



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 05:49 PM BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

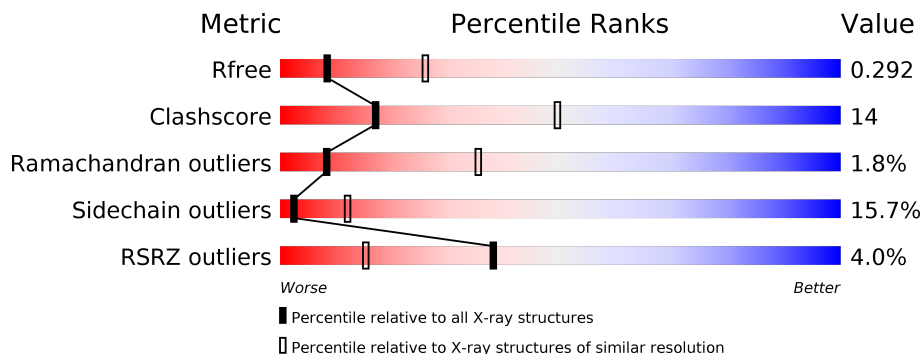
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



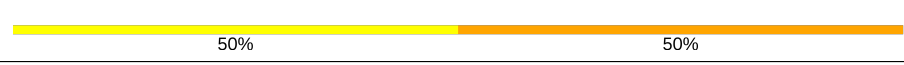

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
2	C	2	
2	D	2	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6305 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-galactosidase A.

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

- 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

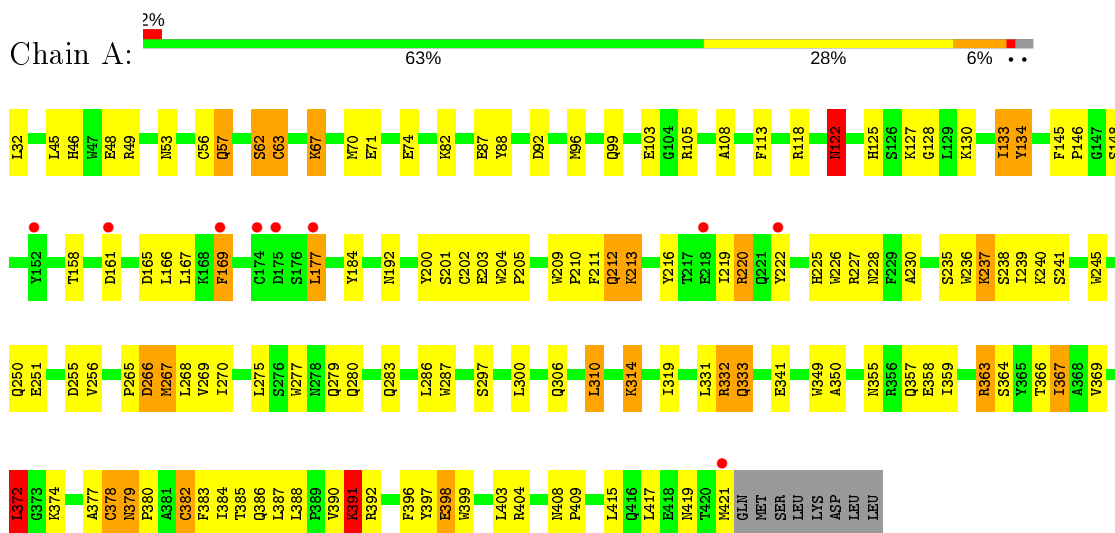


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0

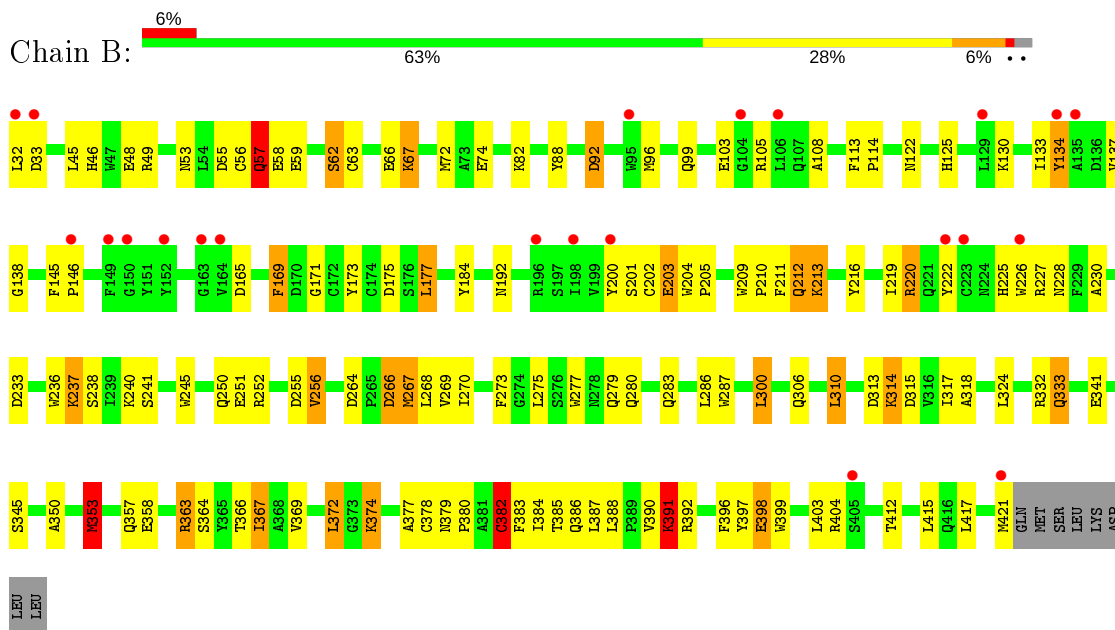
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


