



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 07:08 AM EDT

PDB ID : 7LFN  
Title : Structure of Hyperglycosylated Human IgG1 Fc (Fc267\_329)  
Authors : Fields, J.K.; Sundberg, E.J.  
Deposited on : 2021-01-17  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

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<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>.

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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 : 2.35.1  
buster-report : 1.1.7 (2018)  
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

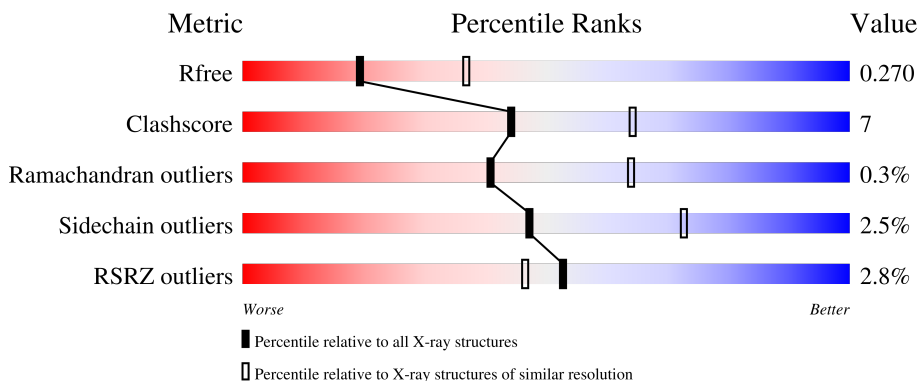
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	233	
1	B	233	
2	C	6	
3	D	7	
3	E	7	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	NAG	A	502	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3315 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.

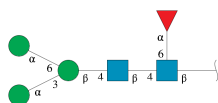
- Molecule 1 is a protein called IgG1 Fc (Fc267\_329).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total 1601	C 1016	N 269	O 309	S 7	0	0	0
1	B	193	Total 1437	C 908	N 240	O 282	S 7	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

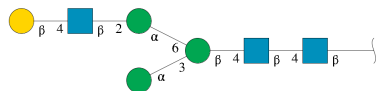
Chain	Residue	Modelled	Actual	Comment	Reference
A	215	GLY	-	expression tag	UNP Q6MZV7
A	267	ASN	SER	conflict	UNP Q6MZV7
A	268	SER	HIS	conflict	UNP Q6MZV7
A	269	THR	GLU	conflict	UNP Q6MZV7
A	329	ASN	PRO	conflict	UNP Q6MZV7
A	330	SER	ALA	conflict	UNP Q6MZV7
A	331	THR	PRO	conflict	UNP Q6MZV7
B	215	GLY	-	expression tag	UNP Q6MZV7
B	267	ASN	SER	conflict	UNP Q6MZV7
B	268	SER	HIS	conflict	UNP Q6MZV7
B	269	THR	GLU	conflict	UNP Q6MZV7
B	329	ASN	PRO	conflict	UNP Q6MZV7
B	330	SER	ALA	conflict	UNP Q6MZV7
B	331	THR	PRO	conflict	UNP Q6MZV7

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



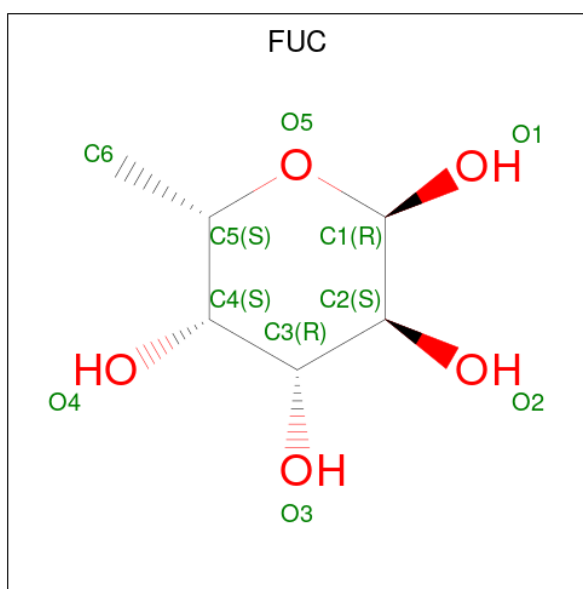
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	6	71	40	2	29	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
			Total	C	N	O			
3	D	7	86	48	3	35	0	0	0
3	E	7	86	48	3	35	0	0	0

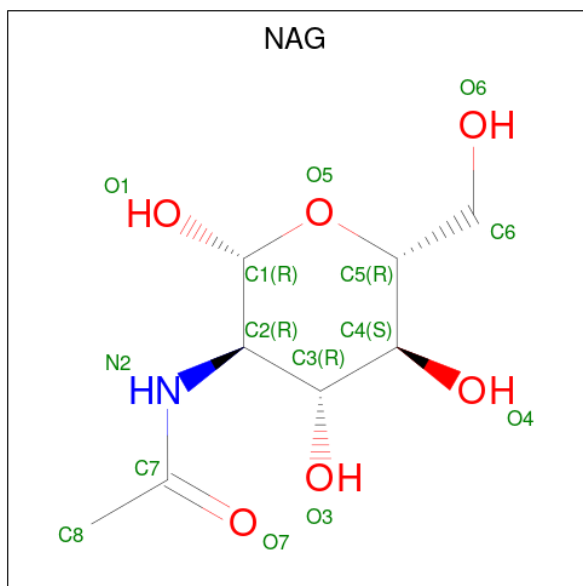
- Molecule 4 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0
4	B	1	10	6	4	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).




