



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 AM UTC

PDB ID : 6J0T / pdb_00006j0t
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

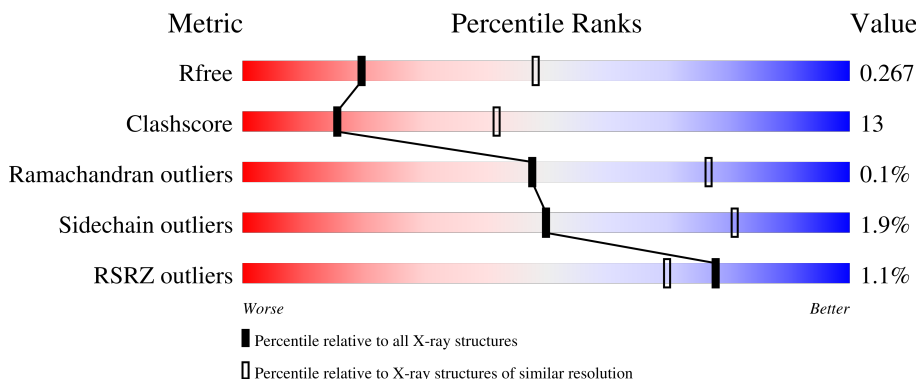
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	556	65% 25% • 9%
1	B	556	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	C	N	O	S	0	0	0
			4066	2608	664	788	6			
1	B	512	Total	C	N	O	S	0	0	0
			4100	2626	669	799	6			

- 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

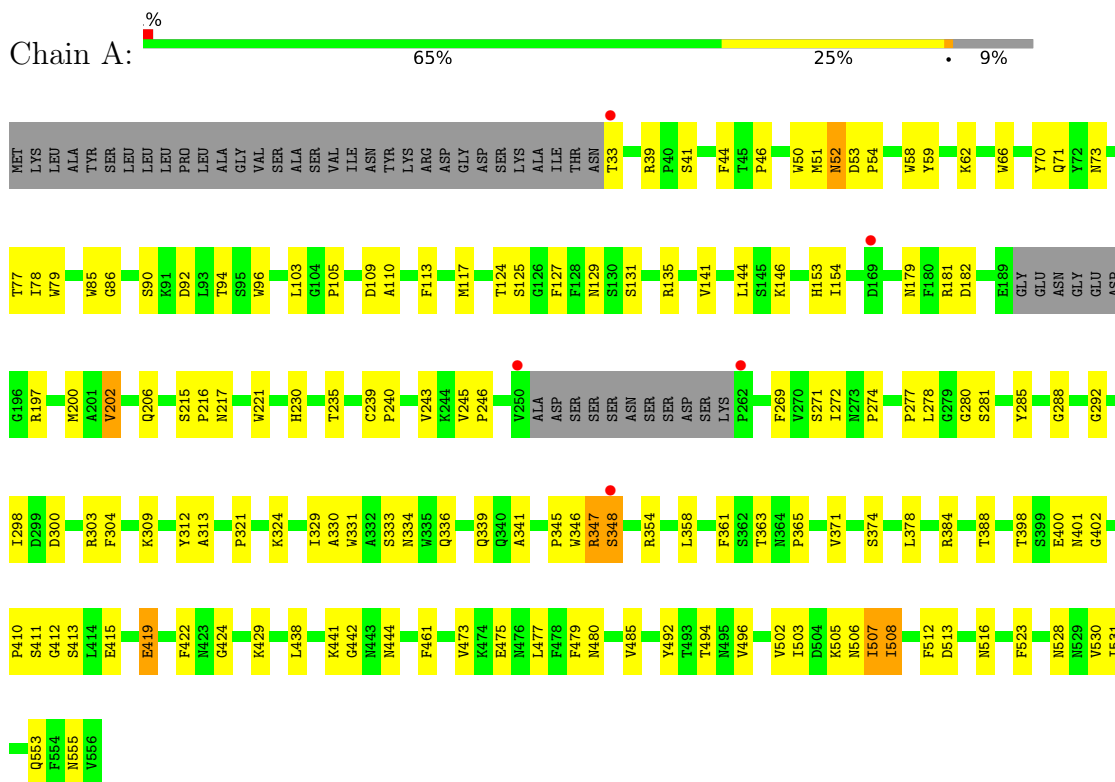
- Molecule 4 is water.

