Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:27 PM JST

PDB ID	:	6J0T
Title	:	The crystal structure of exoinulinase INU1
Authors	:	Hu, X.-J.
Deposited on	:	2018-12-26
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:

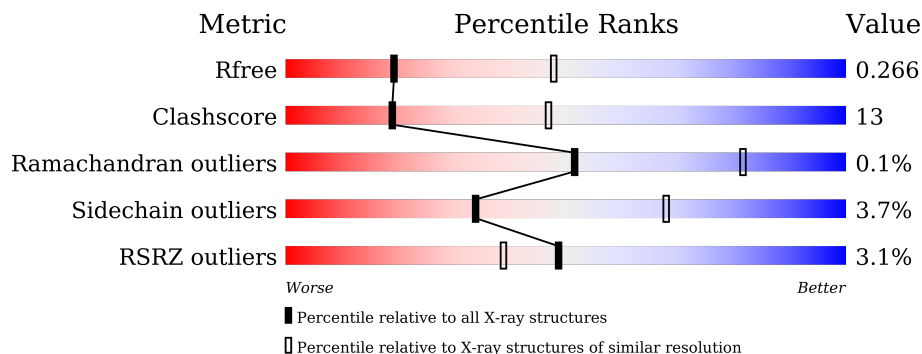|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.266
Clashscore		13
Ramachandran outliers		0.1%
Sidechain outliers		3.7%
RSRZ outliers		3.1%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	556	2% / 65% / 25% / · / 9%
1	B	556	4% / 67% / 24% / · / 8%
2	C	2	50% / 50%
2	D	2	100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8243 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 Inulinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total 4066	C 2608	N 664	O 788	S 6	0	0	0
1	B	512	Total 4100	C 2626	N 669	O 799	S 6	0	0	0

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

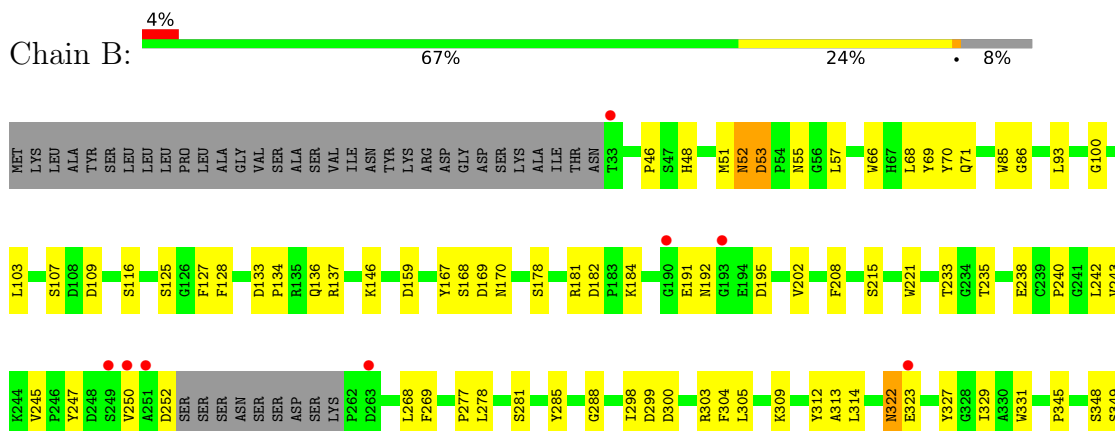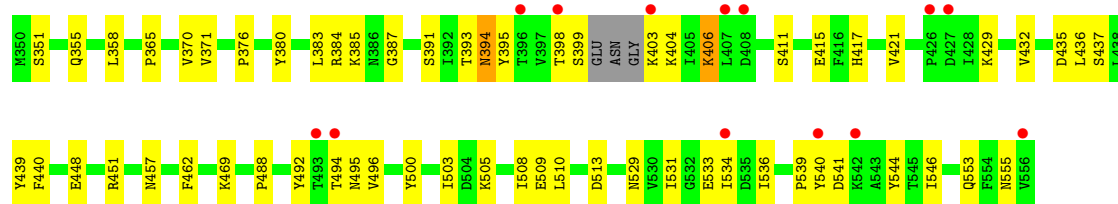| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	7	Total 7	O 7	0	0

