



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 12:28 AM EDT

PDB ID : 3LXA
Title : Interconversion of Human Lysosomal Enzyme Specificities
Authors : Tomasic, I.B.; Metcalf, M.C.; Guce, A.I.; Clark, N.E.; Garman, S.C.
Deposited on : 2010-02-25
Resolution : 3.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

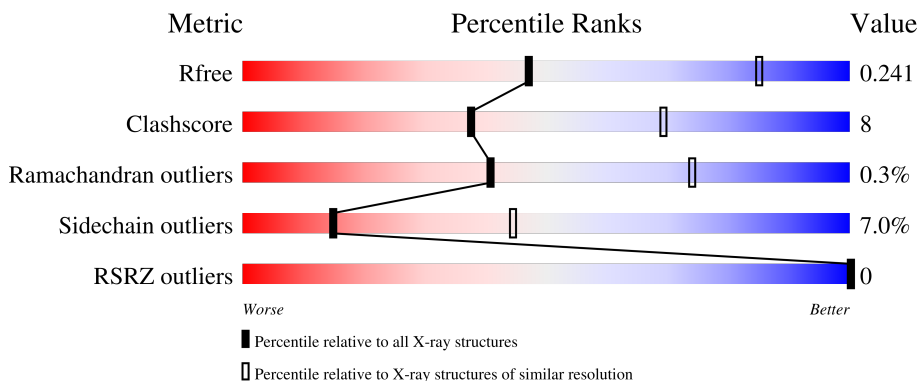
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 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	404	 74% 21% ..
1	B	404	 78% 17% ..
2	C	4	 25% 75%
2	E	4	 25% 25% 50%
3	D	2	 50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6557 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	395	3156	2008	541	580	27	0	0	0
1	B	394	3147	2002	539	579	27	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	GLU	engineered mutation	UNP P06280
A	206	ALA	LEU	engineered mutation	UNP P06280
A	430	HIS	-	expression tag	UNP P06280
A	431	HIS	-	expression tag	UNP P06280
A	432	HIS	-	expression tag	UNP P06280
A	433	HIS	-	expression tag	UNP P06280
A	434	HIS	-	expression tag	UNP P06280
A	435	HIS	-	expression tag	UNP P06280
B	203	SER	GLU	engineered mutation	UNP P06280
B	206	ALA	LEU	engineered mutation	UNP P06280
B	430	HIS	-	expression tag	UNP P06280
B	431	HIS	-	expression tag	UNP P06280
B	432	HIS	-	expression tag	UNP P06280
B	433	HIS	-	expression tag	UNP P06280
B	434	HIS	-	expression tag	UNP P06280
B	435	HIS	-	expression tag	UNP P06280

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



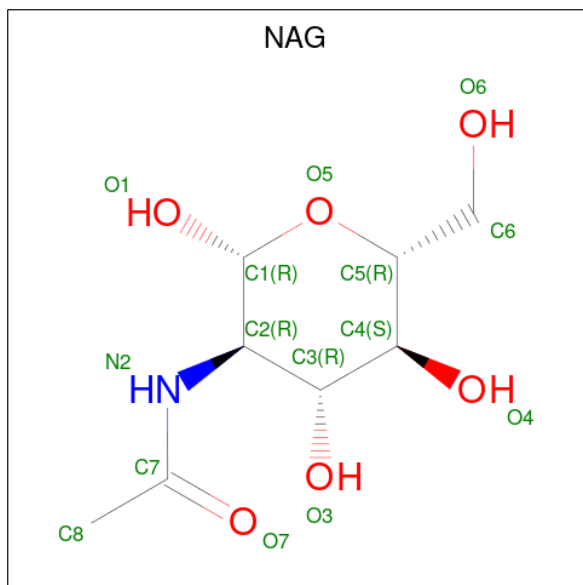
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



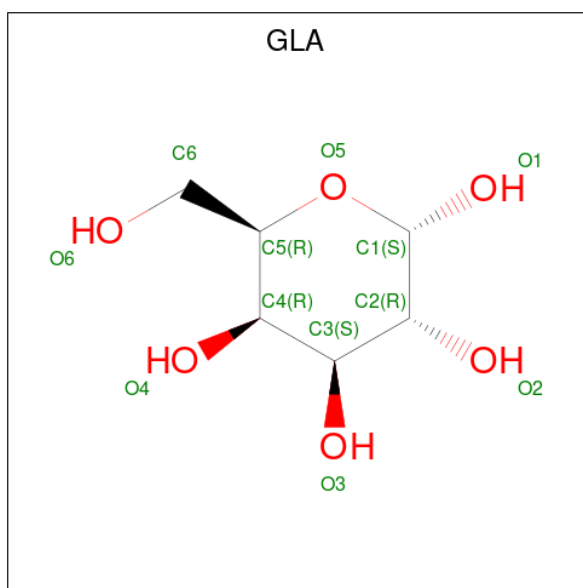
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 5 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 6 6	0	0
5	A	1	Total C O 12 6 6	0	0
5	B	1	Total C O 12 6 6	0	0
5	B	1	Total C O 12 6 6	0	0