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

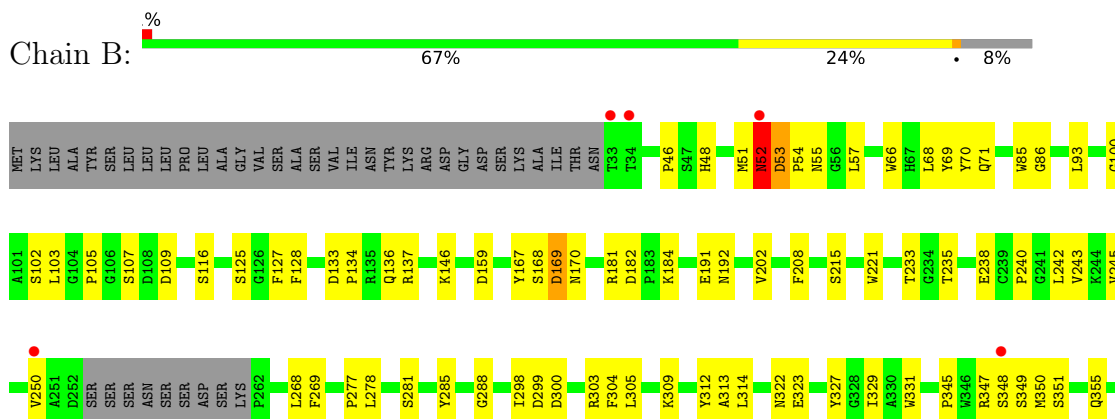
3 Residue-property plots

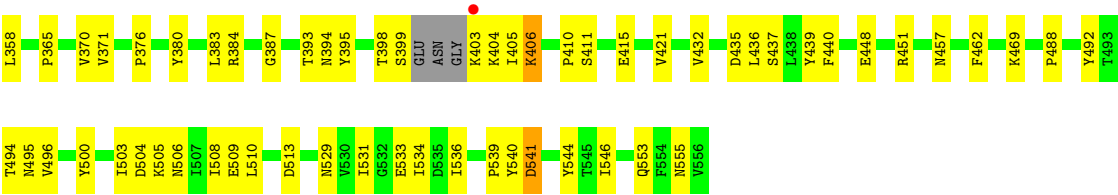
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Inulinase





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



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



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
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.198 , 0.272 0.203 , 0.267	Depositor DCC
R_{free} test set	1715 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)	0.34 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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, MG

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	0.69	4/4198 (0.1%)	0.79	3/5734 (0.1%)
1	B	0.65	5/4232 (0.1%)	0.78	7/5780 (0.1%)
All	All	0.67	9/8430 (0.1%)	0.79	10/11514 (0.1%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	VAL	C-O	-6.95	1.16	1.24
1	B	54	PRO	C-O	-6.41	1.16	1.23
1	A	54	PRO	C-O	-6.28	1.16	1.23
1	B	52	ASN	C-O	-6.21	1.18	1.24
1	B	105	PRO	C-O	-5.90	1.17	1.24
1	A	334	ASN	C-O	-5.57	1.17	1.23
1	B	410	PRO	C-O	-5.42	1.17	1.23
1	A	507	ILE	C-O	-5.22	1.18	1.24
1	B	102	SER	CA-CB	-5.16	1.45	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	LYS	CA-C-N	-9.62	111.44	121.35
1	A	441	LYS	C-N-CA	-9.62	111.44	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ASP	CA-CB-CG	8.49	121.09	112.60
1	B	533	GLU	CB-CA-C	-6.13	96.57	109.38
1	B	169	ASP	CB-CA-C	5.55	120.28	111.51
1	B	541	ASP	CB-CA-C	5.53	118.87	109.53
1	B	347	ARG	CA-C-N	-5.20	113.28	122.74
1	B	347	ARG	C-N-CA	-5.20	113.28	122.74
1	B	52	ASN	CB-CA-C	-5.18	102.49	114.41
1	A	402	GLY	CA-C-O	-5.03	117.06	121.58