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: Inulinase
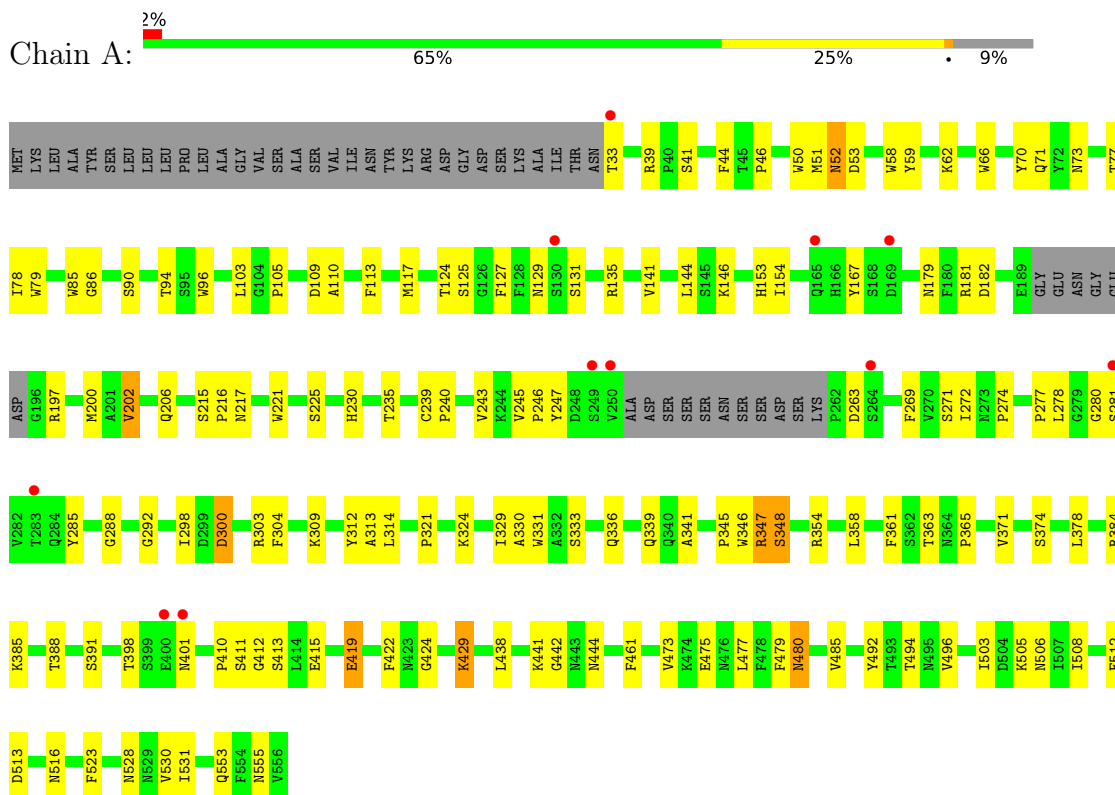
Chain A:

• Molecule 1: Inulinase

Chain B:

M350 S351 Q355 L358 P365 V370 V371 P376 Y380 L383 R384 K385 N386 G387 S391 I392 T393 N394 Y395 T396 V397 T398 S399 GLU ASN GLY K403 K404 I405 K406 L407 D408 S411 E415 F416 H417 V421 P426 D427 I428 K429 V432 D435 L436 S437 L438

Y439 F440 E448 R451 N457 F462 K469 P488 Y492 T493 T494 N495 V496 Y500 I503 D504 K505 I508 E509 L510 D513 N529 V530 I531 G532 E533 I534 D535 I536 P539 Y540 D541 K542 A543 Y544 T545 I546 Q553 F554 N555 V556

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

Chain C:

50%   50%

NAG1 NAG2

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

Chain D:

100%

NAG1 NAG2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	172.65Å 172.65Å 172.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 2.80 49.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.84-2.80) 99.9 (49.84-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.198 , 0.272 0.202 , 0.266	Depositor DCC
R_{free} test set	1714 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å^2)	54.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h 0.018 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8243	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.60	0/4198	0.67	1/5734 (0.0%)
1	B	0.57	0/4232	0.69	1/5780 (0.0%)
All	All	0.58	0/8430	0.68	2/11514 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	533	GLU	CB-CA-C	-6.91	96.57	110.40
1	A	441	LYS	C-N-CA	-5.17	111.44	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	GLY	Peptide

5.2 Too-close contacts (i)

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	4066	0	3754	101	0
1	B	4100	0	3777	109	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	B	1	0	0	0	0
4	A	13	0	0	0	0
4	B	7	0	0	0	0
All	All	8243	0	7581	205	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 13.

