



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:15 AM BST

PDB ID : 5N11
Title : Crystal structure of Human beta1-coronavirus OC43 NL/A/2005 Hemagglutinin-Esterase
Authors : Bakkers, M.J.G.; Feitsma, L.J.; de Groot, R.J.; Huizinga, E.G.
Deposited on : 2017-02-04
Resolution : 2.45 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 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

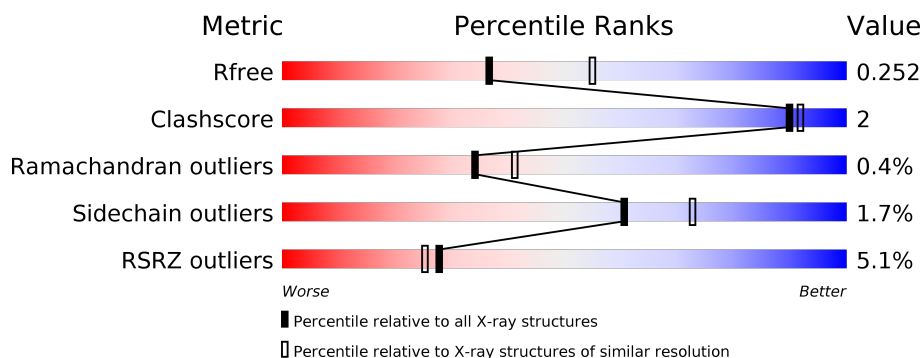
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.




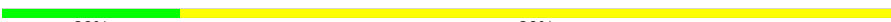
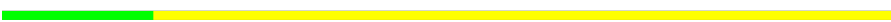

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 ≥ 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	376	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>5% • 9%</div> </div> </div>
1	B	376	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>5% 7%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	G	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	J	2	 50% 50%
3	F	5	 20% 80%
4	I	6	 17% 83%
5	K	3	 67% 33%
6	L	4	 25% 75%

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
2	NAG	C	2	-	-	-	X
3	BMA	F	3	-	-	-	X
7	NAG	A	508	-	-	-	X
7	NAG	B	508	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6081 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 Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2718	1735	449	518	16			
1	B	348	Total	C	N	O	S	0	0	0
			2776	1777	457	526	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	ASP	TYR	conflict	UNP Q4VID6
A	388	SER	-	expression tag	UNP Q4VID6
A	389	ASP	-	expression tag	UNP Q4VID6
A	390	PRO	-	expression tag	UNP Q4VID6
A	391	LEU	-	expression tag	UNP Q4VID6
A	392	VAL	-	expression tag	UNP Q4VID6
A	393	PRO	-	expression tag	UNP Q4VID6
A	394	ARG	-	expression tag	UNP Q4VID6
B	375	ASP	TYR	conflict	UNP Q4VID6
B	388	SER	-	expression tag	UNP Q4VID6
B	389	ASP	-	expression tag	UNP Q4VID6
B	390	PRO	-	expression tag	UNP Q4VID6
B	391	LEU	-	expression tag	UNP Q4VID6
B	392	VAL	-	expression tag	UNP Q4VID6
B	393	PRO	-	expression tag	UNP Q4VID6
B	394	ARG	-	expression tag	UNP Q4VID6

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



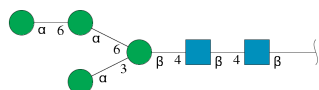
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called 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	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 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.



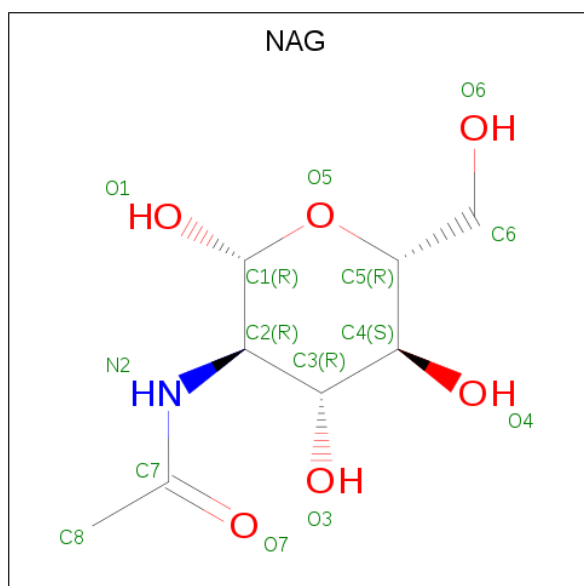
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 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
6	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



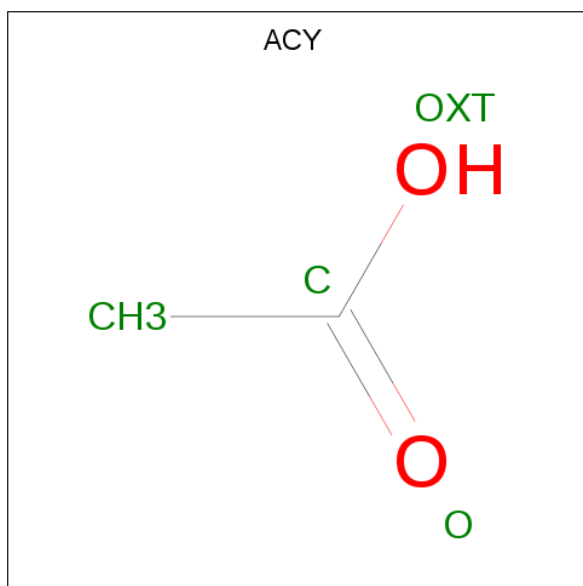
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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


- Molecule 9 is water.

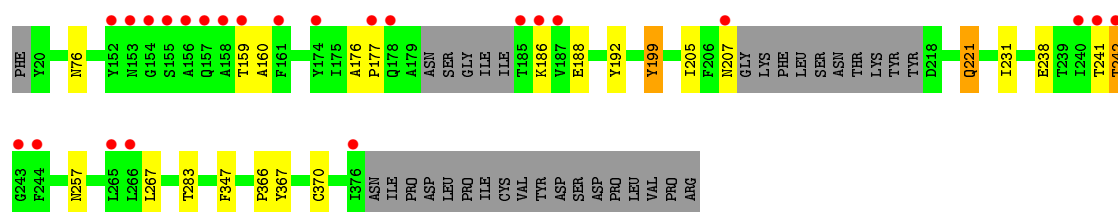
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	27	Total 27	O 27	0	0
9	B	22	Total 22	O 22	0	0

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.

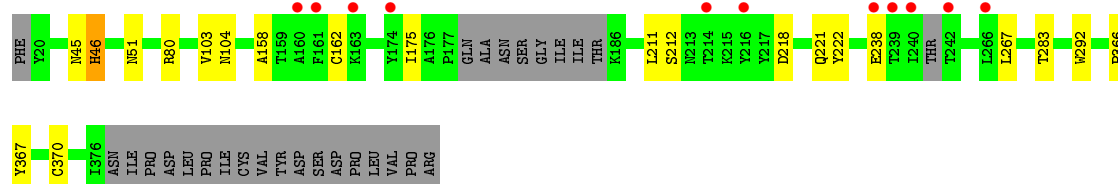
- Molecule 1: Hemagglutinin-esterase

Chain A: 



- Molecule 1: Hemagglutinin-esterase

Chain B: 



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

Chain C: 



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

Chain D: 




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

Chain E:  100%

UAG1
UAG2

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

Chain G:  100%

UAG1
UAG2

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

Chain H:  100%

UAG1
UAG2

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

Chain J:  50%  50%

UAG1
UAG2

- Molecule 3: 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 F:  20%  80%

UAG1
UAG2
BMA3
MAN4
MAN5

- Molecule 4: 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

Chain I:  17%  83%

UAG1
UAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67%  33%



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

Chain L: 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.73 Å 77.73 Å 299.49 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.41 – 2.45 67.32 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (67.41-2.45) 99.9 (67.32-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.211 , 0.249 0.216 , 0.252	Depositor DCC
R_{free} test set	1957 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6081	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0.32	0/2797	0.51	0/3812
1	B	0.32	0/2858	0.51	0/3892
All	All	0.32	0/5655	0.51	0/7704

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2718	0	2516	11	0
1	B	2776	0	2574	10	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
3	F	61	0	52	0	0
4	I	72	0	61	0	0
5	K	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	50	0	43	0	0
7	A	56	0	52	1	0
7	B	84	0	78	0	0
8	A	4	0	3	0	0
8	B	4	0	3	0	0
9	A	27	0	0	0	0
9	B	22	0	0	0	0
All	All	6081	0	5566	21	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:O	1:B:46:HIS:CB	2.50	0.59
1:B:158:ALA:HA	1:B:175:ILE:HD13	1.85	0.58
1:A:231:ILE:HD13	1:B:222:TYR:HE1	1.73	0.53
1:B:211:LEU:HD13	1:B:212:SER:N	2.23	0.53
1:B:45:ASN:O	1:B:46:HIS:HB3	2.08	0.53
1:A:366:PRO:HB2	1:A:370:CYS:SG	2.50	0.50
1:A:221:GLN:OE1	1:A:267:LEU:HD12	2.14	0.48
1:A:241:THR:O	1:A:242:THR:HG23	2.15	0.47
1:A:176:ALA:HB1	1:A:177:PRO:HD2	2.00	0.44
1:A:192:TYR:HD2	1:A:257:ASN:HD22	1.66	0.44
1:A:188:GLU:HG3	7:A:508:NAG:H81	1.99	0.43
1:A:283:THR:HG23	1:A:367:TYR:CZ	2.55	0.42
1:B:283:THR:HG23	1:B:367:TYR:CZ	2.54	0.42
1:B:366:PRO:HB2	1:B:370:CYS:SG	2.60	0.42
1:B:103:VAL:HG22	1:B:292:TRP:CE2	2.55	0.41
1:A:347:PHE:O	1:A:366:PRO:HA	2.21	0.41
1:B:80:ARG:NH1	1:B:104:ASN:O	2.51	0.41
1:A:159:THR:O	1:A:160:ALA:HB3	2.20	0.41
1:A:199:TYR:N	1:A:199:TYR:CD2	2.89	0.41
2:D:2:NAG:O7	2:D:2:NAG:H3	2.21	0.40
1:B:221:GLN:HE22	1:B:267:LEU:HA	1.86	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	336/376 (89%)	319 (95%)	16 (5%)	1 (0%)	41	49
1	B	342/376 (91%)	323 (94%)	17 (5%)	2 (1%)	25	29
All	All	678/752 (90%)	642 (95%)	33 (5%)	3 (0%)	34	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	HIS
1	B	162	CYS
1	A	186	LYS

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	300/332 (90%)	293 (98%)	7 (2%)	50	63
1	B	306/332 (92%)	303 (99%)	3 (1%)	76	84
All	All	606/664 (91%)	596 (98%)	10 (2%)	60	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	199	TYR
1	A	205	ILE

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Mol	Chain	Res	Type
1	A	207	ASN
1	A	221	GLN
1	A	238	GLU
1	A	242	THR
1	B	51	ASN
1	B	218	ASP
1	B	238	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	257	ASN
1	B	51	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