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	104	0
1	B	4100	0	3777	112	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	211	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 (211) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.09
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:B:398:THR:C	1:B:541:ASP:OD2	2.20	0.83
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: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
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:398:THR:HA	1:B:541:ASP:CG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:CD	1:B:192:ASN:H	2.05	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: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:B:399:SER:H	1:B:541:ASP:CG	2.05	0.62
1:A:66:TRP:CH2	1:A:321:PRO:HD3	2.35	0.62
1:B:278:LEU:O	1:B:309:LYS:NZ	2.30	0.61
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:403:LYS:C	1:B:404:LYS:CD	2.64	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:327:TYR:HE1	1:B:355:GLN:HG3	1.68	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:181:ARG:HG3	1:A:182:ASP:CG	2.39	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:403:LYS:O	1:B:404:LYS:HD3	2.11	0.44
1:A:58:TRP:CD1	1:A:117:MET:HG2	2.51	0.44
1:A:109:ASP:HB3	1:A:146:LYS:HZ2	1.82	0.44
1:B:51:MET:HB3	1:B:51:MET:HE2	1.66	0.44
1:A:200:MET:SD	1:A:202:VAL:HG22	2.58	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:SER:HB2	1:A:221:TRP:CE3	2.54	0.43
1:B:243:VAL:HG13	1:B:245:VAL:HG23	2.01	0.43
1:B:504:ASP:O	1:B:505:LYS:C	2.60	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:51:MET:SD	1:B:350:MET:HE2	2.61	0.41
1:B:55:ASN:N	1:B:69:TYR:O	2.41	0.41
1:B:506:ASN:OD1	1:B:506:ASN:C	2.63	0.41
1:A:272:ILE:O	1:A:281:SER:HA	2.20	0.41
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:92:ASP:C	1:A:94:THR:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:51:MET:HE2	1:A:348:SER:O	2.22	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 [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	501/556 (90%)	468 (93%)	33 (7%)	0	100	100
1	B	506/556 (91%)	469 (93%)	36 (7%)	1 (0%)	43	72
All	All	1007/1112 (91%)	937 (93%)	69 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	GLU

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	445/485 (92%)	437 (98%)	8 (2%)	51 82
1	B	448/485 (92%)	439 (98%)	9 (2%)	48 80
All	All	893/970 (92%)	876 (98%)	17 (2%)	50 81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	202	VAL
1	A	347	ARG
1	A	348	SER
1	A	400	GLU
1	A	419	GLU
1	A	507	ILE
1	A	508	ILE
1	B	52	ASN
1	B	53	ASP
1	B	107	SER
1	B	169	ASP
1	B	170	ASN
1	B	202	VAL
1	B	349	SER
1	B	405	ILE
1	B	406	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	165	GLN
1	A	315	GLN
1	A	355	GLN
1	B	48	HIS
1	B	52	ASN
1	B	165	GLN
1	B	336	GLN
1	B	366	ASN
1	B	373	ASN

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	423	ASN
1	B	467	HIS
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	1,2	14,14,15	0.54	0	17,19,21	0.65	0
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.85	1 (7%)	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.56	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	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	-2.56	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	3.44	116.80	112.19
2	D	2	NAG	C1-O5-C5	2.62	115.69	112.19

There are no chirality outliers.