All (205) 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:52:ASN:ND2	1:A:71:GLN:HB2	1.18	1.50
1:B:398:THR:HA	1:B:541:ASP:OD2	1.42	1.19
1:A:52:ASN:HD21	1:A:71:GLN:CB	1.53	1.19
1:A:52:ASN:ND2	1:A:71:GLN:CB	2.09	1.12
1:B:398:THR:CA	1:B:541:ASP:OD2	1.96	1.12
1:B:51:MET:O	1:B:348:SER:OG	1.67	1.12
1:B:399:SER:N	1:B:541:ASP:OD2	1.84	1.09
1:B:403:LYS:C	1:B:404:LYS:HD3	1.75	1.04
1:B:52:ASN:HB3	1:B:71:GLN:HB2	1.05	1.04
1:A:331:TRP:HE1	1:A:348:SER:CB	1.70	1.03
1:B:52:ASN:CB	1:B:71:GLN:HB2	1.90	1.01
1:B:52:ASN:HB3	1:B:71:GLN:CB	1.96	0.93
1:B:278:LEU:HB3	1:B:309:LYS:HE2	1.46	0.93
1:A:52:ASN:HD22	1:A:71:GLN:HB2	1.19	0.91
1:B:331:TRP:HE1	1:B:348:SER:CB	1.85	0.89
1:A:331:TRP:HE1	1:A:348:SER:HB3	1.42	0.82
1:A:41:SER:OG	1:A:505:LYS:NZ	2.12	0.82
1:B:440:PHE:HB3	1:B:531:ILE:HD13	1.59	0.82
1:B:331:TRP:HE1	1:B:348:SER:HB2	1.46	0.79
1:B:278:LEU:HB3	1:B:309:LYS:CE	2.12	0.78
1:B:398:THR:C	1:B:541:ASP:OD2	2.20	0.78
1:A:331:TRP:HE1	1:A:348:SER:HB2	1.48	0.78
1:B:51:MET:HG3	1:B:70:TYR:CD2	2.18	0.78
1:B:358:LEU:HD11	1:B:370:VAL:HG22	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASP:HB3	1:B:136:GLN:HG3	1.65	0.76
1:A:341:ALA:O	1:A:347:ARG:NH2	2.18	0.76
1:B:278:LEU:CB	1:B:309:LYS:HE2	2.15	0.75
1:A:419:GLU:OE1	1:A:496:VAL:HG11	1.88	0.74
1:A:52:ASN:HD21	1:A:71:GLN:HB2	0.91	0.73
1:A:124:THR:HG21	1:A:216:PRO:O	1.88	0.72
1:B:404:LYS:HD3	1:B:404:LYS:N	2.04	0.71
1:B:281:SER:HB2	1:B:312:TYR:CD1	2.27	0.69
1:A:288:GLY:HA2	1:A:298:ILE:HG23	1.74	0.68
1:B:134:PRO:HA	1:B:137:ARG:HD2	1.75	0.68
1:B:327:TYR:CE1	1:B:355:GLN:HG3	2.31	0.66
1:B:288:GLY:HA2	1:B:298:ILE:HG23	1.78	0.66
1:A:277:PRO:HG3	1:A:304:PHE:HE2	1.61	0.65
1:A:52:ASN:HD21	1:A:71:GLN:CG	2.10	0.65
1:B:432:VAL:O	1:B:457:ASN:ND2	2.29	0.65
1:A:361:PHE:HB3	1:A:371:VAL:HG12	1.79	0.64
1:B:57:LEU:HD11	1:B:329:ILE:HG22	1.78	0.64
1:A:271:SER:HB3	1:A:312:TYR:CE1	2.33	0.64
1:A:419:GLU:OE1	1:A:496:VAL:CG1	2.46	0.64
1:A:94:THR:HG23	1:A:378:LEU:HD22	1.80	0.64
1:B:398:THR:HA	1:B:541:ASP:CG	2.18	0.64
1:A:398:THR:HG23	1:A:401:ASN:H	1.62	0.63
1:A:331:TRP:NE1	1:A:348:SER:HB2	2.13	0.63
1:B:181:ARG:NH2	1:B:238:GLU:OE2	2.31	0.62
1:A:66:TRP:CH2	1:A:321:PRO:HD3	2.35	0.62
1:A:281:SER:HB2	1:A:312:TYR:CD1	2.36	0.60
1:A:485:VAL:HG11	1:A:512:PHE:CZ	2.36	0.60
1:B:398:THR:OG1	1:B:541:ASP:OD2	2.19	0.60
1:B:439:TYR:CE2	1:B:451:ARG:HD2	2.37	0.60
1:B:331:TRP:NE1	1:B:348:SER:HB2	2.15	0.60
1:B:380:TYR:HB3	1:B:384:ARG:HE	1.67	0.59
1:B:191:GLU:CD	1:B:192:ASN:H	2.05	0.59
1:A:277:PRO:HG3	1:A:304:PHE:CE2	2.39	0.58
1:A:197:ARG:NH2	1:A:292:GLY:O	2.36	0.58
1:B:376:PRO:HG3	1:B:500:TYR:HE2	1.67	0.58
1:B:278:LEU:O	1:B:309:LYS:NZ	2.30	0.58
1:B:327:TYR:HE1	1:B:355:GLN:HG3	1.68	0.57
1:B:399:SER:H	1:B:541:ASP:CG	2.05	0.57
1:B:384:ARG:NH2	1:B:415:GLU:OE1	2.39	0.56
1:A:513:ASP:OD2	1:A:516:ASN:ND2	2.36	0.56
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:SER:HB2	1:B:221:TRP:CE3	2.40	0.56
1:A:243:VAL:HG13	1:A:245:VAL:HG23	1.88	0.56
1:B:509:GLU:O	1:B:510:LEU:HD23	2.05	0.55
1:B:57:LEU:HD23	1:B:68:LEU:HA	1.88	0.55
1:B:322:ASN:OD1	1:B:322:ASN:N	2.39	0.55
