



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:53 PM UTC

PDB ID : 4DO4 / pdb_00004do4
Title : Pharmacological chaperones for human alpha-N-acetylgalactosaminidase
Authors : Clark, N.E.; Garman, S.C.
Deposited on : 2012-02-09
Resolution : 1.40 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:

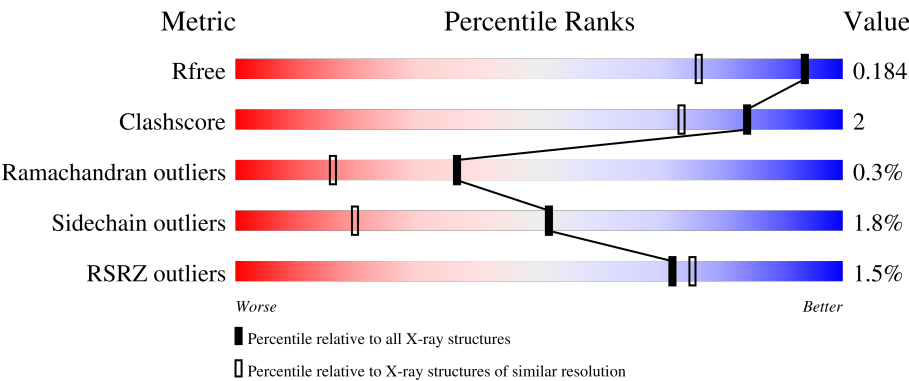
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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.



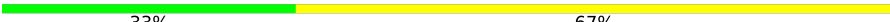
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	400	% 88%8% .
1	B	400	2% 95% ..
2	C	3	33%67%
3	D	5	80%20%
3	F	5	60%40%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	3	 33% 67%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7713 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.

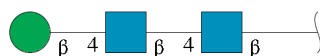
- Molecule 1 is a protein called Alpha-N-acetylgalactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	7	0
			3136	2005	530	573	28			
1	B	400	Total	C	N	O	S	0	5	0
			3223	2059	547	588	29			

There are 14 discrepancies between the modelled and reference sequences:

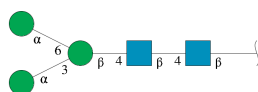
Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLN	ASN	engineered mutation	UNP P17050
A	412	HIS	-	expression tag	UNP P17050
A	413	HIS	-	expression tag	UNP P17050
A	414	HIS	-	expression tag	UNP P17050
A	415	HIS	-	expression tag	UNP P17050
A	416	HIS	-	expression tag	UNP P17050
A	417	HIS	-	expression tag	UNP P17050
B	201	GLN	ASN	engineered mutation	UNP P17050
B	412	HIS	-	expression tag	UNP P17050
B	413	HIS	-	expression tag	UNP P17050
B	414	HIS	-	expression tag	UNP P17050
B	415	HIS	-	expression tag	UNP P17050
B	416	HIS	-	expression tag	UNP P17050
B	417	HIS	-	expression tag	UNP P17050

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



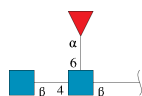
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



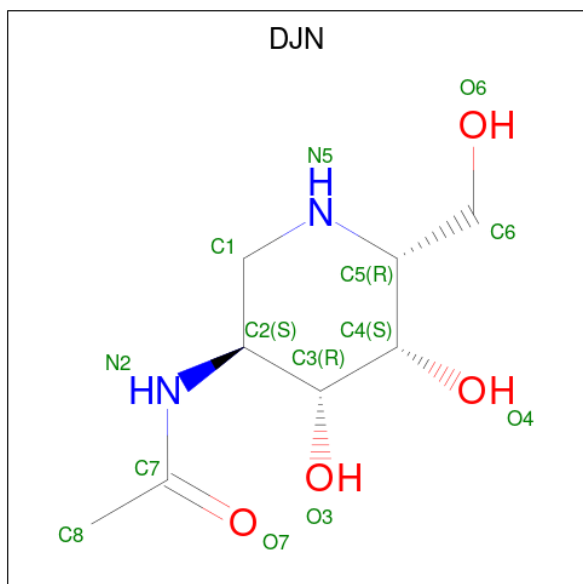
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is N-[(3S,4R,5S,6R)-4,5-dihydroxy-6-(hydroxymethyl)piperidin-3-yl]acetamide (CCD ID: DJN) (formula: C₈H₁₆N₂O₄).



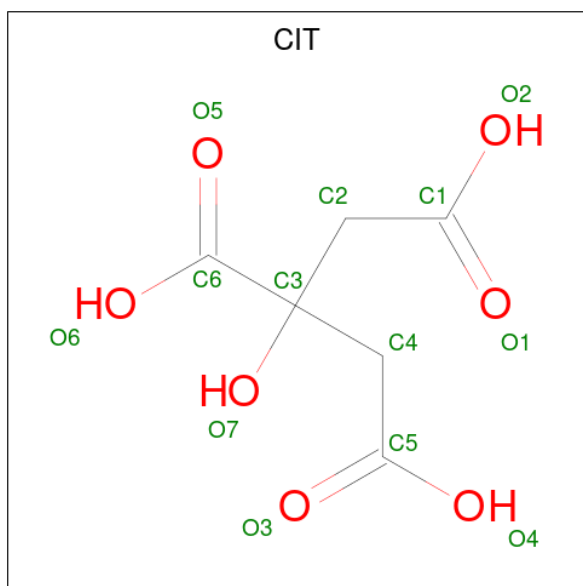
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	2	4		

Continued on next page...

Continued from previous page...