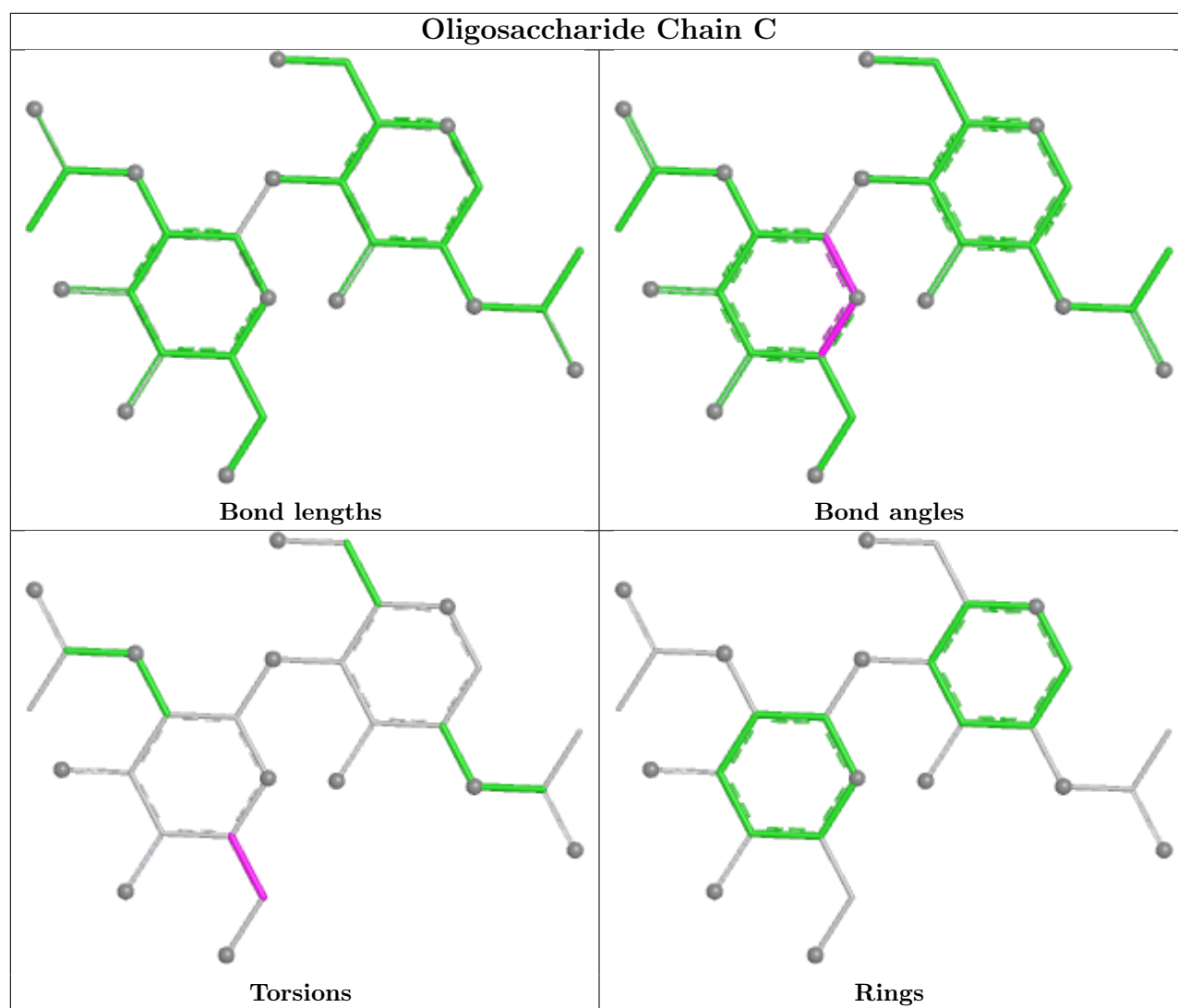
All (2) torsion outliers are listed below:

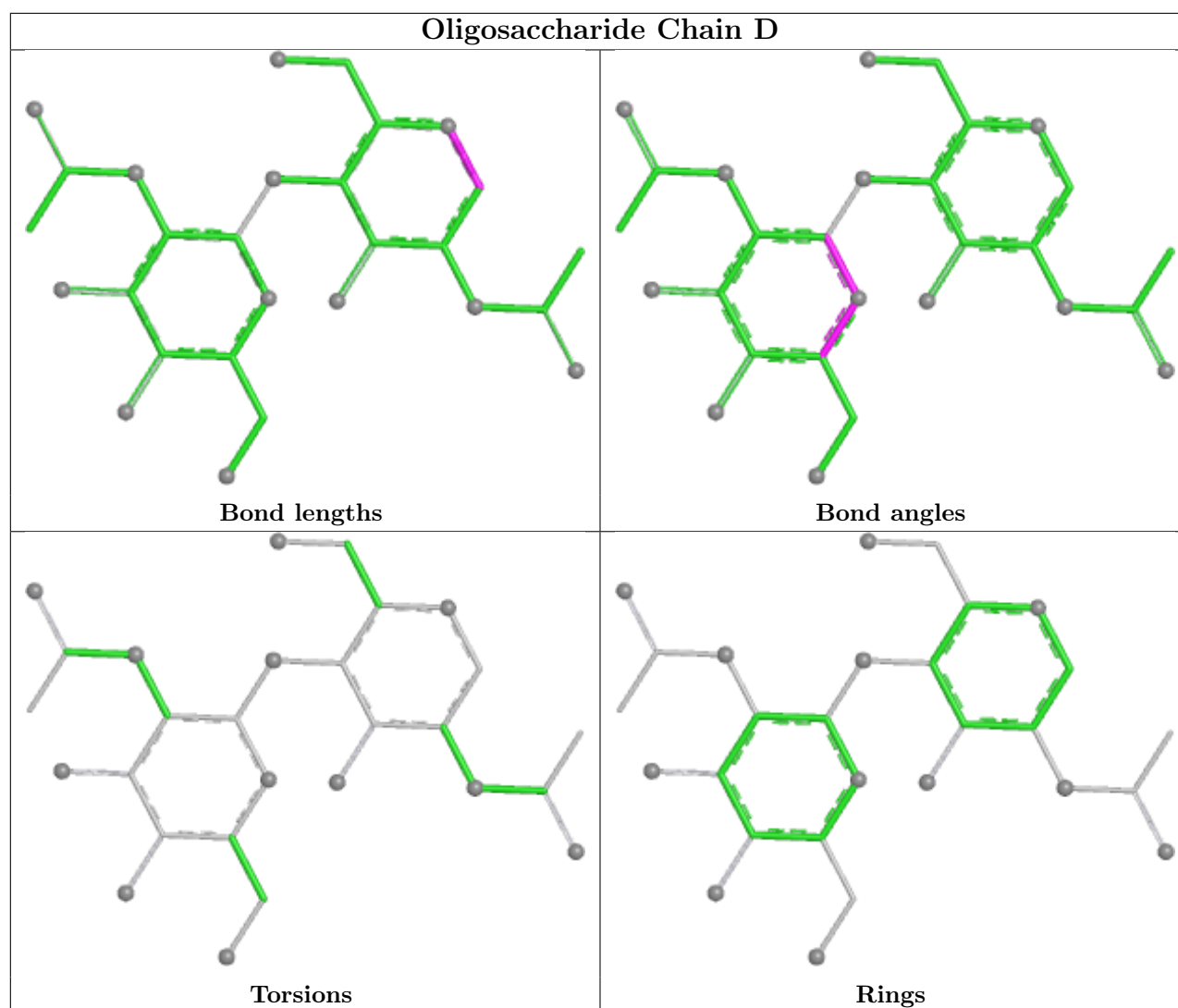
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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.





5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	507/556 (91%)	-0.18	5 (0%) 79 72	34, 46, 64, 84	0
1	B	512/556 (92%)	-0.06	6 (1%) 76 68	35, 50, 75, 102	0
All	All	1019/1112 (91%)	-0.12	11 (1%) 78 70	34, 48, 70, 102	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	SER	3.2
1	B	250	VAL	2.9
1	A	262	PRO	2.7
1	A	250	VAL	2.6
1	B	403	LYS	2.5
1	A	169	ASP	2.4
1	B	52	ASN	2.3
1	B	33	THR	2.1
1	A	348	SER	2.1
1	A	33	THR	2.1
1	B	34	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