1:A:129:ASN:OD1	1:A:131:SER:OG	2.22	0.55
1:B:398:THR:CB	1:B:541:ASP:OD2	2.54	0.55
1:B:403:LYS:C	1:B:404:LYS:CD	2.64	0.55
1:B:53:ASP:OD1	1:B:53:ASP:N	2.32	0.54
1:B:358:LEU:CD1	1:B:370:VAL:HG22	2.36	0.54
1:B:387:GLY:HA2	1:B:555:ASN:OD1	2.07	0.54
1:B:125:SER:HB2	1:B:127:PHE:CD2	2.42	0.54
1:B:46:PRO:HG3	1:B:51:MET:HB2	1.89	0.54
1:B:508:ILE:HD11	1:B:510:LEU:HD21	1.89	0.53
1:A:331:TRP:NE1	1:A:348:SER:CB	2.54	0.53
1:A:503:ILE:HG21	1:A:531:ILE:HD12	1.91	0.53
1:A:46:PRO:HG2	1:A:346:TRP:HB2	1.91	0.52
1:B:358:LEU:HD12	1:B:371:VAL:O	2.10	0.52
1:A:85:TRP:HB2	1:A:103:LEU:HB3	1.91	0.52
1:B:128:PHE:CG	1:B:137:ARG:HG2	2.45	0.52
1:B:539:PRO:HG2	1:B:540:TYR:HD1	1.74	0.52
1:B:404:LYS:N	1:B:404:LYS:CD	2.73	0.51
1:A:44:PHE:HB2	1:A:96:TRP:CD1	2.45	0.51
1:A:422:PHE:CZ	1:A:424:GLY:HA2	2.46	0.51
1:B:376:PRO:HG3	1:B:500:TYR:CE2	2.45	0.50
1:A:53:ASP:OD1	1:A:313:ALA:CB	2.59	0.50
1:B:51:MET:HE2	1:B:348:SER:O	2.11	0.50
1:B:448:GLU:OE1	1:B:529:ASN:ND2	2.40	0.50
1:B:86:GLY:HA2	1:B:100:GLY:O	2.11	0.50
1:B:435:ASP:OD2	1:B:437:SER:OG	2.24	0.50
1:B:52:ASN:CB	1:B:71:GLN:CB	2.72	0.50
1:B:403:LYS:O	1:B:404:LYS:HD3	2.11	0.50
1:B:242:LEU:HD12	1:B:243:VAL:H	1.77	0.50
1:B:85:TRP:HB2	1:B:103:LEU:HB3	1.94	0.50
1:A:50:TRP:NE1	1:A:52:ASN:HB3	2.27	0.49
1:A:215:SER:HB2	1:A:221:TRP:CD2	2.47	0.49
1:B:494:THR:HB	1:B:496:VAL:HG23	1.95	0.49
1:B:365:PRO:HB3	1:B:492:TYR:CG	2.47	0.49
1:A:444:ASN:ND2	1:A:528:ASN:O	2.45	0.49
1:B:250:VAL:HG12	1:B:250:VAL:O	2.12	0.49
1:A:53:ASP:HB2	1:A:71:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:SER:O	1:A:505:LYS:HE3	2.11	0.49
1:B:539:PRO:HG2	1:B:540:TYR:CD1	2.48	0.49
1:A:477:LEU:HD12	1:A:477:LEU:N	2.29	0.48
1:B:116:SER:OG	1:B:184:LYS:HA	2.14	0.48
1:A:365:PRO:HD3	1:A:492:TYR:CE1	2.49	0.48
1:A:503:ILE:HG12	1:A:508:ILE:HG13	1.96	0.48
1:A:300:ASP:HB3	1:B:300:ASP:HB2	1.95	0.47
1:A:278:LEU:HD23	1:B:278:LEU:HD23	1.95	0.47
1:A:46:PRO:HG3	1:A:51:MET:HB2	1.96	0.47
1:A:59:TYR:CZ	1:A:321:PRO:HG3	2.49	0.47
1:A:235:THR:HB	1:A:274:PRO:HD2	1.97	0.47
1:B:53:ASP:HB3	1:B:313:ALA:HB1	1.96	0.47
1:B:421:VAL:HG23	1:B:495:ASN:O	2.15	0.47
1:B:436:LEU:HB2	1:B:544:TYR:CD2	2.48	0.47
1:A:141:VAL:HG22	1:A:154:ILE:HG22	1.95	0.47
1:A:412:GLY:CA	1:A:530:VAL:HG13	2.44	0.47
1:B:411:SER:O	1:B:505:LYS:HE3	2.15	0.47
1:A:230:HIS:HA	1:B:300:ASP:OD1	2.15	0.47
1:B:395:TYR:OH	1:B:403:LYS:HG2	2.15	0.46
1:A:39:ARG:HB2	1:A:346:TRP:CH2	2.50	0.46
1:A:246:PRO:HB3	1:A:324:LYS:HE3	1.98	0.46
1:A:473:VAL:HG13	1:A:479:PHE:CD2	2.50	0.46
1:A:124:THR:HG22	1:A:217:ASN:HA	1.97	0.46
1:B:48:HIS:HB2	1:B:345:PRO:HB2	1.98	0.46
1:B:85:TRP:CD2	1:B:103:LEU:HD23	2.51	0.46
1:A:62:LYS:HB2	1:A:135:ARG:CZ	2.46	0.46
1:B:159:ASP:N	1:B:159:ASP:OD1	2.49	0.46
1:B:331:TRP:NE1	1:B:348:SER:CB	2.67	0.46
1:A:365:PRO:HB3	1:A:492:TYR:CD2	2.50	0.46
1:B:277:PRO:HG3	1:B:304:PHE:HE2	1.81	0.46
1:B:277:PRO:HG3	1:B:304:PHE:CE2	2.51	0.45
1:A:105:PRO:HB2	1:A:110:ALA:HB3	1.98	0.45
1:A:79:TRP:HZ2	1:A:113:PHE:CZ	2.34	0.45
1:A:363:THR:OG1	1:B:235:THR:HA	2.16	0.45
1:B:406:LYS:HE2	1:B:406:LYS:HB3	1.76	0.45