- Molecule 1: Alpha-galactosidase A



- Molecule 1: Alpha-galactosidase A




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

Chain C:  50% 50%

MAG1
MAG2

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

Chain D:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.38Å 90.38Å 217.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.66 – 3.01 44.66 – 3.01	Depositor EDS
% Data completeness (in resolution range)	88.1 (44.66-3.01) 88.1 (44.66-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.01Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.301 0.229 , 0.292	Depositor DCC
R_{free} test set	971 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6305	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NAG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.86	1/3209 (0.0%)	0.92	4/4358 (0.1%)
1	B	0.82	1/3209 (0.0%)	0.88	3/4358 (0.1%)
All	All	0.84	2/6418 (0.0%)	0.90	7/8716 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	CYS	CB-SG	-7.64	1.69	1.82
1	A	382	CYS	CB-SG	-7.38	1.69	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	332	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	286	LEU	CA-CB-CG	-6.59	100.14	115.30
1	B	286	LEU	CA-CB-CG	-6.50	100.36	115.30
1	A	332	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	266	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	353	MET	CG-SD-CE	5.12	108.38	100.20
1	A	388	LEU	CB-CG-CD2	-5.06	102.40	111.00

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	3122	0	2984	91	0
1	B	3122	0	2984	87	1
2	C	28	0	25	3	1
2	D	28	0	25	4	0
3	A	5	0	0	0	0
All	All	6305	0	6018	172	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 14.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:HD21	2:C:1:NAG:C1	1.60	1.15
1:B:192:ASN:HD21	2:D:1:NAG:C1	1.68	1.04
1:B:57:GLN:NE2	1:B:57:GLN:HA	1.88	0.89
1:A:386:GLN:NE2	1:A:390:VAL:HG22	1.90	0.87
1:B:53:ASN:HD22	1:B:62:SER:HB2	1.39	0.87
1:A:386:GLN:O	1:A:391:LYS:HA	1.74	0.86
1:B:53:ASN:ND2	1:B:62:SER:HB2	1.91	0.84
1:B:210:PRO:HD2	1:B:211:PHE:CE2	2.14	0.83
1:B:386:GLN:NE2	1:B:390:VAL:HG22	1.95	0.82
1:A:57:GLN:HA	1:A:57:GLN:NE2	1.96	0.79
1:B:386:GLN:O	1:B:391:LYS:HA	1.81	0.79
1:A:192:ASN:ND2	2:C:1:NAG:C1	2.43	0.79
1:A:386:GLN:HE22	1:A:390:VAL:HG22	1.48	0.78
1:A:366:THR:HG22	1:A:404:ARG:HA	1.63	0.78
1:A:46:HIS:CD2	1:A:92:ASP:H	2.03	0.77
1:A:53:ASN:HD22	1:A:62:SER:HB2	1.53	0.74
1:A:251:GLU:OE1	1:A:251:GLU:N	2.15	0.74
1:A:363:ARG:HG2	1:A:363:ARG:HH11	1.51	0.74
1:B:192:ASN:ND2	2:D:1:NAG:C1	2.48	0.73
1:A:314:LYS:N	1:A:314:LYS:HD3	2.04	0.73
1:A:145:PHE:HB3	1:A:146:PRO:HD2	1.71	0.73
1:A:384:ILE:HG12	1:A:417:LEU:HG	1.70	0.71
1:A:125:HIS:HE1	1:A:165:ASP:OD2	1.71	0.71
1:A:237:LYS:HE3	1:B:237:LYS:HE3	1.71	0.71
1:B:314:LYS:N	1:B:314:LYS:HD3	2.06	0.71
1:B:251:GLU:N	1:B:251:GLU:OE1	2.18	0.70
1:B:384:ILE:HG12	1:B:417:LEU:HG	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:N	1:A:220:ARG:O	2.25	0.70
1:B:46:HIS:CD2	1:B:92:ASP:H	2.09	0.70
1:B:386:GLN:HE22	1:B:390:VAL:HG22	1.58	0.69
1:A:367:ILE:HD12	1:A:403:LEU:HB3	1.74	0.69
1:B:210:PRO:HD2	1:B:211:PHE:CZ	2.28	0.68