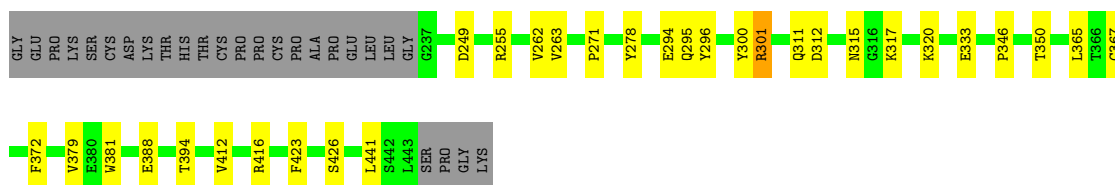
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0

### 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.

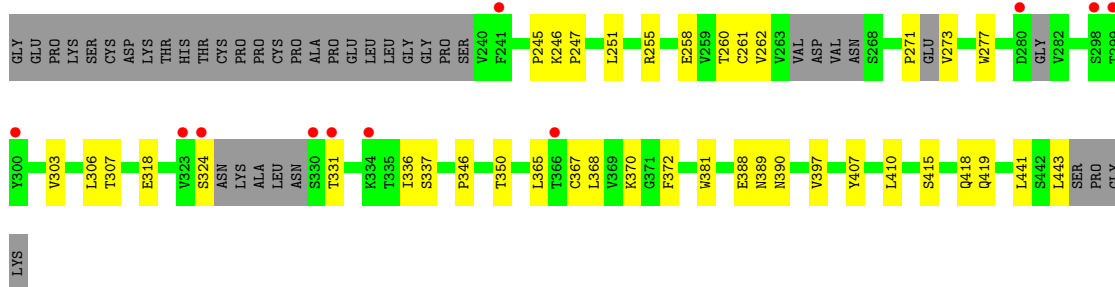
- Molecule 1: IgG1 Fc (Fc267\_329)

Chain A: 

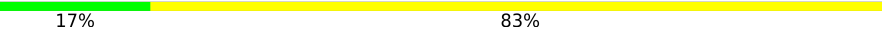


- Molecule 1: IgG1 Fc (Fc267\_329)

Chain B: 



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

Chain D: 

MAG1  
MAG2  
BMA3  
MAN4  
MAG5  
GAL6  
MAN7

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

Chain E:

71%

29%

MAG1  
MAG2  
BMA3  
MAN4  
MAG5  
GAL6  
MAN7



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.48Å 79.25Å 141.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.60 28.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.75-2.60) 98.5 (28.75-2.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.230 , 0.270 0.230 , 0.270	Depositor DCC
$R_{free}$ test set	864 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtrriage
Anisotropy	0.161	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUC, GAL, NAG, BMA

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	0.47	0/1644	0.60	0/2247
1	B	0.46	0/1472	0.63	0/2012
All	All	0.47	0/3116	0.61	0/4259

There are no bond length outliers.

There are no bond angle outliers.

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	1601	0	1503	17	0
1	B	1437	0	1270	22	0
2	C	71	0	61	0	0
3	D	86	0	73	1	0
3	E	86	0	73	6	0
4	A	10	0	10	2	0
4	B	10	0	10	1	0
5	A	14	0	13	0	0
All	All	3315	0	3013	42	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 7.

All (42) 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:262:VAL:HG22	1:B:303:VAL:HG22	1.74	0.70
1:B:245:PRO:HB3	1:B:258:GLU:H	1.56	0.69
1:A:296:TYR:H	4:A:501:FUC:H62	1.60	0.65
1:B:350:THR:HB	1:B:441:LEU:HD13	1.78	0.65
1:A:249:ASP:OD1	1:A:255:ARG:NH2	2.24	0.65
1:B:324:SER:HB3	1:B:331:THR:HG22	1.81	0.63
1:B:271:PRO:O	1:B:273:VAL:N	2.32	0.62
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.82	0.61
3:E:1:NAG:O7	3:E:1:NAG:O3	2.16	0.59
1:A:301:ARG:NH1	3:D:2:NAG:O7	2.38	0.56
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.42	0.54
1:B:277:TRP:CE3	1:B:306:LEU:HD12	2.42	0.54
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.43	0.53
1:A:262:VAL:HG11	1:A:301:ARG:NH1	2.24	0.53
1:A:295:GLN:OE1	4:A:501:FUC:H61	2.09	0.53
1:B:258:GLU:O	3:E:6:GAL:O3	2.20	0.52
1:B:246:LYS:HG2	3:E:6:GAL:O4	2.11	0.51
1:B:415:SER:O	1:B:419:GLN:HG2	2.12	0.49
1:A:312:ASP:OD1	1:A:317:LYS:HE2	2.12	0.49
1:A:388:GLU:OE2	1:A:416:ARG:NH2	2.24	0.48
1:A:294:GLU:HB2	1:A:300:TYR:CZ	2.48	0.48
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.49	0.48
1:A:350:THR:HB	1:A:441:LEU:HD22	1.96	0.47
1:B:365:LEU:HB3	1:B:441:LEU:CD2	2.45	0.47
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.97	0.47
1:A:379:VAL:HA	1:A:426:SER:O	2.15	0.46
1:A:320:LYS:HD2	1:A:333:GLU:OE1	2.15	0.46
1:B:370:LYS:HE2	1:B:370:LYS:HB3	1.82	0.46
1:B:260:THR:HG22	1:B:262:VAL:HG23	1.97	0.45
1:B:247:PRO:O	1:B:251:LEU:HG	2.18	0.44
1:A:394:THR:HG22	1:B:397:VAL:HG21	2.00	0.44
3:E:1:NAG:HO3	3:E:1:NAG:C7	2.20	0.43
1:B:318:GLU:HA	1:B:337:SER:HB3	2.00	0.43
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.54	0.43
1:B:336:ILE:HD12	1:B:336:ILE:HA	1.80	0.43
1:B:390:ASN:O	1:B:410:LEU:HD12	2.19	0.42
1:A:278:TYR:HB2	1:A:320:LYS:HB3	2.02	0.42
4:B:501:FUC:H5	3:E:1:NAG:O6	2.20	0.42
1:A:311:GLN:O	1:A:315:ASN:HB2	2.22	0.40
1:A:412:VAL:HG11	1:A:423:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:MAN:O2	3:E:5:NAG:O7	2.38	0.40
1:B:306:LEU:HD23	1:B:307:THR:N	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	205/233 (88%)	197 (96%)	7 (3%)	1 (0%)	29	52
1	B	183/233 (78%)	174 (95%)	9 (5%)	0	100	100
All	All	388/466 (83%)	371 (96%)	16 (4%)	1 (0%)	41	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	PRO