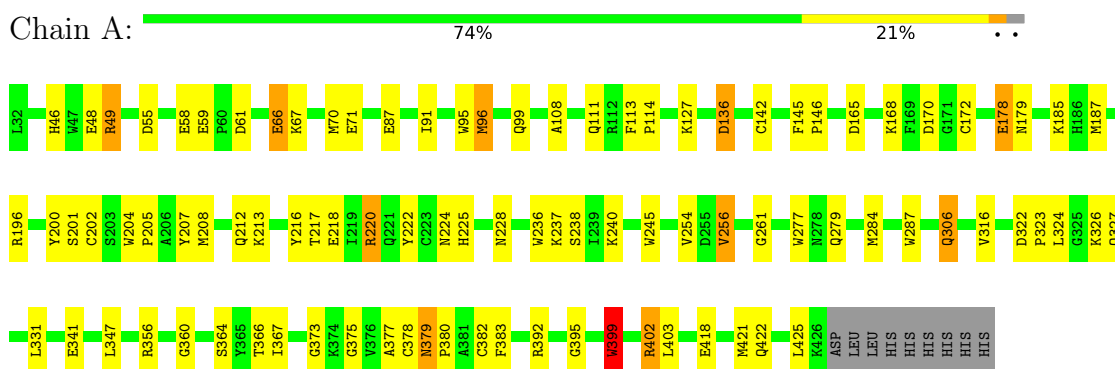
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	19	Total O 19 19	0	0
6	B	17	Total O 17 17	0	0

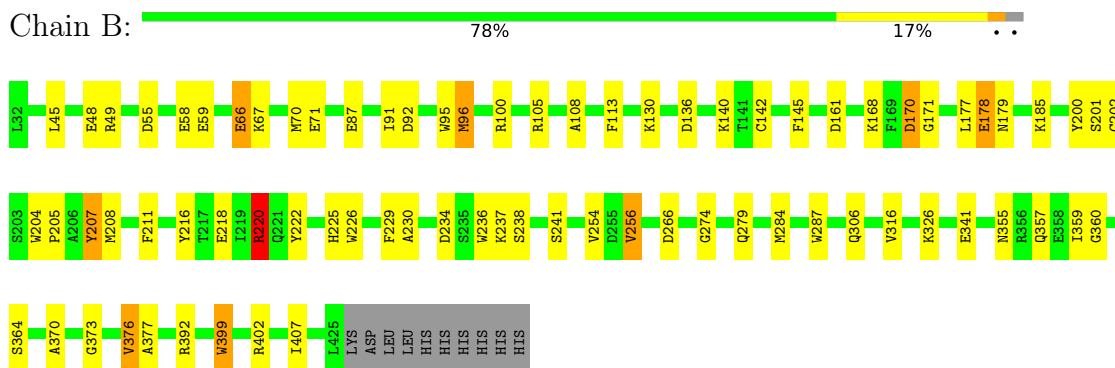
3 Residue-property plots [i](#)

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



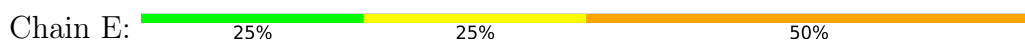
- Molecule 1: Alpha-galactosidase A



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



- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-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

Chain D:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.24Å 104.96Å 181.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.04 49.62 – 3.04	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.63-3.04) 99.5 (49.62-3.04)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.07Å)	Xtrriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.214 , 0.244 0.213 , 0.241	Depositor DCC
R_{free} test set	1128 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6557	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: GLA, NAG, BMA, MAN

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	0.70	7/3243 (0.2%)	0.70	4/4402 (0.1%)
1	B	0.75	8/3234 (0.2%)	0.70	7/4391 (0.2%)
All	All	0.72	15/6477 (0.2%)	0.70	11/8793 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	GLU	CD-OE2	24.13	1.52	1.25
1	A	178	GLU	CD-OE2	21.75	1.49	1.25
1	B	399	TRP	CG-CD1	-8.01	1.25	1.36
1	B	207	TYR	CE1-CZ	-7.16	1.29	1.38
1	A	399	TRP	CG-CD1	-7.00	1.26	1.36
1	A	207	TYR	CE1-CZ	-6.67	1.29	1.38
1	A	207	TYR	CE2-CZ	-6.63	1.29	1.38
1	B	207	TYR	CE2-CZ	-6.55	1.30	1.38
1	B	207	TYR	CG-CD2	-6.39	1.30	1.39
1	B	207	TYR	CG-CD1	-6.25	1.31	1.39
1	A	207	TYR	CG-CD2	-5.80	1.31	1.39
1	A	207	TYR	CG-CD1	-5.50	1.31	1.39
1	A	399	TRP	CB-CG	-5.45	1.40	1.50
1	B	399	TRP	CB-CG	-5.44	1.40	1.50
1	B	220	ARG	CZ-NH1	5.40	1.40	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	399	TRP	CA-CB-CG	-6.78	100.81	113.70
1	A	220	ARG	CG-CD-NE	-6.70	97.72	111.80
1	A	218	GLU	OE1-CD-OE2	-6.11	115.96	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	TRP	CB-CG-CD1	-5.86	119.39	127.00
1	A	66	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	B	399	TRP	CB-CG-CD2	5.72	134.03	126.60
1	B	218	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	B	220	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	136	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	66	GLU	OE1-CD-OE2	-5.04	117.25	123.30

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	3156	0	3020	58	0
1	B	3147	0	3007	41	0
2	C	50	0	43	0	0
2	E	50	0	43	1	0
3	D	28	0	25	3	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
5	A	24	0	24	2	0
5	B	24	0	24	1	0
6	A	19	0	0	1	0
6	B	17	0	0	1	0
All	All	6557	0	6225	98	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 8.