1:B:145:PHE:HB3	1:B:146:PRO:HD2	1.74	0.68
1:B:57:GLN:HE21	1:B:57:GLN:HA	1.59	0.67
1:B:366:THR:HG22	1:B:404:ARG:HA	1.77	0.66
1:A:216:TYR:HA	1:A:219:ILE:HD12	1.77	0.64
1:A:239:ILE:HD12	1:A:275:LEU:HD21	1.80	0.63
1:A:213:LYS:HD2	1:A:213:LYS:H	1.63	0.63
1:B:192:ASN:HD21	2:D:1:NAG:C2	2.10	0.63
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.33	0.62
1:A:367:ILE:CD1	1:A:403:LEU:HB3	2.28	0.62
1:A:409:PRO:HD2	1:B:273:PHE:CD2	2.34	0.62
1:B:367:ILE:HD12	1:B:403:LEU:HB3	1.80	0.62
1:A:32:LEU:HD22	1:A:222:TYR:O	1.98	0.62
1:B:383:PHE:HD1	1:B:396:PHE:CE1	2.18	0.62
1:B:390:VAL:O	1:B:391:LYS:CB	2.47	0.61
1:B:367:ILE:CD1	1:B:403:LEU:HB3	2.30	0.61
1:A:225:HIS:HA	1:A:226:TRP:CE3	2.35	0.61
1:B:177:LEU:H	1:B:177:LEU:HD12	1.64	0.61
1:B:57:GLN:CA	1:B:57:GLN:NE2	2.63	0.61
1:B:213:LYS:H	1:B:213:LYS:HD2	1.66	0.60
1:A:210:PRO:HD2	1:A:211:PHE:CE2	2.36	0.60
1:A:269:VAL:HG23	1:A:275:LEU:HD11	1.84	0.60
1:A:177:LEU:HD12	1:A:177:LEU:H	1.67	0.59
1:A:277:TRP:HA	1:A:280:GLN:HE21	1.67	0.59
1:B:227:ARG:HH11	1:B:227:ARG:HG3	1.67	0.59
1:A:270:ILE:HD13	1:A:310:LEU:HD13	1.86	0.58
1:A:220:ARG:NH1	1:A:256:VAL:O	2.35	0.58
1:A:386:GLN:NE2	1:A:390:VAL:CG2	2.66	0.57
1:A:53:ASN:ND2	1:A:62:SER:HB2	2.19	0.57
1:B:250:GLN:O	1:B:251:GLU:C	2.42	0.57
1:A:363:ARG:HG2	1:A:363:ARG:NH1	2.20	0.56
1:B:277:TRP:HA	1:B:280:GLN:HE21	1.71	0.56
1:A:366:THR:HG22	1:A:404:ARG:CA	2.35	0.56
1:A:57:GLN:NE2	1:A:57:GLN:CA	2.69	0.55
1:B:137:VAL:HG12	1:B:171:GLY:HA2	1.89	0.55
1:A:384:ILE:HD12	1:A:397:TYR:CD1	2.41	0.55
1:B:138:GLY:HA3	1:B:173:TYR:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:HIS:HA	1:B:226:TRP:CE3	2.42	0.54
1:A:237:LYS:CE	1:B:237:LYS:HE3	2.37	0.54
1:B:57:GLN:CA	1:B:57:GLN:HE21	2.21	0.53
1:A:158:THR:O	1:A:161:ASP:HB2	2.08	0.53
1:A:103:GLU:CD	1:A:105:ARG:HH12	2.12	0.53
1:A:125:HIS:O	1:A:128:GLY:N	2.33	0.53
1:B:108:ALA:HB1	1:B:113:PHE:HB2	1.91	0.53
1:B:32:LEU:N	1:B:220:ARG:O	2.41	0.53
1:B:363:ARG:HG2	1:B:363:ARG:HH11	1.74	0.52
1:A:398:GLU:HA	1:A:398:GLU:OE2	2.08	0.52
1:B:66:GLU:OE1	1:B:114:PRO:HG2	2.09	0.52
1:A:355:ASN:HB3	1:A:408:ASN:O	2.10	0.52
1:B:403:LEU:HD21	1:B:415:LEU:HD13	1.92	0.52
1:B:216:TYR:HA	1:B:219:ILE:HD12	1.90	0.51
1:A:366:THR:HA	1:A:403:LEU:O	2.10	0.51
1:B:201:SER:HB2	1:B:225:HIS:CE1	2.46	0.51
1:B:386:GLN:HA	1:B:415:LEU:HD23	1.92	0.51
1:B:269:VAL:HG23	1:B:275:LEU:HD11	1.93	0.50
1:B:270:ILE:HD13	1:B:310:LEU:HD13	1.94	0.50
1:A:211:PHE:O	1:A:212:GLN:HB3	2.11	0.50
1:B:203:GLU:HG3	1:B:227:ARG:HB2	1.93	0.50
1:A:235:SER:OG	1:A:238:SER:HB2	2.12	0.50
1:B:32:LEU:HD22	1:B:222:TYR:O	2.12	0.50
1:A:319:ILE:HD11	1:A:387:LEU:CD2	2.42	0.49
1:B:72:MET:SD	1:B:300:LEU:HB2	2.52	0.49
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.93	0.49
1:A:386:GLN:HA	1:A:415:LEU:HD23	1.95	0.49
1:A:268:LEU:HA	1:A:283:GLN:HE22	1.78	0.49
1:A:390:VAL:O	1:A:391:LYS:CB	2.61	0.48
1:A:108:ALA:HB1	1:A:113:PHE:HB2	1.95	0.48
1:B:125:HIS:HE1	1:B:165:ASP:OD2	1.96	0.48
1:B:382:CYS:HB3	1:B:397:TYR:HB2	1.96	0.48
1:A:236:TRP:NE1	1:A:240:LYS:HD2	2.28	0.48
1:A:359:ILE:HD12	1:B:233:ASP:HB3	1.95	0.48
