



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 01:41 AM EDT

PDB ID : 3KE0
Title : Crystal structure of N370S Glucocerebrosidase at acidic pH.
Authors : Wei, R.R.; Boucher, S.; Pan, C.Q.; Edmunds, T.
Deposited on : 2009-10-23
Resolution : 2.70 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 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 : 2.23.2
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) : 2.23.2

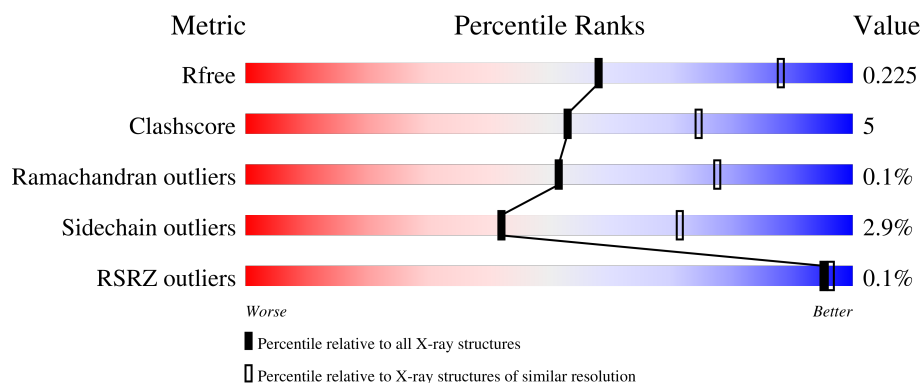
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




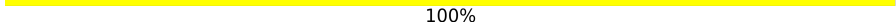
The reported resolution of this entry is 2.70 Å.

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	497	 85% 13% .
1	B	497	 86% 13% .
2	C	2	 100%
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
2	NAG	C	2	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8262 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3928	2531	671	710	16			
1	B	497	Total	C	N	O	S	0	0	0
			3929	2531	671	711	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	SER	ASN	engineered mutation	UNP P04062
B	370	SER	ASN	engineered mutation	UNP P04062

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



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

- 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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

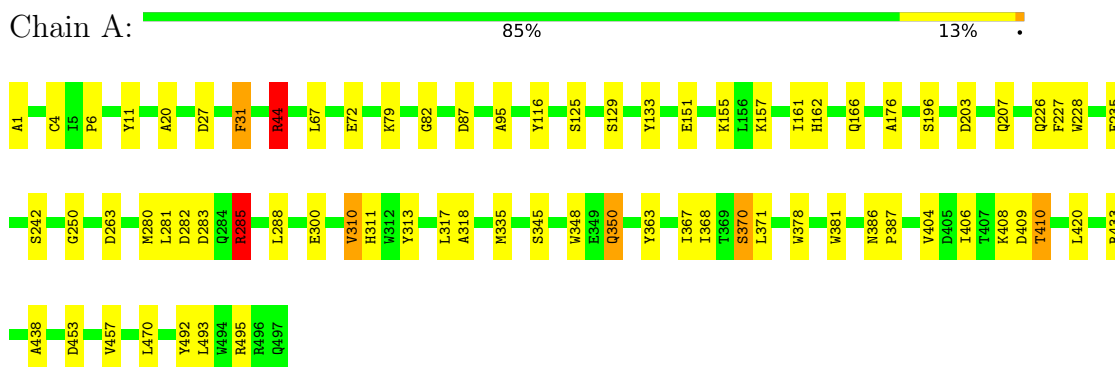
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	118	Total	O	0	0
			118	118		
7	B	134	Total	O	0	0
			134	134		

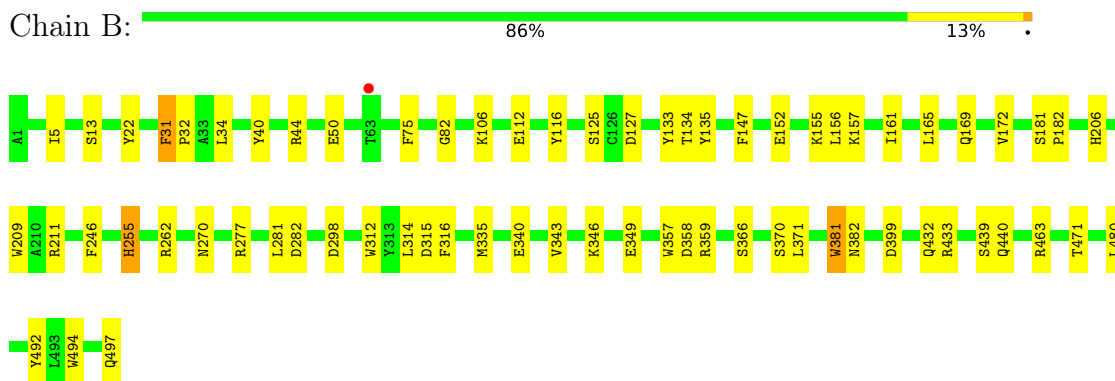
3 Residue-property plots

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.

