



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:03 PM UTC

PDB ID : 2YP1 / pdb_00002yp1
Title : Crystallization of a 45 kDa peroxygenase- peroxidase from the mushroom *Agrocybe aegerita* and structure determination by SAD utilizing only the haem iron
Authors : Piontek, K.; Strittmatter, E.; Ullrich, R.; Plattner, D.A.; Hofrichter, M.
Deposited on : 2012-10-29
Resolution : 2.31 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

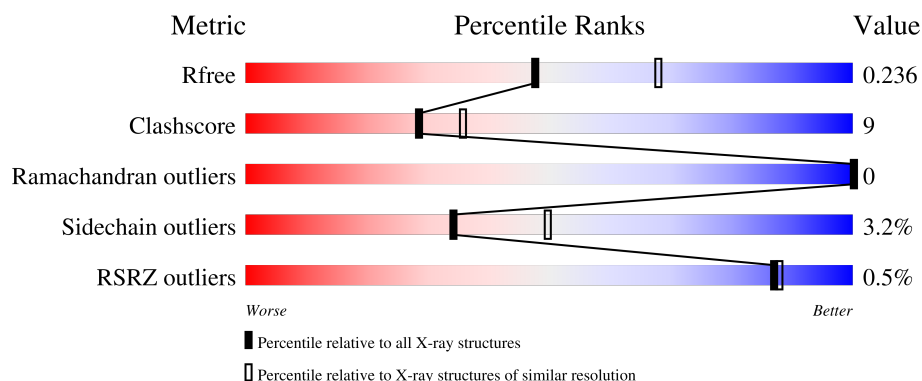
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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.



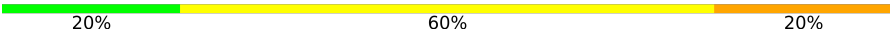
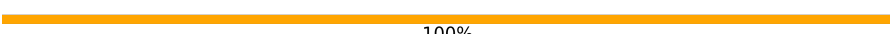
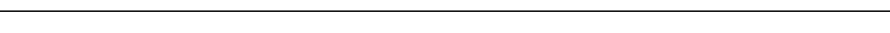
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	325	% 82% 16% ..
1	B	325	% 82% 17% .
1	C	325	89% 11% .
1	D	325	% 76% 22% ..
2	E	6	33% 67%

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Mol	Chain	Length	Quality of chain
3	F	5	
3	J	5	
4	G	2	
4	I	2	
4	K	2	
4	L	2	
4	N	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
5	H	8	
5	M	8	
6	O	3	
6	T	3	

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
10	SO4	A	1331	-	-	X	-
10	SO4	B	1331	-	-	X	-

2 Entry composition [i](#)

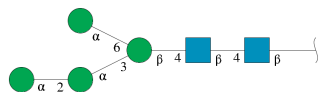
There are 12 unique types of molecules in this entry. The entry contains 12290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AROMATIC PEROXYGENASE.

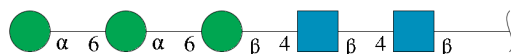
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2506	1589	434	475	8			
1	B	324	Total	C	N	O	S	0	4	0
			2537	1608	442	479	8			
1	C	325	Total	C	N	O	S	0	1	0
			2526	1599	440	479	8			
1	D	323	Total	C	N	O	S	0	1	0
			2507	1590	435	474	8			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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			

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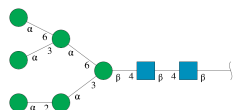
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



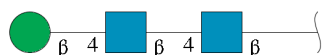
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	8	Total	C	N	O	0	0	0
			94	52	2	40			

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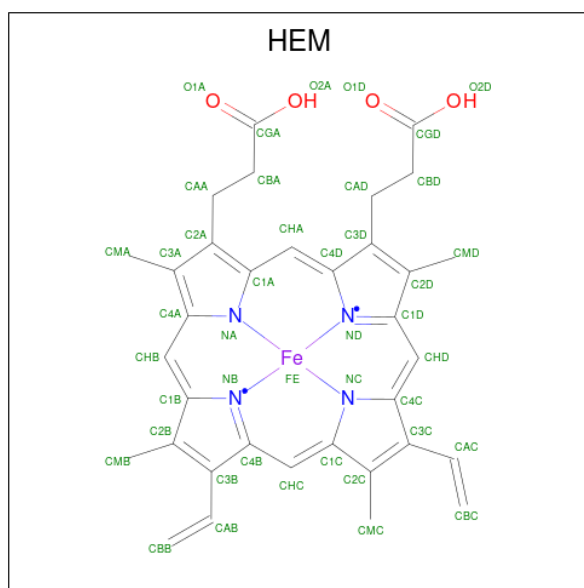
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



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

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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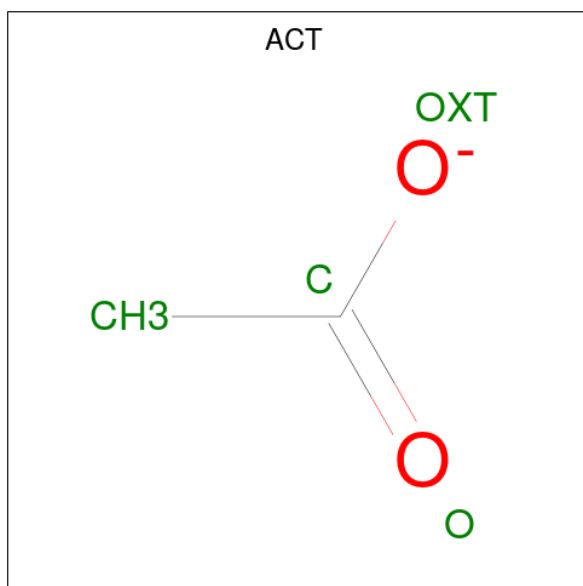
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg		
			1	1	0	0
8	B	1	Total	Mg		
			1	1	0	0
8	C	1	Total	Mg		
			1	1	0	0
8	D	1	Total	Mg		
			1	1	0	0

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



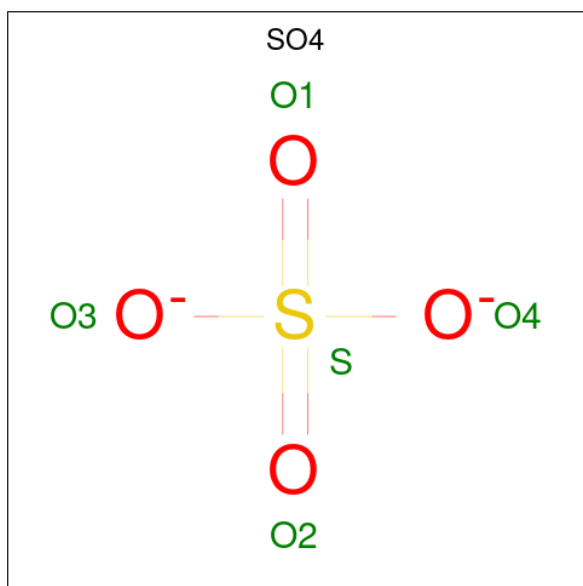
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O		
			4	2	2	0	0
9	B	1	Total	C	O		
			4	2	2	0	0
9	C	1	Total	C	O		
			4	2	2	0	0
9	C	1	Total	C	O		
			4	2	2	0	0

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

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



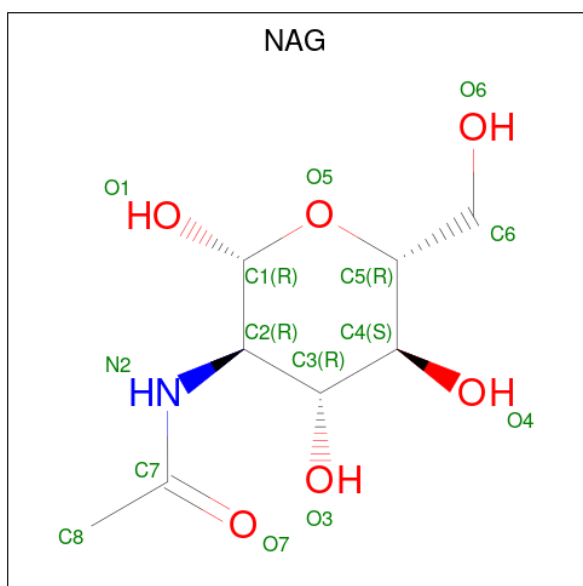
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	327	Total	O	0	0
			327	327		
12	B	369	Total	O	0	0
			369	369		

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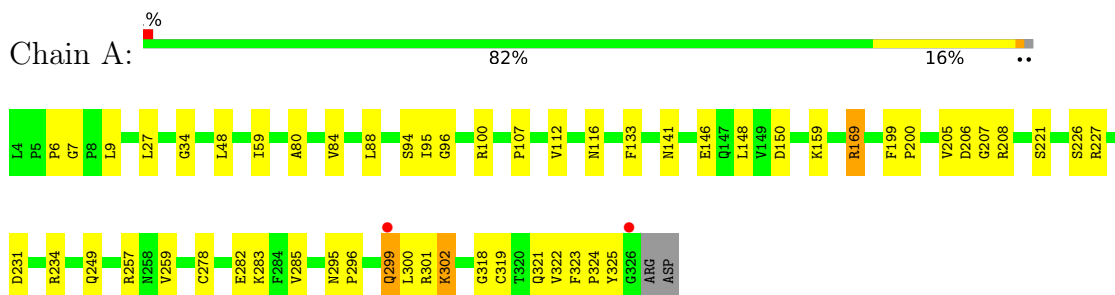
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	291	Total 291	O 291	0	0
12	D	198	Total 198	O 198	0	0

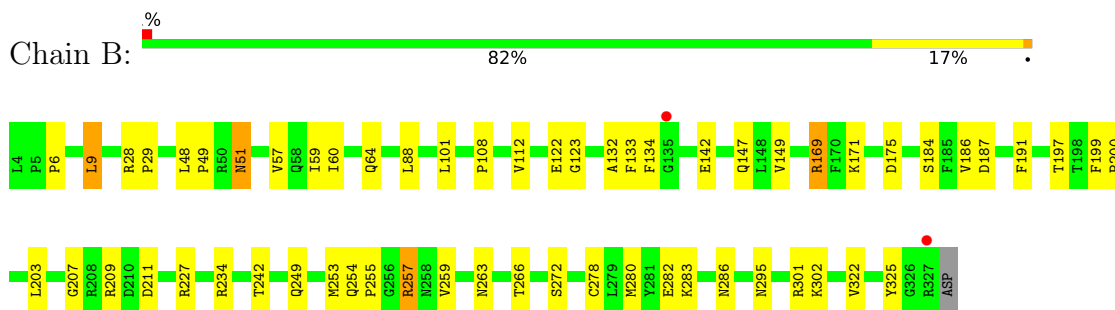
3 Residue-property plots

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.

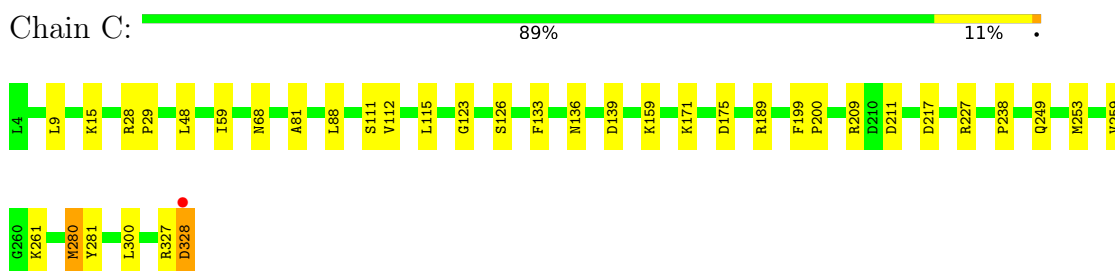
• Molecule 1: AROMATIC PEROXYGENASE



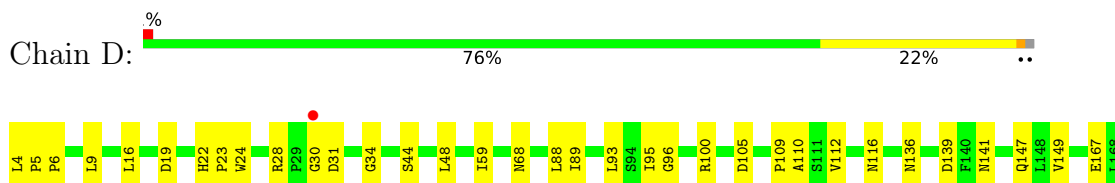
• Molecule 1: AROMATIC PEROXYGENASE

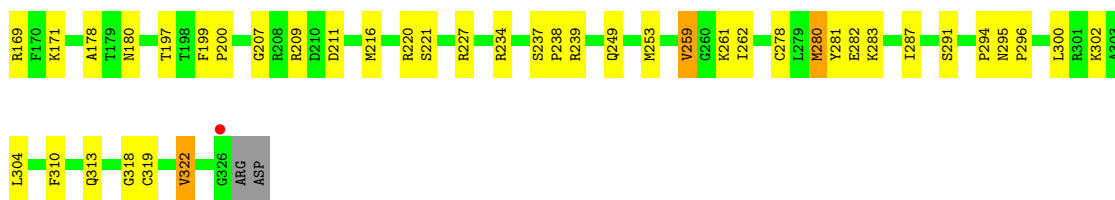


• Molecule 1: AROMATIC PEROXYGENASE



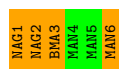
• Molecule 1: AROMATIC PEROXYGENASE





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

Chain E: 33% 67%



- Molecule 3: alpha-D-mannopyranose-(1-6)-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% 60% 20%



- Molecule 3: alpha-D-mannopyranose-(1-6)-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 J: 40% 60%



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

Chain G: 100%



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

Chain I: 100%



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

Chain K:  100%

NAG1
NAG2

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

Chain L:  50% 50%

NAG1
NAG2

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

Chain N:  100%

NAG1
NAG2

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

Chain P:  50% 50%

NAG1
NAG2

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

Chain Q:  50% 50%

NAG1
NAG2

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

Chain R:  100%

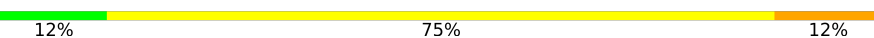
NAG1
NAG2

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

Chain S:  50% 50%

NAG1
NAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 H:  12% 75% 12%

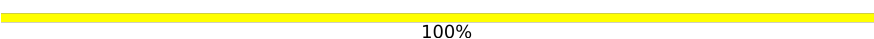


- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  12% 62% 25%

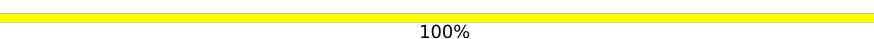


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



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

Chain T:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.75Å 144.88Å 134.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.31 48.91 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-2.31) 99.7 (48.91-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.230 (Not available) , 0.236	Depositor DCC
R_{free} test set	4851 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12290	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.95% 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: BMA, NAG, ACT, MG, MAN, SO4, HEM

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	0.61	0/2579	0.82	4/3512 (0.1%)
1	B	0.66	1/2619 (0.0%)	0.85	0/3564
1	C	0.63	0/2599	0.80	0/3538
1	D	0.56	0/2580	0.78	2/3513 (0.1%)
All	All	0.61	1/10377 (0.0%)	0.81	6/14127 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	PRO	CA-C	5.33	1.54	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	PRO	CA-C-N	6.20	124.19	119.66
1	A	107	PRO	C-N-CA	6.20	124.19	119.66
1	D	105	ASP	CA-C-N	5.31	125.85	120.38
1	D	105	ASP	C-N-CA	5.31	125.85	120.38
1	A	7	GLY	CA-C-N	5.04	125.32	119.92
1	A	7	GLY	C-N-CA	5.04	125.32	119.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	30	GLY	Peptide

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	2506	0	2386	42	0
1	B	2537	0	2426	47	0
1	C	2526	0	2405	24	0
1	D	2507	0	2390	54	0
2	E	72	0	61	2	0
3	F	61	0	52	2	0
3	J	61	0	52	2	0
4	G	28	0	25	3	0
4	I	28	0	25	3	0
4	K	28	0	25	2	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
5	H	94	0	79	4	0
5	M	94	0	79	2	0
6	O	39	0	34	0	0
6	T	39	0	34	0	0
7	A	43	0	30	5	0
7	B	43	0	30	3	0
7	C	43	0	30	3	0
7	D	43	0	30	3	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	4	0	3	0	0
9	B	4	0	3	0	0
9	C	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	4	0	3	0	0
10	A	20	0	0	3	0
10	B	15	0	0	2	0
10	C	20	0	0	0	0
10	D	10	0	0	2	0
11	C	14	0	13	1	0
11	D	42	0	39	0	0
12	A	327	0	0	7	0
12	B	369	0	0	14	0
12	C	291	0	0	5	0
12	D	198	0	0	6	0
All	All	12290	0	10410	189	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 9.

