



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:04 AM UTC

PDB ID : 9VBW / pdb\_00009vbw  
Title : Lectin FRIL from Lablab purpureus complexed to Lewis X tetrasaccharide  
Authors : Nguyen, V.H.T.; Chen, T.H.; Chen, X.; Liu, Y.M.; Ma, C.  
Deposited on : 2025-06-05  
Resolution : 2.49 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

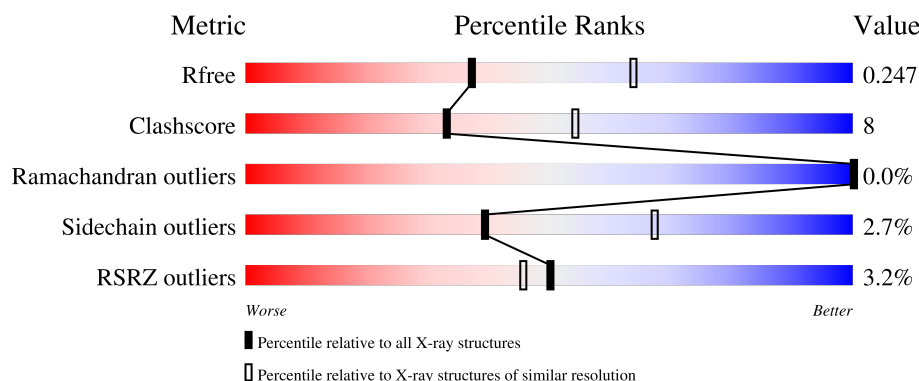
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	264	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	264	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	264	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	264	<div> <div>0%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>



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Mol	Chain	Length	Quality of chain
1	F	264	
1	G	264	
1	H	264	
1	I	264	
1	J	264	
1	K	264	
1	L	264	
1	M	264	
1	N	264	
1	O	264	
1	P	264	
2	a	4	
2	b	4	
2	c	4	
2	d	4	
2	e	4	
2	f	4	
2	g	4	
2	h	4	
2	i	4	
2	j	4	
2	k	4	
2	l	4	
2	m	4	
2	n	4	

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Mol	Chain	Length	Quality of chain
2	o	4	 100%
2	p	4	 75% 25%



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30738 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 Flt3 receptor-interacting lectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	0	0	0
			1817	1160	301	356			
1	E	234	Total	C	N	O	0	0	0
			1822	1163	302	357			
1	C	234	Total	C	N	O	0	0	0
			1822	1163	302	357			
1	G	232	Total	C	N	O	0	0	0
			1812	1157	300	355			
1	I	232	Total	C	N	O	0	0	0
			1812	1157	300	355			
1	M	232	Total	C	N	O	0	0	0
			1812	1157	300	355			
1	H	232	Total	C	N	O	0	0	0
			1812	1157	300	355			
1	D	233	Total	C	N	O	0	0	0
			1817	1160	301	356			
1	J	232	Total	C	N	O	0	0	0
			1812	1157	300	355			
1	P	232	Total	C	N	O	0	1	0
			1823	1163	304	356			
1	L	234	Total	C	N	O	0	0	0
			1822	1163	302	357			
1	O	234	Total	C	N	O	0	0	0
			1822	1163	302	357			
1	B	234	Total	C	N	O	0	1	0
			1830	1167	304	359			
1	F	234	Total	C	N	O	0	0	0
			1822	1163	302	357			
1	N	233	Total	C	N	O	0	0	0
			1817	1160	301	356			
1	K	234	Total	C	N	O	0	0	0
			1822	1163	302	357			

There are 48 discrepancies between the modelled and reference sequences:

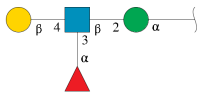
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	LEU	VAL	variant	UNP Q9ZTA9
A	195	THR	SER	variant	UNP Q9ZTA9
A	198	PRO	ALA	variant	UNP Q9ZTA9
E	33	LEU	VAL	variant	UNP Q9ZTA9
E	195	THR	SER	variant	UNP Q9ZTA9
E	198	PRO	ALA	variant	UNP Q9ZTA9
C	33	LEU	VAL	variant	UNP Q9ZTA9
C	195	THR	SER	variant	UNP Q9ZTA9
C	198	PRO	ALA	variant	UNP Q9ZTA9
G	33	LEU	VAL	variant	UNP Q9ZTA9
G	195	THR	SER	variant	UNP Q9ZTA9
G	198	PRO	ALA	variant	UNP Q9ZTA9
I	33	LEU	VAL	variant	UNP Q9ZTA9
I	195	THR	SER	variant	UNP Q9ZTA9
I	198	PRO	ALA	variant	UNP Q9ZTA9
M	33	LEU	VAL	variant	UNP Q9ZTA9
M	195	THR	SER	variant	UNP Q9ZTA9
M	198	PRO	ALA	variant	UNP Q9ZTA9
H	33	LEU	VAL	variant	UNP Q9ZTA9
H	195	THR	SER	variant	UNP Q9ZTA9
H	198	PRO	ALA	variant	UNP Q9ZTA9
D	33	LEU	VAL	variant	UNP Q9ZTA9
D	195	THR	SER	variant	UNP Q9ZTA9
D	198	PRO	ALA	variant	UNP Q9ZTA9
J	33	LEU	VAL	variant	UNP Q9ZTA9
J	195	THR	SER	variant	UNP Q9ZTA9
J	198	PRO	ALA	variant	UNP Q9ZTA9
P	33	LEU	VAL	variant	UNP Q9ZTA9
P	195	THR	SER	variant	UNP Q9ZTA9
P	198	PRO	ALA	variant	UNP Q9ZTA9
L	33	LEU	VAL	variant	UNP Q9ZTA9
L	195	THR	SER	variant	UNP Q9ZTA9
L	198	PRO	ALA	variant	UNP Q9ZTA9
O	33	LEU	VAL	variant	UNP Q9ZTA9
O	195	THR	SER	variant	UNP Q9ZTA9
O	198	PRO	ALA	variant	UNP Q9ZTA9
B	33	LEU	VAL	variant	UNP Q9ZTA9
B	195	THR	SER	variant	UNP Q9ZTA9
B	198	PRO	ALA	variant	UNP Q9ZTA9
F	33	LEU	VAL	variant	UNP Q9ZTA9
F	195	THR	SER	variant	UNP Q9ZTA9
F	198	PRO	ALA	variant	UNP Q9ZTA9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	33	LEU	VAL	variant	UNP Q9ZTA9
N	195	THR	SER	variant	UNP Q9ZTA9
N	198	PRO	ALA	variant	UNP Q9ZTA9
K	33	LEU	VAL	variant	UNP Q9ZTA9
K	195	THR	SER	variant	UNP Q9ZTA9
K	198	PRO	ALA	variant	UNP Q9ZTA9

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	a	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	e	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	c	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	g	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	i	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	m	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	h	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	d	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	j	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	n	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	p	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	l	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	o	4	Total	C	N	O	0	0	0
			47	26	1	20			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	k	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	b	4	Total	C	N	O	0	0	0
			47	26	1	20			
2	f	4	Total	C	N	O	0	0	0
			47	26	1	20			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		
3	M	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	J	1	Total	Ca	0	0
			1	1		
3	P	1	Total	Ca	0	0
			1	1		
3	L	1	Total	Ca	0	0
			1	1		
3	O	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	N	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	E	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	G	1	Total Mn 1 1	0	0
4	I	1	Total Mn 1 1	0	0
4	M	1	Total Mn 1 1	0	0
4	H	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0
4	J	1	Total Mn 1 1	0	0
4	P	1	Total Mn 1 1	0	0
4	L	1	Total Mn 1 1	0	0
4	O	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	F	1	Total Mn 1 1	0	0
4	N	1	Total Mn 1 1	0	0
4	K	1	Total Mn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	E	46	Total O 46 46	0	0

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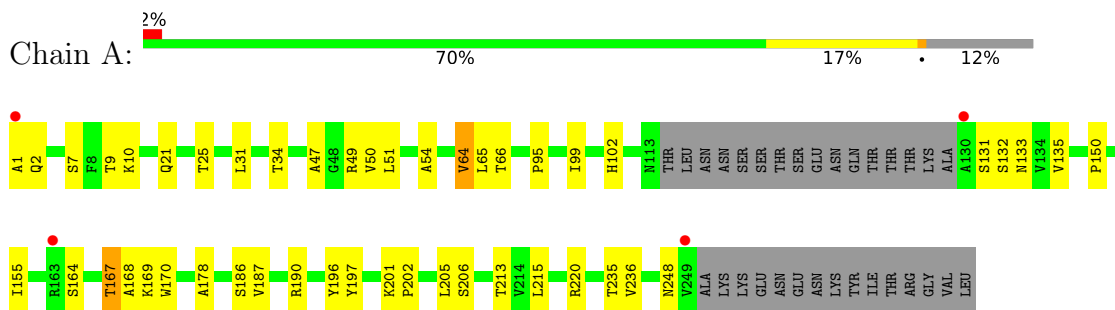
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	51	Total 51	O 51	0	0
5	G	63	Total 63	O 63	0	0
5	I	45	Total 45	O 45	0	0
5	M	74	Total 74	O 74	0	0
5	H	66	Total 66	O 66	0	0
5	D	58	Total 58	O 58	0	0
5	J	79	Total 79	O 79	0	0
5	P	41	Total 41	O 41	0	0
5	L	45	Total 45	O 45	0	0
5	O	51	Total 51	O 51	0	0
5	B	44	Total 44	O 44	0	0
5	F	42	Total 42	O 42	0	0
5	N	78	Total 78	O 78	0	0
5	K	25	Total 25	O 25	0	0

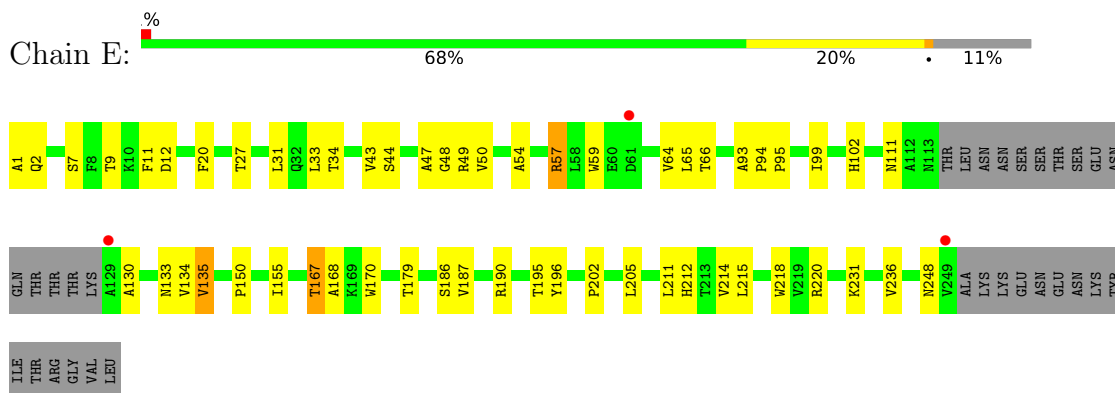
### 3 Residue-property plots [i](#)

