



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:55 AM EDT

PDB ID : 4UNX / pdb_00004unx
Title : Structure of the A_Equine_Newmarket_2_93 H3 haemagglutinin in complex with 3SLN
Authors : Vachieri, S.G.; Collins, P.J.; Haire, L.F.; Ogradowicz, R.W.; Martin, S.R.; Walker, P.A.; Xiong, X.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2014-05-31
Resolution : 3.20 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

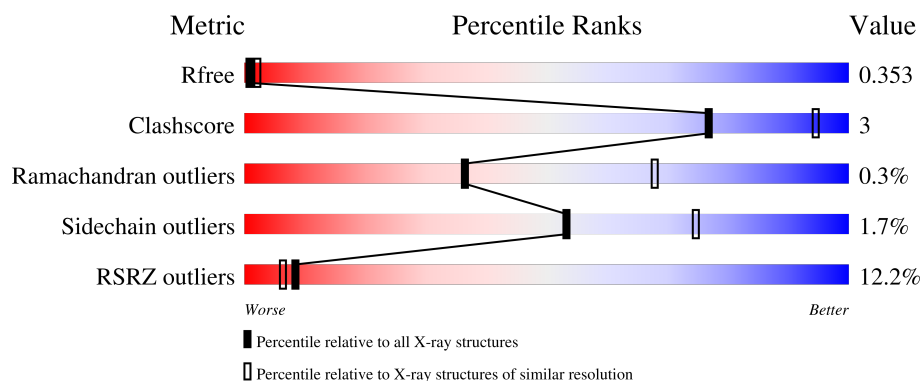
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	323	
1	C	323	
1	E	323	
2	B	173	

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Mol	Chain	Length	Quality of chain
2	D	173	
2	F	173	
3	G	2	
3	H	2	
3	L	2	
3	M	2	
3	P	2	
3	Q	2	
4	I	5	
4	R	5	
5	J	3	
6	K	2	
6	O	2	
6	S	2	
7	N	4	

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
3	NAG	P	2	X	-	-	-
6	FUC	K	2	X	-	-	-
6	FUC	O	2	X	-	-	-
6	FUC	S	2	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12208 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 H3 HAEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2484	1553	438	479	14			
1	C	319	Total	C	N	O	S	0	0	0
			2484	1553	438	479	14			
1	E	319	Total	C	N	O	S	0	0	0
			2484	1553	438	479	14			

- Molecule 2 is a protein called H3 HAEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			
2	D	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			
2	F	172	Total	C	N	O	S	0	0	0
			1396	870	245	275	6			

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



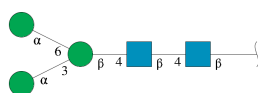
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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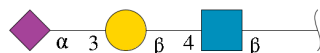
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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
4	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	3	Total	C	N	O	0	0	0
			46	25	2	19			

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



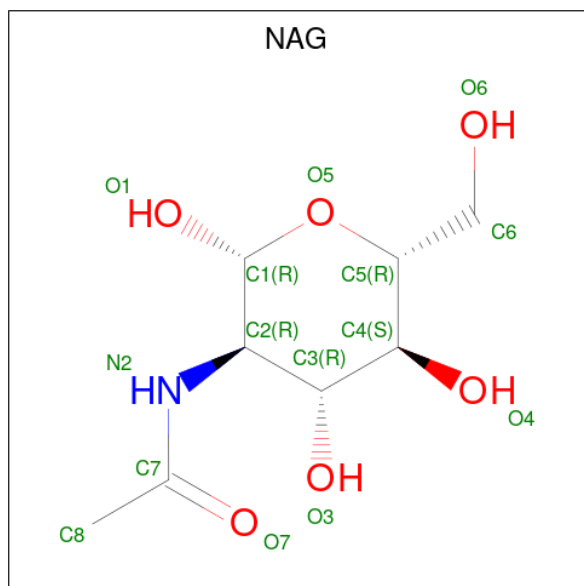
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	O	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	S	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called 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
7	N	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



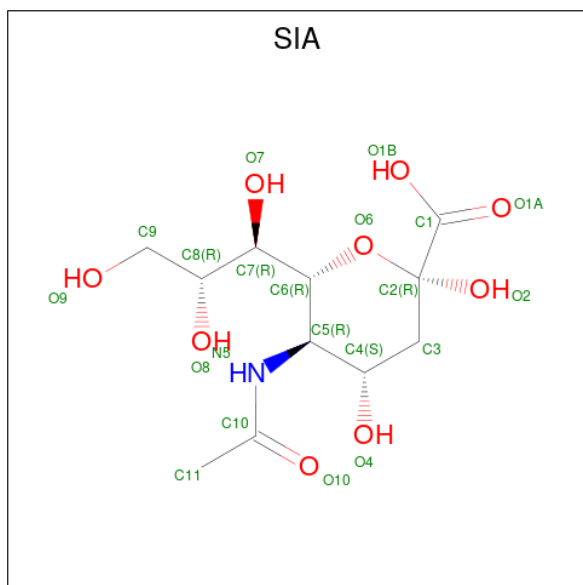
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).

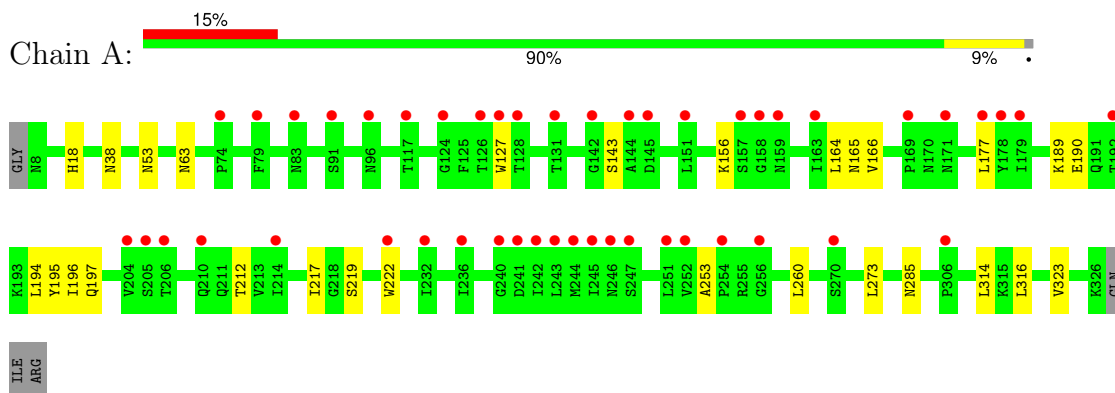


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			20	11	1	8		
9	E	1	Total	C	N	O	0	0
			20	11	1	8		

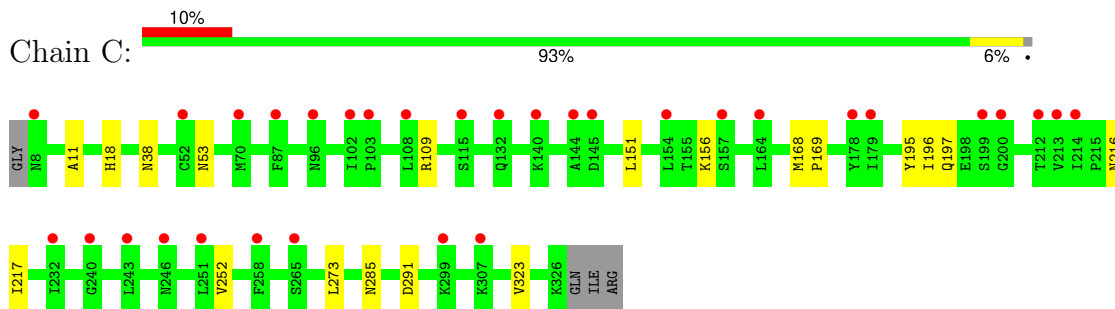
3 Residue-property plots

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.

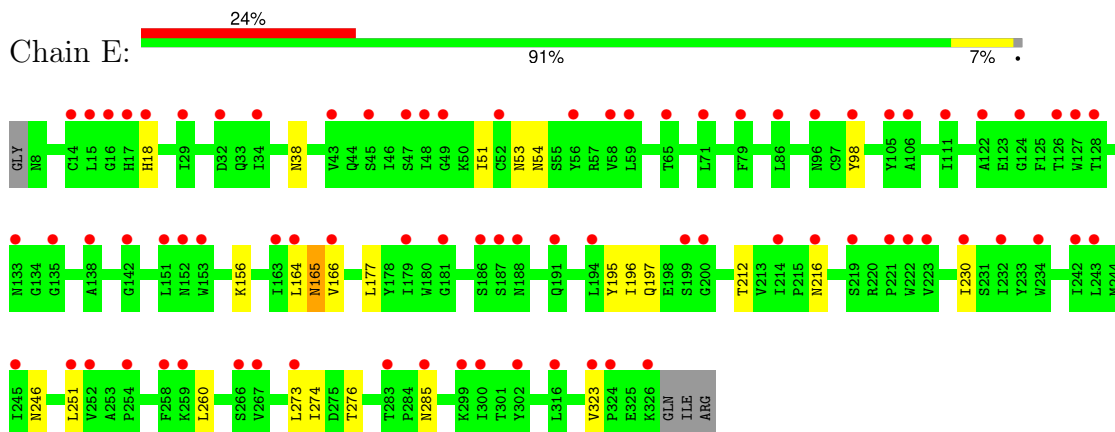
• Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN



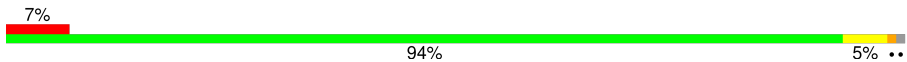
• Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN

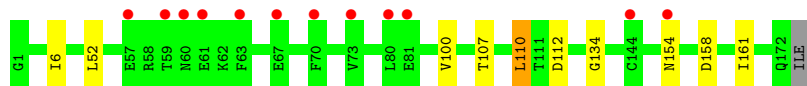


• Molecule 1: H3 HAEMAGGLUTININ HA1 CHAIN

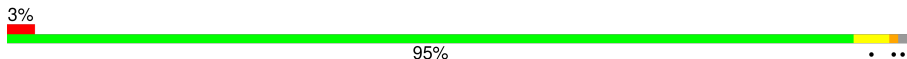


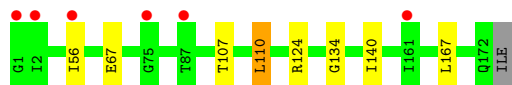
• Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain B:  7% 94% 5% ..

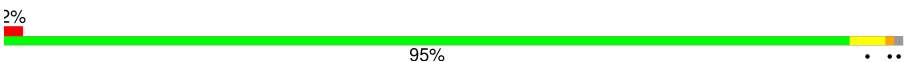


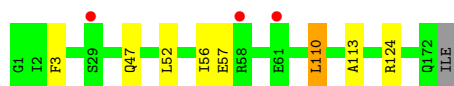
• Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain D:  3% 95%



• Molecule 2: H3 HAEMAGGLUTININ HA2 CHAIN

Chain F:  2% 95%



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

Chain G:  50% 50%



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

Chain H:  50% 50%

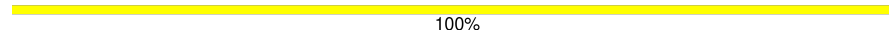


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%



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

Chain M:  100%

MAG1
MAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

- Molecule 4: 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 I:  40% 40% 20%

MAG1
MAG2
MAN3
MAN4
MAN5

- Molecule 4: 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 R:  40% 40% 20%

MAG1
MAG2
MAN3
MAN4
MAN5

- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 33% 33%

MAG1
GAL2
SIA3

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

Chain K:  100%

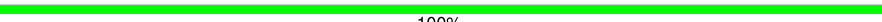
MAG1
FUC2

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

Chain O:  50% 50%

MAG1
FUC2

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

Chain S:  100%

MAG1
FUC2

- Molecule 7: 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 N:  75% 25%

MAG1
MAG2
BNA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.48Å 102.25Å 228.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.19 – 3.20 114.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (114.19-3.20) 99.2 (114.19-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.319 , 0.354 0.316 , 0.353	Depositor DCC
R_{free} test set	1971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	12208	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/2537	0.62	0/3445
1	C	0.37	0/2537	0.61	0/3445
1	E	0.39	0/2537	0.60	0/3445
2	B	0.39	0/1421	0.70	0/1910
2	D	0.38	0/1421	0.70	0/1910
2	F	0.39	0/1421	0.67	0/1910
All	All	0.38	0/11874	0.64	0/16065

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2484	0	2432	20	0
1	C	2484	0	2432	13	0
1	E	2484	0	2432	17	0
2	B	1396	0	1318	8	0
2	D	1396	0	1318	8	0
2	F	1396	0	1318	6	0
3	G	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	1	0
3	L	28	0	25	1	0
3	M	28	0	25	2	0
3	P	28	0	25	3	0
3	Q	28	0	25	2	0
4	I	61	0	52	2	0
4	R	61	0	52	1	0
5	J	46	0	40	2	0
6	K	24	0	22	1	0
6	O	24	0	22	1	0
6	S	24	0	22	0	0
7	N	50	0	43	3	0
8	A	28	0	26	4	0
8	C	28	0	26	3	0
8	E	14	0	13	1	0
9	C	20	0	17	0	0
9	E	20	0	17	0	0
All	All	12208	0	11752	69	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 3.