All (189) 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)
7:D:350:HEM:HMC2	7:D:350:HEM:HBC2	1.29	1.11
1:A:259:VAL:HG23	1:A:259:VAL:O	1.68	0.94
1:A:299:GLN:HG2	12:A:2271:HOH:O	1.73	0.88
1:A:299:GLN:NE2	12:A:2273:HOH:O	2.07	0.88
1:D:89:ILE:HD11	1:D:300:LEU:HD13	1.56	0.88
1:A:283:LYS:NZ	12:A:2252:HOH:O	2.00	0.87
7:D:350:HEM:HBC2	7:D:350:HEM:CMC	2.02	0.85
1:D:100:ARG:N	10:D:1328:SO4:O1	2.13	0.81
1:D:259:VAL:O	1:D:259:VAL:CG1	2.29	0.81
1:B:278:CYS:HB2	10:B:1331:SO4:O2	1.81	0.80
5:H:6:MAN:C6	5:H:8:MAN:H3	2.11	0.80
1:D:296:PRO:HB2	1:D:300:LEU:HB3	1.65	0.79
5:H:6:MAN:H62	5:H:8:MAN:H3	1.66	0.76
7:A:350:HEM:HBC2	7:A:350:HEM:HHD	1.68	0.74
1:B:134:PHE:CD1	3:J:2:NAG:H62	2.21	0.74
1:B:282:GLU:HG3	1:B:322:VAL:HG11	1.69	0.74
1:D:253:MET:HE3	1:D:253:MET:HA	1.70	0.73
1:D:282:GLU:HG2	1:D:322:VAL:HG11	1.71	0.71
1:B:302:LYS:HE3	12:B:2319:HOH:O	1.91	0.70
12:B:2351:HOH:O	4:K:2:NAG:O6	2.08	0.70
1:B:254:GLN:NE2	12:B:2267:HOH:O	2.25	0.69
5:M:6:MAN:H62	5:M:8:MAN:H3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG12	1:B:259:VAL:O	1.90	0.69
1:A:133:PHE:CE1	4:G:1:NAG:H82	2.27	0.68
1:D:5:PRO:O	12:D:2003:HOH:O	2.11	0.68
1:D:31:ASP:N	12:D:2024:HOH:O	2.27	0.67
1:D:259:VAL:O	1:D:259:VAL:HG13	1.94	0.67
1:A:112:VAL:HG12	1:A:112:VAL:O	1.97	0.65
1:D:167:GLU:OE2	12:D:2103:HOH:O	2.14	0.64
1:A:48:LEU:HD21	1:A:59:ILE:HA	1.80	0.64
1:B:263:ASN:ND2	12:B:2277:HOH:O	2.16	0.63
1:D:147:GLN:OE1	1:D:171:LYS:HE3	1.98	0.63
1:D:88:LEU:HD23	1:D:304:LEU:HG	1.80	0.63
1:D:291:SER:HB2	12:D:2158:HOH:O	1.99	0.62
1:A:249:GLN:NE2	1:C:249:GLN:OE1	2.33	0.61
1:C:227:ARG:CD	12:C:2199:HOH:O	2.49	0.61
1:C:280:MET:HE2	1:C:280:MET:C	2.26	0.60
1:A:299:GLN:HE21	1:A:299:GLN:HA	1.66	0.60
1:A:206:ASP:OD2	12:A:2183:HOH:O	2.16	0.60
1:D:96:GLY:HA2	1:D:116:ASN:ND2	2.17	0.59
1:C:259:VAL:HG12	1:C:259:VAL:O	2.02	0.58
1:B:249:GLN:OE1	12:B:2261:HOH:O	2.17	0.58
1:D:180:ASN:C	1:D:180:ASN:OD1	2.45	0.58
1:D:310:PHE:O	1:D:313[A]:GLN:HB2	2.03	0.58
1:B:278:CYS:HB2	10:B:1331:SO4:S	2.44	0.57
1:B:147:GLN:NE2	1:B:171:LYS:HE2	2.19	0.57
1:C:327:ARG:O	1:C:328:ASP:HB2	2.05	0.57
1:C:123:GLY:HA3	1:C:189:ARG:HD3	1.87	0.57
1:C:171:LYS:HE2	1:C:175:ASP:OD1	2.05	0.56
1:C:209:ARG:HD2	1:C:211:ASP:OD2	2.05	0.56
7:C:350:HEM:CMC	7:C:350:HEM:HBC2	2.36	0.56
1:A:208:ARG:NH2	1:A:231:ASP:O	2.39	0.56
1:B:184:SER:HA	1:B:257[A]:ARG:HB3	1.88	0.56
1:D:4:LEU:N	12:D:2002:HOH:O	2.38	0.56
1:A:259:VAL:O	1:A:259:VAL:CG2	2.42	0.55
7:A:350:HEM:HHH	7:A:350:HEM:CBC	2.37	0.55
1:D:5:PRO:HD3	1:D:310:PHE:CE1	2.41	0.55
1:D:209:ARG:HD2	1:D:211:ASP:OD2	2.07	0.54
5:M:6:MAN:H62	5:M:8:MAN:C3	2.36	0.54
1:B:254:GLN:HB3	1:B:255:PRO:HD2	1.89	0.54
4:I:1:NAG:C6	4:I:2:NAG:C1	2.83	0.54
1:C:48:LEU:HD21	1:C:59:ILE:HA	1.90	0.54
1:B:6:PRO:HD3	1:B:57:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:O	1:B:49:PRO:C	2.51	0.53
12:B:2100:HOH:O	1:D:313[B]:GLN:HG3	2.08	0.53
1:B:191:PHE:HB2	12:B:2090:HOH:O	2.07	0.53
1:A:296:PRO:HG2	1:A:301:ARG:HB2	1.89	0.53
1:D:16:LEU:HG	1:D:19:ASP:HB3	1.90	0.53
1:A:282:GLU:HG3	1:A:322:VAL:HG21	1.91	0.53
1:D:278:CYS:HB2	10:D:1329:SO4:O3	2.09	0.53
4:G:1:NAG:H61	4:G:2:NAG:C7	2.39	0.52
4:I:1:NAG:H62	4:I:2:NAG:C1	2.39	0.52
1:A:100:ARG:HD2	12:A:2099:HOH:O	2.10	0.52
1:B:207:GLY:HA3	1:B:234:ARG:O	2.10	0.52
1:A:207:GLY:HA3	1:A:234:ARG:O	2.10	0.51
7:D:350:HEM:HMC2	7:D:350:HEM:CBC	2.20	0.51
7:B:350:HEM:HHC	7:B:350:HEM:HBB2	1.91	0.51
1:D:68:ASN:O	1:D:238:PRO:HA	2.10	0.51
5:H:6:MAN:C6	5:H:8:MAN:C3	2.67	0.51
1:A:278:CYS:HB2	10:A:1331:SO4:O1	2.10	0.51
1:A:285:VAL:CG1	1:A:324:PRO:HD3	2.41	0.51
7:A:350:HEM:HBC2	7:A:350:HEM:CHD	2.37	0.51
1:D:282:GLU:HG2	1:D:322:VAL:CG1	2.39	0.51
1:D:259:VAL:O	1:D:259:VAL:HG12	2.06	0.50
1:D:112:VAL:HG12	1:D:112:VAL:O	2.11	0.50
1:D:48:LEU:HD21	1:D:59:ILE:HA	1.94	0.50
1:D:24:TRP:CG	1:D:227:ARG:HG3	2.47	0.49
1:B:9:LEU:HD13	1:B:64:GLN:HB3	1.94	0.49
1:B:48:LEU:HD21	1:B:59:ILE:HA	1.94	0.49
7:C:350:HEM:HBC2	7:C:350:HEM:HMC1	1.95	0.49
1:D:237:SER:O	1:D:239:ARG:NE	2.43	0.49
4:I:1:NAG:H62	4:I:2:NAG:O5	2.13	0.49
1:A:27:LEU:N	12:A:2028:HOH:O	2.30	0.49
1:B:112:VAL:O	1:B:112:VAL:HG12	2.11	0.48
1:C:126:SER:OG	7:C:350:HEM:O2A	2.31	0.48
1:C:227:ARG:HD2	12:C:2199:HOH:O	2.12	0.48
1:B:51:ASN:H	1:B:51:ASN:HD22	1.60	0.48
1:D:318:GLY:O	1:D:319:CYS:HB2	2.12	0.48
1:B:283:LYS:NZ	12:B:2282:HOH:O	2.34	0.48
1:D:136:ASN:ND2	1:D:139:ASP:OD2	2.35	0.48
1:D:109:PRO:O	1:D:110:ALA:C	2.56	0.48
1:B:28:ARG:HB3	1:B:29:PRO:CD	2.44	0.47
1:D:22:HIS:N	1:D:23:PRO:CD	2.77	0.47
1:D:199:PHE:N	1:D:200:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ARG:O	12:D:2024:HOH:O	2.20	0.47
1:B:259:VAL:O	1:B:259:VAL:CG1	2.61	0.47
1:B:266:THR:HA	12:B:2278:HOH:O	2.14	0.47
1:D:207:GLY:HA3	1:D:234:ARG:O	2.14	0.47
1:B:60:ILE:O	1:B:64:GLN:HG3	2.15	0.47
1:C:28:ARG:HB3	1:C:29:PRO:HD2	1.96	0.47
1:D:280:MET:HE2	1:D:281:TYR:N	2.29	0.47
1:A:301:ARG:NH2	1:A:325:TYR:O	2.43	0.47
1:D:280:MET:CE	1:D:280:MET:C	2.88	0.47
1:B:249:GLN:NE2	1:D:249:GLN:OE1	2.44	0.47
2:E:3:BMA:C6	2:E:6:MAN:O2	2.62	0.47
1:A:133:PHE:CD1	4:G:1:NAG:H82	2.49	0.46
1:B:203:LEU:HD13	7:B:350:HEM:CBC	2.45	0.46
1:B:171:LYS:HE3	1:B:175:ASP:OD1	2.15	0.46
1:A:257:ARG:N	1:A:257:ARG:HD3	2.30	0.46
1:C:111:SER:HB2	12:C:2111:HOH:O	2.16	0.46
10:A:1331:SO4:O1	4:P:1:NAG:O3	2.30	0.45
1:B:301:ARG:NH1	1:B:325:TYR:O	2.50	0.45
1:C:253:MET:HE3	1:C:253:MET:HB3	1.80	0.45
1:C:280:MET:HE2	1:C:281:TYR:N	2.32	0.45
1:A:199:PHE:HB3	7:A:350:HEM:HBC2	1.99	0.45
1:B:191:PHE:HD1	12:B:2090:HOH:O	2.00	0.45
1:A:318:GLY:O	1:A:319:CYS:HB2	2.17	0.45
3:J:4:MAN:O5	3:J:5:MAN:H2	2.17	0.45
1:B:227:ARG:NH2	12:B:2241:HOH:O	2.17	0.45
1:A:80:ALA:O	1:A:84:VAL:HG22	2.17	0.44
1:A:257:ARG:N	1:A:257:ARG:CD	2.81	0.44
3:F:3:BMA:H61	3:F:4:MAN:C5	2.47	0.44
1:A:302:LYS:HA	1:A:302:LYS:HD2	1.48	0.44
1:D:141:ASN:OD1	1:D:141:ASN:C	2.60	0.44
1:C:189:ARG:HA	12:C:2128:HOH:O	2.17	0.44
1:B:203:LEU:HD13	7:B:350:HEM:HBC2	1.99	0.44
1:A:205:VAL:O	1:A:206:ASP:C	2.59	0.43
1:B:28:ARG:HE	1:B:28:ARG:HB2	1.57	0.43
1:C:81:ALA:HB1	1:C:115:LEU:HD21	2.00	0.43
1:D:149:VAL:HG22	1:D:216:MET:SD	2.58	0.43
5:H:6:MAN:H61	5:H:8:MAN:H2	1.37	0.43
1:A:146:GLU:HG2	1:B:149:VAL:HG11	2.00	0.43
1:C:136:ASN:ND2	1:C:139:ASP:OD2	2.45	0.43
1:A:34:GLY:HA3	1:A:95:ILE:O	2.19	0.43
1:A:141:ASN:OD1	1:A:141:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:O	1:C:238:PRO:HA	2.19	0.43
1:B:132:ALA:O	1:B:133:PHE:C	2.61	0.43
1:B:253:MET:HE3	1:B:253:MET:HB3	1.88	0.43
1:A:148:LEU:HD23	1:A:148:LEU:C	2.44	0.43
1:D:24:TRP:HA	1:D:44:SER:O	2.18	0.43
1:B:209:ARG:HD2	1:B:211:ASP:OD2	2.18	0.42
1:C:111:SER:O	1:C:112:VAL:C	2.60	0.42
1:D:283:LYS:O	1:D:287:ILE:HB	2.19	0.42
1:D:220:ARG:O	1:D:221:SER:C	2.60	0.42
1:A:94:SER:C	1:A:96:GLY:H	2.27	0.42
1:D:5:PRO:HA	1:D:6:PRO:HD3	1.90	0.42
1:D:178:ALA:O	1:D:262:ILE:HB	2.19	0.42
1:A:278:CYS:HB2	10:A:1331:SO4:S	2.59	0.42
1:A:150:ASP:OD1	1:B:142:GLU:OE2	2.37	0.42
1:A:323:PHE:HA	1:A:324:PRO:HD2	1.92	0.42
1:C:133:PHE:CE2	11:C:381:NAG:H82	2.55	0.42
1:C:199:PHE:N	1:C:200:PRO:CD	2.83	0.42
1:B:199:PHE:N	1:B:200:PRO:CD	2.82	0.42
2:E:1:NAG:H61	2:E:2:NAG:C1	2.49	0.42
1:B:302:LYS:CE	12:B:2319:HOH:O	2.58	0.41
1:A:169:ARG:HH11	1:A:169:ARG:HD3	1.75	0.41
1:A:96:GLY:HA2	1:A:116:ASN:ND2	2.35	0.41
1:D:24:TRP:CD1	1:D:227:ARG:HG3	2.55	0.41
1:D:34:GLY:HA3	1:D:95:ILE:O	2.20	0.41
1:D:169:ARG:HB2	1:D:197:THR:HG21	2.01	0.41
1:D:294:PRO:O	1:D:295:ASN:HB3	2.20	0.41
1:D:209:ARG:HG2	1:D:211:ASP:OD2	2.21	0.41
1:A:199:PHE:HB3	7:A:350:HEM:CBC	2.50	0.41
1:A:321:GLN:HG2	1:A:323:PHE:CZ	2.56	0.41
1:B:186:VAL:O	1:B:187:ASP:C	2.64	0.41
1:B:242:THR:HG22	12:B:2259:HOH:O	2.21	0.41
1:D:89:ILE:CD1	1:D:300:LEU:HD13	2.40	0.41
1:D:278:CYS:SG	4:K:1:NAG:H83	2.61	0.41
1:B:122:GLU:CD	1:B:123:GLY:N	2.78	0.41
1:B:169:ARG:HB2	1:B:197:THR:HG21	2.03	0.41
1:B:301:ARG:NH2	12:B:2316:HOH:O	2.53	0.41
1:A:6:PRO:HG3	12:A:2057:HOH:O	2.21	0.40
1:B:280:MET:HB3	1:B:280:MET:HE3	1.81	0.40
1:D:280:MET:HE2	1:D:280:MET:C	2.46	0.40
3:F:3:BMA:H61	3:F:4:MAN:H5	2.03	0.40
1:B:272:SER:OG	1:B:280:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:PHE:N	1:A:200:PRO:CD	2.84	0.40
1:C:15:LYS:HE3	12:C:2019:HOH:O	2.20	0.40
1:C:112:VAL:HG12	1:C:112:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/325 (99%)	301 (94%)	21 (6%)	0	100	100
1	B	326/325 (100%)	307 (94%)	19 (6%)	0	100	100
1	C	324/325 (100%)	304 (94%)	20 (6%)	0	100	100
1	D	322/325 (99%)	298 (92%)	24 (8%)	0	100	100
All	All	1294/1300 (100%)	1210 (94%)	84 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/271 (100%)	259 (96%)	11 (4%)	27	40
1	B	274/271 (101%)	265 (97%)	9 (3%)	33	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	272/271 (100%)	264 (97%)	8 (3%)	37	53
1	D	270/271 (100%)	263 (97%)	7 (3%)	40	57
All	All	1086/1084 (100%)	1051 (97%)	35 (3%)	34	50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	88	LEU
1	A	159	LYS
1	A	169	ARG
1	A	221	SER
1	A	226	SER
1	A	227	ARG
1	A	295	ASN
1	A	299	GLN
1	A	300	LEU
1	A	302	LYS
1	B	9	LEU
1	B	51	ASN
1	B	88	LEU
1	B	101	LEU
1	B	169	ARG
1	B	257[A]	ARG
1	B	257[B]	ARG
1	B	286	ASN
1	B	295	ASN
1	C	9	LEU
1	C	88	LEU
1	C	159	LYS
1	C	217	ASP
1	C	261	LYS
1	C	280	MET
1	C	300	LEU
1	C	328	ASP
1	D	9	LEU
1	D	93	LEU
1	D	259	VAL
1	D	261	LYS
1	D	280	MET
1	D	302	LYS

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Mol	Chain	Res	Type
1	D	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	116	ASN
1	A	138	HIS
1	A	174	GLN
1	A	249	GLN
1	A	299	GLN
1	A	313	GLN
1	B	51	ASN
1	B	68	ASN
1	B	147	GLN
1	B	249	GLN
1	B	307	ASN
1	C	249	GLN
1	C	307	ASN
1	C	313	GLN
1	D	116	ASN
1	D	249	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

56 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	E	1	2,1	14,14,15	0.44	0	17,19,21	1.39	3 (17%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.12	1 (5%)
2	BMA	E	3	2	11,11,12	0.55	0	15,15,17	0.94	1 (6%)
2	MAN	E	4	2	11,11,12	0.52	0	15,15,17	0.94	0
2	MAN	E	5	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	E	6	2	11,11,12	0.54	0	15,15,17	1.14	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.69	0	17,19,21	1.26	2 (11%)
3	NAG	F	2	3	14,14,15	0.79	0	17,19,21	1.31	4 (23%)
3	BMA	F	3	3	11,11,12	0.56	0	15,15,17	1.00	0
3	MAN	F	4	3	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
3	MAN	F	5	3	11,11,12	0.54	0	15,15,17	0.87	0
4	NAG	G	1	1,4	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
4	NAG	G	2	4	14,14,15	0.53	0	17,19,21	1.55	4 (23%)
5	NAG	H	1	5,1	14,14,15	0.65	0	17,19,21	1.64	2 (11%)
5	NAG	H	2	5	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
5	BMA	H	3	5	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
5	MAN	H	4	5	11,11,12	0.58	0	15,15,17	1.08	1 (6%)
5	MAN	H	5	5	11,11,12	0.42	0	15,15,17	1.07	1 (6%)
5	MAN	H	6	5	11,11,12	0.57	0	15,15,17	0.83	0
5	MAN	H	7	5	11,11,12	0.53	0	15,15,17	0.87	0
5	MAN	H	8	5	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.49	0	17,19,21	1.94	3 (17%)
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.90	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.60	0	17,19,21	1.18	2 (11%)
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	2.01	5 (29%)
3	BMA	J	3	3	11,11,12	0.56	0	15,15,17	1.22	2 (13%)
3	MAN	J	4	3	11,11,12	0.59	0	15,15,17	1.14	2 (13%)
3	MAN	J	5	3	11,11,12	0.61	0	15,15,17	1.68	3 (20%)
4	NAG	K	1	1,4	14,14,15	0.55	0	17,19,21	1.80	4 (23%)
4	NAG	K	2	4	14,14,15	0.59	0	17,19,21	1.56	2 (11%)
4	NAG	L	1	1,4	14,14,15	0.77	0	17,19,21	1.28	1 (5%)
4	NAG	L	2	4	14,14,15	0.55	0	17,19,21	0.87	0
5	NAG	M	1	5,1	14,14,15	0.65	0	17,19,21	1.80	4 (23%)
5	NAG	M	2	5	14,14,15	0.74	0	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	M	3	5	11,11,12	0.78	0	15,15,17	1.22	1 (6%)
5	MAN	M	4	5	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
5	MAN	M	5	5	11,11,12	0.43	0	15,15,17	1.44	1 (6%)
5	MAN	M	6	5	11,11,12	0.52	0	15,15,17	1.96	4 (26%)
5	MAN	M	7	5	11,11,12	0.48	0	15,15,17	0.81	0
5	MAN	M	8	5	11,11,12	0.73	0	15,15,17	1.41	2 (13%)
4	NAG	N	1	1,4	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
4	NAG	N	2	4	14,14,15	0.51	0	17,19,21	0.76	1 (5%)
6	NAG	O	1	6,1	14,14,15	0.59	0	17,19,21	0.85	1 (5%)
6	NAG	O	2	6	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
6	BMA	O	3	6	11,11,12	0.51	0	15,15,17	1.80	3 (20%)
4	NAG	P	1	1,4	14,14,15	0.71	0	17,19,21	1.78	6 (35%)
4	NAG	P	2	4	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
4	NAG	Q	1	1,4	14,14,15	0.56	0	17,19,21	1.59	3 (17%)
4	NAG	Q	2	4	14,14,15	0.49	0	17,19,21	0.77	0
4	NAG	R	1	1,4	14,14,15	0.59	0	17,19,21	0.74	0
4	NAG	R	2	4	14,14,15	0.57	0	17,19,21	0.70	0
4	NAG	S	1	1,4	14,14,15	0.66	0	17,19,21	1.24	3 (17%)
4	NAG	S	2	4	14,14,15	0.49	0	17,19,21	0.57	0
6	NAG	T	1	6,1	14,14,15	0.64	0	17,19,21	1.49	3 (17%)
6	NAG	T	2	6	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
6	BMA	T	3	6	11,11,12	0.51	0	15,15,17	1.27	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
5	MAN	H	7	5	-	1/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	MAN	M	5	5	-	2/2/19/22	0/1/1/1
5	MAN	M	6	5	-	2/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
6	NAG	O	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2	NAG	C2-N2-C7	-5.23	115.89	122.90
4	I	1	NAG	C1-O5-C5	5.23	119.19	112.19
5	M	1	NAG	C1-O5-C5	4.94	118.81	112.19
4	K	2	NAG	O5-C1-C2	-4.69	104.04	111.29
3	J	5	MAN	C3-C4-C5	4.60	118.57	110.23
4	Q	1	NAG	C1-O5-C5	4.57	118.31	112.19
5	H	1	NAG	C1-O5-C5	4.49	118.20	112.19
6	O	3	BMA	C1-O5-C5	4.48	118.19	112.19
5	M	5	MAN	C1-O5-C5	4.23	117.85	112.19
5	M	6	MAN	C3-C4-C5	4.17	117.79	110.23
5	M	6	MAN	C1-O5-C5	4.11	117.69	112.19
4	K	1	NAG	C2-N2-C7	-3.79	117.82	122.90
6	O	3	BMA	C1-C2-C3	3.66	114.97	109.64
4	P	1	NAG	O5-C1-C2	-3.61	105.71	111.29
5	H	1	NAG	C2-N2-C7	-3.60	118.07	122.90
5	M	6	MAN	C6-C5-C4	-3.52	104.38	113.02
5	M	8	MAN	C1-C2-C3	3.51	114.75	109.64
5	M	3	BMA	C1-O5-C5	3.49	116.87	112.19
3	J	2	NAG	C4-C3-C2	-3.44	105.97	111.02
6	T	1	NAG	O5-C1-C2	-3.34	106.13	111.29
5	H	2	NAG	C1-O5-C5	-3.34	107.72	112.19
4	I	1	NAG	C4-C3-C2	-3.25	106.25	111.02
5	H	8	MAN	C1-C2-C3	-3.25	104.91	109.64
6	T	2	NAG	O5-C1-C2	-3.12	106.46	111.29
3	J	5	MAN	C1-O5-C5	3.11	116.36	112.19
4	G	2	NAG	C1-C2-N2	3.07	115.27	110.43
3	J	1	NAG	C2-N2-C7	-3.04	118.83	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2	NAG	C1-O5-C5	-3.01	108.15	112.19
4	L	1	NAG	C2-N2-C7	-2.98	118.90	122.90
4	K	1	NAG	C1-O5-C5	2.95	116.14	112.19
4	P	2	NAG	C2-N2-C7	-2.94	118.97	122.90
4	G	2	NAG	O5-C1-C2	-2.89	106.82	111.29
4	K	1	NAG	C1-C2-N2	2.86	114.94	110.43
5	M	8	MAN	O2-C2-C3	-2.79	104.36	110.15
2	E	1	NAG	O5-C1-C2	-2.77	107.00	111.29
3	J	2	NAG	C1-C2-N2	2.76	114.79	110.43
5	H	5	MAN	C1-O5-C5	2.76	115.89	112.19
4	Q	1	NAG	C3-C4-C5	-2.75	105.25	110.23
5	M	1	NAG	C6-C5-C4	-2.74	106.28	113.02
3	F	2	NAG	C2-N2-C7	-2.73	119.24	122.90
4	P	1	NAG	C1-C2-N2	2.71	114.71	110.43
5	M	4	MAN	C2-C3-C4	-2.71	106.09	110.86
6	T	1	NAG	O5-C5-C4	2.68	117.35	110.83
4	P	1	NAG	C2-N2-C7	-2.65	119.36	122.90
3	J	2	NAG	C1-O5-C5	2.64	115.72	112.19
4	P	1	NAG	O4-C4-C3	-2.63	104.18	110.38
3	J	3	BMA	C1-O5-C5	2.62	115.70	112.19
4	G	1	NAG	C3-C4-C5	-2.62	105.49	110.23
2	E	6	MAN	C2-C3-C4	-2.59	106.31	110.86
3	J	1	NAG	O5-C1-C2	-2.58	107.31	111.29
4	S	1	NAG	O5-C1-C2	-2.56	107.33	111.29
3	J	5	MAN	O5-C5-C4	2.56	117.05	110.83
3	J	2	NAG	O5-C1-C2	-2.55	107.34	111.29
2	E	3	BMA	C1-O5-C5	2.54	115.59	112.19
3	F	4	MAN	C1-C2-C3	2.49	113.27	109.64
3	J	4	MAN	C1-C2-C3	2.49	113.26	109.64
5	M	2	NAG	C3-C4-C5	-2.48	105.74	110.23
2	E	2	NAG	O5-C1-C2	-2.45	107.51	111.29
4	G	2	NAG	C3-C4-C5	2.44	114.65	110.23
3	J	3	BMA	C1-C2-C3	2.43	113.19	109.64
4	Q	1	NAG	C2-N2-C7	-2.40	119.68	122.90
2	E	1	NAG	C2-N2-C7	-2.39	119.70	122.90
4	K	1	NAG	O5-C1-C2	-2.37	107.62	111.29
4	I	1	NAG	O5-C5-C4	2.37	116.59	110.83
3	F	2	NAG	O5-C1-C2	-2.35	107.65	111.29
3	F	1	NAG	O5-C5-C4	2.35	116.53	110.83
6	T	3	BMA	C1-O5-C5	2.29	115.26	112.19
6	T	1	NAG	C1-C2-N2	2.29	114.04	110.43
5	M	2	NAG	C1-O5-C5	-2.27	109.14	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	BMA	C1-C2-C3	2.27	112.95	109.64
4	N	2	NAG	O5-C1-C2	-2.27	107.79	111.29
6	O	2	NAG	O5-C5-C6	2.26	112.06	107.66
4	G	2	NAG	C4-C3-C2	2.24	114.30	111.02
4	S	1	NAG	C1-O5-C5	2.23	115.17	112.19
4	I	2	NAG	C1-O5-C5	2.18	115.11	112.19
4	P	1	NAG	C4-C3-C2	2.18	114.21	111.02
2	E	1	NAG	O7-C7-C8	-2.18	118.18	122.05
5	M	1	NAG	C3-C4-C5	2.16	114.16	110.23
4	P	1	NAG	O4-C4-C5	-2.15	104.03	109.32
5	H	4	MAN	C2-C3-C4	-2.12	107.13	110.86
4	S	1	NAG	C3-C4-C5	2.11	114.06	110.23
4	N	1	NAG	O5-C5-C6	2.11	111.77	107.66
5	M	6	MAN	O3-C3-C4	-2.08	105.47	110.38
6	T	3	BMA	O5-C5-C6	2.08	111.71	107.66
3	F	2	NAG	C1-C2-N2	2.08	113.70	110.43
5	M	1	NAG	O7-C7-C8	-2.07	118.36	122.05
3	F	2	NAG	C4-C3-C2	2.06	114.04	111.02
3	J	4	MAN	C2-C3-C4	2.06	114.48	110.86
6	O	3	BMA	C2-C3-C4	-2.03	107.28	110.86
6	O	1	NAG	O5-C1-C2	-2.02	108.17	111.29
3	F	1	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C3-C2-N2-C7
3	F	4	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	J	5	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
6	O	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	5	MAN	C4-C5-C6-O6
6	T	3	BMA	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
5	M	6	MAN	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
5	M	6	MAN	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	C8-C7-N2-C2
4	Q	2	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
2	E	3	BMA	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
6	T	3	BMA	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
5	M	5	MAN	C4-C5-C6-O6
5	M	8	MAN	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
5	H	6	MAN	C4-C5-C6-O6
5	H	7	MAN	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	H	3	BMA	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
5	M	5	MAN	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
5	H	6	MAN	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6