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

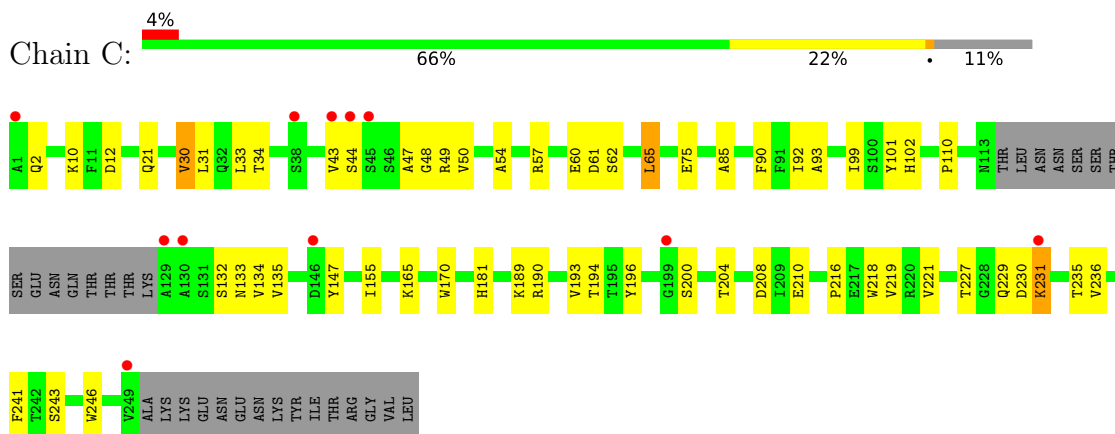
- Molecule 1: Flt3 receptor-interacting lectin



- Molecule 1: Flt3 receptor-interacting lectin

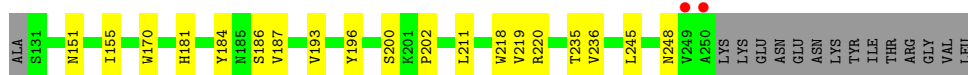


- Molecule 1: Flt3 receptor-interacting lectin



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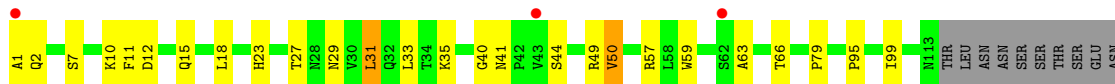




• Molecule 1: Flt3 receptor-interacting lectin



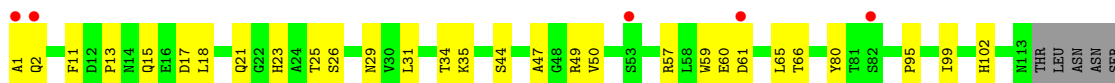
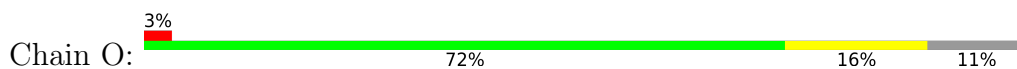
• Molecule 1: Flt3 receptor-interacting lectin



• Molecule 1: Flt3 receptor-interacting lectin

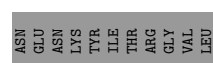
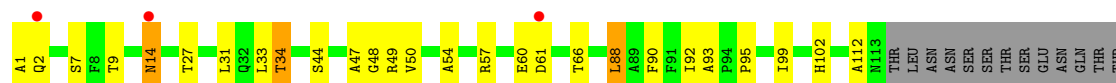


• Molecule 1: Flt3 receptor-interacting lectin

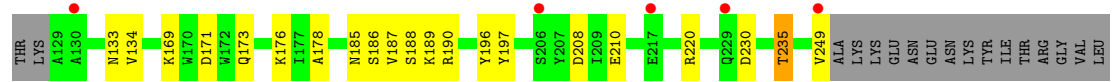




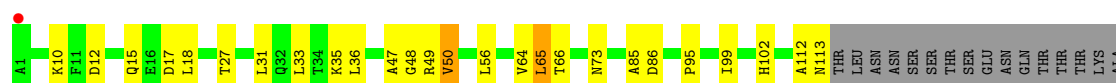
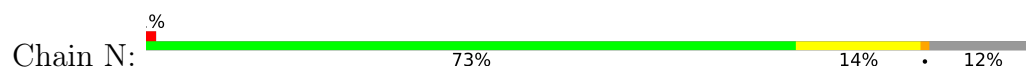
• Molecule 1: Flt3 receptor-interacting lectin



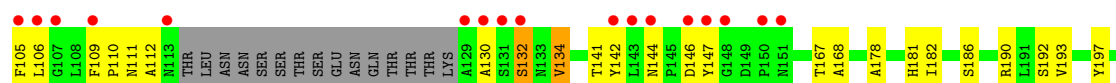
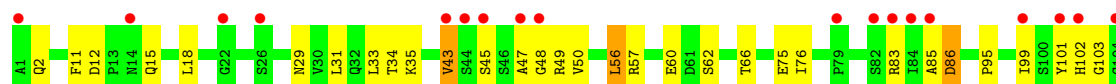
• Molecule 1: Flt3 receptor-interacting lectin



• Molecule 1: Flt3 receptor-interacting lectin



• Molecule 1: Flt3 receptor-interacting lectin





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

Chain a:  100%



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

Chain e:  100%



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

Chain c:  50%



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

Chain g:  25%



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

Chain i:  100%



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

Chain m:  100%



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

Chain h:  100%



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

Chain d:  100%



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

Chain j:  100%



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

Chain n:  75% 25%



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

Chain p:  75% 25%



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

Chain l:  100%



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

Chain o:  100%



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

Chain k:  25% 50% 25%



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

Chain b:  50% 50%



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

Chain f:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.83Å 75.24Å 241.81Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	29.14 – 2.49 29.14 – 2.49	Depositor EDS
% Data completeness (in resolution range)	83.5 (29.14-2.49) 83.5 (29.14-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.207 , 0.246 0.206 , 0.247	Depositor DCC
$R_{free}$ test set	2000 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9897e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.18	0/1867	0.47	0/2554
1	B	0.19	0/1880	0.50	0/2572
1	C	0.27	1/1872 (0.1%)	0.54	1/2561 (0.0%)
1	D	0.18	0/1867	0.48	0/2554
1	E	0.18	0/1872	0.46	0/2561
1	F	0.20	0/1872	0.48	0/2561
1	G	0.17	0/1862	0.48	0/2547
1	H	0.18	0/1862	0.48	0/2547
1	I	0.18	0/1862	0.47	0/2547
1	J	0.19	0/1862	0.53	0/2547
1	K	0.22	0/1872	0.53	0/2561
1	L	0.26	0/1872	0.54	0/2561
1	M	0.18	0/1862	0.49	0/2547
1	N	0.18	0/1867	0.47	0/2554
1	O	0.19	0/1872	0.50	0/2561
1	P	0.21	0/1873	0.52	0/2561
All	All	0.20	1/29896 (0.0%)	0.50	1/40896 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	LYS	CG-CD	-6.51	1.32	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	LYS	N-CA-C	5.32	116.88	108.96

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	1817	0	1744	32	0
1	B	1830	0	1754	42	0
1	C	1822	0	1749	45	1
1	D	1817	0	1744	27	0
1	E	1822	0	1749	33	0
1	F	1822	0	1749	33	0
1	G	1812	0	1739	22	0
1	H	1812	0	1738	32	0
1	I	1812	0	1738	23	1
1	J	1812	0	1738	26	0
1	K	1822	0	1749	42	1
1	L	1822	0	1749	34	1
1	M	1812	0	1738	20	1
1	N	1817	0	1744	21	1
1	O	1822	0	1749	26	1
1	P	1823	0	1750	36	1
2	a	47	0	42	0	0
2	b	47	0	42	2	0
2	c	47	0	42	4	0
2	d	47	0	42	0	0
2	e	47	0	42	0	0
2	f	47	0	42	0	0
2	g	47	0	42	2	0
2	h	47	0	42	0	0
2	i	47	0	42	0	0
2	j	47	0	42	0	0
2	k	47	0	42	4	0
2	l	47	0	42	0	0
2	m	47	0	42	0	0
2	n	47	0	42	0	0
2	o	47	0	42	0	0
2	p	47	0	42	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	A	50	0	0	4	0
5	B	44	0	0	4	0
5	C	51	0	0	1	0
5	D	58	0	0	3	0
5	E	46	0	0	1	0
5	F	42	0	0	0	0
5	G	63	0	0	2	0
5	H	66	0	0	1	0
5	I	45	0	0	2	0
5	J	79	0	0	6	0
5	K	25	0	0	2	0
5	L	45	0	0	2	0
5	M	74	0	0	1	0
5	N	78	0	0	2	0
5	O	51	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	41	0	0	2	0
All	All	30738	0	28593	453	4

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 8.

