



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:43 AM UTC

PDB ID : 1UKC / pdb_00001ukc
Title : Crystal Structure of Aspergillus niger EstA
Authors : Bourne, Y.; Hasper, A.A.; Chahinian, H.; Juin, M.; De Graaff, L.H.; Marchot, P.
Deposited on : 2003-08-19
Resolution : 2.10 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

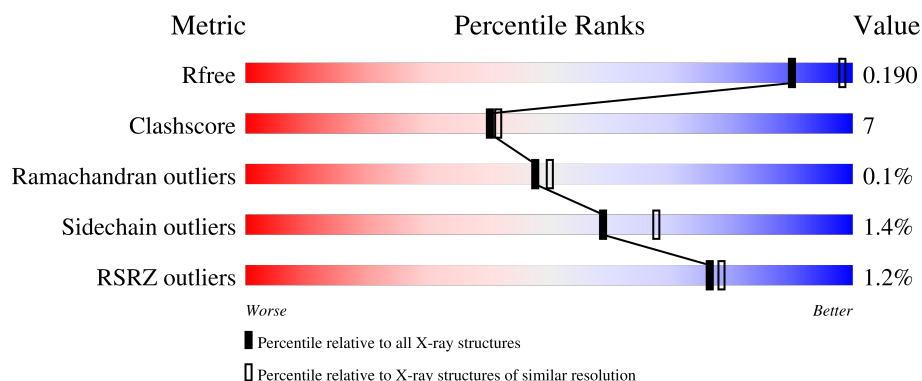
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	522	89% 9% ..
1	B	522	2% 89% 9% .
2	C	3	33% 67%
3	D	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	D	1	-	-	X	-
7	CL	A	2902	-	-	X	-

2 Entry composition [i](#)

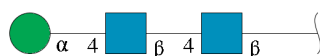
There are 9 unique types of molecules in this entry. The entry contains 9377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EstA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			3986	2520	672	783	11			
1	B	513	Total	C	N	O	S	0	0	0
			3953	2502	664	776	11			

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



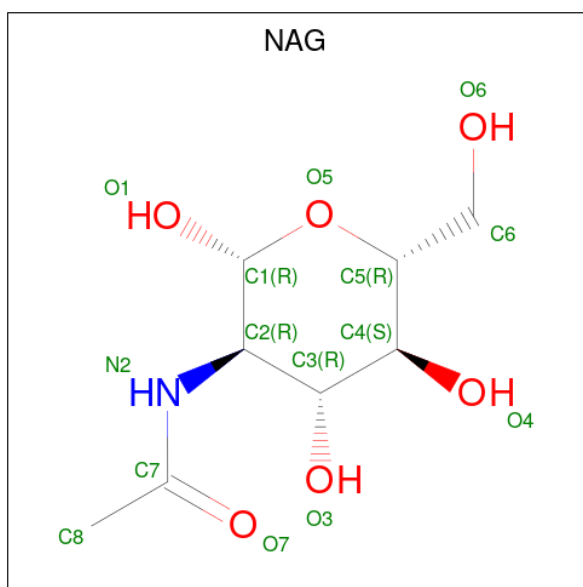
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



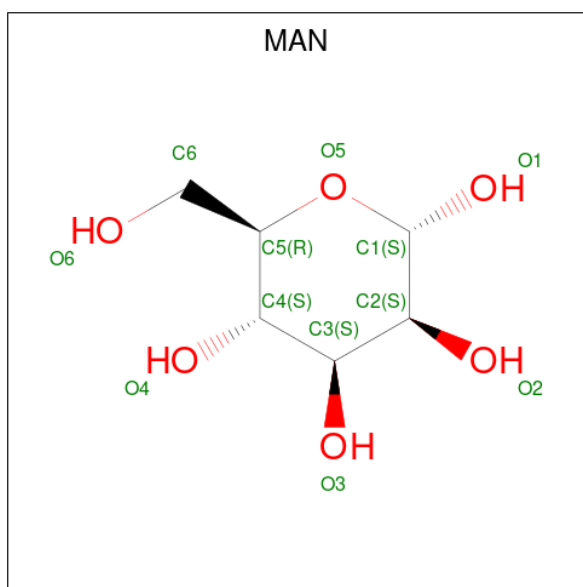
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



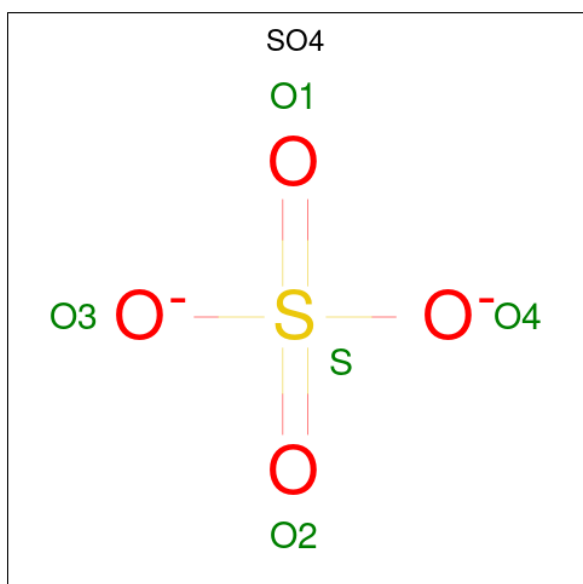
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1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