All (69) 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:E:165:ASN:HD21	3:Q:1:NAG:C1	1.74	1.00
1:C:285:ASN:HD21	7:N:1:NAG:C1	1.91	0.83
2:B:154:ASN:HD22	6:K:1:NAG:C1	1.93	0.80
1:E:165:ASN:ND2	3:Q:1:NAG:C1	2.45	0.79
1:A:53:ASN:HD21	3:G:1:NAG:C1	1.96	0.78
1:A:38:ASN:HD21	8:A:401:NAG:C1	1.98	0.76
1:A:63:ASN:HD21	3:H:1:NAG:C1	2.00	0.73
1:C:38:ASN:HD21	8:C:401:NAG:C1	2.04	0.70
1:A:285:ASN:HD21	4:I:1:NAG:C1	2.06	0.68
1:E:274:ILE:O	3:P:1:NAG:H83	1.97	0.65
1:A:38:ASN:ND2	8:A:401:NAG:C1	2.62	0.62
1:A:165:ASN:HD21	8:A:431:NAG:C1	2.14	0.61
1:A:194:LEU:HD21	5:J:3:SIA:O10	2.04	0.58
1:E:53:ASN:HD22	3:P:1:NAG:C1	2.16	0.58
8:C:421:NAG:C1	8:C:421:NAG:C8	2.82	0.58
1:C:53:ASN:HD21	3:L:1:NAG:C1	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:ND2	4:I:1:NAG:C1	2.67	0.57
1:E:38:ASN:HD21	8:E:401:NAG:C1	2.17	0.57
1:E:53:ASN:OD1	1:E:53:ASN:N	2.37	0.57
1:C:285:ASN:ND2	7:N:1:NAG:C1	2.67	0.56
1:C:168:MET:HE3	1:C:169:PRO:HD2	1.88	0.55
2:F:56:ILE:HG22	2:F:57:GLU:HG2	1.90	0.53
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.45	0.52
2:D:110:LEU:C	2:D:110:LEU:HD22	2.34	0.52
1:E:274:ILE:N	1:E:274:ILE:HD12	2.25	0.52
1:C:291:ASP:O	2:D:56:ILE:HG23	2.10	0.51
1:E:53:ASN:HD21	1:E:276:THR:HA	1.74	0.51
2:F:110:LEU:HD22	2:F:110:LEU:C	2.34	0.51
3:P:1:NAG:H3	3:P:2:NAG:O5	2.10	0.51
1:E:285:ASN:HD21	4:R:1:NAG:C1	2.24	0.51
1:A:165:ASN:ND2	8:A:431:NAG:C1	2.73	0.51
2:D:56:ILE:O	2:D:56:ILE:HG22	2.12	0.49
1:A:53:ASN:ND2	3:G:1:NAG:C1	2.72	0.49
1:A:219:SER:HB3	3:M:1:NAG:H82	1.94	0.49
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.95	0.49
1:E:164:LEU:HD12	1:E:251:LEU:HD23	1.94	0.49
1:A:195:TYR:O	1:A:197:GLN:N	2.46	0.48
1:C:195:TYR:O	1:C:197:GLN:N	2.47	0.48
2:B:134:GLY:HA2	2:D:124:ARG:HD3	1.96	0.47
1:C:285:ASN:OD1	7:N:1:NAG:H83	2.14	0.47
1:C:11:ALA:HB3	2:D:140:ILE:HB	1.97	0.47
1:E:54:ASN:HD22	1:E:54:ASN:N	2.14	0.46
5:J:3:SIA:O6	5:J:3:SIA:O8	2.33	0.46
6:O:1:NAG:O3	6:O:1:NAG:H82	2.14	0.46
1:E:195:TYR:O	1:E:197:GLN:N	2.48	0.45
2:B:107:THR:HA	2:B:110:LEU:HD12	2.00	0.43
8:C:421:NAG:C1	8:C:421:NAG:H83	2.48	0.43
1:A:212:THR:HG21	1:E:216:ASN:CG	2.44	0.43
1:E:51:ILE:HB	1:E:274:ILE:HG13	2.00	0.43
1:A:189:LYS:HG3	1:A:190:GLU:N	2.33	0.42
2:B:158:ASP:HB3	2:B:161:ILE:HD12	2.01	0.42
1:A:177:LEU:HD22	1:A:260:LEU:HD21	2.00	0.42
1:A:222:TRP:CG	3:M:2:NAG:HO3	2.38	0.42
2:F:3:PHE:CE1	2:F:113:ALA:HB2	2.55	0.42
3:G:1:NAG:C1	3:G:1:NAG:O7	2.67	0.41
2:B:110:LEU:HD22	2:B:110:LEU:C	2.45	0.41
1:C:216:ASN:CG	1:E:212:THR:HG21	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:GLY:HA2	2:F:124:ARG:HD3	2.03	0.41
1:A:217:ILE:HD12	1:A:217:ILE:N	2.36	0.41
1:E:177:LEU:HD22	1:E:260:LEU:HD21	2.03	0.41
1:C:151:LEU:HD23	1:C:252:VAL:HG11	2.03	0.40
1:C:217:ILE:HD12	1:C:217:ILE:N	2.37	0.40
1:E:98:TYR:CD2	1:E:230:ILE:HD12	2.57	0.40
1:A:316:LEU:HD23	2:B:52:LEU:HD13	2.04	0.40
1:C:109:ARG:NH1	2:D:67:GLU:OE2	2.53	0.40
2:F:47:GLN:OE1	2:F:110:LEU:HD23	2.21	0.40
1:A:314:LEU:HB3	2:B:100:VAL:HG21	2.04	0.40
2:D:107:THR:HA	2:D:110:LEU:HD12	2.04	0.40
2:F:52:LEU:HG	2:F:56:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	317/323 (98%)	295 (93%)	20 (6%)	2 (1%)	21	56
1	C	317/323 (98%)	296 (93%)	20 (6%)	1 (0%)	36	68
1	E	317/323 (98%)	294 (93%)	22 (7%)	1 (0%)	36	68
2	B	170/173 (98%)	159 (94%)	11 (6%)	0	100	100
2	D	170/173 (98%)	158 (93%)	12 (7%)	0	100	100
2	F	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
All	All	1461/1488 (98%)	1364 (93%)	93 (6%)	4 (0%)	36	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	SER

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Mol	Chain	Res	Type
1	A	196	ILE
1	C	196	ILE
1	E	196	ILE

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	280/283 (99%)	274 (98%)	6 (2%)	47	71
1	C	280/283 (99%)	276 (99%)	4 (1%)	59	77
1	E	280/283 (99%)	273 (98%)	7 (2%)	42	69
2	B	144/145 (99%)	143 (99%)	1 (1%)	76	83
2	D	144/145 (99%)	142 (99%)	2 (1%)	59	77
2	F	144/145 (99%)	143 (99%)	1 (1%)	76	83
All	All	1272/1284 (99%)	1251 (98%)	21 (2%)	53	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	156	LYS
1	A	164	LEU
1	A	166	VAL
1	A	273	LEU
1	A	323	VAL
2	B	110	LEU
1	C	18	HIS
1	C	156	LYS
1	C	273	LEU
1	C	323	VAL
2	D	110	LEU
2	D	167	LEU
1	E	18	HIS
1	E	156	LYS

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Mol	Chain	Res	Type
1	E	165	ASN
1	E	166	VAL
1	E	246	ASN
1	E	273	LEU
1	E	323	VAL
2	F	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	63	ASN
1	A	165	ASN
1	A	216	ASN
1	A	246	ASN
1	A	296	ASN
2	B	78	GLN
2	B	125	GLN
2	B	154	ASN
2	B	159	HIS
1	C	53	ASN
1	C	54	ASN
1	C	159	ASN
1	C	216	ASN
1	C	248	ASN
1	C	285	ASN
2	D	78	GLN
1	E	38	ASN
1	E	54	ASN
1	E	165	ASN
1	E	184	HIS
1	E	211	GLN
1	E	216	ASN
2	F	78	GLN
2	F	159	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 ⓘ

35 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	$\# Z > 2$
3	NAG	G	1	3	14,14,15	0.52	0	17,19,21	1.53	5 (29%)
3	NAG	G	2	3	14,14,15	0.59	0	17,19,21	0.75	0
3	NAG	H	1	3	14,14,15	0.55	0	17,19,21	1.42	2 (11%)
3	NAG	H	2	3	14,14,15	0.69	0	17,19,21	2.46	4 (23%)
4	NAG	I	1	4	14,14,15	0.55	0	17,19,21	1.85	5 (29%)
4	NAG	I	2	4	14,14,15	0.54	0	17,19,21	0.74	0
4	BMA	I	3	4	11,11,12	0.31	0	15,15,17	0.48	0
4	MAN	I	4	4	11,11,12	0.60	0	15,15,17	1.02	1 (6%)
4	MAN	I	5	4	11,11,12	0.54	0	15,15,17	1.08	1 (6%)
5	NAG	J	1	5	15,15,15	0.47	0	21,21,21	1.74	4 (19%)
5	GAL	J	2	5	11,11,12	0.58	0	15,15,17	0.73	0
5	SIA	J	3	5	20,20,21	0.68	0	21,28,31	0.93	2 (9%)
6	NAG	K	1	6	14,14,15	0.52	0	17,19,21	0.81	0
6	FUC	K	2	6	10,10,11	0.83	0	14,14,16	1.49	4 (28%)
3	NAG	L	1	3	14,14,15	0.52	0	17,19,21	1.17	1 (5%)
3	NAG	L	2	3	14,14,15	0.60	0	17,19,21	1.18	3 (17%)
3	NAG	M	1	3	14,14,15	0.55	0	17,19,21	0.83	0
3	NAG	M	2	3	14,14,15	0.54	0	17,19,21	0.70	0
7	NAG	N	1	7	14,14,15	0.57	0	17,19,21	1.86	5 (29%)
7	NAG	N	2	7	14,14,15	0.37	0	17,19,21	1.73	2 (11%)
7	BMA	N	3	7	11,11,12	0.45	0	15,15,17	1.74	2 (13%)
7	MAN	N	4	7	11,11,12	0.56	0	15,15,17	1.15	1 (6%)
6	NAG	O	1	6	14,14,15	0.66	0	17,19,21	1.85	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FUC	O	2	6	10,10,11	0.62	0	14,14,16	0.61	0
3	NAG	P	1	3	14,14,15	0.69	0	17,19,21	1.67	3 (17%)
3	NAG	P	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.66	4 (23%)
3	NAG	Q	1	3	14,14,15	0.58	0	17,19,21	1.22	2 (11%)
3	NAG	Q	2	3	14,14,15	0.49	0	17,19,21	0.71	0
4	NAG	R	1	4	14,14,15	0.52	0	17,19,21	1.35	3 (17%)
4	NAG	R	2	4	14,14,15	0.54	0	17,19,21	0.64	0
4	BMA	R	3	4	11,11,12	0.33	0	15,15,17	0.79	0
4	MAN	R	4	4	11,11,12	0.61	0	15,15,17	0.78	1 (6%)
4	MAN	R	5	4	11,11,12	0.53	0	15,15,17	1.11	1 (6%)
6	NAG	S	1	6	14,14,15	0.52	0	17,19,21	0.73	0
6	FUC	S	2	6	10,10,11	0.67	0	14,14,16	0.74	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
3	NAG	G	1	3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
4	NAG	I	1	4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1
4	MAN	I	4	4	-	1/2/19/22	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	1/1/1/1
5	NAG	J	1	5	-	2/6/26/26	0/1/1/1
5	GAL	J	2	5	-	1/2/19/22	0/1/1/1
5	SIA	J	3	5	-	6/18/34/38	0/1/1/1
6	NAG	K	1	6	-	4/6/23/26	0/1/1/1
6	FUC	K	2	6	1/1/4/5	-	0/1/1/1
3	NAG	L	1	3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
7	NAG	N	1	7	-	2/6/23/26	0/1/1/1
7	NAG	N	2	7	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	N	3	7	-	2/2/19/22	0/1/1/1
7	MAN	N	4	7	-	2/2/19/22	0/1/1/1
6	NAG	O	1	6	-	3/6/23/26	0/1/1/1
6	FUC	O	2	6	1/1/4/5	-	0/1/1/1
3	NAG	P	1	3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	Q	1	3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4	-	4/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	BMA	R	3	4	-	2/2/19/22	0/1/1/1
4	MAN	R	4	4	-	2/2/19/22	0/1/1/1
4	MAN	R	5	4	-	0/2/19/22	1/1/1/1
6	NAG	S	1	6	-	2/6/23/26	0/1/1/1
6	FUC	S	2	6	1/1/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	2	NAG	C1-C2	3.00	1.56	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C2-N2-C7	7.16	132.49	122.90
7	N	2	NAG	C1-O5-C5	5.36	119.37	112.19
7	N	3	BMA	C1-O5-C5	4.94	118.81	112.19
3	H	2	NAG	C8-C7-N2	4.88	124.21	116.12
3	P	1	NAG	C4-C3-C2	4.61	117.77	111.02
5	J	1	NAG	C1-C2-N2	4.19	115.58	110.73
7	N	1	NAG	C8-C7-N2	4.02	122.78	116.12
4	I	1	NAG	C8-C7-N2	3.92	122.63	116.12
7	N	3	BMA	C1-C2-C3	3.84	115.23	109.64
6	O	1	NAG	C2-N2-C7	3.83	128.03	122.90
7	N	1	NAG	C2-N2-C7	3.45	127.53	122.90
4	I	5	MAN	C1-O5-C5	3.45	116.81	112.19
3	H	1	NAG	O5-C1-C2	-3.43	105.98	111.29
4	I	1	NAG	O5-C1-C2	-3.36	106.09	111.29
5	J	1	NAG	C4-C3-C2	3.36	115.29	110.40
7	N	2	NAG	C4-C3-C2	-3.31	106.16	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	5	MAN	C1-O5-C5	3.30	116.61	112.19
7	N	4	MAN	C1-O5-C5	3.30	116.61	112.19
6	O	1	NAG	C8-C7-N2	3.17	121.37	116.12
3	G	1	NAG	C1-C2-N2	3.16	115.41	110.43
3	H	2	NAG	O7-C7-C8	-3.10	116.53	122.05
3	H	1	NAG	C3-C4-C5	3.10	115.86	110.23
4	I	1	NAG	C3-C4-C5	3.04	115.74	110.23
3	P	2	NAG	O5-C1-C2	3.03	115.98	111.29
7	N	1	NAG	C3-C4-C5	3.03	115.72	110.23
3	Q	1	NAG	C3-C4-C5	2.97	115.61	110.23
3	P	2	NAG	C1-C2-N2	2.89	114.99	110.43
5	J	1	NAG	C3-C4-C5	2.89	115.48	110.23
3	G	1	NAG	O5-C1-C2	-2.86	106.86	111.29
4	I	1	NAG	C2-N2-C7	2.85	126.72	122.90
7	N	1	NAG	O7-C7-C8	-2.84	117.00	122.05
3	P	2	NAG	C4-C3-C2	2.83	115.17	111.02
6	O	1	NAG	C1-C2-N2	-2.81	106.01	110.43
4	I	4	MAN	C1-O5-C5	2.74	115.86	112.19
3	P	1	NAG	C3-C4-C5	2.70	115.12	110.23
3	L	1	NAG	C4-C3-C2	2.68	114.95	111.02
3	Q	1	NAG	O5-C1-C2	-2.63	107.22	111.29
6	K	2	FUC	O5-C1-C2	2.62	117.05	110.79
5	J	1	NAG	C3-C2-N2	-2.57	105.88	110.62
4	I	1	NAG	O7-C7-C8	-2.55	117.51	122.05
6	K	2	FUC	C2-C3-C4	2.54	115.33	110.86
3	L	2	NAG	O5-C1-C2	-2.53	107.37	111.29
3	H	2	NAG	C1-C2-N2	-2.52	106.45	110.43
3	P	1	NAG	O5-C1-C2	-2.52	107.39	111.29
6	K	2	FUC	C3-C4-C5	2.52	113.64	109.81
3	L	2	NAG	C3-C4-C5	2.48	114.73	110.23
6	O	1	NAG	O7-C7-C8	-2.47	117.66	122.05
4	R	1	NAG	C4-C3-C2	2.45	114.60	111.02
3	P	2	NAG	O5-C5-C4	-2.41	104.96	110.83
5	J	3	SIA	O1B-C1-C2	2.41	118.97	112.71
6	K	2	FUC	C1-O5-C5	-2.39	107.33	112.97
3	G	1	NAG	C2-N2-C7	2.37	126.08	122.90
6	O	1	NAG	O5-C1-C2	2.35	114.92	111.29
4	R	4	MAN	C1-C2-C3	2.31	113.00	109.64
3	L	2	NAG	C4-C3-C2	2.29	114.37	111.02
7	N	1	NAG	C4-C3-C2	2.28	114.35	111.02
4	R	1	NAG	C3-C4-C5	2.27	114.35	110.23
4	R	1	NAG	C8-C7-N2	2.21	119.78	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	O7-C7-C8	-2.16	118.22	122.05
3	G	1	NAG	C3-C4-C5	2.15	114.12	110.23
6	O	1	NAG	O5-C5-C4	-2.06	105.81	110.83
5	J	3	SIA	O6-C2-C1	2.03	111.55	107.72
6	O	1	NAG	O3-C3-C4	-2.00	105.66	110.38

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	P	2	NAG	C1
6	K	2	FUC	C1
6	O	2	FUC	C1
6	S	2	FUC	C1

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C1-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
5	J	1	NAG	C1-C2-N2-C7
5	J	3	SIA	C6-C7-C8-O8
5	J	3	SIA	O7-C7-C8-O8
6	S	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
7	N	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
5	J	3	SIA	O7-C7-C8-C9
5	J	3	SIA	C6-C7-C8-C9
4	R	1	NAG	O5-C5-C6-O6
7	N	4	MAN	O5-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
7	N	3	BMA	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	R	1	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
4	R	4	MAN	C4-C5-C6-O6
7	N	4	MAN	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
4	R	4	MAN	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	R	3	BMA	C4-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
6	K	1	NAG	C3-C2-N2-C7
7	N	2	NAG	O5-C5-C6-O6
5	J	3	SIA	C7-C8-C9-O9
5	J	1	NAG	C3-C2-N2-C7
3	P	1	NAG	C4-C5-C6-O6
5	J	3	SIA	O8-C8-C9-O9
4	R	3	BMA	O5-C5-C6-O6
6	K	1	NAG	C1-C2-N2-C7
3	G	1	NAG	C4-C5-C6-O6
5	J	2	GAL	C4-C5-C6-O6
3	M	1	NAG	C1-C2-N2-C7
3	P	1	NAG	C1-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	P	2	NAG	C3-C2-N2-C7
6	O	1	NAG	C3-C2-N2-C7
3	M	2	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6

