



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:19 PM BST

PDB ID : 4TVZ  
Title : Crystal Structure of SCARB2 in Neural Condition (pH7.5)  
Authors : Dang, M.H.; Wang, X.X.; Rao, Z.H.  
Deposited on : 2014-06-29  
Resolution : 3.01 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

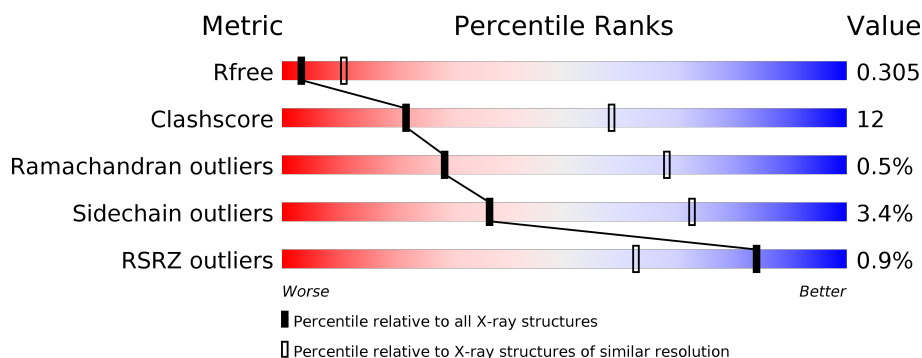
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	394	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>33%</div> <div>.</div> </div> </div>
1	B	394	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>..</div> </div> </div>
2	C	4	<div> <div>75%</div> <div>25%</div> </div>
2	L	4	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>
3	D	2	<div> <div>100%</div> </div>
3	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	J	2	 100%
4	F	9	 11% 78% 11%
5	G	5	 40% 60%
6	H	3	 67% 33%
7	K	10	 20% 80%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	K	10	-	-	-	X
8	NAG	A	501	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6892 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 Scavenger receptor class B member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3148	2031	510	596	11			
1	B	394	Total	C	N	O	S	0	0	0
			3127	2019	505	592	11			

- 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	L	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.



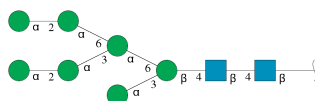
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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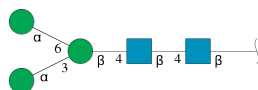
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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
4	F	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 5 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.



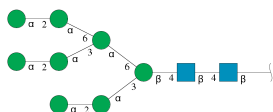
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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.



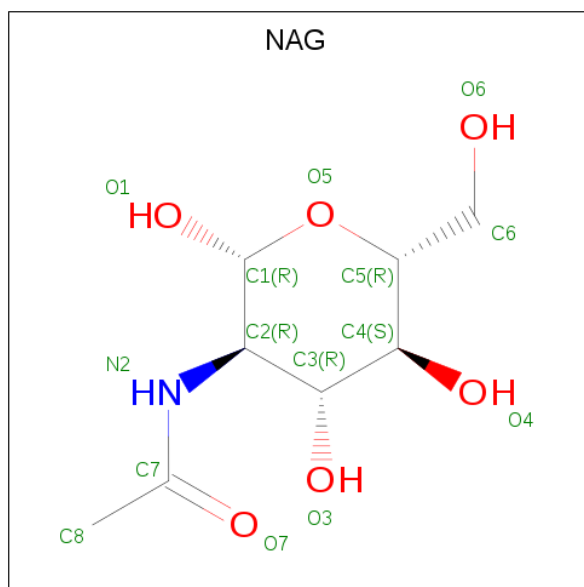
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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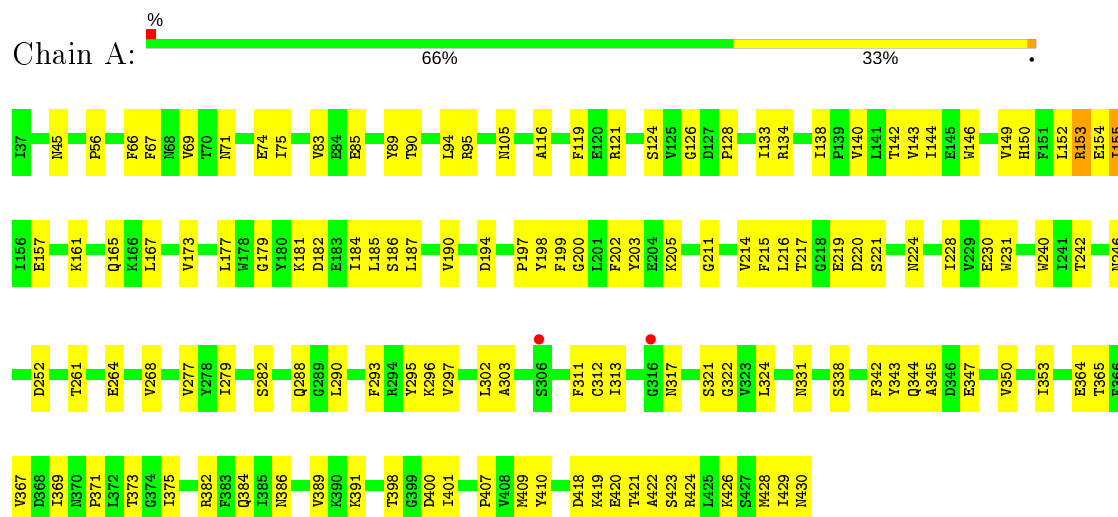
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

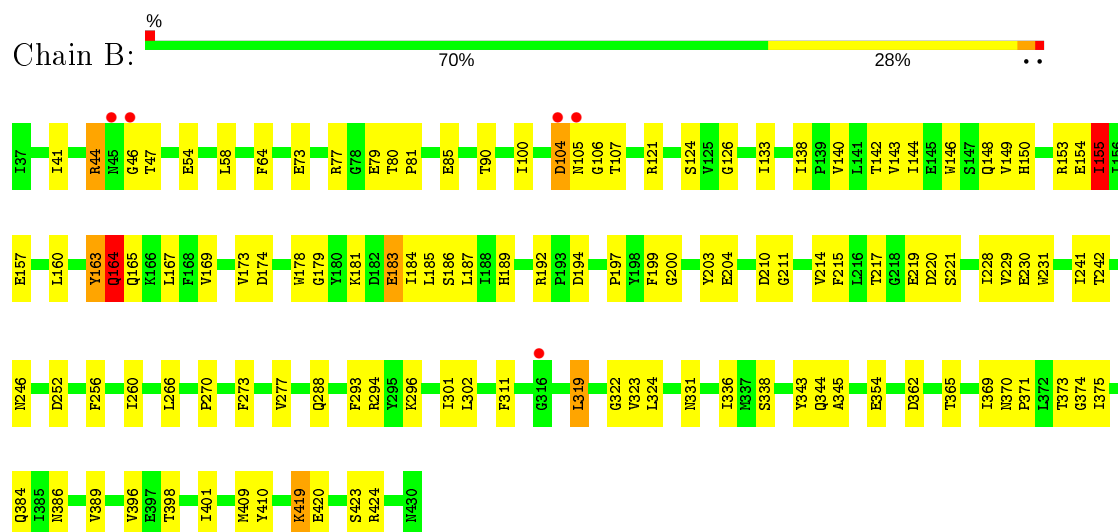
### 3 Residue-property plots

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

#### • Molecule 1: Scavenger receptor class B member 2



#### • Molecule 1: Scavenger receptor class B member 2



#### • 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



- Molecule 3: 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



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



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



- Molecule 5: 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

Chain G:  40% 60%

MAN1  
MAN2  
BMA3  
MAN4  
MAN5

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

MAN1  
MAN2  
BMA3

- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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

Chain K:  20% 80%

MAN1  
MAN2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.96 Å 63.72 Å 219.93 Å 90.00° 99.75° 90.00°	Depositor
Resolution (Å)	34.88 – 3.01 49.26 – 3.01	Depositor EDS
% Data completeness (in resolution range)	69.6 (34.88-3.01) 69.6 (49.26-3.01)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.27 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.259 , 0.304 0.261 , 0.305	Depositor DCC
$R_{free}$ test set	896 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 27.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1791e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.31	1/3231 (0.0%)	0.57	0/4401
1	B	0.28	0/3210	0.61	5/4376 (0.1%)
All	All	0.30	1/6441 (0.0%)	0.59	5/8777 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	347	GLU	CD-OE2	7.01	1.33	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	GLN	N-CA-C	6.06	127.35	111.00
1	B	319	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	106	GLY	N-CA-C	-5.47	99.41	113.10
1	B	149	VAL	C-N-CA	-5.41	108.18	121.70
1	B	155	ILE	CG1-CB-CG2	-5.30	99.74	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	TYR	Peptide

## 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	3148	0	2999	86	0
1	B	3127	0	2957	72	0
2	C	50	0	43	0	0
2	L	50	0	43	1	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
4	F	105	0	88	3	0
5	G	61	0	52	0	0
6	H	39	0	34	0	0
7	K	116	0	97	0	0
8	A	42	0	39	1	0
8	B	42	0	39	0	0
All	All	6892	0	6491	158	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 12.