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

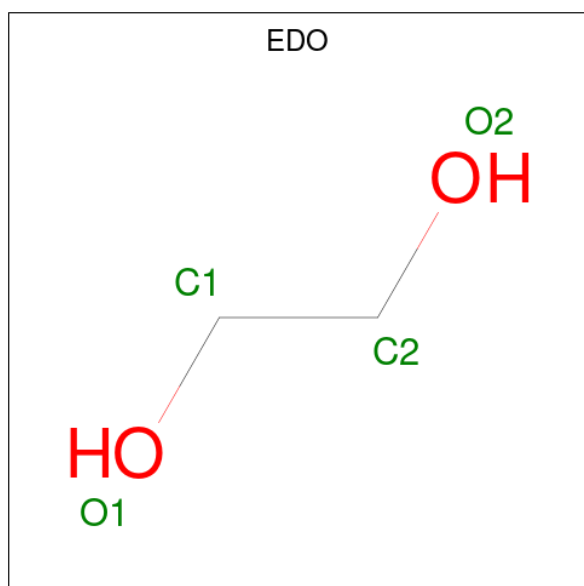


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

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

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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0

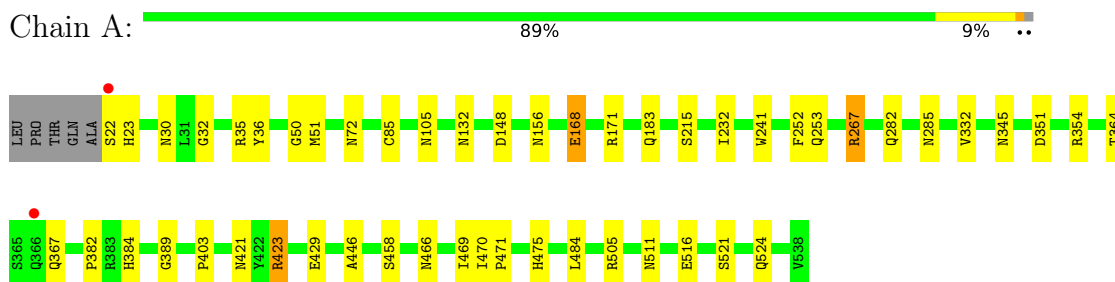
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	643	Total 643	O 643	0	0
9	B	506	Total 506	O 506	0	0

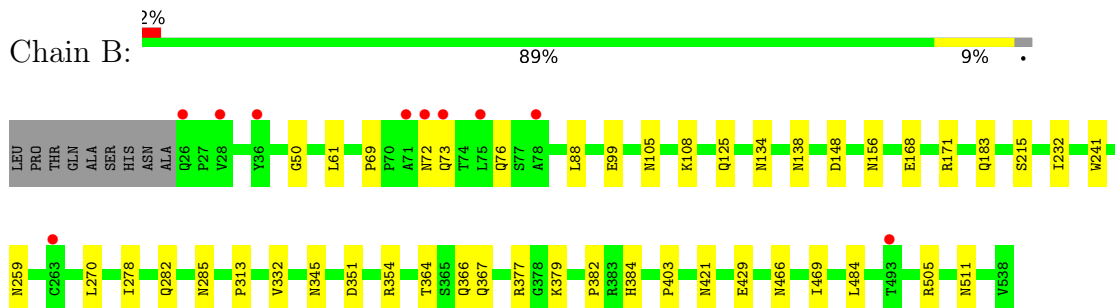
3 Residue-property plots

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: EstA



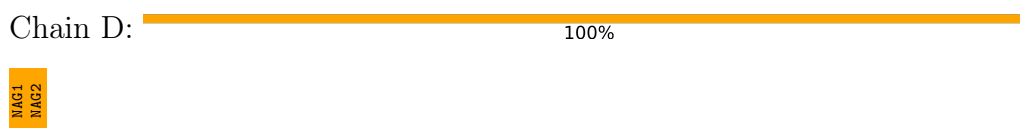
- Molecule 1: EstA



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



- Molecule 3: 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	P 63	Depositor
Cell constants a, b, c, α , β , γ	167.49Å 167.49Å 112.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.10) 99.9 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.158 , 0.184 0.169 , 0.190	Depositor DCC
R_{free} test set	1006 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9377	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG, CL, MAN, 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	0.72	0/4092	0.84	1/5581 (0.0%)
1	B	0.67	0/4058	0.83	1/5535 (0.0%)
All	All	0.69	0/8150	0.84	2/11116 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ARG	NE-CZ-NH2	-7.67	112.30	119.20
1	B	69	PRO	O-C-N	5.54	123.75	121.15

There are no chirality outliers.

There are no planarity outliers.

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	3986	0	3759	45	1
1	B	3953	0	3731	38	0
2	C	39	0	35	2	0
3	D	28	0	26	11	0
4	A	70	0	65	11	0
4	B	70	0	65	12	0
5	A	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	33	0	30	4	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	1	0	0	3	1
8	A	12	0	18	1	0
8	B	4	0	6	0	0
9	A	643	0	0	7	0
9	B	506	0	0	3	0
All	All	9377	0	7755	97	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 7.