1:B:236:TRP:CE3	1:B:279:GLN:HG2	2.48	0.48
1:A:203:GLU:HG3	1:A:227:ARG:HB2	1.96	0.48
1:A:134:TYR:CD2	1:A:134:TYR:C	2.87	0.47
1:B:353:MET:O	1:B:412:THR:HA	2.14	0.47
1:A:88:TYR:CZ	1:A:130:LYS:HD2	2.49	0.47
1:B:67:LYS:HD3	1:B:67:LYS:H	1.79	0.47
1:A:331:LEU:HD22	1:A:341:GLU:OE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLN:NE2	1:B:390:VAL:CG2	2.73	0.47
1:B:55:ASP:OD2	1:B:57:GLN:HB2	2.14	0.47
1:A:166:LEU:HD23	1:A:167:LEU:N	2.29	0.47
1:B:372:LEU:HA	1:B:372:LEU:HD12	1.70	0.47
1:A:403:LEU:HD21	1:A:415:LEU:HD13	1.97	0.47
1:A:67:LYS:HD3	1:A:67:LYS:H	1.80	0.47
1:B:372:LEU:O	1:B:374:LYS:N	2.42	0.47
1:A:202:CYS:O	1:A:226:TRP:HA	2.15	0.46
1:A:372:LEU:HA	1:A:372:LEU:HD12	1.75	0.46
1:B:398:GLU:OE2	1:B:398:GLU:HA	2.15	0.46
1:B:378:CYS:O	1:B:399:TRP:HD1	1.99	0.46
1:B:341:GLU:HA	1:B:350:ALA:O	2.15	0.46
1:B:211:PHE:O	1:B:212:GLN:HB3	2.16	0.46
1:A:210:PRO:HD2	1:A:211:PHE:CZ	2.51	0.45
1:B:228:ASN:HB3	1:B:245:TRP:CH2	2.51	0.45
1:B:88:TYR:CZ	1:B:130:LYS:HD2	2.52	0.45
1:A:250:GLN:O	1:A:251:GLU:C	2.55	0.45
1:B:33:ASP:O	2:D:1:NAG:H4	2.16	0.45
1:B:377:ALA:O	1:B:378:CYS:SG	2.75	0.45
1:A:404:ARG:HH12	1:B:58:GLU:HB3	1.82	0.44
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.53	0.44
1:A:237:LYS:NZ	1:B:237:LYS:HE3	2.33	0.44
1:A:267:MET:SD	1:A:297:SER:HB2	2.57	0.44
1:B:315:ASP:O	1:B:318:ALA:HB3	2.18	0.44
1:A:118:ARG:O	1:A:122:ASN:HB2	2.16	0.44
1:B:268:LEU:HA	1:B:283:GLN:HE22	1.82	0.44
1:B:313:ASP:O	1:B:317:ILE:HG13	2.18	0.44
1:B:236:TRP:CD1	1:B:240:LYS:HD2	2.53	0.44
1:B:366:THR:HG22	1:B:404:ARG:CA	2.46	0.44
1:B:384:ILE:HD12	1:B:397:TYR:CD1	2.52	0.44
1:A:201:SER:HB2	1:A:225:HIS:CE1	2.53	0.44
1:A:378:CYS:O	1:A:399:TRP:HD1	2.01	0.43
1:B:333:GLN:HB2	1:B:333:GLN:HE21	1.55	0.43
1:B:390:VAL:O	1:B:391:LYS:HB2	2.17	0.43
1:A:265:PRO:O	1:A:266:ASP:CB	2.67	0.43
1:A:228:ASN:HB3	1:A:245:TRP:CZ3	2.54	0.43
1:A:277:TRP:HA	1:A:280:GLN:NE2	2.32	0.43
1:A:57:GLN:HA	1:A:57:GLN:HE21	1.81	0.43
1:A:67:LYS:O	1:A:71:GLU:HB2	2.19	0.43
1:B:48:GLU:N	1:B:267:MET:HE1	2.33	0.43
1:A:383:PHE:HD1	1:A:396:PHE:CE1	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ASN:HA	1:B:380:PRO:HA	1.87	0.42
1:A:200:TYR:CE2	1:A:202:CYS:SG	3.12	0.42
1:A:341:GLU:HA	1:A:350:ALA:O	2.19	0.42
1:B:134:TYR:C	1:B:134:TYR:CD2	2.93	0.42
1:B:200:TYR:CE2	1:B:202:CYS:SG	3.12	0.42
1:B:220:ARG:NH1	1:B:256:VAL:O	2.53	0.42
1:A:169:PHE:HB3	1:A:184:TYR:HE1	1.85	0.42
1:A:417:LEU:HD12	1:A:417:LEU:N	2.34	0.42
1:A:192:ASN:ND2	2:C:1:NAG:O7	2.53	0.42
1:A:379:ASN:HA	1:A:380:PRO:HA	1.81	0.41
1:A:48:GLU:N	1:A:267:MET:HE1	2.36	0.41
1:B:366:THR:HA	1:B:403:LEU:O	2.20	0.41
1:A:333:GLN:HE21	1:A:333:GLN:HB2	1.60	0.41
1:B:237:LYS:HB2	1:B:237:LYS:HE2	1.69	0.41
1:A:349:TRP:CD1	1:A:377:ALA:HB2	2.56	0.41
1:B:169:PHE:HB3	1:B:184:TYR:HE1	1.86	0.41
1:B:226:TRP:O	1:B:264:ASP:HB3	2.21	0.41
1:A:378:CYS:O	1:A:399:TRP:CD1	2.74	0.40
1:B:204:TRP:HB3	1:B:205:PRO:HD3	2.02	0.40
1:B:103:GLU:CD	1:B:105:ARG:HH12	2.25	0.40
1:A:133:ILE:HG13	1:A:134:TYR:H	1.86	0.40
1:A:62:SER:O	1:A:63:CYS:C	2.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PRO:CB	2:C:1:NAG:O5[4_545]	2.05	0.15