All (158) 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:152:LEU:HD23	1:A:153:ARG:H	1.35	0.89
1:A:296:LYS:NZ	1:A:364:GLU:OE1	2.20	0.72
1:A:220:ASP:OD2	1:A:221:SER:N	2.25	0.70
1:B:165:GLN:HE21	1:B:184:ILE:HG12	1.56	0.69
1:B:220:ASP:OD2	1:B:221:SER:N	2.25	0.68
1:A:185:LEU:HB3	1:A:197:PRO:HA	1.77	0.67
1:B:167:LEU:HD22	1:B:398:THR:HA	1.75	0.67
1:B:373:THR:HG23	1:B:375:ILE:H	1.59	0.67
1:B:211:GLY:HA3	1:B:231:TRP:HE1	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:HB	1:A:375:ILE:HG13	1.78	0.66
1:B:154:GLU:O	1:B:155:ILE:HG22	1.98	0.64
1:B:311:PHE:HB3	1:B:324:LEU:HD11	1.79	0.64
1:A:313:ILE:HG21	4:F:1:NAG:H61	1.80	0.64
1:A:211:GLY:HA3	1:A:231:TRP:HE1	1.63	0.63
1:B:420:GLU:HA	1:B:423:SER:HB3	1.79	0.63
1:A:152:LEU:HD23	1:A:153:ARG:N	2.13	0.62
1:A:311:PHE:HB3	1:A:324:LEU:HD11	1.83	0.61
1:B:64:PHE:HD1	1:B:409:MET:HE1	1.66	0.60
1:B:90:THR:N	1:B:124:SER:OG	2.30	0.60
1:B:204:GLU:O	1:B:204:GLU:HG2	2.02	0.60
1:A:71:ASN:HB2	1:A:74:GLU:HB2	1.83	0.60
1:A:288:GLN:HB2	1:A:290:LEU:HD12	1.83	0.59
1:B:242:THR:O	1:B:246:ASN:ND2	2.34	0.59
1:B:293:PHE:CE2	1:B:371:PRO:HB3	2.38	0.57
1:B:323:VAL:HG12	1:B:338:SER:HB3	1.85	0.57
1:A:288:GLN:HE22	1:A:419:LYS:HD3	1.70	0.57
1:B:288:GLN:HE22	1:B:419:LYS:HG3	1.70	0.56
1:B:164:GLN:HG2	1:B:165:GLN:HG2	1.87	0.56
1:A:200:GLY:HA3	1:A:203:TYR:HB2	1.87	0.56
1:A:194:ASP:OD1	1:A:194:ASP:N	2.38	0.56
1:A:143:VAL:HA	1:A:146:TRP:HB2	1.88	0.56
1:A:154:GLU:O	1:A:155:ILE:HG22	2.06	0.55
1:A:215:PHE:HE1	1:A:228:ILE:HG12	1.71	0.55
1:A:429:ILE:N	1:A:430:ASN:HA	2.20	0.55
1:B:85:GLU:OE1	1:B:410:TYR:OH	2.15	0.55
1:A:364:GLU:O	1:A:382:ARG:NH1	2.39	0.55
1:B:181:LYS:NZ	1:B:197:PRO:HB2	2.22	0.55
1:A:391:LYS:HD2	1:A:400:ASP:HA	1.89	0.54
1:A:69:VAL:O	1:A:134:ARG:NH2	2.40	0.54
1:A:90:THR:N	1:A:124:SER:OG	2.28	0.54
1:A:293:PHE:CE2	1:A:371:PRO:HB3	2.43	0.54
1:A:121:ARG:CZ	1:A:126:GLY:HA2	2.38	0.53
1:B:44:ARG:HG3	1:B:46:GLY:H	1.73	0.53
1:A:338:SER:O	1:A:384:GLN:N	2.41	0.53
1:A:384:GLN:NE2	1:A:386:ASN:OD1	2.38	0.53
1:A:181:LYS:HG3	1:A:198:TYR:CE1	2.44	0.53
1:A:214:VAL:CG1	1:A:230:GLU:HB3	2.39	0.53
1:A:312:CYS:HB3	1:A:317:ASN:O	2.09	0.52
1:A:242:THR:O	1:A:246:ASN:ND2	2.39	0.52
1:B:185:LEU:HB3	1:B:197:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:CG1	1:B:230:GLU:HB3	2.40	0.52
1:B:370:ASN:HB3	1:B:373:THR:HG22	1.92	0.52
1:B:338:SER:O	1:B:384:GLN:N	2.40	0.51
1:A:94:LEU:HD12	1:A:116:ALA:HB3	1.94	0.50
1:B:215:PHE:HE1	1:B:228:ILE:HG12	1.76	0.50
1:A:422:ALA:O	1:A:426:LYS:HG3	2.12	0.49
1:A:423:SER:HA	1:A:426:LYS:HB2	1.94	0.49
1:B:164:GLN:HE22	1:B:183:GLU:HG2	1.77	0.49
1:A:279:ILE:HB	1:A:295:TYR:HB3	1.94	0.49
1:B:164:GLN:HE22	1:B:183:GLU:CG	2.26	0.49
1:A:75:ILE:HG22	1:A:401:ILE:HG13	1.95	0.49
1:B:181:LYS:HE3	1:B:197:PRO:HB2	1.95	0.49
1:B:336:ILE:HB	1:B:386:ASN:HB2	1.94	0.49
1:A:343:TYR:CE2	1:A:344:GLN:HG3	2.48	0.48
1:B:192:ARG:NH2	1:B:194:ASP:OD2	2.46	0.48
1:B:200:GLY:HA3	1:B:203:TYR:HB2	1.96	0.48
1:A:252:ASP:OD1	1:A:252:ASP:N	2.46	0.47
1:A:420:GLU:O	1:A:424:ARG:HG2	2.14	0.47
1:B:184:ILE:HA	1:B:187:LEU:HD12	1.95	0.47
1:A:418:ASP:OD2	1:A:420:GLU:HG2	2.15	0.47
1:A:367:VAL:HG12	1:A:369:ILE:HG23	1.94	0.47
1:A:342:PHE:HB2	1:A:350:VAL:HG22	1.95	0.47
1:A:165:GLN:HE21	1:A:184:ILE:HG12	1.80	0.47
1:A:167:LEU:HD22	1:A:398:THR:HA	1.97	0.47
1:B:217:THR:HG23	1:B:219:GLU:H	1.79	0.47
1:A:353:ILE:HG21	1:A:407:PRO:HG3	1.96	0.47
1:B:143:VAL:HA	1:B:146:TRP:HB2	1.98	0.46
1:A:179:GLY:HA2	1:A:199:PHE:O	2.15	0.46
1:B:181:LYS:CE	1:B:197:PRO:HB2	2.45	0.46
1:B:420:GLU:O	1:B:424:ARG:N	2.45	0.46
1:A:302:LEU:HD22	1:A:324:LEU:HB2	1.96	0.46
1:B:322:GLY:HA3	1:B:345:ALA:HB2	1.98	0.46
1:A:282:SER:OG	1:A:296:LYS:HE3	2.15	0.46
1:B:189:HIS:CG	1:B:197:PRO:HG3	2.51	0.46
1:A:240:TRP:C	1:A:246:ASN:HD21	2.18	0.46
1:A:418:ASP:OD2	1:A:421:THR:HG23	2.16	0.46
1:A:426:LYS:HB3	1:A:426:LYS:NZ	2.30	0.45
1:B:81:PRO:O	1:B:354:GLU:HB2	2.16	0.45
1:B:273:PHE:HZ	1:B:302:LEU:HD11	1.81	0.45
1:B:73:GLU:O	1:B:77:ARG:HG3	2.17	0.45
1:A:182:ASP:O	1:A:186:SER:OG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:O	1:A:344:GLN:NE2	2.47	0.45
1:B:163:TYR:HB3	1:B:164:GLN:HB3	1.99	0.45
1:A:202:PHE:HA	1:A:205:LYS:HD2	1.98	0.45
1:B:277:VAL:HG13	1:B:301:ILE:HG13	1.99	0.45
1:A:215:PHE:CE1	1:A:228:ILE:HG12	2.52	0.44
1:B:121:ARG:CZ	1:B:126:GLY:HA2	2.47	0.44
1:B:252:ASP:N	1:B:252:ASP:OD1	2.50	0.44
1:B:140:VAL:O	1:B:144:ILE:HG13	2.17	0.44
1:A:133:ILE:HG13	1:A:173:VAL:HG22	1.99	0.44
1:A:261:THR:O	1:A:264:GLU:HG2	2.18	0.44
1:B:104:ASP:HB3	1:B:105:ASN:H	1.31	0.44
1:B:181:LYS:HZ1	1:B:197:PRO:HB2	1.81	0.44
1:A:187:LEU:O	1:A:190:VAL:HB	2.17	0.44
1:A:364:GLU:O	1:A:382:ARG:HD2	2.18	0.44
1:B:164:GLN:HE22	1:B:183:GLU:CD	2.21	0.44
1:B:165:GLN:HG3	1:B:184:ILE:HG13	1.99	0.43
1:B:211:GLY:HA3	1:B:231:TRP:NE1	2.31	0.43
1:A:398:THR:O	1:A:401:ILE:HB	2.18	0.43
1:A:389:VAL:HG21	1:A:401:ILE:HD13	2.00	0.43
1:B:133:ILE:HG13	1:B:173:VAL:HG22	1.99	0.43
1:B:186:SER:HA	1:B:197:PRO:HB3	2.00	0.43
1:A:428:MET:O	1:A:429:ILE:HG13	2.18	0.43
1:B:80:THR:HA	1:B:81:PRO:HD3	1.78	0.43
1:A:149:VAL:HG23	4:F:3:BMA:H62	2.00	0.43
1:A:240:TRP:CE3	1:A:311:PHE:HA	2.54	0.43
1:A:220:ASP:CG	1:A:224:ASN:HD22	2.22	0.43
1:A:85:GLU:OE1	1:A:410:TYR:OH	2.23	0.43
1:B:409:MET:HB2	1:B:409:MET:HE2	1.77	0.43
1:A:303:ALA:HA	1:A:321:SER:HA	2.01	0.43
1:A:353:ILE:HG12	1:A:407:PRO:HD2	2.00	0.43
1:B:389:VAL:HG21	1:B:401:ILE:HD13	2.00	0.43
1:A:313:ILE:HG13	4:F:1:NAG:O6	2.20	0.42
1:A:140:VAL:O	1:A:144:ILE:HG13	2.19	0.42
1:B:294:ARG:HD3	1:B:296:LYS:HE2	2.01	0.42
1:A:138:ILE:O	1:A:142:THR:HG23	2.18	0.42
1:A:217:THR:HG23	1:A:219:GLU:H	1.85	0.42
1:B:157:GLU:O	1:B:160:LEU:HB2	2.19	0.42
1:B:343:TYR:CE2	1:B:344:GLN:HG3	2.55	0.42
1:B:179:GLY:HA2	1:B:199:PHE:O	2.20	0.42
1:A:268:VAL:N	1:A:277:VAL:O	2.47	0.42
1:A:71:ASN:O	1:A:75:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:HD2	1:A:95:ARG:O	2.20	0.41
1:B:256:PHE:CD1	1:B:266:LEU:HD13	2.55	0.41
1:A:161:LYS:HD3	1:A:161:LYS:HA	1.71	0.41
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.93	0.41
1:A:322:GLY:HA3	1:A:345:ALA:CB	2.51	0.41
1:A:119:PHE:CZ	1:A:128:PRO:HD3	2.55	0.41
1:A:89:TYR:HA	1:A:124:SER:HB3	2.01	0.41
1:B:105:ASN:HB3	1:B:107:THR:HB	2.03	0.41
1:B:270:PRO:HG2	1:B:273:PHE:HB3	2.01	0.41
1:A:389:VAL:HG22	1:A:401:ILE:HG21	2.03	0.41
1:A:45:ASN:HD22	8:A:501:NAG:H62	1.85	0.41
1:A:165:GLN:NE2	1:A:184:ILE:HG12	2.36	0.41
1:B:260:ILE:HD11	1:B:374:GLY:HA2	2.03	0.41
1:B:194:ASP:OD1	1:B:194:ASP:N	2.40	0.41
1:B:214:VAL:HG13	1:B:229:VAL:HG23	2.03	0.41
1:A:66:PHE:HB2	1:A:133:ILE:HD12	2.03	0.41
1:B:54:GLU:HG3	1:B:100:ILE:HD11	2.03	0.41
1:B:138:ILE:O	1:B:142:THR:HG23	2.21	0.41
1:A:67:PHE:CD2	1:A:407:PRO:HB2	2.56	0.40
1:B:144:ILE:O	1:B:148:GLN:HG3	2.21	0.40
1:B:174:ASP:OD1	1:B:178:TRP:HD1	2.04	0.40
1:A:67:PHE:HB3	1:A:83:VAL:HB	2.02	0.40
1:A:429:ILE:O	1:A:429:ILE:HD12	2.20	0.40
1:B:58:LEU:HD12	1:B:58:LEU:O	2.22	0.40
1:B:44:ARG:HG2	1:B:47:THR:H	1.85	0.40
1:B:362:ASP:O	2:L:1:NAG:O6	2.40	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	392/394 (100%)	381 (97%)	9 (2%)	2 (0%)	29	68
1	B	392/394 (100%)	383 (98%)	7 (2%)	2 (0%)	29	68
All	All	784/788 (100%)	764 (97%)	16 (2%)	4 (0%)	29	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	B	155	ILE
1	A	331	ASN
1	B	331	ASN

### 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	342/355 (96%)	335 (98%)	7 (2%)	55	83
1	B	336/355 (95%)	320 (95%)	16 (5%)	25	62
All	All	678/710 (96%)	655 (97%)	23 (3%)	37	72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	150	HIS
1	A	153	ARG
1	A	157	GLU
1	A	177	LEU
1	A	365	THR
1	A	409	MET
1	B	41	ILE
1	B	44	ARG
1	B	79	GLU
1	B	104	ASP
1	B	150	HIS

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Mol	Chain	Res	Type
1	B	153	ARG
1	B	164	GLN
1	B	169	VAL
1	B	183	GLU
1	B	210	ASP
1	B	241	ILE
1	B	319	LEU
1	B	365	THR
1	B	369	ILE
1	B	396	VAL
1	B	419	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	GLN
1	B	165	GLN