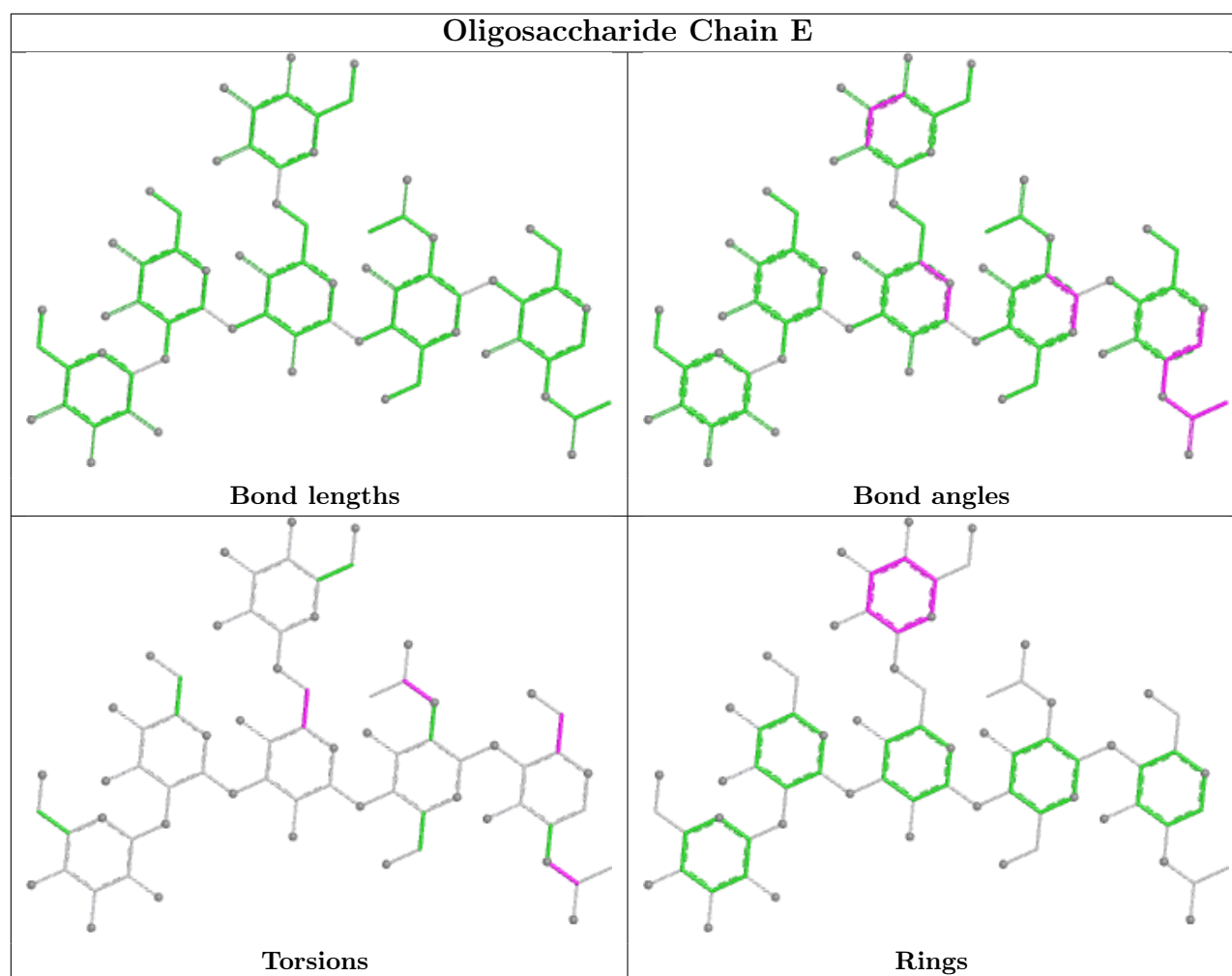
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	MAN	C1-C2-C3-C4-C5-O5

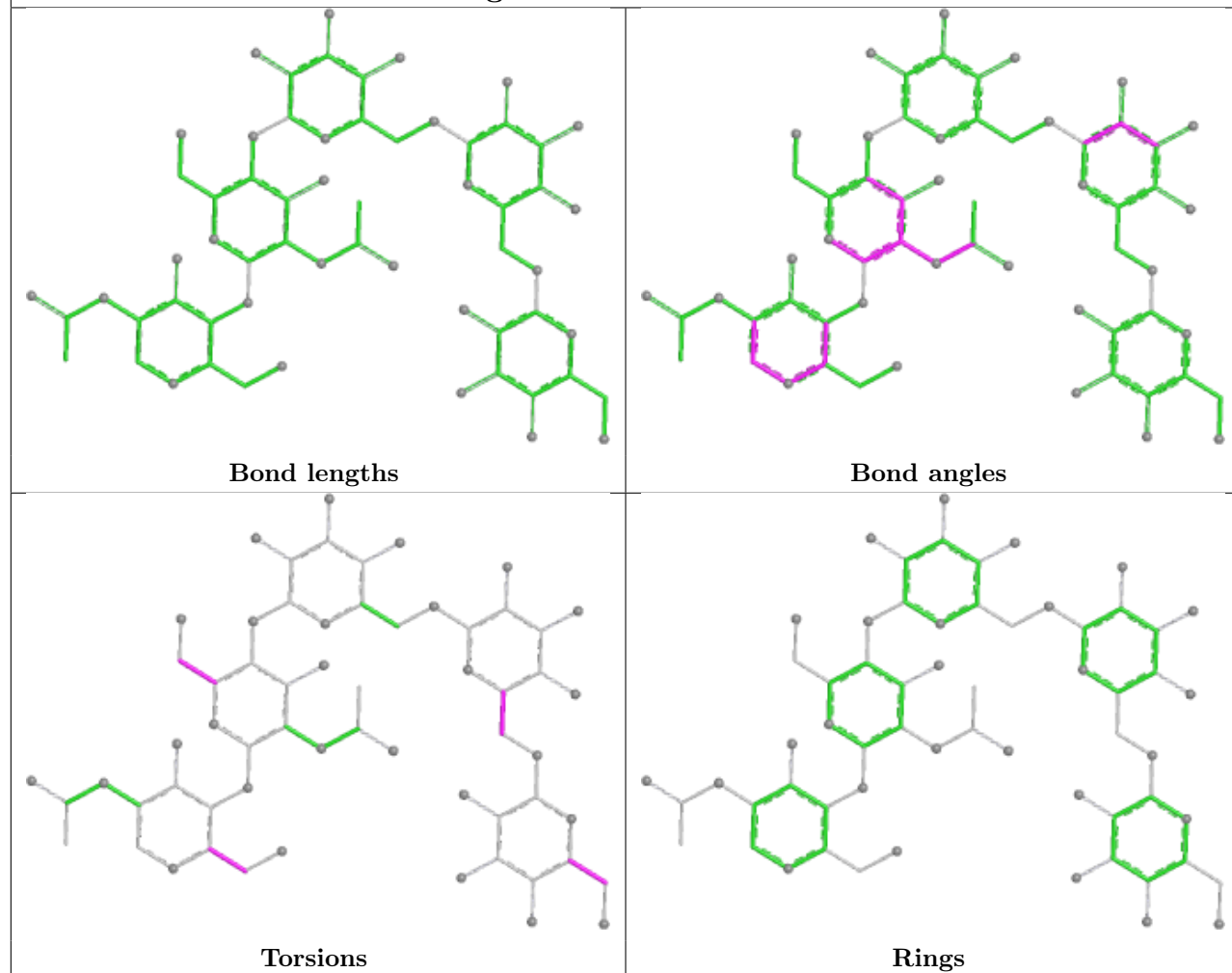
20 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	8	MAN	2	0
4	I	2	NAG	3	0
5	H	6	MAN	4	0
2	E	3	BMA	1	0
4	G	2	NAG	1	0
5	M	6	MAN	2	0
2	E	2	NAG	1	0
3	F	4	MAN	2	0
5	H	8	MAN	4	0
2	E	6	MAN	1	0
3	J	4	MAN	1	0
4	P	1	NAG	1	0
4	K	1	NAG	1	0
2	E	1	NAG	1	0
3	J	5	MAN	1	0
3	F	3	BMA	2	0
4	K	2	NAG	1	0
3	J	2	NAG	1	0
4	I	1	NAG	3	0
4	G	1	NAG	3	0

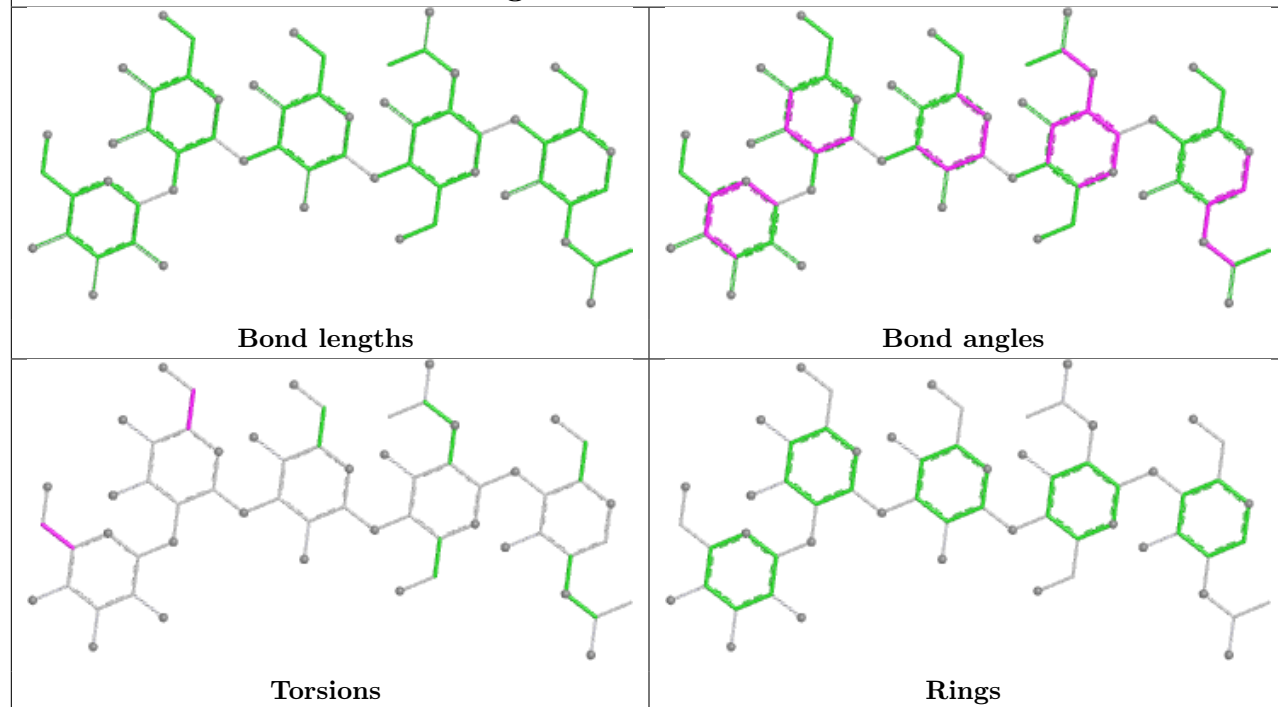
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