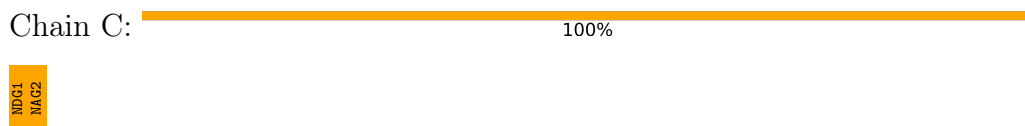
- Molecule 1: Glucosylceramidase




- Molecule 1: Glucosylceramidase



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



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	109.47Å 285.06Å 92.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.5 (47.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.172 , 0.229 0.171 , 0.225	Depositor DCC
R_{free} test set	1997 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8262	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: NDG, NAG, GOL, 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	0.97	7/4048 (0.2%)	0.84	5/5519 (0.1%)
1	B	0.96	5/4049 (0.1%)	0.87	3/5519 (0.1%)
All	All	0.97	12/8097 (0.1%)	0.86	8/11038 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	GLU	CB-CG	7.98	1.67	1.52
1	A	310	VAL	CB-CG1	-7.33	1.37	1.52
1	B	494	TRP	CE3-CZ3	-7.31	1.26	1.38
1	B	492	TYR	CD2-CE2	-7.08	1.28	1.39
1	B	155	LYS	CD-CE	6.92	1.68	1.51
1	A	72	GLU	CG-CD	6.85	1.62	1.51
1	A	300	GLU	CG-CD	6.61	1.61	1.51
1	A	350	GLN	CG-CD	6.60	1.66	1.51
1	B	492	TYR	CD1-CE1	-6.31	1.29	1.39
1	A	310	VAL	CB-CG2	-5.88	1.40	1.52
1	A	350	GLN	CB-CG	5.83	1.68	1.52
1	B	155	LYS	CE-NZ	5.31	1.62	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	285	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	317	LEU	CA-CB-CG	6.66	130.62	115.30
1	A	317	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	A	44	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	155	LYS	CD-CE-NZ	5.37	124.06	111.70
1	B	315	ASP	CB-CG-OD2	-5.24	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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	3928	0	3847	40	0
1	B	3929	0	3847	42	0
2	C	28	0	23	3	0
3	D	28	0	25	0	0
4	A	40	0	0	1	0
4	B	25	0	0	2	0
5	A	12	0	16	0	0
5	B	6	0	8	1	0
6	B	14	0	13	0	0
7	A	118	0	0	3	0
7	B	134	0	0	1	0
All	All	8262	0	7779	85	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 5.