### 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 ⓘ

43 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	0.39	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	0.46	0
2	BMA	C	3	2	11,11,12	0.70	0	15,15,17	0.86	0
2	MAN	C	4	2	11,11,12	0.72	0	15,15,17	1.58	3 (20%)
3	NAG	D	1	1,3	14,14,15	0.31	0	17,19,21	0.44	0
3	NAG	D	2	3	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	E	1	1,3	14,14,15	0.33	0	17,19,21	0.58	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	F	1	1,4	14,14,15	0.51	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.35	0	17,19,21	0.44	0
4	BMA	F	3	4	11,11,12	0.93	1 (9%)	15,15,17	0.83	0
4	MAN	F	4	4	11,11,12	1.04	1 (9%)	15,15,17	0.90	1 (6%)
4	MAN	F	5	4	11,11,12	0.77	0	15,15,17	0.98	1 (6%)
4	MAN	F	6	4	11,11,12	0.77	0	15,15,17	1.36	3 (20%)
4	MAN	F	7	4	11,11,12	1.38	2 (18%)	15,15,17	3.59	6 (40%)
4	MAN	F	8	4	11,11,12	0.86	1 (9%)	15,15,17	1.12	2 (13%)
4	MAN	F	9	4	11,11,12	0.90	1 (9%)	15,15,17	0.93	0
5	NAG	G	1	1,5	14,14,15	0.19	0	17,19,21	1.00	1 (5%)
5	NAG	G	2	5	14,14,15	0.44	0	17,19,21	0.37	0
5	BMA	G	3	5	11,11,12	0.64	0	15,15,17	0.85	0
5	MAN	G	4	5	11,11,12	0.94	1 (9%)	15,15,17	0.97	1 (6%)
5	MAN	G	5	5	11,11,12	0.73	0	15,15,17	1.09	2 (13%)
6	NAG	H	1	1,6	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	H	2	6	14,14,15	0.30	0	17,19,21	0.36	0
6	BMA	H	3	6	11,11,12	0.92	1 (9%)	15,15,17	0.81	0
3	NAG	I	1	1,3	14,14,15	0.30	0	17,19,21	0.35	0
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.37	0
3	NAG	J	1	1,3	14,14,15	0.41	0	17,19,21	0.50	0
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.33	0
7	NAG	K	1	1,7	14,14,15	0.42	0	17,19,21	0.50	0
7	MAN	K	10	7	11,11,12	0.73	0	15,15,17	1.02	2 (13%)
7	NAG	K	2	7	14,14,15	0.17	0	17,19,21	0.52	0
7	BMA	K	3	7	11,11,12	0.81	1 (9%)	15,15,17	0.91	0
7	MAN	K	4	7	11,11,12	1.13	1 (9%)	15,15,17	0.81	1 (6%)
7	MAN	K	5	7	11,11,12	0.99	1 (9%)	15,15,17	1.00	1 (6%)
7	MAN	K	6	7	11,11,12	0.90	1 (9%)	15,15,17	1.64	2 (13%)
7	MAN	K	7	7	11,11,12	1.38	2 (18%)	15,15,17	3.62	8 (53%)
7	MAN	K	8	7	11,11,12	0.90	1 (9%)	15,15,17	1.15	1 (6%)
7	MAN	K	9	7	11,11,12	0.81	0	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	L	1	1,2	14,14,15	0.16	0	17,19,21	0.95	2 (11%)
2	NAG	L	2	2	14,14,15	0.44	0	17,19,21	0.42	0
2	BMA	L	3	2	11,11,12	0.74	1 (9%)	15,15,17	0.84	0
2	MAN	L	4	2	11,11,12	0.94	1 (9%)	15,15,17	0.90	1 (6%)

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	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	1/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	1/2/19/22	0/1/1/1
4	MAN	F	5	4	-	1/2/19/22	0/1/1/1
4	MAN	F	6	4	-	2/2/19/22	1/1/1/1
4	MAN	F	7	4	-	0/2/19/22	1/1/1/1
4	MAN	F	8	4	-	0/2/19/22	0/1/1/1
4	MAN	F	9	4	-	1/2/19/22	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	MAN	G	5	5	-	1/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	K	1	1,7	-	2/6/23/26	0/1/1/1
7	MAN	K	10	7	-	0/2/19/22	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	1/2/19/22	0/1/1/1
7	MAN	K	6	7	-	1/2/19/22	1/1/1/1
7	MAN	K	7	7	-	0/2/19/22	1/1/1/1
7	MAN	K	8	7	-	2/2/19/22	0/1/1/1
7	MAN	K	9	7	-	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	BMA	L	3	2	-	0/2/19/22	0/1/1/1
2	MAN	L	4	2	-	2/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	4	MAN	O5-C1	-3.09	1.38	1.43
4	F	4	MAN	O5-C1	-2.89	1.39	1.43
7	K	7	MAN	O5-C1	-2.79	1.39	1.43
7	K	5	MAN	O5-C1	-2.67	1.39	1.43
4	F	7	MAN	C1-C2	2.59	1.58	1.52
2	L	4	MAN	O5-C1	-2.56	1.39	1.43
4	F	9	MAN	O5-C1	-2.53	1.39	1.43
4	F	7	MAN	O5-C1	-2.52	1.39	1.43
5	G	4	MAN	O5-C1	-2.44	1.39	1.43
7	K	8	MAN	C1-C2	2.41	1.57	1.52
7	K	6	MAN	O5-C5	2.35	1.48	1.43
7	K	7	MAN	C1-C2	2.27	1.57	1.52
6	H	3	BMA	O5-C1	-2.24	1.40	1.43
4	F	3	BMA	O5-C1	-2.14	1.40	1.43
7	K	3	BMA	O5-C1	-2.06	1.40	1.43
4	F	8	MAN	C1-C2	2.02	1.56	1.52
2	L	3	BMA	O5-C1	-2.00	1.40	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	7	MAN	O5-C1-C2	-11.18	93.51	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	7	MAN	O5-C1-C2	-11.02	93.76	110.77
7	K	6	MAN	C1-O5-C5	5.05	119.03	112.19
7	K	7	MAN	C1-O5-C5	5.04	119.02	112.19
4	F	7	MAN	C1-O5-C5	4.80	118.70	112.19
2	C	4	MAN	C1-O5-C5	4.68	118.53	112.19
7	K	7	MAN	C3-C4-C5	-3.86	103.35	110.24
4	F	6	MAN	C1-O5-C5	3.81	117.36	112.19
4	F	7	MAN	C3-C4-C5	-3.57	103.87	110.24
7	K	5	MAN	O2-C2-C3	-3.00	104.12	110.14
5	G	1	NAG	C1-O5-C5	2.83	116.03	112.19
4	F	7	MAN	O5-C5-C4	-2.75	104.13	110.83
4	F	5	MAN	O2-C2-C3	-2.71	104.72	110.14
5	G	5	MAN	C1-O5-C5	2.69	115.84	112.19
4	F	7	MAN	O2-C2-C3	-2.56	105.01	110.14
7	K	7	MAN	O3-C3-C2	2.52	114.82	109.99
7	K	7	MAN	C2-C3-C4	-2.49	106.59	110.89
5	G	4	MAN	O2-C2-C3	-2.43	105.28	110.14
4	F	7	MAN	O3-C3-C2	2.40	114.60	109.99
7	K	7	MAN	O2-C2-C3	-2.40	105.34	110.14
7	K	7	MAN	O5-C5-C4	-2.39	105.02	110.83
4	F	4	MAN	O2-C2-C3	-2.36	105.41	110.14
2	L	1	NAG	C2-N2-C7	2.30	126.17	122.90
7	K	10	MAN	C1-O5-C5	2.25	115.24	112.19
7	K	9	MAN	O2-C2-C3	-2.25	105.64	110.14
7	K	6	MAN	O5-C1-C2	2.23	114.22	110.77
4	F	8	MAN	C1-O5-C5	2.18	115.15	112.19
4	F	8	MAN	O2-C2-C3	-2.18	105.77	110.14
2	L	1	NAG	C1-O5-C5	2.16	115.12	112.19
2	C	4	MAN	O5-C1-C2	2.16	114.10	110.77
5	G	5	MAN	O2-C2-C3	-2.15	105.84	110.14
7	K	8	MAN	O2-C2-C3	-2.12	105.89	110.14
7	K	10	MAN	O2-C2-C3	-2.11	105.91	110.14
7	K	7	MAN	C1-C2-C3	2.08	112.22	109.67
4	F	6	MAN	O2-C2-C3	-2.06	106.01	110.14
2	L	4	MAN	O2-C2-C3	-2.05	106.03	110.14
4	F	6	MAN	O5-C1-C2	2.02	113.89	110.77
7	K	4	MAN	O2-C2-C3	-2.02	106.10	110.14
2	C	4	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	NAG	C3-C2-N2-C7
7	K	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
7	K	9	MAN	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
2	L	4	MAN	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	L	4	MAN	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
4	F	6	MAN	O5-C5-C6-O6
7	K	9	MAN	C4-C5-C6-O6
7	K	5	MAN	O5-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
6	H	1	NAG	O5-C5-C6-O6
7	K	6	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
4	F	9	MAN	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
5	G	1	NAG	C3-C2-N2-C7
7	K	8	MAN	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
5	G	5	MAN	O5-C5-C6-O6
4	F	6	MAN	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
7	K	8	MAN	O5-C5-C6-O6
7	K	4	MAN	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	F	4	MAN	C4-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6

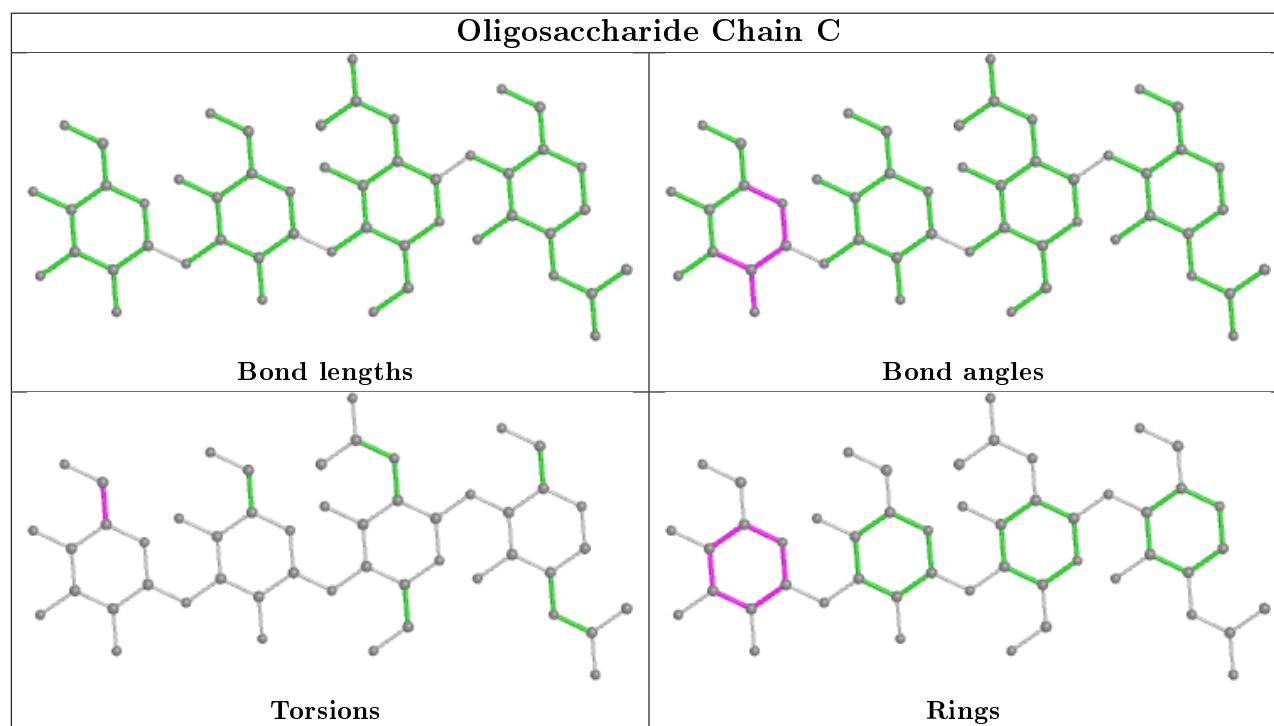
All (5) ring outliers are listed below:

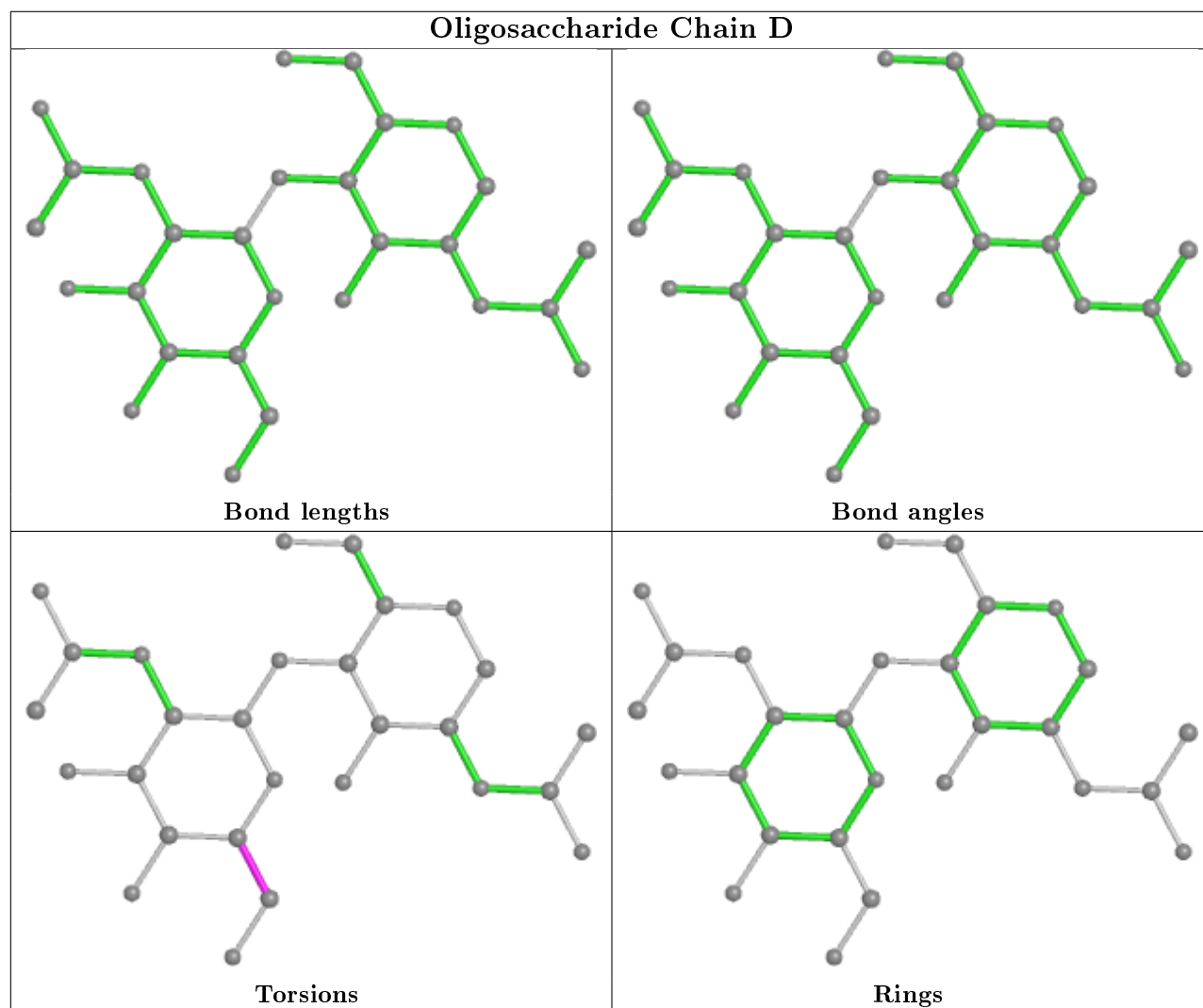
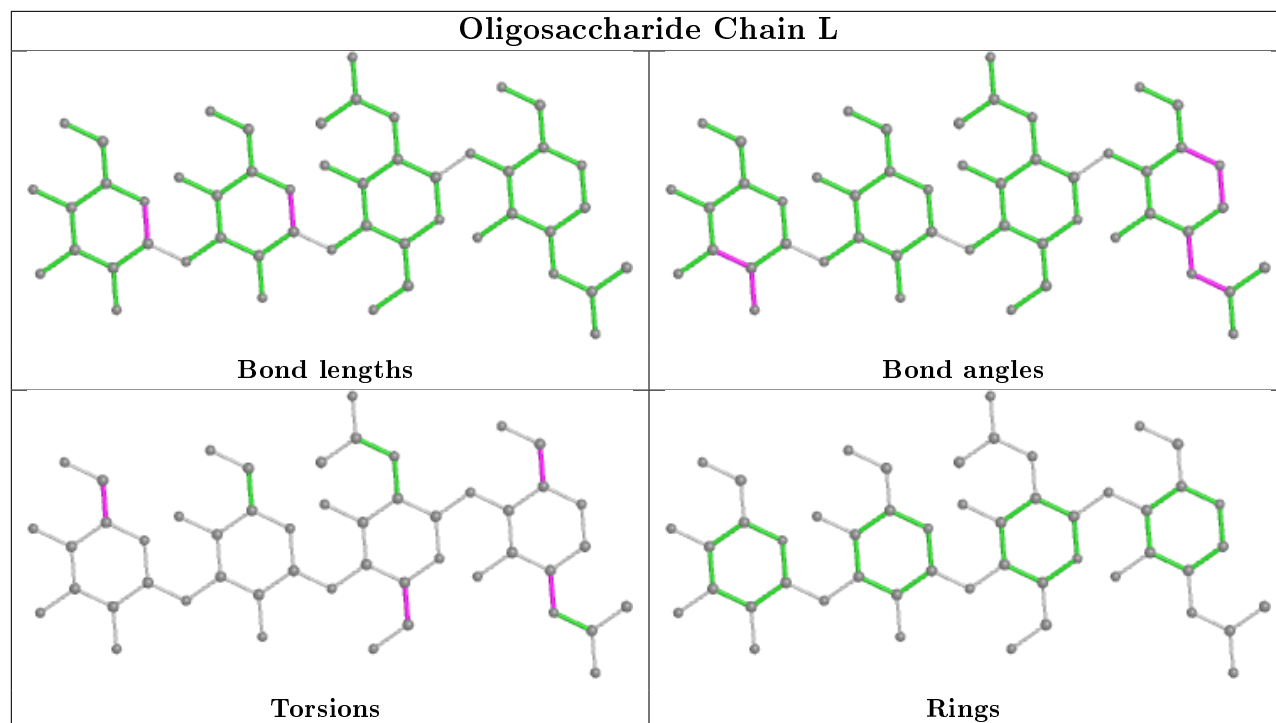
Mol	Chain	Res	Type	Atoms
7	K	6	MAN	C1-C2-C3-C4-C5-O5
4	F	6	MAN	C1-C2-C3-C4-C5-O5
2	C	4	MAN	C1-C2-C3-C4-C5-O5
4	F	7	MAN	C1-C2-C3-C4-C5-O5
7	K	7	MAN	C1-C2-C3-C4-C5-O5

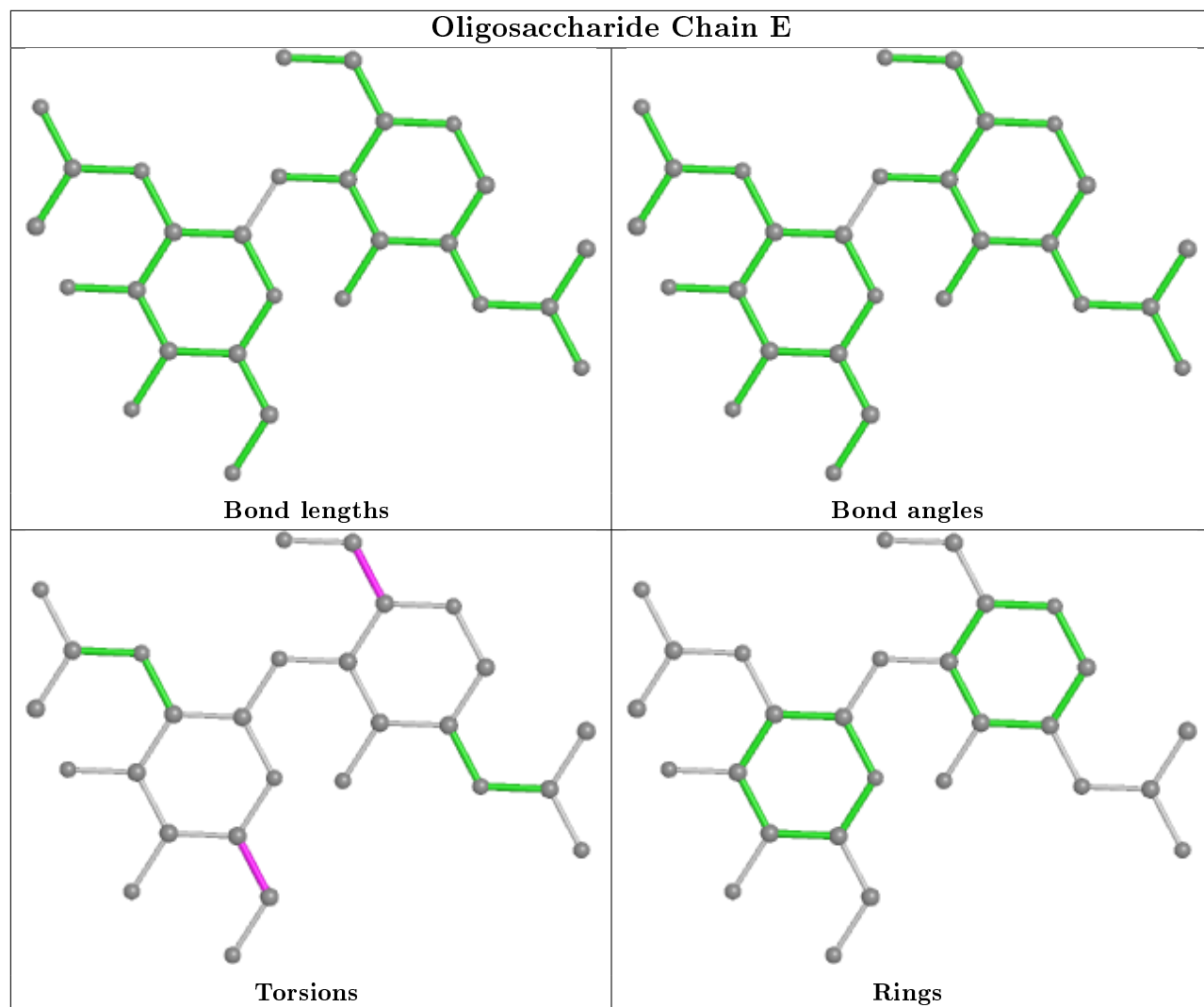
3 monomers are involved in 4 short contacts:

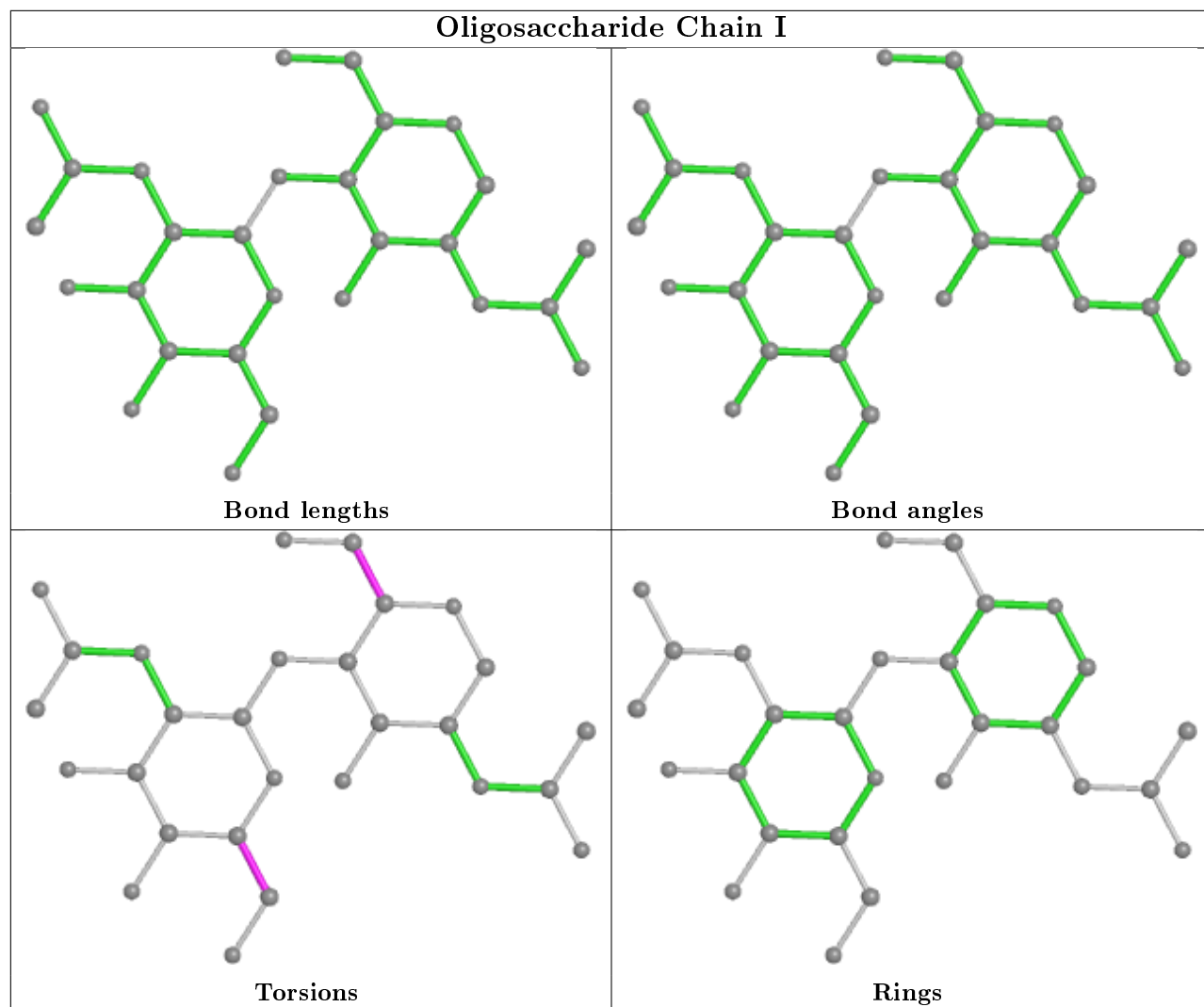
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	1	0
4	F	1	NAG	2	0
4	F	3	BMA	1	0

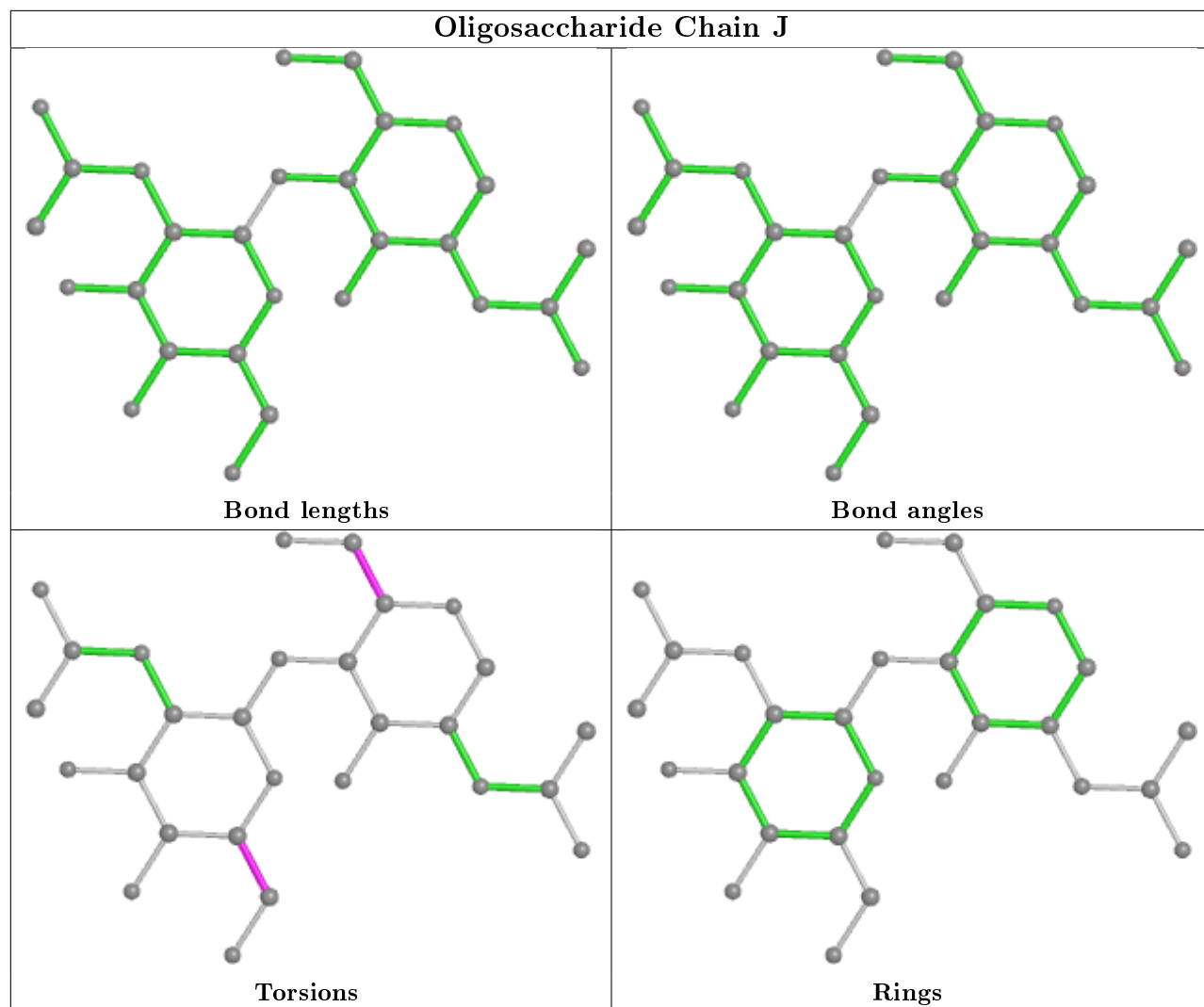
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