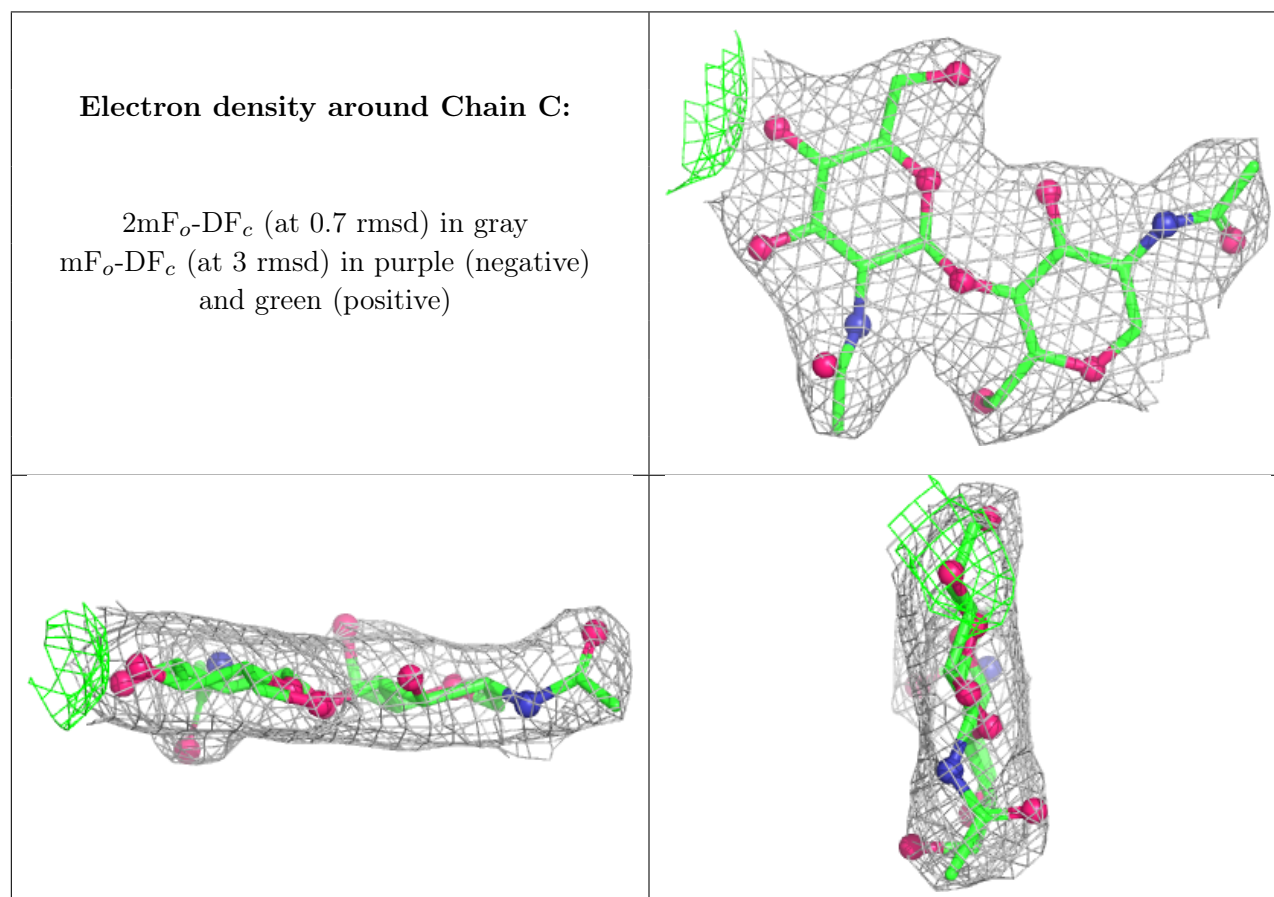
There are no non-standard protein/DNA/RNA residues in this entry.