All (453) 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:F:2:GLN:HE22	1:F:57:ARG:HB3	1.09	1.09
1:B:2:GLN:HE22	1:B:57:ARG:HB3	1.00	1.08
1:F:2:GLN:NE2	1:F:57:ARG:HB3	1.83	0.92
1:B:2:GLN:NE2	1:B:57:ARG:HB3	1.85	0.91
1:A:21:GLN:OE1	1:A:49:ARG:NH1	2.08	0.85
1:C:2:GLN:NE2	1:D:17:ASP:OD2	2.10	0.83
1:F:53:SER:O	1:F:220:ARG:NH1	2.14	0.81
1:E:54:ALA:HB2	1:F:54:ALA:HB2	1.61	0.81
1:A:54:ALA:HB2	1:B:54:ALA:HB2	1.64	0.80
1:D:47:ALA:HB2	1:D:102:HIS:HB3	1.63	0.80
1:H:61:ASP:OD2	1:J:147:TYR:OH	1.99	0.80
1:O:57:ARG:NH2	1:O:217:GLU:OE2	2.16	0.77
1:C:57:ARG:NH2	1:I:146:ASP:OD2	2.20	0.75
1:D:2:GLN:NE2	5:D:402:HOH:O	2.19	0.75
1:D:53:SER:O	1:D:220:ARG:NH1	2.19	0.74
1:E:150:PRO:HG3	1:E:167:THR:HG21	1.67	0.74
1:K:105:PHE:HE2	2:k:2:NAG:H61	1.51	0.74
1:I:143:LEU:HD11	1:I:151:ASN:HA	1.70	0.74
1:G:31:LEU:HB2	1:G:236:VAL:HB	1.69	0.73
1:I:10:LYS:NZ	1:I:12:ASP:OD1	2.22	0.73
1:K:47:ALA:HB2	1:K:102:HIS:HB3	1.69	0.73
1:L:49:ARG:HD3	1:L:99:ILE:HG13	1.71	0.73
1:C:227:THR:HB	1:C:231:LYS:HG2	1.71	0.72
1:J:49:ARG:HD3	1:J:99:ILE:HG13	1.72	0.72
1:K:111:ASN:ND2	1:K:130:ALA:O	2.22	0.71
1:G:111:ASN:ND2	5:G:401:HOH:O	2.15	0.71
1:D:31:LEU:HB2	1:D:236:VAL:HB	1.73	0.71
1:M:10:LYS:NZ	1:M:12:ASP:OD1	2.24	0.70
1:L:26:SER:HB3	1:L:31:LEU:HD23	1.73	0.70
1:C:92:ILE:HD12	1:C:221:VAL:HG12	1.74	0.70
1:L:47:ALA:HB2	1:L:102:HIS:HB3	1.74	0.70
1:I:31:LEU:HB2	1:I:236:VAL:HB	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:95:PRO:O	1:L:220:ARG:NH1	2.25	0.69
1:C:165:LYS:NZ	5:C:401:HOH:O	2.24	0.69
1:B:14[B]:ASN:ND2	5:B:404:HOH:O	2.25	0.69
1:K:66:THR:HG22	1:K:186:SER:HB3	1.75	0.69
1:O:49:ARG:HD3	1:O:99:ILE:HG13	1.74	0.69
1:H:166:VAL:HG22	1:H:205:LEU:HD11	1.73	0.68
1:F:2:GLN:HE22	1:F:57:ARG:CB	1.96	0.68
1:H:49:ARG:HD3	1:H:99:ILE:HG13	1.76	0.68
1:C:133:ASN:HD21	1:C:216:PRO:HD3	1.58	0.68
1:G:49:ARG:HD3	1:G:99:ILE:HG13	1.74	0.67
1:P:169:LYS:NZ	1:P:171:ASP:OD1	2.23	0.67
1:P:10:LYS:NZ	1:P:12:ASP:OD1	2.28	0.67
1:A:47:ALA:HB2	1:A:102:HIS:HB3	1.76	0.67
1:D:49:ARG:HD3	1:D:99:ILE:HG13	1.75	0.66
1:K:31:LEU:HB2	1:K:236:VAL:HB	1.77	0.66
1:K:242:THR:OG1	5:K:401:HOH:O	2.14	0.66
1:M:31:LEU:HB2	1:M:236:VAL:HB	1.77	0.66
1:B:49:ARG:HD3	1:B:99:ILE:HG13	1.78	0.65
1:O:66:THR:HG22	1:O:186:SER:HB3	1.76	0.65
1:P:190[B]:ARG:NE	1:P:208:ASP:OD1	2.30	0.65
1:A:169:LYS:O	5:A:401:HOH:O	2.14	0.65
1:A:201:LYS:NZ	5:A:404:HOH:O	2.25	0.65
1:B:112:ALA:O	1:B:163:ARG:NE	2.28	0.64
1:B:190:ARG:HE	1:B:206:SER:HB3	1.63	0.64
1:D:151:ASN:ND2	5:D:404:HOH:O	2.29	0.64
1:E:47:ALA:HB2	1:E:102:HIS:HB3	1.80	0.64
1:H:44:SER:HB2	1:H:228:GLY:O	1.97	0.64
1:O:61:ASP:OD1	5:O:401:HOH:O	2.15	0.63
1:P:11:PHE:O	1:P:29:ASN:HA	1.99	0.62
1:K:110:PRO:HD3	1:K:132:SER:HB2	1.80	0.62
1:A:150:PRO:HG3	1:A:167:THR:HG21	1.80	0.62
1:L:11:PHE:O	1:L:29:ASN:HA	2.00	0.62
1:A:213:THR:HA	1:O:44:SER:HB2	1.80	0.62
1:G:1:ALA:HA	1:H:9:THR:HG22	1.81	0.62
1:A:248:ASN:ND2	1:C:200:SER:O	2.32	0.61
1:N:10:LYS:NZ	1:N:12:ASP:OD1	2.33	0.61
1:H:66:THR:HG22	1:H:186:SER:HB3	1.82	0.61
1:P:41:ASN:HA	1:P:233:ARG:NH2	2.16	0.61
1:B:92:ILE:HD12	1:B:221:VAL:HG12	1.83	0.61
1:F:66:THR:HG22	1:F:186:SER:HB3	1.82	0.61
1:C:31:LEU:HB3	1:C:236:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ASP:OD2	1:H:2:GLN:NE2	2.34	0.61
1:L:186:SER:O	5:L:401:HOH:O	2.16	0.61
1:K:106:LEU:O	1:K:224:SER:OG	2.19	0.60
1:C:47:ALA:HB2	1:C:102:HIS:HB3	1.82	0.60
1:P:49:ARG:HD3	1:P:99:ILE:HG13	1.82	0.60
1:F:18:LEU:HD13	1:F:50:VAL:HG21	1.84	0.60
1:C:49:ARG:HD3	1:C:99:ILE:HG13	1.83	0.60
1:C:44:SER:HA	1:C:231:LYS:HD3	1.82	0.60
1:J:31:LEU:HD11	1:J:50:VAL:HG21	1.84	0.60
1:K:75:GLU:HG3	1:K:235:THR:HG23	1.82	0.60
1:B:230:ASP:H	2:b:1:MAN:HO6	1.48	0.60
1:E:20:PHE:O	5:E:401:HOH:O	2.16	0.60
1:P:59:TRP:O	1:P:217:GLU:HG3	2.01	0.59
1:E:190:ARG:HG3	1:G:190:ARG:HG3	1.83	0.59
1:P:66:THR:HG22	1:P:186:SER:HB3	1.84	0.59
1:N:49:ARG:HD3	1:N:99:ILE:HG13	1.84	0.59
1:N:47:ALA:HB2	1:N:102:HIS:HB3	1.84	0.59
1:K:49:ARG:HD3	1:K:99:ILE:HG13	1.84	0.59
1:M:47:ALA:HB2	1:M:102:HIS:HB3	1.85	0.58
1:A:135:VAL:HB	1:A:215:LEU:HD11	1.85	0.58
1:B:14[A]:ASN:OD1	1:B:14[A]:ASN:N	2.26	0.58
1:G:47:ALA:HB2	1:G:102:HIS:HB3	1.85	0.58
1:C:54:ALA:HB2	1:D:54:ALA:HB2	1.85	0.58
1:O:13:PRO:HA	1:O:26:SER:OG	2.03	0.58
1:B:232:GLU:OE2	1:B:234:ASN:ND2	2.32	0.57
1:K:18:LEU:HD13	1:K:50:VAL:HG21	1.86	0.57
1:H:112:ALA:O	1:H:163:ARG:HD3	2.04	0.57
1:L:144:ASN:HB3	1:L:147:TYR:HD2	1.69	0.57
1:M:28:ASN:ND2	5:M:404:HOH:O	2.36	0.57
1:F:49:ARG:HD3	1:F:99:ILE:HG13	1.86	0.57
1:M:44:SER:HB2	1:M:228:GLY:O	2.04	0.57
1:C:10:LYS:NZ	1:C:12:ASP:OD1	2.37	0.56
1:K:103:GLY:C	1:K:105:PHE:H	2.12	0.56
1:C:43:VAL:C	1:C:231:LYS:HD3	2.31	0.56
1:P:79:PRO:HD3	1:P:233:ARG:NH1	2.21	0.56
1:D:1:ALA:N	1:D:245:LEU:O	2.34	0.56
1:A:49:ARG:HD3	1:A:99:ILE:HG13	1.88	0.56
1:J:47:ALA:HB2	1:J:102:HIS:HB3	1.88	0.56
1:B:34:THR:HG21	1:B:227:THR:HG23	1.88	0.56
1:G:57:ARG:NH2	1:M:146:ASP:OD2	2.35	0.56
1:G:54:ALA:HB2	1:H:54:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:40:GLY:O	1:P:233:ARG:NE	2.38	0.55
1:I:140:ASP:HB3	1:I:154:HIS:CE1	2.41	0.55
1:K:95:PRO:O	1:K:220:ARG:NH1	2.39	0.55
1:F:169:LYS:NZ	1:F:171:ASP:OD1	2.39	0.55
1:C:133:ASN:ND2	1:C:216:PRO:HD3	2.22	0.55
1:A:65:LEU:HD13	1:A:187:VAL:HG23	1.89	0.54
1:A:66:THR:HG22	1:A:186:SER:HB3	1.89	0.54
1:M:49:ARG:HD3	1:M:99:ILE:HG13	1.88	0.54
1:H:190:ARG:HD2	1:F:188:SER:HB2	1.88	0.54
1:I:47:ALA:HB2	1:I:102:HIS:HB3	1.89	0.54
1:E:196:TYR:HB3	1:E:202:PRO:HB3	1.90	0.54
1:A:190:ARG:HG3	1:C:190:ARG:HG3	1.90	0.54
1:L:66:THR:HG22	1:L:186:SER:HB3	1.90	0.54
1:I:49:ARG:HD3	1:I:99:ILE:HG13	1.90	0.54
1:O:60:GLU:HG2	1:O:61:ASP:N	2.22	0.54
1:J:42:PRO:HG3	1:J:233:ARG:HG3	1.90	0.54
1:D:10:LYS:HE3	1:D:12:ASP:OD1	2.09	0.53
1:K:11:PHE:O	1:K:29:ASN:HA	2.09	0.53
1:K:190:ARG:HD3	1:K:208:ASP:OD1	2.08	0.53
1:L:223:LEU:HD13	1:L:236:VAL:HG21	1.91	0.53
1:H:47:ALA:HB2	1:H:102:HIS:HB3	1.90	0.53
1:B:196:TYR:HB3	1:B:202:PRO:HB3	1.91	0.53
1:N:31:LEU:HB3	1:N:236:VAL:HB	1.90	0.53
1:B:7:SER:HA	1:B:240:SER:HA	1.91	0.53
1:B:66:THR:HG22	1:B:186:SER:HB3	1.90	0.52
1:E:155:ILE:HG23	1:E:170:TRP:HB2	1.91	0.52
1:E:49:ARG:HD3	1:E:99:ILE:HG13	1.90	0.52
1:E:95:PRO:O	1:E:220:ARG:NH1	2.42	0.52
1:K:62:SER:HB2	1:K:248:ASN:OD1	2.10	0.52
1:A:95:PRO:O	1:A:220:ARG:NH1	2.43	0.52
1:C:61:ASP:OD2	1:I:147:TYR:OH	2.17	0.52
1:L:31:LEU:O	1:L:235:THR:HA	2.10	0.52
1:B:31:LEU:HD11	1:B:50:VAL:HG21	1.90	0.52
1:P:95:PRO:O	1:P:220:ARG:NH1	2.43	0.52
1:B:47:ALA:HB2	1:B:102:HIS:HB3	1.91	0.52
1:K:85:ALA:HA	1:K:142:TYR:HB2	1.92	0.52
1:E:196:TYR:CE1	1:G:64:VAL:HG21	2.45	0.52
1:C:65:LEU:HD23	1:C:246:TRP:HB2	1.91	0.52
1:C:60:GLU:OE2	1:C:62:SER:OG	2.29	0.51
1:H:33:LEU:O	1:H:48:GLY:HA3	2.10	0.51
1:P:178:ALA:HB2	1:P:197:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:VAL:CG1	1:J:248:ASN:HB2	2.40	0.51
1:P:44:SER:OG	5:P:401:HOH:O	2.17	0.51
1:E:9:THR:OG1	1:F:1:ALA:HA	2.10	0.51
1:E:168:ALA:HB2	1:E:205:LEU:HD13	1.92	0.51
1:C:57:ARG:HD3	1:C:218:TRP:CZ2	2.45	0.51
1:B:95:PRO:O	1:B:220:ARG:NH1	2.41	0.51
1:J:42:PRO:O	1:J:231:LYS:HD2	2.11	0.51
1:A:7:SER:O	1:B:2:GLN:HA	2.10	0.51
1:A:164:SER:OG	5:A:402:HOH:O	2.19	0.51
1:L:19:ILE:HB	1:L:51:LEU:HB2	1.93	0.51
1:E:57:ARG:HG3	1:E:218:TRP:CZ2	2.45	0.51
1:A:31:LEU:HB3	1:A:236:VAL:HB	1.92	0.51
1:O:190:ARG:HD3	1:O:208:ASP:OD1	2.10	0.51
1:N:15:GLN:HG2	1:N:18:LEU:HD12	1.93	0.51
1:K:229:GLN:HB3	2:k:1:MAN:H62	1.93	0.51
1:F:10:LYS:NZ	1:F:12:ASP:OD1	2.43	0.51
1:E:111:ASN:ND2	1:E:130:ALA:O	2.41	0.50
1:D:33:LEU:O	1:D:48:GLY:HA3	2.10	0.50
1:K:31:LEU:O	1:K:235:THR:HA	2.11	0.50
1:C:189:LYS:HD3	1:C:210:GLU:HG2	1.93	0.50
1:G:66:THR:HG22	1:G:186:SER:HB3	1.92	0.50
1:H:168:ALA:HB2	1:H:205:LEU:HD13	1.92	0.50
1:E:64:VAL:HG21	1:G:196:TYR:CE1	2.46	0.50
1:G:5:SER:OG	1:H:5:SER:HB2	2.11	0.50
1:C:92:ILE:HB	1:C:135:VAL:HG12	1.93	0.50
5:G:407:HOH:O	1:M:145:PRO:HG2	2.10	0.50
1:E:135:VAL:CG1	1:E:215:LEU:HD11	2.42	0.50
1:J:21:GLN:HB2	1:J:49:ARG:HB2	1.94	0.50
1:J:231:LYS:NZ	5:J:410:HOH:O	2.45	0.49
1:H:196:TYR:CE1	1:F:64:VAL:HG21	2.47	0.49
1:A:9:THR:OG1	1:B:1:ALA:HA	2.12	0.49
1:H:31:LEU:HB3	1:H:236:VAL:HB	1.93	0.49
1:P:57:ARG:HD3	1:P:218:TRP:CZ2	2.48	0.49
1:L:43:VAL:C	1:L:231:LYS:HD3	2.37	0.49
1:A:155:ILE:HG23	1:A:170:TRP:HB2	1.93	0.49
1:B:60:GLU:HG2	1:B:61:ASP:N	2.28	0.49
1:J:61:ASP:OD1	5:J:401:HOH:O	2.20	0.49
1:J:33:LEU:O	1:J:48:GLY:HA3	2.13	0.49
1:P:31:LEU:CD2	1:P:33:LEU:HG	2.43	0.49
1:F:94:PRO:HD3	1:F:133:ASN:O	2.13	0.49
1:P:1:ALA:HB2	1:P:247:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:18:LEU:HD13	1:P:50:VAL:HG21	1.95	0.49
1:L:113:ASN:HD21	1:L:131:SER:HB3	1.77	0.48
1:K:234:ASN:N	5:K:404:HOH:O	2.44	0.48
1:O:15:GLN:HG2	1:O:18:LEU:HD12	1.95	0.48
1:A:64:VAL:HG11	1:C:196:TYR:CE1	2.48	0.48
1:F:47:ALA:HB2	1:F:102:HIS:HB3	1.94	0.48
1:C:230:ASP:N	2:c:1:MAN:O6	2.38	0.48
1:C:75:GLU:HG3	1:C:235:THR:HB	1.95	0.48
1:J:217:GLU:OE2	5:J:401:HOH:O	2.20	0.48
1:F:83:ARG:O	1:F:230:ASP:HB3	2.14	0.48
1:F:178:ALA:HB2	1:F:197:TYR:CE1	2.49	0.48
1:J:65:LEU:HD13	1:J:246:TRP:CE3	2.48	0.48
1:E:33:LEU:O	1:E:48:GLY:HA3	2.13	0.48
1:E:65:LEU:HD13	1:E:187:VAL:HG23	1.96	0.48
1:P:31:LEU:HD21	1:P:33:LEU:HG	1.96	0.48
1:J:220:ARG:HG2	5:J:412:HOH:O	2.14	0.47
1:B:190:ARG:HD3	1:B:208:ASP:OD1	2.14	0.47
1:N:66:THR:HG22	1:N:186:SER:HB3	1.95	0.47
1:P:18:LEU:HB3	1:P:50:VAL:HG22	1.96	0.47
1:P:23:HIS:CD2	1:P:35:LYS:HE3	2.49	0.47
1:N:95:PRO:HA	1:N:220:ARG:HB2	1.97	0.47
1:A:133:ASN:HB2	1:O:80:TYR:CD1	2.50	0.47
1:P:79:PRO:HD3	1:P:233:ARG:HH12	1.79	0.47
1:L:248:ASN:CG	1:L:249:VAL:H	2.21	0.47
1:K:45:SER:HA	1:K:102:HIS:CD2	2.49	0.47
1:K:178:ALA:HB2	1:K:197:TYR:CE1	2.49	0.47
1:I:178:ALA:HB2	1:I:197:TYR:CE1	2.49	0.47
1:N:33:LEU:O	1:N:48:GLY:HA3	2.15	0.47
1:E:66:THR:HG22	1:E:186:SER:HB3	1.96	0.47
1:C:227:THR:CB	1:C:231:LYS:HG2	2.41	0.47
1:G:45:SER:HB3	2:g:3:FUC:H61	1.95	0.47
1:D:184:TYR:OH	5:D:401:HOH:O	2.17	0.47
1:L:196:TYR:HB3	1:L:202:PRO:HB3	1.96	0.47
1:C:85:ALA:HB3	1:C:230:ASP:O	2.14	0.47
1:I:132:SER:O	5:I:401:HOH:O	2.20	0.47
1:I:150:PRO:HD2	1:I:154:HIS:CE1	2.49	0.47
1:N:35:LYS:O	5:N:401:HOH:O	2.20	0.47
1:N:181:HIS:O	1:N:193:VAL:HA	2.14	0.47
1:C:190:ARG:HD3	1:C:208:ASP:OD1	2.15	0.47
1:E:11:PHE:CG	1:E:31:LEU:HG	2.50	0.46
1:D:57:ARG:HD3	1:D:218:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:LEU:HB3	1:N:50:VAL:HG22	1.97	0.46
1:E:12:ASP:OD2	1:F:57:ARG:NH1	2.48	0.46
1:C:30:VAL:HG11	1:C:235:THR:HG23	1.96	0.46
1:H:65:LEU:HD13	1:H:187:VAL:HG23	1.98	0.46
1:L:10:LYS:HB2	1:L:29:ASN:HB2	1.96	0.46
1:A:2:GLN:HA	1:B:7:SER:O	2.16	0.46
1:L:44:SER:N	1:L:231:LYS:HD3	2.30	0.46
1:O:1:ALA:O	1:O:2:GLN:HG3	2.16	0.46
1:F:33:LEU:O	1:F:48:GLY:HA3	2.15	0.46
1:N:113:ASN:O	5:N:402:HOH:O	2.21	0.46
1:E:59:TRP:HB2	1:E:212:HIS:HB2	1.97	0.46
1:H:64:VAL:HG11	1:F:196:TYR:CE1	2.51	0.46
1:H:178:ALA:HB2	1:H:197:TYR:CE1	2.50	0.46
1:K:144:ASN:C	1:K:146:ASP:N	2.73	0.46
1:A:190:ARG:HE	1:A:206:SER:HB3	1.79	0.46
1:I:169:LYS:NZ	1:I:171:ASP:OD1	2.45	0.46
1:L:155:ILE:HG23	1:L:170:TRP:HB2	1.96	0.46
1:O:47:ALA:HB2	1:O:102:HIS:HB3	1.98	0.46
1:K:168:ALA:HB2	1:K:205:LEU:HD13	1.97	0.46
1:G:61:ASP:OD2	1:M:147:TYR:OH	2.25	0.46
1:A:178:ALA:HB2	1:A:197:TYR:CE1	2.51	0.46
1:P:31:LEU:HD22	1:P:236:VAL:HB	1.98	0.46
1:K:47:ALA:HB2	1:K:102:HIS:CB	2.42	0.46
1:B:189:LYS:HD3	1:B:210:GLU:HG2	1.98	0.46
1:J:172:TRP:CZ2	1:J:174:ASN:HA	2.51	0.45
1:B:201:LYS:HG3	5:B:444:HOH:O	2.15	0.45
1:D:57:ARG:HD3	1:D:218:TRP:CZ2	2.52	0.45
1:D:181:HIS:O	1:D:193:VAL:HA	2.16	0.45
1:J:92:ILE:HG22	1:J:219:VAL:HG21	1.98	0.45
1:J:179:THR:O	1:J:195:THR:HA	2.16	0.45
1:G:9:THR:OG1	1:H:1:ALA:HA	2.16	0.45
1:D:200:SER:O	1:B:248:ASN:ND2	2.49	0.45
1:K:103:GLY:C	1:K:105:PHE:N	2.74	0.45
1:A:196:TYR:HB3	1:A:202:PRO:HB3	1.99	0.45
1:E:94:PRO:HD3	1:E:133:ASN:O	2.17	0.45
1:O:21:GLN:HB2	1:O:49:ARG:HB2	1.99	0.45
1:D:248:ASN:ND2	1:B:200:SER:O	2.50	0.45
1:O:1:ALA:HB2	1:O:247:THR:OG1	2.16	0.45
1:K:57:ARG:NE	1:K:60:GLU:HG3	2.32	0.45
1:P:31:LEU:O	1:P:235:THR:HA	2.16	0.45
1:M:33:LEU:O	1:M:48:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:LYS:NZ	1:H:12:ASP:OD1	2.49	0.45
1:I:18:LEU:HD22	1:I:50:VAL:HG13	1.99	0.45
1:P:7:SER:HA	1:P:240:SER:HA	1.98	0.45
1:P:15:GLN:HG2	1:P:18:LEU:HD12	1.98	0.45
1:P:230:ASP:OD1	5:P:402:HOH:O	2.21	0.45
1:A:9:THR:O	5:A:403:HOH:O	2.21	0.45
1:E:31:LEU:HB2	1:E:236:VAL:HB	1.98	0.45
1:M:113:ASN:HB2	1:H:28:ASN:OD1	2.17	0.45
1:L:57:ARG:NH2	5:L:402:HOH:O	2.24	0.45
1:B:229:GLN:N	2:b:1:MAN:O6	2.50	0.45
1:K:211:LEU:HD23	1:K:211:LEU:HA	1.79	0.45
1:E:93:ALA:HB2	1:E:134:VAL:HG22	1.99	0.44
1:A:1:ALA:HA	1:B:9:THR:OG1	2.16	0.44
1:G:194:THR:HB	1:G:204:THR:HG22	1.98	0.44
1:L:85:ALA:HA	1:L:86:ASP:HA	1.80	0.44
1:N:112:ALA:O	1:N:163:ARG:NH2	2.50	0.44
1:K:56:LEU:HG	1:K:219:VAL:HG23	2.00	0.44
1:M:181:HIS:O	1:M:193:VAL:HA	2.17	0.44
1:O:60:GLU:HG2	1:O:61:ASP:H	1.83	0.44
1:C:241:PHE:CE1	1:C:243:SER:HB2	2.53	0.44
1:M:56:LEU:HD23	1:M:57:ARG:C	2.42	0.44
1:E:7:SER:O	1:F:2:GLN:HA	2.17	0.44
1:C:229:GLN:N	2:c:1:MAN:O6	2.51	0.44
1:C:231:LYS:HE2	1:C:231:LYS:HB2	1.62	0.44
1:F:15:GLN:HG2	1:F:18:LEU:HD12	1.99	0.44
1:N:64:VAL:CG1	1:N:248:ASN:HB2	2.48	0.44
1:K:33:LEU:O	1:K:48:GLY:HA3	2.18	0.44
1:K:35:LYS:HB3	1:K:43:VAL:HG22	2.00	0.44
1:I:65:LEU:HD13	1:I:187:VAL:HG23	1.98	0.44
1:M:190:ARG:HD3	1:M:208:ASP:OD1	2.18	0.44
1:P:41:ASN:HA	1:P:233:ARG:HH21	1.81	0.44
1:L:63:ALA:HA	1:L:247:THR:HA	2.00	0.44
1:B:33:LEU:O	1:B:48:GLY:HA3	2.18	0.44
1:B:44:SER:HB2	1:B:228:GLY:O	2.16	0.44
1:P:211:LEU:HD23	1:P:211:LEU:HA	1.84	0.44
1:B:90:PHE:CZ	1:B:92:ILE:HD11	2.53	0.44
1:C:101:TYR:CE2	2:c:4:GAL:H3	2.52	0.44
1:I:66:THR:HG22	1:I:186:SER:HB3	1.98	0.44
1:J:190:ARG:NH1	1:J:206:SER:OG	2.51	0.44
1:P:63:ALA:HA	1:P:247:THR:HA	1.99	0.44
1:C:110:PRO:HD3	1:C:132:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ILE:HG23	1:C:170:TRP:HB2	2.00	0.43
1:H:196:TYR:HB3	1:H:202:PRO:HB3	2.00	0.43
1:K:101:TYR:CE2	2:k:4:GAL:H3	2.52	0.43
1:J:64:VAL:HG11	1:J:248:ASN:HB2	2.00	0.43
1:L:70:THR:HB	1:L:241:PHE:HD1	1.83	0.43
1:L:181:HIS:O	1:L:193:VAL:HA	2.19	0.43
1:F:185:ASN:HB3	1:F:188:SER:OG	2.18	0.43
1:N:85:ALA:HA	1:N:86:ASP:HA	1.79	0.43
1:G:33:LEU:O	1:G:48:GLY:HA3	2.17	0.43
1:D:66:THR:HG22	1:D:186:SER:HB3	1.99	0.43
1:F:31:LEU:O	1:F:235:THR:HA	2.17	0.43
1:H:11:PHE:O	1:H:29:ASN:HA	2.18	0.43
1:O:31:LEU:HB3	1:O:236:VAL:HB	2.01	0.43
1:A:31:LEU:O	1:A:235:THR:HA	2.18	0.43
1:O:59:TRP:HB2	1:O:212:HIS:HB2	2.01	0.43
1:N:64:VAL:HG11	1:N:248:ASN:HB2	2.00	0.43
1:P:190[B]:ARG:NH2	1:P:208:ASP:OD1	2.52	0.43
1:O:190:ARG:HA	1:O:190:ARG:HD2	1.88	0.43
1:I:41:ASN:HD21	1:J:80:TYR:HD1	1.66	0.43
1:F:190:ARG:HD3	1:F:208:ASP:OD1	2.18	0.43
1:K:83:ARG:O	1:K:230:ASP:HB3	2.18	0.43
1:E:179:THR:O	1:E:195:THR:HA	2.19	0.43
1:I:33:LEU:O	1:I:48:GLY:HA3	2.18	0.43
1:M:15:GLN:HG2	1:M:18:LEU:HD12	2.01	0.43
1:D:64:VAL:HG11	1:B:196:TYR:CE1	2.54	0.43
1:P:223:LEU:HD13	1:P:236:VAL:HG21	2.01	0.43
1:A:10:LYS:HE2	1:B:249:VAL:HG21	2.01	0.42
1:C:30:VAL:CG1	1:C:235:THR:HG23	2.49	0.42
1:J:66:THR:HG22	1:J:186:SER:HB3	2.01	0.42
1:L:112:ALA:HB2	1:L:147:TYR:CD1	2.54	0.42
1:F:173:GLN:OE1	1:F:176:LYS:HD2	2.19	0.42
1:K:85:ALA:HA	1:K:86:ASP:HA	1.81	0.42
1:A:131:SER:OG	1:A:132:SER:N	2.52	0.42
1:A:168:ALA:HB2	1:A:205:LEU:HD13	2.00	0.42
1:C:33:LEU:O	1:C:48:GLY:HA3	2.19	0.42
1:P:150:PRO:HB2	1:P:152:TYR:CZ	2.53	0.42
1:O:23:HIS:ND1	1:O:35:LYS:HE3	2.34	0.42
1:O:178:ALA:HB2	1:O:197:TYR:CE1	2.54	0.42
1:B:178:ALA:HB2	1:B:197:TYR:CE1	2.54	0.42
1:B:223:LEU:HD13	1:B:236:VAL:HG21	2.01	0.42
1:I:31:LEU:O	1:I:235:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:196:TYR:HB3	1:P:202:PRO:HB3	2.00	0.42
1:L:189:LYS:HE3	1:L:210:GLU:OE2	2.19	0.42
1:E:211:LEU:HD23	1:E:211:LEU:HA	1.88	0.42
1:C:93:ALA:HB2	1:C:134:VAL:HG22	2.02	0.42
1:P:190[B]:ARG:HD3	1:P:190[B]:ARG:HA	1.88	0.42
1:F:85:ALA:HA	1:F:86:ASP:HA	1.78	0.42
1:C:101:TYR:CZ	2:c:4:GAL:H3	2.55	0.42
1:H:56:LEU:HD23	1:H:57:ARG:C	2.44	0.42
1:H:204:THR:HG23	1:F:187:VAL:HG13	2.02	0.42
1:D:155:ILE:HG23	1:D:170:TRP:HB2	2.02	0.42
1:N:163:ARG:CZ	1:N:163:ARG:HB2	2.49	0.42
1:E:57:ARG:NH2	1:F:12:ASP:OD2	2.53	0.42
1:I:75:GLU:HG2	1:I:237:HIS:NE2	2.34	0.42
1:D:11:PHE:O	1:D:29:ASN:HA	2.20	0.42
1:D:31:LEU:O	1:D:235:THR:HA	2.20	0.42
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.81	0.42
1:N:65:LEU:HD13	1:N:246:TRP:CE3	2.55	0.42
1:L:50:VAL:O	1:L:222:GLY:HA3	2.19	0.42
1:K:56:LEU:C	1:K:56:LEU:HD12	2.45	0.42
1:I:57:ARG:HD3	1:I:218:TRP:CZ2	2.54	0.42
1:D:65:LEU:HD13	1:D:187:VAL:HG23	2.02	0.42
1:D:211:LEU:HD23	1:D:211:LEU:HA	1.73	0.42
1:O:95:PRO:O	1:O:220:ARG:NH1	2.51	0.42
1:E:1:ALA:HA	1:F:9:THR:OG1	2.20	0.42
1:E:64:VAL:CG1	1:E:248:ASN:HB2	2.49	0.42
1:L:112:ALA:O	1:L:113:ASN:C	2.62	0.42
1:K:12:ASP:O	1:K:15:GLN:HG2	2.20	0.42
1:K:76:ILE:HG21	1:K:141:THR:HG21	2.01	0.42
1:C:90:PHE:CZ	1:C:92:ILE:HD11	2.55	0.41
1:G:113:ASN:HD21	1:G:131:SER:N	2.17	0.41
1:M:194:THR:HB	1:M:204:THR:HG22	2.02	0.41
1:O:194:THR:HB	1:O:204:THR:HG22	2.01	0.41
1:H:211:LEU:HD23	1:H:211:LEU:HA	1.80	0.41
1:L:194:THR:HB	1:L:204:THR:HG22	2.02	0.41
1:L:21:GLN:HB2	1:L:49:ARG:HB2	2.01	0.41
1:K:228:GLY:C	2:k:2:NAG:H83	2.45	0.41
2:g:2:NAG:H61	2:g:4:GAL:C1	2.51	0.41
1:C:21:GLN:HB2	1:C:49:ARG:HB2	2.02	0.41
1:I:143:LEU:HB2	5:I:440:HOH:O	2.20	0.41
1:H:34:THR:OG1	5:H:401:HOH:O	2.22	0.41
1:H:93:ALA:O	1:H:219:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:SER:OG	1:J:132:SER:N	2.44	0.41
1:O:11:PHE:O	1:O:29:ASN:HA	2.19	0.41
1:B:93:ALA:O	1:B:219:VAL:HG22	2.21	0.41
1:B:249:VAL:O	5:B:401:HOH:O	2.21	0.41
1:L:42:PRO:HB2	1:L:231:LYS:HB3	2.03	0.41
1:L:168:ALA:HB2	1:L:205:LEU:HD13	2.03	0.41
1:O:57:ARG:NH1	5:O:406:HOH:O	2.32	0.41
1:B:34:THR:HB	5:B:406:HOH:O	2.20	0.41
1:N:73:ASN:HB2	1:N:238:SER:OG	2.20	0.41
1:A:51:LEU:HD22	1:A:220:ARG:HB3	2.02	0.41
1:C:194:THR:HB	1:C:204:THR:HG22	2.02	0.41
1:G:150:PRO:HD2	1:G:154:HIS:CE1	2.56	0.41
1:G:211:LEU:HD23	1:G:211:LEU:HA	1.90	0.41
1:L:189:LYS:O	1:L:208:ASP:HA	2.21	0.41
1:O:65:LEU:HD13	1:O:187:VAL:HG23	2.02	0.41
1:B:241:PHE:CE1	1:B:243:SER:HB2	2.55	0.41
1:D:15:GLN:HG2	1:D:18:LEU:HD12	2.01	0.41
1:D:196:TYR:HB3	1:D:202:PRO:HB3	2.02	0.41
1:E:2:GLN:HA	1:F:7:SER:O	2.20	0.41
1:E:44:SER:OG	1:E:231:LYS:HE3	2.21	0.41
1:G:56:LEU:HD23	1:G:57:ARG:C	2.45	0.41
1:I:11:PHE:O	1:I:29:ASN:HA	2.20	0.41
1:I:85:ALA:HA	1:I:86:ASP:HA	1.85	0.41
1:H:205:LEU:HD12	1:H:205:LEU:HA	1.95	0.41
1:L:12:ASP:O	1:L:26:SER:OG	2.33	0.41
1:L:179:THR:O	1:L:195:THR:HA	2.21	0.41
1:H:103:GLY:O	1:H:226:SER:OG	2.38	0.41
1:F:189:LYS:HE2	1:F:210:GLU:OE2	2.21	0.41
1:C:90:PHE:CE2	1:C:92:ILE:HD11	2.56	0.40
1:M:11:PHE:O	1:M:29:ASN:HA	2.21	0.40
1:M:85:ALA:HA	1:M:86:ASP:HA	1.83	0.40
1:N:56:LEU:HD11	1:N:243:SER:OG	2.21	0.40
1:C:57:ARG:HD3	1:C:218:TRP:CE2	2.56	0.40
1:J:31:LEU:HB3	1:J:236:VAL:HB	2.03	0.40
1:P:155:ILE:HG23	1:P:170:TRP:HB2	2.02	0.40
1:B:88:LEU:HD22	1:B:225:ALA:HB2	2.04	0.40
1:K:109:PHE:CE1	1:K:134:VAL:HG13	2.56	0.40
1:K:112:ALA:HB2	1:K:147:TYR:CD1	2.57	0.40
1:M:158:ASP:HB3	1:M:161:SER:O	2.21	0.40
1:F:15:GLN:HG3	1:F:17:ASP:OD1	2.20	0.40
1:K:181:HIS:O	1:K:193:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LEU:HD22	1:D:220:ARG:HB3	2.02	0.40
1:J:98:VAL:O	5:J:402:HOH:O	2.22	0.40
1:J:181:HIS:O	1:J:193:VAL:HA	2.21	0.40
1:J:243:SER:OG	5:J:403:HOH:O	2.22	0.40
1:C:181:HIS:O	1:C:193:VAL:HA	2.22	0.40
1:M:12:ASP:O	1:M:26:SER:OG	2.39	0.40
1:H:73:ASN:HA	1:H:178:ALA:O	2.22	0.40
1:P:57:ARG:NH2	1:P:217:GLU:OE2	2.54	0.40
1:O:31:LEU:O	1:O:235:THR:HA	2.22	0.40
1:N:36:LEU:HD21	1:N:233:ARG:HG2	2.03	0.40
1:K:182:ILE:HA	1:K:192:SER:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:GLN:NE2	1:N:17:ASP:OD2[1_465]	2.12	0.08
1:P:2:GLN:NE2	1:O:17:ASP:OD2[1_565]	2.16	0.04
1:C:147:TYR:OH	1:I:61:ASP:OD2[1_545]	2.19	0.01
1:L:17:ASP:OD2	1:K:2:GLN:NE2[1_565]	2.19	0.01