All (98) 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:379:ASN:HB2	1:A:399:TRP:HE3	1.40	0.85
1:A:399:TRP:C	1:A:399:TRP:CD1	2.50	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASN:HB2	1:A:399:TRP:CE3	2.17	0.80
1:B:370:ALA:HA	1:B:399:TRP:HE1	1.46	0.79
1:A:378:CYS:O	1:A:399:TRP:HB2	1.83	0.78
1:A:67:LYS:HE3	1:A:71:GLU:OE2	1.85	0.76
1:B:67:LYS:HE3	1:B:71:GLU:OE2	1.86	0.75
1:A:375:GLY:O	1:A:399:TRP:HZ3	1.73	0.71
1:A:379:ASN:HD22	1:A:380:PRO:HA	1.56	0.71
1:B:177:LEU:HD11	1:B:211:PHE:HB3	1.74	0.70
1:B:177:LEU:HD11	1:B:211:PHE:CB	2.22	0.69
1:B:399:TRP:CD1	1:B:399:TRP:O	2.49	0.66
1:B:136:ASP:OD1	1:B:140:LYS:O	2.15	0.64
1:A:220:ARG:NH1	1:A:256:VAL:O	2.30	0.64
1:B:177:LEU:HD11	1:B:211:PHE:CG	2.33	0.63
1:B:399:TRP:CD1	1:B:399:TRP:C	2.68	0.62
1:B:67:LYS:O	1:B:71:GLU:HG3	1.98	0.62
1:A:331:LEU:HD22	1:A:341:GLU:OE2	2.01	0.61
1:A:67:LYS:O	1:A:71:GLU:HG3	2.01	0.61
1:A:375:GLY:O	1:A:399:TRP:CZ3	2.52	0.61
2:E:3:BMA:H2	2:E:4:MAN:H3	1.83	0.59
1:A:399:TRP:C	1:A:399:TRP:HD1	2.05	0.59
1:A:217:THR:CG2	3:D:1:NAG:H5	2.32	0.59
1:A:204:TRP:HB3	1:A:205:PRO:HD3	1.85	0.59
1:A:367:ILE:HG13	6:A:19:HOH:O	2.04	0.57
1:B:204:TRP:HB3	1:B:205:PRO:HD3	1.88	0.55
1:A:66:GLU:OE2	1:A:114:PRO:HG2	2.07	0.55
1:A:216:TYR:HB3	1:A:256:VAL:HG21	1.89	0.54
1:A:142:CYS:HB2	5:A:801:GLA:O6	2.07	0.54
1:B:236:TRP:CE3	1:B:279:GLN:HG2	2.43	0.54
1:A:378:CYS:HA	1:A:382:CYS:HB3	1.89	0.53
1:A:379:ASN:CB	1:A:399:TRP:CE3	2.91	0.53
1:B:168:LYS:HA	1:B:201:SER:HB3	1.90	0.53
1:B:96:MET:HG3	1:B:145:PHE:HB3	1.92	0.52
1:B:100:ARG:HA	1:B:105:ARG:O	2.10	0.52
1:A:108:ALA:HB1	1:A:113:PHE:HB2	1.92	0.51
1:B:357:GLN:HE21	1:B:359:ILE:HG23	1.75	0.51
1:B:108:ALA:HB1	1:B:113:PHE:HB2	1.92	0.51
1:B:142:CYS:SG	1:B:170:ASP:OD2	2.70	0.50
1:A:228:ASN:HB3	1:A:245:TRP:CH2	2.47	0.49
1:B:161:ASP:HB2	6:B:9:HOH:O	2.11	0.49
1:A:96:MET:HG3	1:A:145:PHE:HB3	1.94	0.49
1:A:208:MET:O	1:A:212:GLN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:HA	1:A:201:SER:HB3	1.94	0.48
1:A:217:THR:HG22	3:D:1:NAG:H5	1.95	0.48
1:A:224:ASN:O	1:A:261:GLY:HA2	2.14	0.48
1:A:55:ASP:OD2	1:A:58:GLU:HB2	2.14	0.48
1:B:58:GLU:C	1:B:59:GLU:HG2	2.34	0.47
1:B:216:TYR:HB3	1:B:256:VAL:HG21	1.96	0.47
1:A:216:TYR:O	1:A:220:ARG:HB2	2.14	0.47
1:B:229:PHE:CG	1:B:230:ALA:N	2.83	0.47
1:A:200:TYR:CE2	1:A:202:CYS:SG	3.08	0.46
1:A:236:TRP:CE3	1:A:279:GLN:HG2	2.51	0.46
1:B:216:TYR:O	1:B:220:ARG:HB3	2.16	0.46
1:A:379:ASN:CB	1:A:399:TRP:HE3	2.19	0.46
1:A:136:ASP:OD1	1:A:172:CYS:HB2	2.16	0.45
1:A:185:LYS:HG2	1:A:222:TYR:CZ	2.51	0.45
1:B:66:GLU:O	1:B:70:MET:HG3	2.17	0.45
1:B:341:GLU:OE1	1:B:373:GLY:N	2.44	0.45
1:A:49:ARG:HD2	1:A:49:ARG:HA	1.51	0.45
1:A:324:LEU:HD22	1:A:326:LYS:HB2	1.99	0.45
1:A:324:LEU:CD2	1:A:326:LYS:HB2	2.47	0.45
1:A:284:MET:HG3	1:A:316:VAL:HG11	1.99	0.44
1:B:185:LYS:HG2	1:B:222:TYR:CZ	2.52	0.44
1:A:48:GLU:O	1:B:360:GLY:HA2	2.17	0.44
1:B:200:TYR:CE2	1:B:202:CYS:SG	3.10	0.44
1:B:202:CYS:O	1:B:226:TRP:HA	2.18	0.44
1:A:402:ARG:HE	1:A:402:ARG:HB3	1.61	0.43
1:A:58:GLU:C	1:A:59:GLU:HG2	2.37	0.43
1:B:55:ASP:OD2	1:B:58:GLU:HB2	2.19	0.43
1:B:171:GLY:HA3	1:B:207:TYR:CD2	2.54	0.43
1:A:165:ASP:OD1	1:A:196:ARG:NH2	2.51	0.43
1:A:366:THR:HG22	1:A:402:ARG:HH21	1.84	0.43
1:A:66:GLU:O	1:A:70:MET:HG3	2.19	0.42
1:B:236:TRP:CD2	1:B:279:GLN:HG2	2.55	0.42
1:B:373:GLY:O	1:B:376:VAL:HG23	2.19	0.42
1:A:217:THR:HG21	3:D:1:NAG:H5	2.02	0.42
1:A:383:PHE:CE1	1:A:395:GLY:HA2	2.54	0.42
1:B:91:ILE:HG21	1:B:95:TRP:HB3	2.00	0.42
1:A:403:LEU:C	1:A:403:LEU:HD23	2.40	0.42
1:A:360:GLY:HA2	1:B:48:GLU:O	2.20	0.42
1:B:284:MET:HG3	1:B:316:VAL:HG11	2.02	0.42
1:B:234:ASP:O	1:B:274:GLY:HA3	2.20	0.41
1:A:91:ILE:HG21	1:A:95:TRP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:PHE:HB3	1:A:146:PRO:HD2	2.01	0.41
1:A:254:VAL:HG13	1:A:327:GLN:HG2	2.02	0.41
1:A:277:TRP:CZ3	1:A:306:GLN:HB3	2.55	0.41
1:A:236:TRP:CD2	1:A:279:GLN:HG2	2.56	0.41
1:B:45:LEU:HD11	1:B:92:ASP:OD2	2.21	0.41
1:B:254:VAL:HB	5:B:804:GLA:O4	2.21	0.41
1:A:378:CYS:O	1:A:399:TRP:CB	2.63	0.41
1:A:373:GLY:HA3	1:A:377:ALA:HB2	2.03	0.41
1:A:322:ASP:HA	1:A:323:PRO:HD3	1.98	0.40
1:A:170:ASP:OD1	5:A:801:GLA:H2	2.21	0.40
1:B:205:PRO:CG	1:B:226:TRP:HB2	2.51	0.40
1:B:355:ASN:HB2	1:B:407:ILE:HB	2.02	0.40
1:B:373:GLY:HA3	1:B:377:ALA:HB2	2.03	0.40
1:A:240:LYS:HD2	1:A:356:ARG:NH2	2.37	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	393/404 (97%)	372 (95%)	20 (5%)	1 (0%)	41	74
1	B	392/404 (97%)	375 (96%)	16 (4%)	1 (0%)	41	74
All	All	785/808 (97%)	747 (95%)	36 (5%)	2 (0%)	41	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	LEU
1	B	266	ASP