All (97) 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:B:345:ASN:HD21	4:B:1751:NAG:C1	1.08	1.64
1:B:138:ASN:HD21	3:D:1:NAG:C1	1.04	1.59
1:B:511:ASN:HD21	4:B:1851:NAG:C1	1.00	1.55
1:A:72:ASN:HD21	4:A:1501:NAG:C1	1.09	1.54
1:A:345:ASN:HD21	4:A:1701:NAG:C1	1.15	1.51
1:A:511:ASN:HD21	4:A:1801:NAG:C1	0.92	1.51
1:B:259:ASN:HD21	4:B:1951:NAG:C1	1.38	1.37
1:A:35:ARG:NH1	9:A:3524:HOH:O	1.73	1.20
1:A:23:HIS:N	7:A:2902:CL:CL	2.14	1.16
1:B:259:ASN:ND2	4:B:1951:NAG:C1	2.24	0.99
1:A:23:HIS:ND1	7:A:2902:CL:CL	2.41	0.91
1:A:22:SER:N	7:A:2902:CL:CL	2.41	0.90
1:A:282:GLN:HE22	1:A:285:ASN:HD22	1.28	0.82
1:B:282:GLN:HE22	1:B:285:ASN:HD22	1.27	0.81
4:A:1801:NAG:O4	4:A:1802:NAG:C1	2.32	0.78
3:D:1:NAG:HO4	3:D:2:NAG:C1	1.94	0.77
1:B:511:ASN:HD21	4:B:1851:NAG:C2	1.96	0.76
1:B:138:ASN:HD21	3:D:1:NAG:C2	1.95	0.76
1:A:351:ASP:OD1	1:A:354:ARG:NH1	2.20	0.75
3:D:1:NAG:C4	3:D:2:NAG:C1	2.67	0.72
1:A:364:THR:H	1:A:367:GLN:NE2	1.89	0.71
1:A:511:ASN:HD21	4:A:1801:NAG:C2	1.98	0.70
1:B:50:GLY:H	1:B:105:ASN:HD22	1.40	0.70
1:A:511:ASN:CG	4:A:1801:NAG:C1	2.63	0.69
4:B:1851:NAG:O4	4:B:1852:NAG:C1	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:NAG:C4	2:C:3:MAN:C1	2.72	0.67
1:B:364:THR:H	1:B:367:GLN:NE2	1.93	0.66
1:A:50:GLY:H	1:A:105:ASN:HD22	1.44	0.66
1:A:364:THR:H	1:A:367:GLN:HE21	1.44	0.64
1:A:429:GLU:HG2	9:B:3203:HOH:O	1.98	0.63
1:B:168:GLU:OE1	1:B:171:ARG:HD2	2.00	0.61
1:B:50:GLY:H	1:B:105:ASN:ND2	1.99	0.60
1:A:423:ARG:HD3	1:A:516:GLU:OE2	2.03	0.59
1:B:345:ASN:HD21	4:B:1751:NAG:C2	2.06	0.59
1:B:138:ASN:CG	3:D:1:NAG:C1	2.73	0.58
1:B:332:VAL:O	1:B:421:ASN:HA	2.03	0.58
1:B:511:ASN:CG	4:B:1851:NAG:C1	2.72	0.58
1:B:72:ASN:HD21	4:B:1551:NAG:C1	2.16	0.58
1:B:421:ASN:HD22	1:B:505:ARG:HB3	1.70	0.56
1:B:232:ILE:HD12	1:B:484:LEU:HD11	1.87	0.56
1:A:30:ASN:ND2	1:A:32:GLY:H	2.03	0.55
1:A:30:ASN:HD22	1:A:32:GLY:H	1.55	0.55
1:A:72:ASN:HD21	4:A:1501:NAG:C2	2.07	0.54
5:B:1652:MAN:C1	3:D:2:NAG:O4	2.56	0.53
1:B:384:HIS:HE1	9:B:3245:HOH:O	1.92	0.53
1:A:332:VAL:O	1:A:421:ASN:HA	2.09	0.53
1:A:421:ASN:HD22	1:A:505:ARG:HB3	1.72	0.53
1:A:521:SER:HA	1:A:524:GLN:HE21	1.75	0.52
1:B:364:THR:H	1:B:367:GLN:HE21	1.57	0.52
1:A:382:PRO:O	1:A:384:HIS:HD2	1.92	0.52
1:B:511:ASN:ND2	4:B:1851:NAG:C2	2.63	0.51
1:A:50:GLY:H	1:A:105:ASN:ND2	2.06	0.51
1:B:241:TRP:CD2	1:B:403:PRO:HB3	2.45	0.51
1:A:72:ASN:CG	4:A:1501:NAG:C1	2.76	0.51
1:B:511:ASN:ND2	4:B:1851:NAG:O5	2.40	0.51
2:C:2:NAG:HO4	2:C:3:MAN:C1	2.22	0.51
1:A:511:ASN:ND2	4:A:1801:NAG:C2	2.67	0.50
1:A:423:ARG:NH2	9:A:3183:HOH:O	2.37	0.50
1:A:389:GLY:HA3	9:A:3353:HOH:O	2.12	0.50
1:A:267:ARG:HH11	1:A:267:ARG:HB3	1.77	0.50
1:B:345:ASN:ND2	4:B:1751:NAG:C2	2.70	0.50
1:B:138:ASN:ND2	3:D:1:NAG:O5	2.43	0.49
1:B:183:GLN:OE1	1:B:215:SER:HB3	2.12	0.49
3:D:1:NAG:O4	3:D:2:NAG:C2	2.58	0.49
8:A:1932:EDO:H12	9:A:3508:HOH:O	2.12	0.49
5:B:1652:MAN:O3	5:B:1651:MAN:H5	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:HIS:HE1	9:A:3004:HOH:O	1.94	0.49
5:B:1652:MAN:C1	3:D:2:NAG:C4	2.91	0.48
1:A:241:TRP:CD2	1:A:403:PRO:HB3	2.49	0.48
1:B:382:PRO:O	1:B:384:HIS:HD2	1.96	0.48
1:A:470:ILE:HB	1:A:471:PRO:HD3	1.97	0.47
9:A:3396:HOH:O	1:B:379:LYS:HE3	2.14	0.47
1:A:30:ASN:HD22	1:A:30:ASN:C	2.23	0.47
1:B:125:GLN:HB2	1:B:134:ASN:HB2	1.97	0.46
4:A:1501:NAG:O4	4:A:1502:NAG:C1	2.64	0.46
1:A:168:GLU:OE1	1:A:171:ARG:CD	2.64	0.46
1:A:132:ASN:ND2	1:A:156:ASN:HB3	2.30	0.46
1:A:446:ALA:HA	1:A:470:ILE:HG12	1.98	0.45
1:A:85:CYS:H	1:A:132:ASN:ND2	2.15	0.44
1:B:138:ASN:ND2	3:D:1:NAG:C2	2.66	0.44
1:B:313:PRO:HD2	9:B:3037:HOH:O	2.16	0.44
1:B:125:GLN:NE2	1:B:156:ASN:HD22	2.16	0.44
5:B:1652:MAN:C1	3:D:2:NAG:H4	2.48	0.43
1:B:466:ASN:O	1:B:469:ILE:HG22	2.18	0.43
1:B:351:ASP:OD1	1:B:354:ARG:NH1	2.48	0.43
9:A:3395:HOH:O	1:B:429:GLU:HG2	2.17	0.42
1:A:168:GLU:OE1	1:A:171:ARG:HD2	2.19	0.42
1:A:132:ASN:HD21	1:A:156:ASN:HB3	1.85	0.42
1:A:232:ILE:HD12	1:A:484:LEU:HD11	2.02	0.42
1:A:252:PHE:CG	1:A:253:GLN:N	2.88	0.42
1:B:125:GLN:HE22	1:B:156:ASN:HD22	1.67	0.42
1:A:183:GLN:OE1	1:A:215:SER:HB3	2.20	0.41
1:B:99:GLU:HG3	1:B:278:ILE:HD13	2.02	0.41
4:A:1801:NAG:C4	4:A:1802:NAG:C1	2.98	0.41
1:A:466:ASN:O	1:A:469:ILE:HG22	2.21	0.40
1:A:36:TYR:CD2	1:A:51:MET:HG2	2.57	0.40
1:A:367:GLN:HE21	1:A:367:GLN:HB2	1.70	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:A:475:HIS:NE2	7:A:2902:CL:CL[2_665]	2.12	0.08