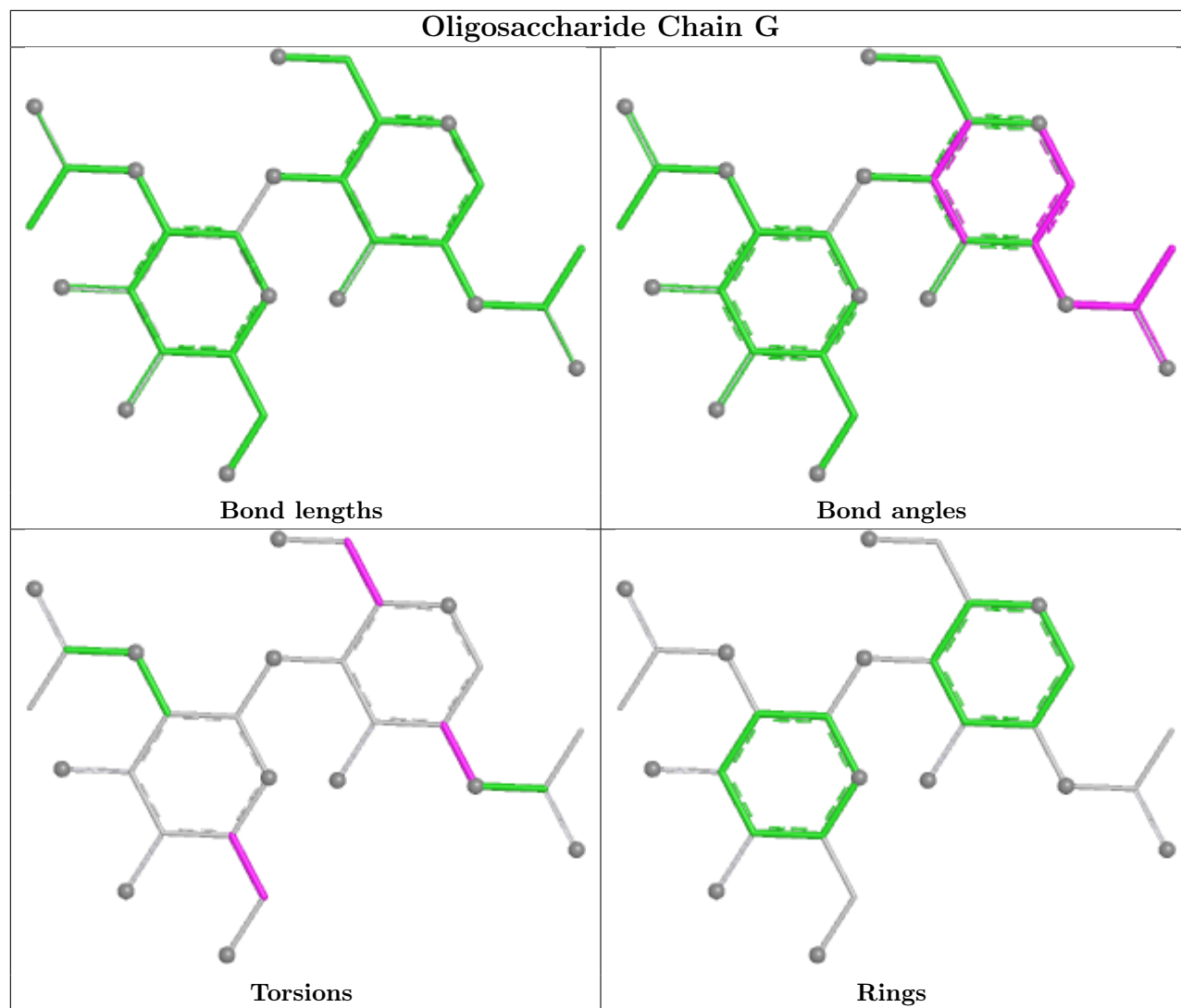
All (2) ring outliers are listed below:

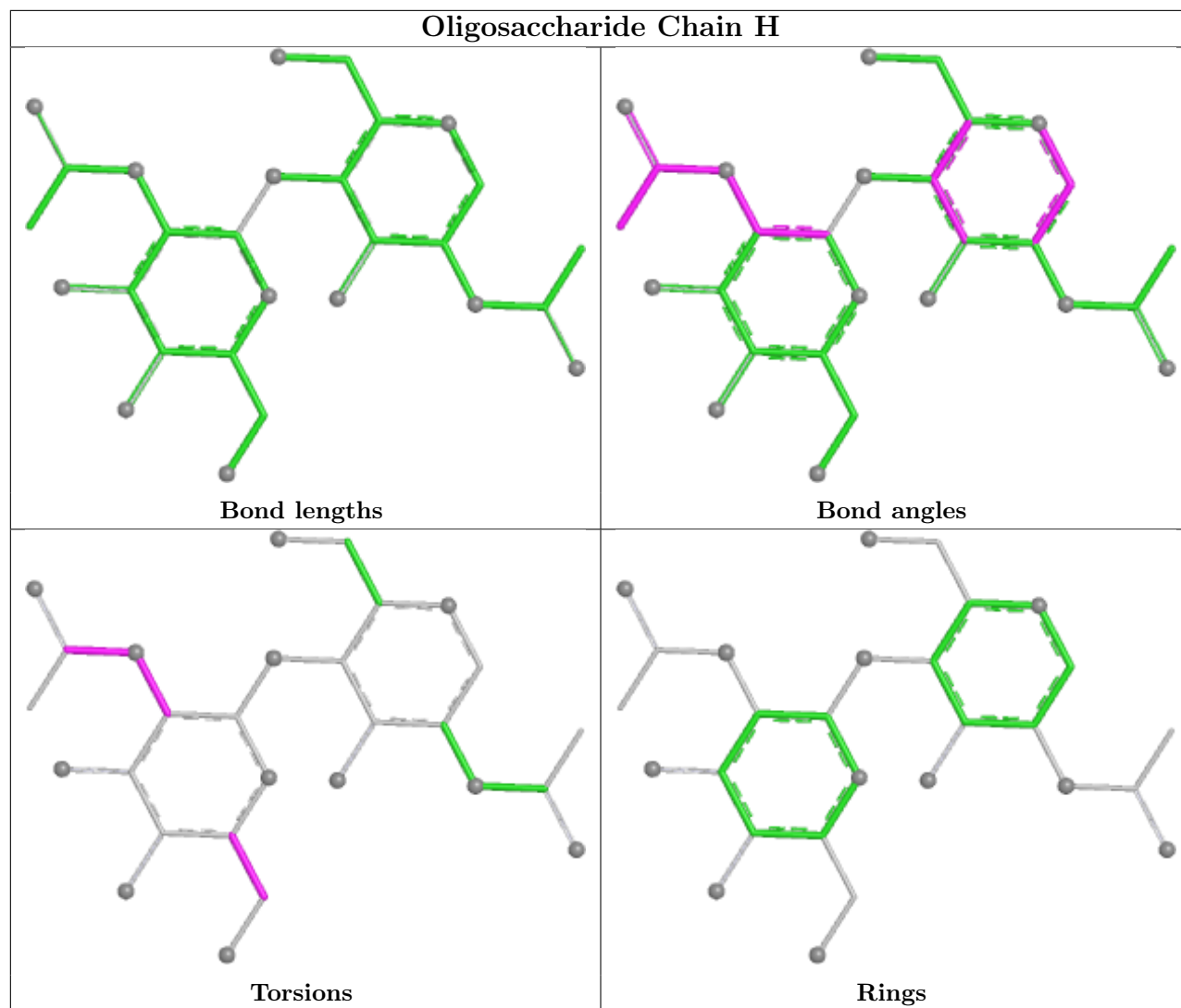
Mol	Chain	Res	Type	Atoms
4	R	5	MAN	C1-C2-C3-C4-C5-O5
4	I	5	MAN	C1-C2-C3-C4-C5-O5

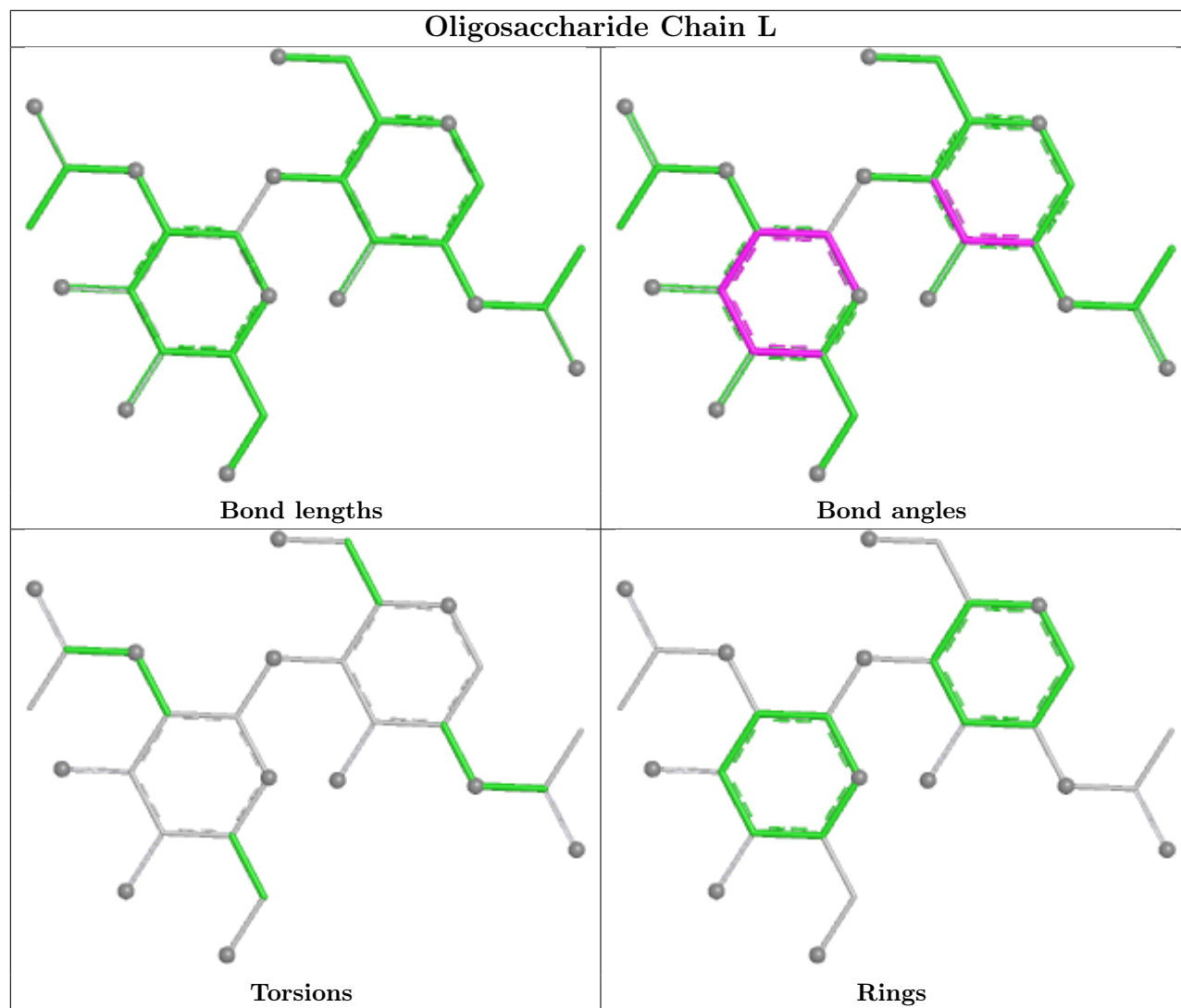
14 monomers are involved in 22 short contacts:

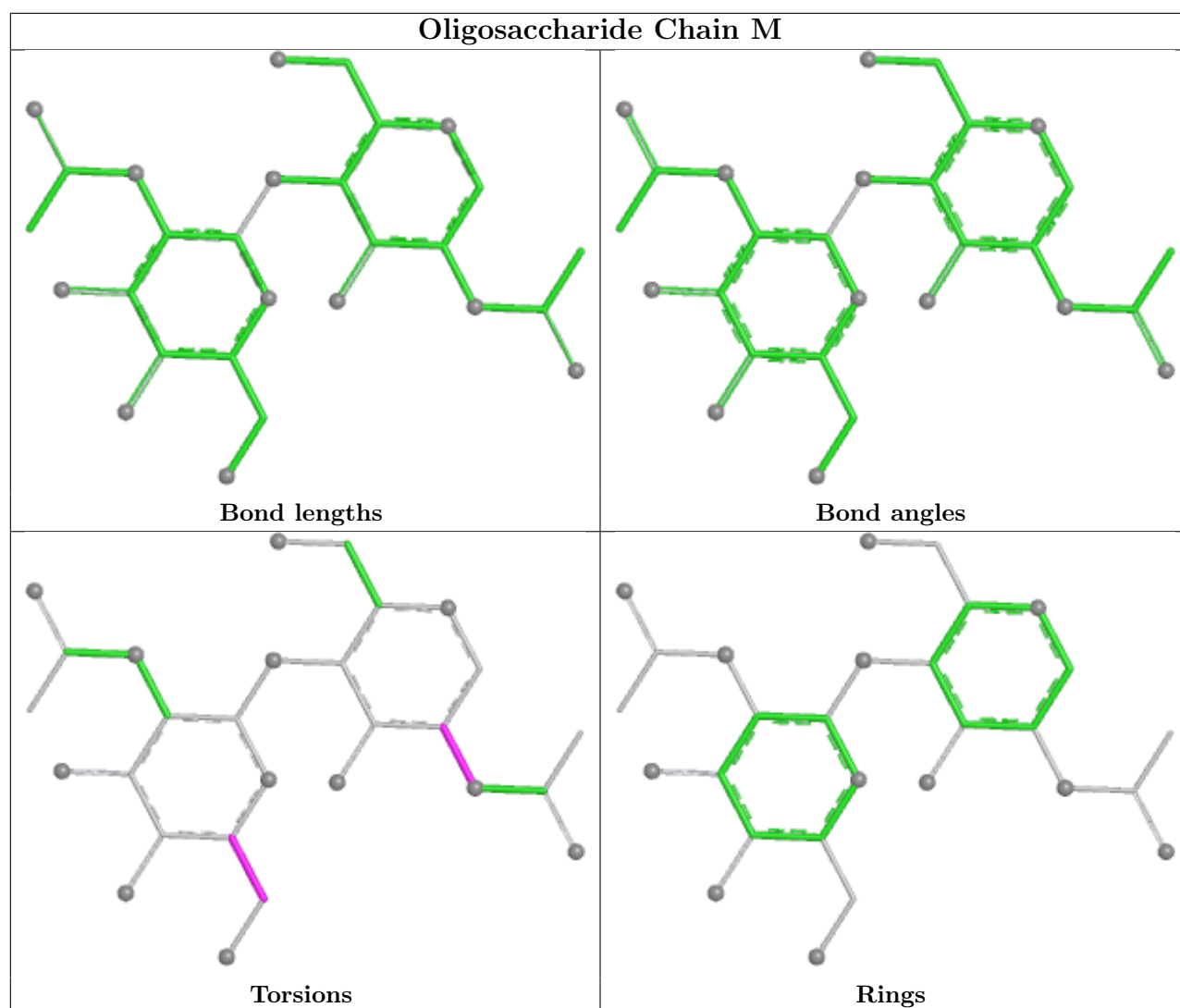
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	1	NAG	2	0
6	O	1	NAG	1	0
3	L	1	NAG	1	0
6	K	1	NAG	1	0
3	M	1	NAG	1	0
3	P	1	NAG	3	0
3	P	2	NAG	1	0
3	G	1	NAG	3	0
5	J	3	SIA	2	0
7	N	1	NAG	3	0
3	H	1	NAG	1	0
4	R	1	NAG	1	0
3	M	2	NAG	1	0
4	I	1	NAG	2	0