36 non-standard protein/DNA/RNA residues 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	J	1	1,2	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
2	NAG	H	2	2	14,14,15	0.61	0	17,19,21	0.87	0
7	NAG	A	508	1	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
7	NAG	B	501	1	14,14,15	0.57	0	17,19,21	1.18	2 (11%)
4	NAG	I	2	4	14,14,15	0.59	0	17,19,21	0.85	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.53	0	17,19,21	0.97	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	1,3	14,14,15	0.63	0	17,19,21	1.41	1 (5%)
7	NAG	B	515	1	14,14,15	0.42	0	17,19,21	1.49	2 (11%)
6	MAN	L	4	6	11,11,12	0.65	0	15,15,17	1.32	1 (6%)
2	NAG	G	2	2	14,14,15	0.56	0	17,19,21	1.26	2 (11%)
7	NAG	B	521	1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
7	NAG	A	509	1	14,14,15	0.54	0	17,19,21	1.20	0
3	MAN	F	4	3	11,11,12	0.43	0	15,15,17	2.07	2 (13%)
7	NAG	B	514	1	14,14,15	0.44	0	17,19,21	1.49	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
7	NAG	A	510	1	14,14,15	0.61	0	17,19,21	0.91	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.69	0	17,19,21	1.28	1 (5%)
4	MAN	I	5	4	11,11,12	0.59	0	15,15,17	0.99	1 (6%)
2	NAG	J	2	2	14,14,15	0.47	0	17,19,21	0.75	0
7	NAG	A	505	1	14,14,15	0.59	0	17,19,21	0.84	0
2	NAG	H	1	1,2	14,14,15	0.44	0	17,19,21	0.87	0
4	MAN	I	4	4	11,11,12	0.61	0	15,15,17	0.66	0
4	MAN	I	6	4	11,11,12	0.67	0	15,15,17	1.59	3 (20%)
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	0.95	0
5	NAG	K	1	1,5	14,14,15	0.63	0	17,19,21	1.23	2 (11%)
3	MAN	F	5	3	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
5	NAG	K	2	5	14,14,15	0.48	0	17,19,21	0.74	0
7	NAG	B	508	1	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
6	NAG	L	2	6	14,14,15	0.54	0	17,19,21	0.93	0
2	NAG	C	1	1,2	14,14,15	0.49	0	17,19,21	1.00	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.48	3 (17%)
7	NAG	B	520	1	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
6	NAG	L	1	1,6	14,14,15	0.59	0	17,19,21	1.12	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
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
7	NAG	A	508	1	-	0/6/23/26	0/1/1/1
7	NAG	B	501	1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
7	NAG	B	515	1	-	0/6/23/26	0/1/1/1
6	MAN	L	4	6	-	1/2/19/22	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
7	NAG	B	521	1	-	2/6/23/26	0/1/1/1
7	NAG	A	509	1	-	4/6/23/26	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
7	NAG	B	514	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
7	NAG	A	510	1	-	1/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
7	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	0/1/1/1
4	MAN	I	6	4	-	2/2/19/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
7	NAG	B	508	1	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
7	NAG	B	520	1	-	0/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	6.91	121.56	112.19
7	B	514	NAG	C1-O5-C5	4.86	118.78	112.19
3	F	1	NAG	C1-O5-C5	4.43	118.19	112.19
7	B	515	NAG	C1-O5-C5	4.29	118.00	112.19
6	L	4	MAN	C1-C2-C3	4.10	114.70	109.67
2	C	2	NAG	O5-C1-C2	-3.84	105.22	111.29
6	L	1	NAG	C1-O5-C5	3.45	116.86	112.19
7	B	521	NAG	O5-C1-C2	-3.44	105.86	111.29
4	I	1	NAG	O5-C1-C2	-3.38	105.95	111.29
4	I	6	MAN	C2-C3-C4	3.30	116.61	110.89
7	B	508	NAG	C1-O5-C5	3.27	116.62	112.19
7	B	501	NAG	C1-O5-C5	3.26	116.61	112.19
4	I	6	MAN	C3-C4-C5	3.25	116.04	110.24
2	C	2	NAG	C1-C2-N2	3.06	115.71	110.49
2	G	2	NAG	O5-C1-C2	-3.03	106.50	111.29
4	I	6	MAN	C1-C2-C3	2.99	113.34	109.67
5	K	1	NAG	O5-C1-C2	-2.86	106.77	111.29
2	E	1	NAG	C1-O5-C5	2.82	116.01	112.19
2	E	2	NAG	C1-O5-C5	2.65	115.79	112.19
5	K	1	NAG	C1-O5-C5	2.56	115.66	112.19
3	F	2	NAG	O5-C1-C2	-2.51	107.32	111.29
2	G	1	NAG	O5-C1-C2	-2.49	107.36	111.29
4	I	2	NAG	O5-C1-C2	-2.40	107.49	111.29
7	B	501	NAG	O7-C7-C8	-2.37	117.66	122.06
7	B	515	NAG	C4-C3-C2	-2.33	107.61	111.02
7	A	508	NAG	C1-O5-C5	2.31	115.33	112.19
2	C	2	NAG	C3-C4-C5	2.31	114.36	110.24
7	A	510	NAG	C1-O5-C5	2.27	115.27	112.19
3	F	5	MAN	C1-O5-C5	2.26	115.25	112.19
4	I	5	MAN	C1-O5-C5	2.25	115.24	112.19
2	J	1	NAG	C1-O5-C5	2.21	115.18	112.19
2	G	2	NAG	C4-C3-C2	-2.19	107.81	111.02
3	F	5	MAN	C1-C2-C3	2.19	112.36	109.67
3	F	4	MAN	C6-C5-C4	-2.17	107.92	113.00
2	C	1	NAG	O5-C1-C2	-2.16	107.88	111.29
2	D	2	NAG	C2-N2-C7	2.08	125.86	122.90
7	B	520	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
7	B	521	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
7	B	521	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
7	A	509	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
7	A	509	NAG	C1-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
7	A	509	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
4	I	5	MAN	C4-C5-C6-O6
7	A	505	NAG	O5-C5-C6-O6
4	I	6	MAN	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
4	I	4	MAN	C4-C5-C6-O6
4	I	5	MAN	O5-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
7	A	510	NAG	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
7	A	505	NAG	C4-C5-C6-O6
7	A	509	NAG	C3-C2-N2-C7
7	B	508	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0

5.5 Carbohydrates

30 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	0.49	0	17,19,21	1.00	1 (5%)
2	NAG	C	2	2	14,14,15	0.51	0	17,19,21	1.48	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	0.95	0
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	1.14	1 (5%)
2	NAG	E	1	1,2	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
2	NAG	E	2	2	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.63	0	17,19,21	1.41	1 (5%)
3	NAG	F	2	3	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
3	BMA	F	3	3	11,11,12	0.39	0	15,15,17	0.51	0
3	MAN	F	4	3	11,11,12	0.43	0	15,15,17	2.07	2 (13%)
3	MAN	F	5	3	11,11,12	0.61	0	15,15,17	1.14	2 (13%)
2	NAG	G	1	1,2	14,14,15	0.53	0	17,19,21	0.97	1 (5%)
2	NAG	G	2	2	14,14,15	0.56	0	17,19,21	1.26	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.44	0	17,19,21	0.87	0
2	NAG	H	2	2	14,14,15	0.61	0	17,19,21	0.87	0
4	NAG	I	1	1,4	14,14,15	0.69	0	17,19,21	1.28	1 (5%)
4	NAG	I	2	4	14,14,15	0.59	0	17,19,21	0.85	1 (5%)
4	BMA	I	3	4	11,11,12	0.32	0	15,15,17	0.77	1 (6%)
4	MAN	I	4	4	11,11,12	0.61	0	15,15,17	0.66	0
4	MAN	I	5	4	11,11,12	0.59	0	15,15,17	0.99	1 (6%)
4	MAN	I	6	4	11,11,12	0.67	0	15,15,17	1.59	3 (20%)
2	NAG	J	1	1,2	14,14,15	0.54	0	17,19,21	1.02	1 (5%)
2	NAG	J	2	2	14,14,15	0.47	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	1	1,5	14,14,15	0.63	0	17,19,21	1.23	2 (11%)
5	NAG	K	2	5	14,14,15	0.48	0	17,19,21	0.74	0
5	BMA	K	3	5	11,11,12	0.44	0	15,15,17	0.89	0
6	NAG	L	1	1,6	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
6	NAG	L	2	6	14,14,15	0.54	0	17,19,21	0.93	0
6	BMA	L	3	6	11,11,12	0.53	0	15,15,17	1.50	1 (6%)
6	MAN	L	4	6	11,11,12	0.65	0	15,15,17	1.32	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	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	-	2/2/19/22	0/1/1/1
4	MAN	I	5	4	-	2/2/19/22	0/1/1/1
4	MAN	I	6	4	-	2/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	6.91	121.56	112.19
6	L	3	BMA	C1-C2-C3	4.47	115.16	109.67
3	F	1	NAG	C1-O5-C5	4.43	118.19	112.19
6	L	4	MAN	C1-C2-C3	4.10	114.70	109.67
2	C	2	NAG	O5-C1-C2	-3.84	105.22	111.29
6	L	1	NAG	C1-O5-C5	3.45	116.86	112.19
4	I	1	NAG	O5-C1-C2	-3.38	105.95	111.29
4	I	6	MAN	C2-C3-C4	3.30	116.61	110.89
4	I	6	MAN	C3-C4-C5	3.25	116.04	110.24
2	C	2	NAG	C1-C2-N2	3.06	115.71	110.49
2	G	2	NAG	O5-C1-C2	-3.03	106.50	111.29
4	I	6	MAN	C1-C2-C3	2.99	113.34	109.67
5	K	1	NAG	O5-C1-C2	-2.86	106.77	111.29
2	E	1	NAG	C1-O5-C5	2.82	116.01	112.19
2	E	2	NAG	C1-O5-C5	2.65	115.79	112.19
5	K	1	NAG	C1-O5-C5	2.56	115.66	112.19
3	F	2	NAG	O5-C1-C2	-2.51	107.32	111.29
2	G	1	NAG	O5-C1-C2	-2.49	107.36	111.29
4	I	2	NAG	O5-C1-C2	-2.40	107.49	111.29
2	C	2	NAG	C3-C4-C5	2.31	114.36	110.24
3	F	5	MAN	C1-O5-C5	2.26	115.25	112.19
4	I	5	MAN	C1-O5-C5	2.25	115.24	112.19
4	I	3	BMA	C1-O5-C5	2.21	115.19	112.19
2	J	1	NAG	C1-O5-C5	2.21	115.18	112.19
2	G	2	NAG	C4-C3-C2	-2.19	107.81	111.02
3	F	5	MAN	C1-C2-C3	2.19	112.36	109.67
3	F	4	MAN	C6-C5-C4	-2.17	107.92	113.00
2	C	1	NAG	O5-C1-C2	-2.16	107.88	111.29
2	D	2	NAG	C2-N2-C7	2.08	125.86	122.90

There are no chirality outliers.