1:B:536:ILE:HD13	1:B:546:ILE:CD1	2.47	0.45
1:B:503:ILE:HG12	1:B:508:ILE:HG13	1.98	0.45
1:A:354:ARG:HD3	1:A:374:SER:HB3	1.99	0.45
1:A:477:LEU:HD22	1:B:462:PHE:CE1	2.52	0.45
1:A:58:TRP:CD1	1:A:117:MET:HG2	2.51	0.44
1:A:200:MET:SD	1:A:202:VAL:HG22	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:CE2	1:A:303:ARG:HD3	2.52	0.44
1:A:245:VAL:HG12	1:A:246:PRO:O	2.17	0.44
1:B:109:ASP:OD2	1:B:146:LYS:NZ	2.51	0.44
1:A:475:GLU:O	1:A:477:LEU:CD1	2.66	0.44
1:A:506:ASN:O	1:A:523:PHE:N	2.46	0.44
1:B:448:GLU:OE2	1:B:469:LYS:HB2	2.17	0.44
1:A:182:ASP:HB3	1:A:239:CYS:HA	2.01	0.43
1:A:33:THR:HG22	1:A:33:THR:O	2.18	0.43
1:A:246:PRO:HB3	1:A:324:LYS:CE	2.48	0.43
1:A:78:ILE:HG22	1:A:339:GLN:HB3	1.99	0.43
1:A:77:THR:CG2	1:A:345:PRO:O	2.66	0.43
1:A:475:GLU:O	1:A:477:LEU:HD12	2.19	0.43
1:B:439:TYR:O	1:B:534:ILE:HA	2.18	0.43
1:A:413:SER:HA	1:A:503:ILE:O	2.19	0.43
1:B:393:THR:HG22	1:B:394:ASN:N	2.33	0.43
1:A:51:MET:HG3	1:A:70:TYR:CD2	2.53	0.43
1:A:215:SER:HB2	1:A:221:TRP:CE3	2.54	0.43
1:A:181:ARG:HG3	1:A:182:ASP:CG	2.39	0.43
1:B:243:VAL:HG13	1:B:245:VAL:HG23	2.01	0.43
1:B:553:GLN:HE21	1:B:555:ASN:ND2	2.17	0.42
1:A:179:ASN:ND2	1:A:206:GLN:HG3	2.34	0.42
1:B:240:PRO:HA	1:B:269:PHE:O	2.20	0.42
1:A:50:TRP:HB3	1:A:73:ASN:HB3	2.00	0.42
1:A:144:LEU:HB2	1:A:153:HIS:CD2	2.54	0.42
1:A:461:PHE:HB3	1:A:485:VAL:HG13	2.01	0.42
1:A:384:ARG:NH2	1:A:415:GLU:OE1	2.53	0.42
1:B:305:LEU:CD2	1:B:314:LEU:HD13	2.49	0.42
1:A:70:TYR:CZ	1:A:86:GLY:HA3	2.54	0.42
1:A:429:LYS:HE3	1:A:429:LYS:HB3	1.79	0.42
1:B:329:ILE:HD11	1:B:351:SER:O	2.20	0.42
1:B:358:LEU:HD21	1:B:370:VAL:HG21	2.02	0.42
1:A:125:SER:HB2	1:A:127:PHE:CE2	2.55	0.41
1:B:299:ASP:OD1	1:B:303:ARG:NH1	2.52	0.41
1:A:109:ASP:HB3	1:A:146:LYS:NZ	2.34	0.41
1:A:438:LEU:HD12	1:A:438:LEU:N	2.35	0.41
1:B:208:PHE:CD1	1:B:233:THR:HB	2.56	0.41
1:A:53:ASP:O	1:A:70:TYR:HA	2.19	0.41
1:A:329:ILE:HG12	1:A:330:ALA:H	1.85	0.41
1:A:410:PRO:HA	1:A:553:GLN:OE1	2.20	0.41
1:B:55:ASN:N	1:B:69:TYR:O	2.41	0.41
1:A:272:ILE:O	1:A:281:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASN:HD22	1:B:52:ASN:HA	1.59	0.41
1:B:268:LEU:O	1:B:285:TYR:HA	2.21	0.41
1:A:240:PRO:HA	1:A:269:PHE:O	2.21	0.40
1:B:167:TYR:CE2	1:B:168:SER:HB3	2.55	0.40
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.93	0.40
1:B:398:THR:OG1	1:B:541:ASP:HB3	2.20	0.40
1:B:488:PRO:HG2	1:B:513:ASP:HB2	2.03	0.40
1:A:358:LEU:HD12	1:A:358:LEU:HA	1.90	0.40
1:B:66:TRP:CD2	1:B:93:LEU:HD21	2.56	0.40
1:B:182:ASP:O	1:B:240:PRO:HD2	2.21	0.40
1:A:309:LYS:HD2	1:A:480:ASN:OD1	2.21	0.40
1:A:331:TRP:CZ2	1:A:333:SER:HB3	2.57	0.40
1:A:388:THR:HG23	1:A:555:ASN:HD21	1.86	0.40
1:A:494:THR:HB	1:A:496:VAL:HG23	2.02	0.40
1:B:365:PRO:HD3	1:B:492:TYR:CE1	2.57	0.40
1:B:553:GLN:HE21	1:B:555:ASN:HD21	1.69	0.40
1:A:280:GLY:HA3	1:A:336:GLN:HG3	2.02	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	501/556 (90%)	468 (93%)	33 (7%)	0	100	100
1	B	506/556 (91%)	469 (93%)	36 (7%)	1 (0%)	47	78
All	All	1007/1112 (91%)	937 (93%)	69 (7%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	GLU