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	335/344 (97%)	308 (92%)	27 (8%)	11	37
1	B	334/344 (97%)	314 (94%)	20 (6%)	19	51
All	All	669/688 (97%)	622 (93%)	47 (7%)	15	44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	49	ARG
1	A	61	ASP
1	A	87	GLU
1	A	96	MET
1	A	99	GLN
1	A	111	GLN
1	A	127	LYS
1	A	178	GLU
1	A	179	ASN
1	A	187	MET
1	A	213	LYS
1	A	225	HIS
1	A	237	LYS
1	A	238	SER
1	A	256	VAL
1	A	287	TRP
1	A	306	GLN
1	A	347	LEU
1	A	364	SER
1	A	379	ASN
1	A	392	ARG
1	A	399	TRP
1	A	402	ARG
1	A	418	GLU
1	A	421	MET
1	A	422	GLN

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Mol	Chain	Res	Type
1	B	49	ARG
1	B	87	GLU
1	B	96	MET
1	B	130	LYS
1	B	178	GLU
1	B	179	ASN
1	B	208	MET
1	B	220	ARG
1	B	225	HIS
1	B	237	LYS
1	B	238	SER
1	B	241	SER
1	B	256	VAL
1	B	287	TRP
1	B	306	GLN
1	B	326	LYS
1	B	364	SER
1	B	376	VAL
1	B	392	ARG
1	B	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	122	ASN
1	A	336	ASN
1	A	379	ASN
1	B	111	GLN
1	B	122	ASN
1	B	157	GLN
1	B	228	ASN
1	B	357	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](#)

10 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	0.53	0	17,19,21	0.87	1 (5%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
2	BMA	C	3	2	11,11,12	0.44	0	15,15,17	1.10	1 (6%)
2	MAN	C	4	2	11,11,12	0.61	0	15,15,17	0.95	0
3	NAG	D	1	1,3	14,14,15	0.55	0	17,19,21	1.04	2 (11%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.53	0	17,19,21	0.82	0
2	NAG	E	2	2	14,14,15	0.60	0	17,19,21	1.00	2 (11%)
2	BMA	E	3	2	11,11,12	0.52	0	15,15,17	1.48	2 (13%)
2	MAN	E	4	2	11,11,12	0.59	0	15,15,17	2.28	2 (13%)

