
1	A	155	ASP	N-CA-C	5.37	117.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	TRP	N-CA-C	5.27	118.15	109.72
1	A	389	PRO	CA-C-N	-5.22	117.62	123.16
1	A	389	PRO	C-N-CA	-5.22	117.62	123.16
1	B	390	VAL	N-CA-C	5.20	120.16	109.34
1	A	99	GLN	N-CA-C	5.07	116.01	108.86
1	A	305	PRO	N-CA-C	-5.07	107.13	114.18
1	A	97	ALA	CA-C-N	5.07	126.17	119.84
1	A	97	ALA	C-N-CA	5.07	126.17	119.84
1	A	392	ARG	N-CA-C	-5.07	101.43	109.59
1	A	235	SER	N-CA-C	5.01	116.86	108.99
1	B	384	ILE	N-CA-C	5.00	115.29	107.99

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	3122	0	2984	97	0
1	B	3122	0	2984	93	1
2	C	28	0	25	3	1
2	D	28	0	25	4	0
3	A	5	0	0	0	0
All	All	6305	0	6018	184	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 15.

All (184) 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:192:ASN:HD21	2:C:1:NAG:C1	1.60	1.15
1:B:192:ASN:HD21	2:D:1:NAG:C1	1.68	1.04
1:B:57:GLN:NE2	1:B:57:GLN:HA	1.88	0.89
1:A:386:GLN:NE2	1:A:390:VAL:HG22	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASN:HD22	1:B:62:SER:HB2	1.39	0.87
1:A:386:GLN:O	1:A:391:LYS:HA	1.74	0.86
1:B:53:ASN:ND2	1:B:62:SER:HB2	1.91	0.84
1:B:210:PRO:HD2	1:B:211:PHE:CE2	2.14	0.83
1:B:386:GLN:NE2	1:B:390:VAL:HG22	1.95	0.82
1:A:57:GLN:NE2	1:A:57:GLN:HA	1.96	0.79
1:B:386:GLN:O	1:B:391:LYS:HA	1.81	0.79
1:A:192:ASN:ND2	2:C:1:NAG:C1	2.43	0.79
1:A:366:THR:HG22	1:A:404:ARG:HA	1.63	0.78
1:A:386:GLN:HE22	1:A:390:VAL:HG22	1.48	0.78
1:A:46:HIS:CD2	1:A:92:ASP:H	2.03	0.77
1:A:53:ASN:HD22	1:A:62:SER:HB2	1.53	0.74
1:A:251:GLU:OE1	1:A:251:GLU:N	2.15	0.74
1:A:363:ARG:HH11	1:A:363:ARG:HG2	1.51	0.74
1:B:192:ASN:ND2	2:D:1:NAG:C1	2.48	0.73
1:A:314:LYS:N	1:A:314:LYS:HD3	2.04	0.73
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.71	0.73
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.70	0.71
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.71	0.71
1:A:237:LYS:HE3	1:B:237:LYS:HE3	1.71	0.71
1:B:47:TRP:HB3	1:B:267:MET:HE1	1.73	0.71
1:B:314:LYS:N	1:B:314:LYS:HD3	2.06	0.71
1:B:251:GLU:OE1	1:B:251:GLU:N	2.18	0.70
1:B:384:ILE:HG12	1:B:417:LEU:HG	1.73	0.70
1:A:32:LEU:N	1:A:220:ARG:O	2.25	0.70
1:B:46:HIS:CD2	1:B:92:ASP:H	2.09	0.70
1:B:386:GLN:HE22	1:B:390:VAL:HG22	1.58	0.69
1:A:367:ILE:HD12	1:A:403:LEU:HB3	1.74	0.69
1:B:210:PRO:HD2	1:B:211:PHE:CZ	2.28	0.68
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.74	0.68
1:B:57:GLN:HA	1:B:57:GLN:HE21	1.59	0.67
1:A:47:TRP:HB3	1:A:267:MET:HE1	1.77	0.67
1:B:366:THR:HG22	1:B:404:ARG:HA	1.77	0.66
1:A:216:TYR:HA	1:A:219:ILE:HD12	1.77	0.64
1:A:239:ILE:HD12	1:A:275:LEU:HD21	1.80	0.63
1:A:213:LYS:H	1:A:213:LYS:HD2	1.63	0.63
1:B:192:ASN:HD21	2:D:1:NAG:C2	2.10	0.63
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.33	0.62
1:A:367:ILE:CD1	1:A:403:LEU:HB3	2.28	0.62
1:A:409:PRO:HD2	1:B:273:PHE:CD2	2.34	0.62
1:B:367:ILE:HD12	1:B:403:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD22	1:A:222:TYR:O	1.98	0.62
1:B:383:PHE:HD1	1:B:396:PHE:CE1	2.18	0.62
1:B:250:GLN:O	1:B:251:GLU:C	2.42	0.61
1:B:367:ILE:CD1	1:B:403:LEU:HB3	2.30	0.61