All (85) 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:31:PHE:HD2	1:B:32:PRO:HD2	1.22	1.03
1:B:31:PHE:CD2	1:B:32:PRO:HD2	2.09	0.88
1:B:206:HIS:NE2	1:B:255:HIS:HE1	1.84	0.77
1:A:31:PHE:HB2	1:A:495:ARG:HH21	1.53	0.74
1:A:408:LYS:O	1:A:410:THR:HG23	1.90	0.70
1:B:314:LEU:HB2	1:B:343:VAL:CG1	2.22	0.70
1:A:95:ALA:HB1	1:A:406:ILE:HD12	1.74	0.70
1:B:340:GLU:OE2	5:B:498:GOL:H11	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:TRP:HA	1:B:381:TRP:CE3	2.34	0.61
1:B:314:LEU:HB2	1:B:343:VAL:HG13	1.83	0.60
1:A:371:LEU:O	1:A:433:ARG:HD2	2.01	0.60
7:A:572:HOH:O	2:C:1:NDG:H2	2.03	0.59
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.85	0.59
1:B:381:TRP:HA	1:B:381:TRP:HE3	1.67	0.58
1:B:125:SER:HB3	1:B:133:TYR:CE2	2.38	0.58
1:B:82:GLY:HA2	1:B:116:TYR:CD1	2.39	0.57
1:A:408:LYS:O	1:A:410:THR:CG2	2.54	0.56
1:B:40:TYR:HA	1:B:50:GLU:O	2.07	0.55
1:B:358:ASP:HB2	4:B:1500:SO4:O4	2.08	0.53
1:A:1:ALA:HB2	1:A:27:ASP:OD1	2.08	0.53
1:B:314:LEU:HB2	1:B:343:VAL:HG12	1.90	0.53
1:A:67:LEU:HD23	1:A:438:ALA:HA	1.90	0.53
1:A:79:LYS:HE2	1:A:228:TRP:CE2	2.44	0.52
2:C:1:NDG:H6C1	2:C:2:NAG:H2	1.92	0.52
1:A:125:SER:HB3	1:A:133:TYR:CE2	2.45	0.52
1:B:371:LEU:O	1:B:433:ARG:HD2	2.10	0.51
1:A:207:GLN:NE2	1:A:263:ASP:OD1	2.41	0.50
1:B:314:LEU:HD12	1:B:343:VAL:HG13	1.94	0.49
1:A:235:GLU:OE2	1:A:313:TYR:OH	2.19	0.49
1:B:471:THR:HA	1:B:480:LEU:O	2.13	0.49
1:A:44:ARG:NH1	4:A:1503:SO4:O2	2.31	0.48
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.94	0.48
1:A:226:GLN:NE2	7:A:580:HOH:O	2.44	0.48
1:A:82:GLY:HA2	1:A:116:TYR:CD1	2.48	0.48
1:B:134:THR:HG21	1:B:182:PRO:HA	1.96	0.48
1:B:206:HIS:NE2	1:B:255:HIS:CE1	2.73	0.48
2:C:1:NDG:C6	2:C:2:NAG:H2	2.44	0.47
1:A:453:ASP:OD1	1:A:453:ASP:C	2.52	0.47
1:B:5:ILE:HG12	1:B:22:TYR:CE2	2.49	0.47
1:B:44:ARG:NH2	4:B:1501:SO4:O1	2.45	0.46
1:B:312:TRP:HD1	1:B:314:LEU:HD23	1.81	0.46
1:A:4:CYS:O	1:A:6:PRO:HD3	2.16	0.46
1:B:82:GLY:HA2	1:B:116:TYR:CG	2.51	0.46
1:A:281:LEU:HD22	1:A:288:LEU:HD21	1.98	0.46
1:A:157:LYS:O	1:A:161:ILE:HG13	2.17	0.45
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.52	0.45
1:B:480:LEU:HD12	1:B:480:LEU:N	2.32	0.45
1:A:235:GLU:OE2	1:A:311:HIS:ND1	2.48	0.45
1:B:255:HIS:HD2	7:B:541:HOH:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:TYR:OH	1:A:350:GLN:HG2	2.18	0.44
1:A:363:TYR:CD2	1:A:378:TRP:CH2	3.06	0.44
1:A:285:ARG:CZ	1:A:318:ALA:HB3	2.48	0.44
1:B:157:LYS:O	1:B:161:ILE:HG13	2.18	0.44
1:B:298:ASP:C	1:B:298:ASP:OD1	2.57	0.44
1:B:181:SER:HA	1:B:209:TRP:CZ3	2.53	0.44
1:A:67:LEU:HD12	1:A:470:LEU:HD11	1.99	0.43
1:A:285:ARG:H	1:A:285:ARG:HG2	1.60	0.43
1:A:280:MET:O	1:A:281:LEU:HB3	2.19	0.43
1:A:116:TYR:OH	1:A:420:LEU:HD13	2.19	0.43
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.53	0.43
1:B:135:TYR:O	1:B:147:PHE:HA	2.17	0.43
1:B:439:SER:O	1:B:440:GLN:HB3	2.18	0.43
1:B:13:SER:HB2	1:B:357:TRP:HB2	2.01	0.43
1:A:387:PRO:HD3	1:A:404:VAL:O	2.19	0.43
1:B:281:LEU:O	1:B:282:ASP:C	2.57	0.43
1:B:106:LYS:HE2	1:B:112:GLU:OE2	2.19	0.42
1:A:20:ALA:HB2	1:A:409:ASP:OD2	2.19	0.42
1:A:151:GLU:HB2	7:A:558:HOH:O	2.19	0.42
1:A:162:HIS:O	1:A:166:GLN:HG3	2.19	0.42
1:A:367:ILE:O	1:A:370:SER:HB2	2.19	0.42
1:B:463:ARG:HE	1:B:463:ARG:HB2	1.65	0.42
1:A:378:TRP:CZ3	1:A:420:LEU:HD21	2.55	0.41
1:A:386:ASN:OD1	1:A:386:ASN:C	2.59	0.41
1:A:87:ASP:HB2	1:A:129:SER:HA	2.01	0.41
1:A:196:SER:HB3	1:A:250:GLY:O	2.20	0.41
1:B:359:ARG:NH1	1:B:399:ASP:OD2	2.44	0.41
1:A:368:ILE:HG21	1:A:368:ILE:HD13	1.77	0.41
1:B:75:PHE:O	1:B:432:GLN:HG3	2.20	0.41
1:B:181:SER:HA	1:B:209:TRP:CH2	2.56	0.41
1:A:457:VAL:HA	1:A:492:TYR:O	2.21	0.41
1:B:316:PHE:CE2	1:B:346:LYS:HE3	2.56	0.41
1:B:382:ASN:ND2	1:B:382:ASN:H	2.18	0.40
1:A:281:LEU:O	1:A:283:ASP:HB2	2.22	0.40
1:A:203:ASP:OD1	1:A:203:ASP:C	2.60	0.40
1:B:270:ASN:O	1:B:270:ASN:CG	2.60	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	495/497 (100%)	468 (94%)	26 (5%)	1 (0%)	47	73
1	B	495/497 (100%)	467 (94%)	28 (6%)	0	100	100
All	All	990/994 (100%)	935 (94%)	54 (6%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/424 (100%)	411 (97%)	13 (3%)	40	69
1	B	424/424 (100%)	412 (97%)	12 (3%)	43	73
All	All	848/848 (100%)	823 (97%)	25 (3%)	42	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	44	ARG
1	A	155	LYS
1	A	242	SER
1	A	285	ARG