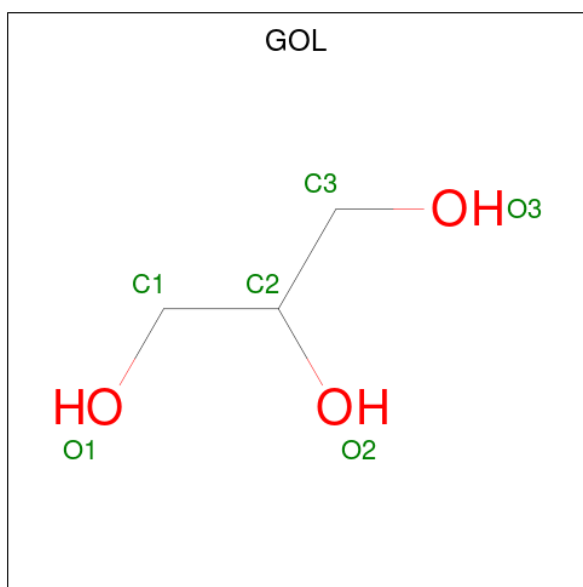
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	2	4		

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



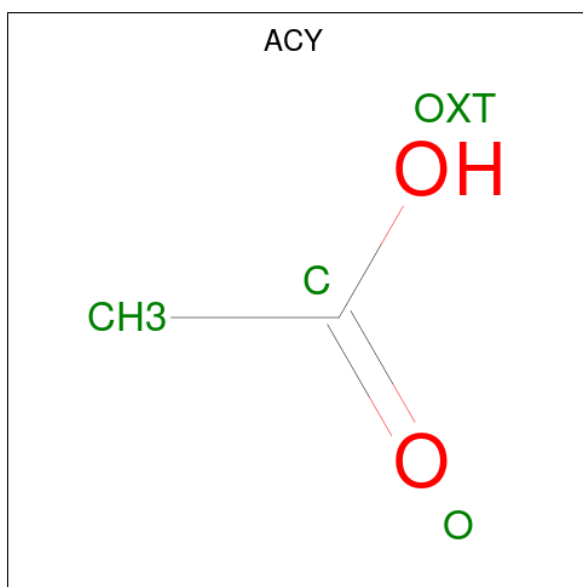
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		
7	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 9 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	531	Total	O	0	0
			531	531		
10	B	460	Total	O	0	0
			460	460		

Chain F:  60% 40%

MAG1
MAG2
BGL3
MAN4
MAN5

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  33% 67%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.06Å 114.62Å 68.63Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	26.63 – 1.40 26.63 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.63-1.40) 98.5 (26.63-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.141 , 0.178 0.151 , 0.184	Depositor DCC
R_{free} test set	11645 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7713	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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: CIT, DJN, MAN, NAG, FUC, GOL, BMA, ACY

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	2/3227 (0.1%)	0.83	3/4388 (0.1%)
1	B	0.69	0/3326	0.80	4/4523 (0.1%)
All	All	0.70	2/6553 (0.0%)	0.81	7/8911 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	PRO	CA-C	5.39	1.54	1.51
1	A	197	PRO	CA-C	5.20	1.54	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PRO	O-C-N	6.21	124.17	121.31
1	A	168	GLY	N-CA-C	6.16	120.66	112.77
1	A	76	ASN	N-CA-C	5.58	117.62	108.52
1	B	66	GLY	N-CA-C	5.43	122.28	115.21
1	B	25	THR	CA-C-N	-5.26	115.82	119.66
1	B	25	THR	C-N-CA	-5.26	115.82	119.66
1	B	26	PRO	O-C-N	5.03	123.62	121.31

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	3136	0	3044	18	0
1	B	3223	0	3116	13	0
2	C	39	0	34	0	0
3	D	61	0	52	0	0
3	F	61	0	52	0	0
4	E	38	0	34	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	14	0	16	0	0
6	B	14	0	16	0	0
7	A	13	0	5	0	0
7	B	13	0	5	0	0
8	A	36	0	48	1	0
8	B	42	0	56	0	0
9	A	4	0	3	0	0
10	A	531	0	0	8	0
10	B	460	0	0	3	0
All	All	7713	0	6507	31	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 2.

All (31) 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:200:VAL:HG23	10:A:1105:HOH:O	1.43	1.17
1:A:233[A]:VAL:HG23	10:A:715:HOH:O	1.44	1.15
1:A:229[B]:LEU:O	1:A:233[B]:VAL:HG13	1.70	0.89
1:A:233[B]:VAL:HG12	10:A:715:HOH:O	1.76	0.84
1:B:55:PHE:HD1	1:B:75[A]:LEU:HD11	1.55	0.72
1:B:110:HIS:HD2	10:B:640:HOH:O	1.74	0.70
1:B:110:HIS:HE1	1:B:151:ASP:OD2	1.77	0.67
1:A:275[A]:VAL:HG11	1:A:339:VAL:HG23	1.79	0.65
1:B:52:GLU:OE2	1:B:100:HIS:HD2	1.83	0.61
1:A:109:VAL:HG13	1:A:114:LEU:HB2	1.82	0.61
1:A:230:ASN:HB2	8:A:517:GOL:O3	2.01	0.60
1:A:237:ASP:OD1	1:A:315[A]:ARG:NH2	2.37	0.57
1:A:233[B]:VAL:CG1	10:A:715:HOH:O	2.44	0.56
1:B:75[A]:LEU:HD13	1:B:75[A]:LEU:C	2.32	0.55
1:B:75[A]:LEU:C	1:B:75[A]:LEU:CD1	2.81	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:HIS:C	10:B:997:HOH:O	2.50	0.54
1:A:240:GLN:HG3	1:A:315[A]:ARG:HG2	1.92	0.51
1:A:118:ILE:HG22	1:A:150:VAL:HG11	1.94	0.49
1:A:275[A]:VAL:HG11	1:A:339:VAL:CG2	2.43	0.49
10:A:794:HOH:O	1:B:392:PRO:HB2	2.13	0.47
1:B:297:LEU:HD11	10:B:1036:HOH:O	2.14	0.47
1:A:235:HIS:HE1	10:A:1015:HOH:O	1.99	0.46
1:B:30:TRP:CE3	1:B:75[B]:LEU:HD12	2.52	0.45
1:B:318:HIS:ND1	1:B:320:GLU:OE2	2.50	0.45
1:A:201:GLN:NE2	10:A:811:HOH:O	2.35	0.44
1:B:239:LEU:O	1:B:242:VAL:HG22	2.18	0.44
1:A:360:PHE:CE1	1:A:400:LEU:CD2	3.01	0.43
1:A:239:LEU:O	1:A:242:VAL:HG22	2.19	0.42
1:B:233[A]:VAL:HG21	1:B:327:TYR:OH	2.19	0.41
1:A:360:PHE:CE1	1:A:400:LEU:HD23	2.54	0.41
1:A:90:ARG:HD3	10:A:682:HOH:O	2.20	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	392/400 (98%)	379 (97%)	12 (3%)	1 (0%)	36	16
1	B	403/400 (101%)	390 (97%)	12 (3%)	1 (0%)	43	19
All	All	795/800 (99%)	769 (97%)	24 (3%)	2 (0%)	36	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ASP
1	B	252	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	340/346 (98%)	332 (98%)	8 (2%)	43	12
1	B	351/346 (101%)	346 (99%)	5 (1%)	59	28
All	All	691/692 (100%)	678 (98%)	13 (2%)	51	18