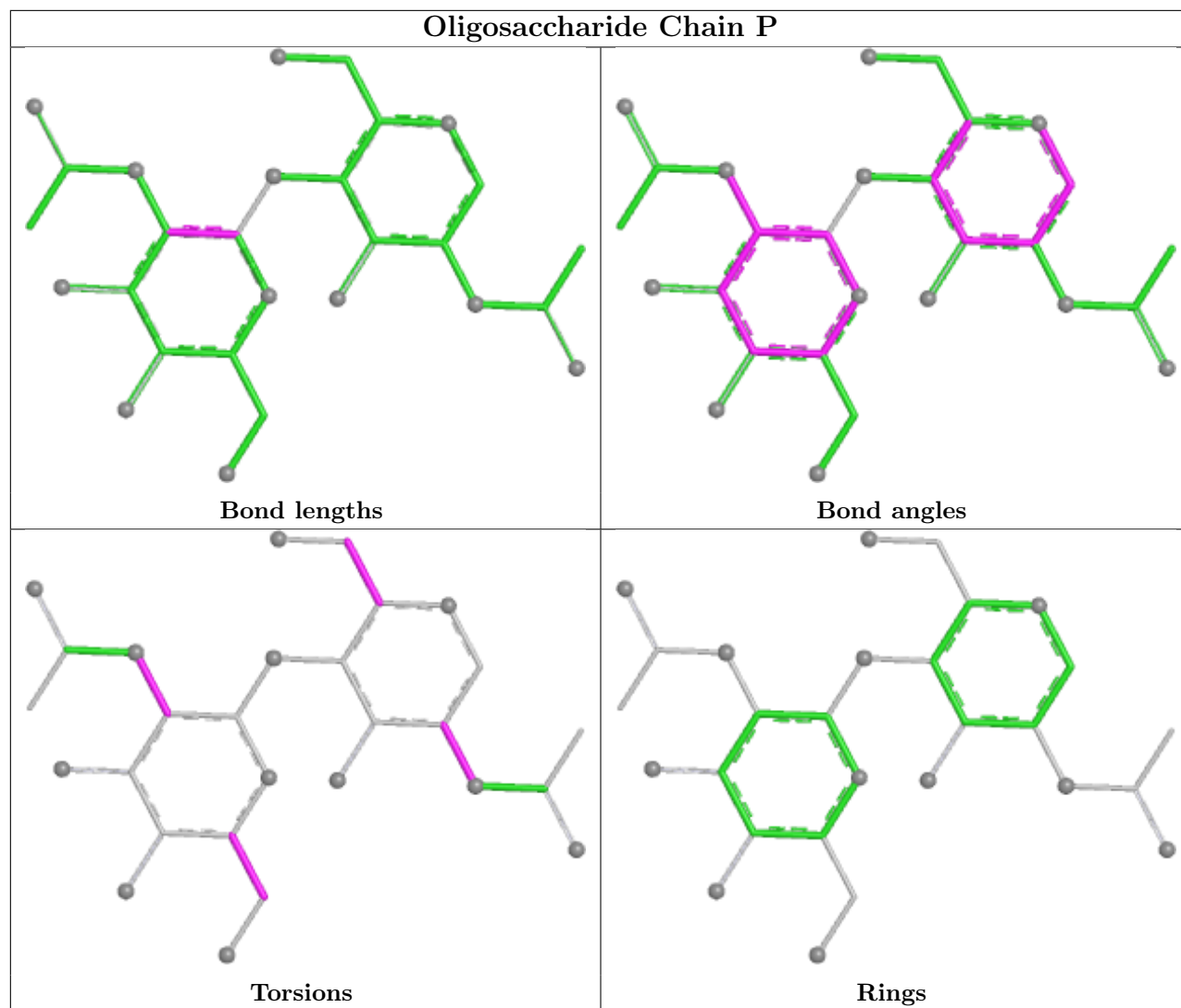
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