### 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	177/216 (82%)	174 (98%)	3 (2%)	60	81
1	B	149/216 (69%)	144 (97%)	5 (3%)	37	63
All	All	326/432 (76%)	318 (98%)	8 (2%)	47	73

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	VAL
1	A	301	ARG
1	A	365	LEU
1	B	255	ARG
1	B	388	GLU
1	B	389	ASN
1	B	418	GLN
1	B	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

20 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	0.23	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
2	BMA	C	3	2	11,11,12	1.36	1 (9%)	15,15,17	0.93	0
2	MAN	C	4	2	11,11,12	1.50	2 (18%)	15,15,17	1.20	3 (20%)
2	MAN	C	5	2	11,11,12	1.39	1 (9%)	15,15,17	1.79	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FUC	C	6	2	10,10,11	1.35	2 (20%)	14,14,16	0.90	1 (7%)
3	NAG	D	1	3,1	14,14,15	0.91	1 (7%)	17,19,21	0.78	0
3	NAG	D	2	3	14,14,15	0.49	0	17,19,21	0.62	0
3	BMA	D	3	3	11,11,12	0.82	0	15,15,17	1.27	2 (13%)
3	MAN	D	4	3	11,11,12	1.20	1 (9%)	15,15,17	1.09	1 (6%)
3	NAG	D	5	3	14,14,15	0.86	1 (7%)	17,19,21	0.44	0
3	GAL	D	6	3	11,11,12	1.36	2 (18%)	15,15,17	1.01	1 (6%)
3	MAN	D	7	3	11,11,12	1.64	3 (27%)	15,15,17	1.02	1 (6%)
3	NAG	E	1	3,1	14,14,15	0.49	0	17,19,21	0.82	0
3	NAG	E	2	3	14,14,15	0.58	0	17,19,21	0.64	1 (5%)
3	BMA	E	3	3	11,11,12	1.11	1 (9%)	15,15,17	1.25	2 (13%)
3	MAN	E	4	3	11,11,12	0.96	0	15,15,17	1.04	1 (6%)
3	NAG	E	5	3	14,14,15	0.60	0	17,19,21	0.84	0
3	GAL	E	6	3	11,11,12	1.12	1 (9%)	15,15,17	1.19	0
3	MAN	E	7	3	11,11,12	1.61	3 (27%)	15,15,17	1.15	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	-	3/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	FUC	C	6	2	-	-	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	NAG	D	5	3	-	0/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	1/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	5	3	-	2/6/23/26	0/1/1/1
3	GAL	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	1/2/19/22	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	7	MAN	O5-C1	-3.84	1.37	1.43
2	C	4	MAN	C1-C2	3.57	1.60	1.52
3	D	7	MAN	O5-C1	-3.40	1.38	1.43
3	E	3	BMA	C1-C2	3.36	1.59	1.52
2	C	5	MAN	C1-C2	3.15	1.59	1.52
2	C	3	BMA	C1-C2	3.10	1.59	1.52
3	D	6	GAL	C1-C2	2.99	1.59	1.52
3	D	5	NAG	O5-C1	-2.81	1.39	1.43
3	D	1	NAG	C1-C2	2.76	1.56	1.52
3	E	6	GAL	C1-C2	2.60	1.58	1.52
3	D	7	MAN	O5-C5	2.56	1.48	1.43
3	D	4	MAN	O5-C5	2.50	1.48	1.43
3	D	6	GAL	O5-C1	-2.37	1.39	1.43
2	C	6	FUC	C2-C3	2.31	1.55	1.52
3	E	7	MAN	C4-C5	2.27	1.57	1.53
3	E	7	MAN	C4-C3	2.14	1.57	1.52
3	D	7	MAN	C4-C5	2.11	1.57	1.53
2	C	4	MAN	C4-C5	2.07	1.57	1.53
2	C	6	FUC	C1-C2	2.01	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	MAN	C1-O5-C5	4.45	118.22	112.19
2	C	5	MAN	O5-C1-C2	3.59	116.31	110.77
2	C	2	NAG	C1-O5-C5	3.24	116.58	112.19
3	D	4	MAN	O2-C2-C3	-3.12	103.89	110.14
3	D	3	BMA	O2-C2-C3	-3.08	103.97	110.14
3	D	6	GAL	C1-C2-C3	2.68	112.96	109.67
3	D	3	BMA	C1-C2-C3	2.65	112.93	109.67
3	E	3	BMA	O2-C2-C3	-2.64	104.85	110.14
3	E	4	MAN	O2-C2-C3	-2.41	105.31	110.14
3	E	7	MAN	O2-C2-C3	-2.41	105.32	110.14
2	C	4	MAN	O2-C2-C3	-2.30	105.53	110.14
3	E	7	MAN	C3-C4-C5	2.23	114.22	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	C1-O5-C5	2.21	115.19	112.19
2	C	6	FUC	O2-C2-C1	2.15	113.54	109.15
2	C	4	MAN	C1-C2-C3	2.10	112.24	109.67
3	D	7	MAN	O2-C2-C3	-2.08	105.97	110.14
2	C	4	MAN	O2-C2-C1	2.04	113.33	109.15
3	E	2	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
2	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	5	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	E	7	MAN	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	D	3	BMA	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
2	C	2	NAG	C3-C2-N2-C7
3	D	7	MAN	O5-C5-C6-O6