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	163	GLU
1	A	193	GLU
1	A	203	SER
1	A	318	HIS
1	A	320	GLU
1	A	333	ASN
1	A	404	LYS
1	B	75[A]	LEU
1	B	75[B]	LEU
1	B	275	VAL
1	B	318	HIS
1	B	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	HIS
1	A	240	GLN
1	B	48	ASN
1	B	100	HIS
1	B	110	HIS
1	B	143	GLN
1	B	167	GLN
1	B	357	GLN
1	B	359	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	416	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 ⓘ

16 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	0.75	0	17,19,21	1.60	4 (23%)
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	1.02	1 (5%)
2	BMA	C	3	2	11,11,12	0.39	0	15,15,17	0.67	0
3	NAG	D	1	1,3	14,14,15	0.61	0	17,19,21	0.70	0
3	NAG	D	2	3	14,14,15	0.60	0	17,19,21	0.73	0
3	BMA	D	3	3	11,11,12	0.39	0	15,15,17	0.72	0
3	MAN	D	4	3	11,11,12	0.56	0	15,15,17	0.73	0
3	MAN	D	5	3	11,11,12	0.72	0	15,15,17	1.03	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
4	NAG	E	2	4	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
4	FUC	E	3	4	10,10,11	0.59	0	14,14,16	0.79	0
3	NAG	F	1	1,3	14,14,15	0.64	0	17,19,21	0.90	0
3	NAG	F	2	3	14,14,15	0.65	0	17,19,21	0.68	0
3	BMA	F	3	3	11,11,12	0.44	0	15,15,17	0.73	0
3	MAN	F	4	3	11,11,12	0.54	0	15,15,17	0.95	1 (6%)
3	MAN	F	5	3	11,11,12	0.54	0	15,15,17	1.03	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	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	3.30	127.33	122.90
3	F	5	MAN	C1-O5-C5	3.14	116.40	112.19
3	F	4	MAN	C1-O5-C5	2.95	116.14	112.19
4	E	1	NAG	C1-O5-C5	2.90	116.07	112.19
2	C	1	NAG	O7-C7-C8	-2.89	116.91	122.05
3	D	5	MAN	C1-C2-C3	2.82	113.75	109.64
2	C	1	NAG	O7-C7-N2	2.73	126.81	121.98
2	C	2	NAG	C1-O5-C5	2.35	115.33	112.19
4	E	2	NAG	C4-C3-C2	2.34	114.44	111.02
2	C	1	NAG	O5-C5-C4	-2.14	105.62	110.83
3	F	5	MAN	C1-C2-C3	2.10	112.71	109.64

There are no chirality outliers.

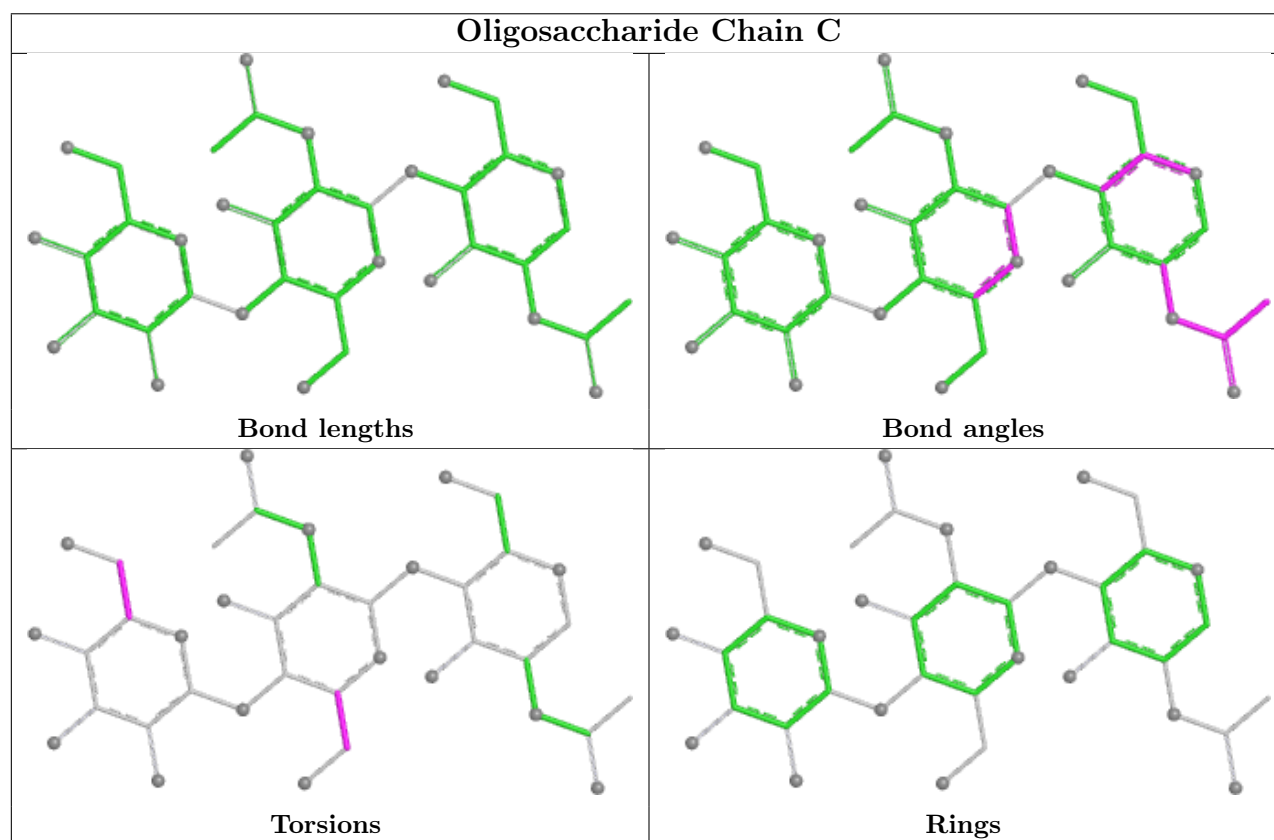
All (10) torsion outliers are listed below:

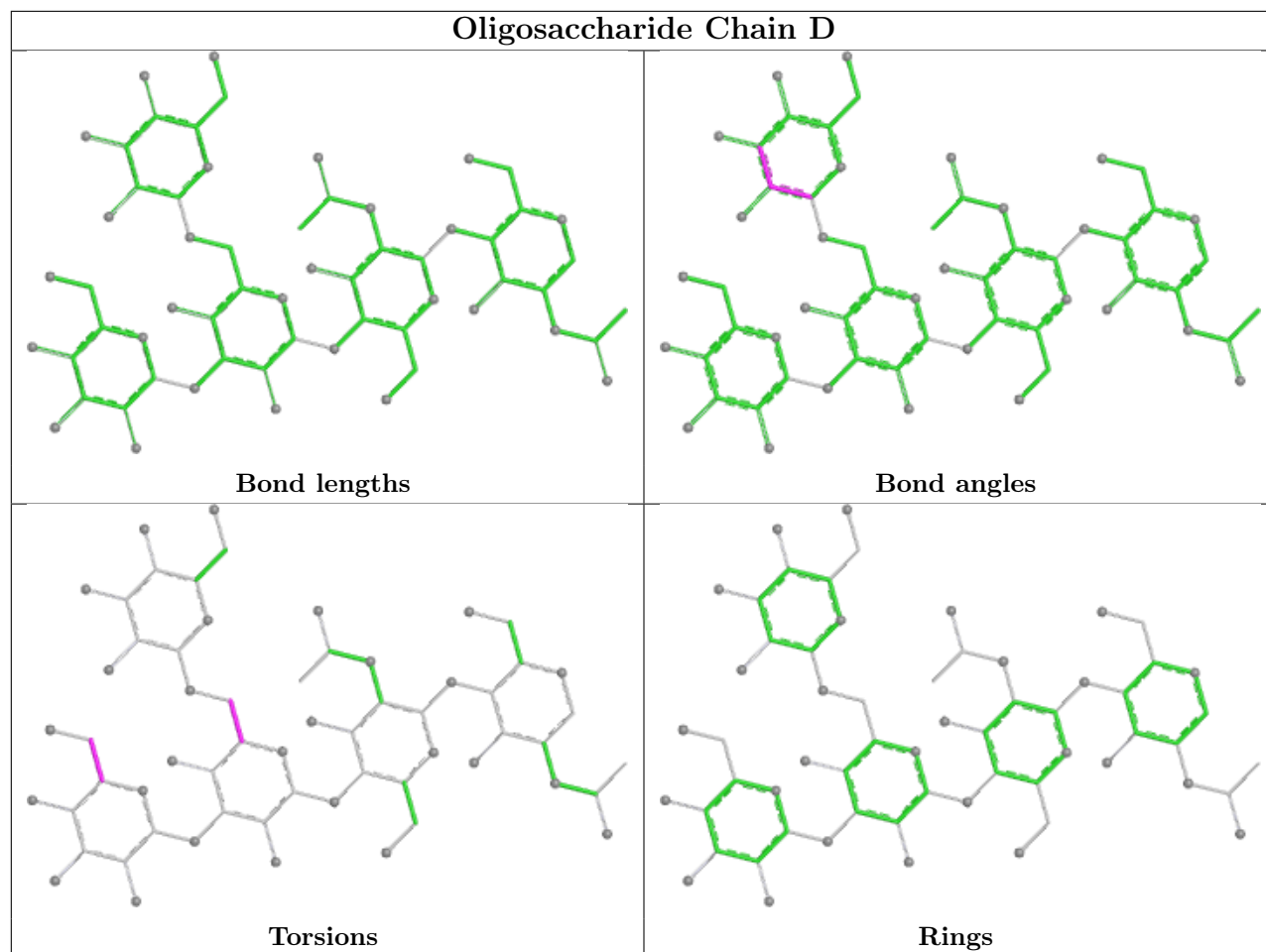
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

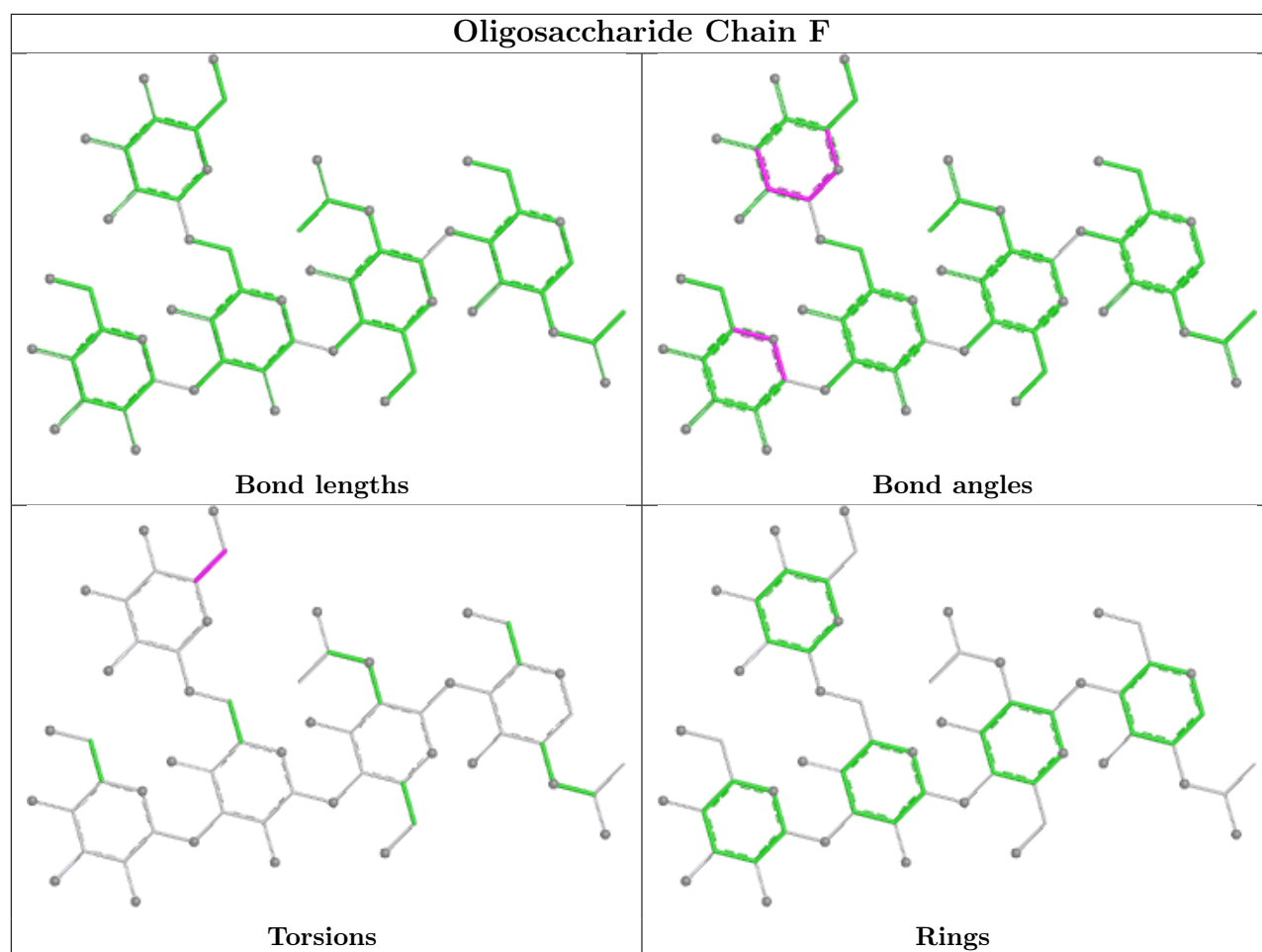
There are no ring outliers.