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	515/522 (99%)	492 (96%)	23 (4%)	0	100	100
1	B	511/522 (98%)	493 (96%)	17 (3%)	1 (0%)	43	44
All	All	1026/1044 (98%)	985 (96%)	40 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	377	ARG

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	425/429 (99%)	421 (99%)	4 (1%)	70	78
1	B	421/429 (98%)	413 (98%)	8 (2%)	50	58
All	All	846/858 (99%)	834 (99%)	12 (1%)	59	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	A	168	GLU
1	A	267	ARG
1	A	458	SER
1	B	61	LEU

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Mol	Chain	Res	Type
1	B	73	GLN
1	B	76	GLN
1	B	88	LEU
1	B	108	LYS
1	B	148	ASP
1	B	270	LEU
1	B	366	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	72	ASN
1	A	105	ASN
1	A	132	ASN
1	A	156	ASN
1	A	172	GLN
1	A	282	GLN
1	A	341	ASN
1	A	345	ASN
1	A	367	GLN
1	A	384	HIS
1	A	421	ASN
1	A	504	GLN
1	A	509	GLN
1	A	511	ASN
1	A	524	GLN
1	B	30	ASN
1	B	67	GLN
1	B	72	ASN
1	B	73	GLN
1	B	105	ASN
1	B	132	ASN
1	B	138	ASN
1	B	156	ASN
1	B	172	GLN
1	B	259	ASN
1	B	282	GLN
1	B	341	ASN
1	B	345	ASN
1	B	366	GLN
1	B	367	GLN

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Mol	Chain	Res	Type
1	B	384	HIS
1	B	421	ASN
1	B	509	GLN
1	B	511	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 ⓘ

5 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	0.55	0	17,19,21	1.33	3 (17%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	1.27	3 (17%)
2	MAN	C	3	2	11,11,12	0.80	0	15,15,17	1.59	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.68	0	17,19,21	1.66	2 (11%)
3	NAG	D	2	3	14,14,15	0.63	0	17,19,21	1.51	3 (17%)

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

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

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	MAN	C1-O5-C5	-4.11	106.68	112.19
3	D	1	NAG	C1-O5-C5	-3.82	107.07	112.19
3	D	2	NAG	C1-O5-C5	-3.79	107.11	112.19
3	D	1	NAG	C3-C4-C5	3.38	116.35	110.23
2	C	2	NAG	O4-C4-C3	-2.75	103.88	110.38
2	C	2	NAG	C1-O5-C5	-2.58	108.73	112.19
2	C	1	NAG	O5-C1-C2	2.53	115.21	111.29
2	C	3	MAN	C2-C3-C4	2.36	115.01	110.86
2	C	2	NAG	C3-C4-C5	2.35	114.49	110.23
3	D	2	NAG	O4-C4-C3	-2.31	104.94	110.38
2	C	3	MAN	C3-C4-C5	2.28	114.37	110.23
2	C	1	NAG	C2-N2-C7	-2.23	119.91	122.90
3	D	2	NAG	O5-C5-C6	2.22	111.98	107.66
2	C	1	NAG	C3-C4-C5	2.20	114.23	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