## 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	229/264 (87%)	221 (96%)	8 (4%)	0	100	100
1	B	231/264 (88%)	222 (96%)	9 (4%)	0	100	100
1	C	230/264 (87%)	224 (97%)	6 (3%)	0	100	100
1	D	229/264 (87%)	223 (97%)	6 (3%)	0	100	100
1	E	230/264 (87%)	222 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	230/264 (87%)	225 (98%)	5 (2%)	0	100	100
1	G	228/264 (86%)	224 (98%)	4 (2%)	0	100	100
1	H	228/264 (86%)	223 (98%)	5 (2%)	0	100	100
1	I	228/264 (86%)	223 (98%)	5 (2%)	0	100	100
1	J	228/264 (86%)	222 (97%)	6 (3%)	0	100	100
1	K	230/264 (87%)	223 (97%)	7 (3%)	0	100	100
1	L	230/264 (87%)	219 (95%)	10 (4%)	1 (0%)	30	49
1	M	228/264 (86%)	223 (98%)	5 (2%)	0	100	100
1	N	229/264 (87%)	222 (97%)	7 (3%)	0	100	100
1	O	230/264 (87%)	223 (97%)	7 (3%)	0	100	100
1	P	229/264 (87%)	222 (97%)	7 (3%)	0	100	100
All	All	3667/4224 (87%)	3561 (97%)	105 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	249	VAL