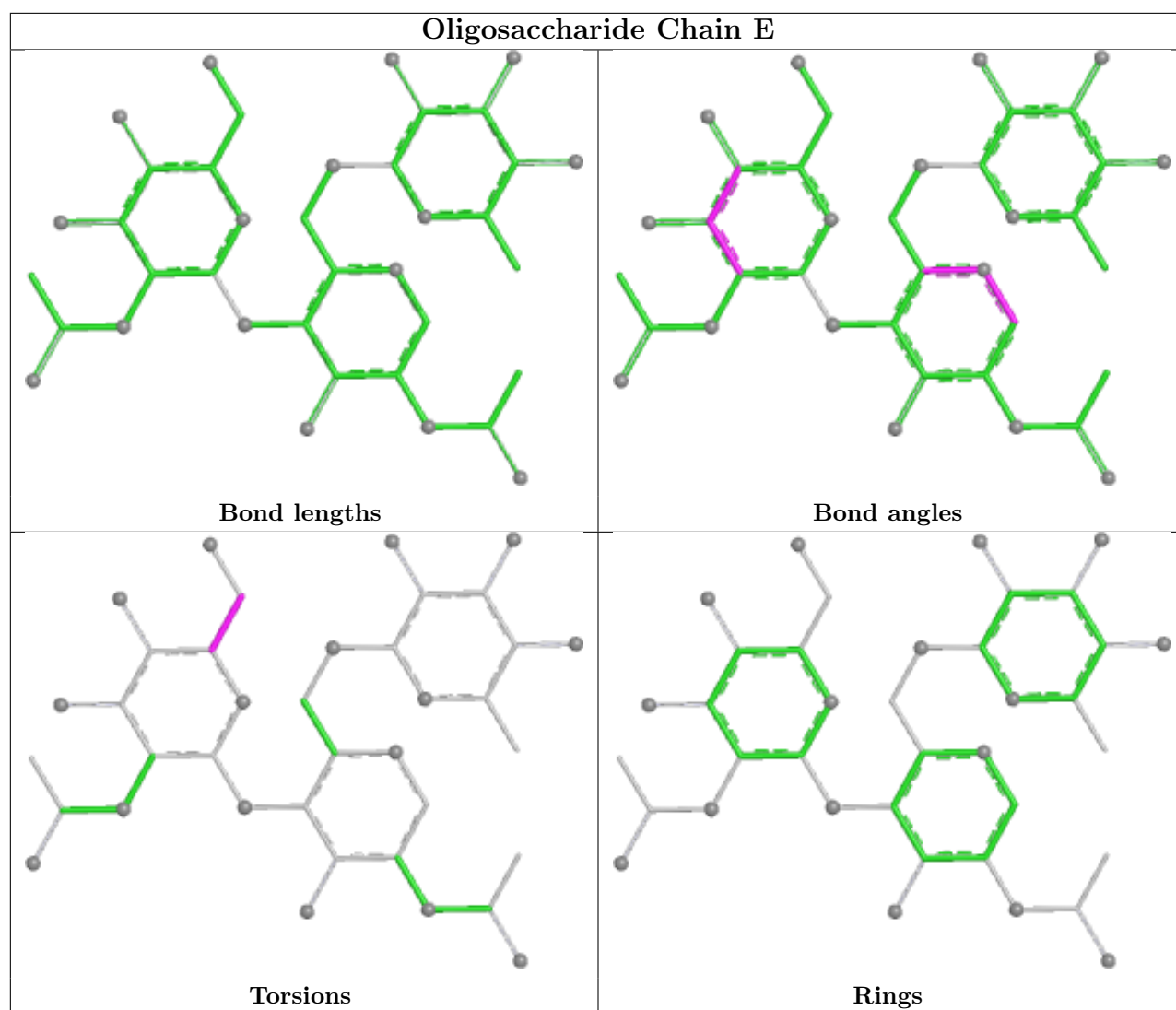
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
8	GOL	B	515	-	5,5,5	0.49	0	5,5,5	0.47	0
7	CIT	B	511	-	12,12,12	0.96	0	17,17,17	1.47	2 (11%)
8	GOL	A	513	-	5,5,5	0.42	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DJN	B	510	-	14,14,14	0.65	0	15,19,19	1.42	2 (13%)
8	GOL	A	516	-	5,5,5	0.34	0	5,5,5	0.40	0
8	GOL	A	517	-	5,5,5	0.43	0	5,5,5	0.26	0
6	DJN	A	510	-	14,14,14	0.66	0	15,19,19	1.34	2 (13%)
5	NAG	B	509	1	14,14,15	0.47	0	17,19,21	1.24	1 (5%)
9	ACY	A	515	-	3,3,3	0.84	0	3,3,3	0.81	0
8	GOL	A	512	-	5,5,5	0.45	0	5,5,5	0.25	0
8	GOL	A	518	-	5,5,5	0.44	0	5,5,5	0.24	0
5	NAG	A	509	1	14,14,15	0.49	0	17,19,21	0.91	0
7	CIT	A	511	-	12,12,12	1.00	0	17,17,17	1.36	4 (23%)
8	GOL	B	518	-	5,5,5	0.35	0	5,5,5	0.39	0
8	GOL	B	516	-	5,5,5	0.41	0	5,5,5	0.46	0
8	GOL	B	517	-	5,5,5	0.40	0	5,5,5	0.20	0
8	GOL	B	513	-	5,5,5	0.40	0	5,5,5	0.35	0
8	GOL	B	512	-	5,5,5	0.35	0	5,5,5	0.31	0
8	GOL	A	514	-	5,5,5	0.29	0	5,5,5	0.54	0
8	GOL	B	514	-	5,5,5	0.39	0	5,5,5	0.29	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
8	GOL	B	515	-	-	2/4/4/4	-
7	CIT	B	511	-	-	2/16/16/16	-
8	GOL	A	513	-	-	2/4/4/4	-
6	DJN	B	510	-	-	1/6/23/23	0/1/1/1
8	GOL	A	516	-	-	0/4/4/4	-
8	GOL	A	517	-	-	2/4/4/4	-
6	DJN	A	510	-	-	1/6/23/23	0/1/1/1
5	NAG	B	509	1	-	0/6/23/26	0/1/1/1
8	GOL	A	512	-	-	0/4/4/4	-
8	GOL	A	518	-	-	3/4/4/4	-
5	NAG	A	509	1	-	2/6/23/26	0/1/1/1
7	CIT	A	511	-	-	4/16/16/16	-
8	GOL	B	518	-	-	0/4/4/4	-
8	GOL	B	516	-	-	2/4/4/4	-
8	GOL	B	517	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	513	-	-	2/4/4/4	-
8	GOL	B	512	-	-	0/4/4/4	-
8	GOL	A	514	-	-	0/4/4/4	-
8	GOL	B	514	-	-	2/4/4/4	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	509	NAG	C1-O5-C5	4.52	118.25	112.19