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	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	7.39	122.20	112.19
2	E	3	BMA	C1-C2-C3	4.23	114.86	109.67
2	E	4	MAN	O5-C1-C2	3.05	115.47	110.77
2	C	3	BMA	O5-C5-C6	2.89	111.73	107.20
2	C	2	NAG	O5-C5-C6	2.44	111.03	107.20
2	E	2	NAG	C4-C3-C2	2.38	114.51	111.02
2	E	3	BMA	C3-C4-C5	2.32	114.37	110.24
3	D	1	NAG	O5-C1-C2	-2.14	107.91	111.29
2	E	2	NAG	O5-C5-C6	2.04	110.41	107.20
3	D	2	NAG	C4-C3-C2	2.04	114.01	111.02
3	D	1	NAG	C1-O5-C5	2.01	114.91	112.19
2	C	1	NAG	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	MAN	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
2	C	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

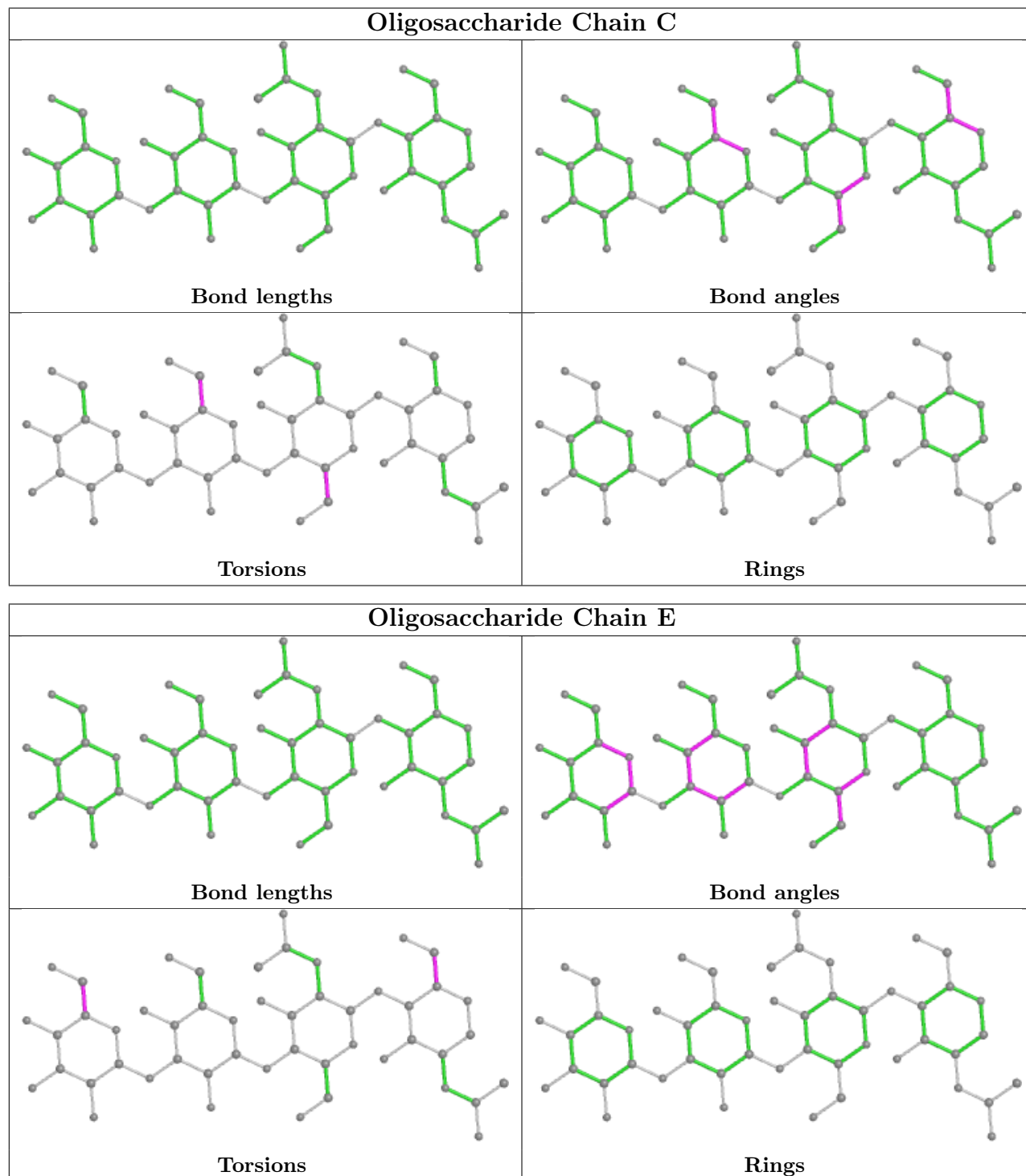
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	BMA	1	0