1:A:225:HIS:HA	1:A:226:TRP:CE3	2.35	0.61
1:B:177:LEU:H	1:B:177:LEU:HD12	1.64	0.61
1:B:57:GLN:NE2	1:B:57:GLN:CA	2.63	0.61
1:B:213:LYS:H	1:B:213:LYS:HD2	1.66	0.60
1:B:390:VAL:O	1:B:391:LYS:CB	2.47	0.60
1:A:209:TRP:H	1:A:209:TRP:CD1	2.18	0.60
1:A:210:PRO:HD2	1:A:211:PHE:CE2	2.36	0.60
1:A:269:VAL:HG23	1:A:275:LEU:HD11	1.84	0.60
1:A:177:LEU:HD12	1:A:177:LEU:H	1.67	0.59
1:A:277:TRP:HA	1:A:280:GLN:HE21	1.67	0.59
1:B:227:ARG:HG3	1:B:227:ARG:HH11	1.67	0.59
1:A:270:ILE:HD13	1:A:310:LEU:HD13	1.86	0.58
1:A:220:ARG:NH1	1:A:256:VAL:O	2.35	0.58
1:A:103:GLU:CD	1:A:105:ARG:HH12	2.12	0.58
1:A:386:GLN:NE2	1:A:390:VAL:CG2	2.66	0.57
1:A:53:ASN:ND2	1:A:62:SER:HB2	2.19	0.57
1:A:363:ARG:HG2	1:A:363:ARG:NH1	2.20	0.56
1:B:277:TRP:HA	1:B:280:GLN:HE21	1.71	0.56
1:A:366:THR:HG22	1:A:404:ARG:CA	2.35	0.56
1:A:57:GLN:NE2	1:A:57:GLN:CA	2.69	0.55
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.89	0.55
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.41	0.55
1:B:138:GLY:HA3	1:B:173:TYR:O	2.07	0.55
1:B:225:HIS:HA	1:B:226:TRP:CE3	2.42	0.54
1:A:237:LYS:CE	1:B:237:LYS:HE3	2.37	0.54
1:B:57:GLN:HE21	1:B:57:GLN:CA	2.21	0.53
1:A:158:THR:O	1:A:161:ASP:HB2	2.08	0.53
1:A:125:HIS:O	1:A:128:GLY:N	2.33	0.53
1:B:108:ALA:HB1	1:B:113:PHE:HB2	1.91	0.53
1:B:32:LEU:N	1:B:220:ARG:O	2.41	0.53
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.74	0.52
1:A:134:TYR:C	1:A:134:TYR:CD2	2.87	0.52
1:A:398:GLU:OE2	1:A:398:GLU:HA	2.08	0.52
1:B:66:GLU:OE1	1:B:114:PRO:HG2	2.09	0.52
1:A:355:ASN:HB3	1:A:408:ASN:O	2.10	0.52
1:B:403:LEU:HD21	1:B:415:LEU:HD13	1.92	0.52
1:B:216:TYR:HA	1:B:219:ILE:HD12	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:THR:HA	1:A:403:LEU:O	2.10	0.51
1:B:201:SER:HB2	1:B:225:HIS:CE1	2.46	0.51
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.92	0.51
1:B:269:VAL:HG23	1:B:275:LEU:HD11	1.93	0.50
1:B:270:ILE:HD13	1:B:310:LEU:HD13	1.94	0.50
1:A:211:PHE:O	1:A:212:GLN:HB3	2.11	0.50
1:B:203:GLU:HG3	1:B:227:ARG:HB2	1.93	0.50
1:A:235:SER:OG	1:A:238:SER:HB2	2.12	0.50
1:B:32:LEU:HD22	1:B:222:TYR:O	2.12	0.50
1:A:250:GLN:O	1:A:251:GLU:C	2.55	0.50
1:A:319:ILE:HD11	1:A:387:LEU:CD2	2.42	0.49
1:B:72:MET:SD	1:B:300:LEU:HB2	2.52	0.49
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.93	0.49
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.95	0.49
1:A:268:LEU:HA	1:A:283:GLN:HE22	1.78	0.49
1:A:390:VAL:O	1:A:391:LYS:CB	2.61	0.48
1:A:108:ALA:HB1	1:A:113:PHE:HB2	1.95	0.48
1:B:125:HIS:HE1	1:B:165:ASP:OD2	1.96	0.48
1:B:382:CYS:HB3	1:B:397:TYR:HB2	1.96	0.48
1:A:236:TRP:NE1	1:A:240:LYS:HD2	2.28	0.48
1:A:359:ILE:HD12	1:B:233:ASP:HB3	1.95	0.48
1:B:236:TRP:CE3	1:B:279:GLN:HG2	2.48	0.48
1:A:203:GLU:HG3	1:A:227:ARG:HB2	1.96	0.48
1:B:353:MET:O	1:B:412:THR:HA	2.14	0.47
1:A:88:TYR:CZ	1:A:130:LYS:HD2	2.49	0.47
1:B:67:LYS:HD3	1:B:67:LYS:H	1.79	0.47
1:A:331:LEU:HD22	1:A:341:GLU:OE2	2.15	0.47
1:B:55:ASP:OD2	1:B:57:GLN:HB2	2.14	0.47
1:B:386:GLN:NE2	1:B:390:VAL:CG2	2.73	0.47
1:A:166:LEU:HD23	1:A:167:LEU:N	2.29	0.47
1:B:134:TYR:CD2	1:B:134:TYR:C	2.93	0.47