5.3 Torsion angles [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	388/398 (98%)	347 (89%)	33 (8%)	8 (2%)	7	31
1	B	388/398 (98%)	342 (88%)	40 (10%)	6 (2%)	10	40
All	All	776/796 (98%)	689 (89%)	73 (9%)	14 (2%)	8	35

All (14) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/339 (98%)	282 (85%)	49 (15%)	3	13
1	B	331/339 (98%)	276 (83%)	55 (17%)	2	10
All	All	662/678 (98%)	558 (84%)	104 (16%)	2	12

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	49	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	56	CYS
1	A	62	SER
1	A	63	CYS
1	A	67	LYS
1	A	70	MET
1	A	74	GLU
1	A	82	LYS
1	A	87	GLU
1	A	96	MET
1	A	99	GLN
1	A	122	ASN
1	A	127	LYS
1	A	133	ILE
1	A	134	TYR
1	A	148	SER
1	A	169	PHE
1	A	177	LEU
1	A	209	TRP
1	A	213	LYS
1	A	220	ARG
1	A	237	LYS
1	A	241	SER
1	A	255	ASP
1	A	267	MET
1	A	287	TRP
1	A	300	LEU
1	A	306	GLN
1	A	310	LEU
1	A	314	LYS
1	A	332	ARG
1	A	333	GLN
1	A	357	GLN
1	A	358	GLU
1	A	363	ARG
1	A	364	SER
1	A	367	ILE
1	A	369	VAL
1	A	372	LEU
1	A	374	LYS
1	A	379	ASN
1	A	382	CYS
1	A	385	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	391	LYS
1	A	392	ARG
1	A	398	GLU
1	A	419	ASN
1	A	421	MET
1	B	45	LEU
1	B	49	ARG
1	B	56	CYS
1	B	57	GLN
1	B	59	GLU
1	B	62	SER
1	B	63	CYS
1	B	67	LYS
1	B	74	GLU
1	B	82	LYS
1	B	92	ASP
1	B	96	MET
1	B	99	GLN
1	B	122	ASN
1	B	133	ILE
1	B	134	TYR
1	B	169	PHE
1	B	177	LEU
1	B	203	GLU
1	B	209	TRP
1	B	213	LYS
1	B	220	ARG
1	B	237	LYS
1	B	238	SER
1	B	241	SER
1	B	252	ARG
1	B	255	ASP
1	B	256	VAL
1	B	267	MET
1	B	287	TRP
1	B	300	LEU
1	B	306	GLN
1	B	310	LEU
1	B	314	LYS
1	B	324	LEU
1	B	332	ARG
1	B	333	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	345	SER
1	B	353	MET
1	B	357	GLN
1	B	358	GLU
1	B	363	ARG
1	B	364	SER
1	B	367	ILE
1	B	369	VAL
1	B	372	LEU
1	B	374	LYS
1	B	382	CYS
1	B	385	THR
1	B	387	LEU
1	B	388	LEU
1	B	391	LYS
1	B	392	ARG
1	B	398	GLU
1	B	421	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	57	GLN
1	A	125	HIS
1	A	192	ASN
1	A	212	GLN
1	A	280	GLN
1	A	333	GLN
1	A	379	ASN
1	A	386	GLN
1	B	46	HIS
1	B	57	GLN
1	B	125	HIS
1	B	179	ASN
1	B	186	HIS
1	B	192	ASN
1	B	212	GLN
1	B	280	GLN
1	B	333	GLN
1	B	379	ASN
1	B	386	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2	14,14,15	0.69	0	17,19,21	2.07	3 (17%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	2.68	6 (35%)
2	NAG	D	1	2	14,14,15	0.68	0	17,19,21	1.21	1 (5%)
2	NAG	D	2	2	14,14,15	0.86	0	17,19,21	2.37	5 (29%)

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

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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	7.91	122.91	112.19
2	D	2	NAG	O5-C5-C6	-4.84	99.62	107.20
2	C	1	NAG	O5-C1-C2	-4.68	103.91	111.29
2	C	1	NAG	C2-N2-C7	-4.61	116.34	122.90
2	D	2	NAG	C1-O5-C5	4.50	118.29	112.19
2	C	1	NAG	O5-C5-C6	4.20	113.79	107.20
2	C	2	NAG	O7-C7-N2	3.71	128.77	121.95
2	D	2	NAG	C2-N2-C7	-3.50	117.92	122.90
2	D	2	NAG	O5-C1-C2	-3.48	105.80	111.29
2	C	2	NAG	O5-C1-C2	3.47	116.77	111.29
2	C	2	NAG	C2-N2-C7	3.39	127.73	122.90
2	D	2	NAG	C3-C4-C5	3.23	116.01	110.24
2	D	1	NAG	C2-N2-C7	3.14	127.38	122.90
2	C	2	NAG	C8-C7-N2	-2.57	111.75	116.10
2	C	2	NAG	O5-C5-C4	2.20	116.18	110.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