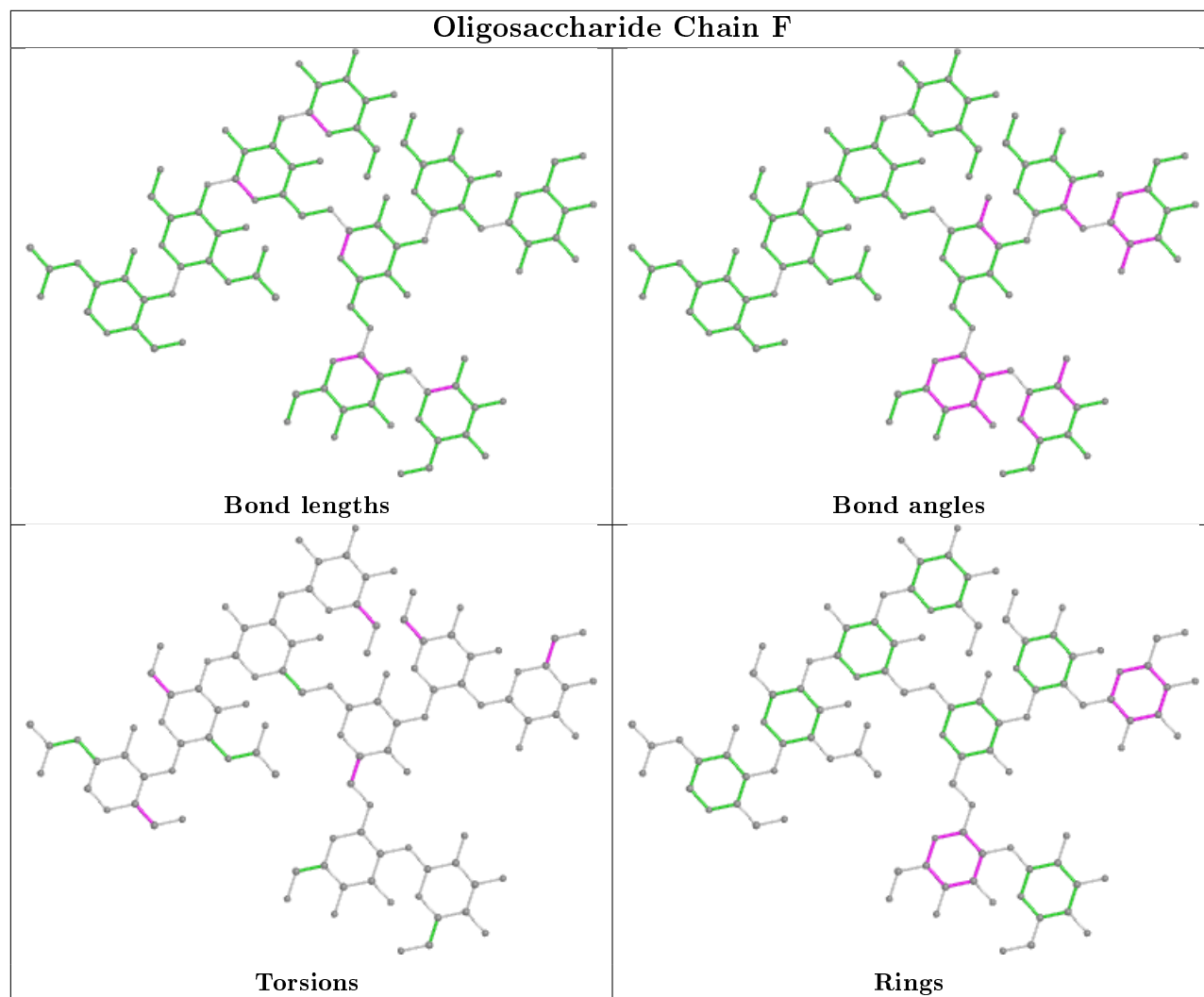




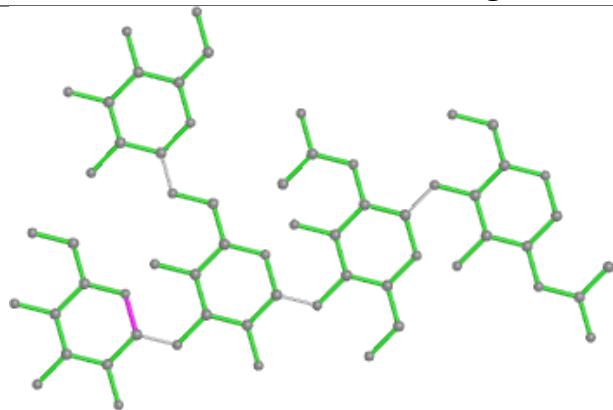




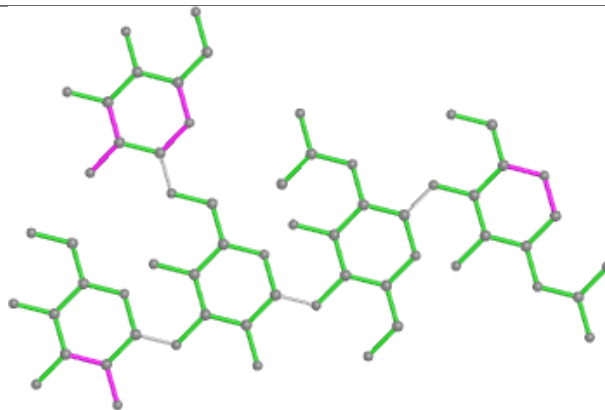




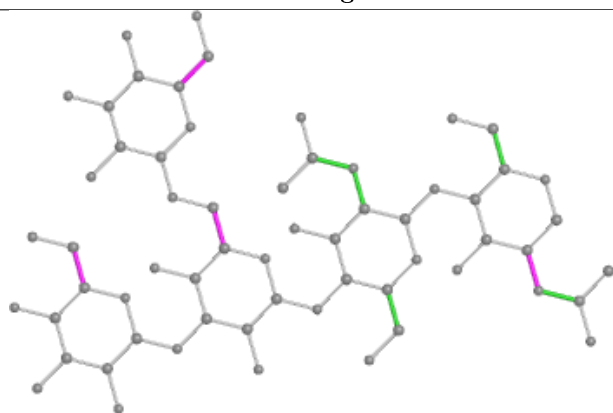
## Oligosaccharide Chain G



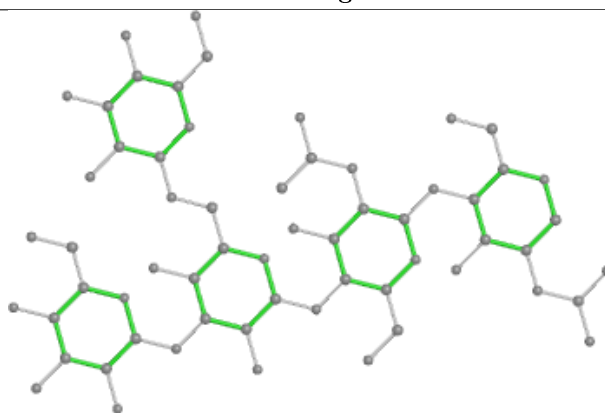
Bond lengths



Bond angles

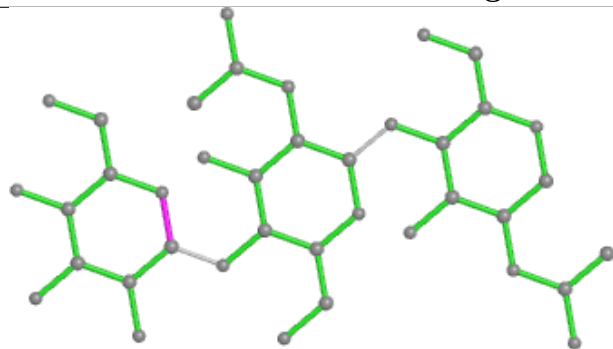


Torsions

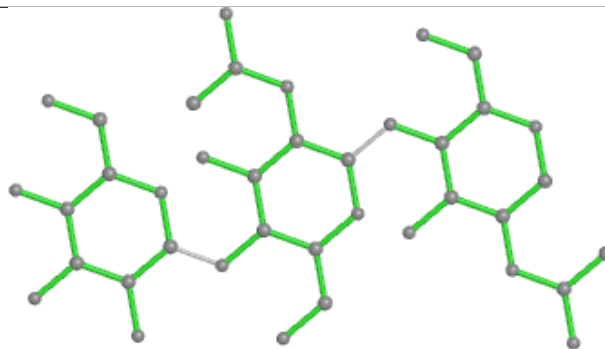


Rings

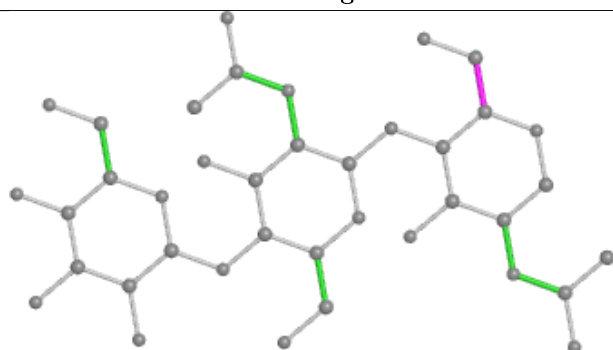
## Oligosaccharide Chain H



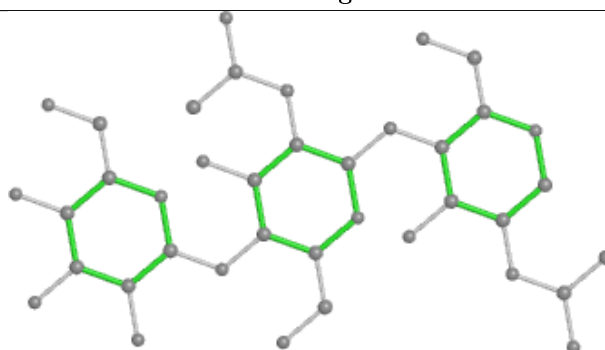
Bond lengths



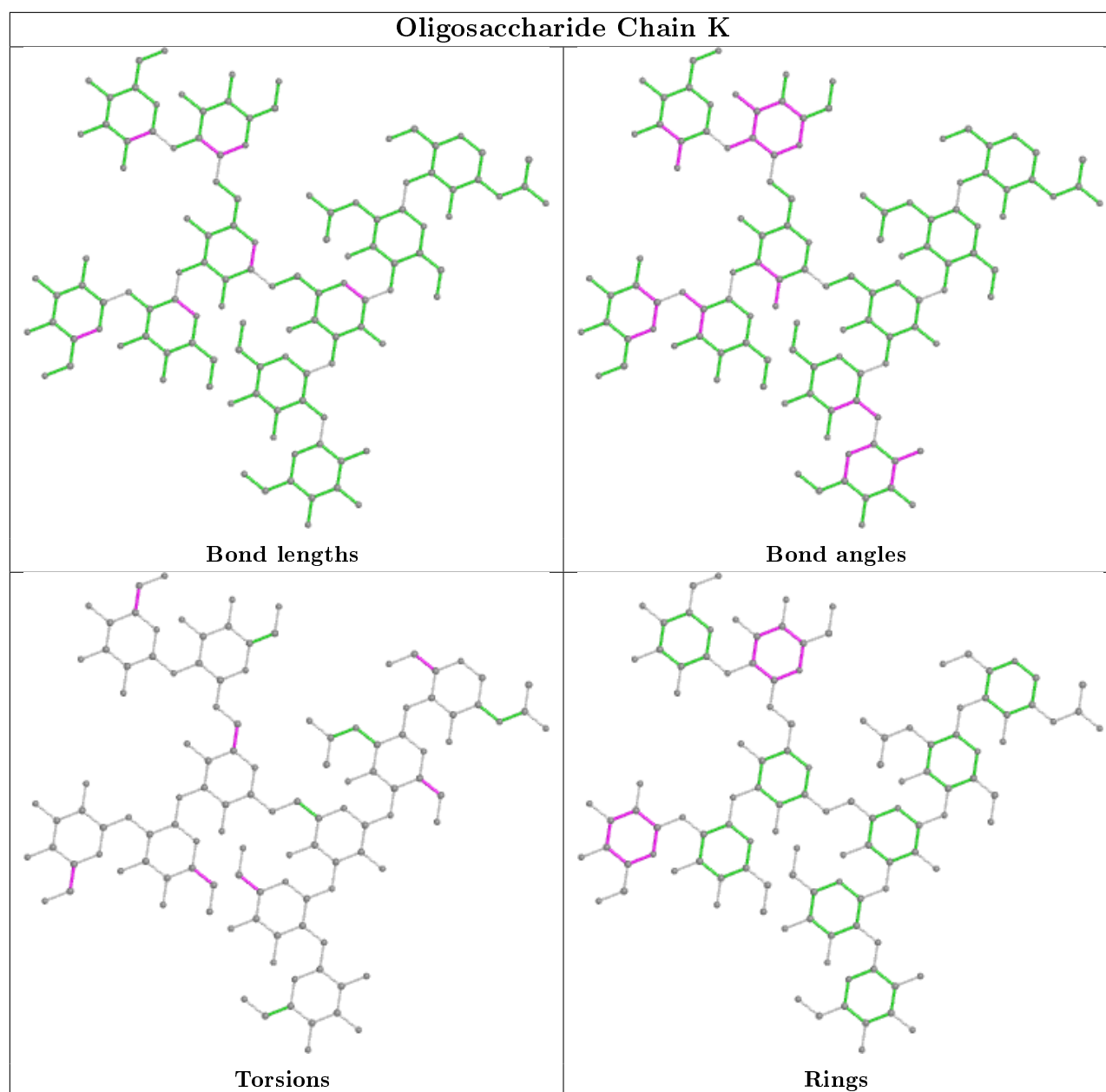
Bond angles



Torsions



Rings



## 5.6 Ligand geometry [i](#)

6 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	NAG	B	507	1	14,14,15	0.71	1 (7%)	17,19,21	1.00	1 (5%)
8	NAG	A	511	1	14,14,15	0.30	0	17,19,21	0.65	0
8	NAG	B	510	1	14,14,15	0.19	0	17,19,21	0.44	0
8	NAG	A	501	1	14,14,15	0.71	1 (7%)	17,19,21	0.97	1 (5%)
8	NAG	B	501	1	14,14,15	0.85	1 (7%)	17,19,21	0.93	1 (5%)
8	NAG	A	508	1	14,14,15	0.96	1 (7%)	17,19,21	1.08	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
8	NAG	B	507	1	-	2/6/23/26	0/1/1/1
8	NAG	A	511	1	-	2/6/23/26	0/1/1/1
8	NAG	B	510	1	-	2/6/23/26	0/1/1/1
8	NAG	A	501	1	-	1/6/23/26	0/1/1/1
8	NAG	B	501	1	-	1/6/23/26	0/1/1/1
8	NAG	A	508	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	508	NAG	O5-C1	3.47	1.49	1.43
8	B	501	NAG	O5-C1	2.97	1.48	1.43
8	B	507	NAG	O5-C1	2.48	1.47	1.43
8	A	501	NAG	O5-C1	2.41	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	508	NAG	C1-O5-C5	4.23	117.93	112.19
8	A	501	NAG	C1-O5-C5	3.75	117.28	112.19
8	B	507	NAG	C1-O5-C5	3.69	117.19	112.19
8	B	501	NAG	C1-O5-C5	3.59	117.06	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	508	NAG	C4-C5-C6-O6
8	B	507	NAG	C4-C5-C6-O6
8	A	508	NAG	O5-C5-C6-O6
8	B	510	NAG	C4-C5-C6-O6
8	B	507	NAG	O5-C5-C6-O6
8	A	511	NAG	O5-C5-C6-O6
8	A	511	NAG	C4-C5-C6-O6
8	A	501	NAG	O5-C5-C6-O6
8	B	510	NAG	O5-C5-C6-O6
8	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	501	NAG	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, 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	394/394 (100%)	-0.30	2 (0%) 91 75	10, 28, 57, 99	0
1	B	394/394 (100%)	-0.11	5 (1%) 77 51	20, 41, 70, 95	0
All	All	788/788 (100%)	-0.21	7 (0%) 84 63	10, 35, 65, 99	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	104	ASP	3.6
1	B	105	ASN	3.5
1	B	316	GLY	3.5
1	B	46	GLY	3.1
1	A	316	GLY	2.9
1	A	306	SER	2.5
1	B	45	ASN	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, 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
7	MAN	K	10	11/12	0.54	0.42	94,115,126,128	0
2	MAN	C	4	11/12	0.63	0.22	68,83,92,92	0