### 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	203/231 (88%)	198 (98%)	5 (2%)	42	69
1	B	204/231 (88%)	196 (96%)	8 (4%)	28	55
1	C	203/231 (88%)	198 (98%)	5 (2%)	42	69
1	D	203/231 (88%)	198 (98%)	5 (2%)	42	69
1	E	203/231 (88%)	195 (96%)	8 (4%)	28	55
1	F	203/231 (88%)	199 (98%)	4 (2%)	48	75
1	G	203/231 (88%)	199 (98%)	4 (2%)	48	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	203/231 (88%)	196 (97%)	7 (3%)	32	60
1	I	203/231 (88%)	199 (98%)	4 (2%)	48	75
1	J	203/231 (88%)	193 (95%)	10 (5%)	22	45
1	K	203/231 (88%)	195 (96%)	8 (4%)	28	55
1	L	203/231 (88%)	198 (98%)	5 (2%)	42	69
1	M	203/231 (88%)	200 (98%)	3 (2%)	57	80
1	N	203/231 (88%)	198 (98%)	5 (2%)	42	69
1	O	203/231 (88%)	199 (98%)	4 (2%)	48	75
1	P	204/231 (88%)	199 (98%)	5 (2%)	42	69
All	All	3250/3696 (88%)	3160 (97%)	90 (3%)	39	66