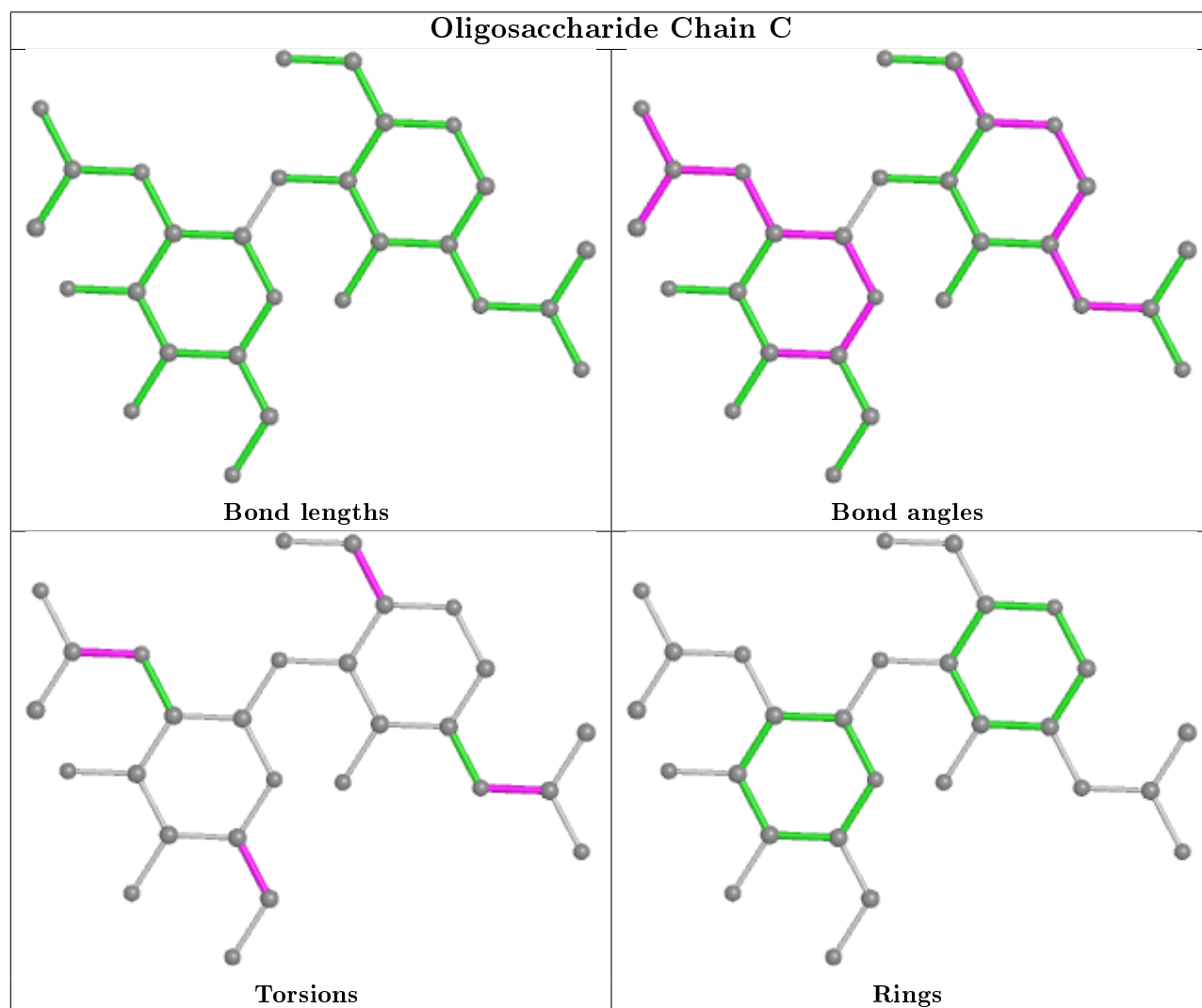
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2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