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	445/485 (92%)	430 (97%)	15 (3%)	37	71
1	B	448/485 (92%)	430 (96%)	18 (4%)	31	65
All	All	893/970 (92%)	860 (96%)	33 (4%)	34	68

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	167	TYR
1	A	202	VAL
1	A	225	SER
1	A	247	TYR
1	A	263	ASP
1	A	300	ASP
1	A	314	LEU
1	A	347	ARG
1	A	348	SER
1	A	385	LYS
1	A	391	SER
1	A	419	GLU
1	A	429	LYS
1	A	480	ASN
1	B	52	ASN
1	B	53	ASP
1	B	107	SER
1	B	169	ASP
1	B	170	ASN
1	B	178	SER
1	B	195	ASP
1	B	202	VAL
1	B	247	TYR
1	B	252	ASP
1	B	322	ASN
1	B	349	SER

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Mol	Chain	Res	Type
1	B	385	LYS
1	B	391	SER
1	B	394	ASN
1	B	406	LYS
1	B	417	HIS
1	B	429	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	B	52	ASN
1	B	394	ASN
1	B	555	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 ⓘ

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	2,1	14,14,15	0.50	0	17,19,21	0.63	0
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	0.99	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.86	1 (7%)	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	D	2	2	14,14,15	0.55	0	17,19,21	0.91	1 (5%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	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)