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	34	THR
1	A	50	VAL
1	A	64	VAL
1	A	167	THR
1	E	27	THR
1	E	34	THR
1	E	43	VAL
1	E	50	VAL
1	E	57	ARG
1	E	135	VAL
1	E	167	THR
1	E	214	VAL
1	C	30	VAL
1	C	34	THR
1	C	50	VAL
1	C	65	LEU
1	C	219	VAL
1	G	34	THR
1	G	50	VAL
1	G	134	VAL
1	G	159	VAL
1	I	50	VAL
1	I	143	LEU
1	I	190	ARG

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Mol	Chain	Res	Type
1	I	219	VAL
1	M	25	THR
1	M	34	THR
1	M	50	VAL
1	H	9	THR
1	H	34	THR
1	H	50	VAL
1	H	167	THR
1	H	219	VAL
1	H	223	LEU
1	H	249	VAL
1	D	34	THR
1	D	43	VAL
1	D	50	VAL
1	D	64	VAL
1	D	219	VAL
1	J	27	THR
1	J	65	LEU
1	J	81	THR
1	J	134	VAL
1	J	190	ARG
1	J	201	LYS
1	J	204	THR
1	J	219	VAL
1	J	223	LEU
1	J	249	VAL
1	P	27	THR
1	P	31	LEU
1	P	50	VAL
1	P	159	VAL
1	P	235	THR
1	L	27	THR
1	L	34	THR
1	L	50	VAL
1	L	134	VAL
1	L	235	THR
1	O	25	THR
1	O	34	THR
1	O	50	VAL
1	O	235	THR
1	B	14[A]	ASN
1	B	14[B]	ASN

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Mol	Chain	Res	Type
1	B	27	THR
1	B	34	THR
1	B	88	LEU
1	B	191	LEU
1	B	219	VAL
1	B	249	VAL
1	F	27	THR
1	F	134	VAL
1	F	235	THR
1	F	249	VAL
1	N	27	THR
1	N	50	VAL
1	N	65	LEU
1	N	131	SER
1	N	219	VAL
1	K	34	THR
1	K	43	VAL
1	K	56	LEU
1	K	86	ASP
1	K	132	SER
1	K	134	VAL
1	K	167	THR
1	K	235	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	212	HIS
1	C	41	ASN
1	C	133	ASN
1	G	2	GLN
1	G	41	ASN
1	I	41	ASN
1	M	14	ASN
1	H	41	ASN
1	H	133	ASN
1	D	41	ASN
1	J	41	ASN
1	J	181	HIS
1	P	14	ASN
1	P	212	HIS

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Mol	Chain	Res	Type
1	L	113	ASN
1	B	2	GLN
1	F	2	GLN
1	F	229	GLN
1	N	14	ASN
1	N	41	ASN
1	K	133	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