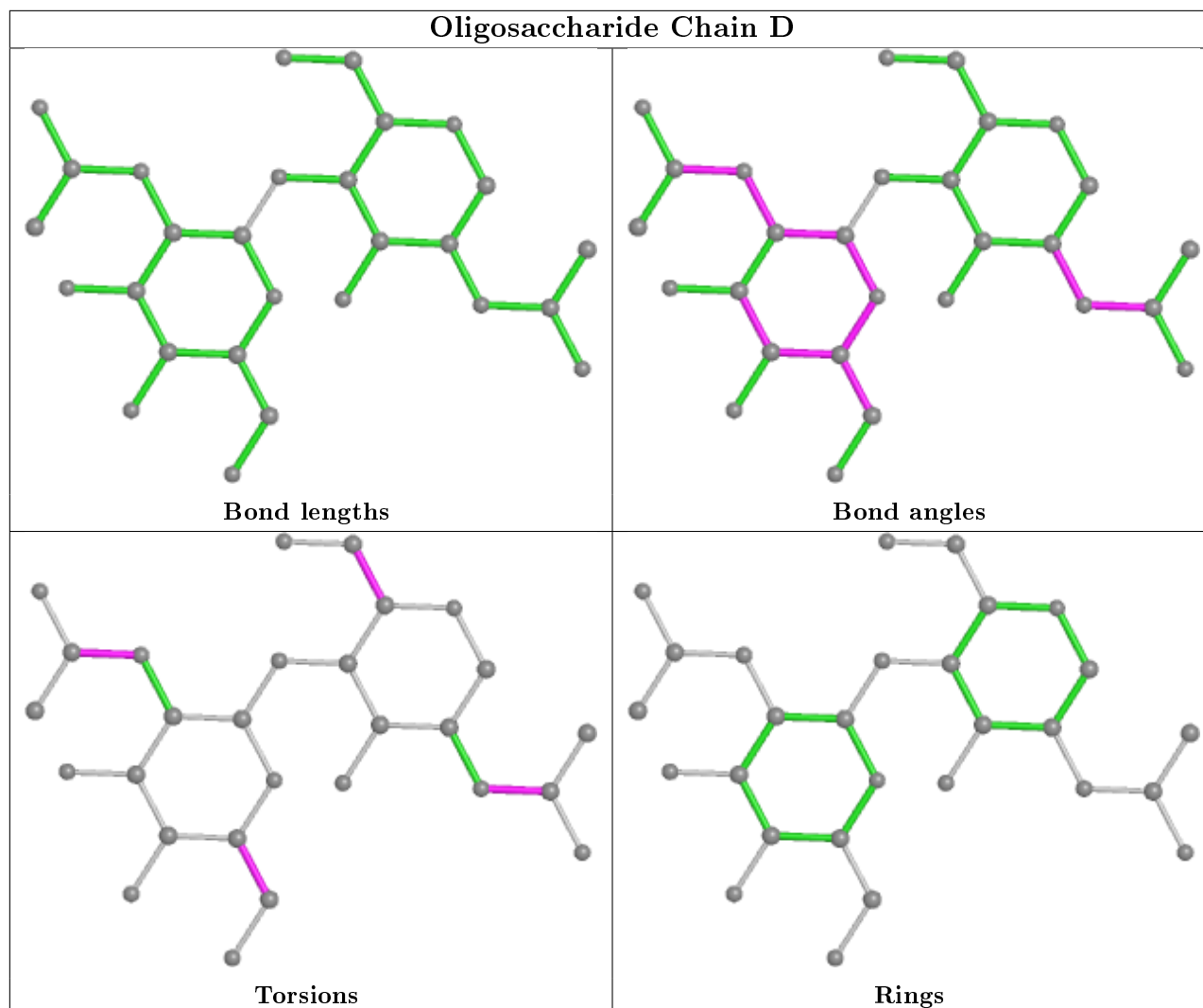
There are no ring outliers.

2 monomers are involved in 8 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.12	0	6,6,6	0.84	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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(Å ²)	Q<0.9
1	A	390/398 (97%)	0.05	9 (2%) 60 31	117, 121, 123, 128	0
1	B	390/398 (97%)	0.19	22 (5%) 24 8	117, 121, 123, 128	0
All	All	780/796 (97%)	0.12	31 (3%) 38 15	117, 121, 123, 128	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	GLY	5.2
1	A	222	TYR	4.3
1	A	177	LEU	3.8
1	B	405	SER	3.5
1	B	223	CYS	3.4
1	B	95	TRP	3.3
1	B	421	MET	3.2
1	B	149	PHE	3.0
1	B	163	GLY	2.8
1	B	196	ARG	2.7
1	B	222	TYR	2.7
1	B	32	LEU	2.7
1	B	129	LEU	2.7
1	B	164	VAL	2.6
1	A	421	MET	2.5
1	B	33	ASP	2.5
1	A	152	TYR	2.5
1	B	150	GLY	2.4
1	B	152	TYR	2.4
1	A	175	ASP	2.4
1	B	146	PRO	2.4
1	B	226	TRP	2.3
1	B	198	ILE	2.2
1	A	218	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	161	ASP	2.1
1	A	169	PHE	2.1
1	A	174	CYS	2.1
1	B	135	ALA	2.1
1	B	106	LEU	2.0
1	B	134	TYR	2.0
1	B	200	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](#)