1:B:372:LEU:HD12	1:B:372:LEU:HA	1.70	0.47
1:A:95:TRP:CZ2	1:A:96:MET:HE2	2.49	0.47
1:A:403:LEU:HD21	1:A:415:LEU:HD13	1.97	0.47
1:A:67:LYS:HD3	1:A:67:LYS:H	1.80	0.47
1:B:372:LEU:O	1:B:374:LYS:N	2.42	0.47
1:A:202:CYS:O	1:A:226:TRP:HA	2.15	0.46
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.75	0.46
1:B:398:GLU:OE2	1:B:398:GLU:HA	2.15	0.46
1:B:378:CYS:O	1:B:399:TRP:HD1	1.99	0.46
1:B:341:GLU:HA	1:B:350:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:PHE:O	1:B:212:GLN:HB3	2.16	0.46
1:A:210:PRO:HD2	1:A:211:PHE:CZ	2.51	0.45
1:B:88:TYR:CZ	1:B:130:LYS:HD2	2.52	0.45
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.51	0.45
1:B:209:TRP:CD1	1:B:209:TRP:H	2.35	0.45
1:B:33:ASP:O	2:D:1:NAG:H4	2.16	0.45
1:B:103:GLU:CD	1:B:105:ARG:HH12	2.25	0.45
1:A:62:SER:O	1:A:63:CYS:C	2.60	0.45
1:A:51:MET:HE2	1:A:51:MET:HB3	1.90	0.45
1:B:377:ALA:O	1:B:378:CYS:SG	2.75	0.45
1:A:404:ARG:HH12	1:B:58:GLU:HB3	1.82	0.44
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.53	0.44
1:A:237:LYS:NZ	1:B:237:LYS:HE3	2.33	0.44
1:A:267:MET:SD	1:A:297:SER:HB2	2.57	0.44
1:B:315:ASP:O	1:B:318:ALA:HB3	2.18	0.44
1:A:118:ARG:O	1:A:122:ASN:HB2	2.16	0.44
1:A:251:GLU:H	1:A:251:GLU:CD	2.18	0.44
1:B:268:LEU:HA	1:B:283:GLN:HE22	1.82	0.44
1:B:313:ASP:O	1:B:317:ILE:HG13	2.18	0.44
1:B:236:TRP:CD1	1:B:240:LYS:HD2	2.53	0.44
1:B:366:THR:HG22	1:B:404:ARG:CA	2.46	0.44
1:B:384:ILE:HD12	1:B:397:TYR:CD1	2.52	0.44
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.53	0.44
1:A:378:CYS:O	1:A:399:TRP:HD1	2.01	0.43
1:B:72:MET:HE1	1:B:299:ASP:OD1	2.18	0.43
1:B:290:MET:O	1:B:291:ALA:C	2.60	0.43
1:B:333:GLN:HE21	1:B:333:GLN:HB2	1.55	0.43
1:B:390:VAL:O	1:B:391:LYS:HB2	2.17	0.43
1:A:265:PRO:O	1:A:266:ASP:CB	2.67	0.43
1:A:57:GLN:HA	1:A:57:GLN:HE21	1.81	0.43
1:A:228:ASN:HB3	1:A:245:TRP:CZ3	2.54	0.43
1:A:277:TRP:HA	1:A:280:GLN:NE2	2.32	0.43
1:A:67:LYS:O	1:A:71:GLU:HB2	2.19	0.43
1:A:383:PHE:HD1	1:A:396:PHE:CE1	2.37	0.42
1:B:379:ASN:HA	1:B:380:PRO:HA	1.87	0.42
1:A:123:TYR:O	1:A:126:SER:OG	2.29	0.42
1:A:200:TYR:CE2	1:A:202:CYS:SG	3.12	0.42
1:A:341:GLU:HA	1:A:350:ALA:O	2.19	0.42
1:B:200:TYR:CE2	1:B:202:CYS:SG	3.12	0.42
1:B:220:ARG:NH1	1:B:256:VAL:O	2.53	0.42
1:A:169:PHE:HB3	1:A:184:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:N	1:A:417:LEU:HD12	2.34	0.42
1:A:192:ASN:ND2	2:C:1:NAG:O7	2.53	0.42
1:A:379:ASN:HA	1:A:380:PRO:HA	1.81	0.41
1:B:321:GLN:O	1:B:322:ASP:C	2.61	0.41
1:B:366:THR:HA	1:B:403:LEU:O	2.20	0.41
1:A:333:GLN:HE21	1:A:333:GLN:HB2	1.60	0.41
1:B:237:LYS:HB2	1:B:237:LYS:HE2	1.69	0.41
1:B:166:LEU:HD23	1:B:166:LEU:C	2.46	0.41
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.56	0.41
1:B:48:GLU:HB2	1:B:267:MET:HE3	2.03	0.41
1:B:169:PHE:HB3	1:B:184:TYR:HE1	1.86	0.41
1:B:226:TRP:O	1:B:264:ASP:HB3	2.21	0.41
1:A:117:ILE:O	1:A:118:ARG:C	2.63	0.40
1:A:378:CYS:O	1:A:399:TRP:CD1	2.74	0.40
1:B:204:TRP:HB3	1:B:205:PRO:HD3	2.02	0.40
1:A:133:ILE:HG13	1:A:134:TYR:H	1.86	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)
1:B:210:PRO:CB	2:C:1:NAG:O5[4_545]	2.05	0.15