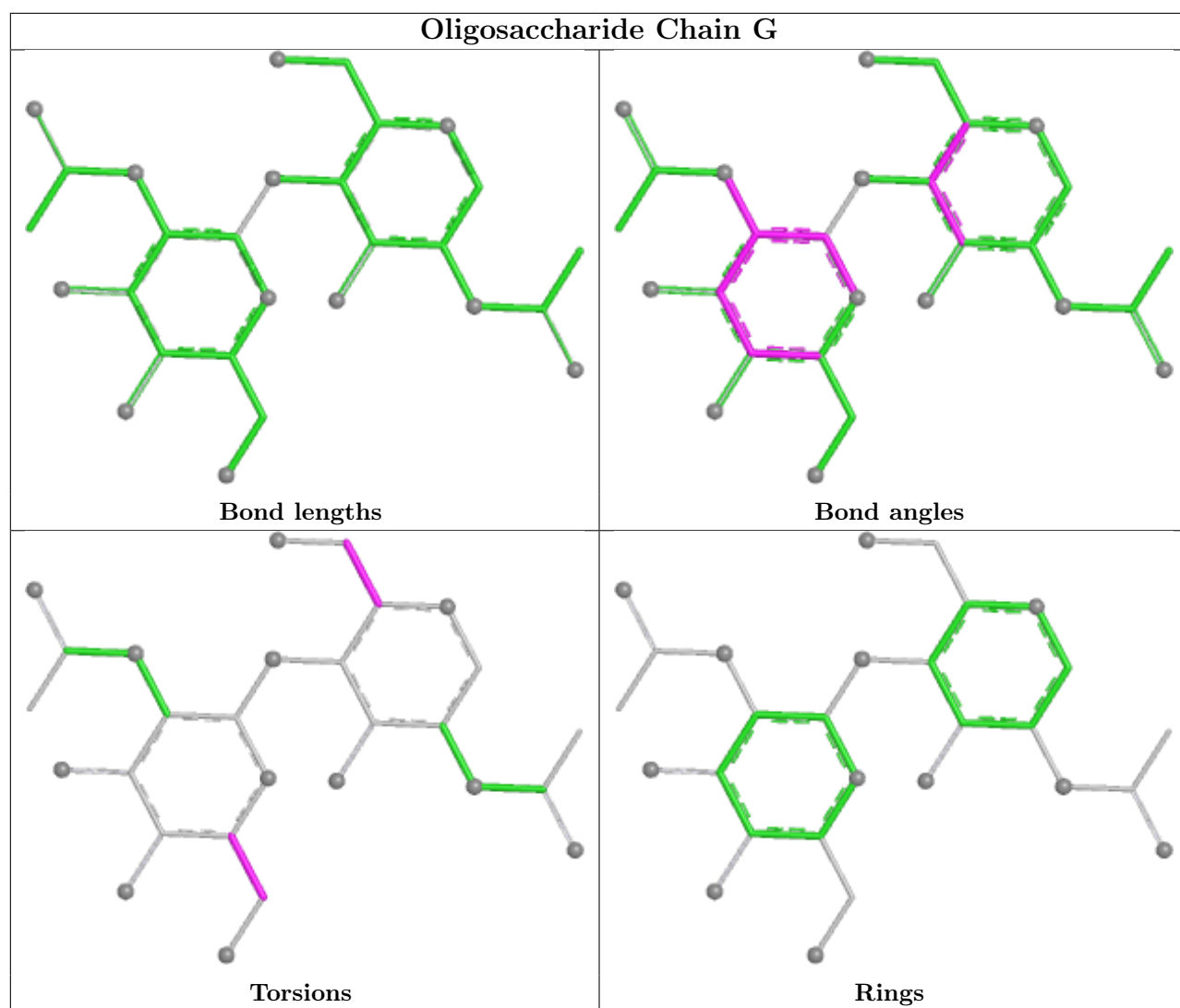


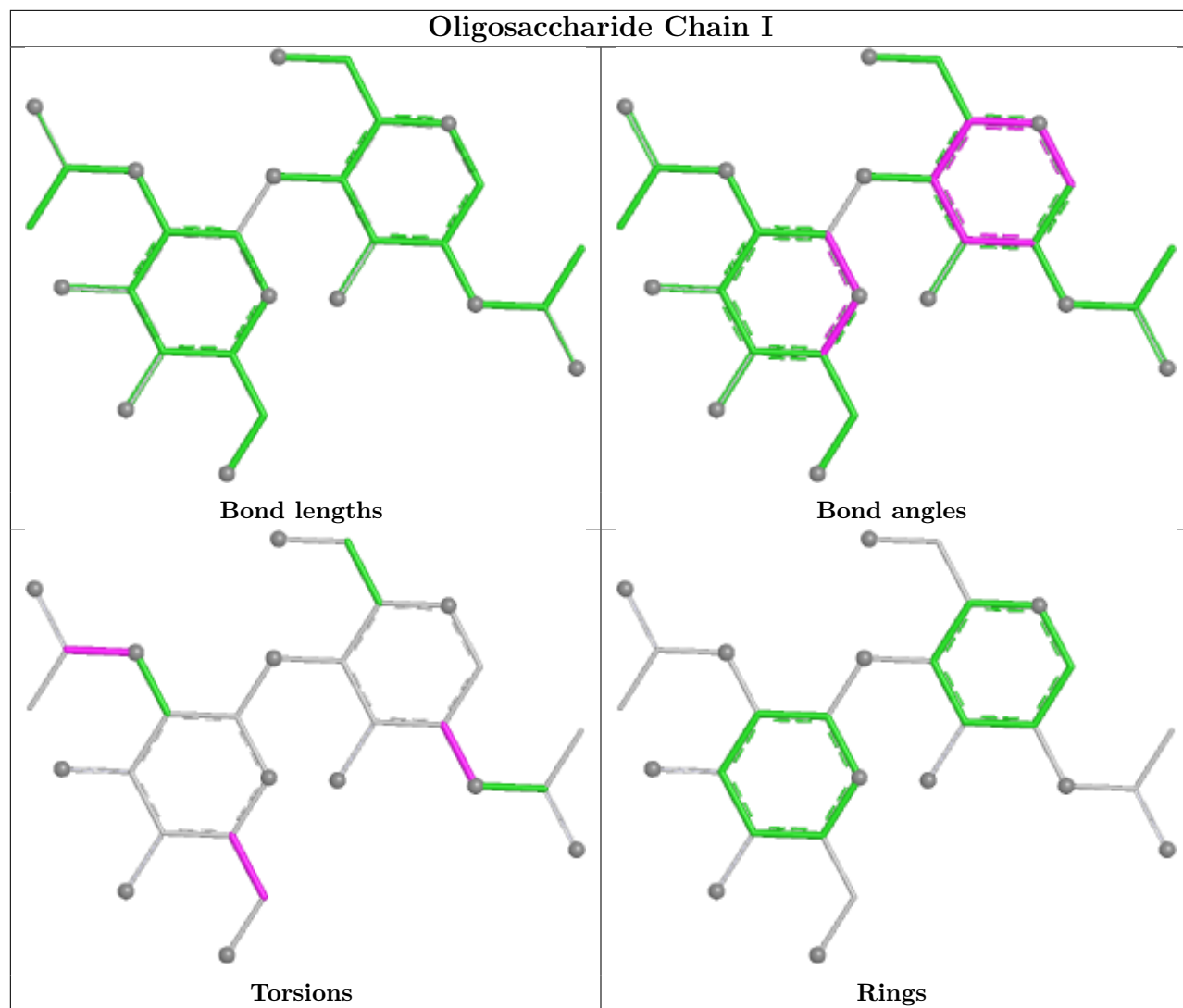
Oligosaccharide Chain F

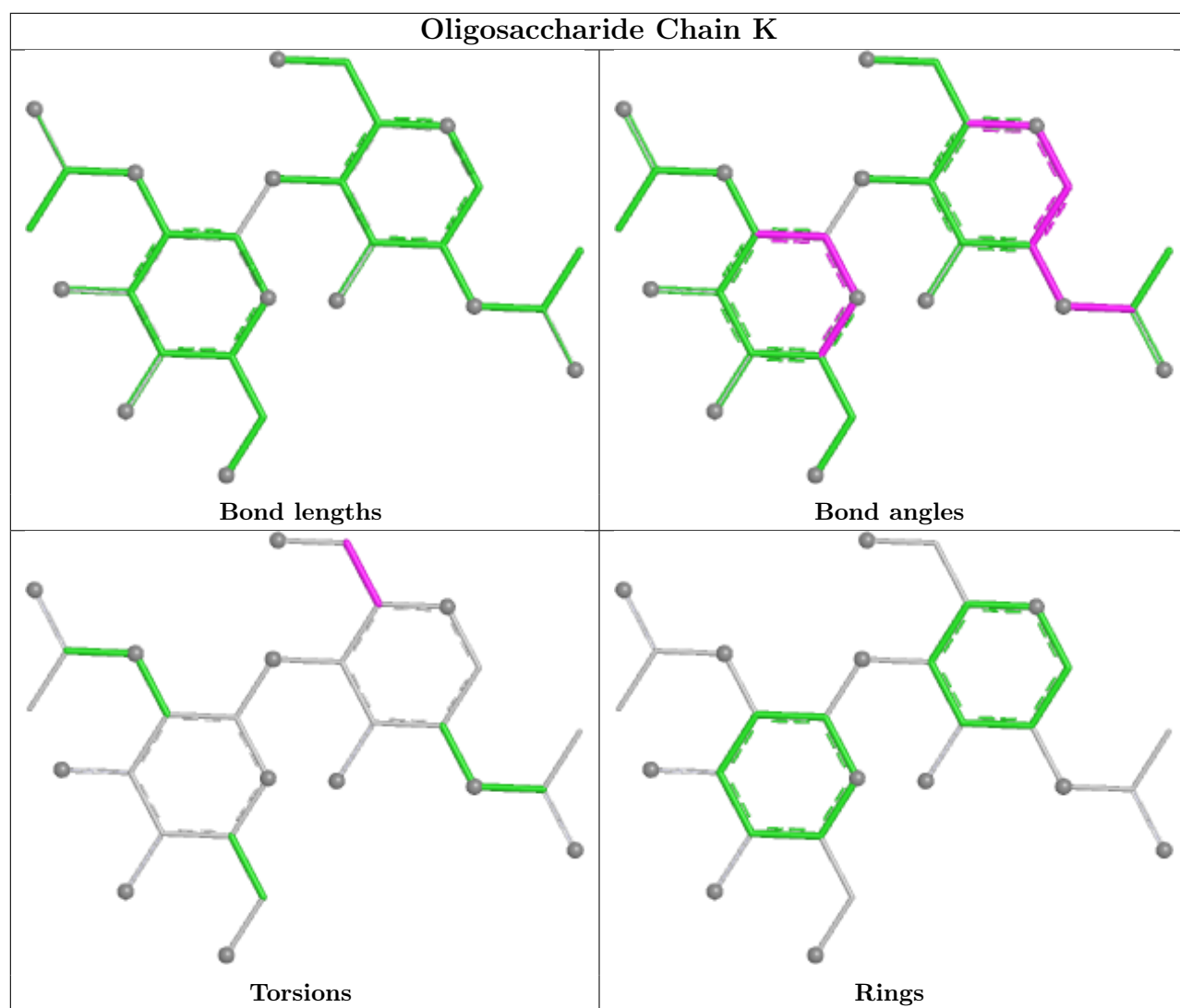


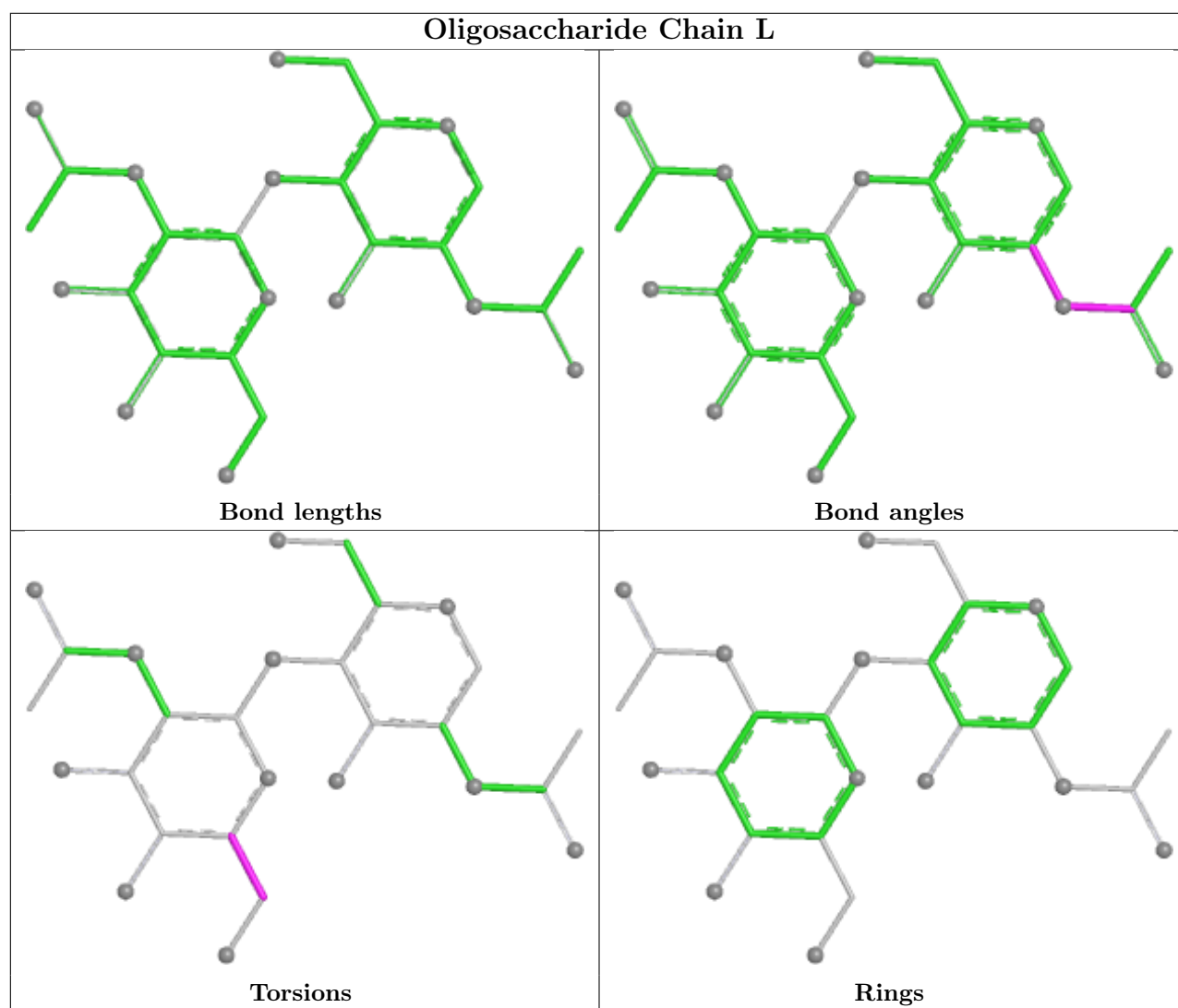
Oligosaccharide Chain J

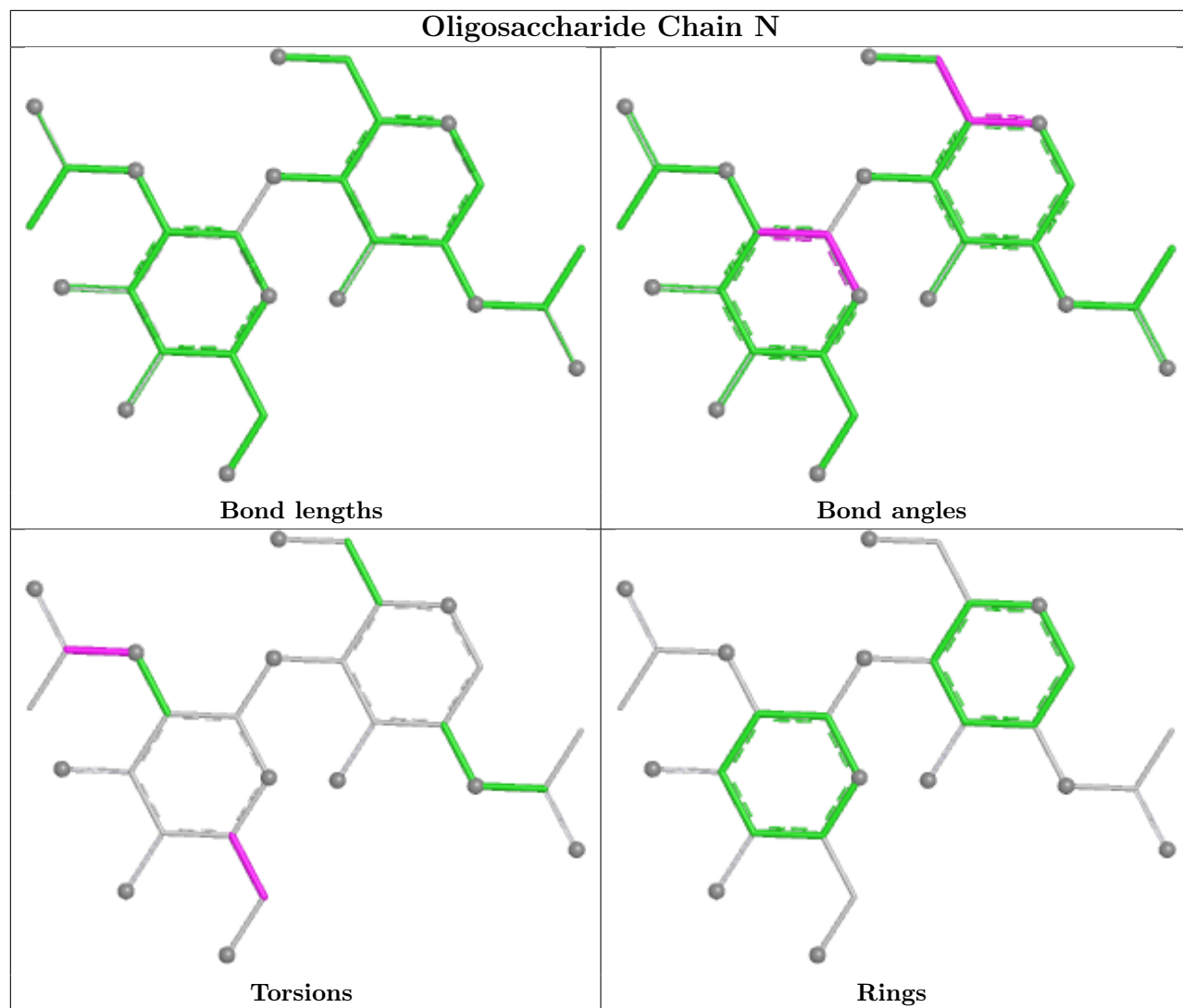


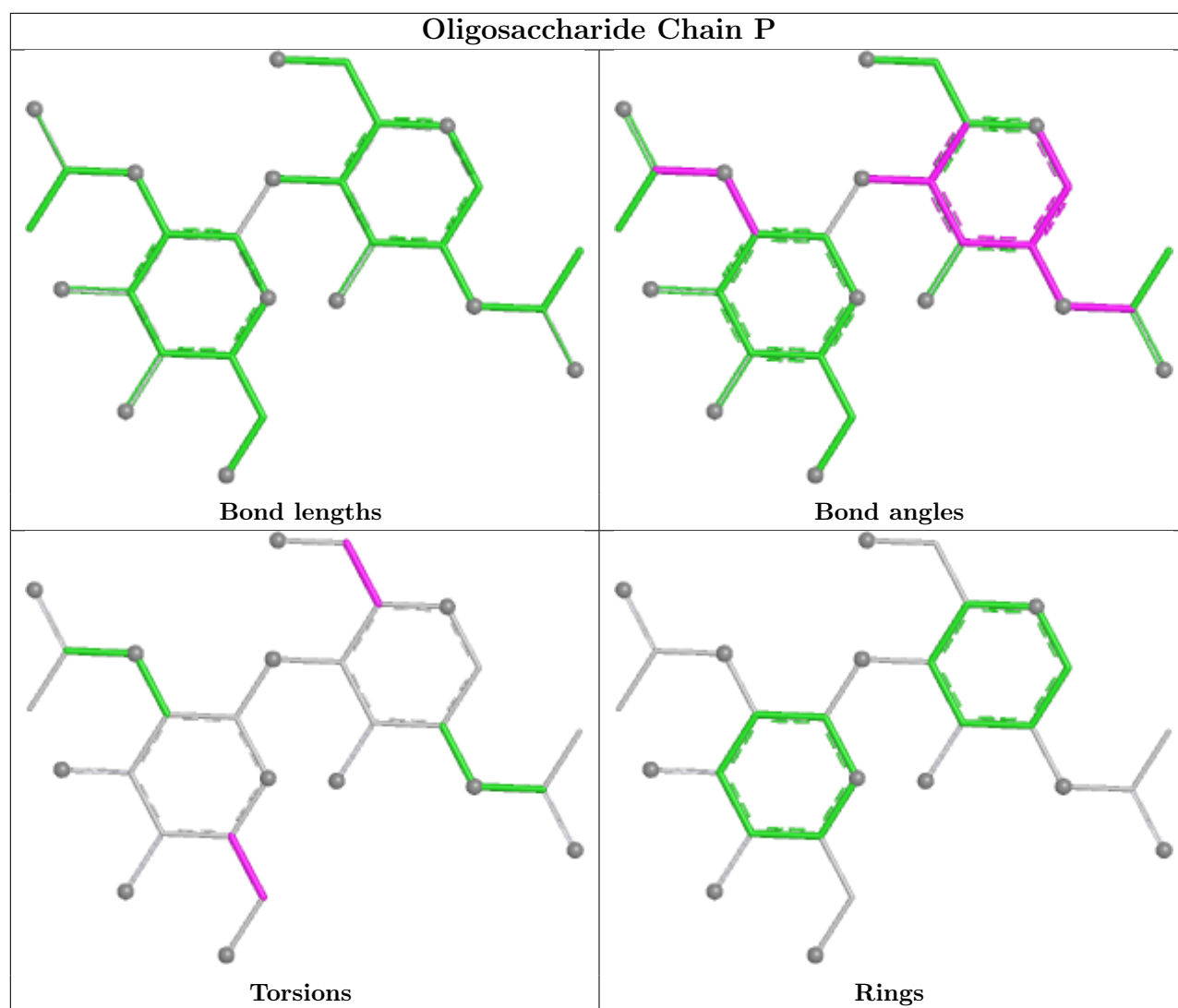


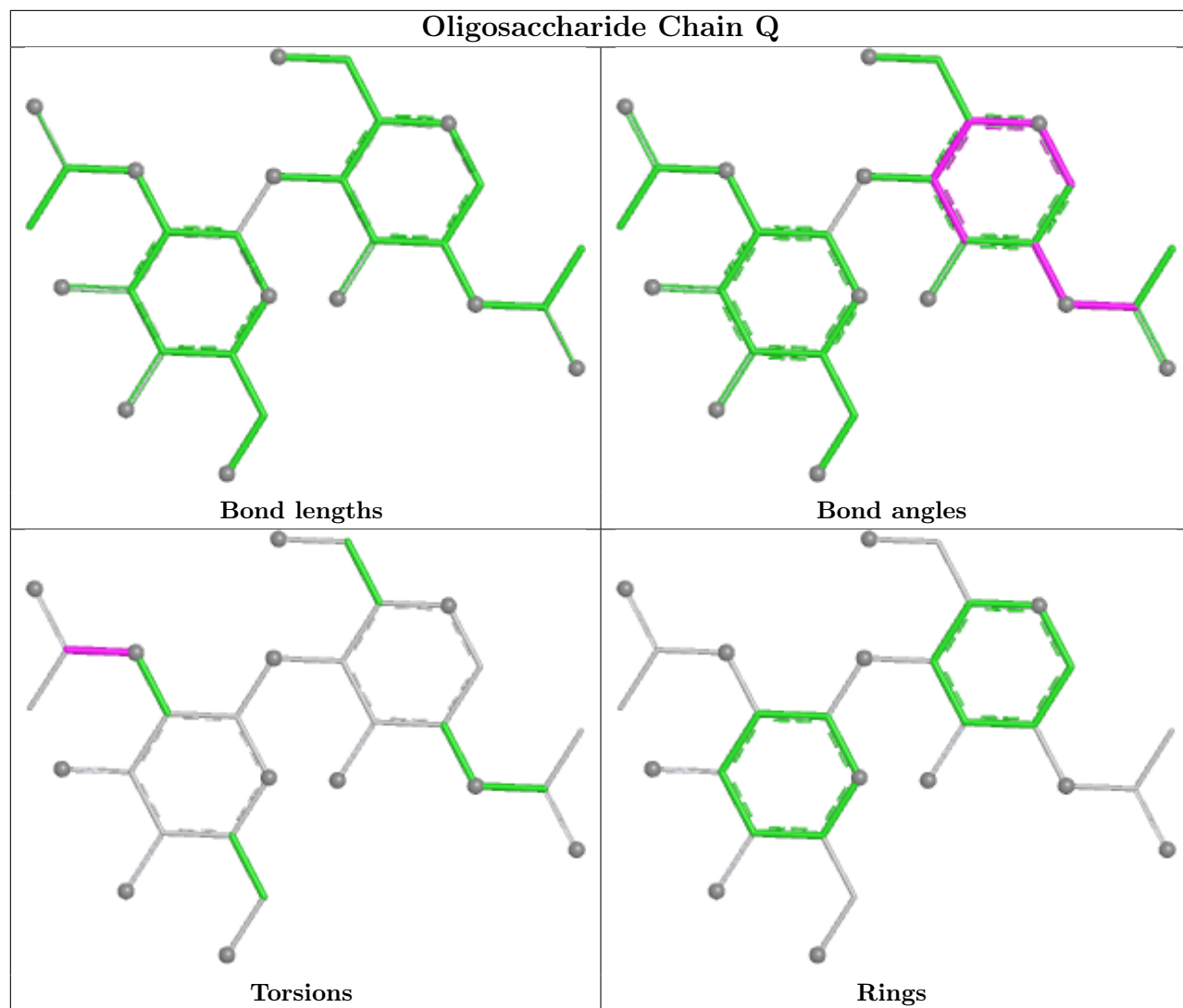


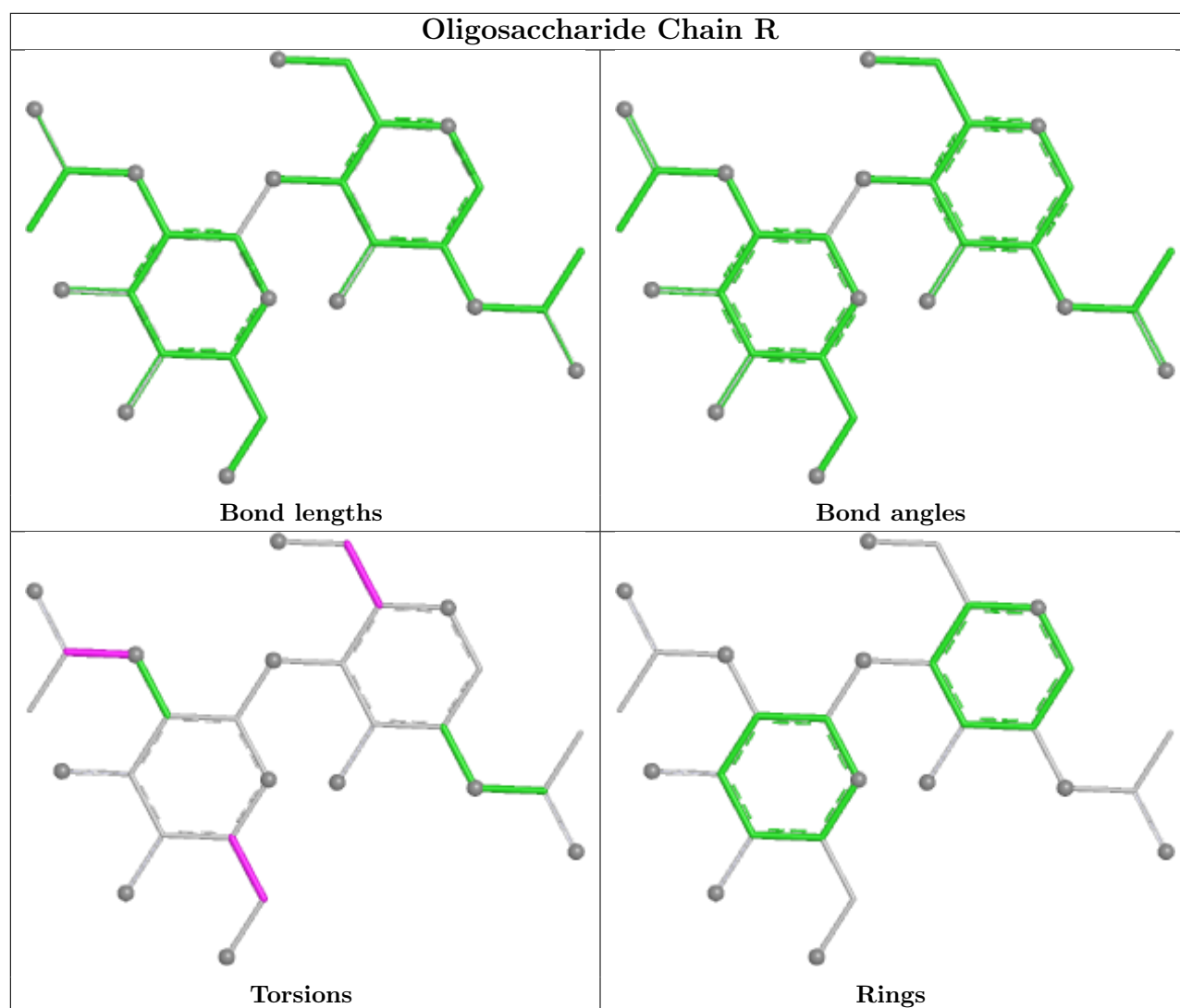


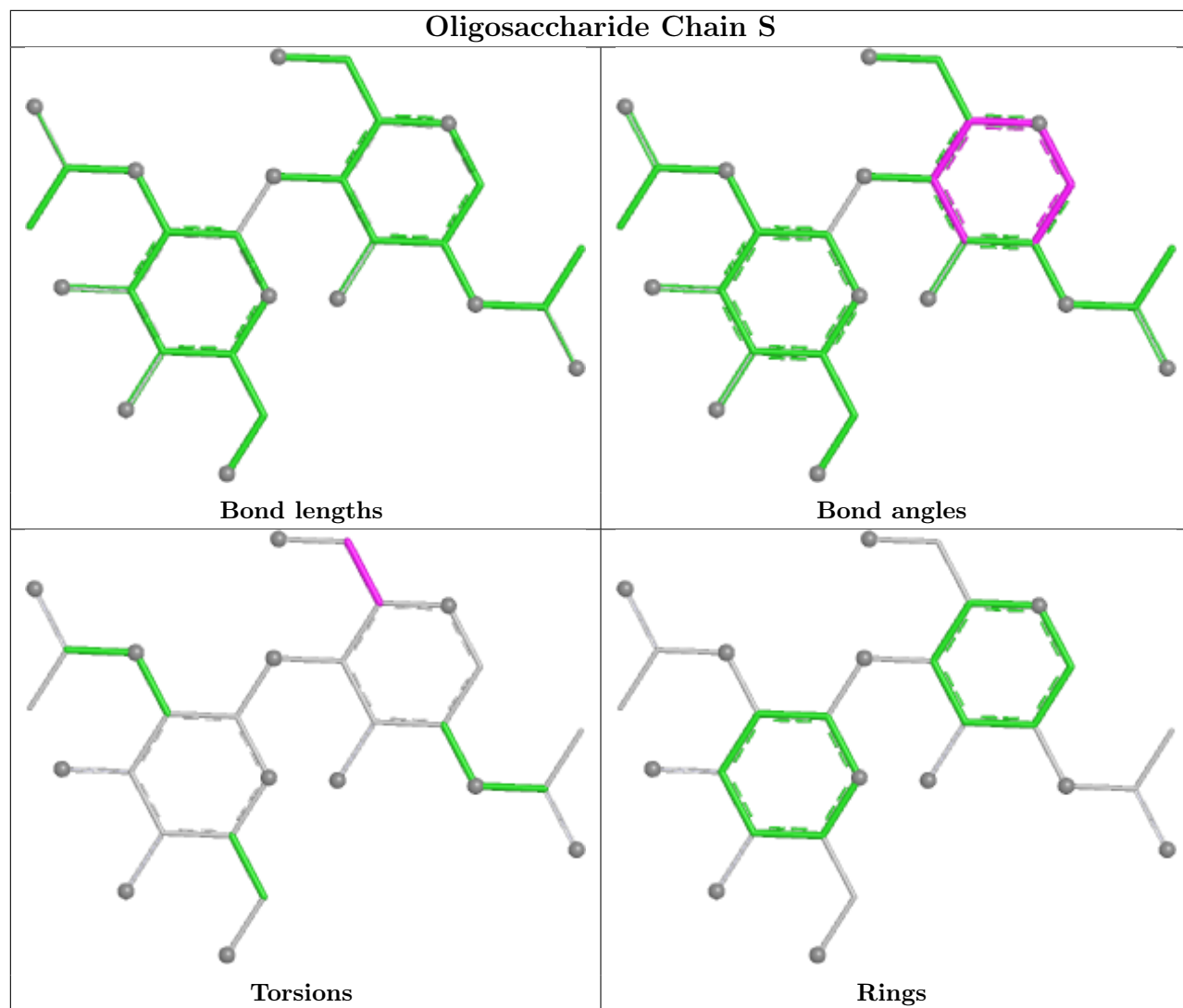


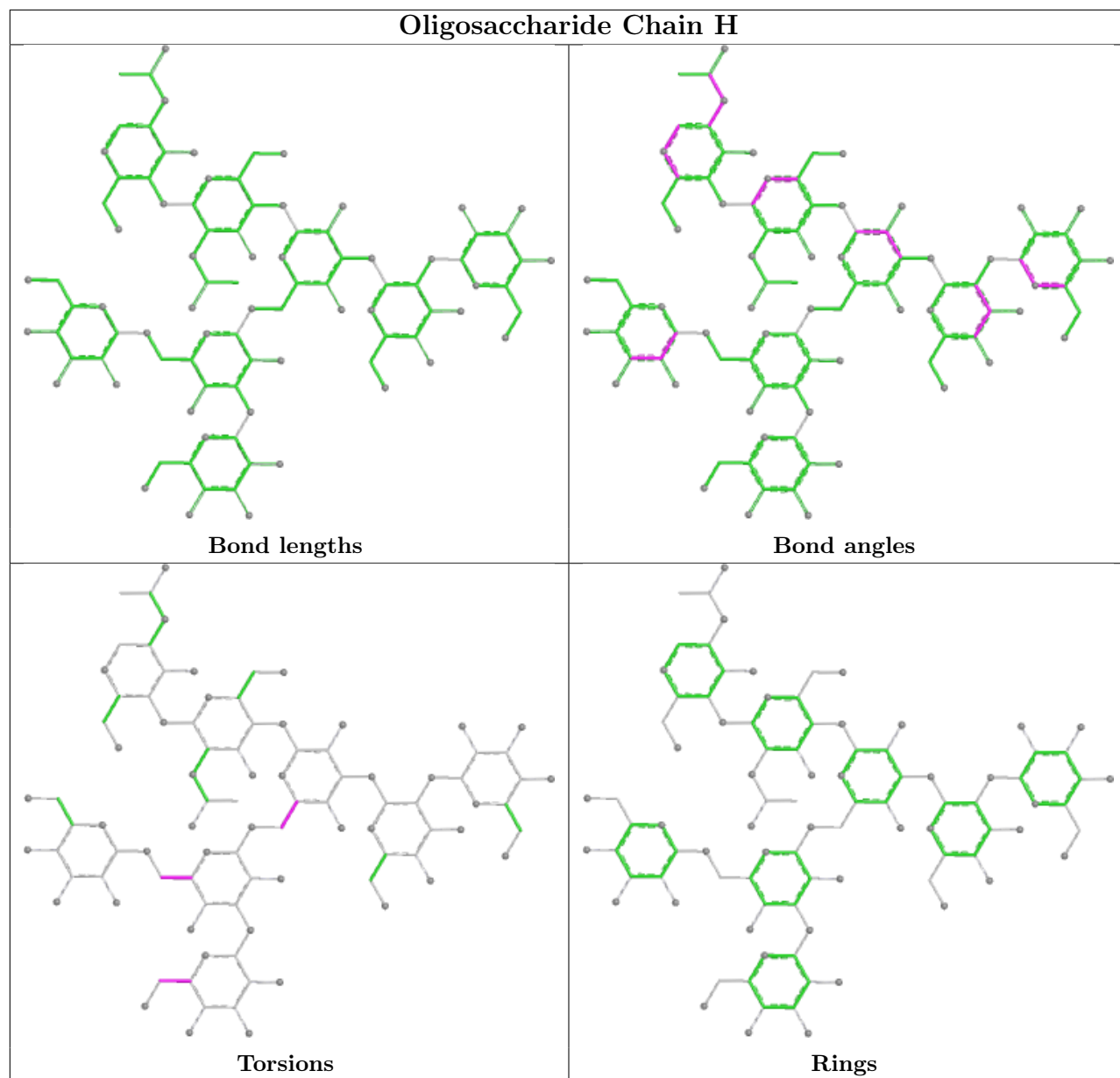


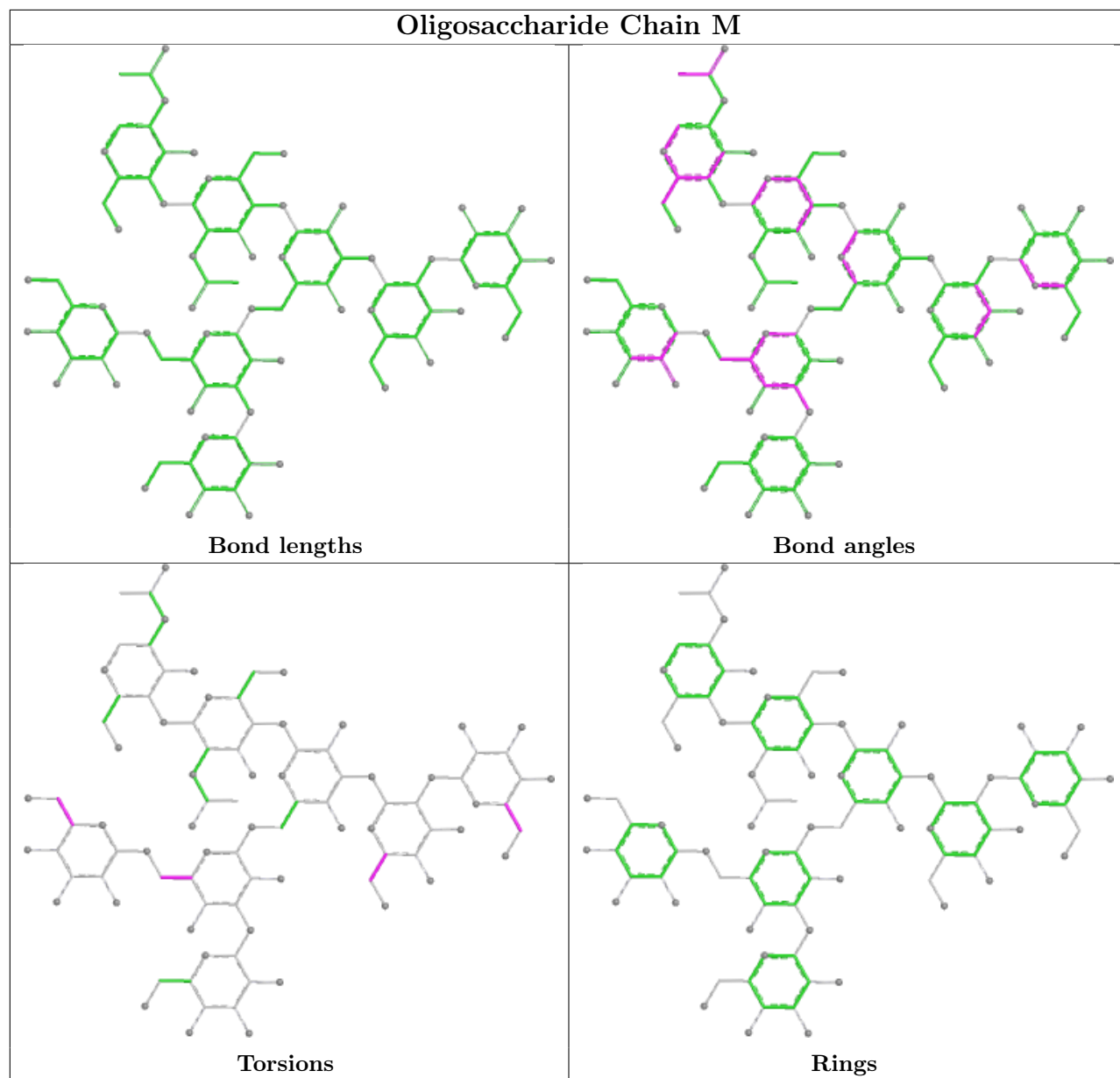


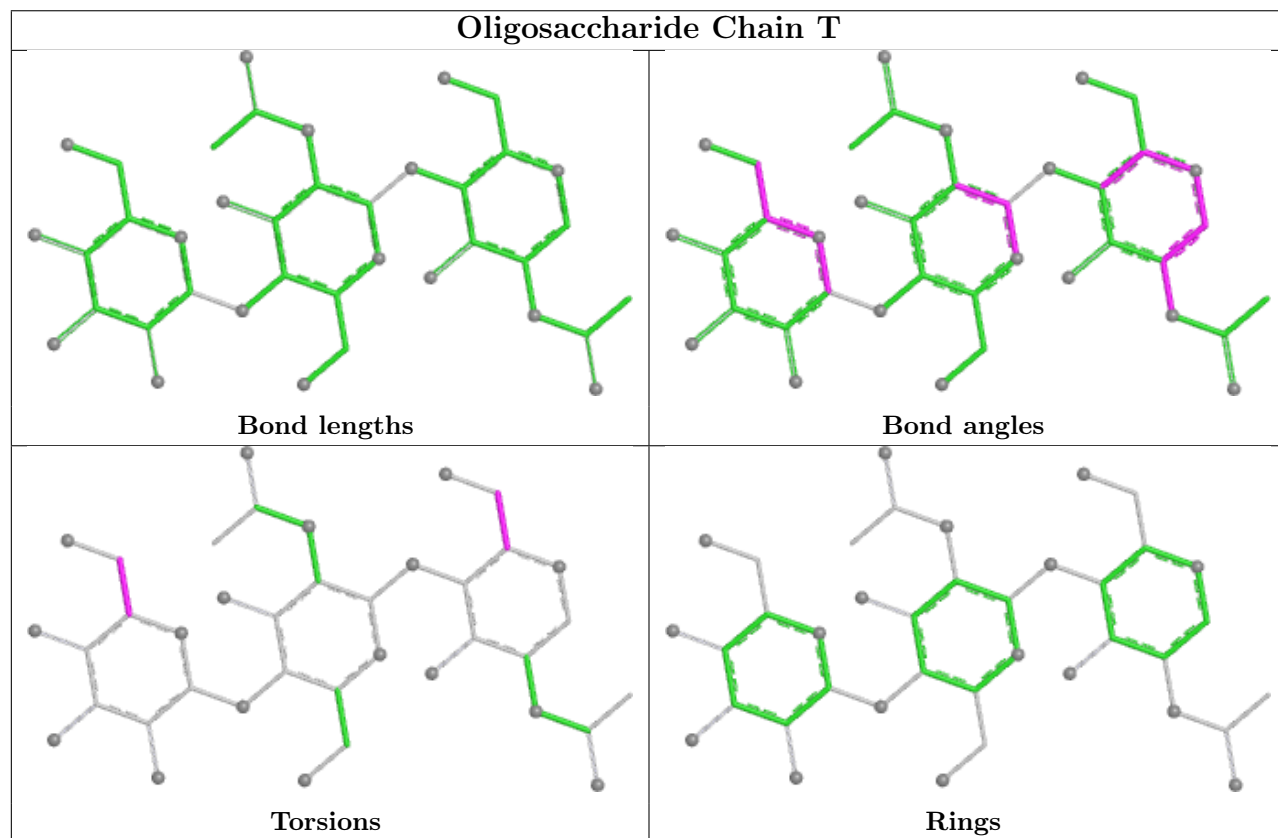
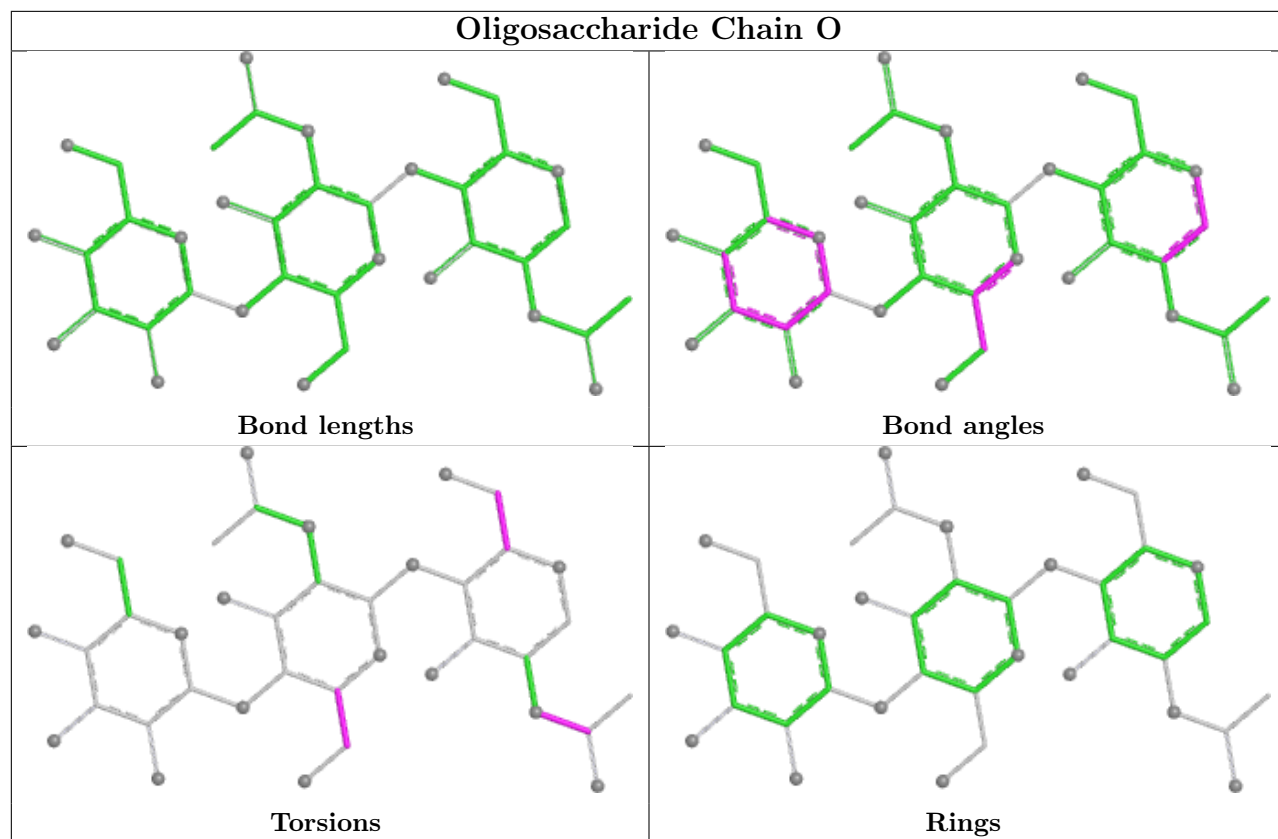












5.6 Ligand geometry

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 for Mogul analysis.

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$
9	ACT	A	1327	-	3,3,3	0.72	0	3,3,3	1.26	0
10	SO4	C	1332	-	4,4,4	0.29	0	6,6,6	0.21	0
10	SO4	A	1328	-	4,4,4	0.31	0	6,6,6	0.19	0
9	ACT	C	1334	-	3,3,3	0.76	0	3,3,3	1.35	0
10	SO4	A	1329	-	4,4,4	0.24	0	6,6,6	0.27	0
7	HEM	C	350	1,8	50,50,50	1.79	9 (18%)	67,82,82	1.33	7 (10%)
11	NAG	D	411	1	14,14,15	0.55	0	17,19,21	0.83	0
11	NAG	D	381	1	14,14,15	0.65	0	17,19,21	0.70	0
10	SO4	A	1330	-	4,4,4	0.27	0	6,6,6	0.18	0
10	SO4	D	1328	-	4,4,4	0.20	0	6,6,6	0.28	0
7	HEM	A	350	1,8	50,50,50	1.82	10 (20%)	67,82,82	1.26	6 (8%)
7	HEM	B	350	1,8,9	50,50,50	1.83	10 (20%)	67,82,82	1.28	6 (8%)
9	ACT	B	1328	7	3,3,3	0.80	0	3,3,3	1.25	0
9	ACT	C	1329	-	3,3,3	0.71	0	3,3,3	1.48	0
9	ACT	D	1327	-	3,3,3	0.71	0	3,3,3	1.39	0
11	NAG	C	381	1	14,14,15	0.63	0	17,19,21	1.37	2 (11%)
10	SO4	B	1329	-	4,4,4	0.27	0	6,6,6	0.32	0
10	SO4	C	1330	-	4,4,4	0.22	0	6,6,6	0.21	0
10	SO4	D	1329	-	4,4,4	0.27	0	6,6,6	0.18	0
10	SO4	B	1330	-	4,4,4	0.23	0	6,6,6	0.17	0
10	SO4	A	1331	-	4,4,4	0.28	0	6,6,6	0.17	0
7	HEM	D	350	1,8	50,50,50	1.70	9 (18%)	67,82,82	1.39	10 (14%)
10	SO4	C	1331	-	4,4,4	0.24	0	6,6,6	0.13	0
11	NAG	D	391	1	14,14,15	0.54	0	17,19,21	1.45	4 (23%)
10	SO4	B	1331	-	4,4,4	0.27	0	6,6,6	0.19	0
10	SO4	C	1333	-	4,4,4	0.21	0	6,6,6	0.07	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
7	HEM	A	350	1,8	-	4/14/54/54	-
11	NAG	C	381	1	-	2/6/23/26	0/1/1/1
7	HEM	B	350	1,8,9	-	3/14/54/54	-
7	HEM	D	350	1,8	-	3/14/54/54	-
11	NAG	D	411	1	-	0/6/23/26	0/1/1/1
7	HEM	C	350	1,8	-	4/14/54/54	-
11	NAG	D	391	1	-	2/6/23/26	0/1/1/1
11	NAG	D	381	1	-	0/6/23/26	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	350	HEM	C3D-C2D	7.43	1.52	1.36
7	A	350	HEM	C3D-C2D	7.41	1.52	1.36
7	D	350	HEM	C3D-C2D	7.29	1.52	1.36
7	B	350	HEM	C3D-C2D	6.88	1.51	1.36
7	C	350	HEM	FE-ND	5.80	2.12	1.94
7	A	350	HEM	FE-ND	4.96	2.10	1.94
7	B	350	HEM	FE-ND	4.44	2.08	1.94
7	B	350	HEM	FE-NB	4.40	2.08	1.94
7	A	350	HEM	CMC-C2C	3.23	1.57	1.50