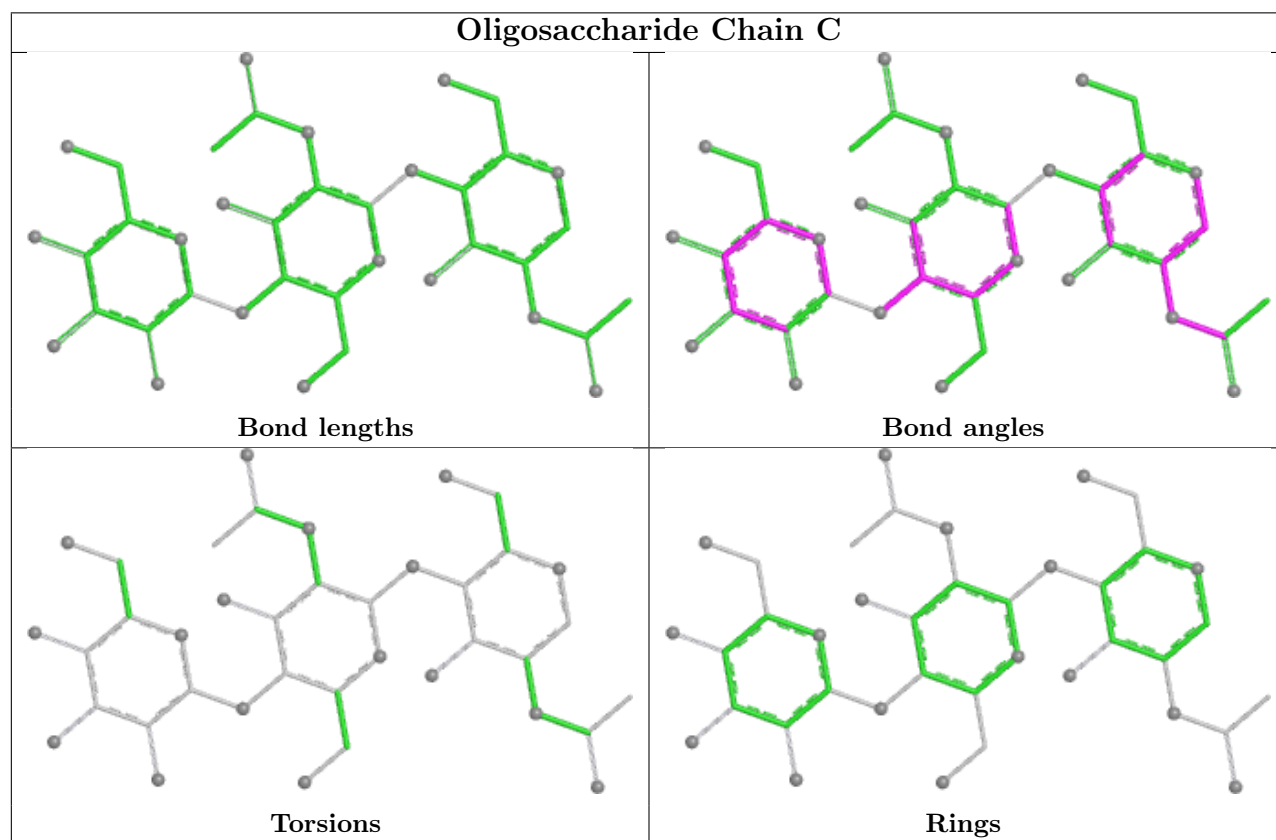
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

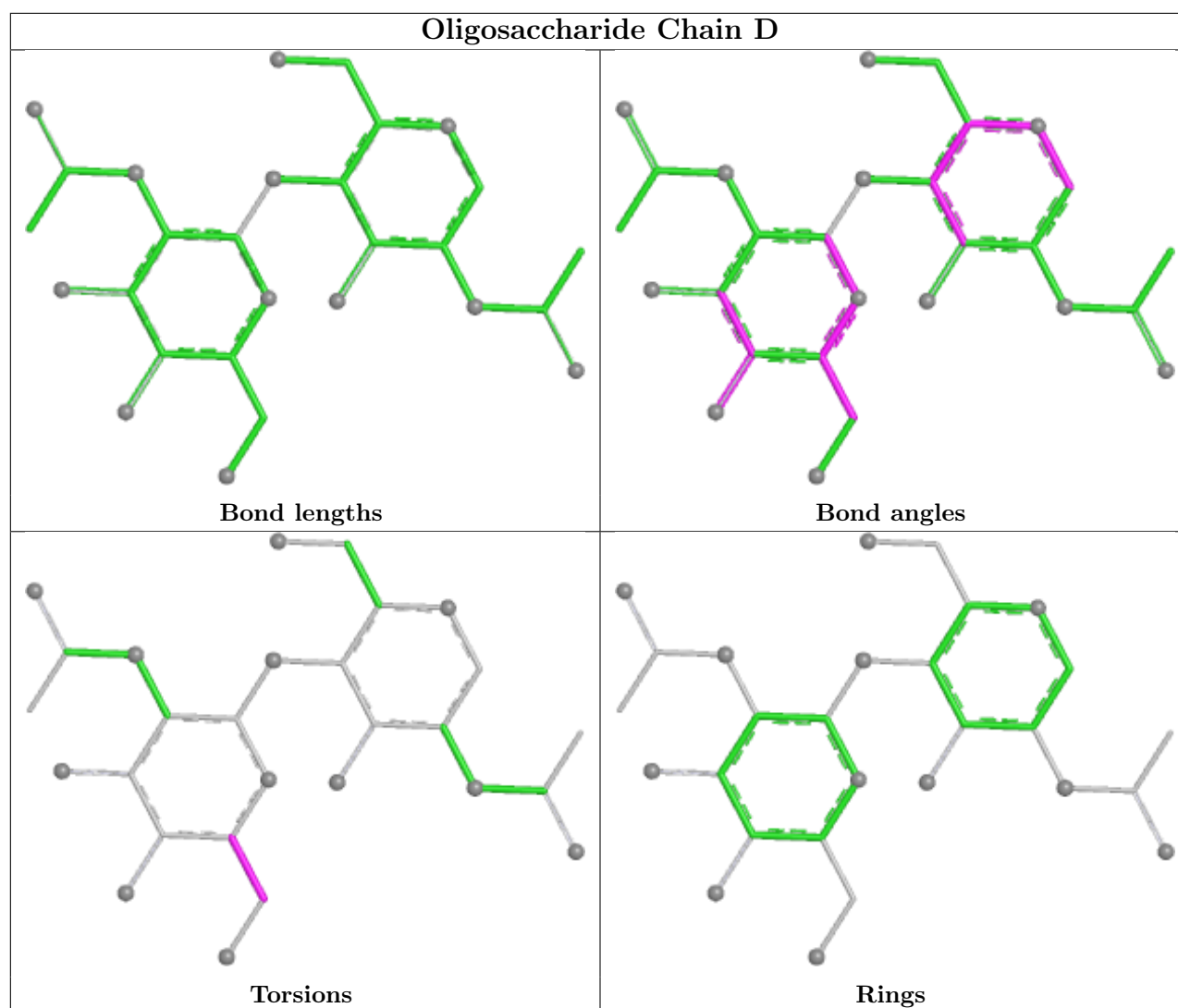
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	C	3	MAN	2	0
3	D	2	NAG	6	0
3	D	1	NAG	8	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 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	$\# Z > 2$
4	NAG	A	1802	-	14,14,15	0.59	0	17,19,21	0.98	0
8	EDO	A	1922	-	3,3,3	0.26	0	2,2,2	0.47	0
8	EDO	B	1912	-	3,3,3	0.33	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	B	1651	-	11,11,12	0.57	0	15,15,17	1.21	2 (13%)
4	NAG	B	1852	-	14,14,15	0.61	0	17,19,21	1.27	3 (17%)
6	SO4	B	2951	-	4,4,4	0.32	0	6,6,6	0.48	0
4	NAG	A	1501	1	14,14,15	0.62	0	17,19,21	1.12	2 (11%)
5	MAN	A	1601	-	11,11,12	0.70	0	15,15,17	1.28	3 (20%)
5	MAN	B	1652	-	11,11,12	0.73	0	15,15,17	1.40	3 (20%)
8	EDO	A	1902	-	3,3,3	0.34	0	2,2,2	0.15	0
4	NAG	B	1751	1	14,14,15	0.63	0	17,19,21	0.77	0
5	MAN	B	1653	-	11,11,12	0.86	1 (9%)	15,15,17	1.83	2 (13%)
4	NAG	B	1851	1	14,14,15	0.63	0	17,19,21	1.03	0
4	NAG	A	1801	1	14,14,15	0.54	0	17,19,21	1.13	2 (11%)
4	NAG	B	1551	-	14,14,15	0.62	0	17,19,21	0.95	1 (5%)
5	MAN	A	1603	-	11,11,12	0.79	0	15,15,17	1.79	4 (26%)
4	NAG	A	1701	1	14,14,15	0.64	0	17,19,21	0.90	0
6	SO4	A	2901	-	4,4,4	0.15	0	6,6,6	0.64	0
4	NAG	A	1502	-	14,14,15	0.59	0	17,19,21	1.12	2 (11%)
8	EDO	A	1932	-	3,3,3	0.36	0	2,2,2	0.27	0
4	NAG	B	1951	-	14,14,15	0.62	0	17,19,21	1.14	2 (11%)