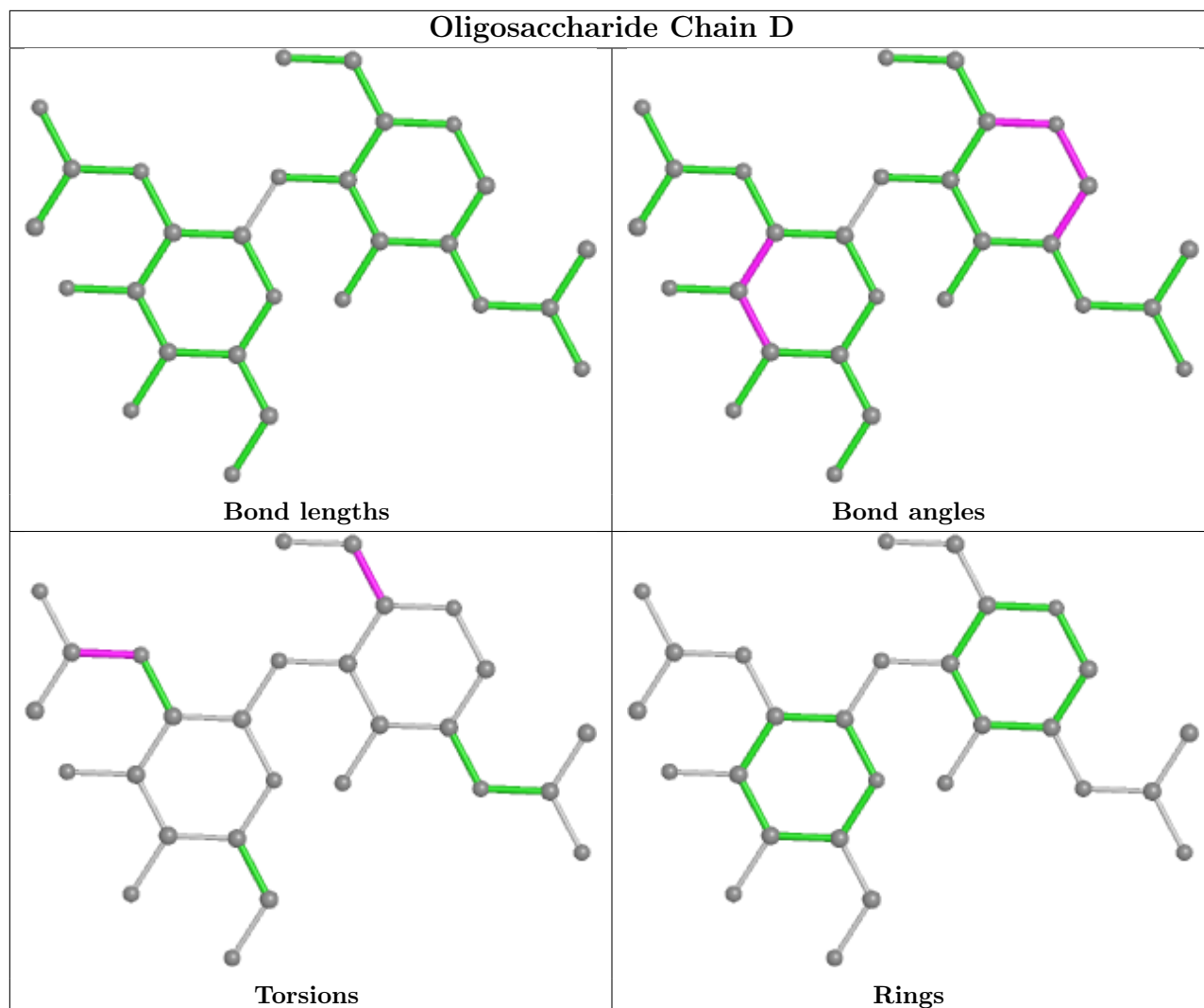
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
2	E	4	MAN	1	0

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](#)

7 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	NAG	B	715	1	14,14,15	0.57	0	17,19,21	0.84	0
4	NAG	A	639	1	14,14,15	0.67	0	17,19,21	1.90	4 (23%)
5	GLA	B	804	-	12,12,12	0.61	0	17,17,17	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLA	A	801	-	12,12,12	0.39	0	17,17,17	1.04	1 (5%)
5	GLA	B	802	-	12,12,12	0.64	0	17,17,17	0.89	0
4	NAG	B	639	1	14,14,15	0.57	0	17,19,21	1.35	2 (11%)
5	GLA	A	803	-	12,12,12	0.82	0	17,17,17	1.16	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
4	NAG	B	715	1	-	2/6/23/26	0/1/1/1
4	NAG	A	639	1	-	0/6/23/26	0/1/1/1
5	GLA	B	804	-	-	0/2/22/22	0/1/1/1
5	GLA	A	801	-	-	0/2/22/22	0/1/1/1
5	GLA	B	802	-	-	0/2/22/22	0/1/1/1
4	NAG	B	639	1	-	1/6/23/26	0/1/1/1
5	GLA	A	803	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	639	NAG	C1-O5-C5	5.45	119.57	112.19
5	A	803	GLA	C1-O5-C5	2.85	119.04	113.66
5	A	801	GLA	C1-O5-C5	2.83	119.00	113.66
4	B	639	NAG	O5-C5-C6	2.79	111.58	107.20
4	A	639	NAG	C3-C4-C5	-2.53	105.72	110.24
4	A	639	NAG	O5-C5-C6	2.46	111.06	107.20
5	B	804	GLA	C1-O5-C5	2.24	117.90	113.66
4	A	639	NAG	O7-C7-C8	-2.18	118.00	122.06
4	B	639	NAG	C1-C2-N2	2.12	114.10	110.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	715	NAG	C4-C5-C6-O6
4	B	715	NAG	O5-C5-C6-O6
5	A	803	GLA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	639	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	GLA	1	0
5	A	801	GLA	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	395/404 (97%)	-0.28	0 100 100	13, 32, 56, 79	0
1	B	394/404 (97%)	-0.28	0 100 100	12, 31, 53, 75	0
All	All	789/808 (97%)	-0.28	0 100 100	12, 31, 55, 79	0

There are no RSRZ outliers to report.