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Mol	Chain	Res	Type
1	A	310	VAL
1	A	335	MET
1	A	345	SER
1	A	348	TRP
1	A	370	SER
1	A	381	TRP
1	A	410	THR
1	A	493	LEU
1	B	31	PHE
1	B	34	LEU
1	B	169	GLN
1	B	211	ARG
1	B	255	HIS
1	B	262	ARG
1	B	335	MET
1	B	349	GLU
1	B	366	SER
1	B	370	SER
1	B	381	TRP
1	B	497	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	226	GLN
1	A	362	GLN
1	A	365	HIS
1	B	223	HIS
1	B	255	HIS
1	B	365	HIS
1	B	374	HIS

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	NDG	C	1	2	14,14,15	0.86	0	17,19,21	1.93	5 (29%)
2	NAG	C	2	2	14,14,15	1.47	3 (21%)	17,19,21	2.46	8 (47%)
3	NAG	D	1	1,3	14,14,15	0.67	0	17,19,21	1.76	2 (11%)
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	2.24	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
2	NDG	C	1	2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	3.50	1.57	1.52
2	C	2	NAG	C2-N2	2.48	1.50	1.46
2	C	2	NAG	O7-C7	2.34	1.28	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	7.72	122.66	112.19
3	D	1	NAG	C2-N2-C7	-5.24	115.44	122.90
2	C	2	NAG	C3-C4-C5	-4.76	101.74	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C5-C6	4.23	113.83	107.20
2	C	2	NAG	C1-O5-C5	4.07	117.71	112.19
2	C	1	NDG	O5-C1-C2	-3.62	105.57	111.29
2	C	1	NDG	C2-N2-C7	-3.55	117.84	122.90
3	D	1	NAG	O5-C1-C2	-3.39	105.93	111.29
2	C	2	NAG	C1-C2-N2	3.26	116.05	110.49
2	C	1	NDG	O4-C4-C5	3.14	117.08	109.30
2	C	1	NDG	C1-C2-N2	-2.90	105.54	110.49
3	D	2	NAG	C1-C2-N2	2.78	115.25	110.49
2	C	1	NDG	C1-O5-C5	2.72	115.88	112.19
2	C	2	NAG	O5-C1-C2	2.34	114.98	111.29
2	C	2	NAG	O4-C4-C5	2.33	115.08	109.30
2	C	2	NAG	C4-C3-C2	-2.08	107.97	111.02
2	C	2	NAG	O3-C3-C2	2.06	113.74	109.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