All (31) torsion outliers are listed below:

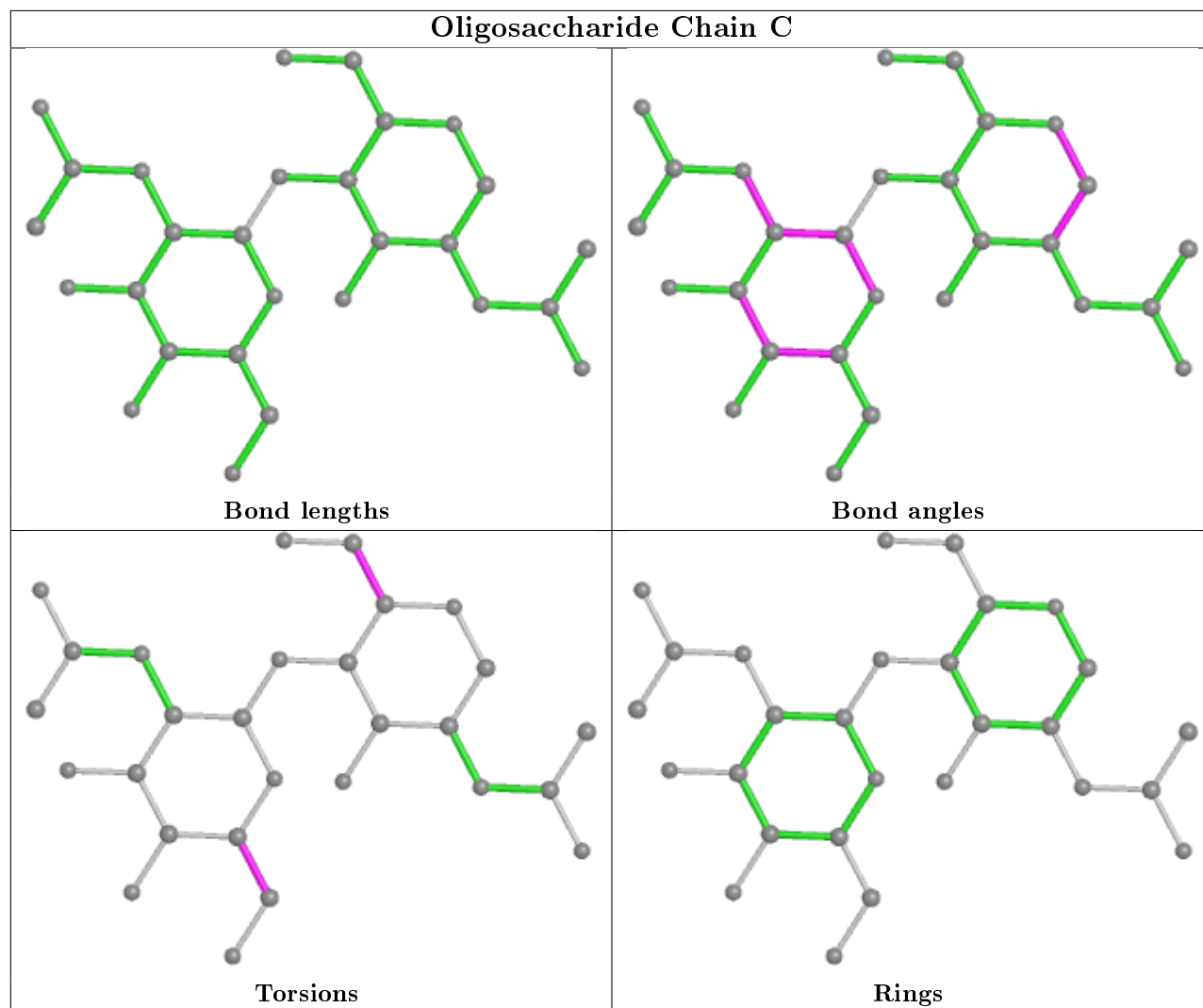
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C3-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	K	3	BMA	O5-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	I	6	MAN	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6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

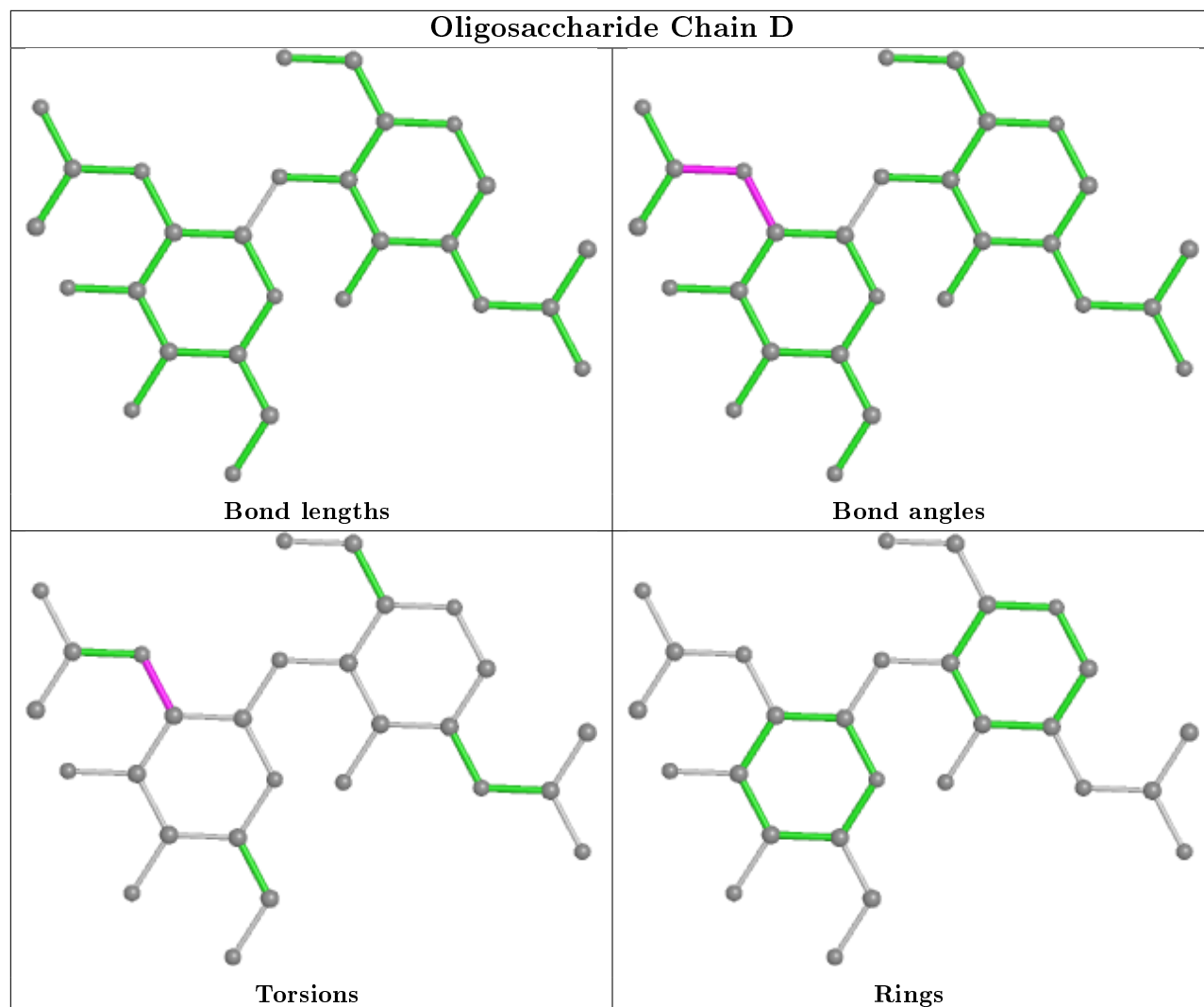
There are no ring outliers.

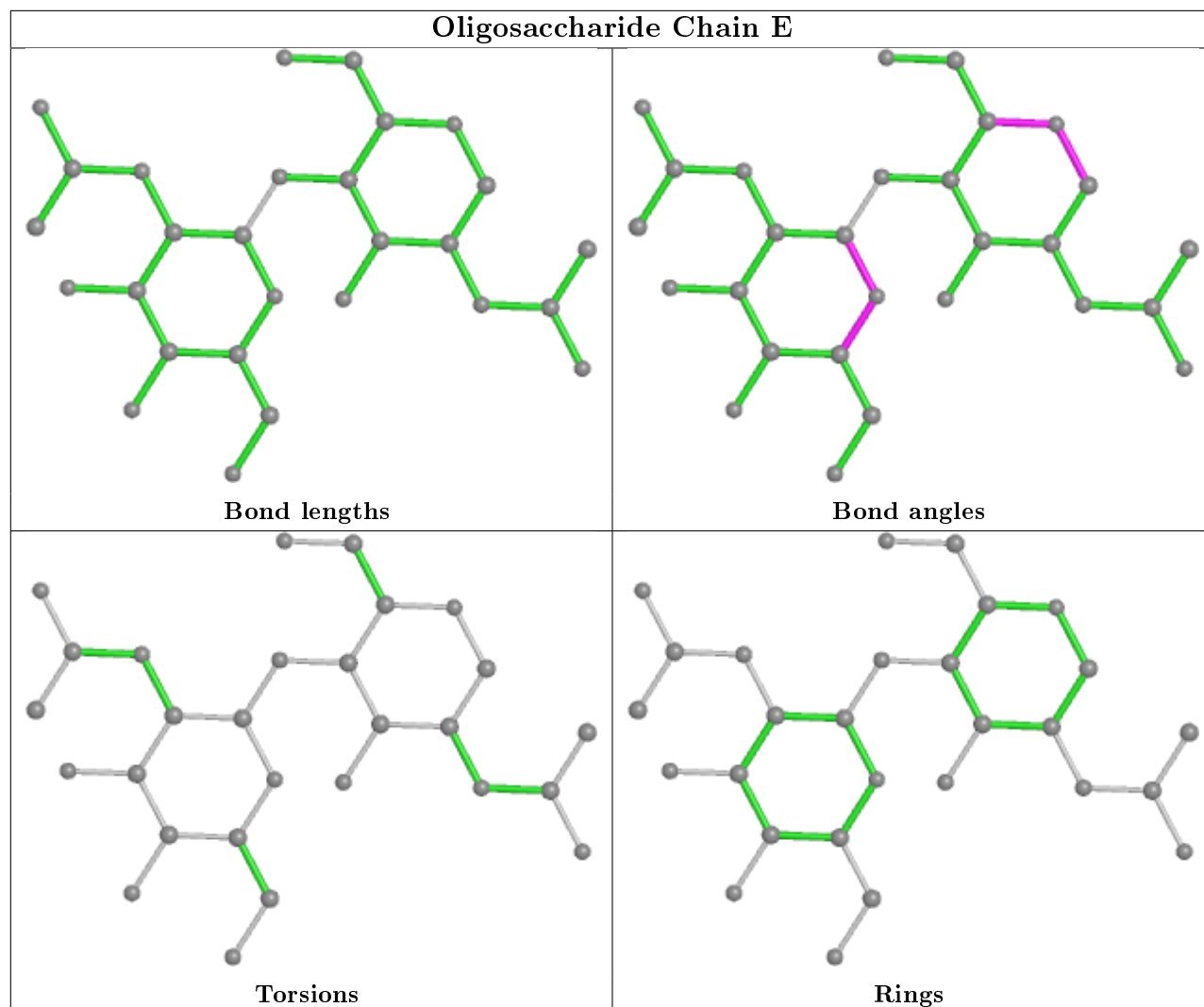
1 monomer is involved in 1 short contact:

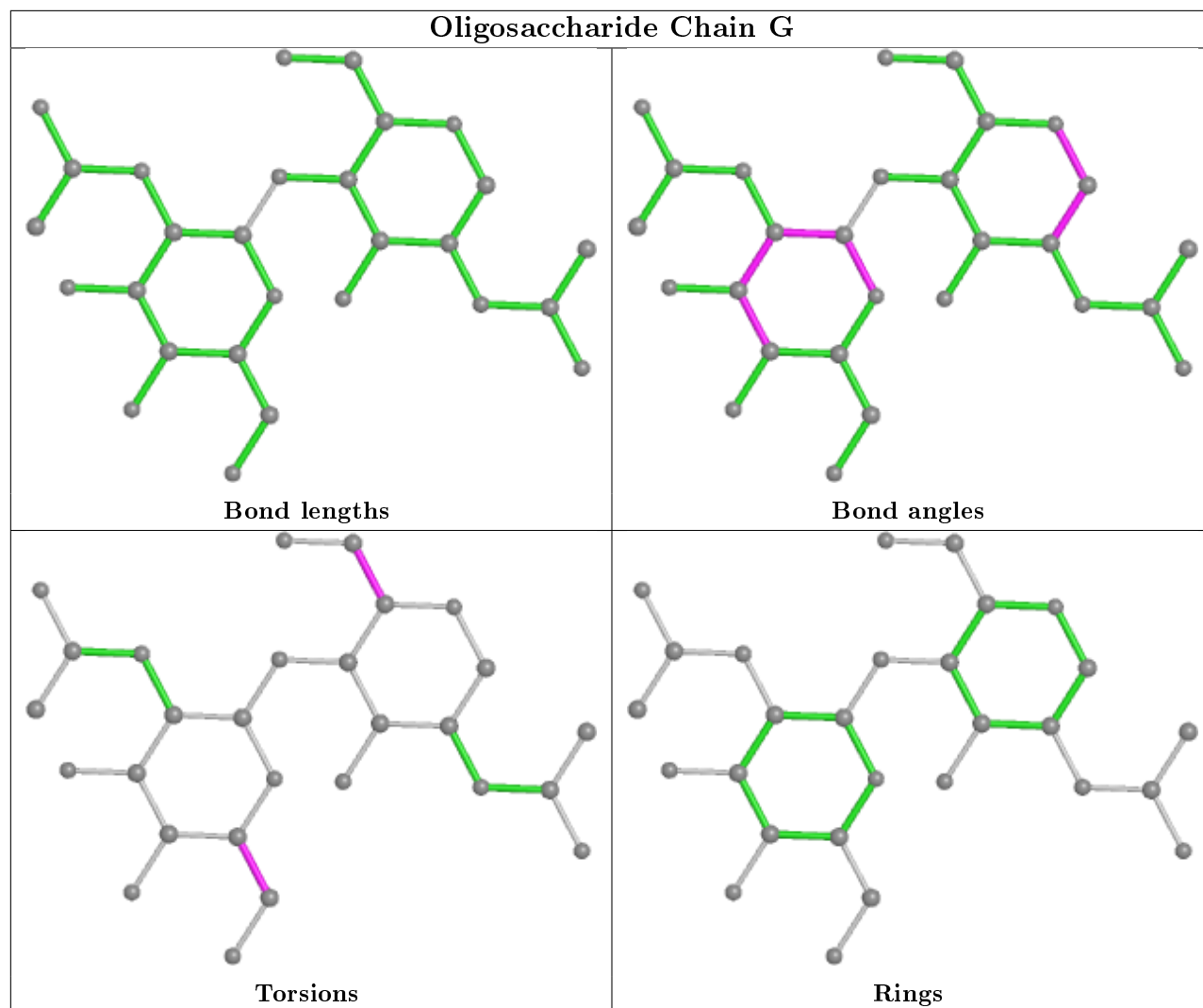
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0

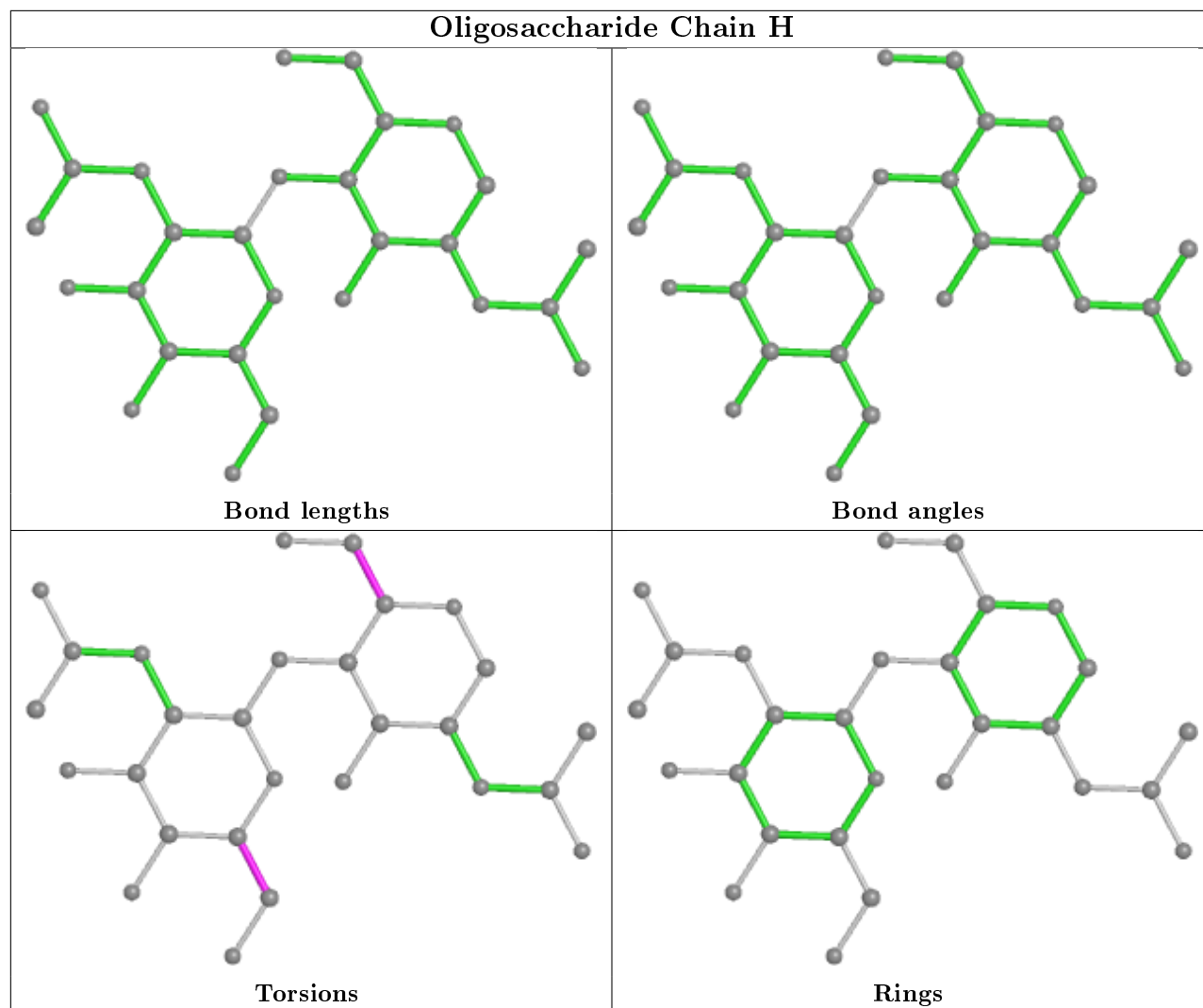
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