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	388/398 (98%)	347 (89%)	33 (8%)	8 (2%)	5	25
1	B	388/398 (98%)	342 (88%)	40 (10%)	6 (2%)	8	33
All	All	776/796 (98%)	689 (89%)	73 (9%)	14 (2%)	6	29

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	230	ALA
1	B	266	ASP
1	A	266	ASP
1	A	391	LYS
1	B	212	GLN
1	B	230	ALA
1	B	391	LYS
1	A	122	ASN
1	B	57	GLN
1	B	175	ASP
1	A	57	GLN
1	A	372	LEU
1	A	378	CYS

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	331/339 (98%)	279 (84%)	52 (16%)	2	12
1	B	331/339 (98%)	275 (83%)	56 (17%)	2	10
All	All	662/678 (98%)	554 (84%)	108 (16%)	2	11

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	56	CYS
1	A	57	GLN
1	A	62	SER
1	A	63	CYS
1	A	66	GLU
1	A	67	LYS
1	A	70	MET
1	A	74	GLU

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Mol	Chain	Res	Type
1	A	82	LYS
1	A	87	GLU
1	A	96	MET
1	A	99	GLN
1	A	122	ASN
1	A	127	LYS
1	A	133	ILE
1	A	134	TYR
1	A	148	SER
1	A	169	PHE
1	A	177	LEU
1	A	209	TRP
1	A	220	ARG
1	A	237	LYS
1	A	241	SER
1	A	255	ASP
1	A	267	MET
1	A	281	VAL
1	A	286	LEU
1	A	300	LEU
1	A	306	GLN
1	A	310	LEU
1	A	314	LYS
1	A	319	ILE
1	A	324	LEU
1	A	332	ARG
1	A	333	GLN
1	A	357	GLN
1	A	358	GLU
1	A	363	ARG
1	A	364	SER
1	A	367	ILE
1	A	369	VAL
1	A	372	LEU
1	A	374	LYS
1	A	382	CYS
1	A	385	THR
1	A	387	LEU
1	A	391	LYS
1	A	392	ARG
1	A	398	GLU
1	A	407	ILE

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Mol	Chain	Res	Type
1	A	421	MET
1	B	41	THR
1	B	45	LEU
1	B	56	CYS
1	B	57	GLN
1	B	59	GLU
1	B	62	SER
1	B	63	CYS
1	B	66	GLU
1	B	67	LYS
1	B	70	MET
1	B	74	GLU
1	B	82	LYS
1	B	96	MET
1	B	99	GLN
1	B	122	ASN
1	B	127	LYS
1	B	133	ILE
1	B	134	TYR
1	B	177	LEU
1	B	180	LEU
1	B	203	GLU
1	B	209	TRP
1	B	220	ARG
1	B	237	LYS
1	B	240	LYS
1	B	241	SER
1	B	255	ASP
1	B	256	VAL
1	B	267	MET
1	B	281	VAL
1	B	286	LEU
1	B	300	LEU
1	B	306	GLN
1	B	310	LEU
1	B	314	LYS
1	B	324	LEU
1	B	332	ARG
1	B	333	GLN
1	B	345	SER
1	B	353	MET
1	B	357	GLN