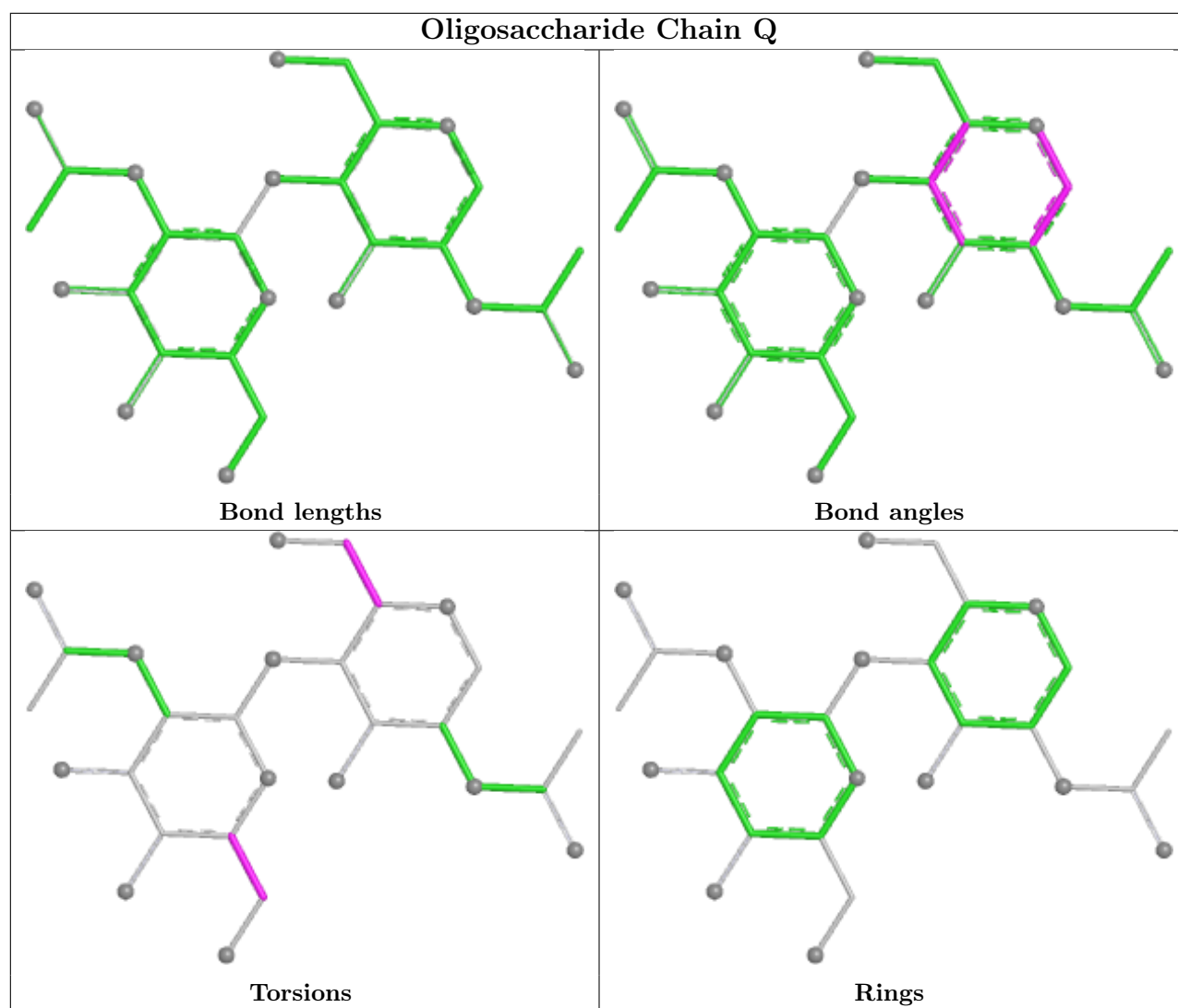


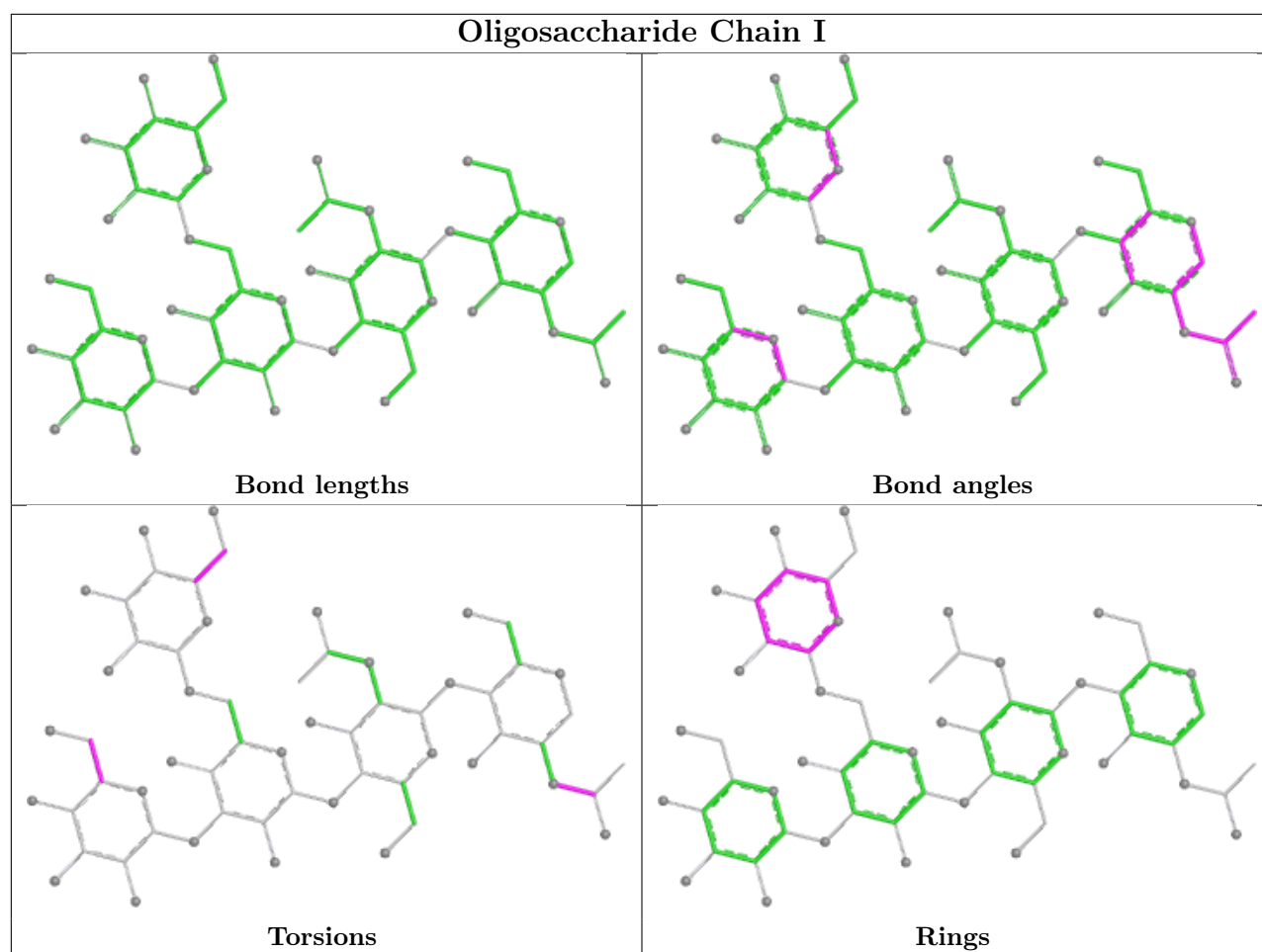


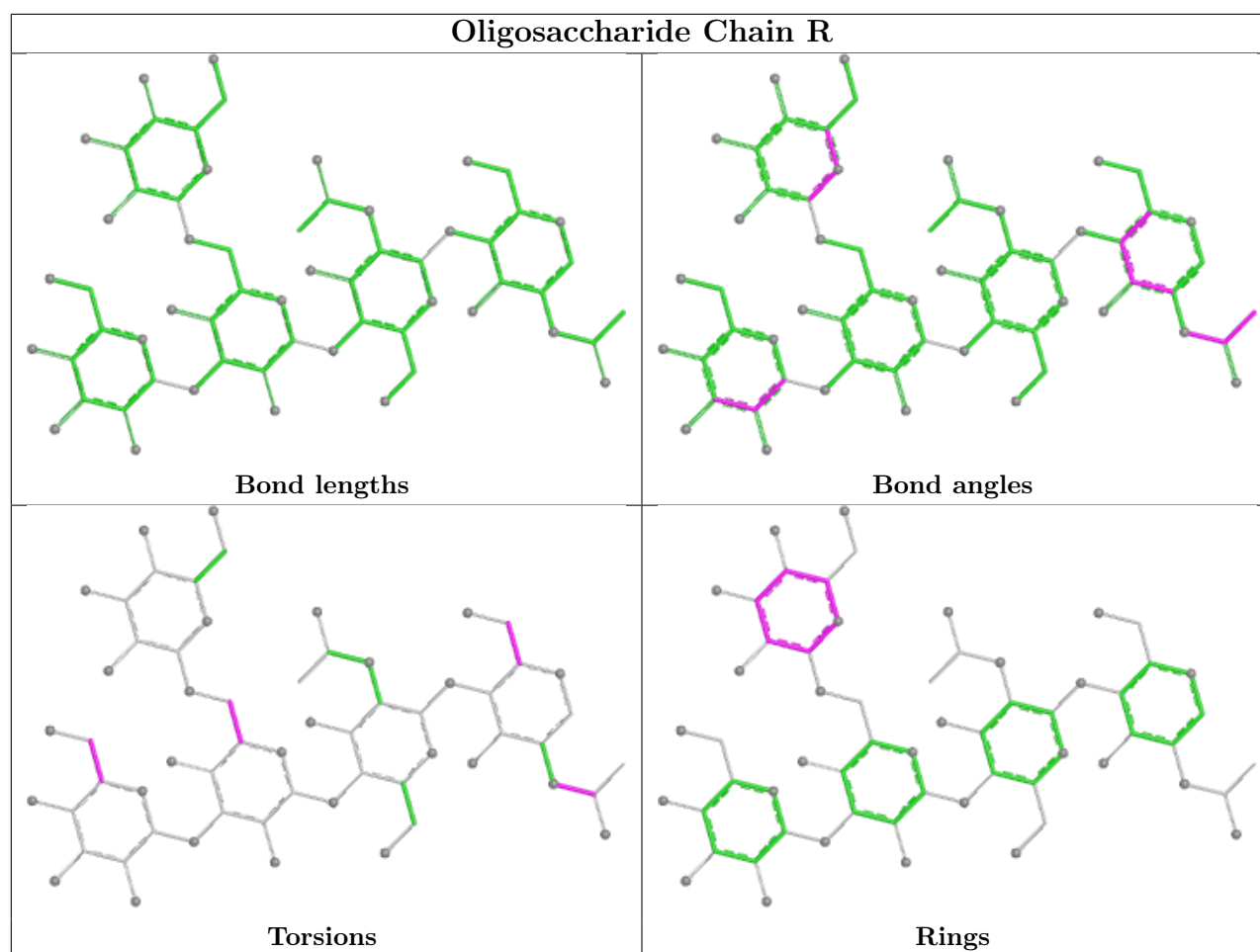


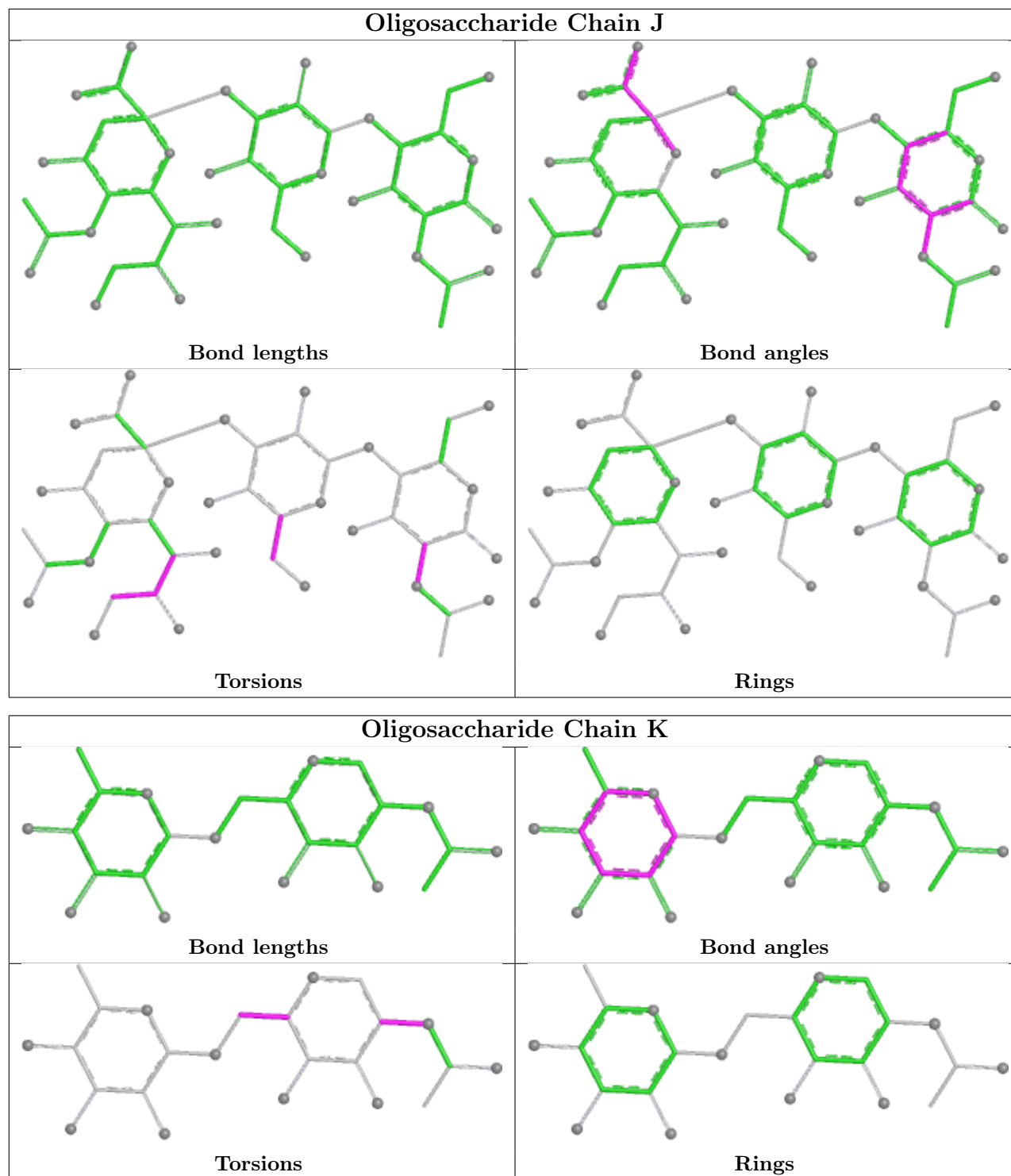


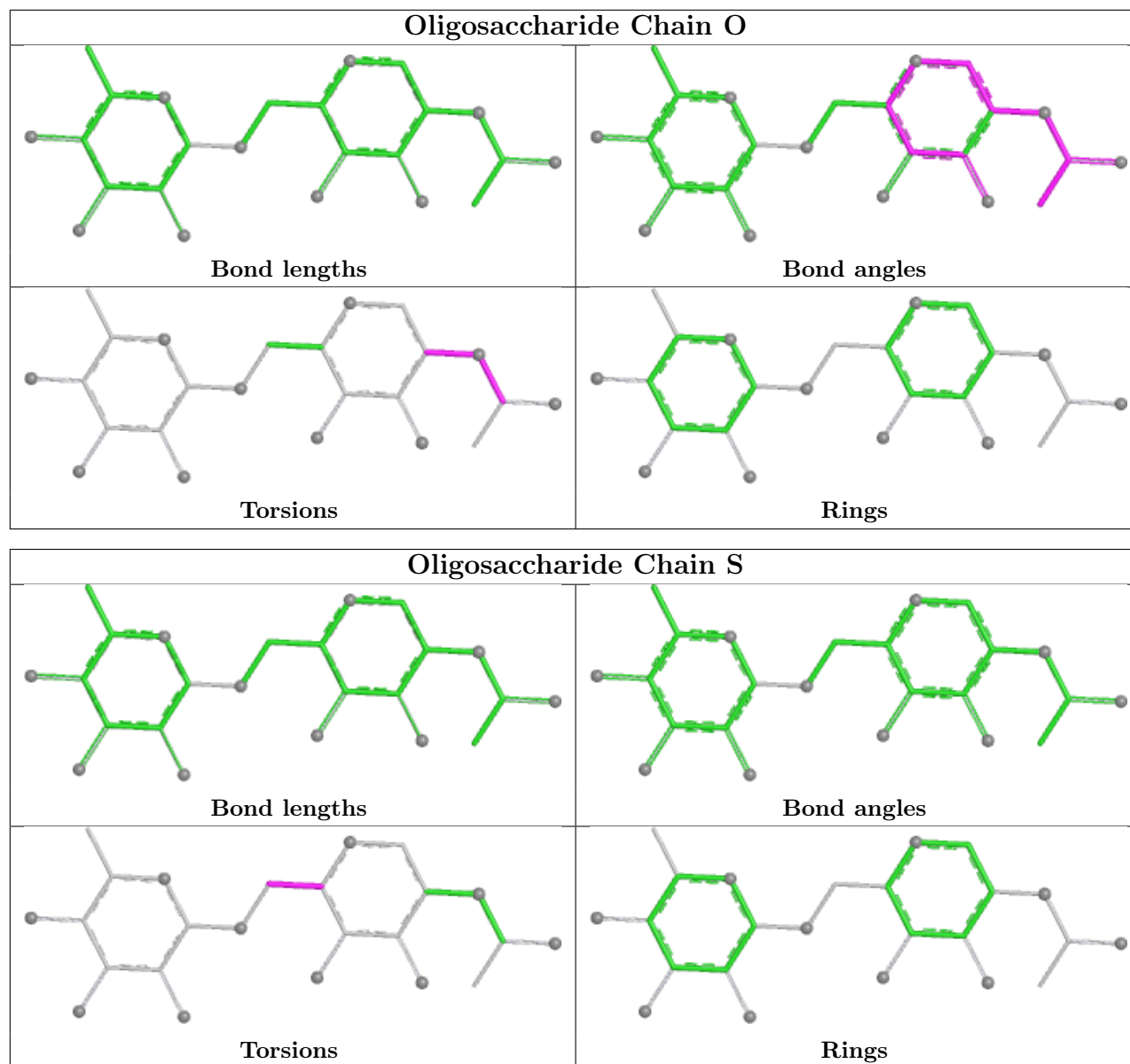


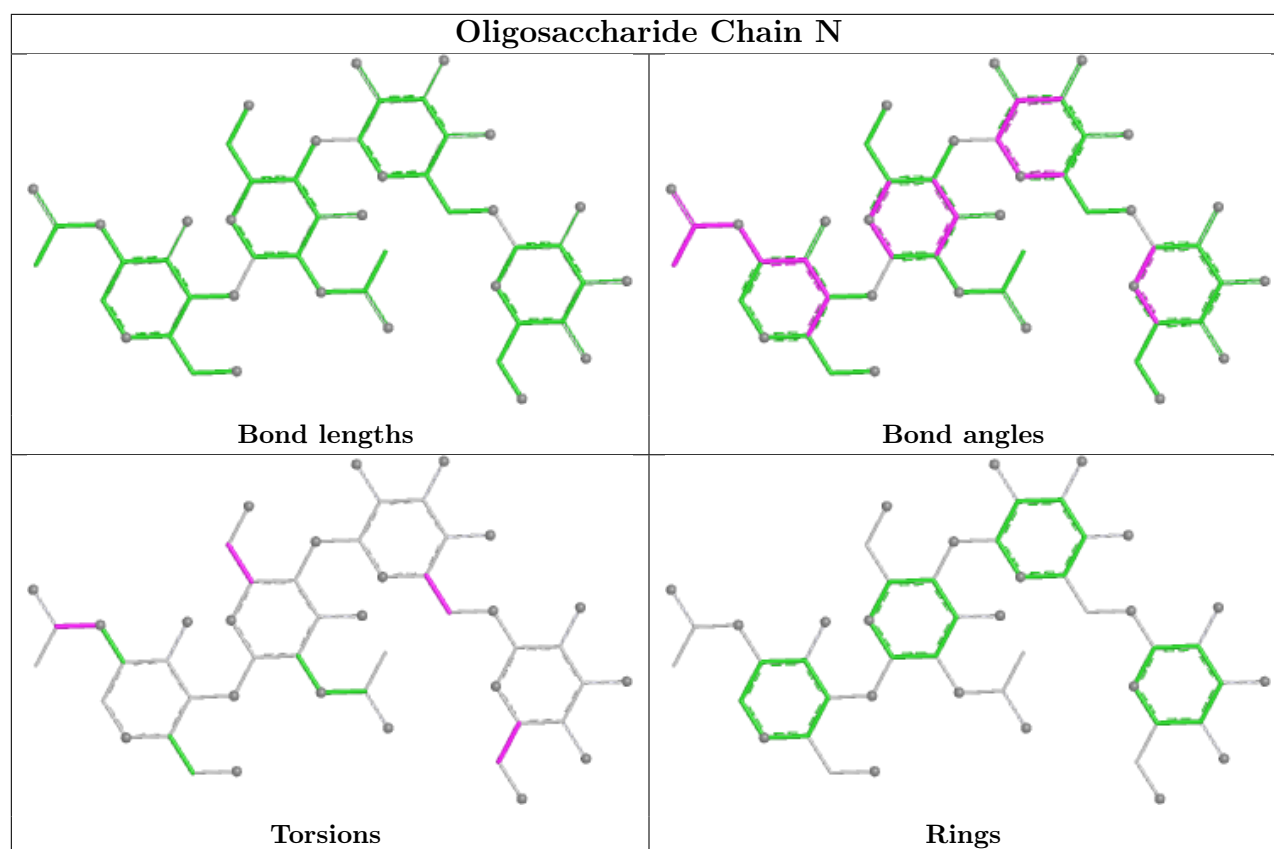












5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	C	421	-	14,14,15	0.54	0	17,19,21	2.11	4 (23%)
8	NAG	A	401	-	14,14,15	0.65	0	17,19,21	1.33	2 (11%)
8	NAG	C	401	-	14,14,15	0.46	0	17,19,21	1.29	2 (11%)
9	SIA	C	701	-	20,20,21	0.50	0	21,28,31	1.16	3 (14%)
8	NAG	E	401	-	14,14,15	0.56	0	17,19,21	0.79	0
8	NAG	A	431	-	14,14,15	0.48	0	17,19,21	1.07	1 (5%)
9	SIA	E	701	-	20,20,21	0.51	0	21,28,31	1.10	3 (14%)

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	C	421	-	-	3/6/23/26	0/1/1/1
8	NAG	A	401	-	-	2/6/23/26	0/1/1/1
8	NAG	C	401	-	-	1/6/23/26	0/1/1/1
9	SIA	C	701	-	-	1/18/34/38	0/1/1/1
8	NAG	E	401	-	-	0/6/23/26	0/1/1/1
8	NAG	A	431	-	-	2/6/23/26	0/1/1/1
9	SIA	E	701	-	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	421	NAG	C2-N2-C7	5.07	129.69	122.90
8	C	421	NAG	C8-C7-N2	4.18	123.06	116.12
8	C	421	NAG	C1-C2-N2	3.96	116.67	110.43
8	C	401	NAG	C1-O5-C5	3.74	117.20	112.19
9	C	701	SIA	O6-C2-C1	3.33	114.00	107.72
8	A	401	NAG	C4-C3-C2	3.30	115.85	111.02
9	E	701	SIA	O6-C2-C1	2.94	113.26	107.72
8	C	421	NAG	O7-C7-C8	-2.91	116.88	122.05
9	C	701	SIA	O1B-C1-C2	2.74	119.85	112.71
8	A	401	NAG	C3-C4-C5	2.62	114.99	110.23
9	E	701	SIA	O1B-C1-C2	2.61	119.51	112.71
8	A	431	NAG	O5-C1-C2	-2.42	107.55	111.29
8	C	401	NAG	C3-C4-C5	2.41	114.61	110.23
9	C	701	SIA	O1A-C1-C2	-2.05	118.43	122.85
9	E	701	SIA	O1A-C1-C2	-2.01	118.51	122.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	421	NAG	C1-C2-N2-C7
8	A	431	NAG	O5-C5-C6-O6
8	A	431	NAG	C4-C5-C6-O6
8	A	401	NAG	O5-C5-C6-O6
8	A	401	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	421	NAG	C8-C7-N2-C2
8	C	421	NAG	O7-C7-N2-C2
8	C	401	NAG	O5-C5-C6-O6
9	C	701	SIA	C4-C5-N5-C10

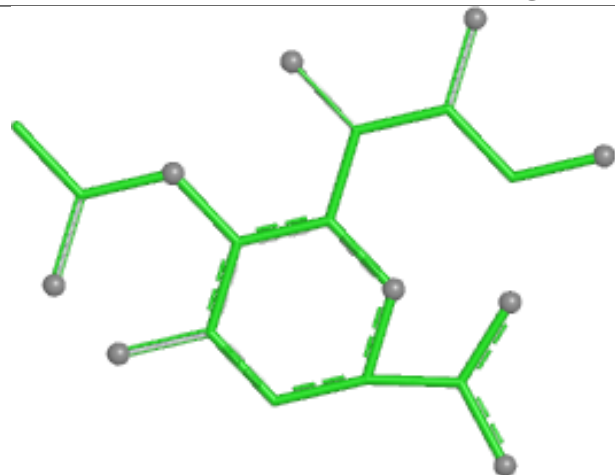
There are no ring outliers.

5 monomers are involved in 8 short contacts:

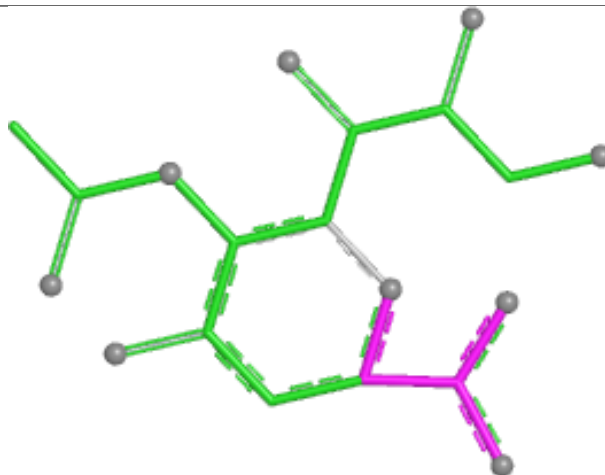
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	421	NAG	2	0
8	A	401	NAG	2	0
8	C	401	NAG	1	0
8	E	401	NAG	1	0
8	A	431	NAG	2	0

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.