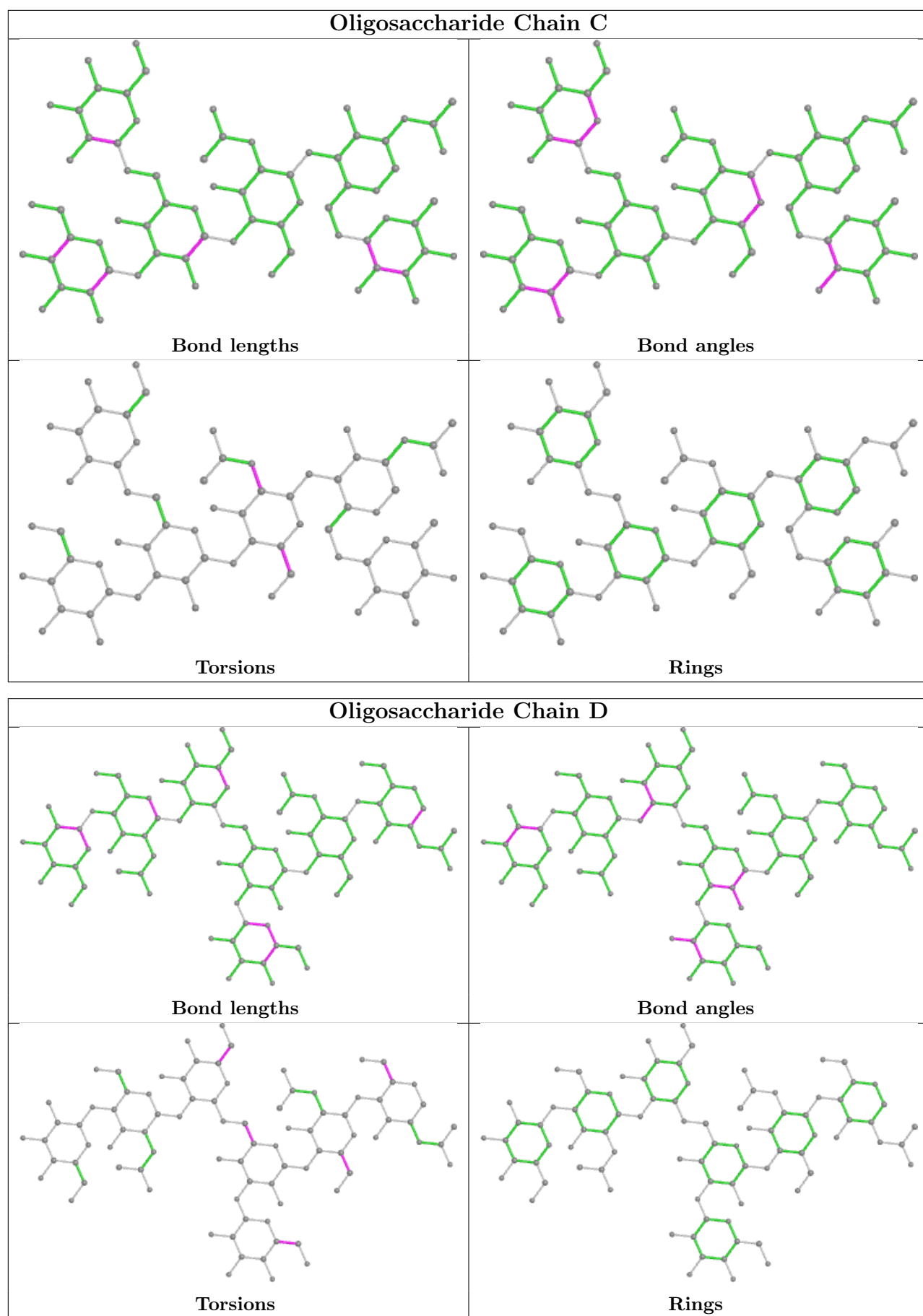
There are no ring outliers.