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Mol	Chain	Res	Type
1	B	358	GLU
1	B	363	ARG
1	B	364	SER
1	B	367	ILE
1	B	369	VAL
1	B	372	LEU
1	B	374	LYS
1	B	382	CYS
1	B	385	THR
1	B	387	LEU
1	B	388	LEU
1	B	391	LYS
1	B	392	ARG
1	B	398	GLU
1	B	421	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	53	ASN
1	A	57	GLN
1	A	119	GLN
1	A	125	HIS
1	A	192	ASN
1	A	280	GLN
1	A	330	GLN
1	A	333	GLN
1	A	379	ASN
1	A	386	GLN
1	B	46	HIS
1	B	57	GLN
1	B	115	HIS
1	B	125	HIS
1	B	179	ASN
1	B	186	HIS
1	B	192	ASN
1	B	280	GLN
1	B	327	GLN
1	B	330	GLN
1	B	333	GLN
1	B	336	ASN

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Mol	Chain	Res	Type
1	B	357	GLN
1	B	379	ASN
1	B	386	GLN
1	B	406	HIS
1	B	416	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 ⓘ

4 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	C	1	2	14,14,15	0.67	0	17,19,21	2.01	3 (17%)
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	2.73	6 (35%)
2	NAG	D	1	2	14,14,15	0.66	0	17,19,21	1.24	1 (5%)
2	NAG	D	2	2	14,14,15	0.86	0	17,19,21	2.32	5 (29%)

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	C	1	2	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	8.00	122.91	112.19
2	C	1	NAG	C2-N2-C7	-4.89	116.34	122.90
2	C	1	NAG	O5-C1-C2	-4.77	103.91	111.29
2	D	2	NAG	C1-O5-C5	4.55	118.29	112.19
2	D	2	NAG	O5-C5-C6	-4.13	99.62	107.66
2	C	2	NAG	O7-C7-N2	3.84	128.77	121.98
2	D	2	NAG	C2-N2-C7	-3.72	117.92	122.90
2	C	2	NAG	C2-N2-C7	3.60	127.73	122.90
2	D	2	NAG	O5-C1-C2	-3.55	105.80	111.29
2	C	2	NAG	O5-C1-C2	3.54	116.77	111.29
2	D	1	NAG	C2-N2-C7	3.34	127.38	122.90
2	D	2	NAG	C3-C4-C5	3.18	116.01	110.23
2	C	1	NAG	O5-C5-C6	3.15	113.79	107.66
2	C	2	NAG	C8-C7-N2	-2.64	111.75	116.12
2	C	2	NAG	O5-C5-C4	2.20	116.18	110.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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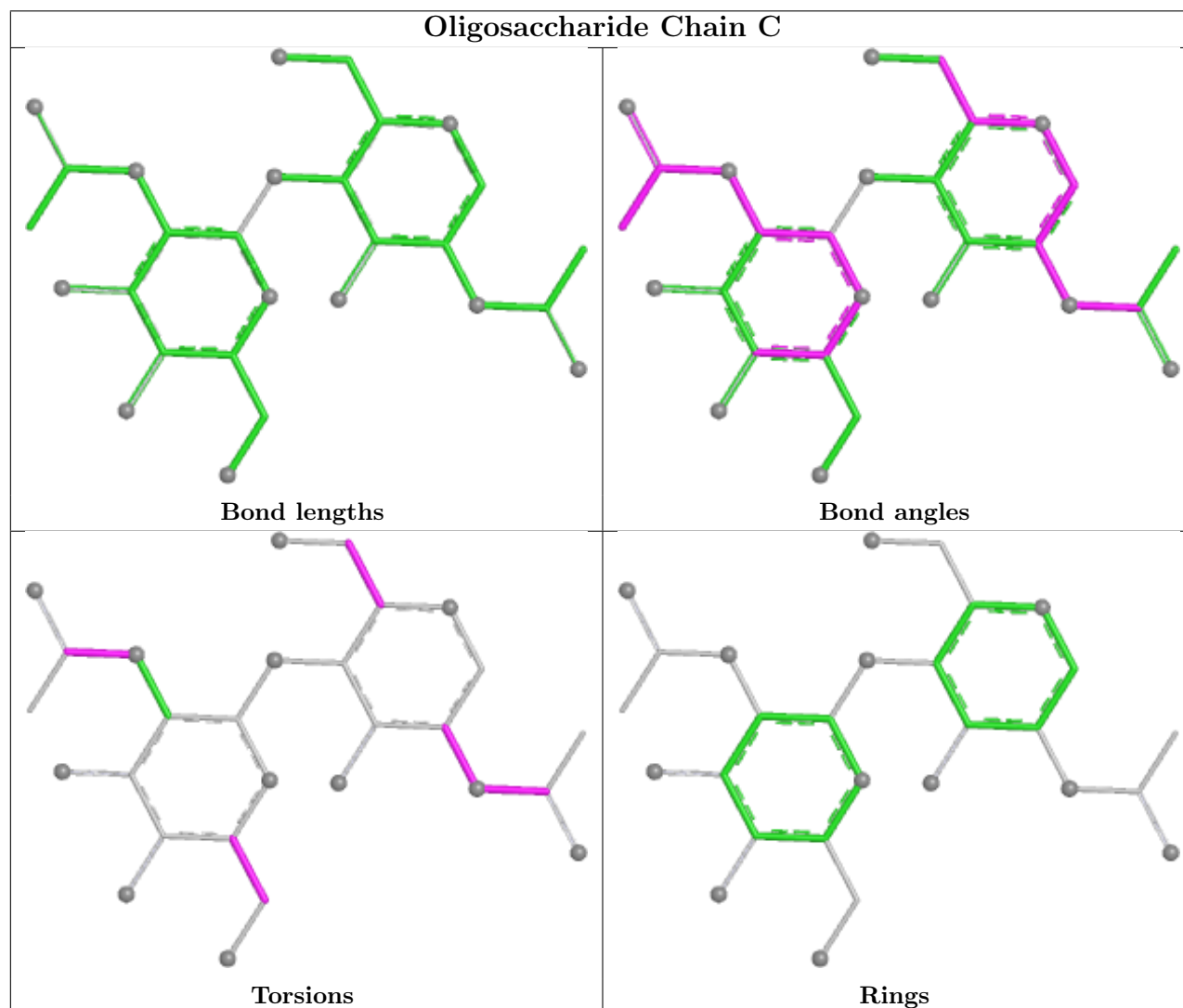
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C1-C2-N2-C7