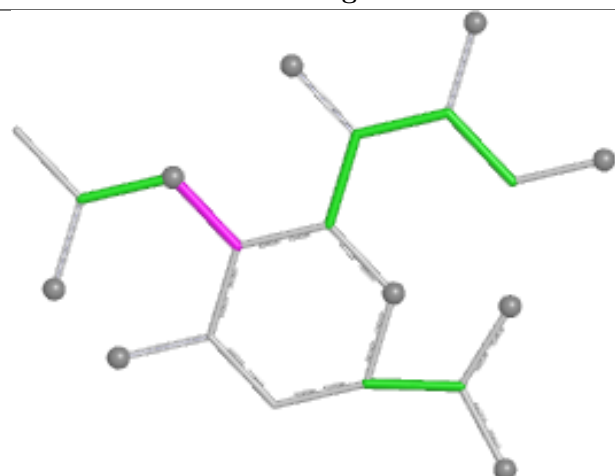
Ligand SIA C 701



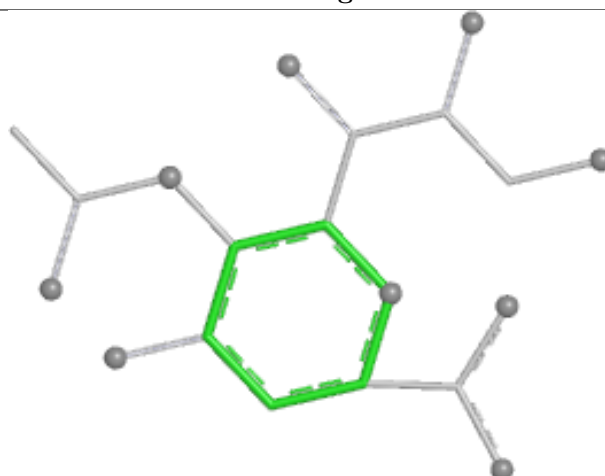
Bond lengths



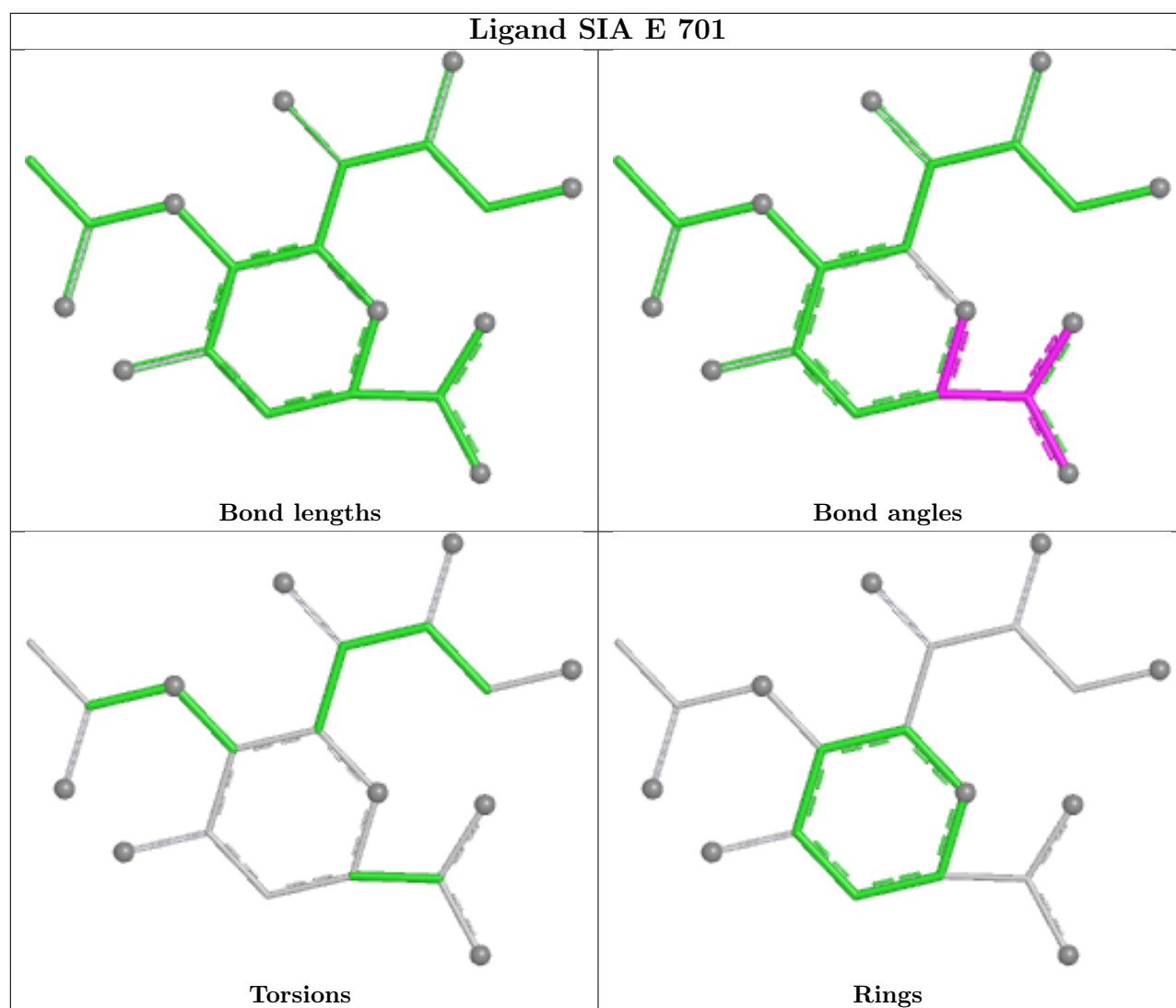
Bond angles



Torsions



Rings



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/323 (98%)	1.11	47 (14%) 6 4	73, 109, 145, 155	0
1	C	319/323 (98%)	1.13	32 (10%) 12 8	91, 120, 162, 175	0
1	E	319/323 (98%)	1.57	79 (24%) 2 2	108, 150, 173, 186	0
2	B	172/173 (99%)	0.75	12 (6%) 22 14	64, 79, 108, 121	0
2	D	172/173 (99%)	0.68	6 (3%) 47 29	64, 76, 108, 122	0
2	F	172/173 (99%)	0.62	3 (1%) 69 49	68, 86, 110, 124	0
All	All	1473/1488 (98%)	1.07	179 (12%) 8 6	64, 108, 163, 186	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	179	ILE	5.5
1	E	58	VAL	4.9
1	E	223	VAL	4.4
1	E	126	THR	3.8
1	A	222	TRP	3.8
1	E	164	LEU	3.7
1	A	242	ILE	3.6
1	E	151	LEU	3.5
2	B	61	GLU	3.5
1	E	79	PHE	3.5
2	B	81	GLU	3.4
1	E	243	LEU	3.4
2	B	59	THR	3.4
1	E	254	PRO	3.4
1	E	194	LEU	3.4
1	E	47	SER	3.4
1	A	252	VAL	3.4
1	E	49	GLY	3.4
1	A	205	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	199	SER	3.3
1	E	230	ILE	3.3
2	F	29	SER	3.2
1	A	243	LEU	3.2
1	E	59	LEU	3.2
1	C	179	ILE	3.2
1	E	221	PRO	3.2
1	E	106	ALA	3.2
1	C	299	LYS	3.1
1	E	234	TRP	3.1
1	E	163	ILE	3.0
1	C	240	GLY	3.0
1	E	152	ASN	3.0
1	E	219	SER	3.0
1	A	142	GLY	3.0
1	A	245	ILE	3.0
1	A	131	THR	2.9
1	A	206	THR	2.9
1	E	222	TRP	2.9
1	E	267	VAL	2.9
1	A	232	ILE	2.9
1	A	171	ASN	2.9
1	C	200	GLY	2.9
1	E	316	LEU	2.9
1	A	210	GLN	2.8
1	E	127	TRP	2.8
1	E	242	ILE	2.8
1	E	45	SER	2.8
1	E	199	SER	2.8
1	C	212	THR	2.8
1	E	15	LEU	2.8
1	A	179	ILE	2.8
1	A	204	VAL	2.7
1	C	154	LEU	2.7
1	C	251	LEU	2.7
1	A	256	GLY	2.7
1	E	214	ILE	2.7
1	E	18	HIS	2.7
1	E	252	VAL	2.7
1	A	236	ILE	2.7
1	E	188	ASN	2.7
1	C	70	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	65	THR	2.6
1	A	159	ASN	2.6
1	A	240	GLY	2.6
1	E	128	THR	2.6
2	B	80	LEU	2.6
1	E	153	TRP	2.6
1	E	17	HIS	2.5
1	A	270	SER	2.5
2	D	1	GLY	2.5
1	C	108	LEU	2.5
2	F	58	ARG	2.5
2	B	73	VAL	2.5
1	E	52	CYS	2.5
1	E	122	ALA	2.5
1	E	96	ASN	2.5
1	C	115	SER	2.5
1	E	258	PHE	2.5
1	A	74	PRO	2.5
1	E	71	LEU	2.5
1	E	135	GLY	2.5
1	A	83	ASN	2.4
2	B	144	CYS	2.4
1	A	192	THR	2.4
1	A	79	PHE	2.4
1	A	157	SER	2.4
1	E	86	LEU	2.4
1	C	213	VAL	2.4
1	E	187	SER	2.4
1	A	254	PRO	2.4
1	A	96	ASN	2.4
1	C	246	ASN	2.4
1	A	145	ASP	2.4
1	E	48	ILE	2.4
1	E	299	LYS	2.4
1	E	273	LEU	2.4
1	A	124	GLY	2.3
1	E	283	THR	2.3
1	C	178	TYR	2.3
2	B	67	GLU	2.3
1	A	117	THR	2.3
1	E	232	ILE	2.3
1	E	56	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	285	ASN	2.3
1	A	177	LEU	2.3
1	E	191	GLN	2.3
1	E	323	VAL	2.3
1	E	245	ILE	2.3
1	A	169	PRO	2.3
1	A	151	LEU	2.3
1	A	306	PRO	2.3
1	A	144	ALA	2.3
1	A	158	GLY	2.3
1	A	251	LEU	2.3
1	C	214	ILE	2.2
1	E	111	ILE	2.2
2	D	161	ILE	2.2
1	A	127	TRP	2.2
1	C	87	PHE	2.2
2	B	63	PHE	2.2
1	C	307	LYS	2.2
1	A	246	ASN	2.2
1	C	8	ASN	2.2
1	E	16	GLY	2.2
1	E	138	ALA	2.2
1	E	200	GLY	2.2
1	E	266	SER	2.2
1	A	244	MET	2.2
2	B	70	PHE	2.2
1	A	91	SER	2.2
1	E	186	SER	2.2
1	C	232	ILE	2.2
1	E	300	ILE	2.2
1	C	52	CYS	2.2
1	A	178	TYR	2.2
1	A	247	SER	2.2
1	E	34	ILE	2.2
1	C	243	LEU	2.2
2	B	60	ASN	2.2
1	C	96	ASN	2.1
1	C	103	PRO	2.1
1	E	181	GLY	2.1
1	E	43	VAL	2.1
1	E	105	TYR	2.1
2	D	56	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	164	LEU	2.1
1	E	259	LYS	2.1
1	E	124	GLY	2.1
2	B	57	GLU	2.1
1	A	126	THR	2.1
1	C	102	ILE	2.1
2	D	87	THR	2.1
1	C	132	GLN	2.1
1	C	265	SER	2.1
1	E	166	VAL	2.1
1	A	241	ASP	2.1
1	E	326	LYS	2.1
1	A	128	THR	2.1
1	C	144	ALA	2.1
1	E	142	GLY	2.1
2	D	75	GLY	2.1
1	E	133	ASN	2.1
1	E	216	ASN	2.1
1	A	214	ILE	2.1
2	D	2	ILE	2.1
1	C	157	SER	2.0
2	B	154	ASN	2.0
1	E	32	ASP	2.0
1	E	98	TYR	2.0
1	E	14	CYS	2.0
2	F	61	GLU	2.0
1	A	163	ILE	2.0
1	E	29	ILE	2.0
1	E	302	TYR	2.0
1	C	145	ASP	2.0
1	C	258	PHE	2.0
1	C	140	LYS	2.0
1	E	324	PRO	2.0
1	E	251	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

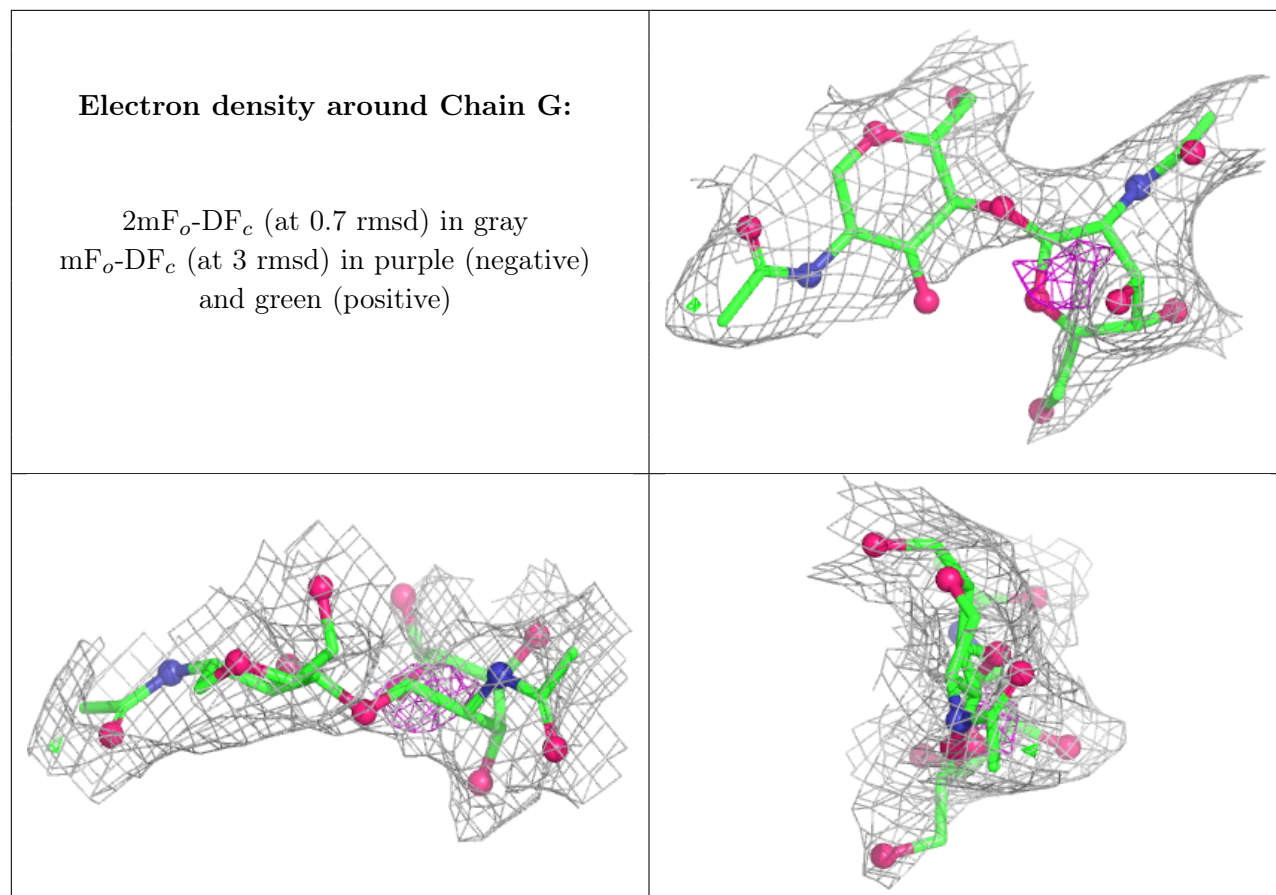
6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	P	1	14/15	0.22	0.19	159,163,167,167	0
3	NAG	P	2	14/15	0.25	0.15	170,174,179,179	0
3	NAG	H	2	14/15	0.29	0.17	125,130,136,137	0
4	MAN	R	5	11/12	0.29	0.15	130,133,136,138	0
3	NAG	L	2	14/15	0.30	0.15	134,140,143,145	0
3	NAG	G	2	14/15	0.30	0.17	121,126,129,129	0
7	MAN	N	4	11/12	0.33	0.14	122,127,134,135	0
7	BMA	N	3	11/12	0.34	0.14	128,131,137,139	0
6	NAG	S	1	14/15	0.38	0.19	99,102,107,108	0
7	NAG	N	2	14/15	0.42	0.17	118,121,125,128	0
6	FUC	S	2	10/11	0.44	0.18	96,101,103,104	0
3	NAG	L	1	14/15	0.45	0.15	120,125,130,133	0
4	BMA	R	3	11/12	0.47	0.13	135,138,142,143	0
4	MAN	I	5	11/12	0.49	0.17	92,95,99,99	0
4	MAN	R	4	11/12	0.50	0.16	143,147,149,151	0
4	MAN	I	4	11/12	0.52	0.14	102,104,106,107	0
5	NAG	J	1	15/15	0.56	0.18	137,142,148,148	0
6	NAG	O	1	14/15	0.60	0.15	85,91,99,102	0
3	NAG	Q	1	14/15	0.60	0.17	165,167,169,169	0
3	NAG	Q	2	14/15	0.61	0.20	164,170,175,176	0
3	NAG	G	1	14/15	0.63	0.16	109,112,118,118	0
4	NAG	R	2	14/15	0.64	0.13	130,134,138,138	0
4	BMA	I	3	11/12	0.65	0.12	96,99,102,103	0
5	GAL	J	2	11/12	0.65	0.12	130,133,135,135	0
6	FUC	O	2	10/11	0.68	0.18	83,88,92,94	0
7	NAG	N	1	14/15	0.71	0.14	112,116,119,120	0
4	NAG	I	2	14/15	0.75	0.12	89,91,94,95	0
3	NAG	H	1	14/15	0.75	0.12	114,116,121,122	0
4	NAG	R	1	14/15	0.75	0.15	132,133,136,137	0
6	FUC	K	2	10/11	0.75	0.19	90,98,102,103	0
5	SIA	J	3	20/21	0.76	0.14	125,129,132,133	0
4	NAG	I	1	14/15	0.76	0.13	84,87,89,90	0
3	NAG	M	1	14/15	0.78	0.14	135,138,142,143	0
3	NAG	M	2	14/15	0.84	0.18	133,141,146,147	0
6	NAG	K	1	14/15	0.85	0.14	93,98,105,106	0