2	D	1	NAG	O5-C1	-2.70	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	3.40	116.80	112.19
2	D	2	NAG	C1-O5-C5	2.59	115.69	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
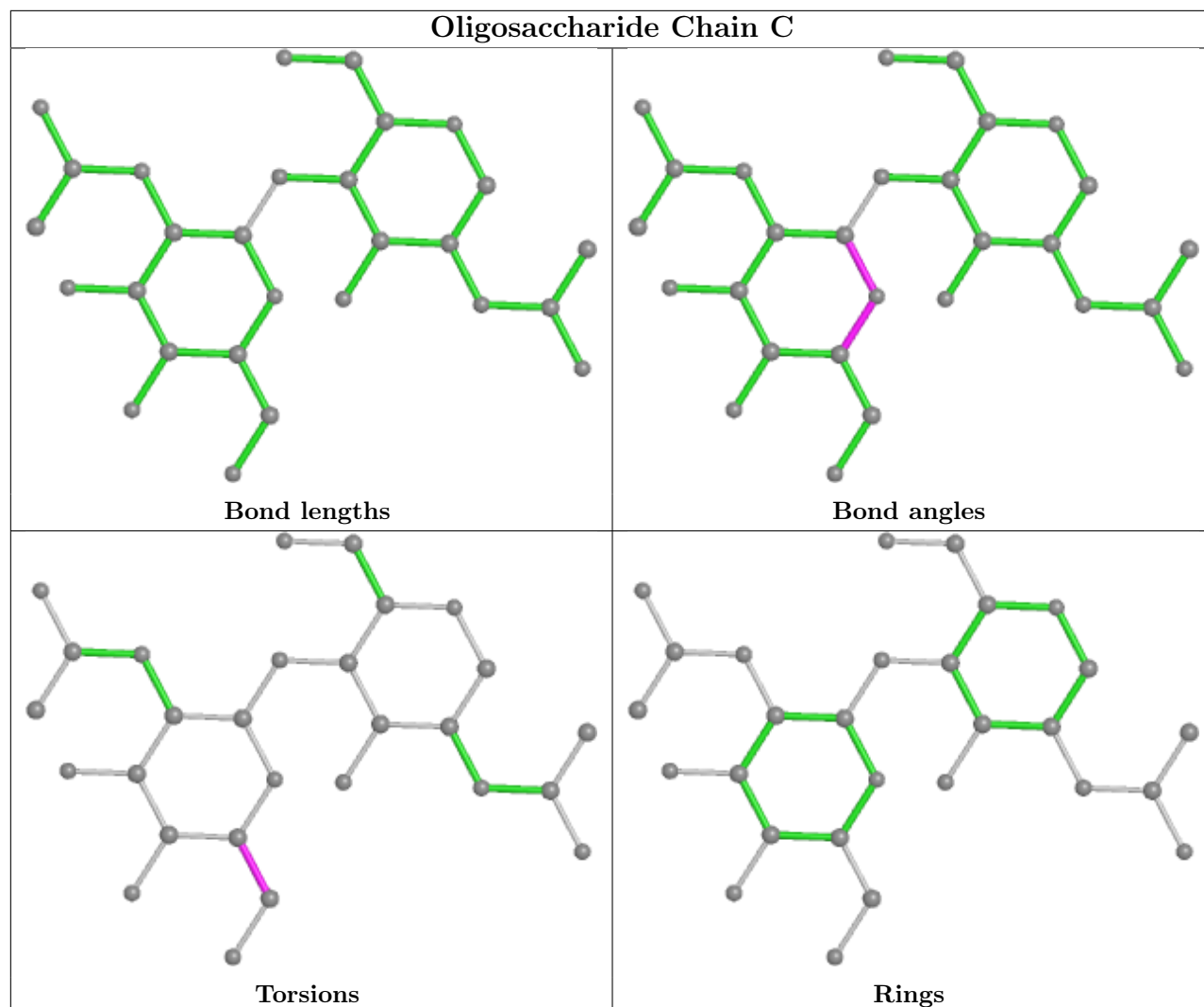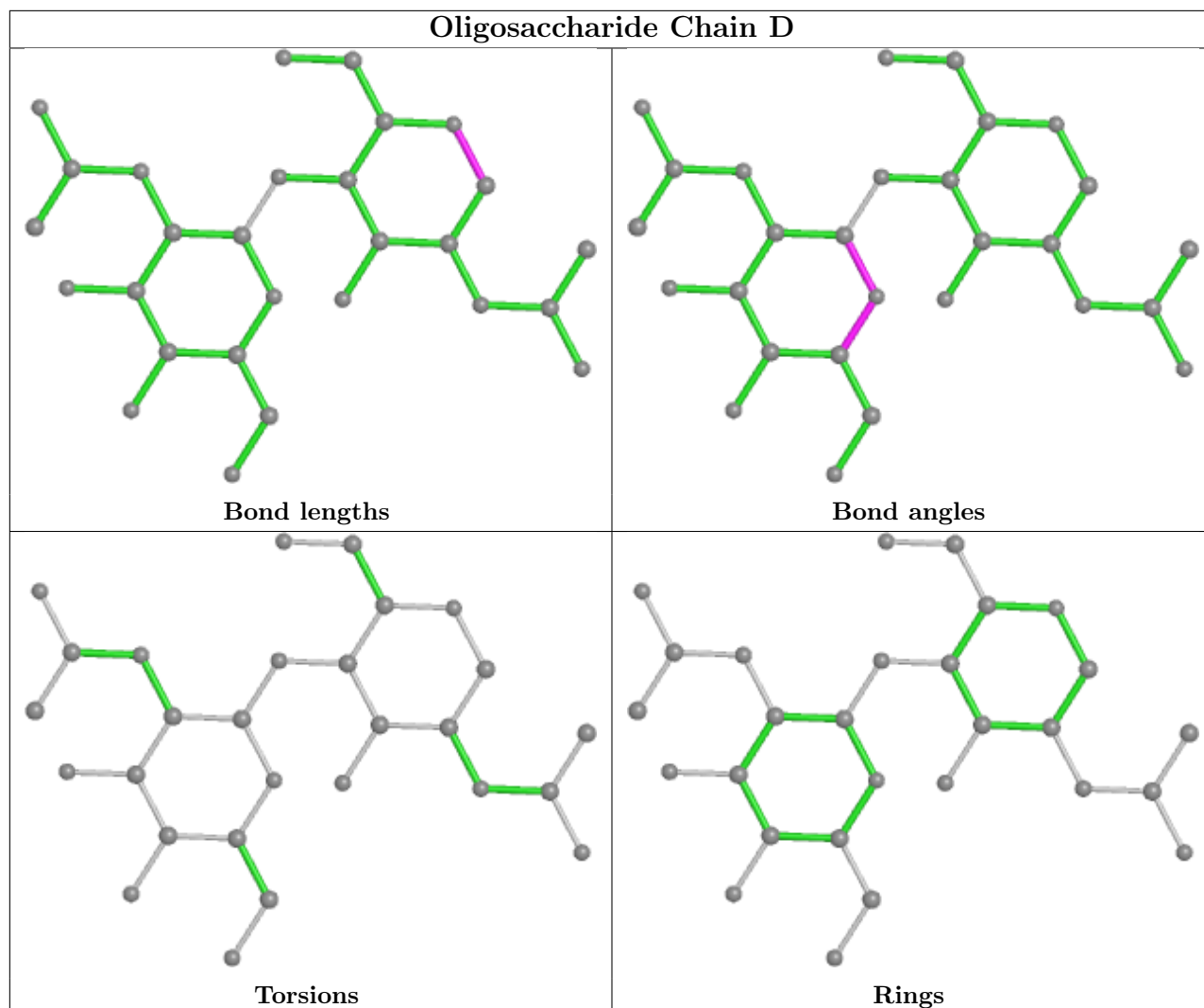
5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	507/556 (91%)	0.11	11 (2%)	62	52	34, 46, 64, 84	0
1	B	512/556 (92%)	0.09	21 (4%)	37	27	35, 50, 75, 102	0
All	All	1019/1112 (91%)	0.10	32 (3%)	49	39	34, 48, 70, 102	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	ALA	6.0
1	B	250	VAL	6.0
1	A	130	SER	4.5
1	B	33	THR	4.5
1	A	401	ASN	4.3
1	B	407	LEU	3.8
1	A	169	ASP	3.8
1	A	33	THR	3.6
1	B	403	LYS	3.3
1	A	264	SER	2.8
1	A	400	GLU	2.8
1	B	556	VAL	2.7
1	B	426	PRO	2.6
1	B	323	GLU	2.5
1	B	494	THR	2.5
1	B	408	ASP	2.4
1	B	427	ASP	2.4
1	B	190	GLY	2.4
1	B	493	THR	2.3
1	B	263	ASP	2.3
1	B	542	LYS	2.3
1	A	250	VAL	2.3
1	A	249	SER	2.2
1	A	281	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	540	TYR	2.2
1	B	193	GLY	2.1
1	B	249	SER	2.1
1	A	165	GLN	2.1
1	B	534	ILE	2.0
1	A	283	THR	2.0
1	B	396	THR	2.0
1	B	398	THR	2.0