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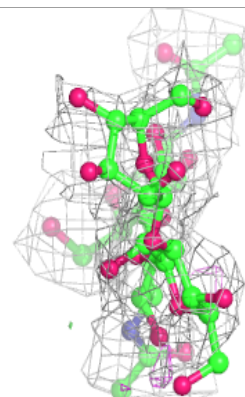
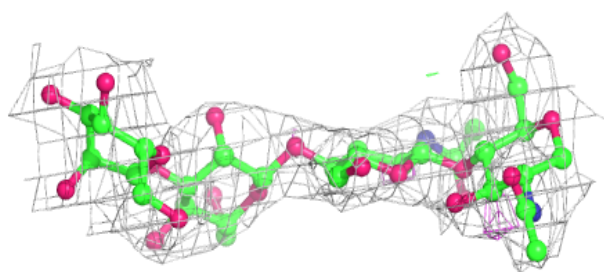
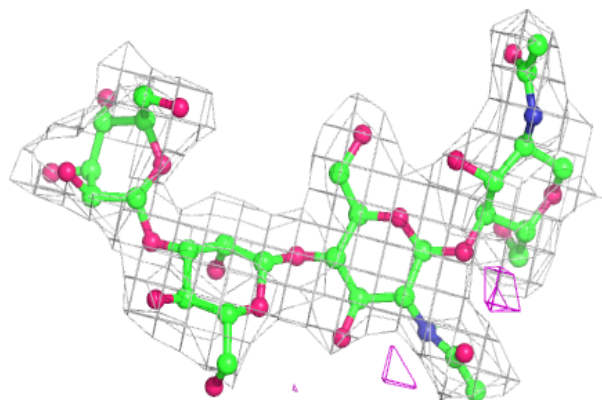
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	F	7	11/12	0.63	0.34	70,74,87,97	0
4	MAN	F	9	11/12	0.68	0.28	108,117,123,126	0
5	MAN	G	5	11/12	0.70	0.31	81,86,96,112	0
4	MAN	F	6	11/12	0.77	0.29	80,88,98,108	0
4	MAN	F	8	11/12	0.78	0.27	56,73,92,92	0
2	MAN	L	4	11/12	0.78	0.31	83,88,94,100	0
3	NAG	E	2	14/15	0.80	0.28	64,72,82,85	0
4	MAN	F	4	11/12	0.80	0.18	63,76,84,91	0
3	NAG	I	2	14/15	0.81	0.30	83,89,104,121	0
2	BMA	L	3	11/12	0.81	0.24	69,77,83,89	0
5	MAN	G	4	11/12	0.81	0.22	57,77,90,91	0
3	NAG	J	2	14/15	0.82	0.24	73,86,95,99	0
7	MAN	K	8	11/12	0.82	0.31	96,102,109,132	0
7	MAN	K	6	11/12	0.82	0.23	83,89,95,101	0
7	MAN	K	5	11/12	0.82	0.20	76,87,98,98	0
7	MAN	K	7	11/12	0.83	0.24	50,70,80,82	0
6	BMA	H	3	11/12	0.83	0.28	75,86,95,106	0
3	NAG	D	2	14/15	0.84	0.31	60,82,91,98	0
4	MAN	F	5	11/12	0.84	0.22	72,79,89,92	0
2	BMA	C	3	11/12	0.86	0.24	70,83,103,106	0
7	MAN	K	4	11/12	0.87	0.17	66,73,89,90	0
7	MAN	K	9	11/12	0.88	0.20	87,98,104,104	0
7	BMA	K	3	11/12	0.89	0.17	61,68,78,82	0
5	BMA	G	3	11/12	0.89	0.15	51,64,74,75	0
4	BMA	F	3	11/12	0.90	0.15	66,73,91,100	0
3	NAG	J	1	14/15	0.90	0.21	37,48,62,69	0
2	NAG	L	1	14/15	0.90	0.21	29,39,46,47	0
6	NAG	H	2	14/15	0.91	0.22	39,59,69,90	0
3	NAG	D	1	14/15	0.91	0.18	30,43,52,54	0
6	NAG	H	1	14/15	0.91	0.18	29,38,46,52	0
5	NAG	G	1	14/15	0.91	0.21	24,29,42,53	0
3	NAG	E	1	14/15	0.92	0.20	34,38,54,59	0
7	NAG	K	1	14/15	0.92	0.16	36,50,57,61	0
7	NAG	K	2	14/15	0.93	0.18	41,52,68,77	0
2	NAG	C	2	14/15	0.93	0.23	26,37,57,64	0
4	NAG	F	2	14/15	0.93	0.16	35,48,61,67	0
2	NAG	L	2	14/15	0.94	0.18	26,46,54,60	0
5	NAG	G	2	14/15	0.94	0.17	19,33,40,48	0
2	NAG	C	1	14/15	0.94	0.17	15,24,32,34	0
3	NAG	I	1	14/15	0.94	0.18	42,53,71,85	0
4	NAG	F	1	14/15	0.96	0.16	15,29,37,44	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.

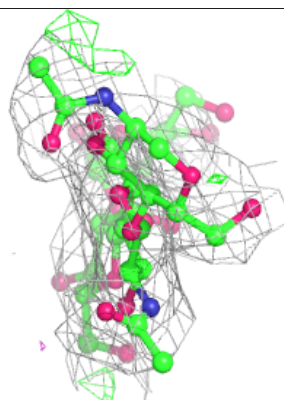
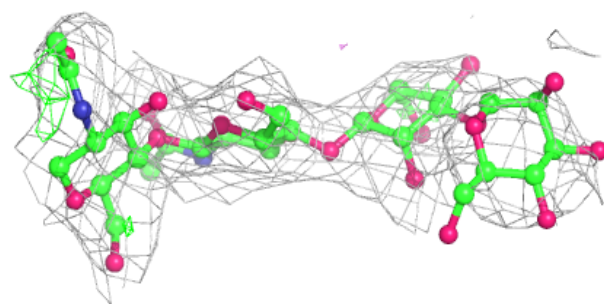
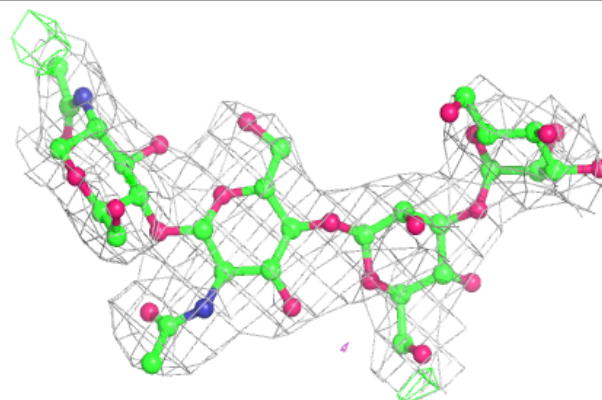
**Electron density around Chain C:**

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



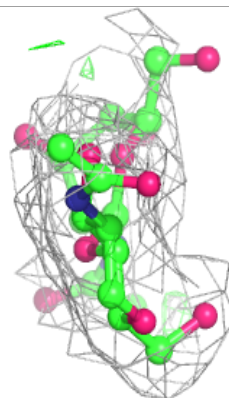
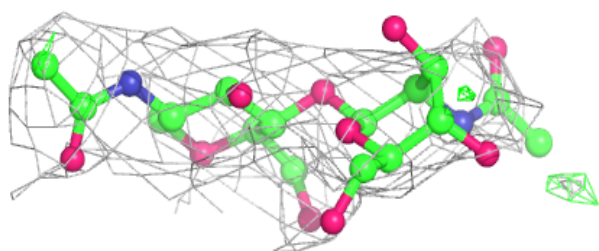
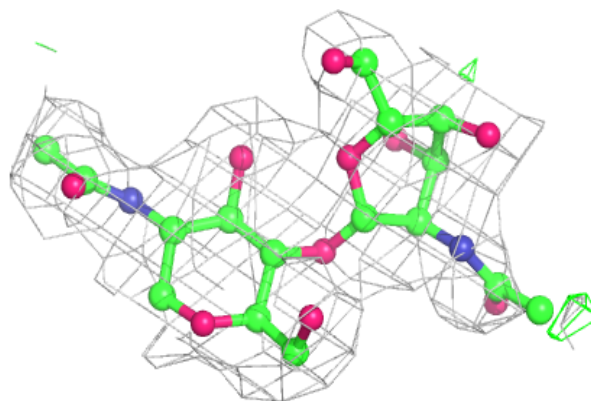
**Electron density around Chain L:**

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

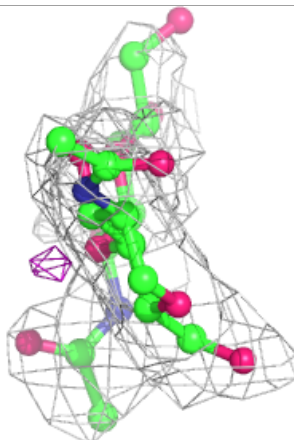
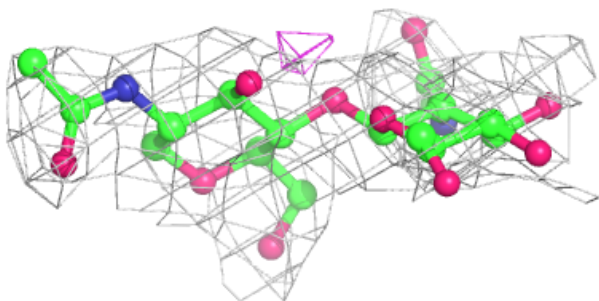
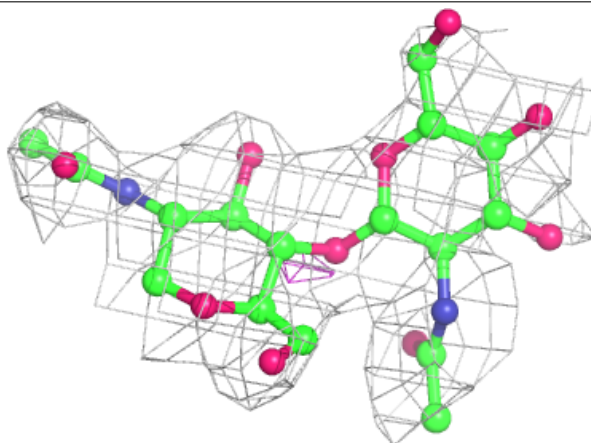