7	A	350	HEM	FE-NB	3.03	2.04	1.94
7	D	350	HEM	FE-ND	3.00	2.04	1.94
7	B	350	HEM	CAC-C3C	2.90	1.55	1.47
7	A	350	HEM	CAC-C3C	2.83	1.54	1.47
7	C	350	HEM	CAB-C3B	2.83	1.54	1.47
7	D	350	HEM	FE-NA	2.75	2.04	1.95
7	B	350	HEM	CAB-C3B	2.74	1.54	1.47
7	A	350	HEM	CMB-C2B	2.72	1.56	1.50
7	A	350	HEM	CAB-C3B	2.68	1.54	1.47
7	A	350	HEM	CMA-C3A	2.67	1.56	1.50
7	D	350	HEM	CAB-C3B	2.61	1.54	1.47
7	D	350	HEM	CAC-C3C	2.61	1.54	1.47
7	C	350	HEM	CMB-C2B	2.57	1.56	1.50
7	B	350	HEM	CMC-C2C	2.54	1.56	1.50
7	D	350	HEM	FE-NB	2.54	2.02	1.94
7	C	350	HEM	CAC-C3C	2.53	1.54	1.47
7	D	350	HEM	CMC-C2C	2.40	1.55	1.50
7	D	350	HEM	CMA-C3A	2.36	1.55	1.50
7	B	350	HEM	CMA-C3A	2.35	1.55	1.50
7	D	350	HEM	FE-NC	2.23	2.02	1.95
7	B	350	HEM	CMB-C2B	2.23	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	350	HEM	FE-NB	2.10	2.01	1.94
7	C	350	HEM	CMC-C2C	2.10	1.55	1.50
7	A	350	HEM	C3C-C2C	-2.08	1.32	1.37
7	B	350	HEM	FE-NA	2.06	2.02	1.95
7	B	350	HEM	C3C-C2C	-2.06	1.33	1.37
7	C	350	HEM	CAA-C2A	2.06	1.56	1.51
7	C	350	HEM	CMD-C2D	2.04	1.55	1.50
7	A	350	HEM	C2A-C3A	-2.02	1.33	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	350	HEM	C4D-ND-C1D	4.56	110.60	105.21
7	D	350	HEM	C4D-ND-C1D	4.52	110.56	105.21
7	B	350	HEM	C4D-ND-C1D	4.40	110.42	105.21
7	C	350	HEM	CHD-C4C-NC	4.28	129.11	124.45
7	C	350	HEM	C4D-ND-C1D	3.95	109.88	105.21
11	C	381	NAG	C4-C3-C2	3.67	116.39	111.02
7	B	350	HEM	C3B-C4B-NB	-3.32	107.08	109.47
11	D	391	NAG	C1-O5-C5	3.17	116.44	112.19
7	D	350	HEM	CHD-C4C-NC	3.13	127.86	124.45
7	B	350	HEM	C1B-NB-C4B	2.85	108.58	105.21
7	D	350	HEM	CAD-CBD-CGD	-2.84	106.12	113.67
7	C	350	HEM	CMD-C2D-C1D	2.83	129.46	125.03
7	A	350	HEM	CAD-C3D-C4D	2.79	129.56	124.70
11	D	391	NAG	C1-C2-N2	2.78	114.81	110.43
7	C	350	HEM	C4C-C3C-C2C	2.69	109.15	106.81
11	D	391	NAG	C4-C3-C2	-2.69	107.08	111.02
7	A	350	HEM	CMD-C2D-C1D	2.66	129.19	125.03
7	A	350	HEM	C4C-C3C-C2C	2.65	109.11	106.81
7	D	350	HEM	C4C-C3C-C2C	2.61	109.08	106.81
7	D	350	HEM	CHD-C1D-ND	2.57	127.19	124.42
7	D	350	HEM	C3B-C2B-C1B	2.55	108.33	106.41
7	B	350	HEM	C2B-C1B-NB	-2.49	106.98	109.84
7	D	350	HEM	CHB-C1B-NB	2.45	127.40	124.37
7	B	350	HEM	CHD-C4C-NC	2.37	127.03	124.45
7	B	350	HEM	C3B-C2B-C1B	2.29	108.13	106.41
11	C	381	NAG	C3-C4-C5	2.23	114.27	110.23
7	D	350	HEM	CAD-C3D-C4D	2.21	128.54	124.70
7	D	350	HEM	CBC-CAC-C3C	-2.18	116.62	127.53
7	C	350	HEM	CBD-CAD-C3D	-2.15	106.59	112.53
7	A	350	HEM	CHD-C4C-NC	2.15	126.79	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	350	HEM	CMC-C2C-C1C	2.14	128.50	124.73
7	D	350	HEM	C3B-C4B-NB	-2.11	107.96	109.47
7	C	350	HEM	C1D-C2D-C3D	-2.09	104.79	106.98
11	D	391	NAG	C3-C4-C5	-2.07	106.47	110.23
7	C	350	HEM	C4A-C3A-C2A	2.06	109.17	106.82