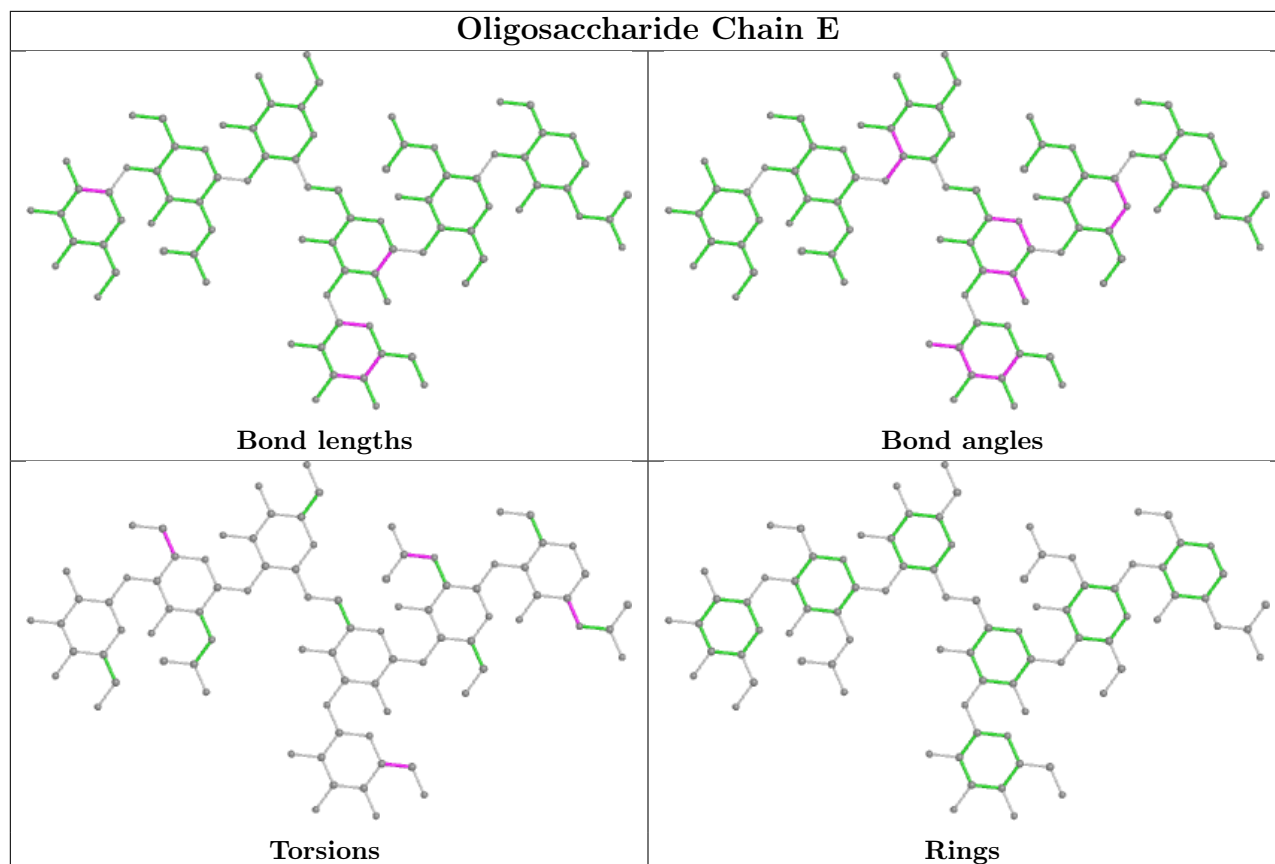
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	NAG	1	0
3	E	6	GAL	2	0
3	E	4	MAN	1	0
3	D	2	NAG	1	0
3	E	1	NAG	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](#)

3 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	FUC	A	501	-	10,10,11	1.57	3 (30%)	14,14,16	1.78	3 (21%)
5	NAG	A	502	1	14,14,15	0.42	0	17,19,21	0.48	0
4	FUC	B	501	-	10,10,11	0.59	0	14,14,16	1.04	1 (7%)

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	FUC	A	501	-	-	-	0/1/1/1
5	NAG	A	502	1	-	1/6/23/26	0/1/1/1
4	FUC	B	501	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	FUC	O5-C5	3.26	1.50	1.43
4	A	501	FUC	O5-C1	2.41	1.47	1.43
4	A	501	FUC	C6-C5	2.40	1.57	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	FUC	C1-O5-C5	4.45	122.86	112.78
4	A	501	FUC	O5-C5-C4	3.19	115.24	109.52
4	A	501	FUC	O5-C1-C2	2.56	114.72	110.77
4	B	501	FUC	C1-O5-C5	2.25	117.87	112.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	NAG	C1-C2-N2-C7