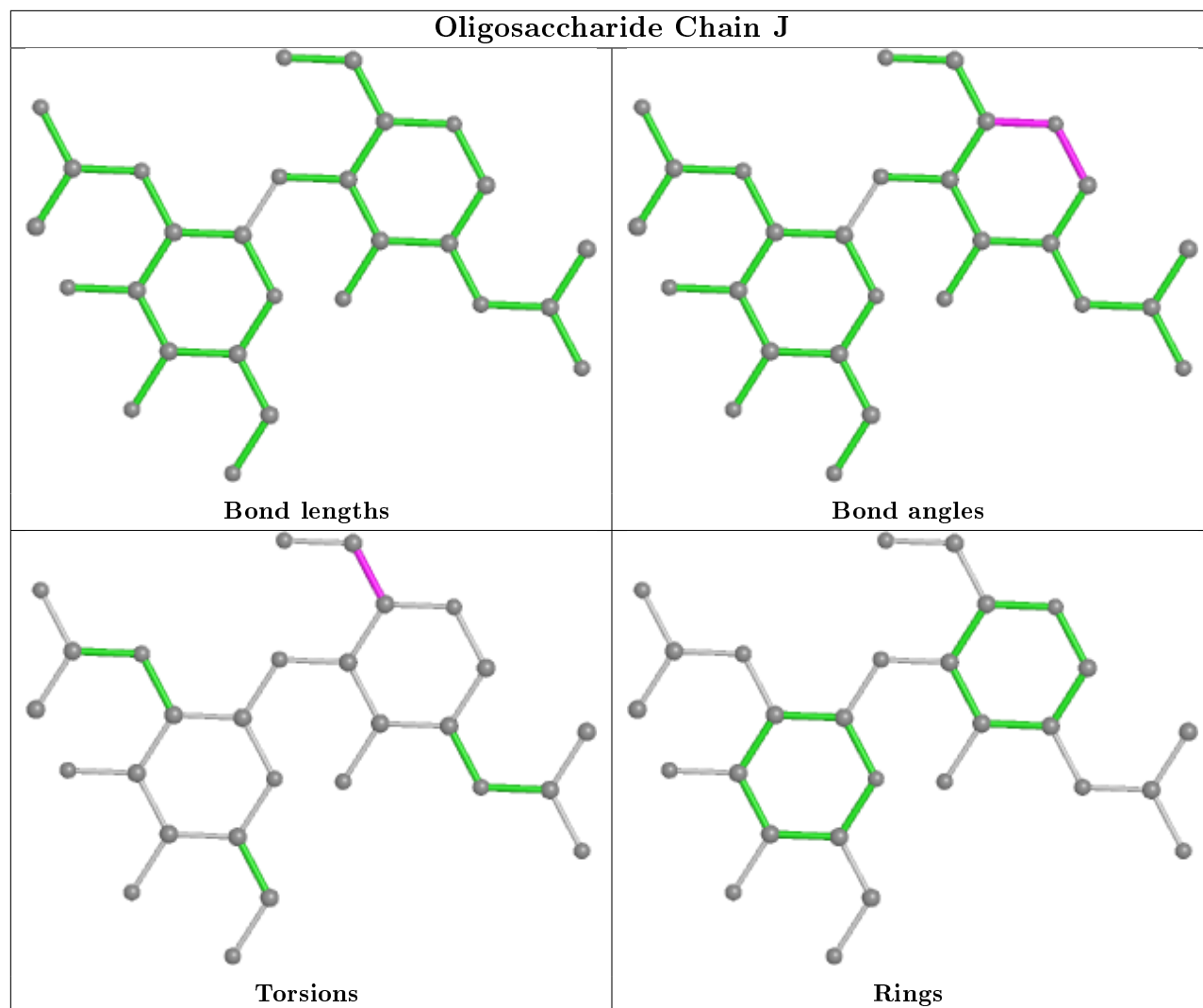


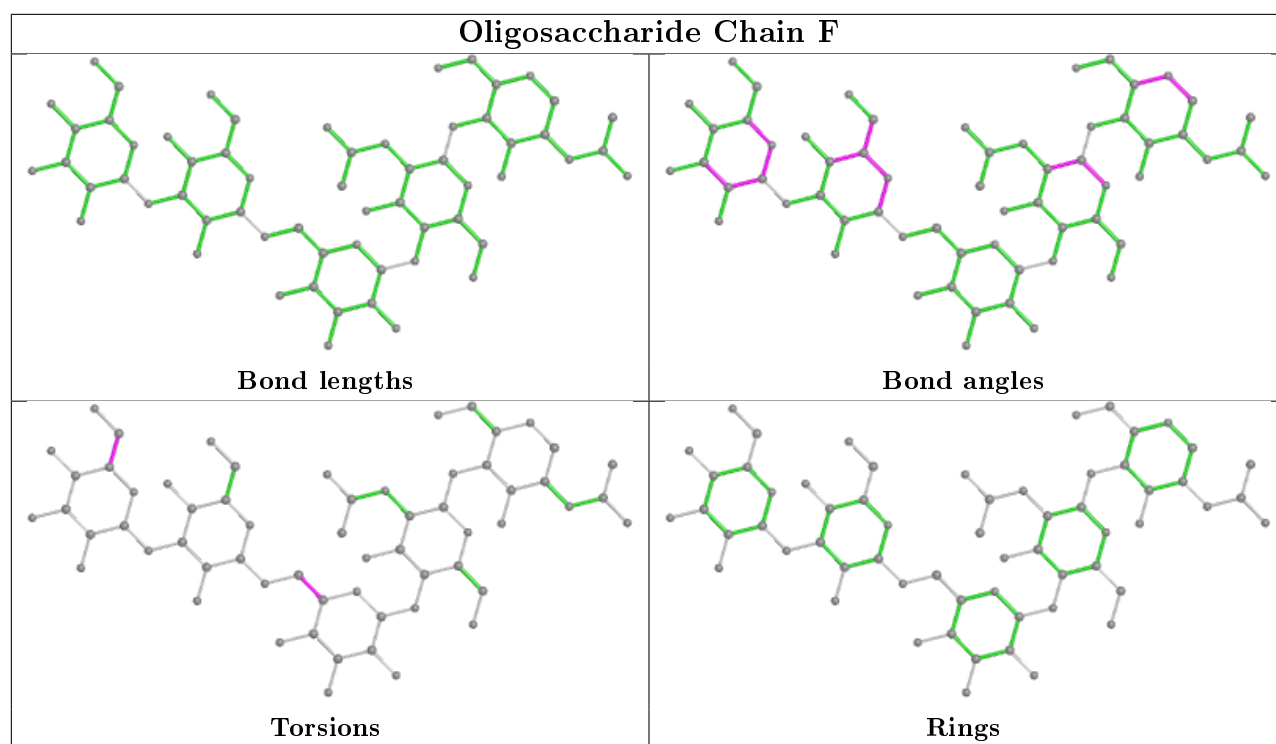


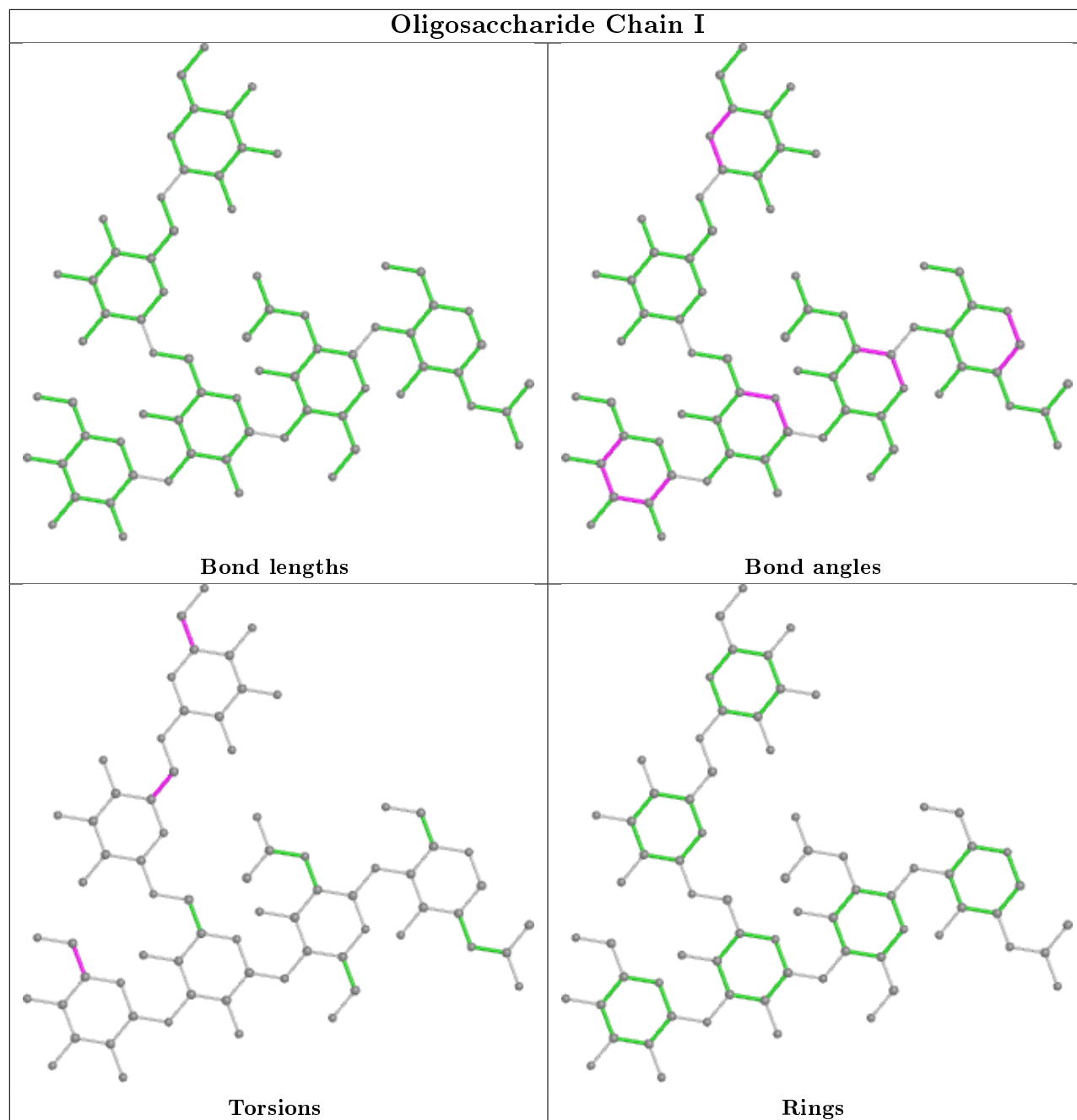


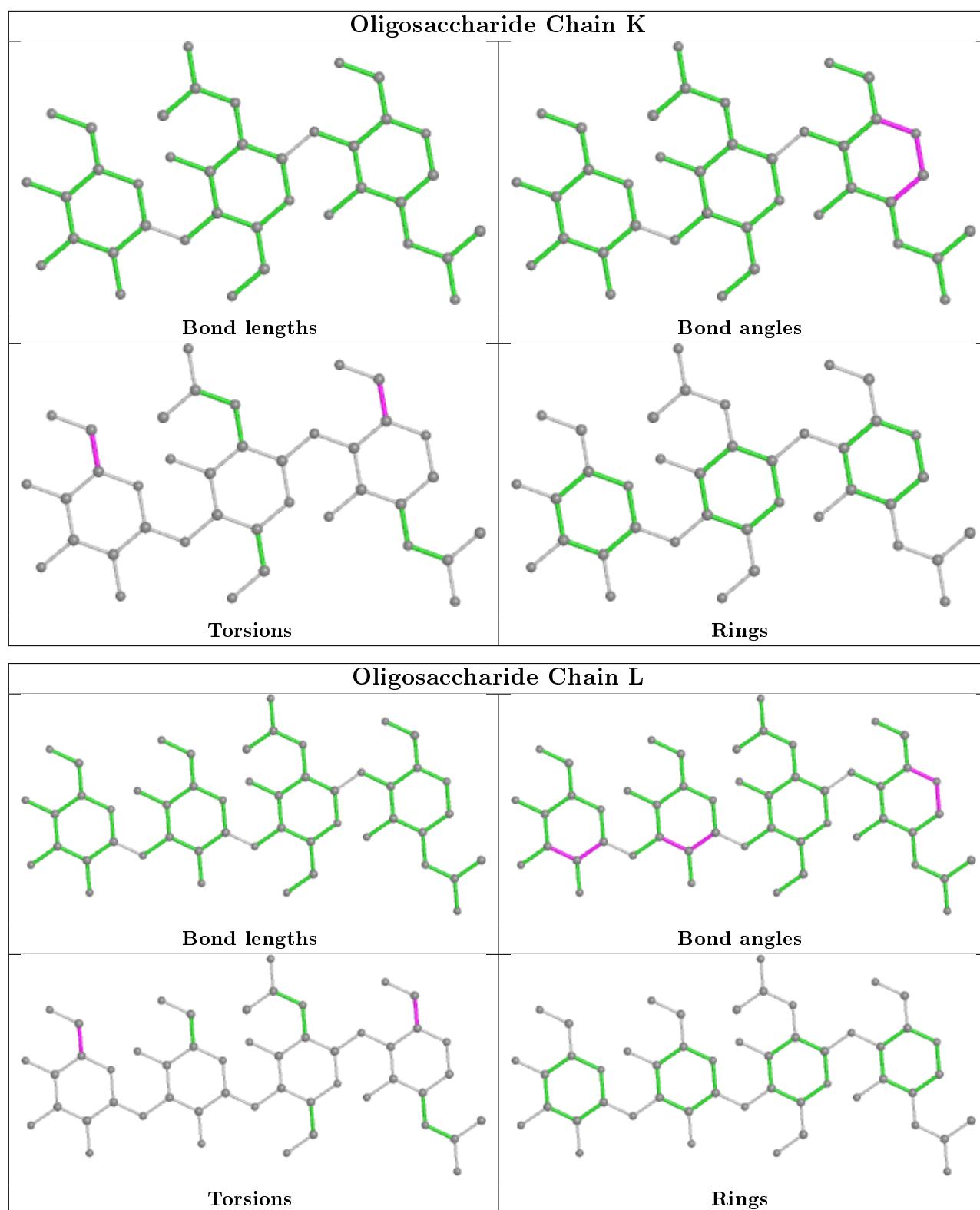












5.6 Ligand geometry [i](#)

12 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$
7	NAG	A	510	1	14,14,15	0.61	0	17,19,21	0.91	1 (5%)
7	NAG	B	515	1	14,14,15	0.42	0	17,19,21	1.49	2 (11%)
7	NAG	B	508	1	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
7	NAG	A	505	1	14,14,15	0.59	0	17,19,21	0.84	0
7	NAG	A	508	1	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
7	NAG	B	501	1	14,14,15	0.57	0	17,19,21	1.18	2 (11%)
7	NAG	B	521	1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
7	NAG	A	509	1	14,14,15	0.54	0	17,19,21	1.20	0
8	ACY	A	520	-	1,3,3	1.22	0	0,3,3	0.00	-
7	NAG	B	514	1	14,14,15	0.44	0	17,19,21	1.49	1 (5%)
7	NAG	B	520	1	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
8	ACY	B	522	-	1,3,3	1.41	0	0,3,3	0.00	-

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
7	NAG	A	510	1	-	1/6/23/26	0/1/1/1
7	NAG	B	515	1	-	0/6/23/26	0/1/1/1
7	NAG	B	508	1	-	1/6/23/26	0/1/1/1
7	NAG	A	505	1	-	2/6/23/26	0/1/1/1
7	NAG	A	508	1	-	0/6/23/26	0/1/1/1
7	NAG	B	501	1	-	0/6/23/26	0/1/1/1
7	NAG	B	521	1	-	2/6/23/26	0/1/1/1
7	NAG	A	509	1	-	4/6/23/26	0/1/1/1
7	NAG	B	514	1	-	0/6/23/26	0/1/1/1
7	NAG	B	520	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	514	NAG	C1-O5-C5	4.86	118.78	112.19
7	B	515	NAG	C1-O5-C5	4.29	118.00	112.19
7	B	521	NAG	O5-C1-C2	-3.44	105.86	111.29
7	B	508	NAG	C1-O5-C5	3.27	116.62	112.19
7	B	501	NAG	C1-O5-C5	3.26	116.61	112.19
7	B	501	NAG	O7-C7-C8	-2.37	117.66	122.06
7	B	515	NAG	C4-C3-C2	-2.33	107.61	111.02
7	A	508	NAG	C1-O5-C5	2.31	115.33	112.19
7	A	510	NAG	C1-O5-C5	2.27	115.27	112.19
7	B	520	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	521	NAG	C4-C5-C6-O6
7	B	521	NAG	O5-C5-C6-O6
7	A	509	NAG	C4-C5-C6-O6
7	A	509	NAG	C1-C2-N2-C7
7	A	509	NAG	O5-C5-C6-O6
7	A	505	NAG	O5-C5-C6-O6
7	A	510	NAG	O5-C5-C6-O6
7	A	505	NAG	C4-C5-C6-O6
7	A	509	NAG	C3-C2-N2-C7
7	B	508	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	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 ⓘ

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	342/376 (90%)	0.45	24 (7%) 16 13	28, 48, 105, 131	0
1	B	348/376 (92%)	0.33	11 (3%) 47 44	33, 52, 96, 139	0
All	All	690/752 (91%)	0.39	35 (5%) 28 25	28, 50, 103, 139	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ILE	15.6
1	A	241	THR	8.0
1	A	240	ILE	7.1
1	B	174	TYR	6.0
1	A	161	PHE	5.8
1	A	156	ALA	5.8
1	A	265	LEU	5.8
1	A	174	TYR	5.4
1	A	154	GLY	5.3
1	B	242	THR	4.9
1	A	242	THR	4.6
1	A	159	THR	4.0
1	B	266	LEU	3.8
1	B	160	ALA	3.8
1	A	155	SER	3.7
1	A	157	GLN	3.5
1	A	186	LYS	3.5
1	A	178	GLN	3.5
1	B	161	PHE	3.4
1	A	244	PHE	3.3
1	A	207	ASN	3.1
1	A	243	GLY	3.1
1	A	158	ALA	2.9