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	NAG	C4-C5-C6-O6
11	C	381	NAG	O5-C5-C6-O6
11	D	391	NAG	O5-C5-C6-O6
11	D	391	NAG	C4-C5-C6-O6
7	A	350	HEM	C2A-CAA-CBA-CGA
7	D	350	HEM	C2A-CAA-CBA-CGA
7	B	350	HEM	C2A-CAA-CBA-CGA
7	C	350	HEM	C2A-CAA-CBA-CGA
7	A	350	HEM	CAA-CBA-CGA-O2A
7	C	350	HEM	CAA-CBA-CGA-O1A
7	B	350	HEM	CAA-CBA-CGA-O1A
7	A	350	HEM	C2B-C3B-CAB-CBB
7	D	350	HEM	CAA-CBA-CGA-O1A
7	C	350	HEM	C4B-C3B-CAB-CBB
7	A	350	HEM	CAA-CBA-CGA-O1A
7	B	350	HEM	CAA-CBA-CGA-O2A
7	C	350	HEM	CAA-CBA-CGA-O2A
7	D	350	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

9 monomers are involved in 22 short contacts:

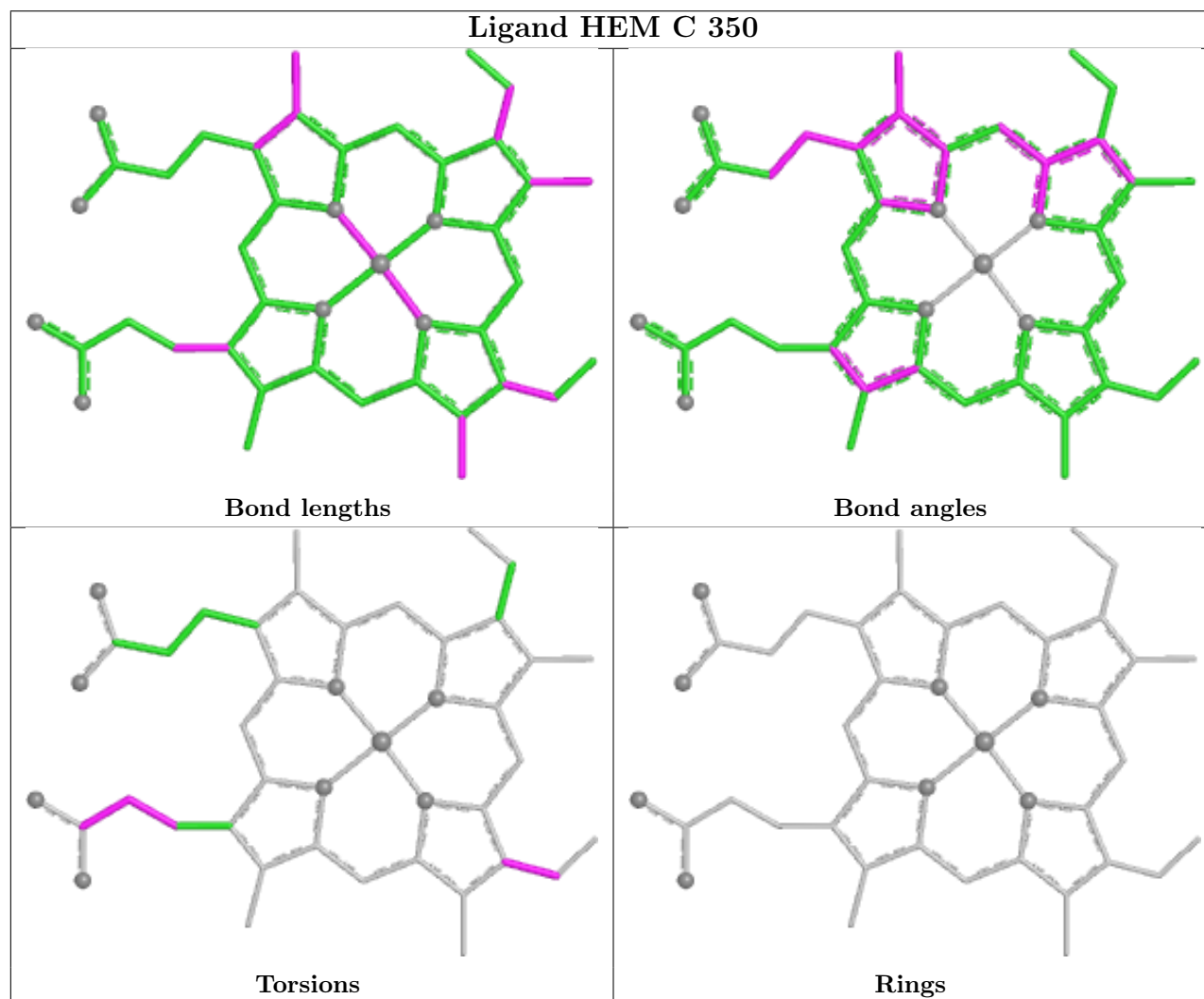
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	350	HEM	3	0
10	D	1328	SO4	1	0
7	A	350	HEM	5	0
7	B	350	HEM	3	0
11	C	381	NAG	1	0
10	D	1329	SO4	1	0
10	A	1331	SO4	3	0
7	D	350	HEM	3	0

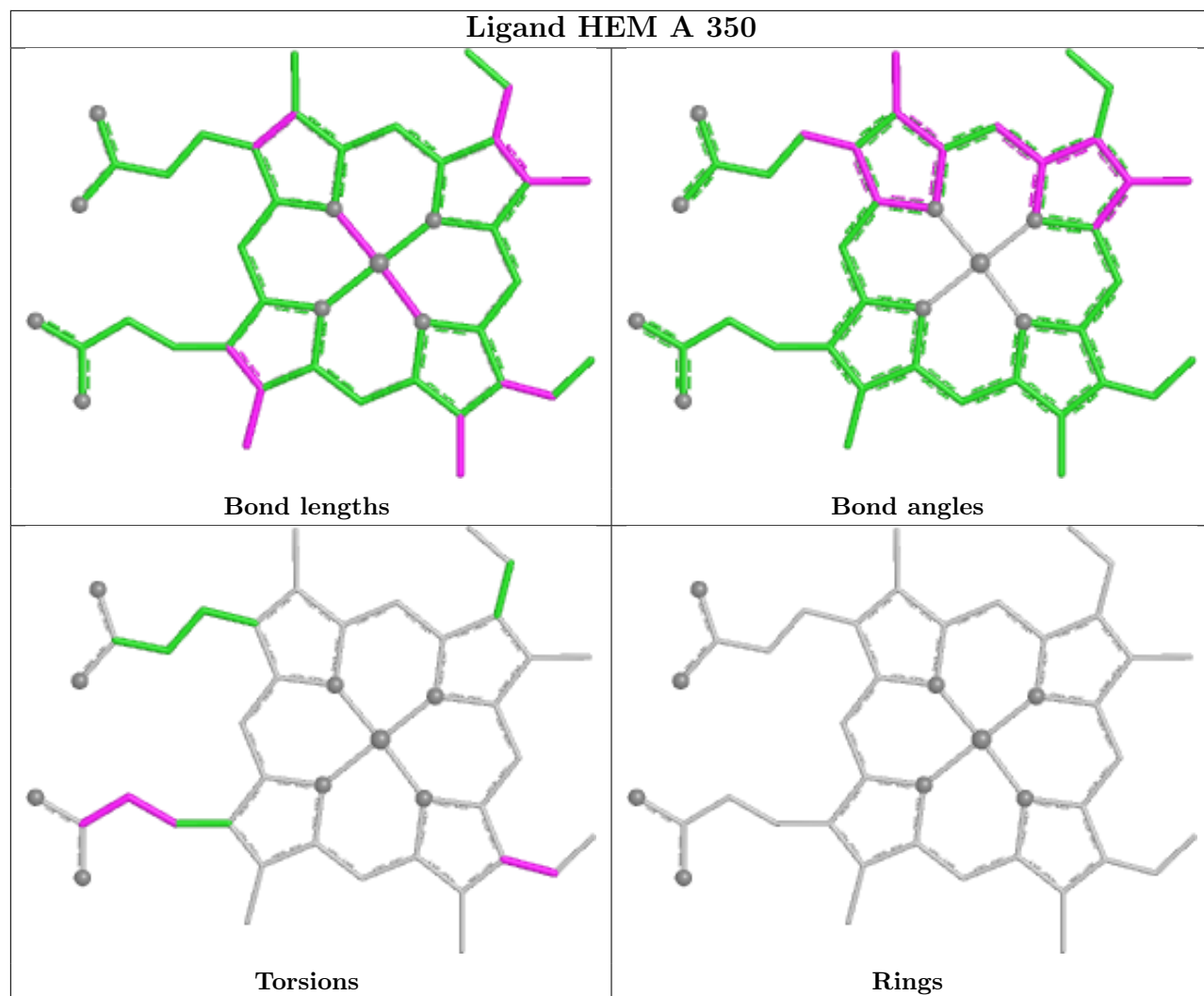
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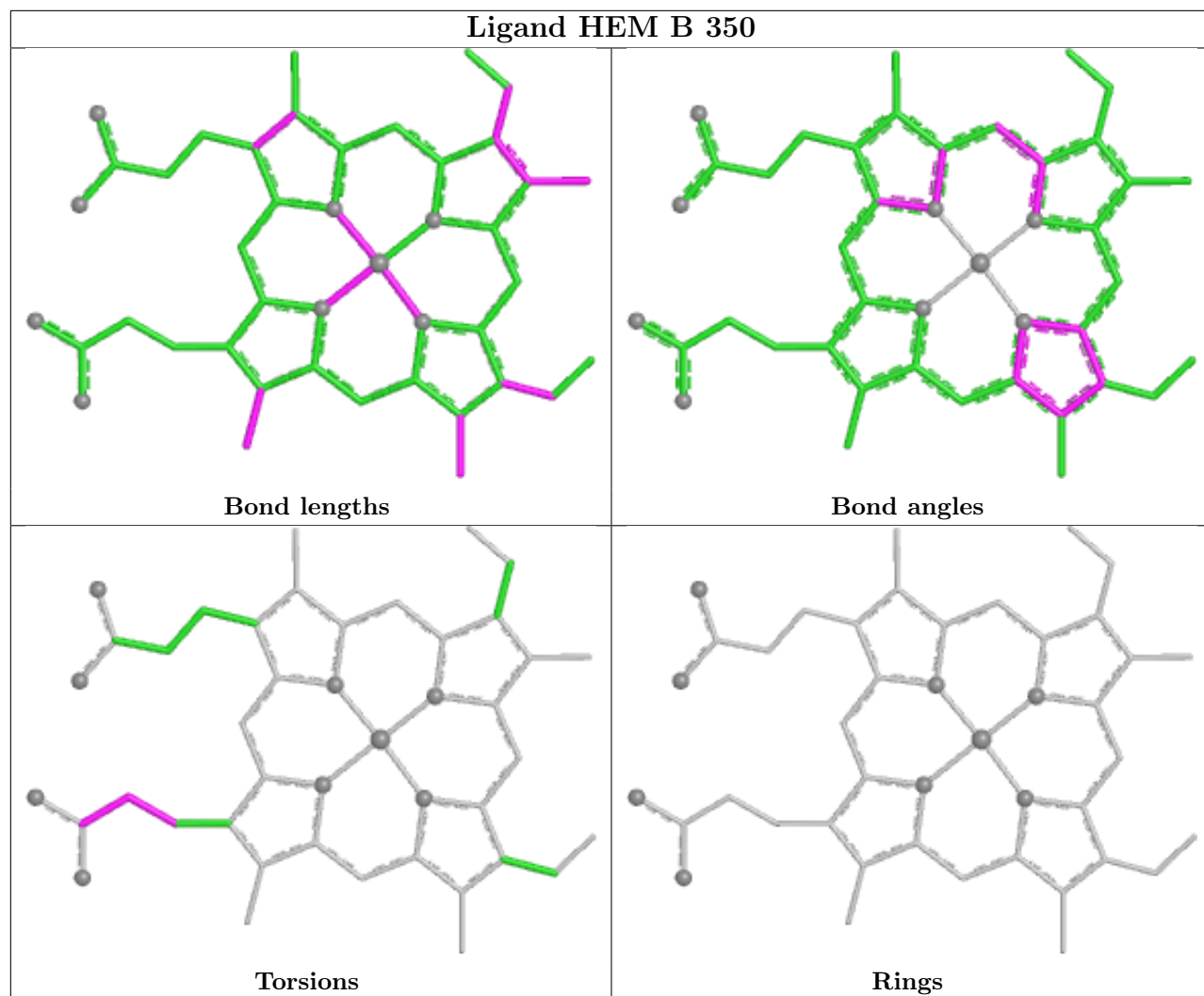
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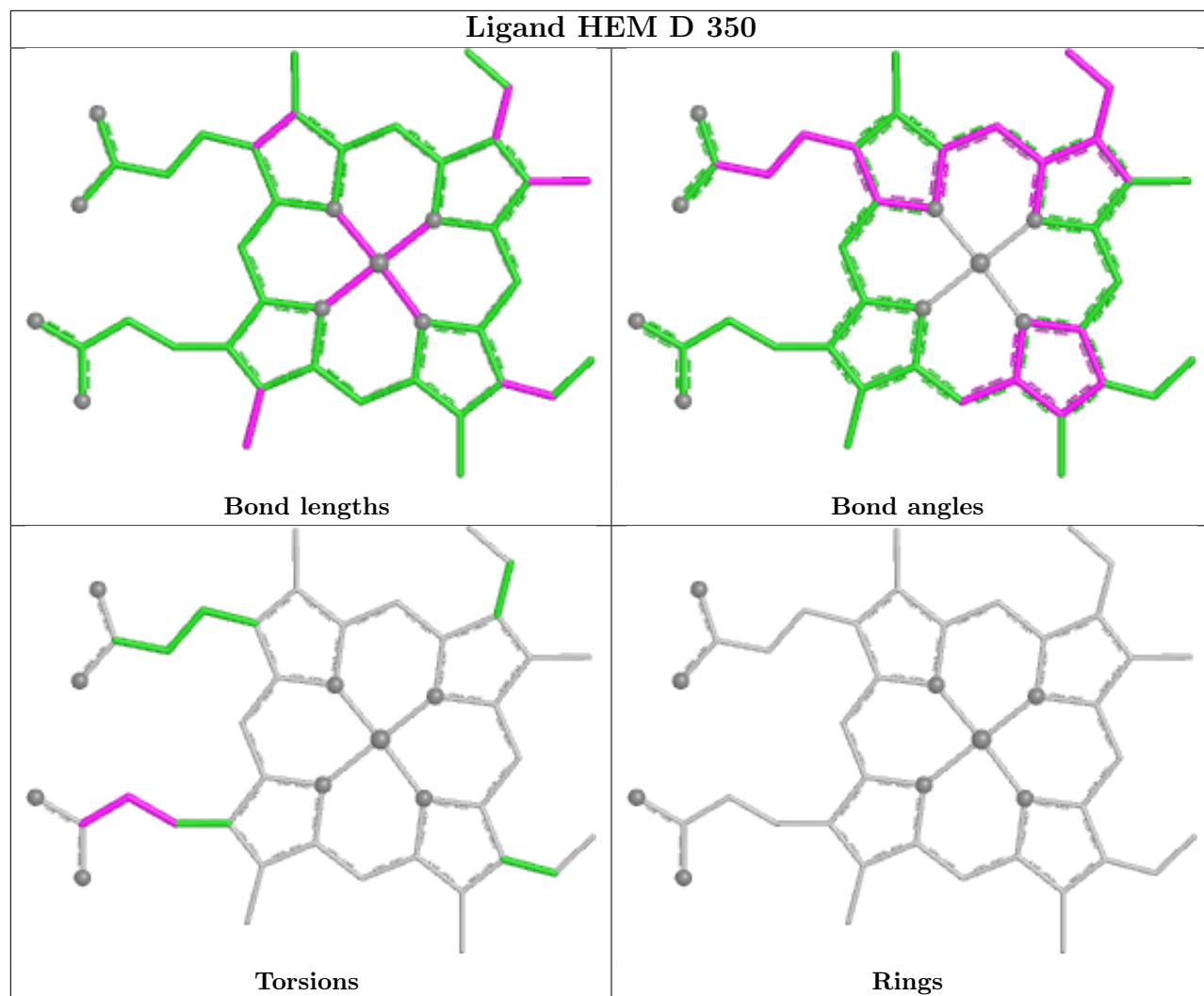
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1331	SO4	2	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/325 (99%)	-0.33	2 (0%) 85 86	12, 26, 42, 56	1 (0%)
1	B	324/325 (99%)	-0.61	2 (0%) 85 86	10, 21, 34, 53	4 (1%)
1	C	325/325 (100%)	-0.47	1 (0%) 90 90	14, 24, 37, 68	1 (0%)
1	D	323/325 (99%)	-0.06	2 (0%) 85 86	15, 32, 47, 59	1 (0%)
All	All	1295/1300 (99%)	-0.37	7 (0%) 87 88	10, 26, 43, 68	7 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	328	ASP	3.4
1	A	326	GLY	2.8
1	B	327	ARG	2.5
1	D	30	GLY	2.5
1	A	299	GLN	2.3
1	B	135	GLY	2.3
1	D	326	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	O	3	11/12	0.43	0.19	75,78,79,79	0
3	MAN	J	5	11/12	0.45	0.23	78,80,81,81	0
2	MAN	E	5	11/12	0.55	0.17	66,68,70,71	0
2	MAN	E	6	11/12	0.63	0.20	64,65,66,67	0
4	NAG	I	2	14/15	0.63	0.18	75,78,81,81	0
3	MAN	F	5	11/12	0.63	0.17	88,90,90,91	0
4	NAG	N	2	14/15	0.65	0.17	74,77,79,81	0
3	MAN	F	4	11/12	0.68	0.17	79,81,84,88	0
3	BMA	J	3	11/12	0.69	0.16	59,62,64,66	0
3	MAN	J	4	11/12	0.73	0.17	67,69,72,75	0
3	BMA	F	3	11/12	0.74	0.16	56,58,68,74	0
6	BMA	T	3	11/12	0.74	0.13	58,60,62,62	0
4	NAG	R	2	14/15	0.76	0.15	73,76,77,78	0
4	NAG	G	2	14/15	0.78	0.15	57,61,65,66	0
3	NAG	J	2	14/15	0.78	0.14	45,50,52,56	0
5	MAN	H	5	11/12	0.79	0.18	58,64,65,65	0
5	MAN	H	8	11/12	0.80	0.16	60,61,63,64	0
4	NAG	S	2	14/15	0.80	0.14	60,62,65,66	0
4	NAG	Q	2	14/15	0.80	0.15	56,60,63,65	0
5	MAN	H	4	11/12	0.81	0.14	55,59,60,62	0
4	NAG	L	2	14/15	0.82	0.15	57,59,63,64	0
4	NAG	K	2	14/15	0.82	0.15	43,49,52,53	0
3	NAG	F	2	14/15	0.84	0.12	37,42,46,52	0
6	NAG	O	2	14/15	0.84	0.13	58,61,65,70	0
5	MAN	M	8	11/12	0.85	0.12	47,50,52,52	0
4	NAG	P	2	14/15	0.85	0.15	47,53,55,58	0
4	NAG	R	1	14/15	0.86	0.13	55,60,64,69	0
2	NAG	E	2	14/15	0.87	0.12	40,46,53,56	0
5	MAN	M	5	11/12	0.87	0.15	52,55,57,58	0
4	NAG	I	1	14/15	0.88	0.12	56,64,68,70	0
2	BMA	E	3	11/12	0.88	0.10	49,54,59,62	0
6	NAG	T	2	14/15	0.88	0.12	48,52,58,58	0
4	NAG	Q	1	14/15	0.88	0.11	31,42,48,51	0
5	MAN	H	6	11/12	0.89	0.12	46,49,55,59	0
2	MAN	E	4	11/12	0.89	0.10	51,54,58,63	0
4	NAG	N	1	14/15	0.89	0.10	51,57,62,69	0
4	NAG	S	1	14/15	0.89	0.12	50,54,56,59	0
5	MAN	M	4	11/12	0.91	0.09	40,43,45,50	0
6	NAG	O	1	14/15	0.91	0.09	41,46,49,54	0
5	NAG	H	1	14/15	0.91	0.08	34,39,42,43	0
5	MAN	H	7	11/12	0.92	0.12	52,53,54,55	0
4	NAG	G	1	14/15	0.92	0.08	39,43,47,54	0
5	NAG	H	2	14/15	0.93	0.09	42,45,47,47	0