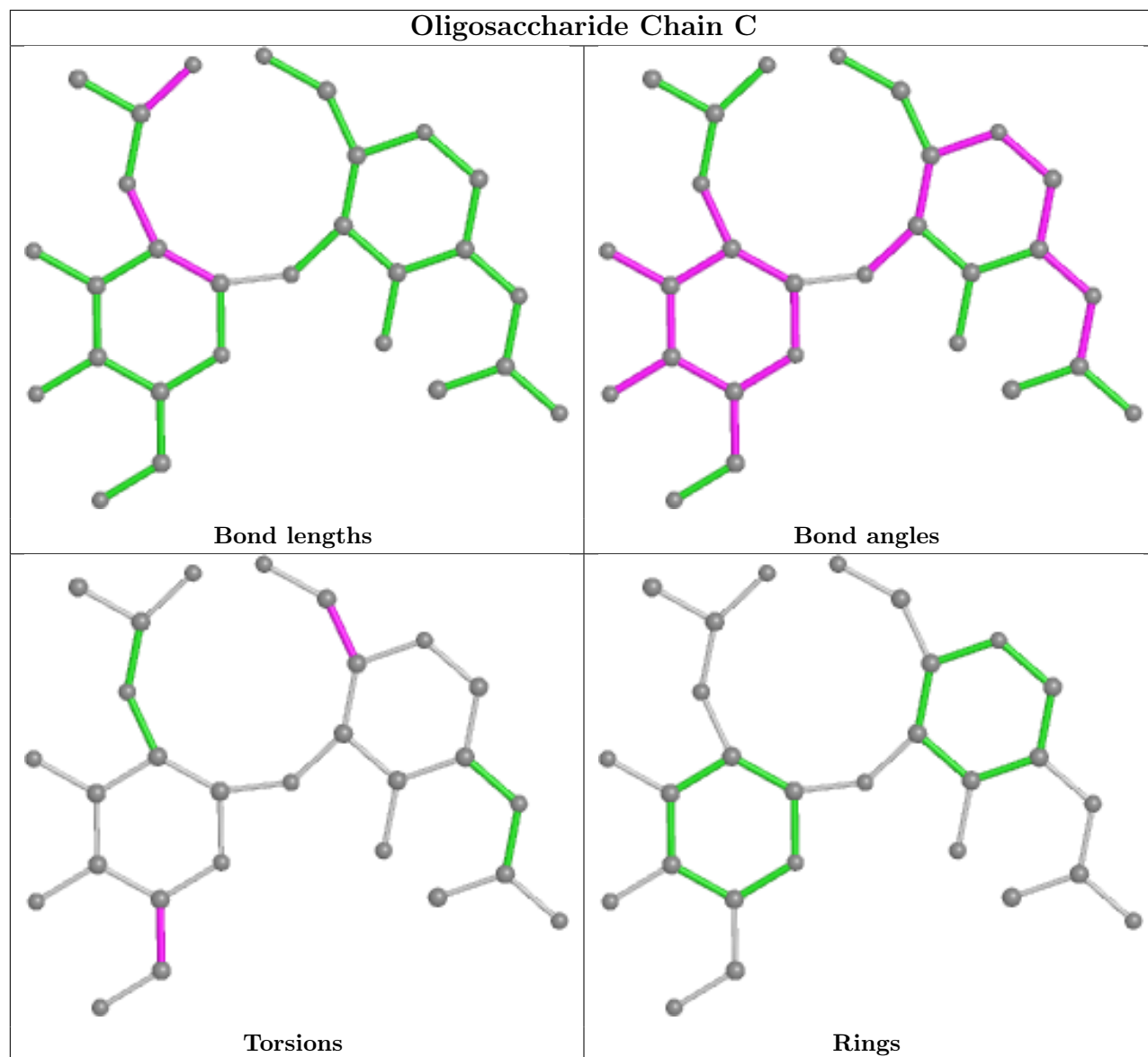
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NDG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NDG	C4-C5-C6-O6