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
4	NAG	A	1802	-	-	2/6/23/26	0/1/1/1
8	EDO	A	1922	-	-	0/1/1/1	-
8	EDO	B	1912	-	-	1/1/1/1	-
5	MAN	B	1651	-	-	2/2/19/22	0/1/1/1
4	NAG	B	1852	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1501	1	-	0/6/23/26	0/1/1/1
5	MAN	A	1601	-	-	0/2/19/22	0/1/1/1
5	MAN	B	1652	-	-	2/2/19/22	0/1/1/1
8	EDO	A	1902	-	-	1/1/1/1	-
4	NAG	B	1751	1	-	2/6/23/26	0/1/1/1
5	MAN	B	1653	-	-	2/2/19/22	0/1/1/1
4	NAG	B	1851	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1801	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1551	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	A	1603	-	-	2/2/19/22	0/1/1/1
4	NAG	A	1701	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1502	-	-	4/6/23/26	0/1/1/1
8	EDO	A	1932	-	-	1/1/1/1	-
4	NAG	B	1951	-	-	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)
5	B	1653	MAN	C2-C3	2.03	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1653	MAN	C1-C2-C3	5.47	117.61	109.64
5	A	1603	MAN	C1-C2-C3	5.07	117.03	109.64
5	A	1603	MAN	C1-O5-C5	3.05	116.27	112.19
4	B	1852	NAG	C1-O5-C5	-2.92	108.27	112.19
5	B	1652	MAN	C3-C4-C5	2.90	115.49	110.23
5	B	1653	MAN	C2-C3-C4	2.81	115.80	110.86
5	B	1652	MAN	C1-O5-C5	-2.80	108.43	112.19
4	B	1951	NAG	C3-C4-C5	2.66	115.06	110.23
5	A	1601	MAN	C1-C2-C3	2.65	113.50	109.64
5	A	1601	MAN	C2-C3-C4	2.62	115.47	110.86
5	B	1651	MAN	C1-C2-C3	2.57	113.38	109.64
5	B	1651	MAN	C1-O5-C5	2.55	115.61	112.19
5	B	1652	MAN	C2-C3-C4	2.51	115.27	110.86
4	A	1801	NAG	C3-C4-C5	2.45	114.68	110.23
5	A	1603	MAN	C2-C3-C4	2.33	114.95	110.86
5	A	1603	MAN	O5-C1-C2	2.26	116.17	110.79
4	A	1502	NAG	C3-C4-C5	2.22	114.26	110.23
4	A	1501	NAG	C3-C4-C5	2.18	114.19	110.23
4	A	1801	NAG	C1-O5-C5	-2.14	109.32	112.19
4	B	1951	NAG	O5-C1-C2	-2.10	108.04	111.29
4	B	1551	NAG	C3-C4-C5	2.10	114.04	110.23
4	A	1501	NAG	O4-C4-C3	-2.09	105.46	110.38
4	B	1852	NAG	C4-C3-C2	2.06	114.04	111.02
4	A	1502	NAG	O5-C1-C2	-2.05	108.12	111.29
4	B	1852	NAG	O5-C1-C2	-2.04	108.13	111.29
5	A	1601	MAN	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1551	NAG	C8-C7-N2-C2
4	B	1551	NAG	O7-C7-N2-C2
5	A	1603	MAN	O5-C5-C6-O6
5	B	1651	MAN	O5-C5-C6-O6
4	B	1751	NAG	O5-C5-C6-O6
5	B	1652	MAN	O5-C5-C6-O6
5	B	1653	MAN	O5-C5-C6-O6
5	B	1653	MAN	C4-C5-C6-O6
5	B	1651	MAN	C4-C5-C6-O6
5	A	1603	MAN	C4-C5-C6-O6
4	A	1802	NAG	C8-C7-N2-C2
4	B	1751	NAG	C4-C5-C6-O6
5	B	1652	MAN	C4-C5-C6-O6
4	A	1802	NAG	O7-C7-N2-C2
4	A	1502	NAG	C8-C7-N2-C2
4	A	1701	NAG	O5-C5-C6-O6
4	A	1701	NAG	C4-C5-C6-O6
4	A	1502	NAG	C4-C5-C6-O6
4	A	1502	NAG	O7-C7-N2-C2
4	B	1852	NAG	C8-C7-N2-C2
8	A	1932	EDO	O1-C1-C2-O2
4	B	1852	NAG	O7-C7-N2-C2
4	A	1502	NAG	O5-C5-C6-O6
8	A	1902	EDO	O1-C1-C2-O2
8	B	1912	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1802	NAG	2	0
5	B	1651	MAN	1	0
4	B	1852	NAG	1	0
4	A	1501	NAG	4	0
5	B	1652	MAN	4	0
4	B	1751	NAG	3	0
4	B	1851	NAG	6	0
4	A	1801	NAG	6	0
4	B	1551	NAG	1	0
4	A	1701	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1502	NAG	1	0
8	A	1932	EDO	1	0
4	B	1951	NAG	2	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	517/522 (99%)	-0.26	2 (0%) 88 90	23, 32, 47, 69	0
1	B	513/522 (98%)	-0.00	10 (1%) 66 69	25, 36, 61, 86	0
All	All	1030/1044 (98%)	-0.13	12 (1%) 76 78	23, 34, 55, 86	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	GLN	4.1
1	B	493	THR	3.0
1	B	263	CYS	2.7
1	B	75	LEU	2.4
1	B	73	GLN	2.3
1	B	78	ALA	2.2
1	B	28	VAL	2.1
1	B	72	ASN	2.0
1	A	366	GLN	2.0
1	A	22	SER	2.0
1	B	71	ALA	2.0
1	B	36	TYR	2.0