64 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	MAN	a	1	2	12,12,12	0.37	0	17,17,17	0.49	0
2	NAG	a	2	2	14,14,15	0.42	0	17,19,21	0.75	0
2	FUC	a	3	2	10,10,11	0.43	0	14,14,16	0.32	0
2	GAL	a	4	2	11,11,12	0.43	0	15,15,17	0.42	0
2	MAN	b	1	2	12,12,12	0.40	0	17,17,17	0.38	0
2	NAG	b	2	2	14,14,15	0.41	0	17,19,21	1.27	3 (17%)
2	FUC	b	3	2	10,10,11	0.43	0	14,14,16	0.36	0
2	GAL	b	4	2	11,11,12	0.51	0	15,15,17	0.59	0
2	MAN	c	1	2	12,12,12	0.10	0	17,17,17	0.43	0
2	NAG	c	2	2	14,14,15	0.43	0	17,19,21	0.74	0
2	FUC	c	3	2	10,10,11	0.42	0	14,14,16	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GAL	c	4	2	11,11,12	0.45	0	15,15,17	0.54	0
2	MAN	d	1	2	12,12,12	0.25	0	17,17,17	0.51	0
2	NAG	d	2	2	14,14,15	0.42	0	17,19,21	0.83	0
2	FUC	d	3	2	10,10,11	0.46	0	14,14,16	0.36	0
2	GAL	d	4	2	11,11,12	0.54	0	15,15,17	0.47	0
2	MAN	e	1	2	12,12,12	0.30	0	17,17,17	0.49	0
2	NAG	e	2	2	14,14,15	0.44	0	17,19,21	0.85	0
2	FUC	e	3	2	10,10,11	0.45	0	14,14,16	0.35	0
2	GAL	e	4	2	11,11,12	0.48	0	15,15,17	0.42	0
2	MAN	f	1	2	12,12,12	0.18	0	17,17,17	0.53	0
2	NAG	f	2	2	14,14,15	0.38	0	17,19,21	1.05	2 (11%)
2	FUC	f	3	2	10,10,11	0.43	0	14,14,16	0.39	0
2	GAL	f	4	2	11,11,12	0.49	0	15,15,17	0.40	0
2	MAN	g	1	2	12,12,12	0.31	0	17,17,17	0.47	0
2	NAG	g	2	2	14,14,15	0.44	0	17,19,21	1.06	0
2	FUC	g	3	2	10,10,11	0.81	1 (10%)	14,14,16	0.65	0
2	GAL	g	4	2	11,11,12	0.42	0	15,15,17	0.55	0
2	MAN	h	1	2	12,12,12	0.25	0	17,17,17	0.53	0
2	NAG	h	2	2	14,14,15	0.45	0	17,19,21	0.76	0
2	FUC	h	3	2	10,10,11	0.44	0	14,14,16	0.32	0
2	GAL	h	4	2	11,11,12	0.60	0	15,15,17	0.41	0
2	MAN	i	1	2	12,12,12	0.20	0	17,17,17	0.48	0
2	NAG	i	2	2	14,14,15	0.43	0	17,19,21	0.89	0
2	FUC	i	3	2	10,10,11	0.49	0	14,14,16	0.39	0
2	GAL	i	4	2	11,11,12	0.47	0	15,15,17	0.41	0
2	MAN	j	1	2	12,12,12	0.30	0	17,17,17	0.54	0
2	NAG	j	2	2	14,14,15	0.45	0	17,19,21	0.78	0
2	FUC	j	3	2	10,10,11	0.40	0	14,14,16	0.35	0
2	GAL	j	4	2	11,11,12	0.39	0	15,15,17	0.59	0
2	MAN	k	1	2	12,12,12	0.36	0	17,17,17	0.44	0
2	NAG	k	2	2	14,14,15	0.32	0	17,19,21	1.11	1 (5%)
2	FUC	k	3	2	10,10,11	0.56	0	14,14,16	0.33	0
2	GAL	k	4	2	11,11,12	0.51	0	15,15,17	0.45	0
2	MAN	l	1	2	12,12,12	0.12	0	17,17,17	0.46	0
2	NAG	l	2	2	14,14,15	0.42	0	17,19,21	0.68	0
2	FUC	l	3	2	10,10,11	0.41	0	14,14,16	0.37	0
2	GAL	l	4	2	11,11,12	0.41	0	15,15,17	0.45	0
2	MAN	m	1	2	12,12,12	0.31	0	17,17,17	0.53	0
2	NAG	m	2	2	14,14,15	0.45	0	17,19,21	0.88	0
2	FUC	m	3	2	10,10,11	0.47	0	14,14,16	0.37	0
2	GAL	m	4	2	11,11,12	0.42	0	15,15,17	0.60	0
2	MAN	n	1	2	12,12,12	0.30	0	17,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	n	2	2	14,14,15	0.39	0	17,19,21	1.22	3 (17%)
2	FUC	n	3	2	10,10,11	0.50	0	14,14,16	0.32	0
2	GAL	n	4	2	11,11,12	0.54	0	15,15,17	0.41	0
2	MAN	o	1	2	12,12,12	0.23	0	17,17,17	0.44	0
2	NAG	o	2	2	14,14,15	0.44	0	17,19,21	0.69	0
2	FUC	o	3	2	10,10,11	0.46	0	14,14,16	0.31	0
2	GAL	o	4	2	11,11,12	0.52	0	15,15,17	0.46	0
2	MAN	p	1	2	12,12,12	0.23	0	17,17,17	0.48	0
2	NAG	p	2	2	14,14,15	0.43	0	17,19,21	0.96	1 (5%)
2	FUC	p	3	2	10,10,11	0.46	0	14,14,16	0.33	0
2	GAL	p	4	2	11,11,12	0.38	0	15,15,17	0.41	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
2	MAN	a	1	2	-	2/2/22/22	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1
2	FUC	a	3	2	-	-	0/1/1/1
2	GAL	a	4	2	-	1/2/19/22	0/1/1/1
2	MAN	b	1	2	-	2/2/22/22	0/1/1/1
2	NAG	b	2	2	-	0/6/23/26	0/1/1/1
2	FUC	b	3	2	-	-	0/1/1/1
2	GAL	b	4	2	-	0/2/19/22	0/1/1/1
2	MAN	c	1	2	-	2/2/22/22	0/1/1/1
2	NAG	c	2	2	-	0/6/23/26	0/1/1/1
2	FUC	c	3	2	-	-	0/1/1/1
2	GAL	c	4	2	-	2/2/19/22	0/1/1/1
2	MAN	d	1	2	-	0/2/22/22	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1
2	FUC	d	3	2	-	-	0/1/1/1
2	GAL	d	4	2	-	0/2/19/22	0/1/1/1
2	MAN	e	1	2	-	0/2/22/22	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	FUC	e	3	2	-	-	0/1/1/1
2	GAL	e	4	2	-	1/2/19/22	0/1/1/1
2	MAN	f	1	2	-	2/2/22/22	0/1/1/1
2	NAG	f	2	2	-	0/6/23/26	0/1/1/1
2	FUC	f	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	f	4	2	-	2/2/19/22	0/1/1/1
2	MAN	g	1	2	-	0/2/22/22	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	FUC	g	3	2	-	-	0/1/1/1
2	GAL	g	4	2	-	2/2/19/22	0/1/1/1
2	MAN	h	1	2	-	0/2/22/22	0/1/1/1
2	NAG	h	2	2	-	0/6/23/26	0/1/1/1
2	FUC	h	3	2	-	-	0/1/1/1
2	GAL	h	4	2	-	2/2/19/22	0/1/1/1
2	MAN	i	1	2	-	0/2/22/22	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
2	FUC	i	3	2	-	-	0/1/1/1
2	GAL	i	4	2	-	2/2/19/22	0/1/1/1
2	MAN	j	1	2	-	0/2/22/22	0/1/1/1
2	NAG	j	2	2	-	0/6/23/26	0/1/1/1
2	FUC	j	3	2	-	-	0/1/1/1
2	GAL	j	4	2	-	0/2/19/22	0/1/1/1
2	MAN	k	1	2	-	0/2/22/22	0/1/1/1
2	NAG	k	2	2	-	3/6/23/26	0/1/1/1
2	FUC	k	3	2	-	-	0/1/1/1
2	GAL	k	4	2	-	0/2/19/22	0/1/1/1
2	MAN	l	1	2	-	0/2/22/22	0/1/1/1
2	NAG	l	2	2	-	1/6/23/26	0/1/1/1
2	FUC	l	3	2	-	-	0/1/1/1
2	GAL	l	4	2	-	2/2/19/22	0/1/1/1
2	MAN	m	1	2	-	0/2/22/22	0/1/1/1
2	NAG	m	2	2	-	0/6/23/26	0/1/1/1
2	FUC	m	3	2	-	-	0/1/1/1
2	GAL	m	4	2	-	0/2/19/22	0/1/1/1
2	MAN	n	1	2	-	0/2/22/22	0/1/1/1
2	NAG	n	2	2	-	0/6/23/26	0/1/1/1
2	FUC	n	3	2	-	-	0/1/1/1
2	GAL	n	4	2	-	2/2/19/22	0/1/1/1
2	MAN	o	1	2	-	1/2/22/22	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	FUC	o	3	2	-	-	0/1/1/1
2	GAL	o	4	2	-	1/2/19/22	0/1/1/1
2	MAN	p	1	2	-	0/2/22/22	0/1/1/1
2	NAG	p	2	2	-	0/6/23/26	0/1/1/1
2	FUC	p	3	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	p	4	2	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	g	3	FUC	C2-C3	-2.34	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	2	NAG	O5-C1-C2	3.49	116.69	111.29
2	b	2	NAG	O5-C1-C2	3.48	116.67	111.29
2	p	2	NAG	O3-C3-C2	-2.96	103.25	109.40
2	k	2	NAG	C2-N2-C7	2.88	126.76	122.90
2	f	2	NAG	O5-C1-C2	2.79	115.61	111.29
2	b	2	NAG	O4-C4-C3	-2.39	104.74	110.38
2	n	2	NAG	O4-C4-C3	-2.23	105.12	110.38
2	b	2	NAG	O3-C3-C2	-2.08	105.07	109.40
2	f	2	NAG	O4-C4-C3	-2.07	105.49	110.38
2	n	2	NAG	O3-C3-C2	-2.00	105.24	109.40

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	2	NAG	C4-C5-C6-O6
2	c	1	MAN	O5-C5-C6-O6
2	n	4	GAL	O5-C5-C6-O6
2	b	1	MAN	O5-C5-C6-O6
2	i	4	GAL	C4-C5-C6-O6
2	l	4	GAL	C4-C5-C6-O6
2	g	4	GAL	C4-C5-C6-O6
2	c	1	MAN	C4-C5-C6-O6
2	a	2	NAG	O5-C5-C6-O6
2	c	4	GAL	C4-C5-C6-O6
2	n	4	GAL	C4-C5-C6-O6
2	h	4	GAL	O5-C5-C6-O6
2	g	4	GAL	O5-C5-C6-O6
2	b	1	MAN	C4-C5-C6-O6
2	c	4	GAL	O5-C5-C6-O6
2	h	4	GAL	C4-C5-C6-O6

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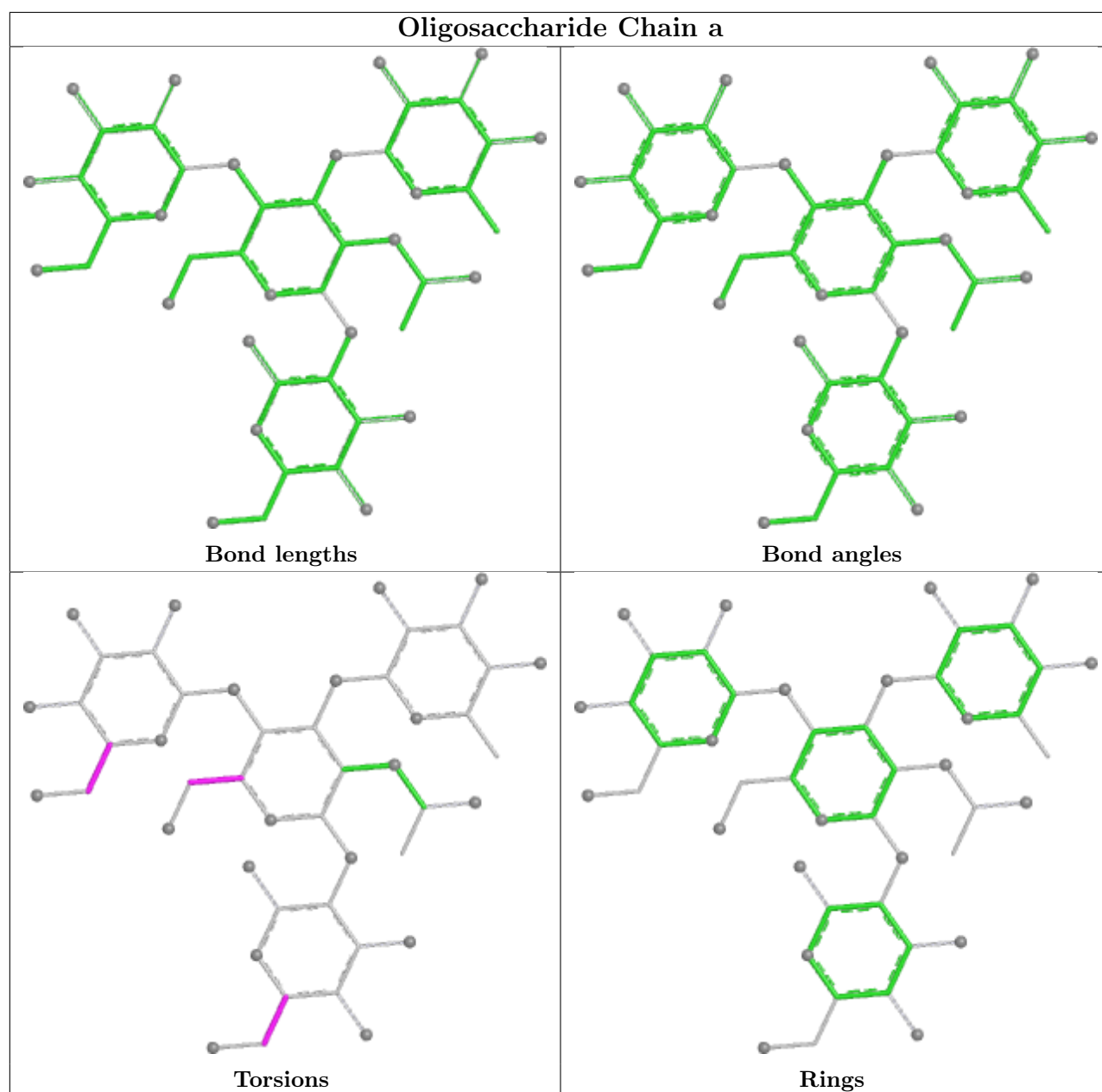
Mol	Chain	Res	Type	Atoms
2	i	4	GAL	O5-C5-C6-O6
2	l	4	GAL	O5-C5-C6-O6
2	e	4	GAL	O5-C5-C6-O6
2	o	4	GAL	O5-C5-C6-O6
2	p	4	GAL	O5-C5-C6-O6
2	k	2	NAG	C3-C2-N2-C7
2	i	2	NAG	C4-C5-C6-O6
2	a	4	GAL	O5-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	f	4	GAL	C4-C5-C6-O6
2	o	2	NAG	C4-C5-C6-O6
2	d	2	NAG	C4-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
2	f	4	GAL	O5-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
2	f	1	MAN	C4-C5-C6-O6
2	k	2	NAG	C1-C2-N2-C7
2	a	1	MAN	C4-C5-C6-O6
2	f	1	MAN	O5-C5-C6-O6
2	l	2	NAG	C4-C5-C6-O6
2	a	1	MAN	O5-C5-C6-O6
2	o	1	MAN	C4-C5-C6-O6
2	k	2	NAG	C8-C7-N2-C2

There are no ring outliers.