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

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

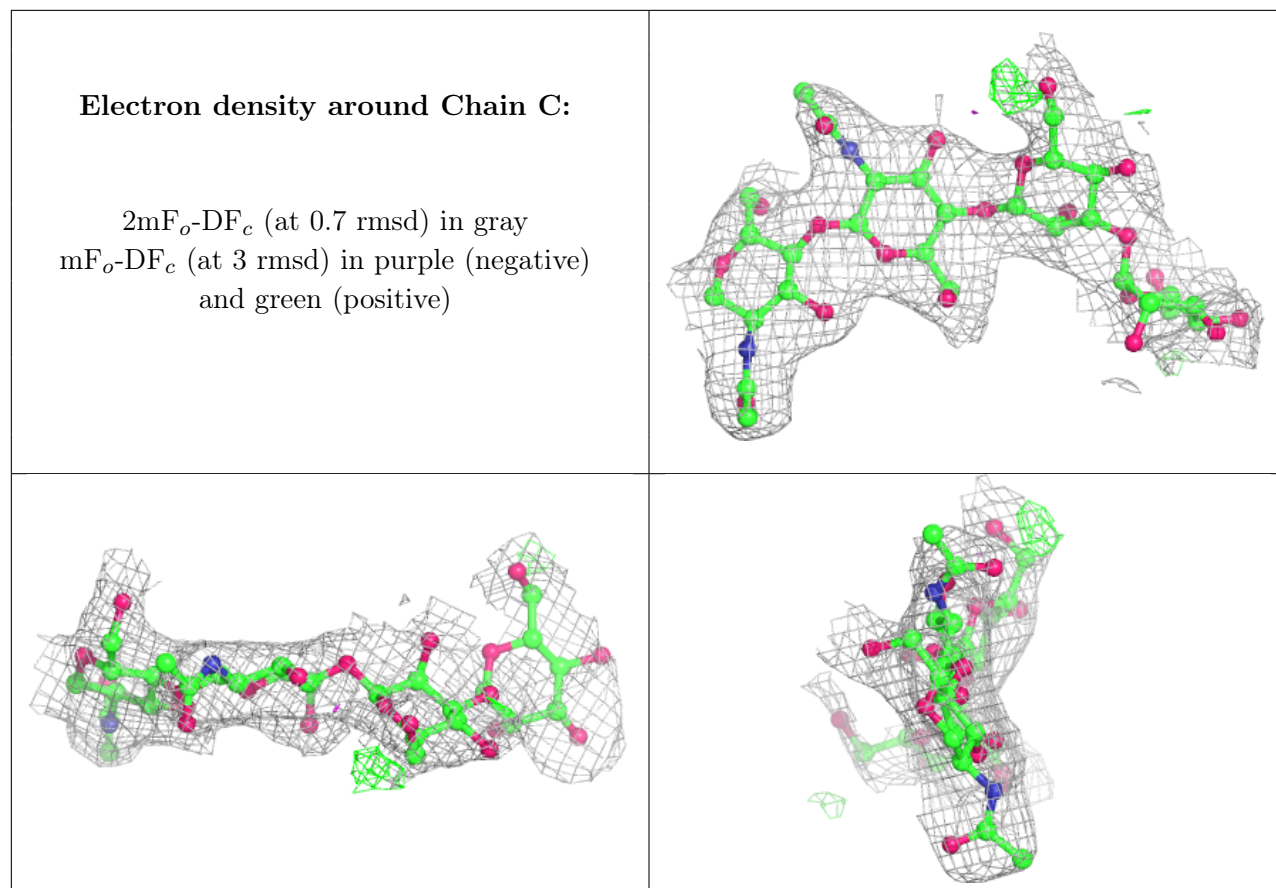
6.3 Carbohydrates [i](#)

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	MAN	C	4	11/12	0.72	0.30	78,79,81,83	0
2	MAN	E	4	11/12	0.72	0.26	68,71,73,74	0
3	NAG	D	2	14/15	0.80	0.35	76,79,85,87	0
2	BMA	C	3	11/12	0.83	0.24	63,67,72,74	0
3	NAG	D	1	14/15	0.84	0.26	53,60,66,72	0
2	BMA	E	3	11/12	0.87	0.34	61,64,67,68	0
2	NAG	C	2	14/15	0.92	0.30	43,50,54,55	0
2	NAG	E	2	14/15	0.92	0.20	43,52,56,57	0
2	NAG	E	1	14/15	0.94	0.18	35,39,46,48	0
2	NAG	C	1	14/15	0.95	0.22	32,35,40,43	0