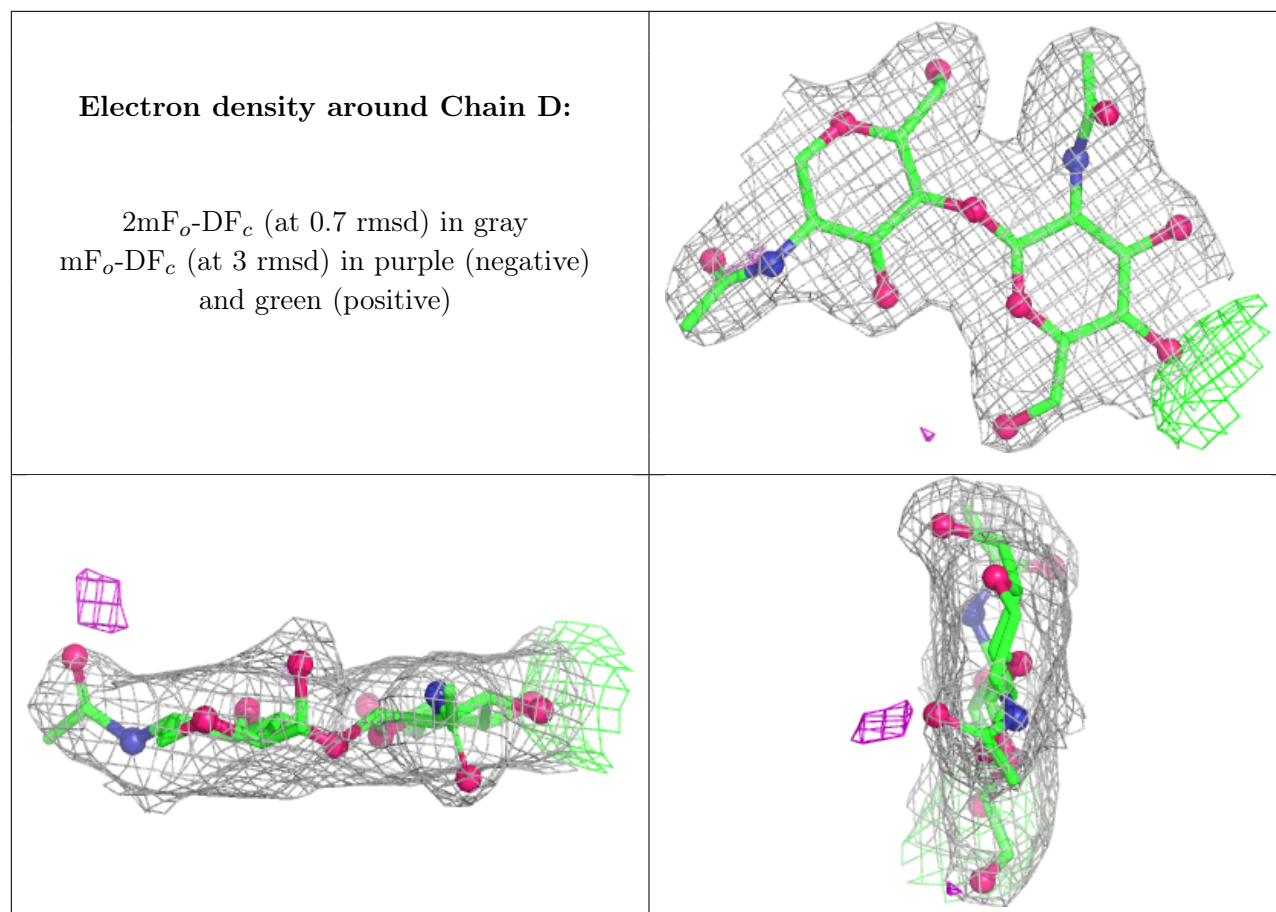
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.90	0.10	42,47,55,57	0
2	NAG	D	2	14/15	0.90	0.10	31,43,48,50	0
2	NAG	D	1	14/15	0.91	0.10	40,48,51,55	0
2	NAG	C	1	14/15	0.94	0.08	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.





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	MG	B	603	1/1	0.90	0.29	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.