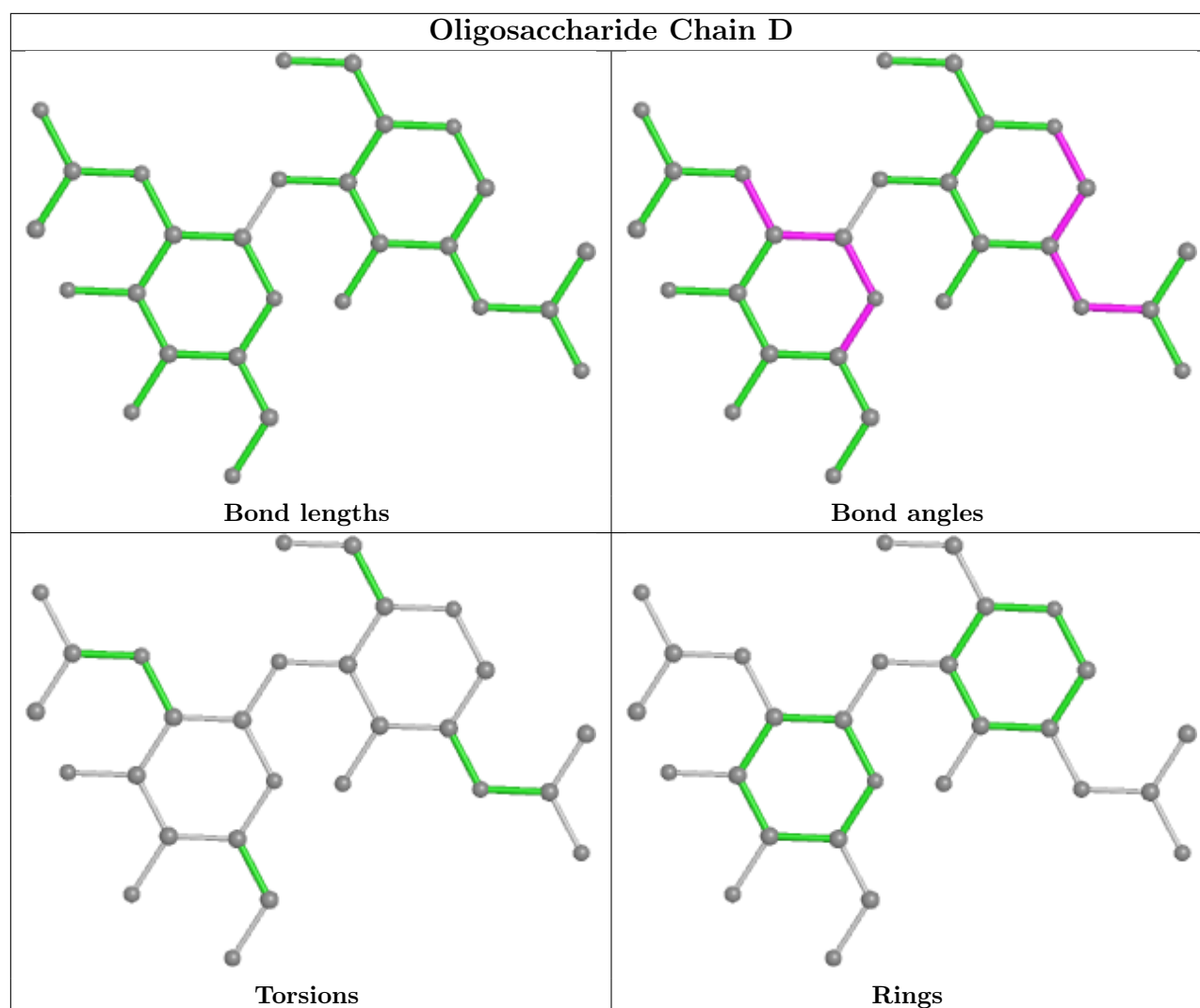
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	C	1	NDG	3	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](#)

17 ligands 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	$\# Z > 2$
4	SO4	B	1499	-	4,4,4	0.21	0	6,6,6	0.85	0
4	SO4	B	1501	-	4,4,4	0.19	0	6,6,6	0.48	0
4	SO4	B	1498	-	4,4,4	0.22	0	6,6,6	0.28	0
4	SO4	A	1505	-	4,4,4	0.12	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	1508	-	5,5,5	0.58	0	5,5,5	0.51	0
6	NAG	B	1505	1	14,14,15	0.86	0	17,19,21	2.36	5 (29%)
4	SO4	A	1506	-	4,4,4	0.23	0	6,6,6	0.83	0
4	SO4	A	1507	-	4,4,4	0.11	0	6,6,6	0.68	0
5	GOL	B	498	-	5,5,5	0.56	0	5,5,5	0.50	0
4	SO4	A	1500	-	4,4,4	0.15	0	6,6,6	0.42	0
4	SO4	A	1501	-	4,4,4	0.20	0	6,6,6	0.48	0
4	SO4	B	1500	-	4,4,4	0.24	0	6,6,6	1.03	0
4	SO4	A	1504	-	4,4,4	0.19	0	6,6,6	0.65	0
5	GOL	A	1509	-	5,5,5	0.40	0	5,5,5	0.59	0
4	SO4	B	1502	-	4,4,4	0.22	0	6,6,6	0.44	0
4	SO4	A	1503	-	4,4,4	0.25	0	6,6,6	0.52	0
4	SO4	A	1502	-	4,4,4	0.12	0	6,6,6	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	498	-	-	2/4/4/4	-
6	NAG	B	1505	1	-	2/6/23/26	0/1/1/1
5	GOL	A	1509	-	-	4/4/4/4	-
5	GOL	A	1508	-	-	2/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1505	NAG	C1-O5-C5	7.34	122.14	112.19
6	B	1505	NAG	C4-C3-C2	3.10	115.56	111.02
6	B	1505	NAG	O4-C4-C5	2.79	116.22	109.30
6	B	1505	NAG	O5-C5-C6	2.58	111.25	107.20
6	B	1505	NAG	O5-C1-C2	-2.29	107.67	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1509	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	1508	GOL	C1-C2-C3-O3
5	A	1508	GOL	O2-C2-C3-O3
5	B	498	GOL	O1-C1-C2-C3
5	A	1509	GOL	O1-C1-C2-C3
5	A	1509	GOL	O2-C2-C3-O3
6	B	1505	NAG	C4-C5-C6-O6
5	B	498	GOL	O1-C1-C2-O2
5	A	1509	GOL	O1-C1-C2-O2
6	B	1505	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1501	SO4	1	0
5	B	498	GOL	1	0
4	B	1500	SO4	1	0
4	A	1503	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/497 (100%)	-0.61	0 100 100	3, 13, 25, 37	5 (1%)
1	B	497/497 (100%)	-0.66	1 (0%) 95 96	5, 12, 26, 44	7 (1%)
All	All	994/994 (100%)	-0.63	1 (0%) 95 96	3, 12, 26, 44	12 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	THR	3.2