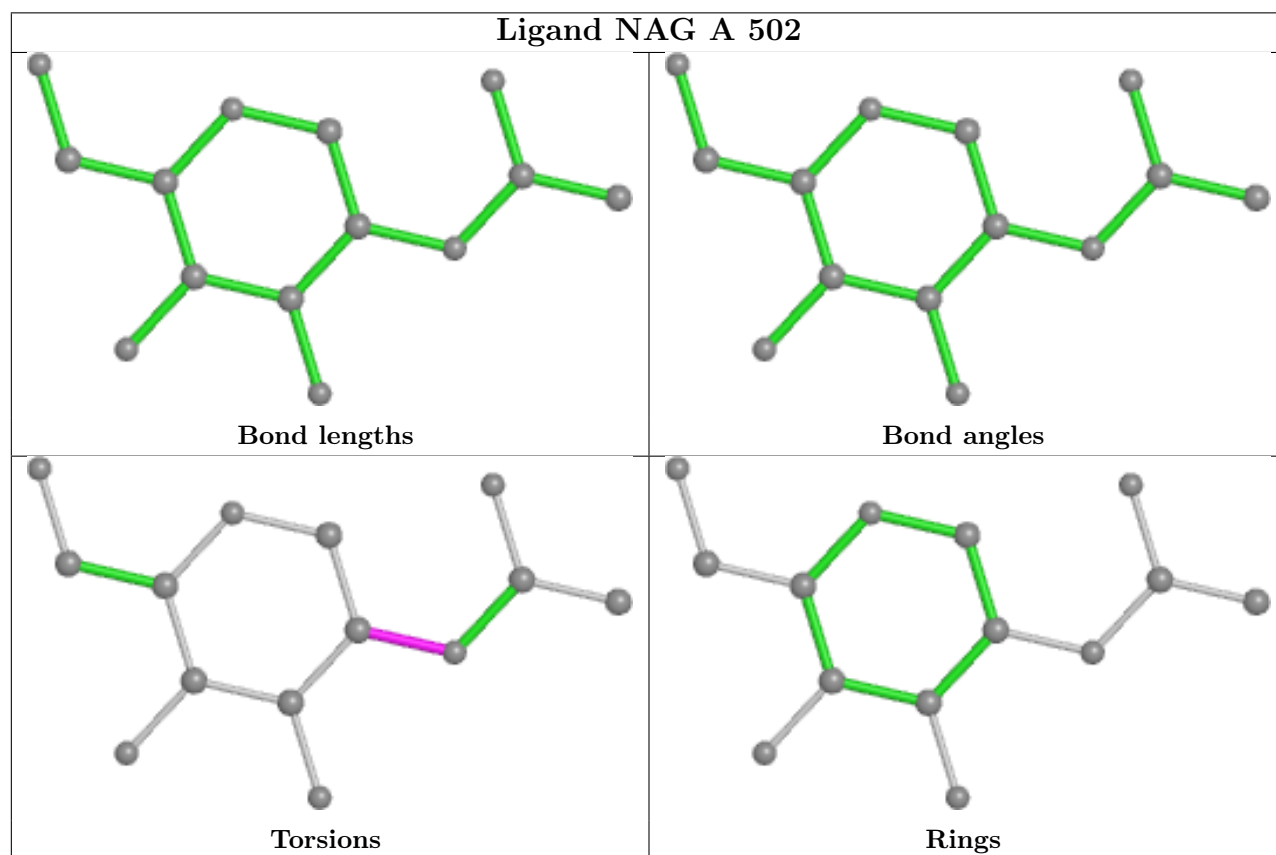
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	FUC	2	0
4	B	501	FUC	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	207/233 (88%)	-0.09	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	39, 52, 79, 104	0
1	B	193/233 (82%)	0.33	11 (5%) <span style="border: 1px solid red; padding: 2px;">23</span> <span style="border: 1px solid red; padding: 2px;">18</span>	39, 66, 115, 136	0
All	All	400/466 (85%)	0.11	11 (2%) <span style="border: 1px solid gray; padding: 2px;">53</span> <span style="border: 1px solid gray; padding: 2px;">46</span>	39, 56, 103, 136	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	SER	4.2
1	B	300	TYR	3.6
1	B	330	SER	3.6
1	B	280	ASP	3.5
1	B	331	THR	3.5
1	B	323	VAL	3.0
1	B	241	PHE	2.8
1	B	298	SER	2.8
1	B	366	THR	2.7
1	B	334	LYS	2.5
1	B	299	THR	2.3

### 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](#)

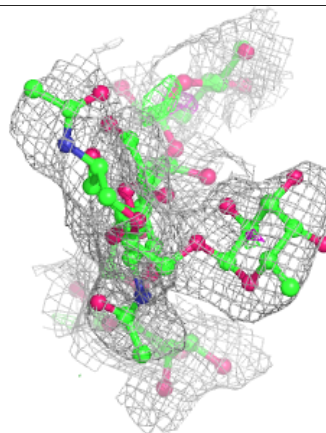
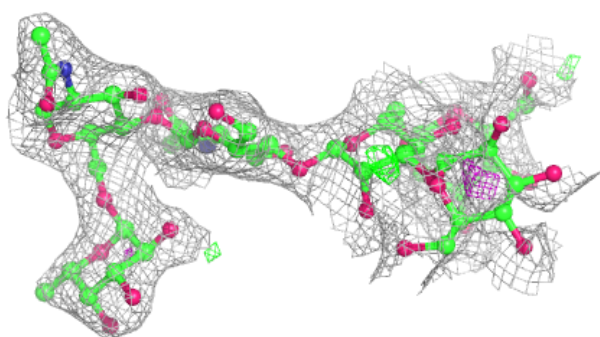
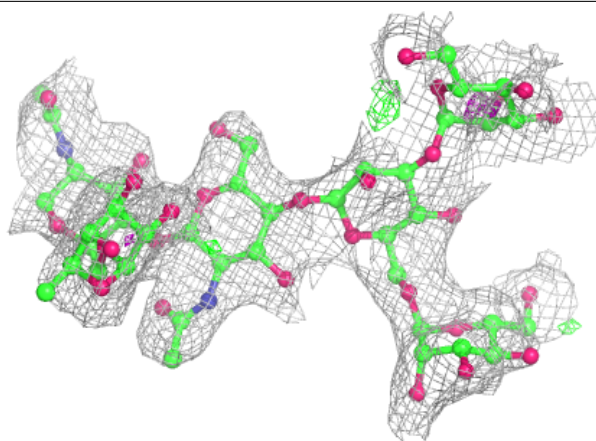
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	C	4	11/12	0.09	0.31	115,124,128,130	0
3	GAL	E	6	11/12	0.65	0.35	104,109,115,116	0
3	NAG	E	2	14/15	0.70	0.33	108,119,125,128	0
3	NAG	E	1	14/15	0.74	0.30	138,141,144,145	0
3	MAN	E	7	11/12	0.75	0.24	92,103,108,109	0
2	MAN	C	5	11/12	0.78	0.25	91,95,100,101	0
3	MAN	D	7	11/12	0.78	0.21	81,87,97,97	0
3	NAG	E	5	14/15	0.80	0.26	96,106,109,110	0
3	BMA	E	3	11/12	0.81	0.28	98,108,111,112	0
2	BMA	C	3	11/12	0.81	0.23	92,98,108,115	0
3	MAN	E	4	11/12	0.82	0.26	87,104,107,107	0
3	GAL	D	6	11/12	0.82	0.29	74,82,87,88	0
2	FUC	C	6	10/11	0.83	0.27	86,93,96,100	0
2	NAG	C	2	14/15	0.87	0.25	76,80,87,90	0
2	NAG	C	1	14/15	0.88	0.17	65,73,80,83	0
3	NAG	D	5	14/15	0.90	0.17	58,68,71,71	0
3	BMA	D	3	11/12	0.92	0.13	60,65,71,75	0
3	MAN	D	4	11/12	0.92	0.13	60,63,66,66	0
3	NAG	D	1	14/15	0.92	0.13	51,56,58,60	0
3	NAG	D	2	14/15	0.95	0.14	49,54,58,59	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.