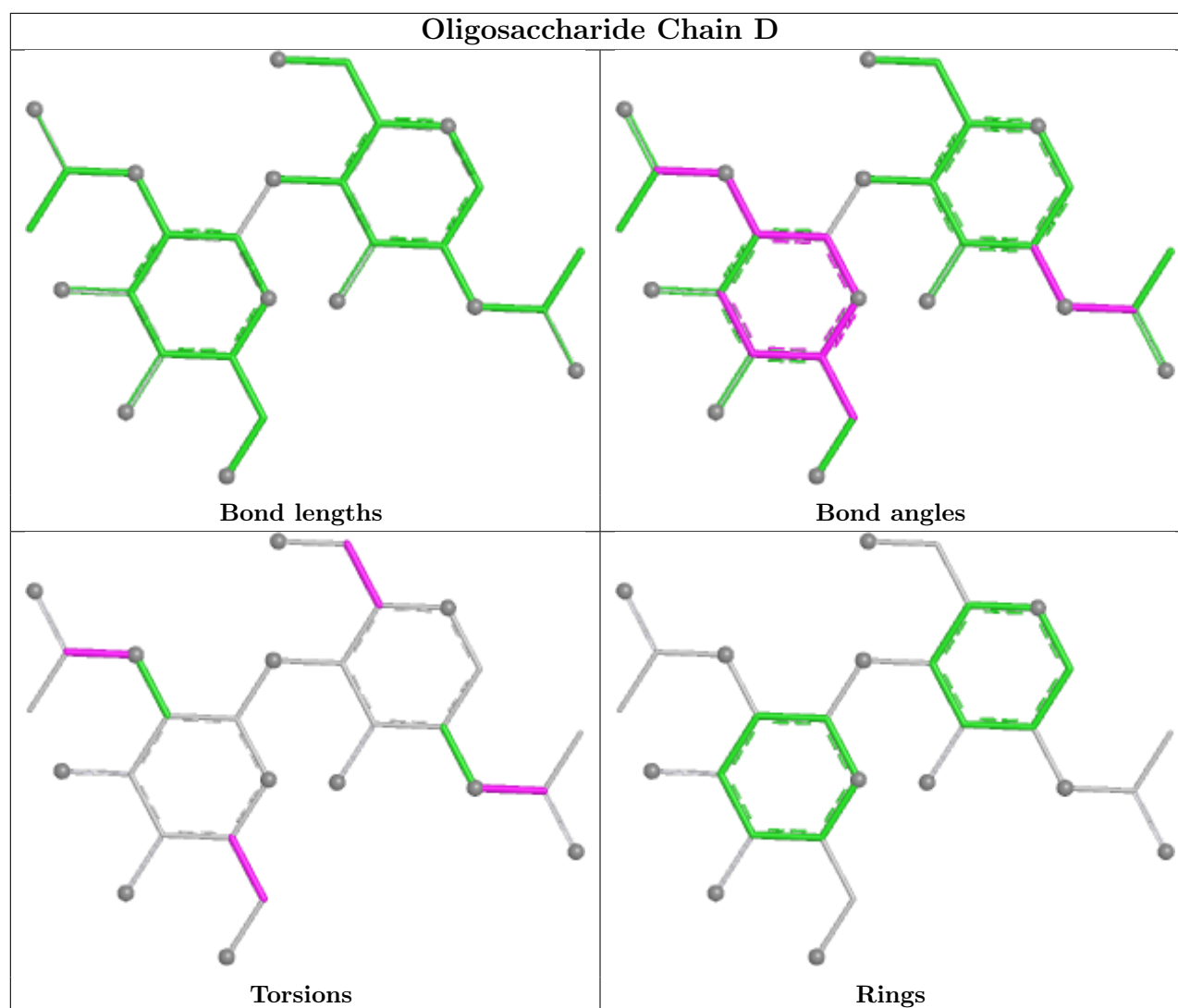
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	0
2	C	1	NAG	3	1