**Electron density around Chain D:**

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

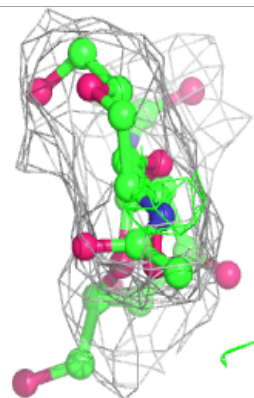
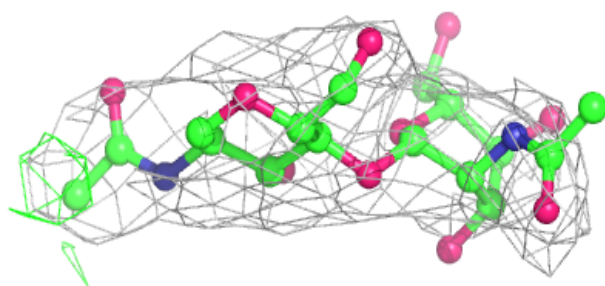
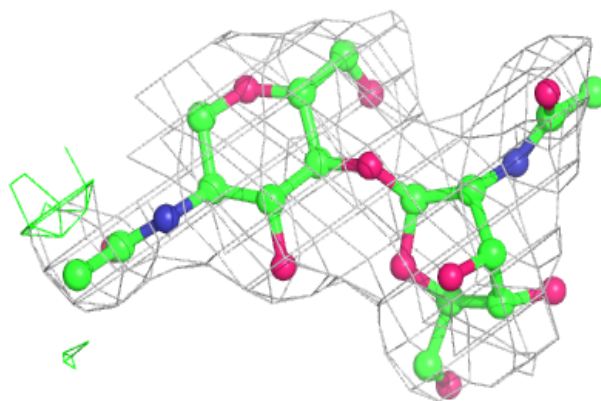
**Electron density around Chain E:**

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

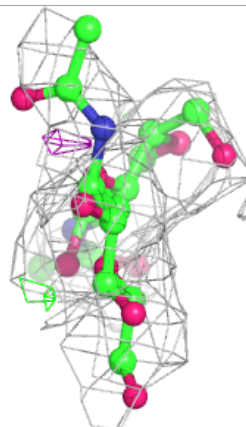
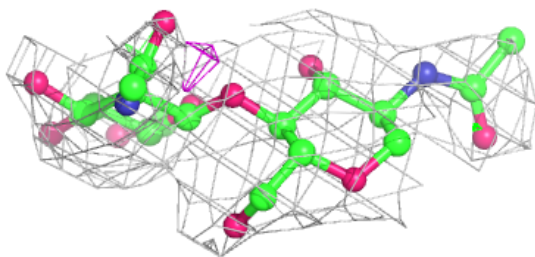
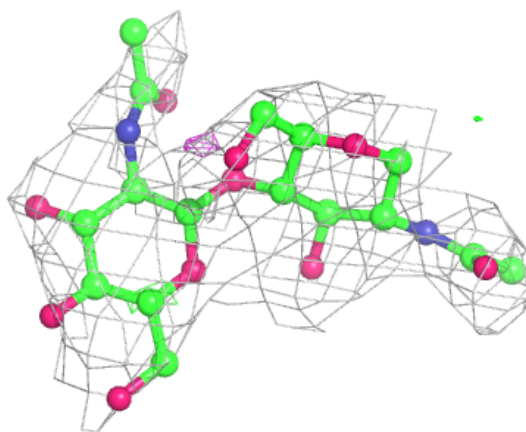


**Electron density around Chain I:**

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

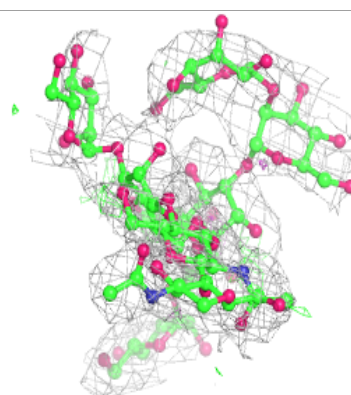
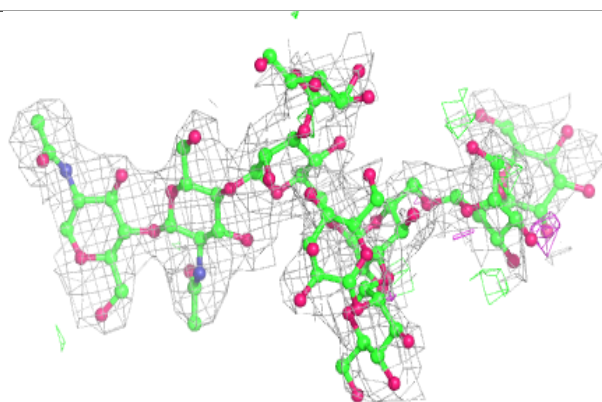
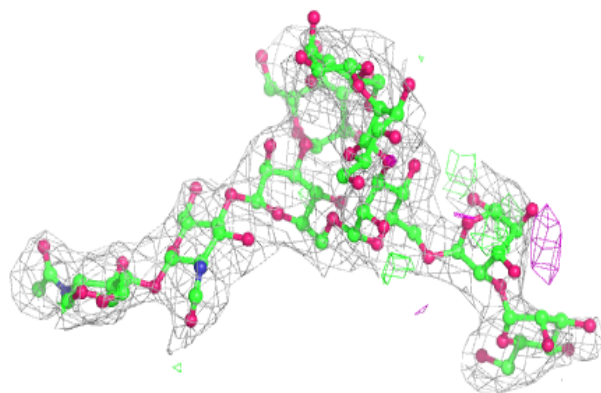
**Electron density around Chain J:**

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

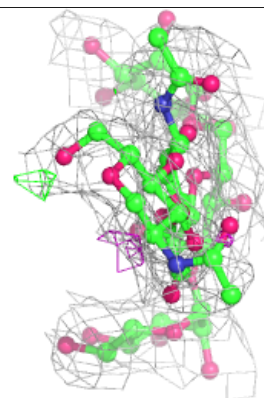
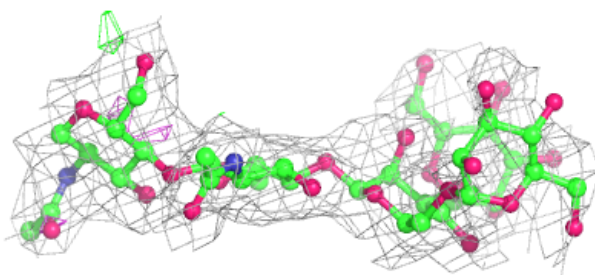
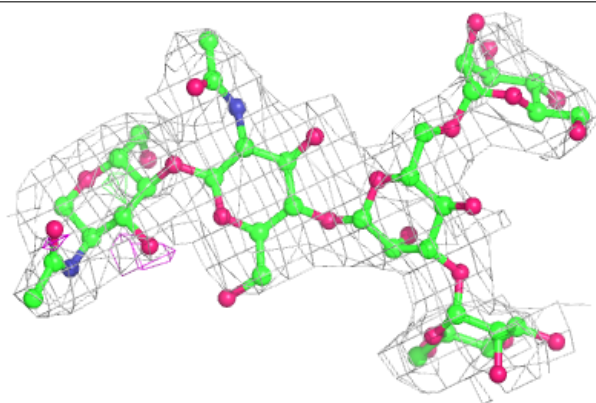


**Electron density around Chain F:**

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

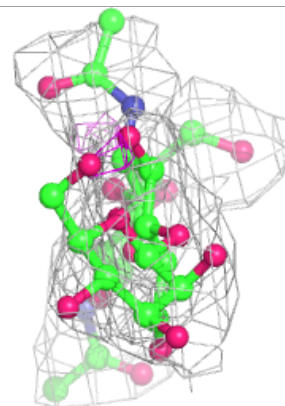
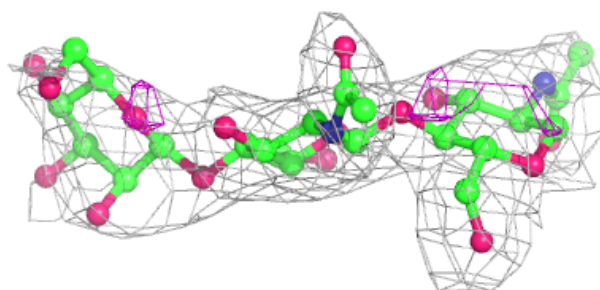
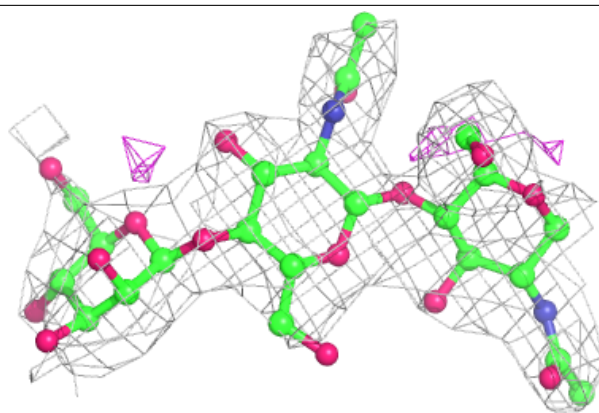
**Electron density around Chain G:**

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

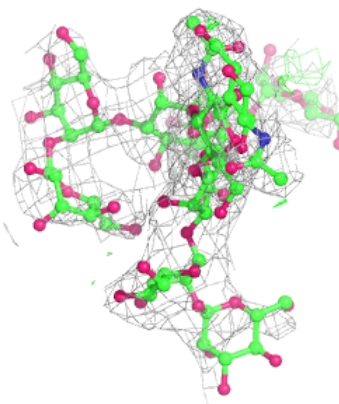
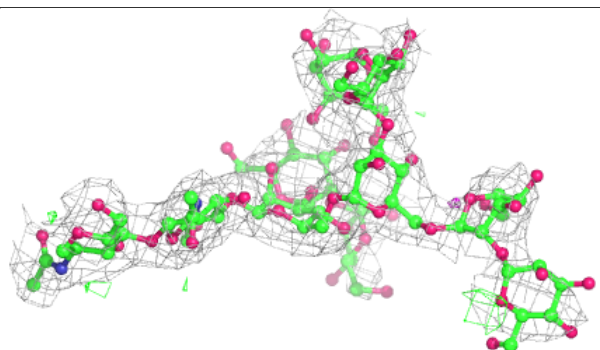
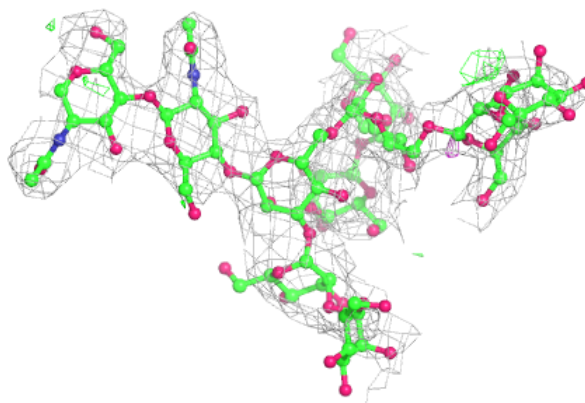


**Electron density around Chain H:**

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

**Electron density around Chain K:**

$2mF_o-DF_c$  (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
8	NAG	A	501	14/15	0.68	0.43	94,106,112,117	0
8	NAG	B	501	14/15	0.73	0.39	73,94,113,117	0
8	NAG	A	508	14/15	0.73	0.28	61,71,77,80	0
8	NAG	A	511	14/15	0.79	0.22	58,76,97,97	0
8	NAG	B	507	14/15	0.83	0.29	65,72,87,96	0
8	NAG	B	510	14/15	0.84	0.23	78,80,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.