7	B	511	CIT	O6-C6-C3	3.86	120.54	113.14
6	A	510	DJN	C4-C5-N5	3.73	116.64	109.12
6	B	510	DJN	C4-C3-C2	-3.61	105.73	111.02
7	A	511	CIT	O6-C6-C3	2.81	118.54	113.14
6	A	510	DJN	C4-C3-C2	-2.66	107.11	111.02
7	A	511	CIT	O2-C1-C2	2.29	121.59	114.35
7	A	511	CIT	O1-C1-C2	-2.18	116.78	122.95
7	B	511	CIT	O2-C1-C2	2.17	121.21	114.35
7	A	511	CIT	O3-C5-C4	-2.07	117.08	122.95
6	B	510	DJN	C2-N2-C7	-2.05	120.15	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	517	GOL	O1-C1-C2-O2
8	A	517	GOL	O1-C1-C2-C3
8	B	514	GOL	O1-C1-C2-C3
8	B	515	GOL	O1-C1-C2-O2
8	B	515	GOL	O1-C1-C2-C3
8	B	517	GOL	O1-C1-C2-O2
8	B	517	GOL	O1-C1-C2-C3
8	B	517	GOL	C1-C2-C3-O3
5	A	509	NAG	O5-C5-C6-O6
5	A	509	NAG	C4-C5-C6-O6
8	A	518	GOL	O1-C1-C2-C3
8	B	513	GOL	C1-C2-C3-O3
8	B	517	GOL	O2-C2-C3-O3
7	A	511	CIT	O2-C1-C2-C3
8	B	513	GOL	O2-C2-C3-O3
8	B	514	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	511	CIT	O1-C1-C2-C3
8	A	513	GOL	O1-C1-C2-O2
8	A	513	GOL	O1-C1-C2-C3
8	B	516	GOL	C1-C2-C3-O3
8	A	518	GOL	O1-C1-C2-O2
6	B	510	DJN	C1-C2-N2-C7
8	B	516	GOL	O2-C2-C3-O3
7	B	511	CIT	O2-C1-C2-C3
8	A	518	GOL	O2-C2-C3-O3
7	A	511	CIT	C3-C4-C5-O3
7	B	511	CIT	O1-C1-C2-C3
6	A	510	DJN	C1-C2-N2-C7
7	A	511	CIT	C3-C4-C5-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	517	GOL	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	387/400 (96%)	-0.38	4 (1%) 79 83	9, 21, 39, 63	7 (1%)
1	B	400/400 (100%)	-0.02	8 (2%) 65 68	11, 26, 52, 93	5 (1%)
All	All	787/800 (98%)	-0.20	12 (1%) 72 75	9, 23, 47, 93	12 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	361	THR	3.5
1	A	362	GLY	3.4
1	B	42	CYS	3.0
1	B	409	SER	2.9
1	B	412	HIS	2.8
1	A	363	SER	2.7
1	B	408	MET	2.7
1	B	415	HIS	2.5
1	A	404	LYS	2.4
1	B	363	SER	2.3
1	B	417	HIS	2.2
1	B	414	HIS	2.1