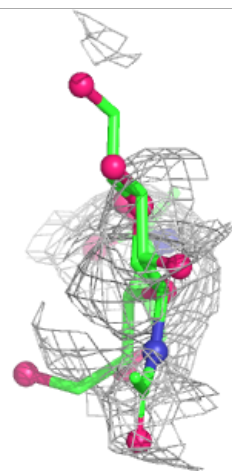
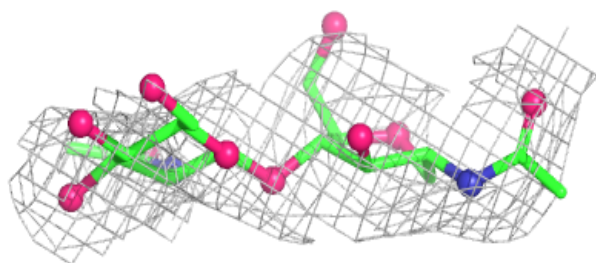
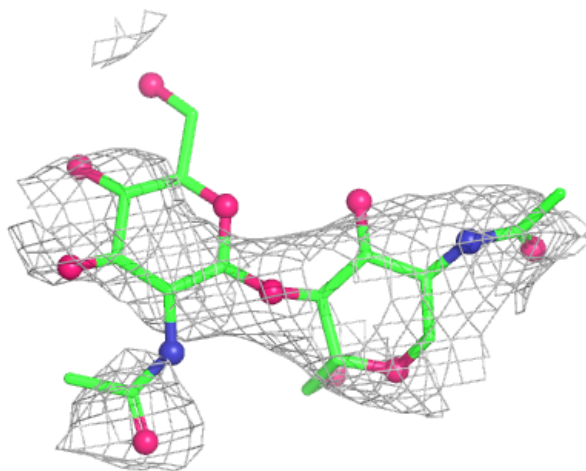
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

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



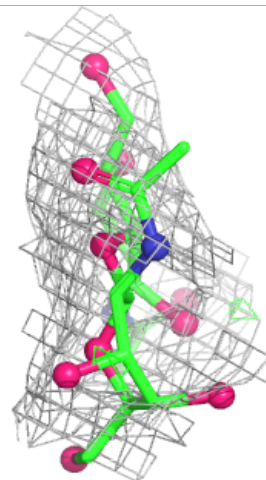
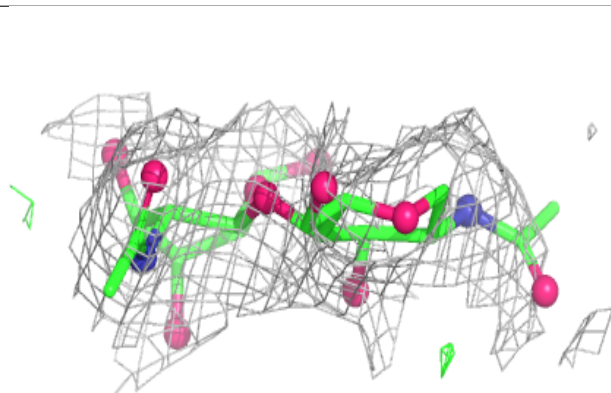
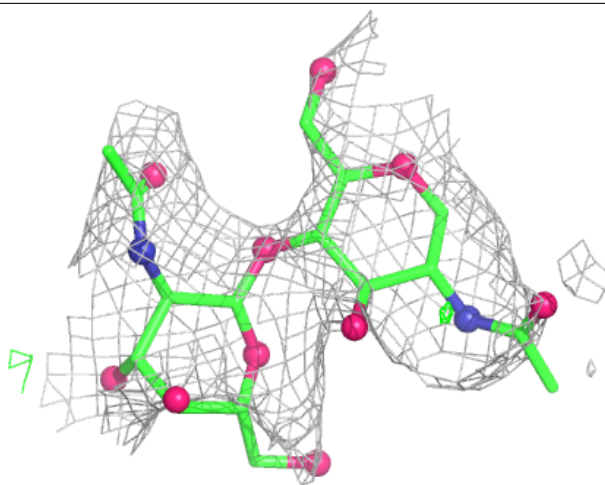
Electron density around Chain H:

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



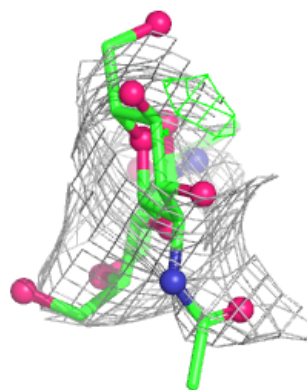
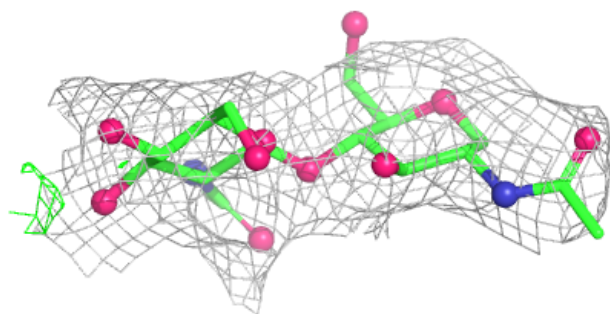
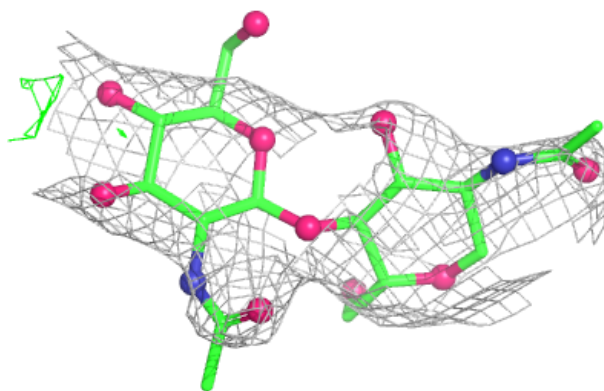
Electron density around Chain L:

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



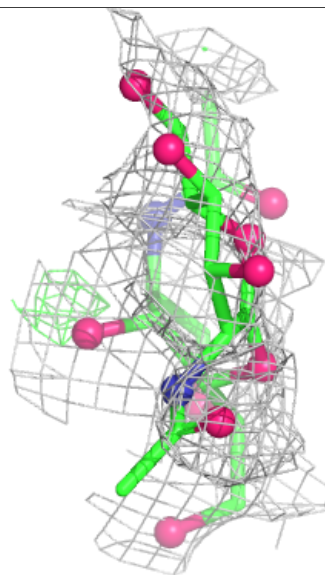
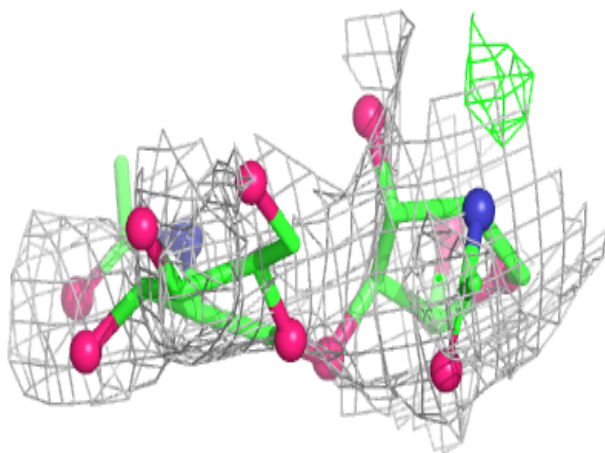
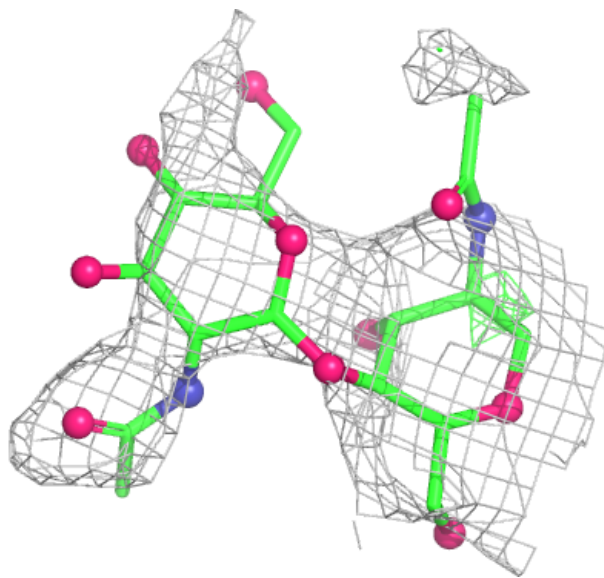
Electron density around Chain M:

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



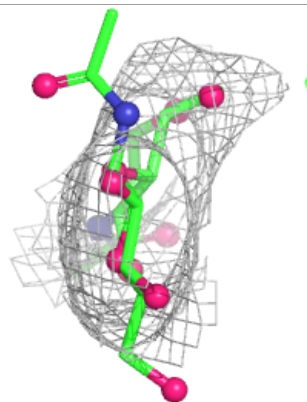
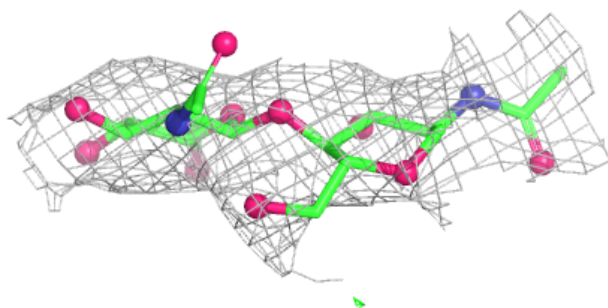
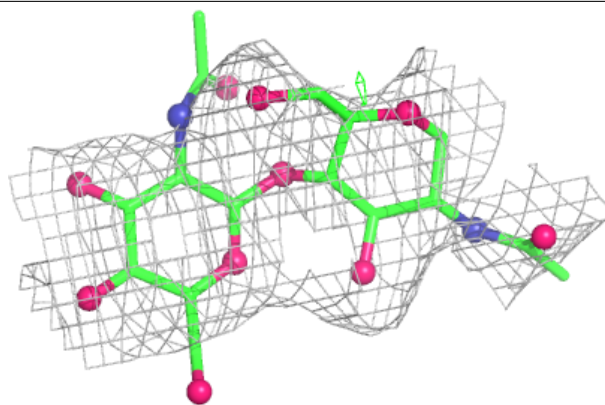
Electron density around Chain P:

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



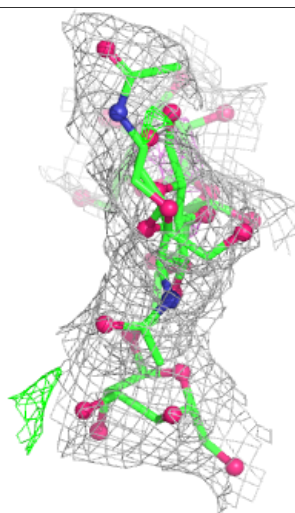
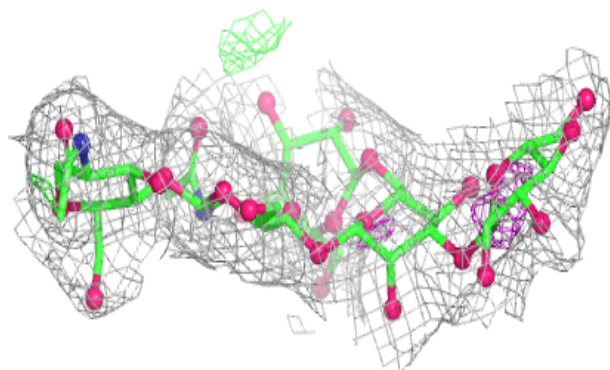
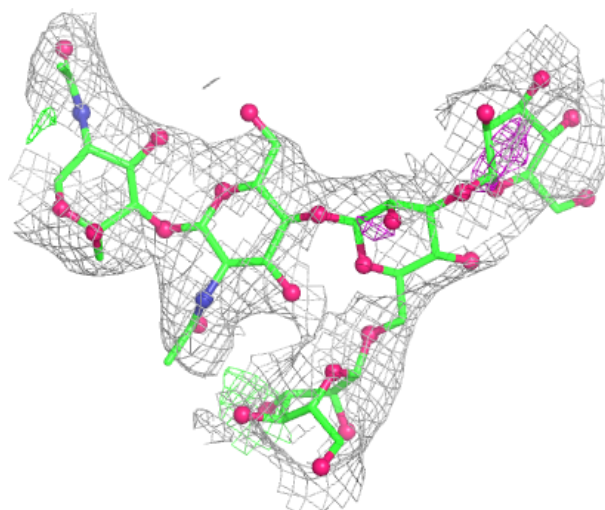
Electron density around Chain Q:

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



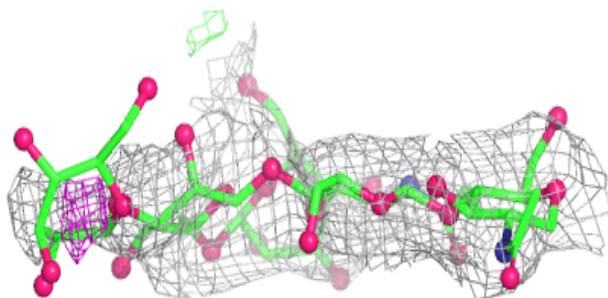
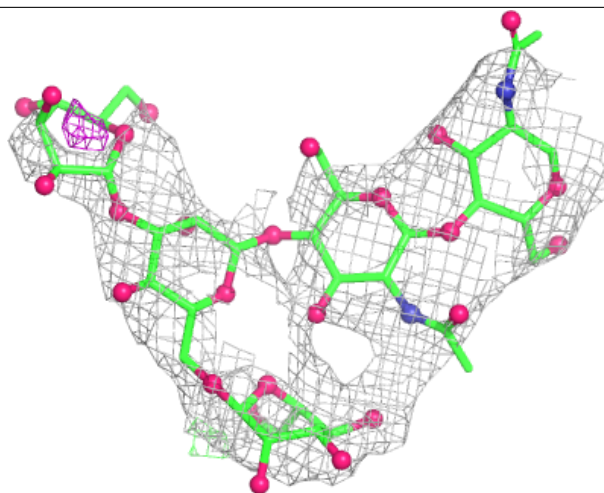
Electron density around Chain I:

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



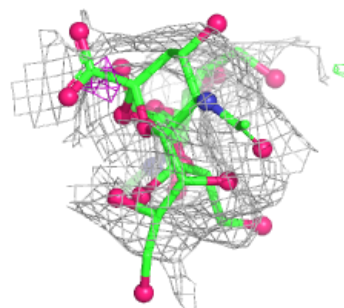
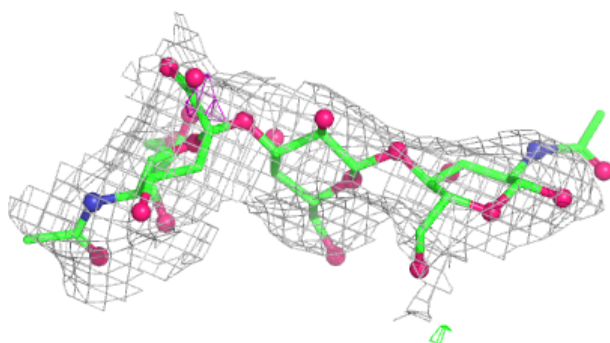
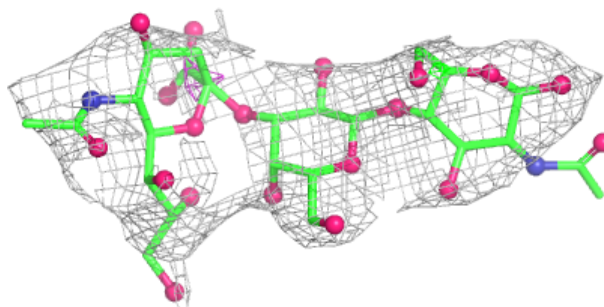
Electron density around Chain R:

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

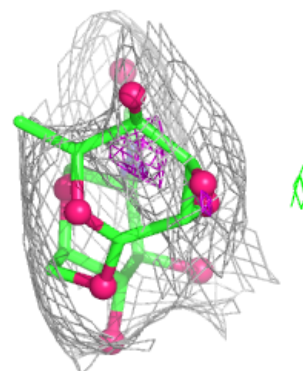
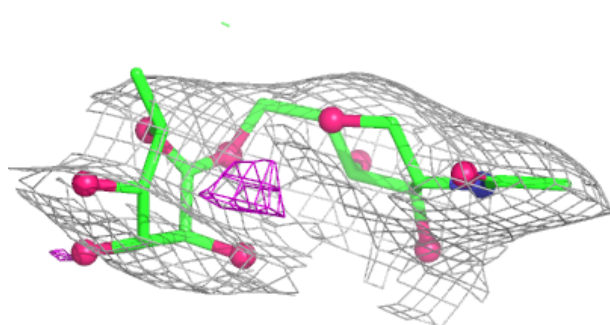
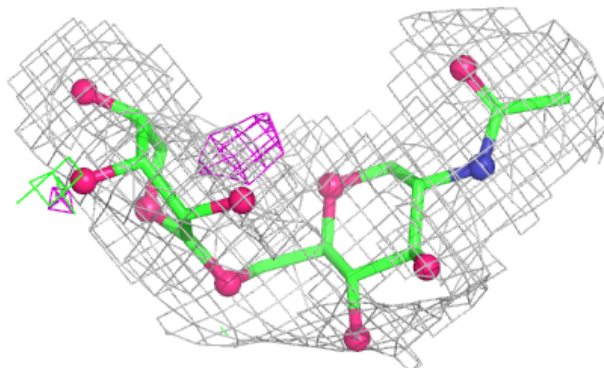


Electron density around Chain J:

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

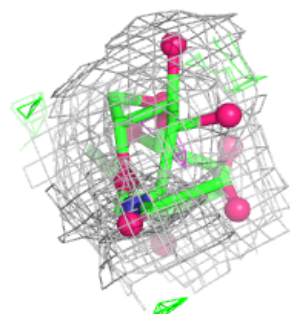
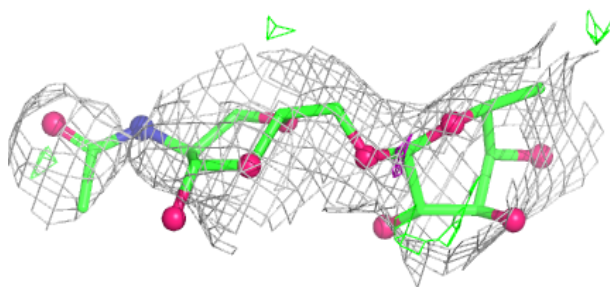
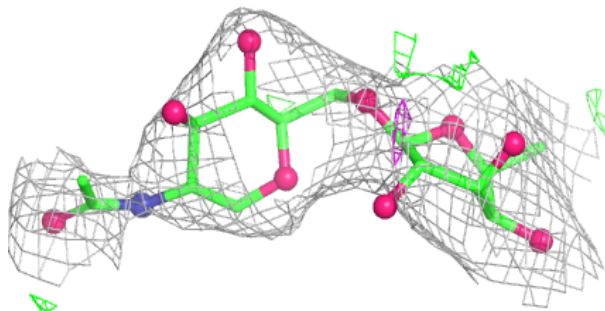
**Electron density around Chain K:**

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

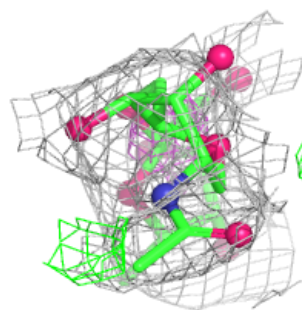
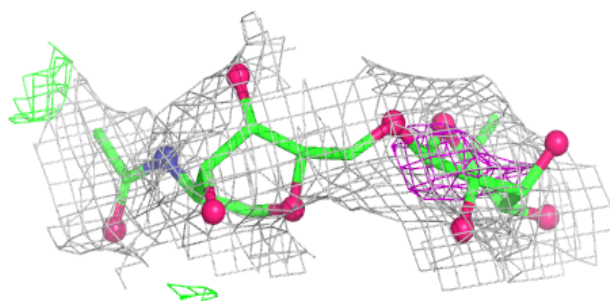
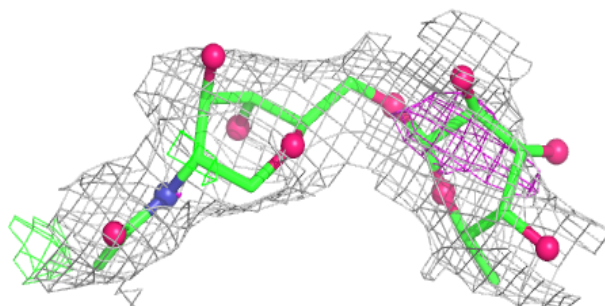


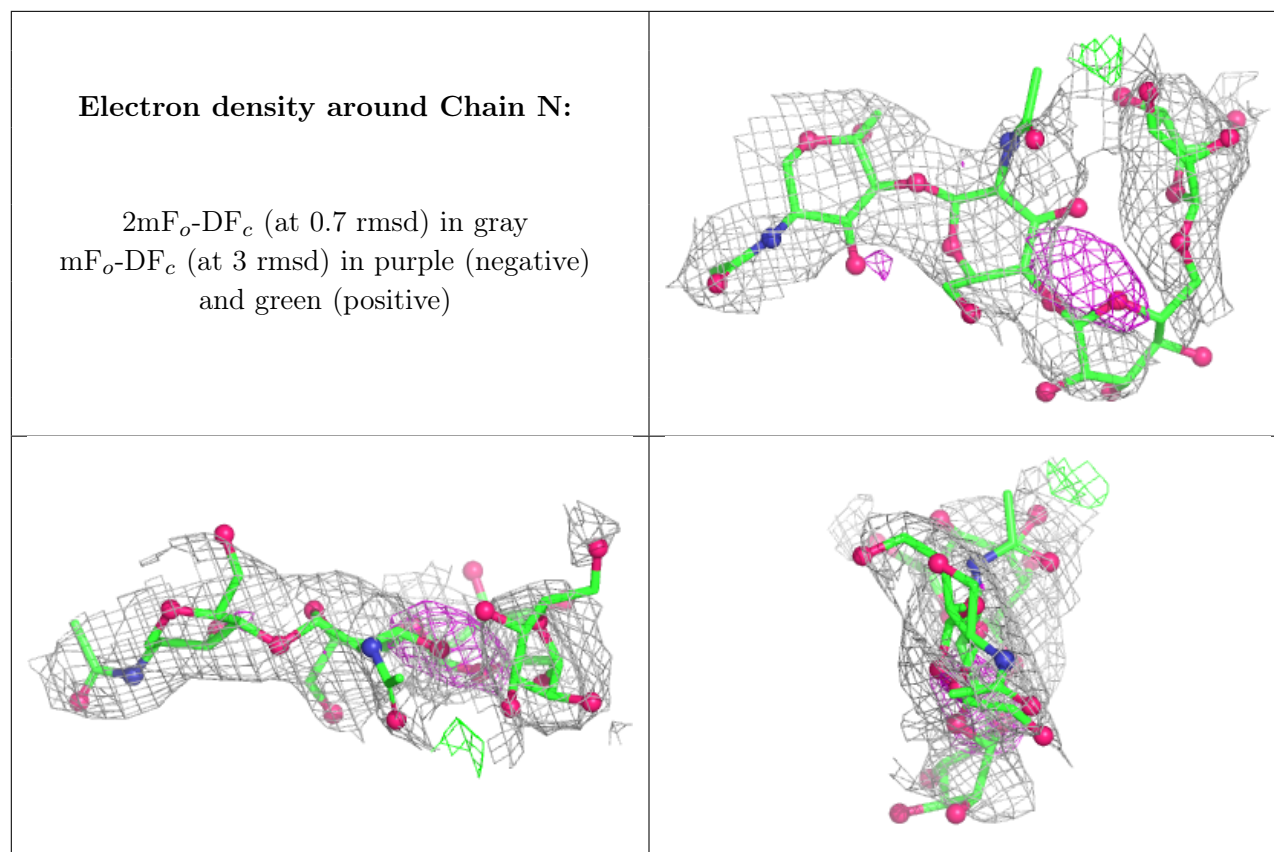
Electron density around Chain O:

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

**Electron density around Chain S:**

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





6.4 Ligands [i](#)

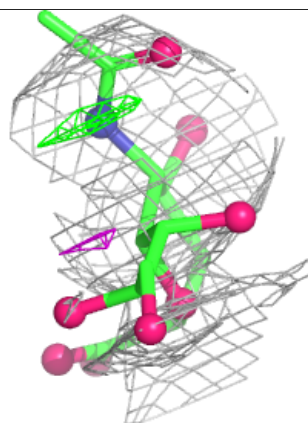
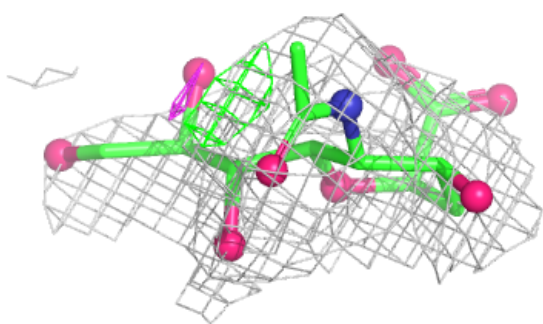
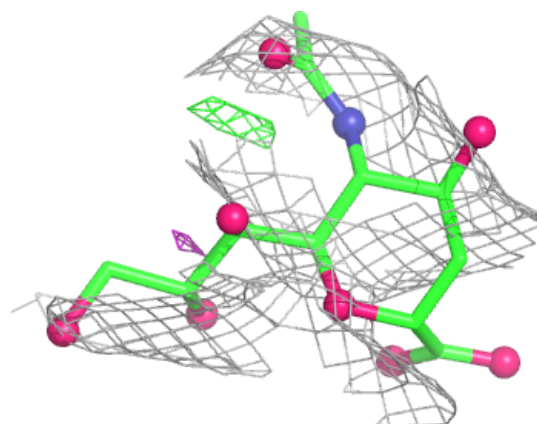
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SIA	E	701	20/21	0.53	0.20	164,170,175,175	0
8	NAG	A	431	14/15	0.61	0.22	157,161,164,167	0
9	SIA	C	701	20/21	0.63	0.16	151,156,161,162	0
8	NAG	C	421	14/15	0.66	0.16	137,145,152,155	0
8	NAG	E	401	14/15	0.67	0.17	127,130,134,137	0
8	NAG	C	401	14/15	0.81	0.14	93,96,97,98	0
8	NAG	A	401	14/15	0.88	0.12	77,79,81,82	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.

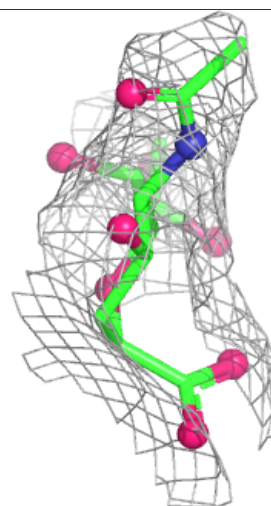
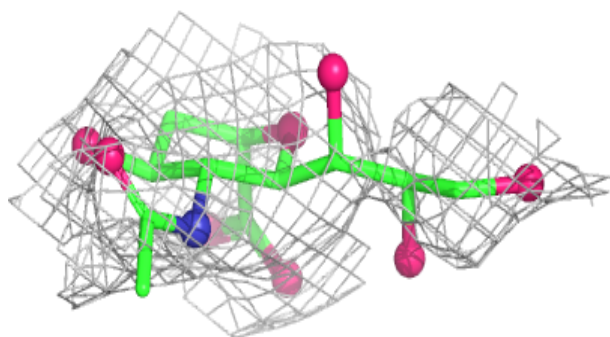
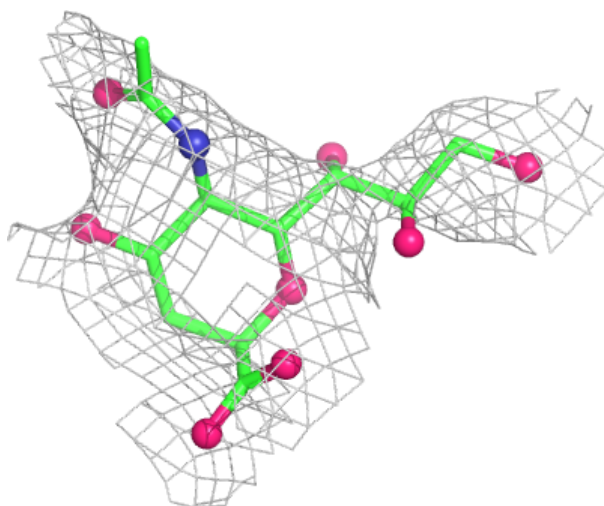
Electron density around SIA E 701:

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



Electron density around SIA C 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.