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](#)

1 ligand is 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	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.22	0	6,6,6	0.81	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	390/398 (97%)	-0.19	4 (1%)	79 59	117, 121, 123, 128	0
1	B	390/398 (97%)	-0.12	4 (1%)	79 59	117, 121, 123, 128	0
All	All	780/796 (97%)	-0.16	8 (1%)	79 59	117, 121, 123, 128	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	GLU	3.1
1	A	327	GLN	2.7
1	B	182	ASP	2.4
1	B	104	GLY	2.4
1	A	406	HIS	2.3
1	A	167	LEU	2.3
1	B	129	LEU	2.2
1	B	370	ALA	2.2

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.

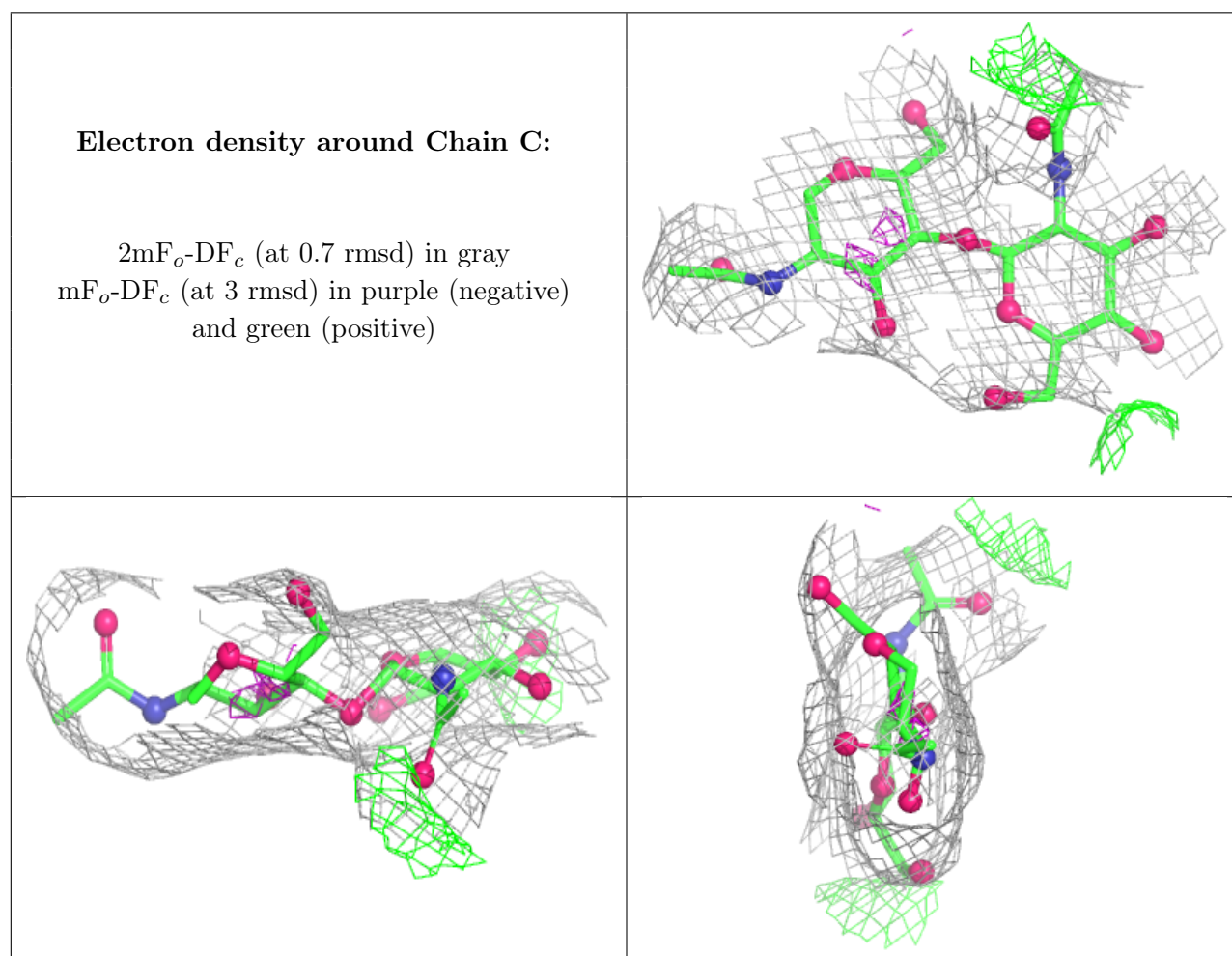
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.56	0.13	141,143,144,144	0