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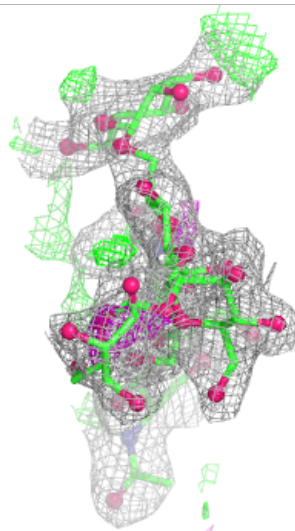
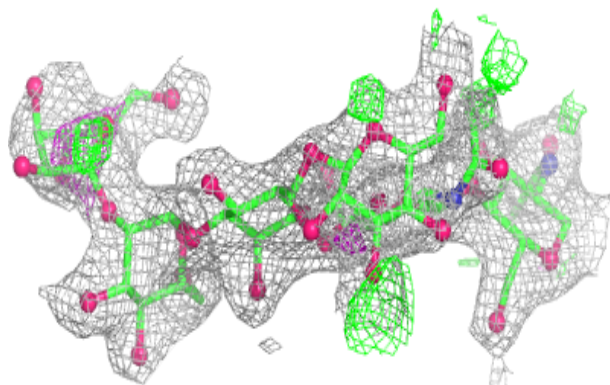
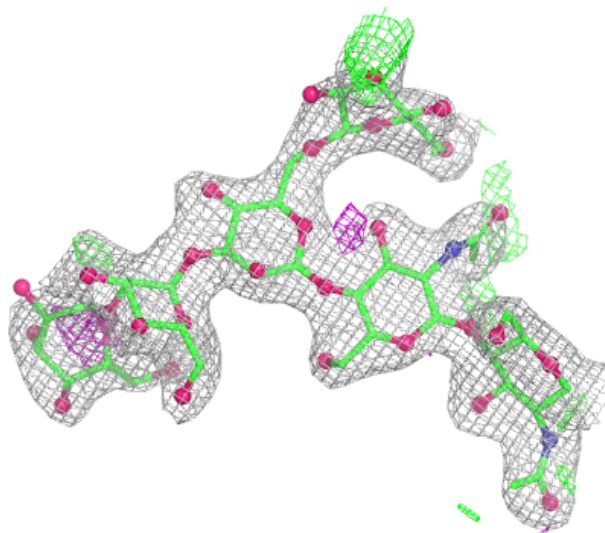
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	M	6	11/12	0.93	0.09	26,30,36,45	0
6	NAG	T	1	14/15	0.93	0.09	26,34,39,43	0
5	NAG	M	2	14/15	0.93	0.09	23,31,34,40	0
5	BMA	H	3	11/12	0.93	0.11	40,44,47,48	0
5	MAN	M	7	11/12	0.94	0.08	27,31,32,34	0
2	NAG	E	1	14/15	0.94	0.07	33,36,41,41	0
4	NAG	L	1	14/15	0.94	0.07	39,42,46,53	0
3	NAG	J	1	14/15	0.94	0.07	30,34,41,45	0
5	NAG	M	1	14/15	0.95	0.07	26,30,32,37	0
4	NAG	P	1	14/15	0.96	0.07	25,30,36,42	0
5	BMA	M	3	11/12	0.97	0.06	30,33,36,37	0
4	NAG	K	1	14/15	0.97	0.06	16,23,29,36	0
3	NAG	F	1	14/15	0.98	0.06	18,21,26,30	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.

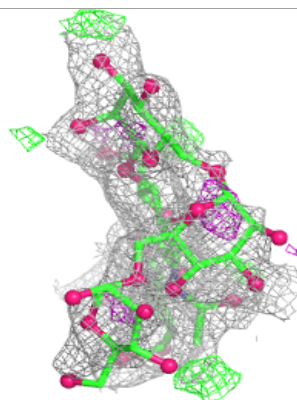
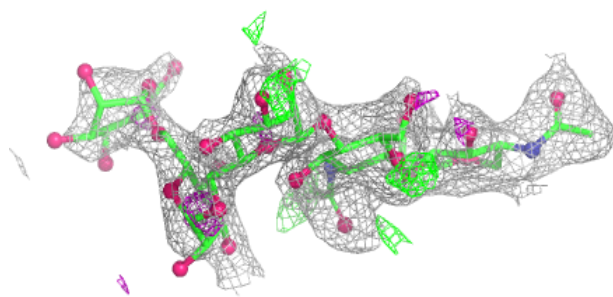
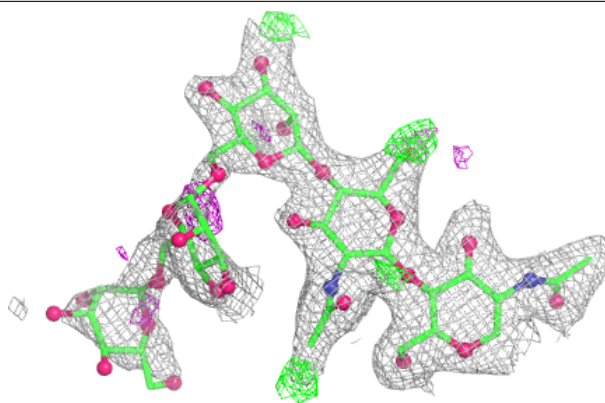
Electron density around Chain E:

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and green (positive)

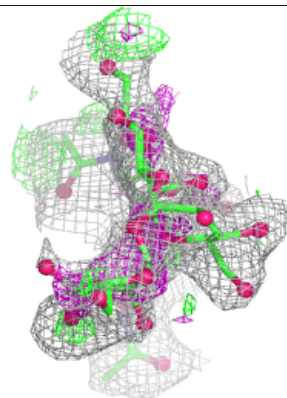
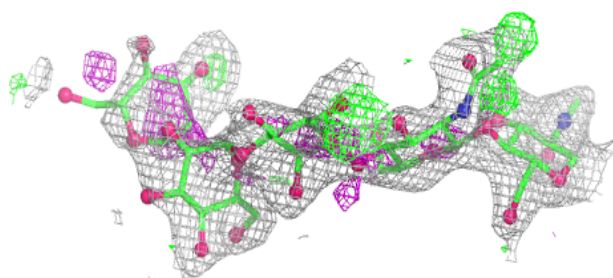
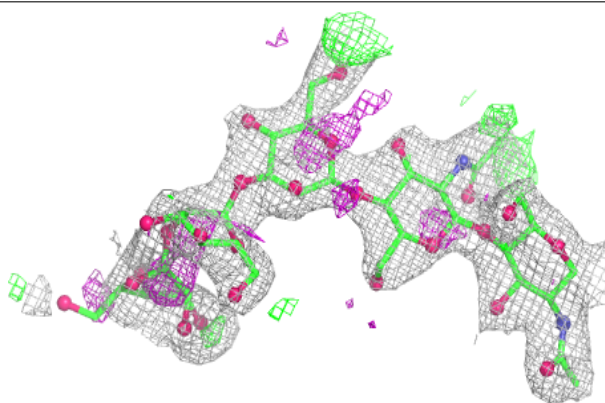


Electron density around Chain F:

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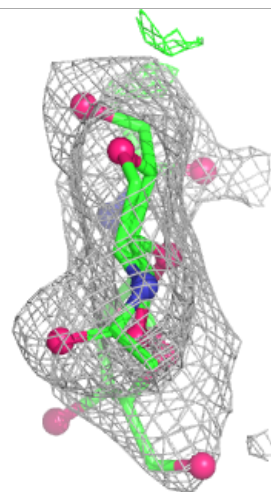
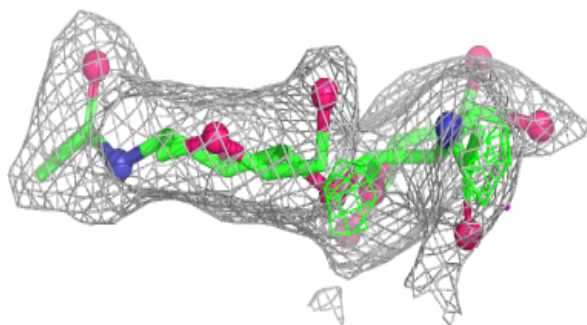
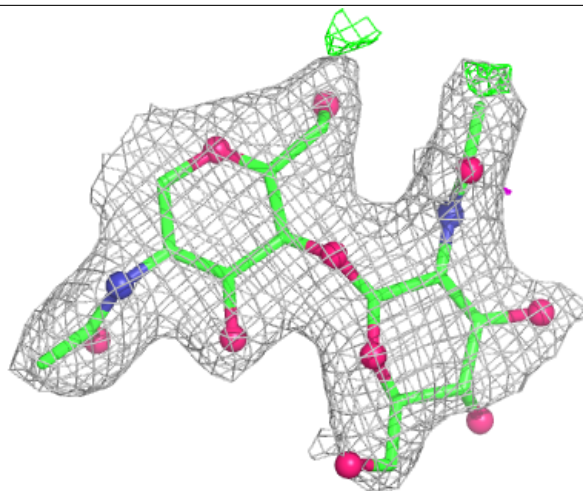
**Electron density around Chain J:**

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and green (positive)



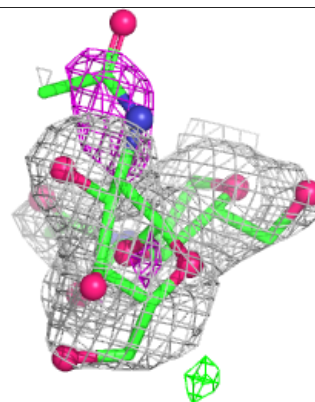
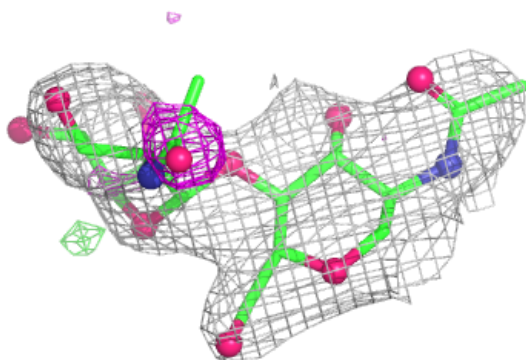
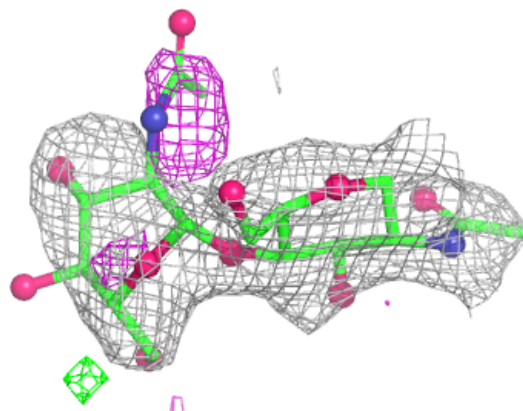
Electron density around Chain G:

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and green (positive)



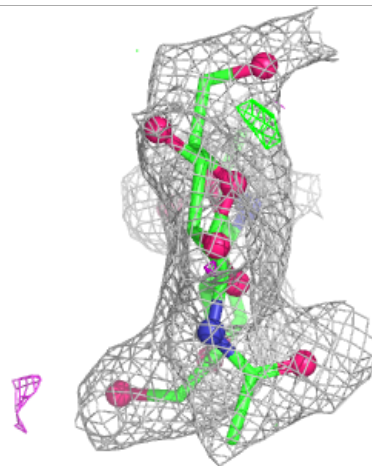
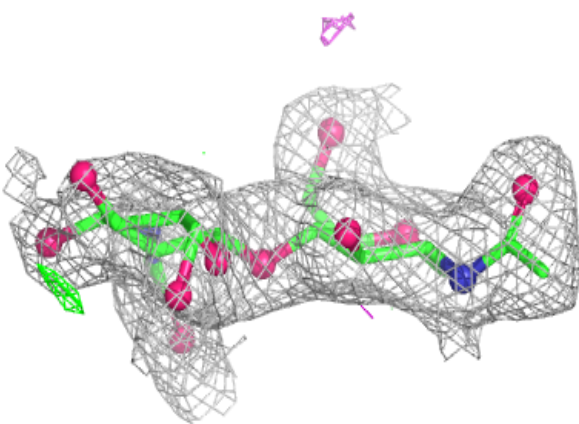
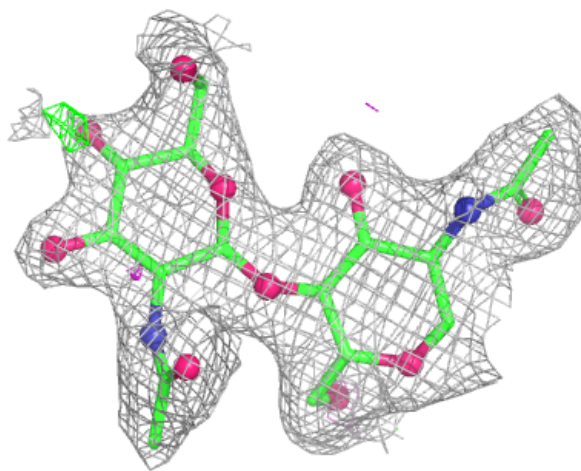
Electron density around Chain I:

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and green (positive)



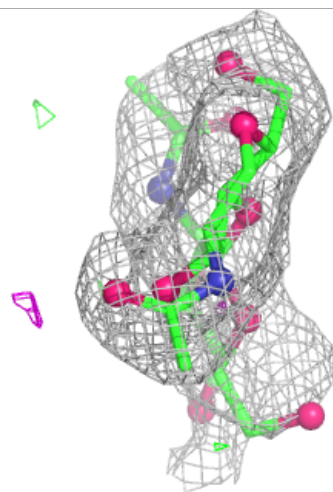
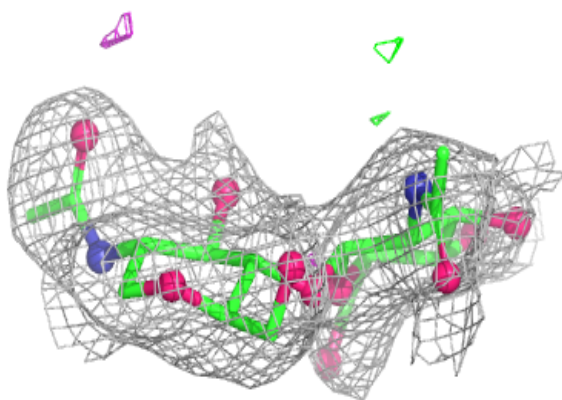
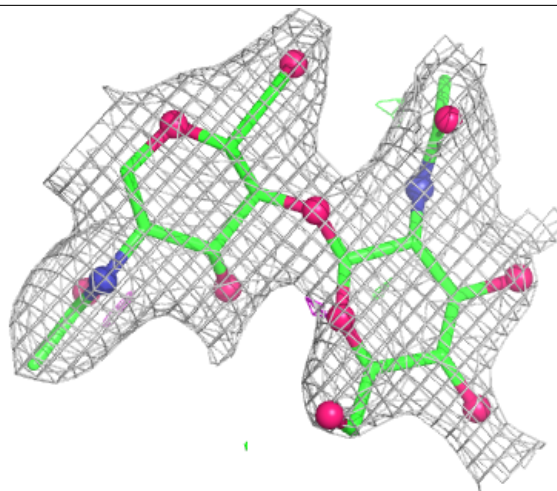
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



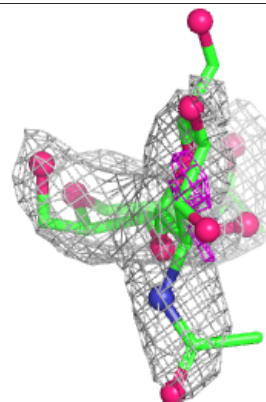
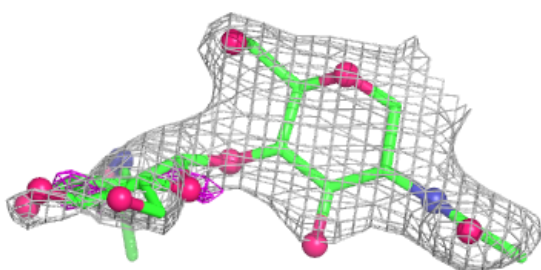
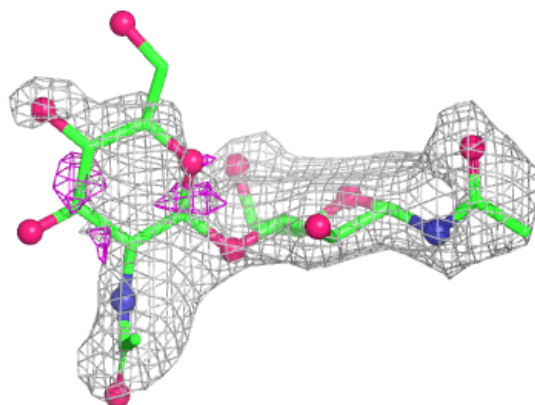
Electron density around Chain L:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



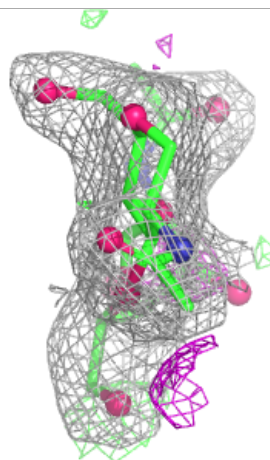
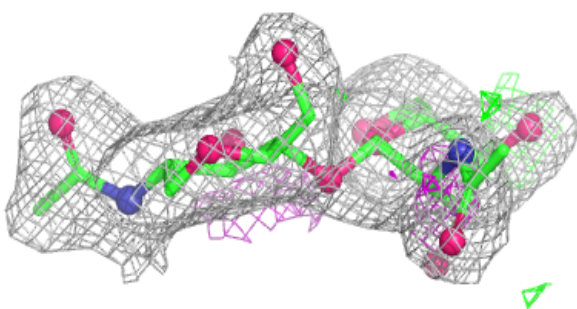
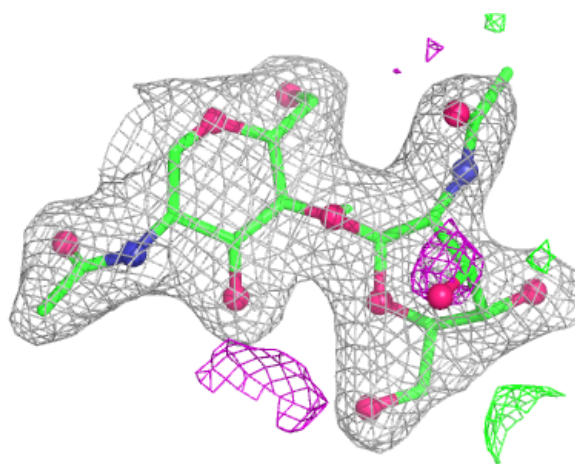
Electron density around Chain N:

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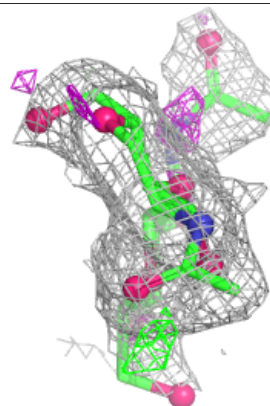
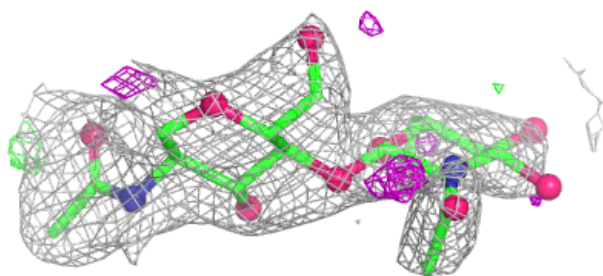
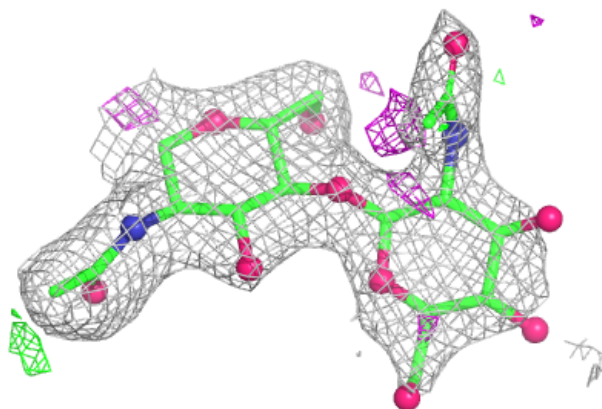
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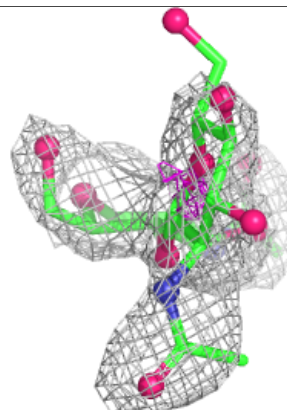
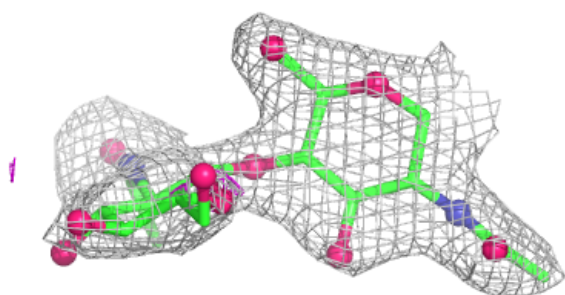
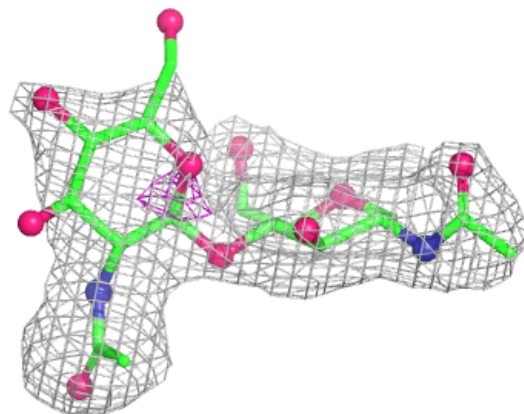


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and green (positive)