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](#)

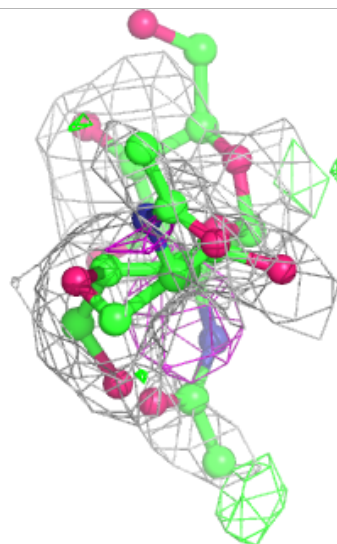
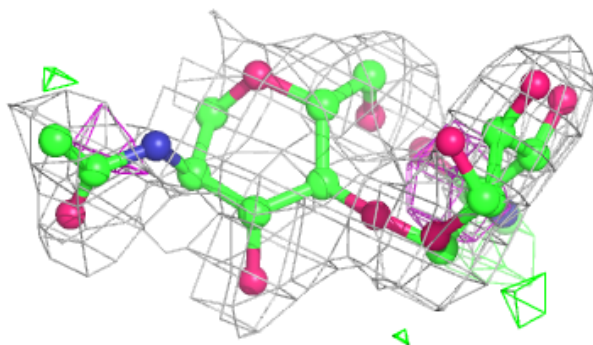
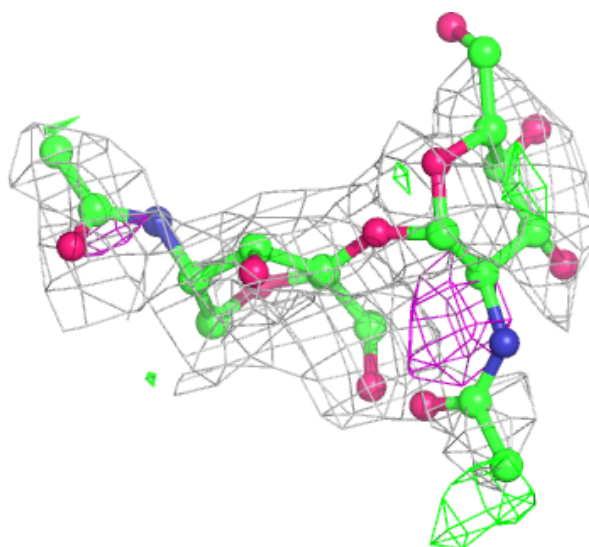
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