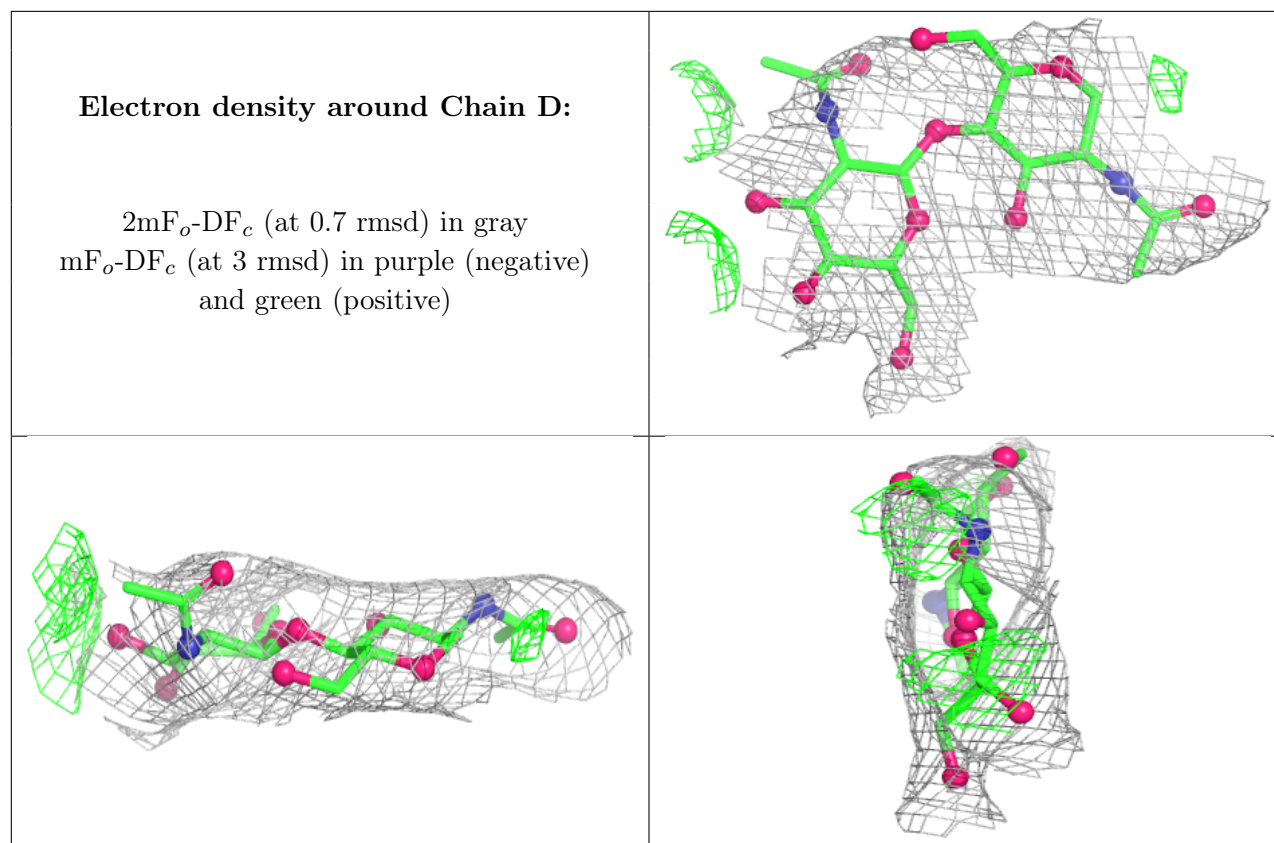
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.65	0.12	136,138,140,141	0
2	NAG	D	1	14/15	0.88	0.09	142,144,147,150	0
2	NAG	C	1	14/15	0.90	0.07	126,130,134,136	0

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
3	SO4	A	1	5/5	0.87	0.10	125,126,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.