1	A	152	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	239	THR	2.8
1	A	177	PRO	2.7
1	A	376	ILE	2.6
1	A	266	LEU	2.5
1	A	185	THR	2.5
1	A	153	ASN	2.5
1	B	216	TYR	2.3
1	B	214	THR	2.2
1	A	187	VAL	2.1
1	B	238	GLU	2.0
1	B	163	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	508	14/15	0.42	0.51	109,114,122,124	0
7	NAG	A	509	14/15	0.49	0.23	90,95,102,104	0
2	NAG	H	2	14/15	0.63	0.21	89,101,111,113	0
6	MAN	L	4	11/12	0.66	0.21	106,111,117,118	0
7	NAG	A	505	14/15	0.68	0.38	95,109,119,119	0
2	NAG	C	1	14/15	0.69	0.38	96,100,108,112	0
4	MAN	I	6	11/12	0.75	0.16	69,73,76,78	0
7	NAG	A	508	14/15	0.77	0.42	100,109,119,121	0
4	MAN	I	5	11/12	0.77	0.32	78,79,85,86	0
2	NAG	D	2	14/15	0.77	0.27	70,80,85,86	0
2	NAG	C	2	14/15	0.78	0.97	116,123,129,130	0
7	NAG	B	514	14/15	0.79	0.22	77,83,89,89	0
3	MAN	F	4	11/12	0.81	0.23	103,108,112,114	0
2	NAG	E	2	14/15	0.83	0.44	74,84,92,92	0
2	NAG	H	1	14/15	0.83	0.14	85,92,98,98	0
7	NAG	B	501	14/15	0.83	0.14	72,75,78,78	0
3	MAN	F	5	11/12	0.84	0.23	94,98,102,104	0
7	NAG	B	521	14/15	0.84	0.24	93,96,101,102	0
2	NAG	G	2	14/15	0.84	0.26	67,75,83,85	0
2	NAG	J	2	14/15	0.85	0.19	67,74,79,80	0
4	MAN	I	4	11/12	0.88	0.16	69,74,76,77	0
3	NAG	F	2	14/15	0.89	0.19	70,75,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	L	2	14/15	0.89	0.20	77,81,89,90	0
7	NAG	A	510	14/15	0.90	0.15	57,64,74,77	0
5	NAG	K	2	14/15	0.90	0.21	76,83,89,92	0
2	NAG	J	1	14/15	0.92	0.21	63,66,69,69	0
7	NAG	B	515	14/15	0.92	0.15	61,69,76,77	0
2	NAG	E	1	14/15	0.92	0.34	63,69,74,75	0
7	NAG	B	520	14/15	0.92	0.15	59,62,65,65	0
2	NAG	G	1	14/15	0.94	0.13	62,65,69,69	0
2	NAG	D	1	14/15	0.95	0.15	46,49,56,61	0
5	NAG	K	1	14/15	0.96	0.13	70,75,83,83	0
4	NAG	I	2	14/15	0.96	0.17	48,51,54,57	0
4	NAG	I	1	14/15	0.96	0.15	44,47,49,49	0
6	NAG	L	1	14/15	0.96	0.13	55,62,67,72	0
3	NAG	F	1	14/15	0.97	0.14	47,53,60,65	0

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.

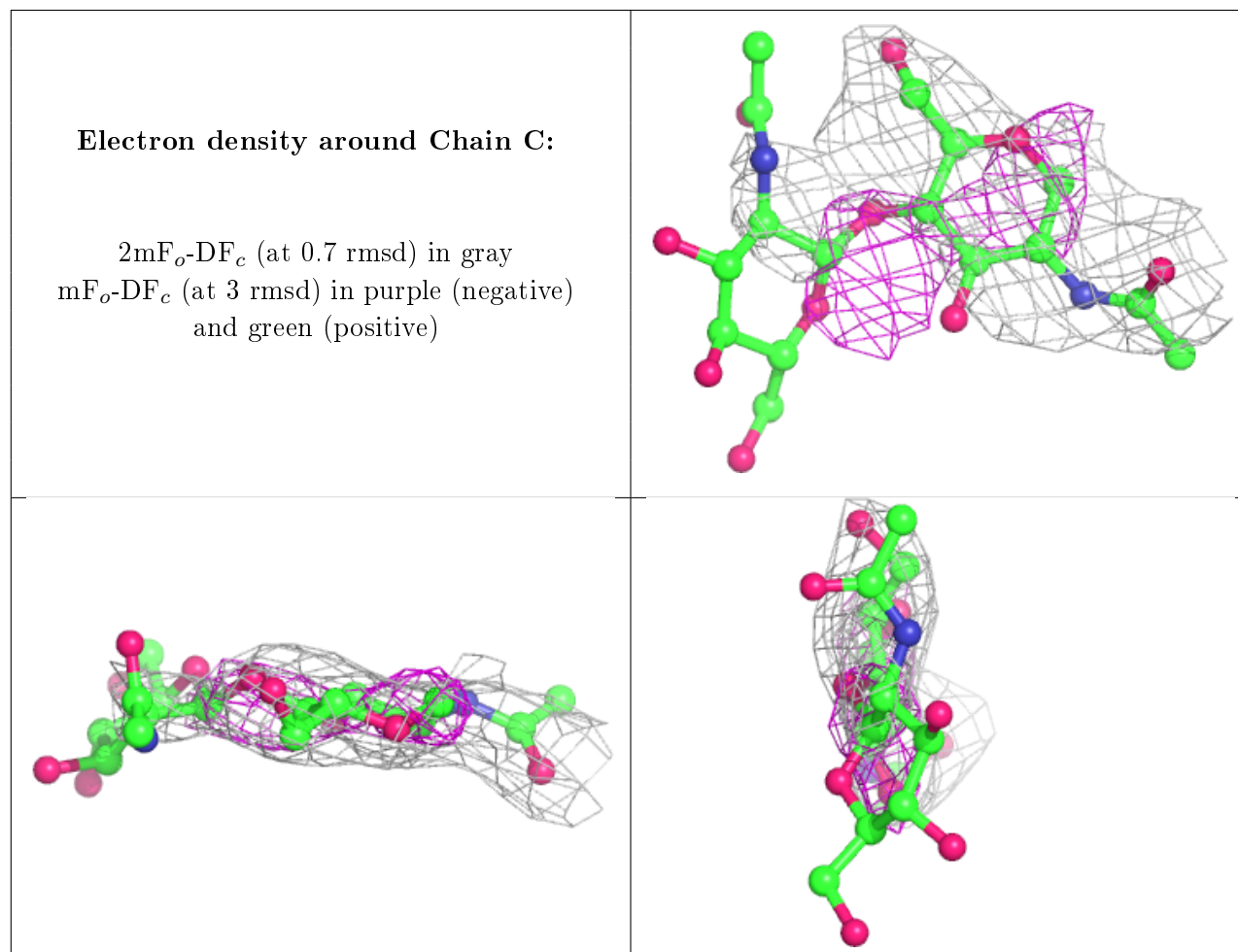
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BMA	F	3	11/12	0.55	0.40	94,102,108,110	0
2	NAG	H	2	14/15	0.63	0.21	89,101,111,113	0
6	MAN	L	4	11/12	0.66	0.21	106,111,117,118	0
2	NAG	C	1	14/15	0.69	0.38	96,100,108,112	0
6	BMA	L	3	11/12	0.71	0.17	95,103,107,111	0
5	BMA	K	3	11/12	0.74	0.21	82,85,92,95	0
4	MAN	I	6	11/12	0.75	0.16	69,73,76,78	0
2	NAG	D	2	14/15	0.77	0.27	70,80,85,86	0
4	MAN	I	5	11/12	0.77	0.32	78,79,85,86	0
2	NAG	C	2	14/15	0.78	0.97	116,123,129,130	0
3	MAN	F	4	11/12	0.81	0.23	103,108,112,114	0
2	NAG	H	1	14/15	0.83	0.14	85,92,98,98	0
2	NAG	E	2	14/15	0.83	0.44	74,84,92,92	0
2	NAG	G	2	14/15	0.84	0.26	67,75,83,85	0
3	MAN	F	5	11/12	0.84	0.23	94,98,102,104	0
2	NAG	J	2	14/15	0.85	0.19	67,74,79,80	0
4	MAN	I	4	11/12	0.88	0.16	69,74,76,77	0
3	NAG	F	2	14/15	0.89	0.19	70,75,83,87	0
6	NAG	L	2	14/15	0.89	0.20	77,81,89,90	0