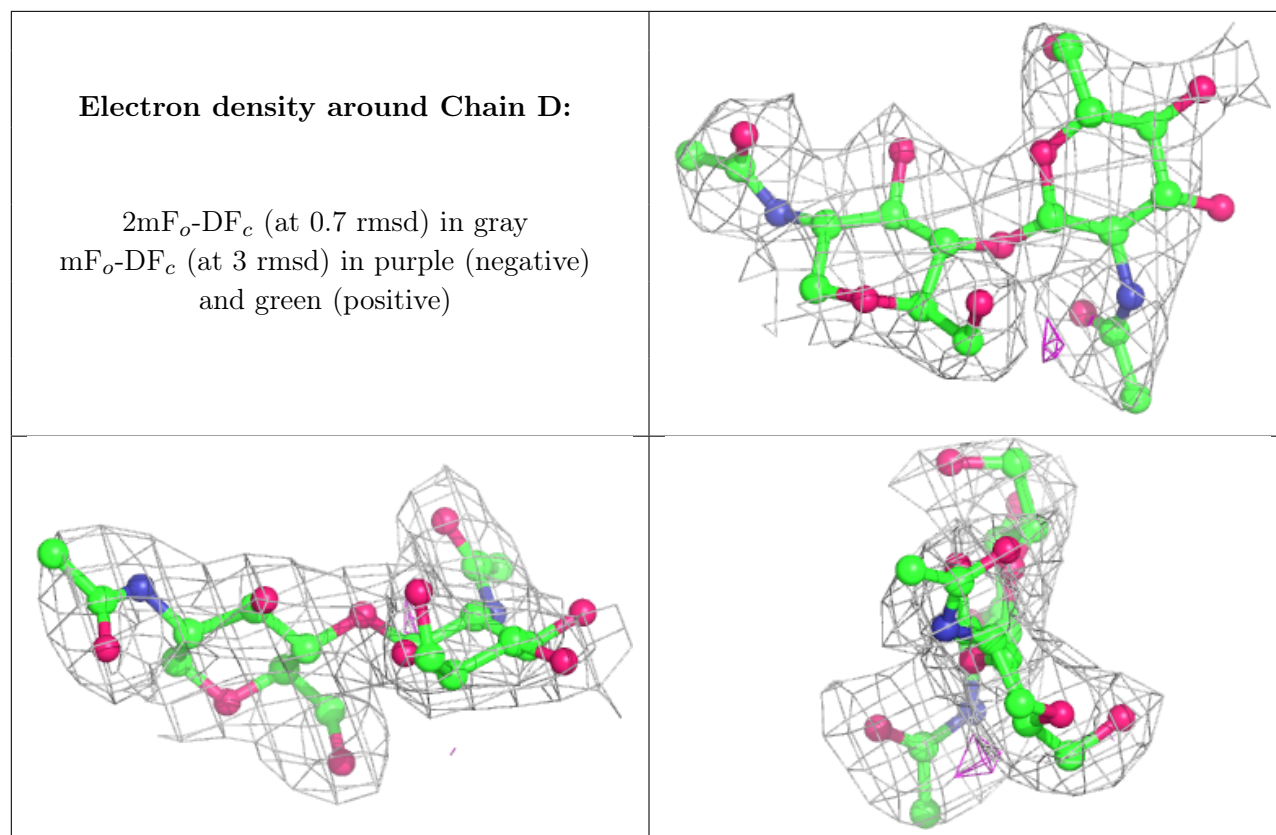
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.70	0.45	62,66,71,72	0
2	NDG	C	1	14/15	0.82	0.23	43,48,54,54	0
3	NAG	D	2	14/15	0.88	0.28	41,44,48,51	0
3	NAG	D	1	14/15	0.95	0.16	25,29,31,36	0

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

Electron density around Chain C:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	1500	5/5	0.83	0.45	75,76,77,78	0
6	NAG	B	1505	14/15	0.84	0.21	40,44,49,49	0
4	SO4	B	1502	5/5	0.85	0.29	69,70,71,71	0
4	SO4	A	1501	5/5	0.88	0.32	78,79,79,79	0
4	SO4	A	1502	5/5	0.90	0.33	86,86,86,87	0
4	SO4	A	1507	5/5	0.91	0.20	53,53,54,55	0
4	SO4	B	1501	5/5	0.92	0.22	50,51,53,53	0
4	SO4	A	1503	5/5	0.93	0.30	49,50,52,54	0
5	GOL	A	1509	6/6	0.94	0.26	31,32,33,34	0
4	SO4	A	1505	5/5	0.94	0.26	65,65,66,67	0
4	SO4	A	1506	5/5	0.95	0.15	33,37,37,38	0
4	SO4	B	1498	5/5	0.95	0.18	60,60,61,62	0
5	GOL	A	1508	6/6	0.96	0.17	19,21,21,22	0
5	GOL	B	498	6/6	0.97	0.14	14,18,21,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	1499	5/5	0.98	0.13	33,34,37,39	0
4	SO4	A	1504	5/5	0.99	0.10	15,16,17,18	0
4	SO4	B	1500	5/5	0.99	0.10	13,13,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.