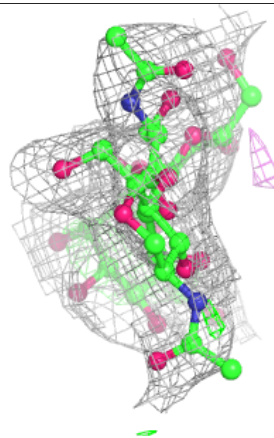
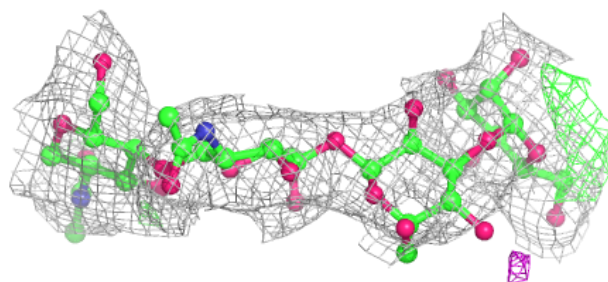
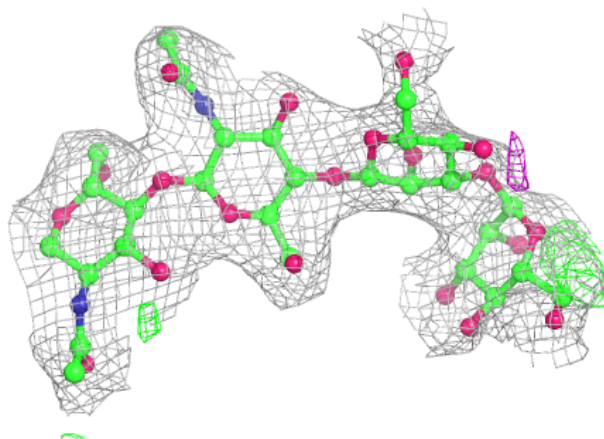
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

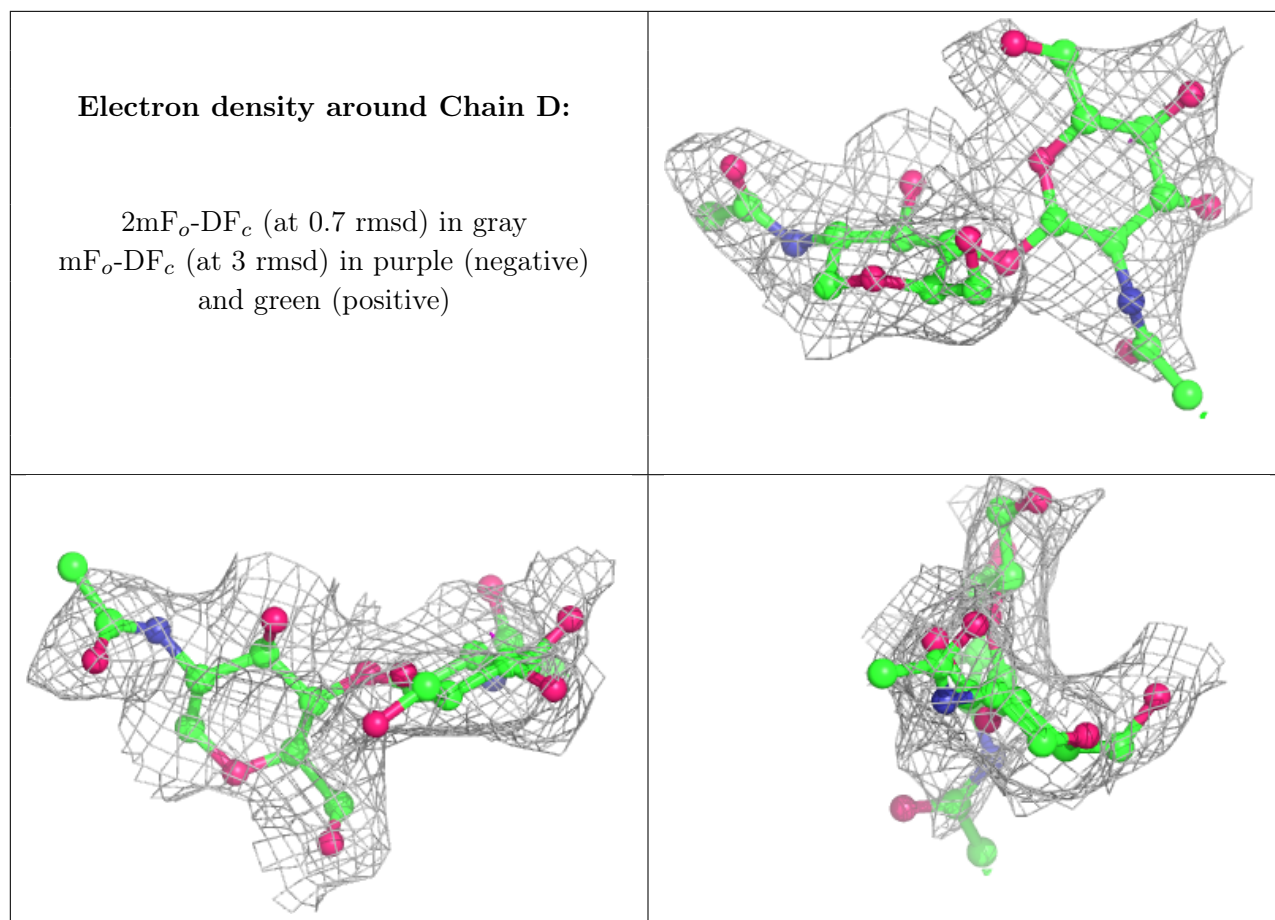
charide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

$2mF_o-DF_c$ (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
4	NAG	B	715	14/15	0.75	0.34	59,68,71,74	0
4	NAG	A	639	14/15	0.80	0.24	51,55,58,60	0
5	GLA	A	803	12/12	0.81	0.39	46,51,53,54	0
4	NAG	B	639	14/15	0.84	0.21	47,54,56,58	0
5	GLA	B	804	12/12	0.85	0.51	52,54,55,58	0
5	GLA	B	802	12/12	0.93	0.18	25,32,36,38	0
5	GLA	A	801	12/12	0.96	0.17	16,19,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.