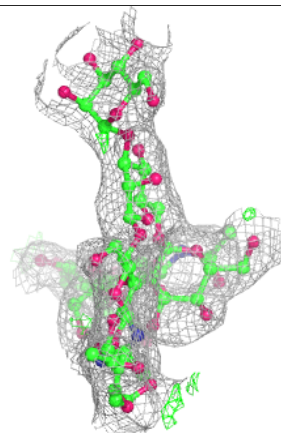
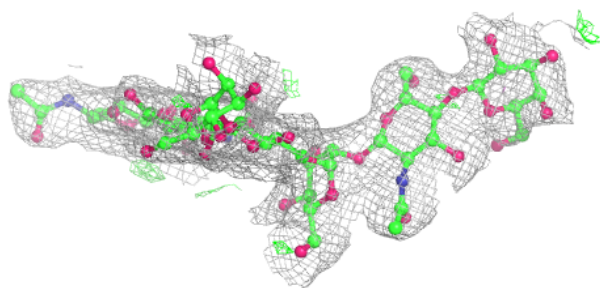
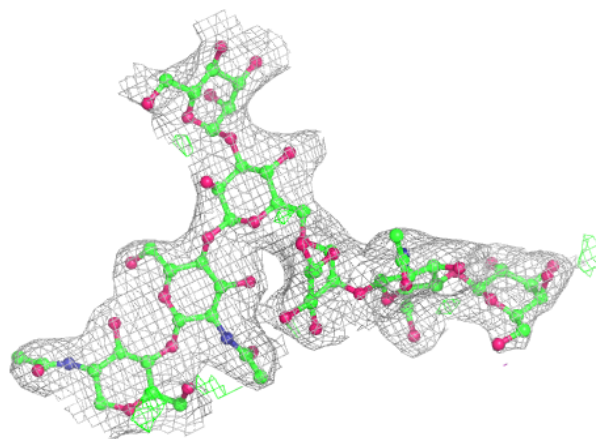
**Electron density around Chain C:**