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

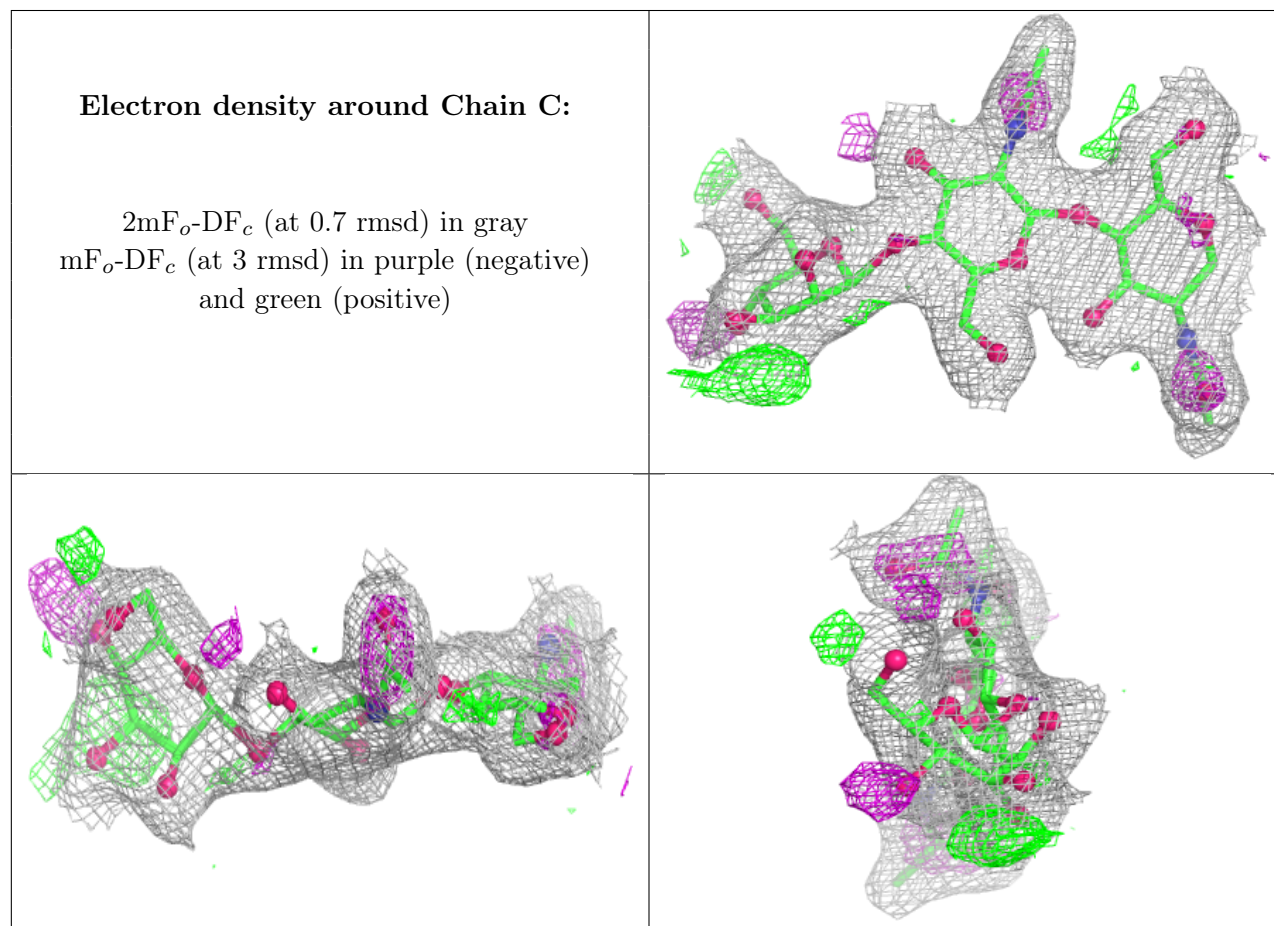
There are no non-standard protein/DNA/RNA residues in this entry.