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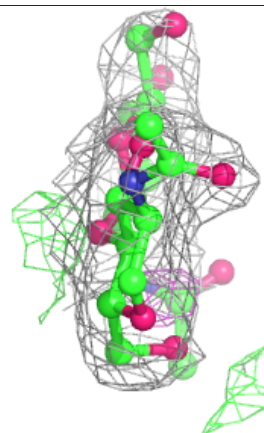
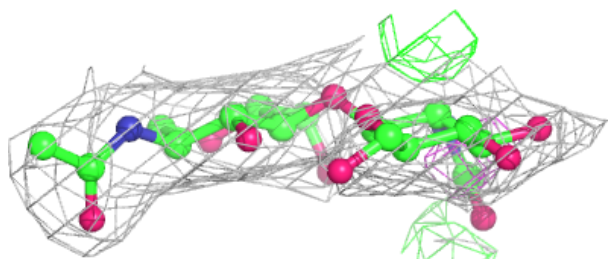
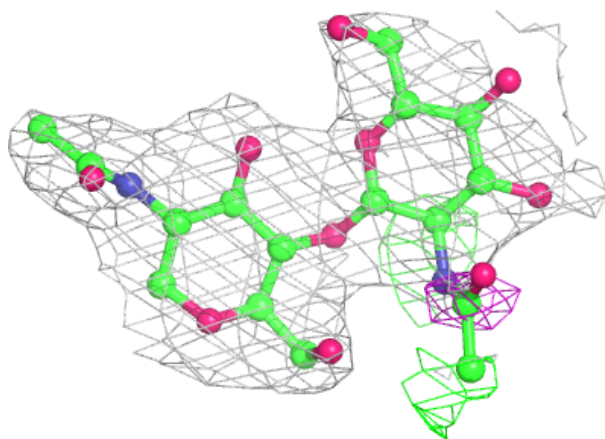
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	K	2	14/15	0.90	0.21	76,83,89,92	0
2	NAG	E	1	14/15	0.92	0.34	63,69,74,75	0
2	NAG	J	1	14/15	0.92	0.21	63,66,69,69	0
4	BMA	I	3	11/12	0.93	0.14	59,63,67,67	0
2	NAG	G	1	14/15	0.94	0.13	62,65,69,69	0
2	NAG	D	1	14/15	0.95	0.15	46,49,56,61	0
5	NAG	K	1	14/15	0.96	0.13	70,75,83,83	0
4	NAG	I	1	14/15	0.96	0.15	44,47,49,49	0
4	NAG	I	2	14/15	0.96	0.17	48,51,54,57	0
6	NAG	L	1	14/15	0.96	0.13	55,62,67,72	0
3	NAG	F	1	14/15	0.97	0.14	47,53,60,65	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



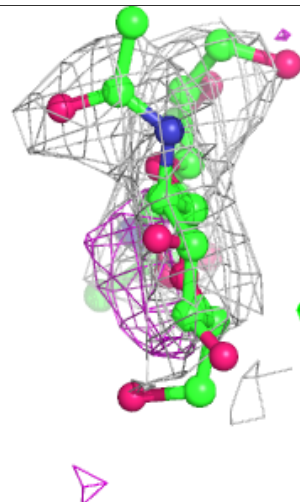
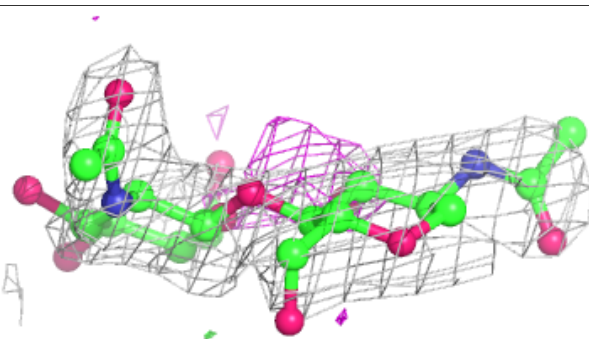
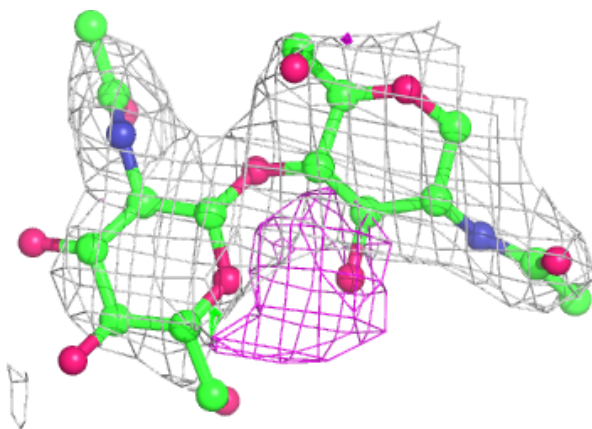
Electron density around Chain D:

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



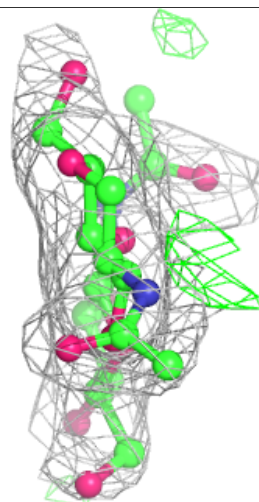
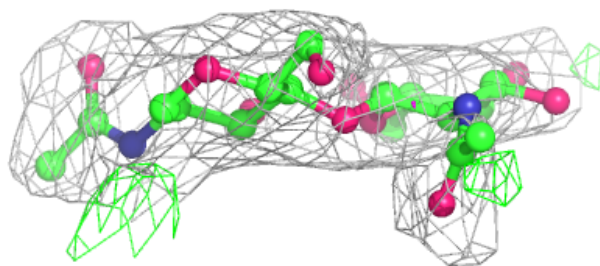
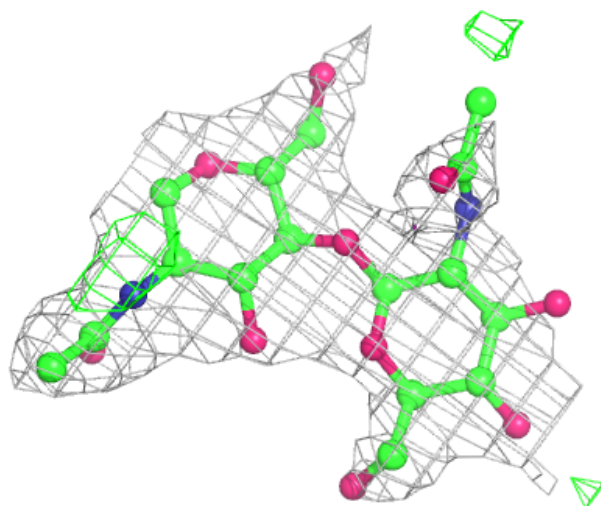
Electron density around Chain E:

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



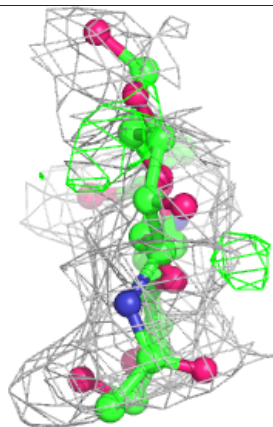
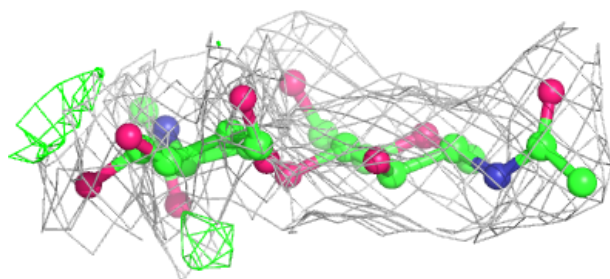
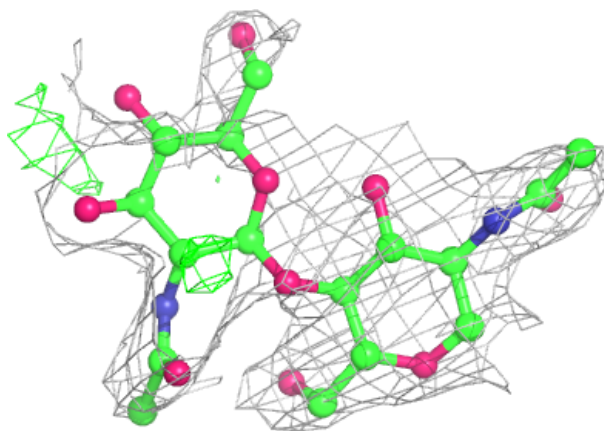
Electron density around Chain G:

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



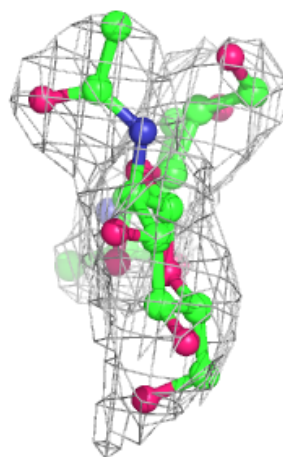
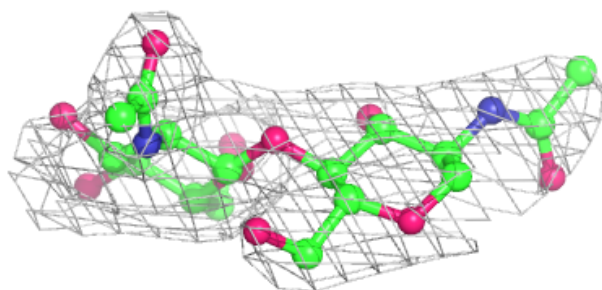
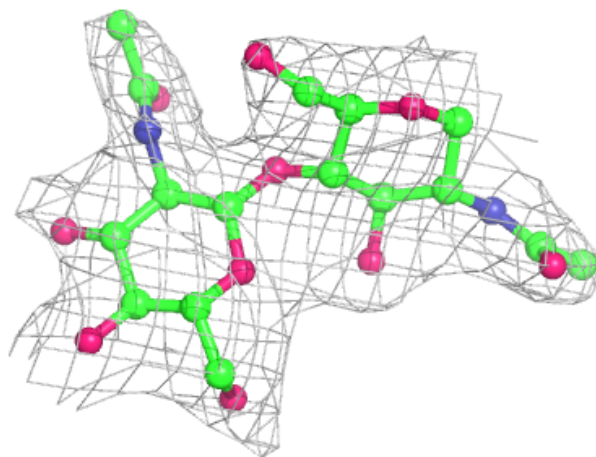
Electron density around Chain H:

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



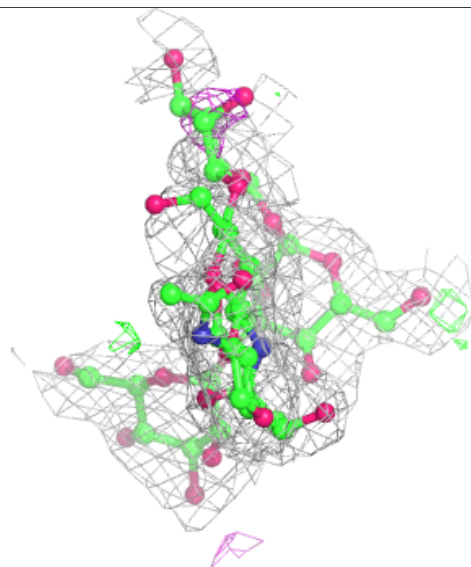
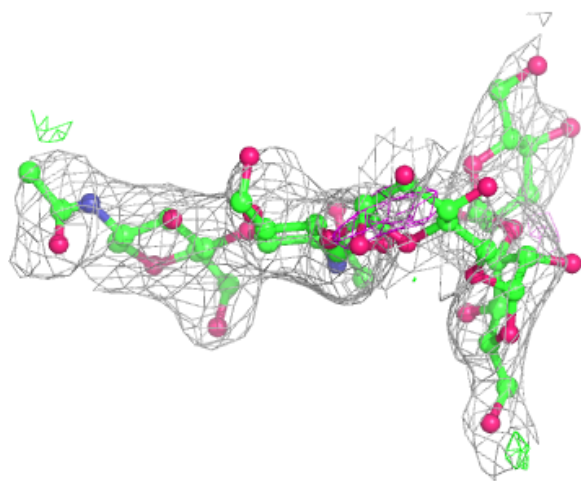
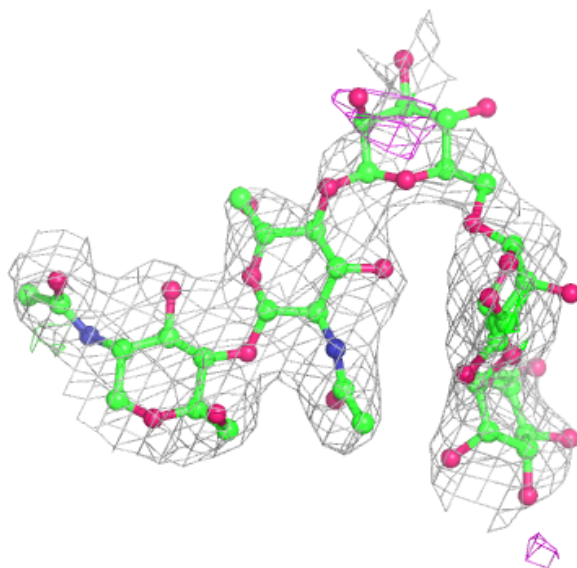
Electron density around Chain J:

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



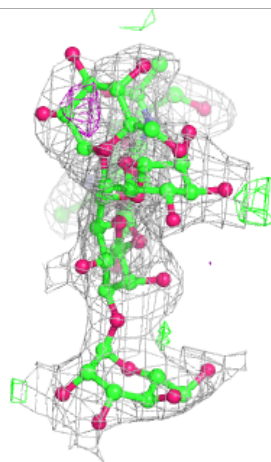
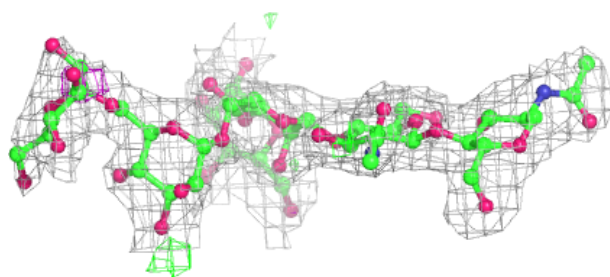
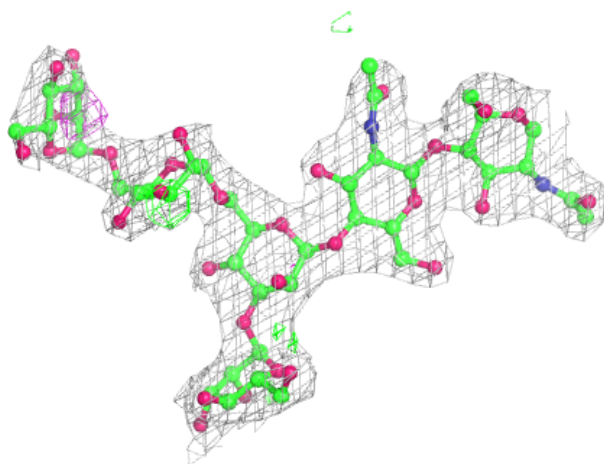
Electron density around Chain F:

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



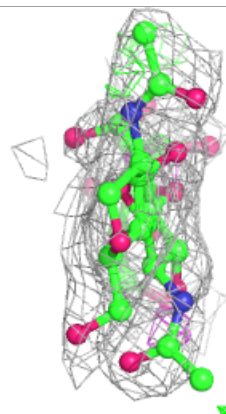
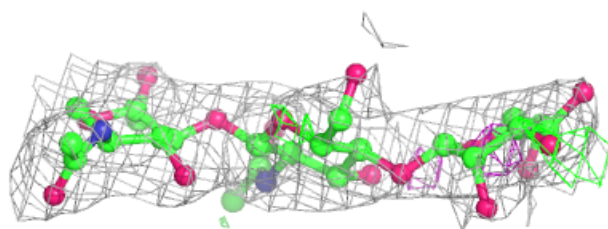
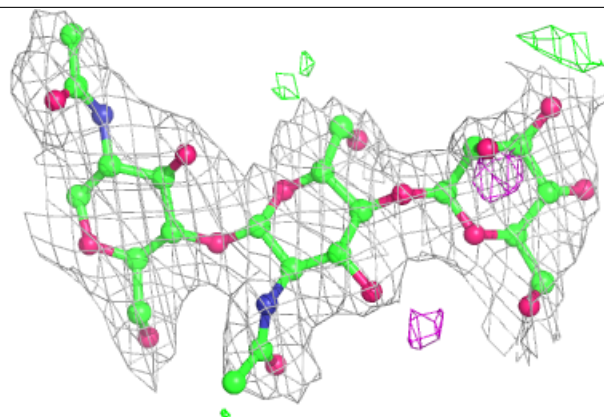
Electron density around Chain I:

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

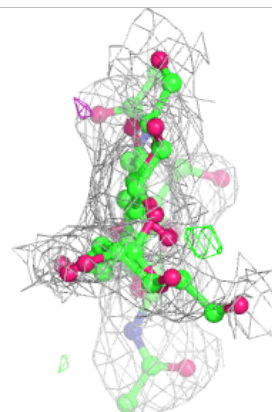
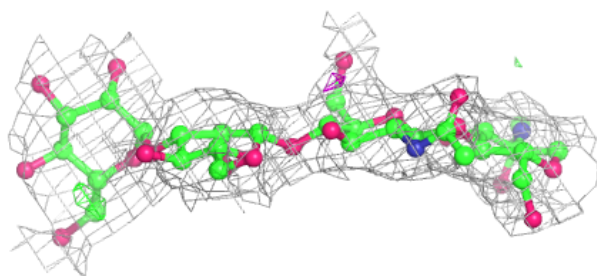
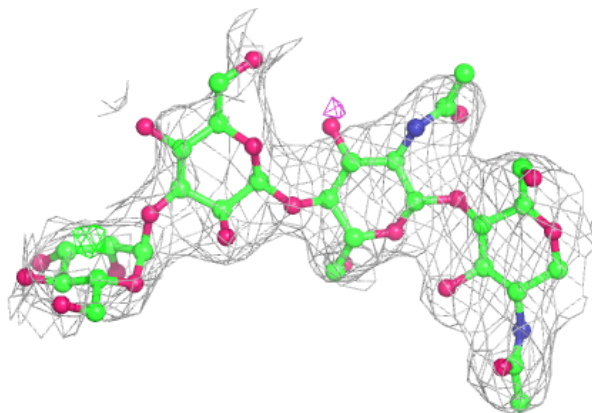


Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	508	14/15	0.42	0.51	109,114,122,124	0
7	NAG	A	509	14/15	0.49	0.23	90,95,102,104	0
7	NAG	A	505	14/15	0.68	0.38	95,109,119,119	0
7	NAG	A	508	14/15	0.77	0.42	100,109,119,121	0
7	NAG	B	514	14/15	0.79	0.22	77,83,89,89	0
7	NAG	B	501	14/15	0.83	0.14	72,75,78,78	0
7	NAG	B	521	14/15	0.84	0.24	93,96,101,102	0
7	NAG	A	510	14/15	0.90	0.15	57,64,74,77	0
7	NAG	B	515	14/15	0.92	0.15	61,69,76,77	0
7	NAG	B	520	14/15	0.92	0.15	59,62,65,65	0
8	ACY	B	522	4/4	0.95	0.26	44,45,45,45	0
8	ACY	A	520	4/4	0.97	0.20	32,32,33,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.