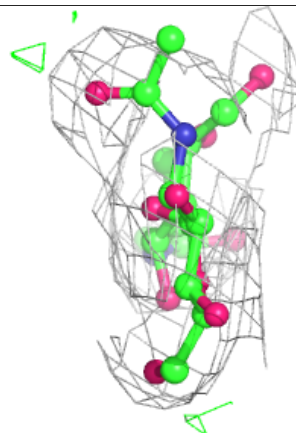
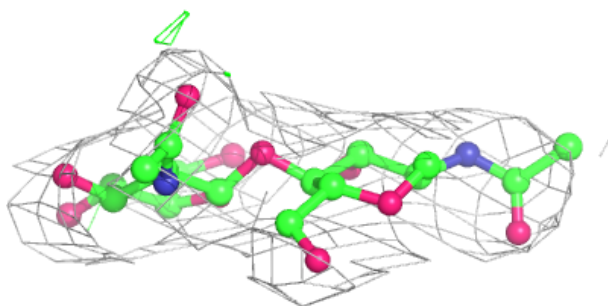
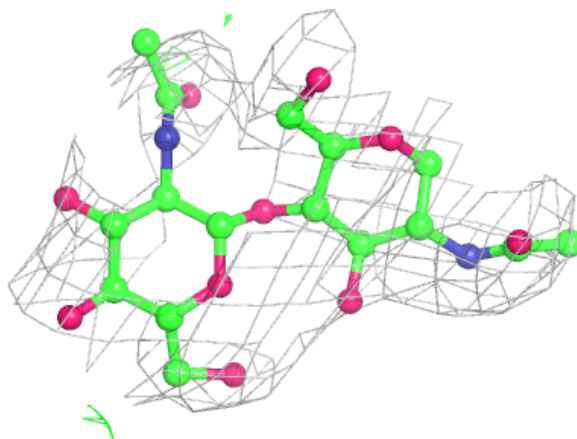
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

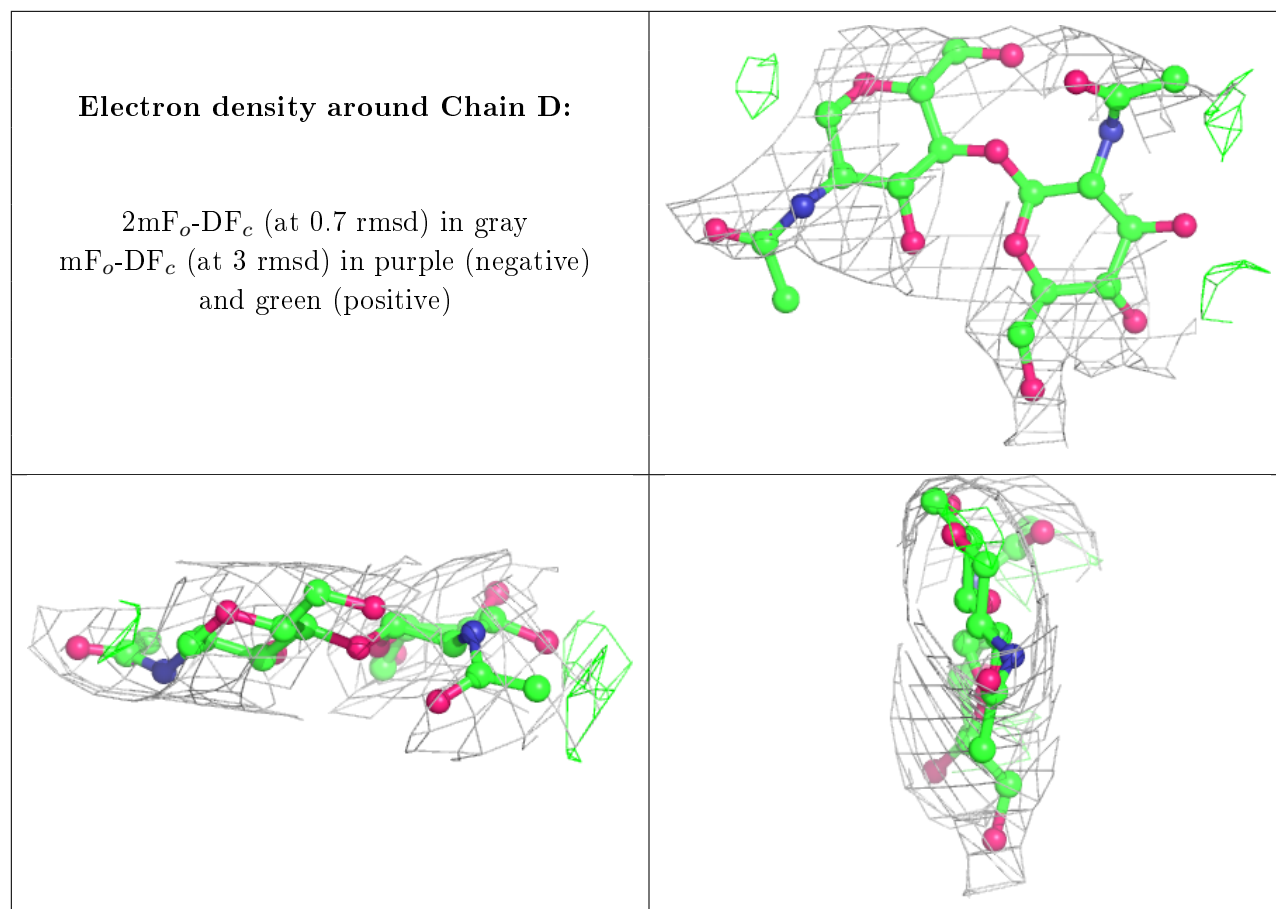
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.87	0.19	141,143,144,144	0
2	NAG	C	2	14/15	0.89	0.20	136,138,140,141	0
2	NAG	D	1	14/15	0.91	0.29	142,144,147,150	0
2	NAG	C	1	14/15	0.94	0.12	126,130,134,136	0

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

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(Å ²)	Q<0.9
3	SO4	A	1	5/5	0.97	0.07	125,126,127,127	0

6.5 Other polymers [i](#)

There are no such residues in this entry.