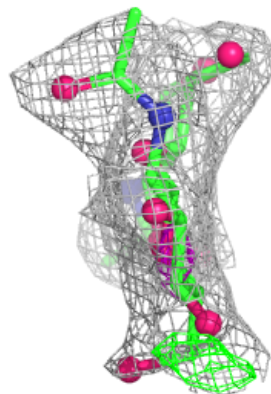
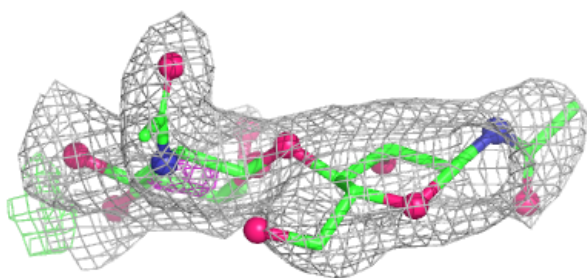
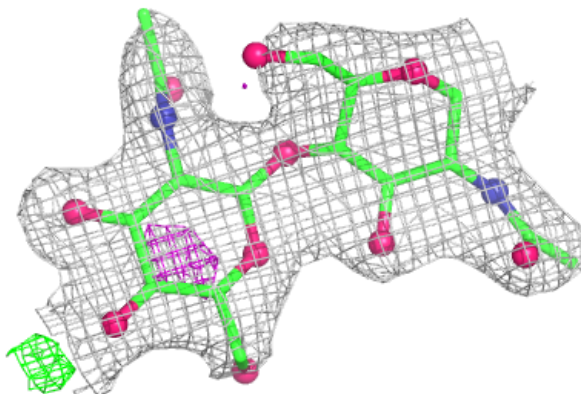
**Electron density around Chain R:**

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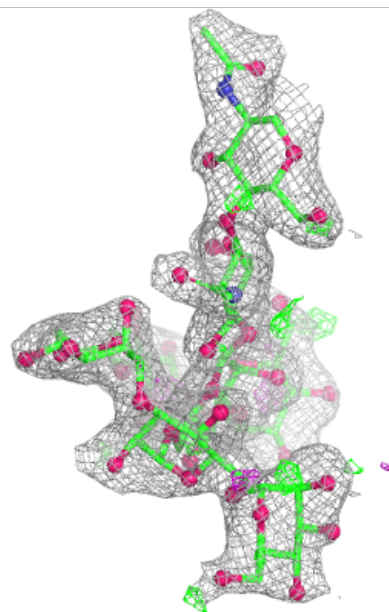
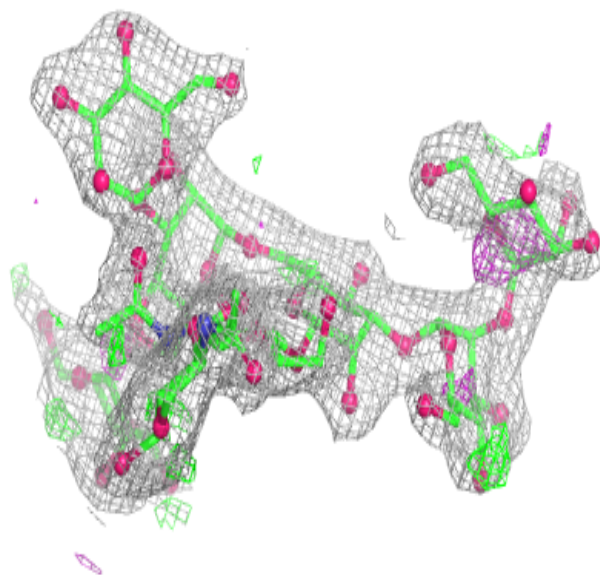
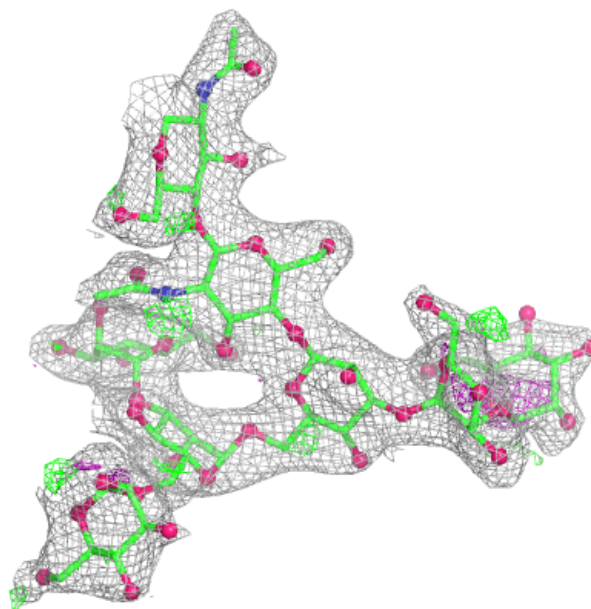
Electron density around Chain S:

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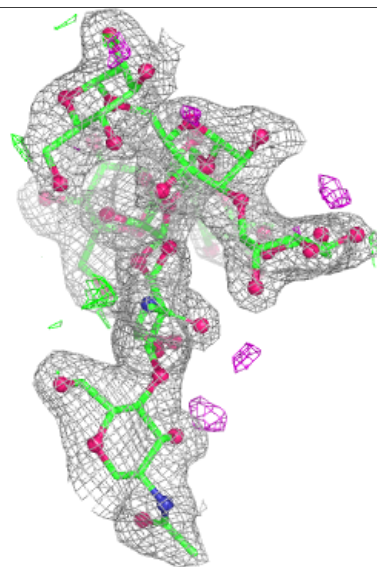
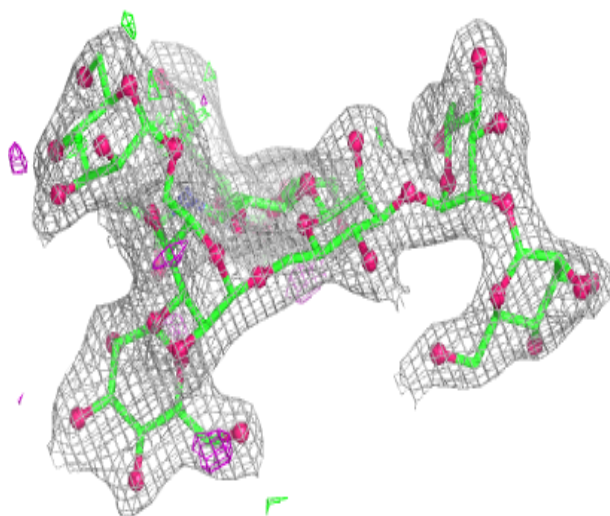
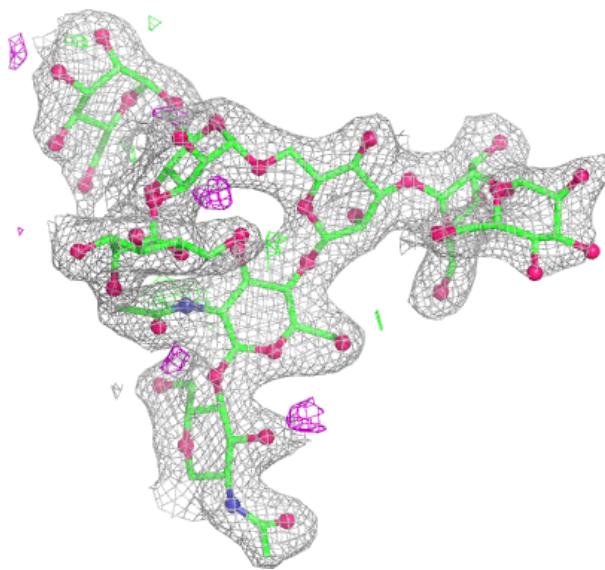
Electron density around Chain H:

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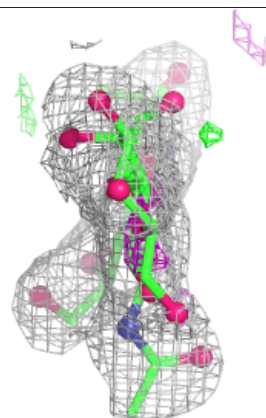
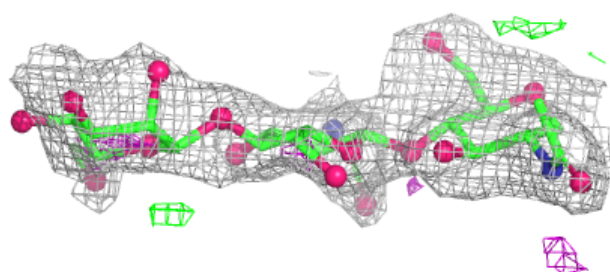
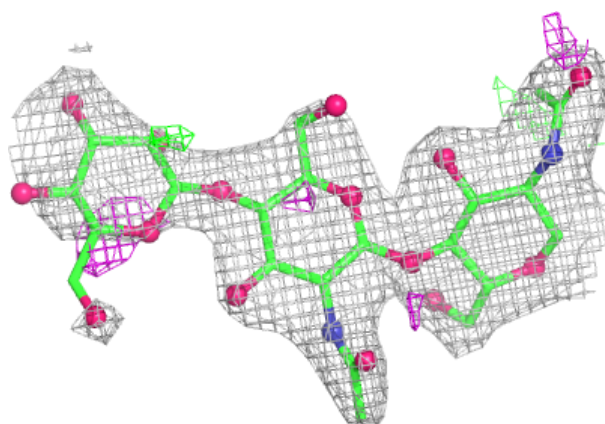
Electron density around Chain M:

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and green (positive)

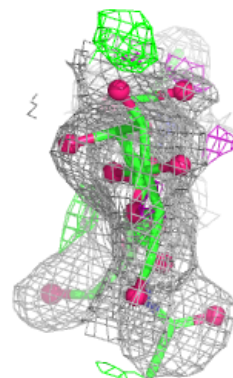
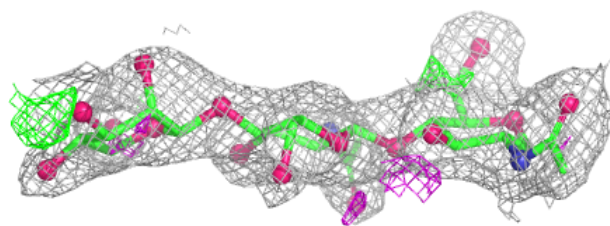
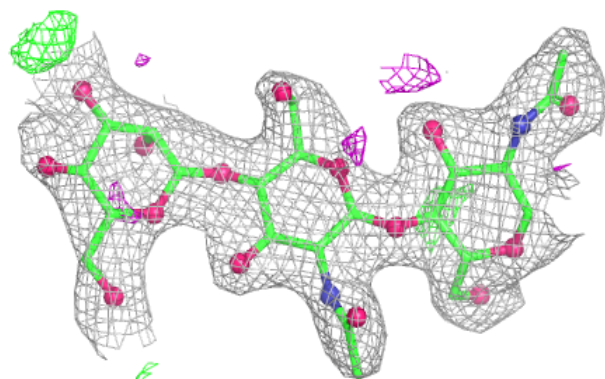


Electron density around Chain O:

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and green (positive)

**Electron density around Chain T:**

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and green (positive)



6.4 Ligands ⓘ

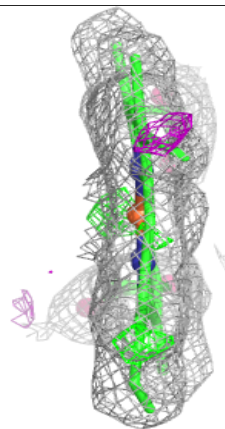
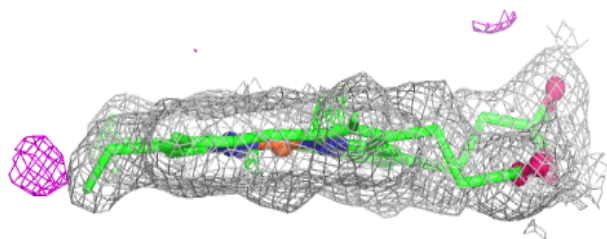
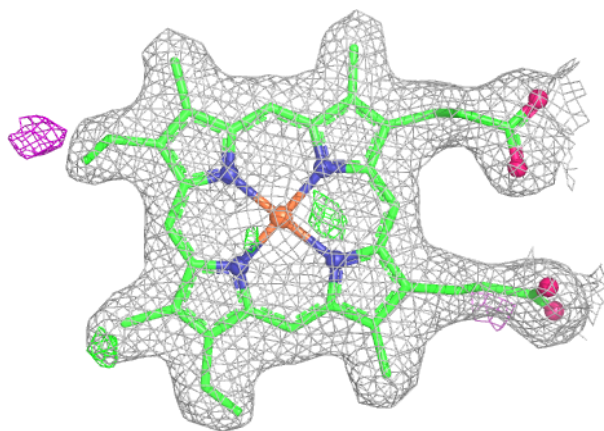
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	D	381	14/15	0.81	0.13	54,57,61,62	0
11	NAG	C	381	14/15	0.83	0.12	50,54,57,58	0
10	SO4	C	1331	5/5	0.84	0.14	87,88,88,89	0
10	SO4	B	1330	5/5	0.85	0.15	65,65,65,66	0
10	SO4	A	1329	5/5	0.87	0.12	70,71,71,72	0
10	SO4	B	1329	5/5	0.87	0.14	57,58,61,62	0
11	NAG	D	391	14/15	0.89	0.10	46,48,51,53	0
10	SO4	C	1333	5/5	0.90	0.19	74,75,75,75	0
10	SO4	A	1328	5/5	0.90	0.12	56,56,58,59	0
11	NAG	D	411	14/15	0.90	0.11	53,56,58,59	0
10	SO4	C	1330	5/5	0.91	0.10	61,62,63,63	0
10	SO4	D	1328	5/5	0.91	0.12	60,60,61,62	0
9	ACT	C	1329	4/4	0.92	0.13	31,34,37,38	0
9	ACT	D	1327	4/4	0.92	0.15	48,49,49,50	0
10	SO4	A	1331	5/5	0.93	0.19	60,60,61,63	0
9	ACT	A	1327	4/4	0.93	0.17	30,32,32,32	0
10	SO4	A	1330	5/5	0.93	0.15	59,62,63,63	0
10	SO4	B	1331	5/5	0.93	0.19	68,69,69,71	0
10	SO4	C	1332	5/5	0.94	0.16	62,62,63,63	0
9	ACT	B	1328	4/4	0.95	0.10	25,25,30,32	0
10	SO4	D	1329	5/5	0.95	0.15	55,56,58,58	0
8	MG	A	353	1/1	0.97	0.05	18,18,18,18	0
7	HEM	A	350	43/43	0.98	0.07	12,19,21,27	0
9	ACT	C	1334	4/4	0.98	0.05	24,27,29,30	0
8	MG	D	353	1/1	0.98	0.04	26,26,26,26	0
7	HEM	C	350	43/43	0.98	0.06	13,17,22,26	0
7	HEM	D	350	43/43	0.98	0.07	18,23,28,33	0
7	HEM	B	350	43/43	0.99	0.05	6,13,16,22	0
8	MG	C	353	1/1	1.00	0.02	19,19,19,19	0
8	MG	B	353	1/1	1.00	0.02	12,12,12,12	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.

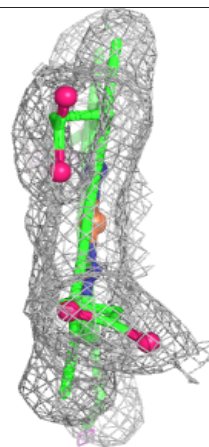
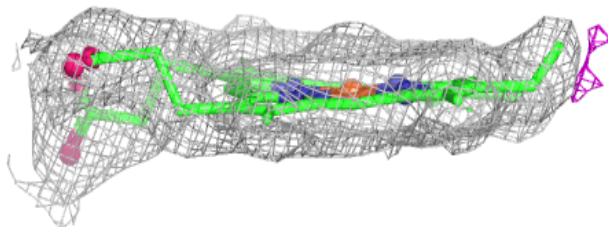
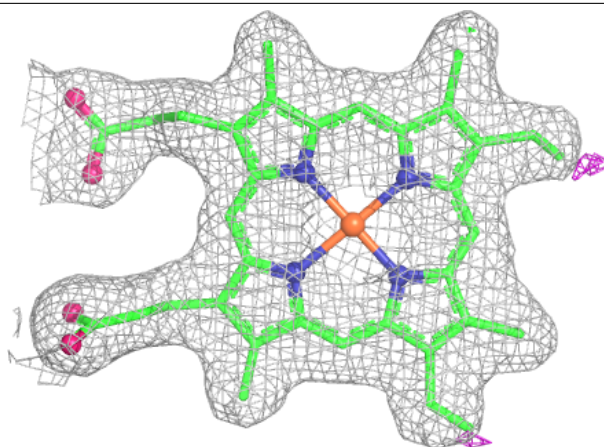
Electron density around HEM A 350:

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



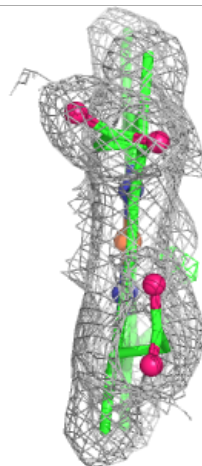
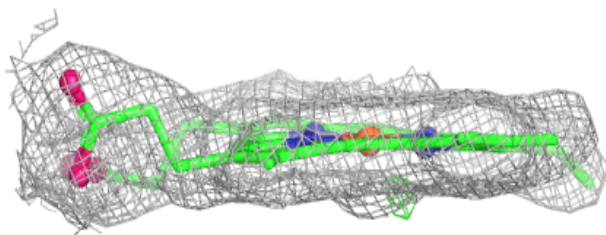
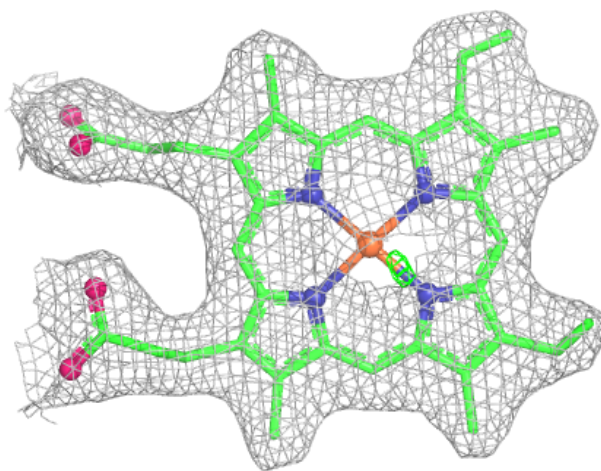
Electron density around HEM C 350:

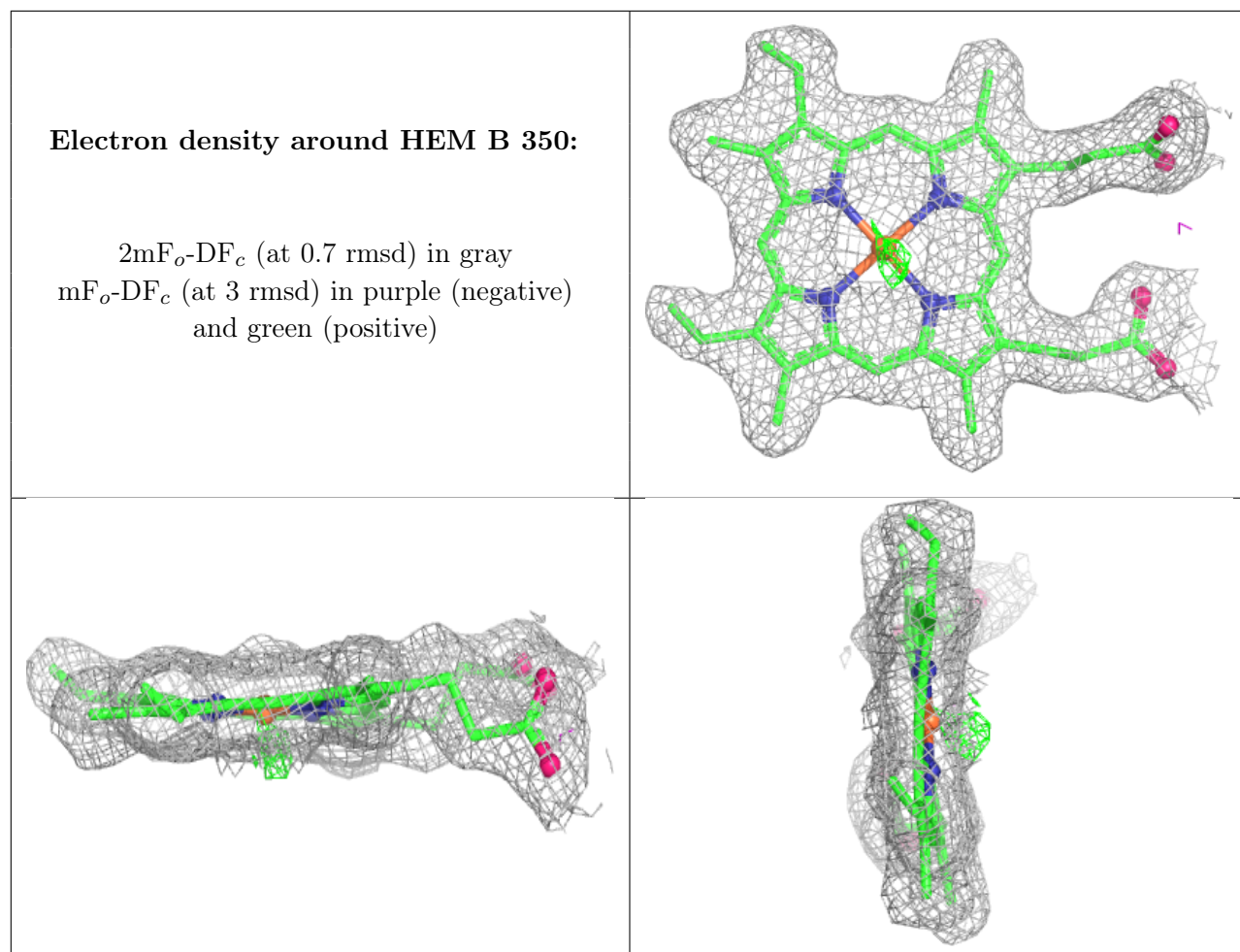
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 350:

$2mF_o-DF_c$ (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.