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

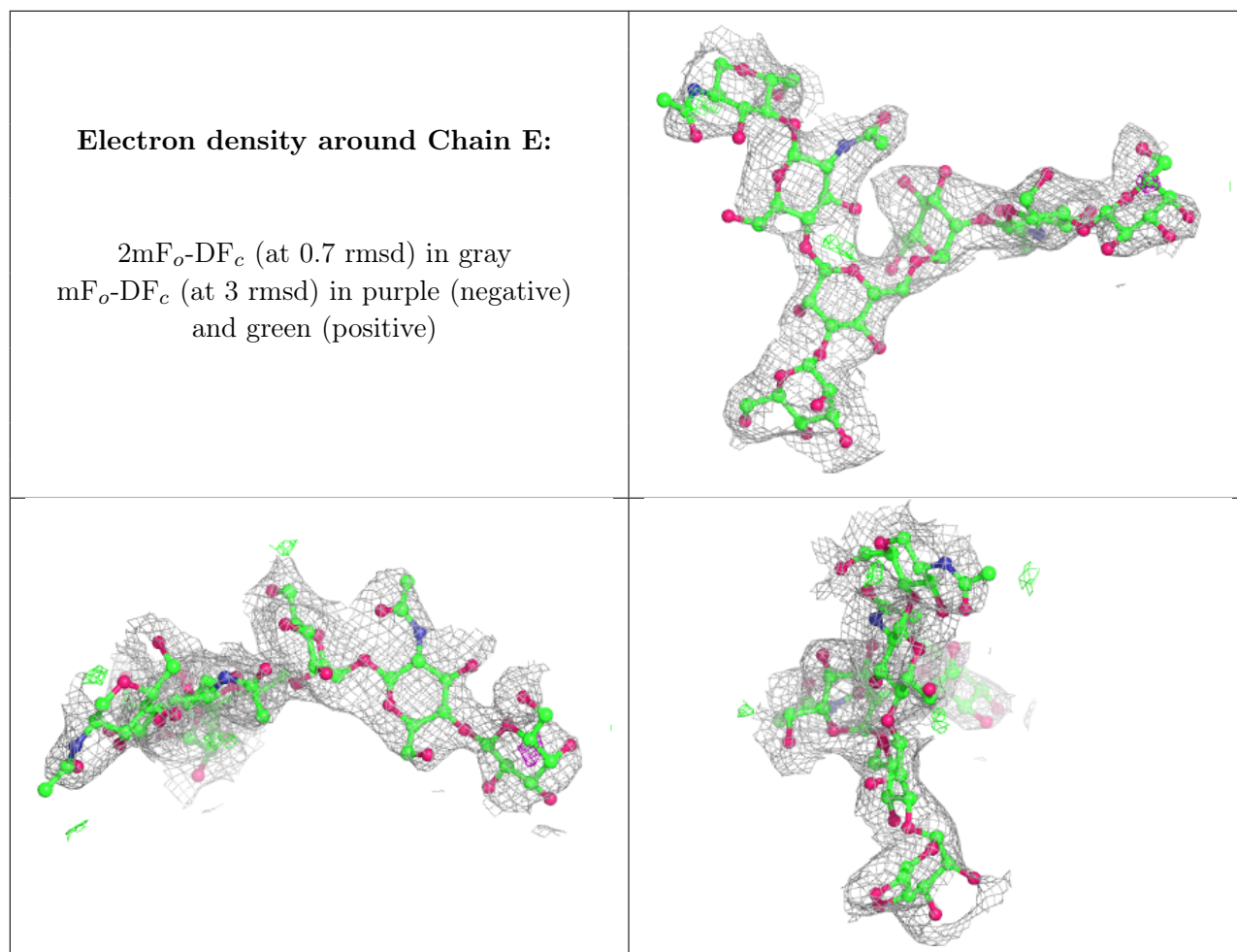


**Electron density around Chain D:**

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





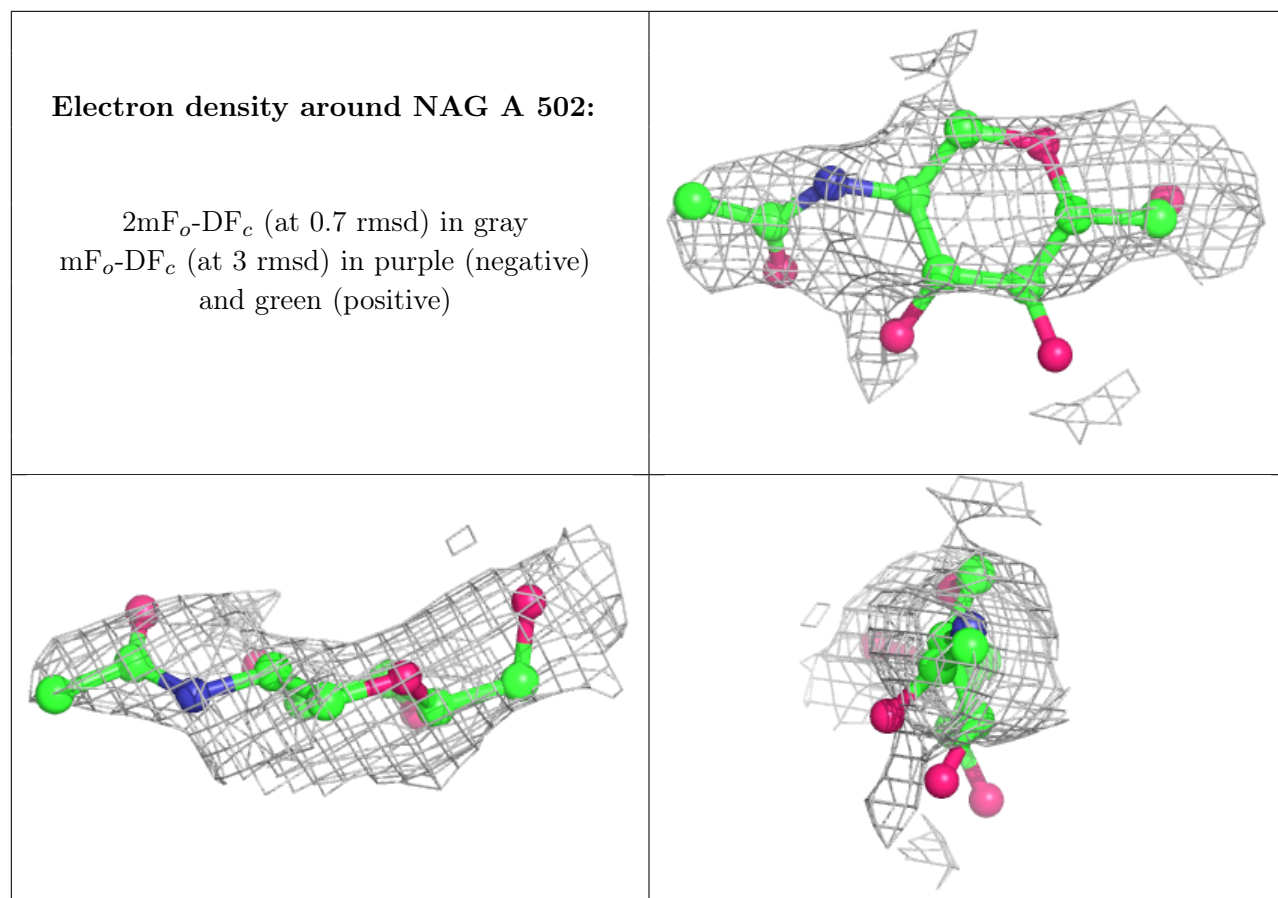


## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	A	502	14/15	0.57	0.48	105,119,122,128	0
4	FUC	A	501	10/11	0.67	0.26	58,64,71,72	0
4	FUC	B	501	10/11	0.76	0.35	116,119,122,122	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.