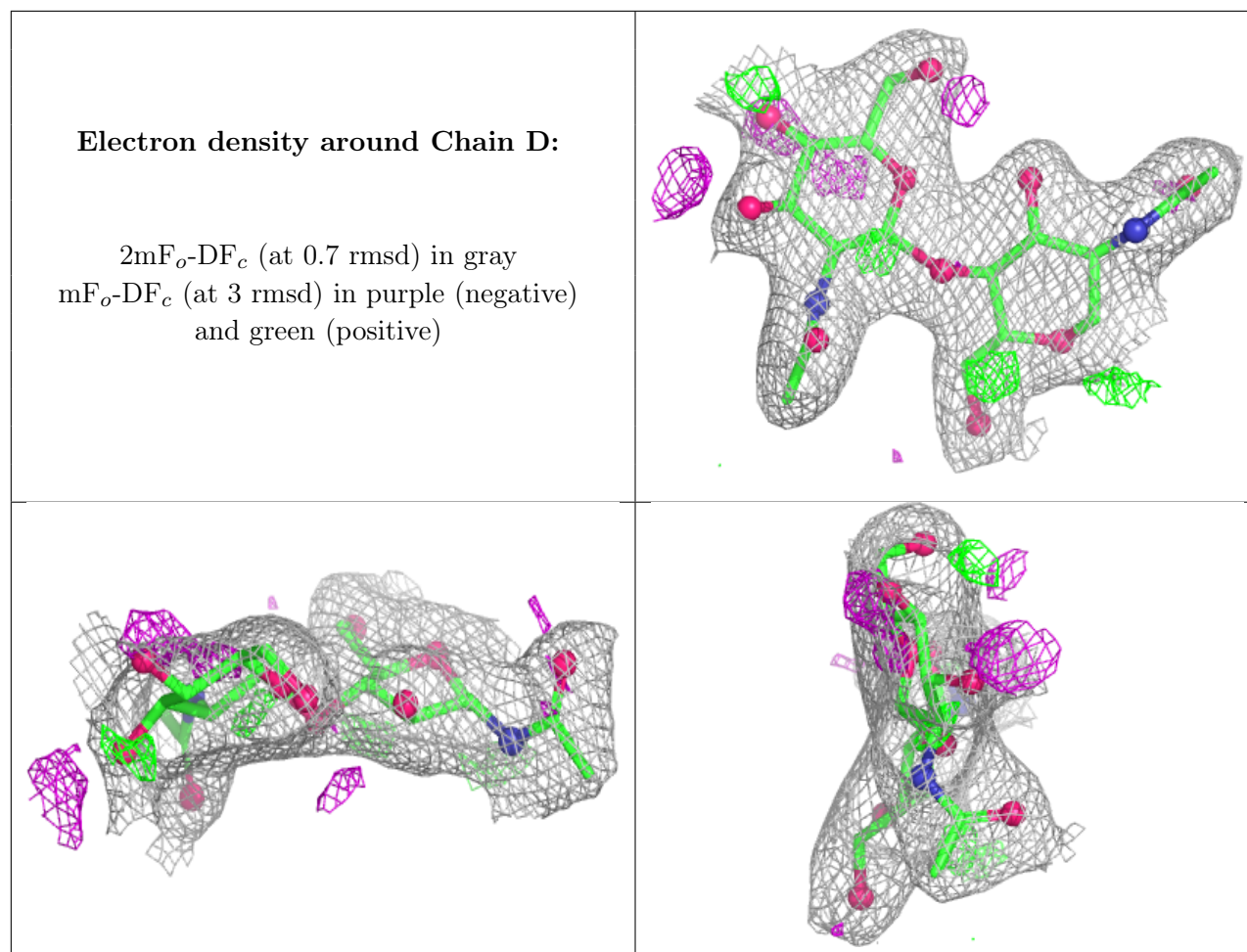
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	MAN	C	3	11/12	0.81	0.12	63,65,68,68	0
3	NAG	D	2	14/15	0.88	0.12	55,63,66,67	0
3	NAG	D	1	14/15	0.93	0.09	47,49,51,52	0
2	NAG	C	2	14/15	0.94	0.08	33,35,40,42	0
2	NAG	C	1	14/15	0.96	0.08	28,30,34,35	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
5	MAN	B	1651	11/12	0.59	0.15	89,89,90,90	0
5	MAN	A	1603	11/12	0.60	0.16	85,85,86,86	0
5	MAN	B	1653	11/12	0.61	0.15	85,86,86,86	0
4	NAG	B	1951	14/15	0.62	0.17	80,81,81,81	0
4	NAG	A	1802	14/15	0.64	0.19	79,80,82,83	0
4	NAG	A	1502	14/15	0.67	0.19	91,92,92,93	0
5	MAN	A	1601	11/12	0.69	0.14	88,88,89,89	0
4	NAG	B	1852	14/15	0.71	0.16	82,84,84,85	0
4	NAG	B	1551	14/15	0.75	0.16	83,83,84,84	0
5	MAN	B	1652	11/12	0.76	0.15	89,90,91,91	0
4	NAG	A	1701	14/15	0.84	0.13	56,58,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	1751	14/15	0.85	0.13	56,59,62,62	0
8	EDO	A	1902	4/4	0.86	0.16	47,49,50,52	0
4	NAG	B	1851	14/15	0.89	0.10	36,46,52,54	0
4	NAG	A	1501	14/15	0.89	0.11	56,59,61,62	0
4	NAG	A	1801	14/15	0.91	0.09	34,42,49,51	0
8	EDO	B	1912	4/4	0.91	0.15	48,52,52,55	0
8	EDO	A	1922	4/4	0.93	0.16	34,39,41,44	0
8	EDO	A	1932	4/4	0.96	0.14	31,37,39,44	0
6	SO4	A	2901	5/5	0.98	0.10	30,30,32,37	0
6	SO4	B	2951	5/5	0.98	0.10	35,36,38,41	0
7	CL	A	2902	1/1	0.99	0.21	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.