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

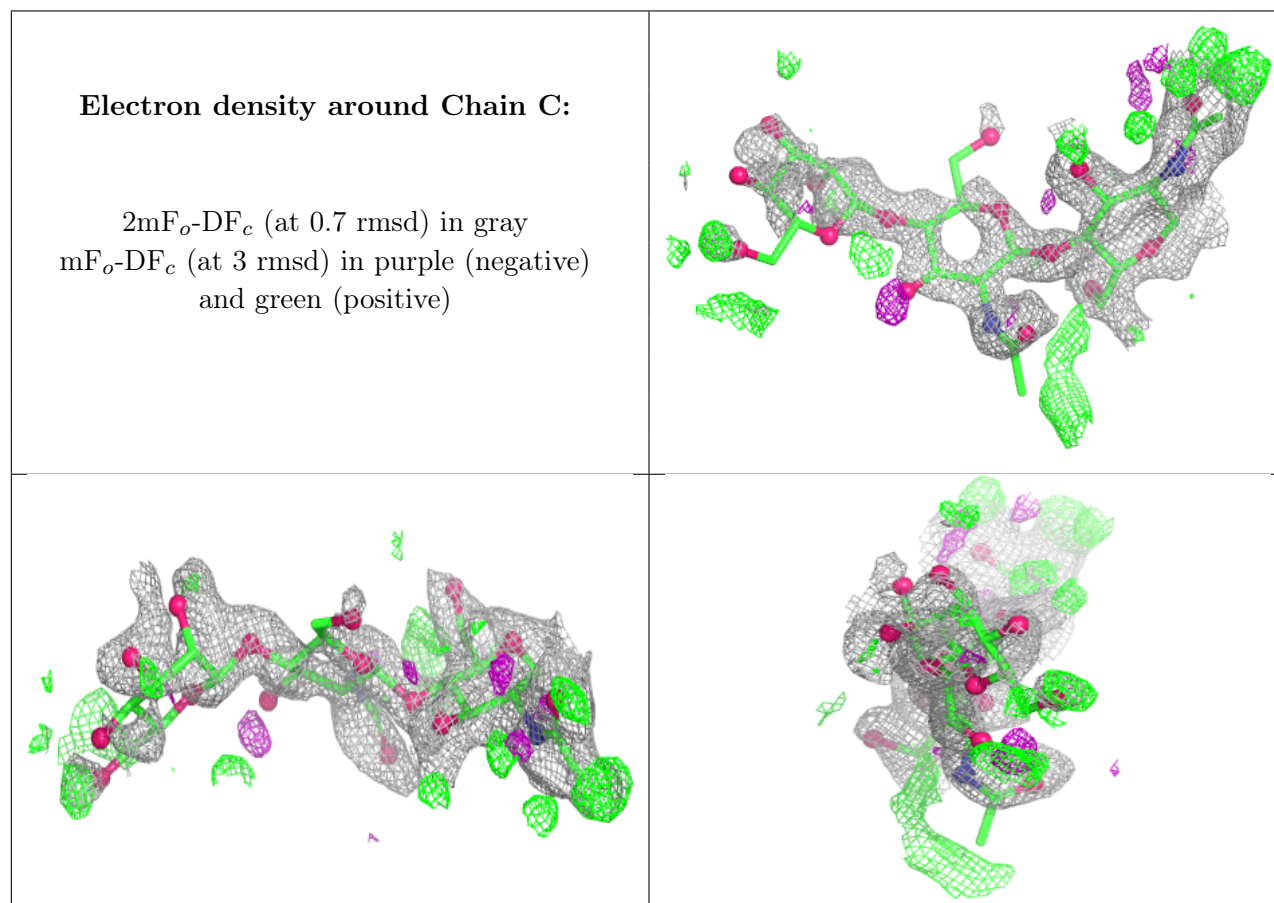
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

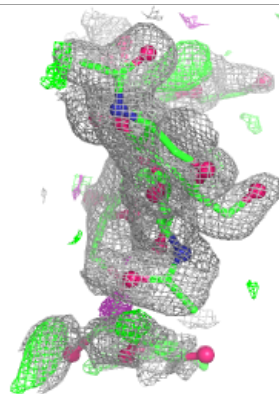
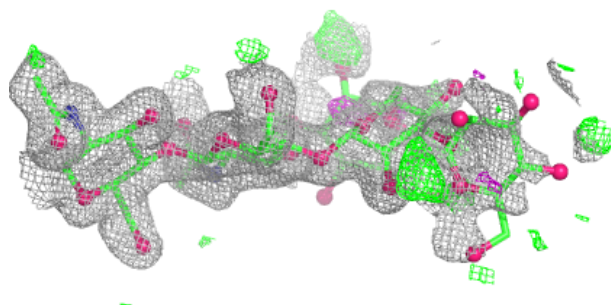
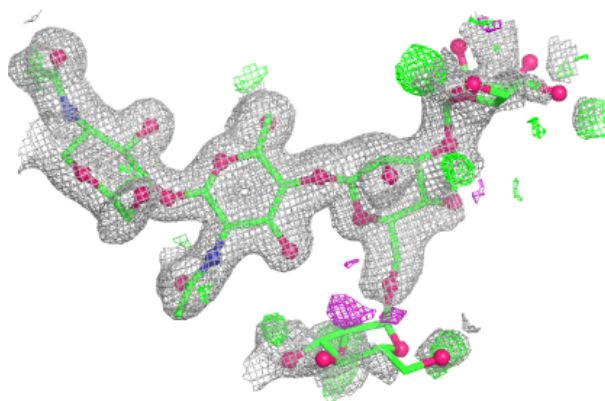
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	F	5	11/12	0.60	0.18	124,126,130,130	0
4	FUC	E	3	10/11	0.63	0.19	99,118,124,127	0
3	MAN	D	5	11/12	0.68	0.20	103,108,115,115	0
3	MAN	F	4	11/12	0.71	0.18	87,104,112,113	0
3	MAN	D	4	11/12	0.72	0.21	79,98,103,103	0
2	BMA	C	3	11/12	0.73	0.20	87,122,123,128	0
2	NAG	C	2	14/15	0.74	0.21	82,94,107,116	0
4	NAG	E	2	14/15	0.76	0.17	97,113,118,121	0
2	NAG	C	1	14/15	0.85	0.13	51,64,78,83	0
4	NAG	E	1	14/15	0.90	0.14	51,68,97,100	0
3	BMA	F	3	11/12	0.91	0.12	54,68,96,111	0
3	BMA	D	3	11/12	0.94	0.12	36,58,70,80	0
3	NAG	D	2	14/15	0.96	0.08	32,38,55,63	0
3	NAG	D	1	14/15	0.96	0.07	25,31,40,45	0
3	NAG	F	2	14/15	0.96	0.07	29,40,53,61	0
3	NAG	F	1	14/15	0.98	0.06	26,28,33,38	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.

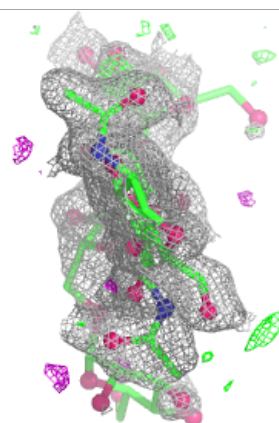
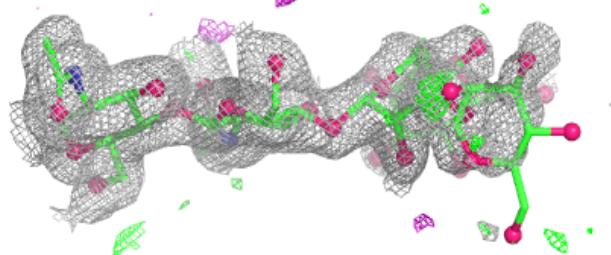
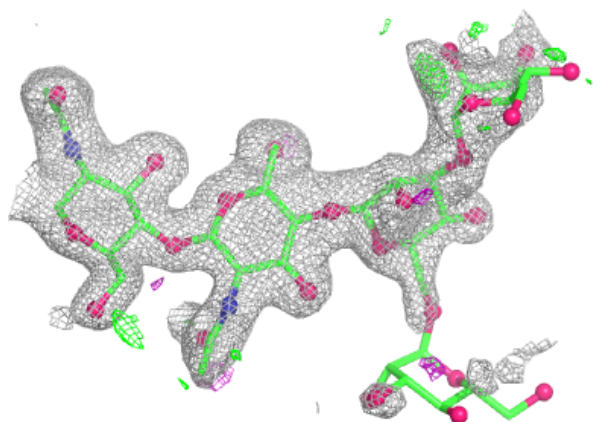