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

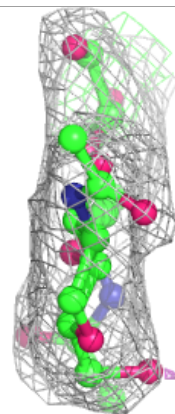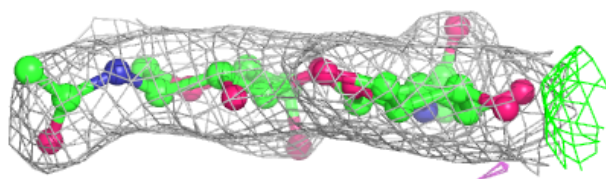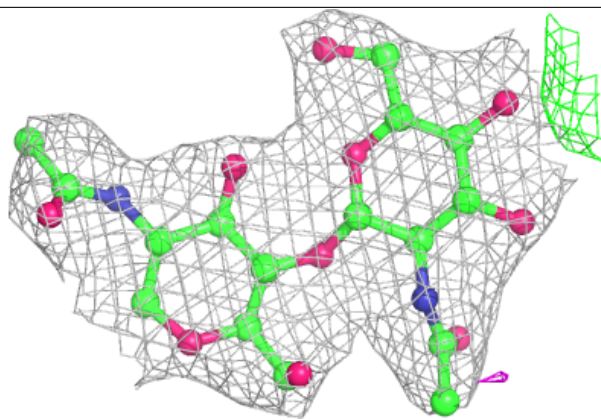There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	0.88	0.16	31,43,48,50	0
2	NAG	C	2	14/15	0.92	0.20	42,47,55,57	0
2	NAG	D	1	14/15	0.96	0.20	40,48,51,55	0
2	NAG	C	1	14/15	0.98	0.17	44,47,55,59	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.

Electron density around Chain C:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
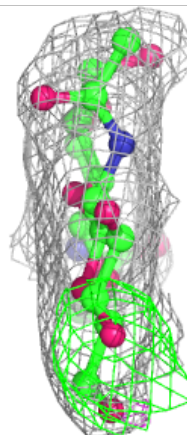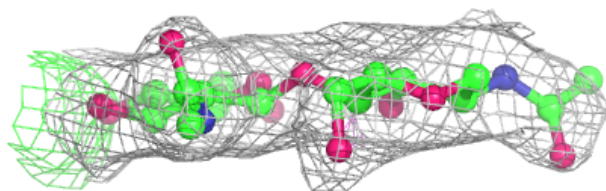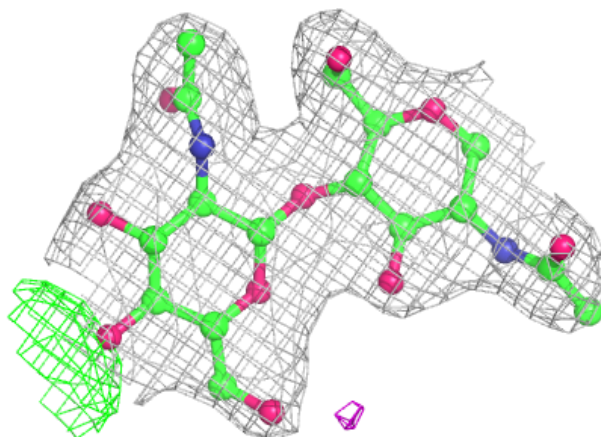
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	MG	B	603	1/1	0.83	0.52	50,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.