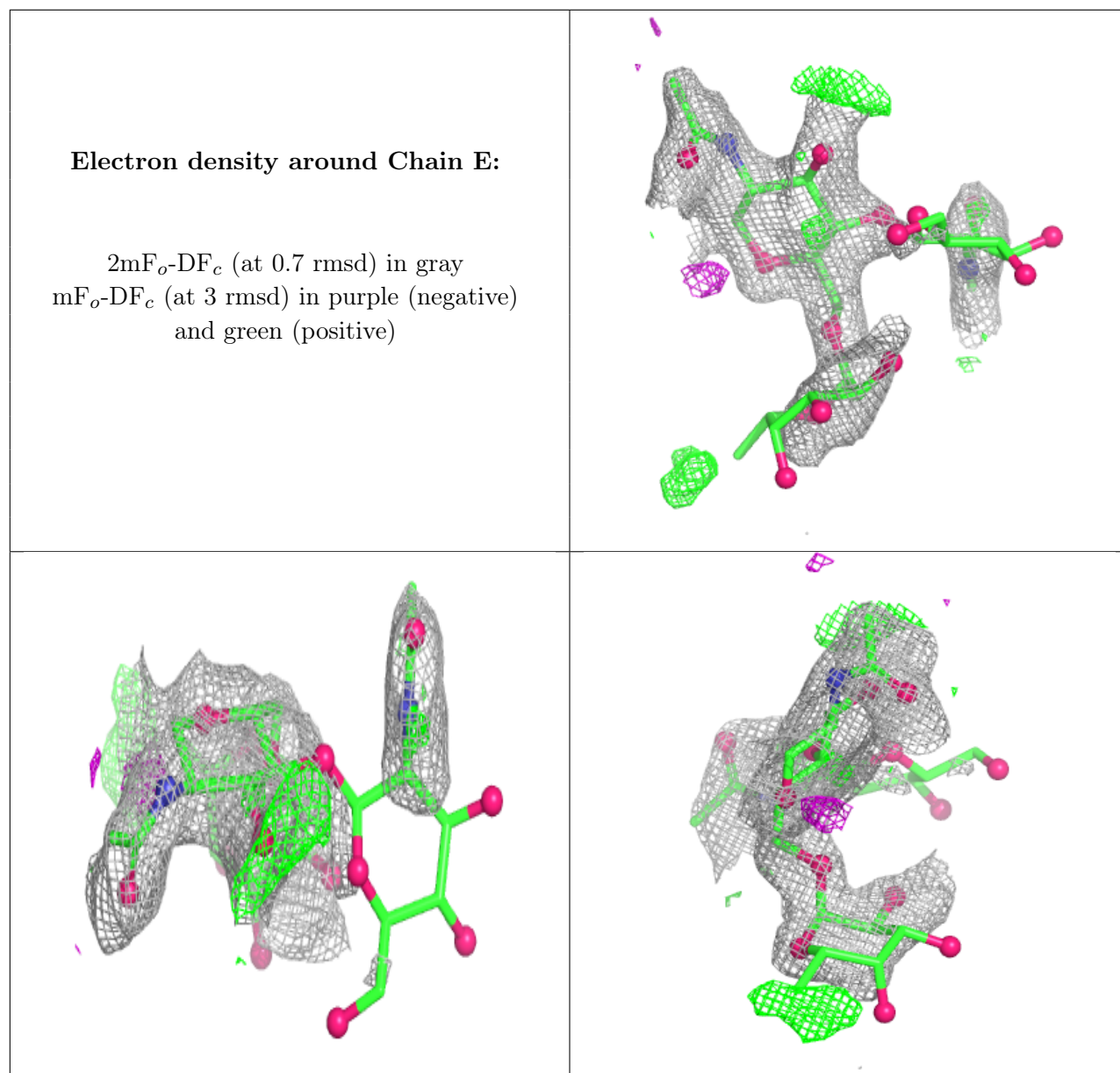
Electron density around Chain D:

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

**Electron density around Chain F:**

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





6.4 Ligands ⓘ

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
8	GOL	B	517	6/6	0.79	0.19	41,71,96,100	0
5	NAG	B	509	14/15	0.80	0.14	85,103,114,115	0
5	NAG	A	509	14/15	0.82	0.15	79,97,107,109	0
8	GOL	B	512	6/6	0.87	0.13	43,52,66,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	GOL	B	514	6/6	0.88	0.14	73,89,90,91	0
8	GOL	B	515	6/6	0.88	0.17	32,52,55,62	0
8	GOL	A	514	6/6	0.88	0.15	26,46,47,50	0
9	ACY	A	515	4/4	0.89	0.18	27,42,54,59	0
8	GOL	A	513	6/6	0.90	0.19	64,83,83,85	0
8	GOL	B	513	6/6	0.90	0.18	86,93,97,98	0
8	GOL	A	512	6/6	0.90	0.15	35,60,78,80	0
7	CIT	B	511	13/13	0.91	0.11	48,65,73,74	0
8	GOL	A	518	6/6	0.91	0.16	28,65,71,74	0
8	GOL	A	517	6/6	0.92	0.11	44,57,65,65	0
8	GOL	A	516	6/6	0.93	0.12	30,53,66,78	0
8	GOL	B	518	6/6	0.93	0.12	26,47,51,59	0
8	GOL	B	516	6/6	0.93	0.12	29,52,65,76	0
7	CIT	A	511	13/13	0.95	0.08	33,43,53,55	0
6	DJN	A	510	14/14	0.98	0.05	15,17,19,20	0
6	DJN	B	510	14/14	0.98	0.05	21,23,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.