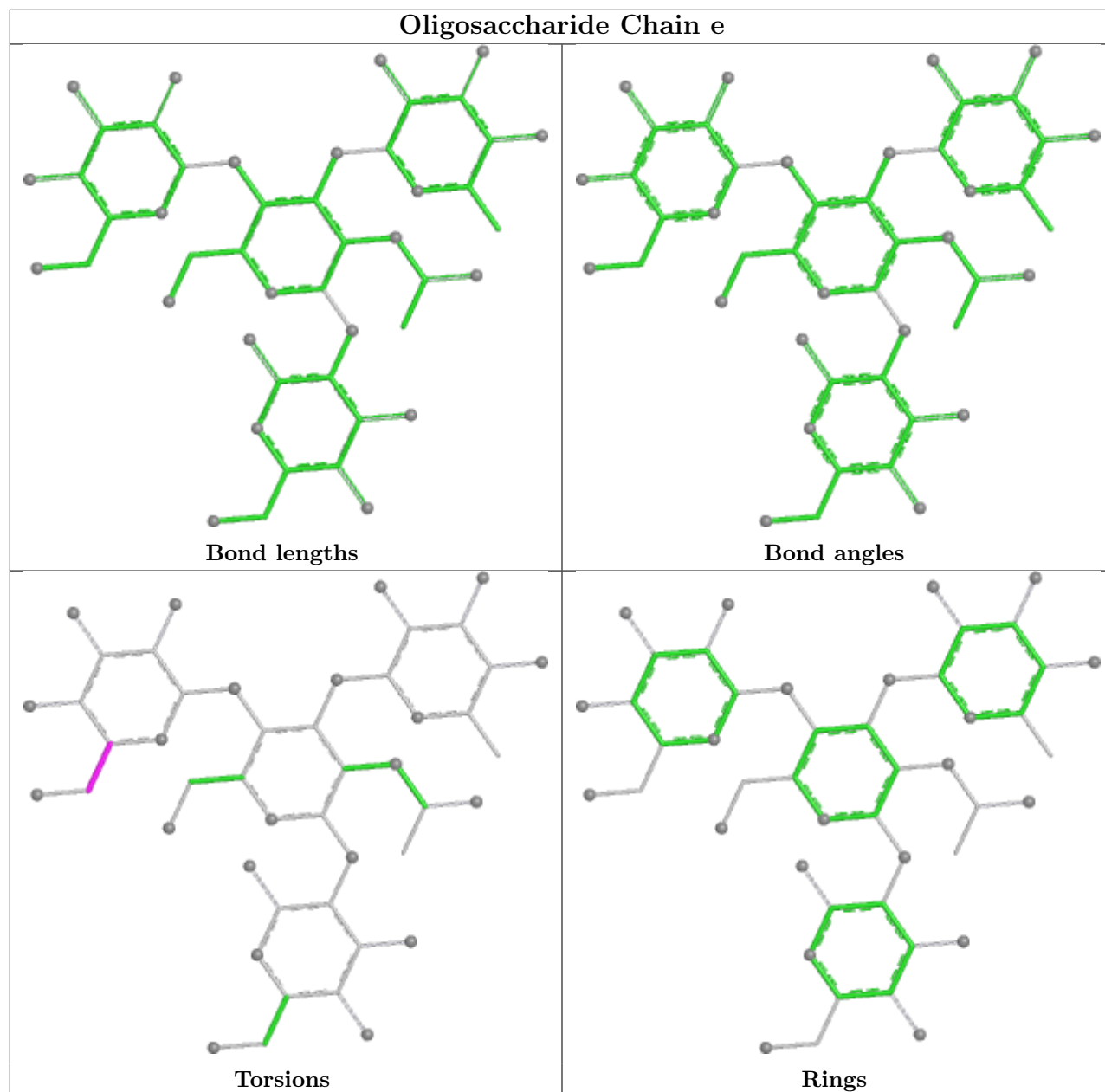
9 monomers are involved in 12 short contacts:

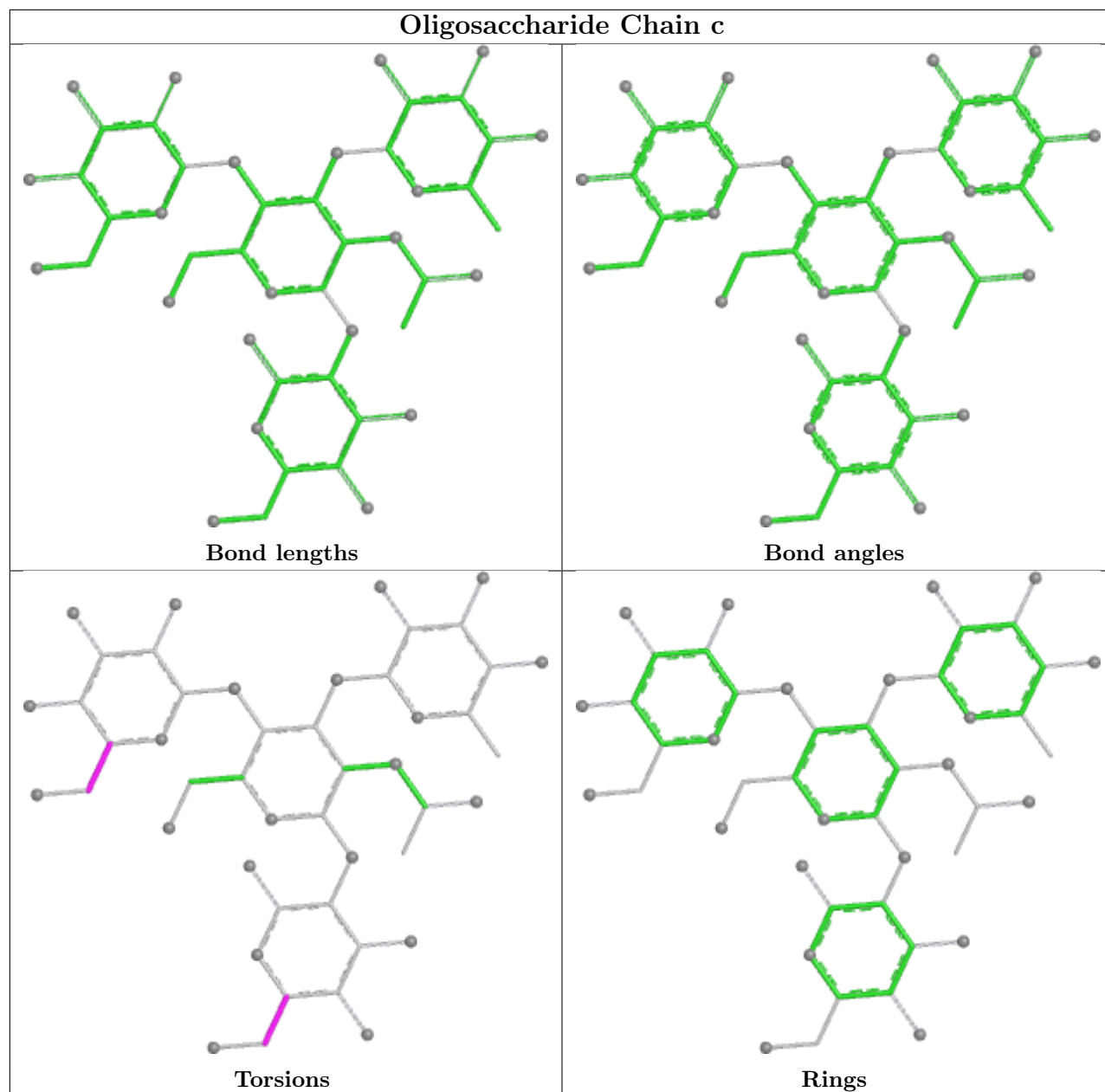
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	g	4	GAL	1	0
2	c	4	GAL	2	0
2	g	2	NAG	1	0
2	c	1	MAN	2	0
2	g	3	FUC	1	0
2	k	1	MAN	1	0
2	k	2	NAG	2	0
2	b	1	MAN	2	0
2	k	4	GAL	1	0

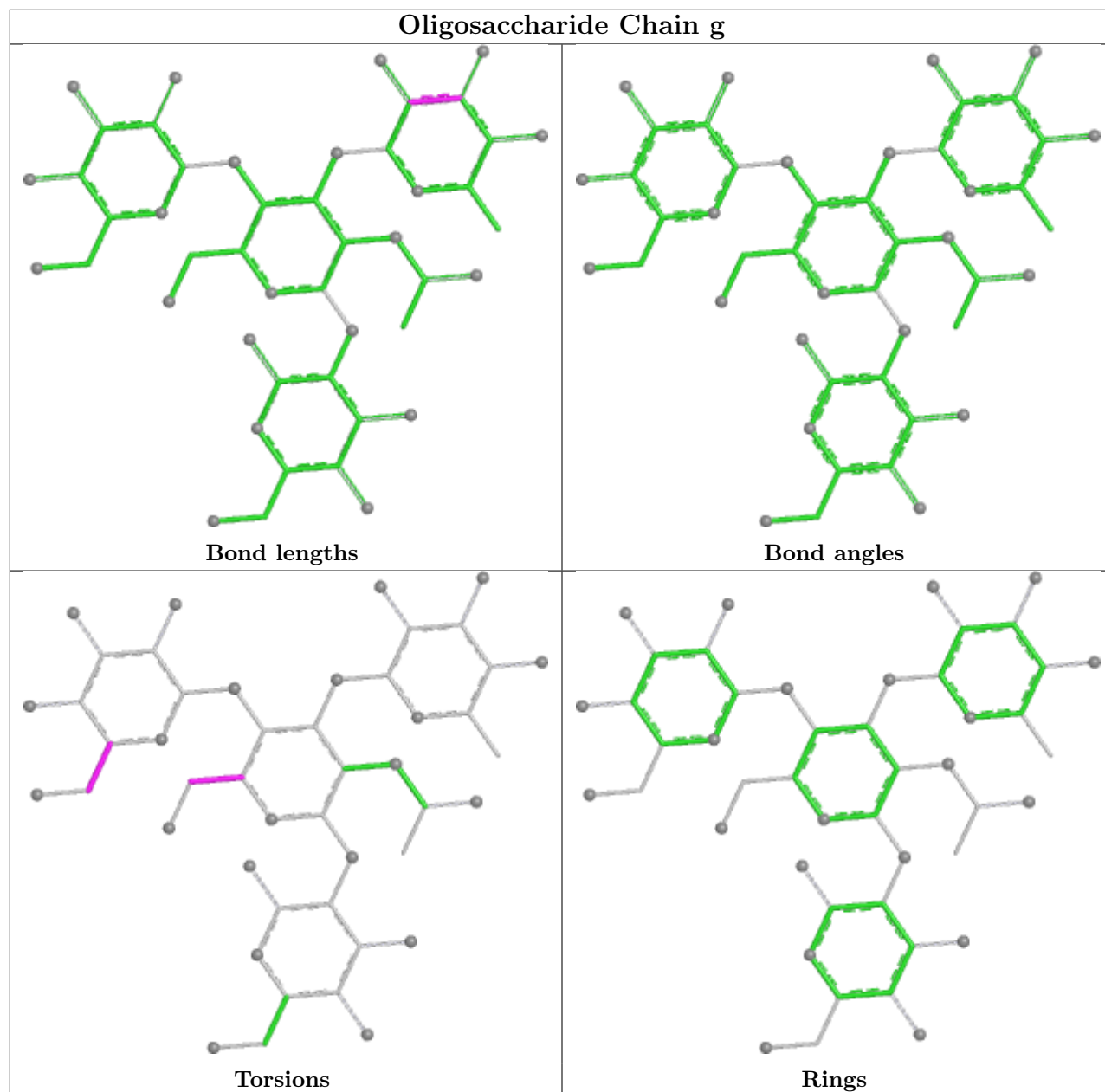
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

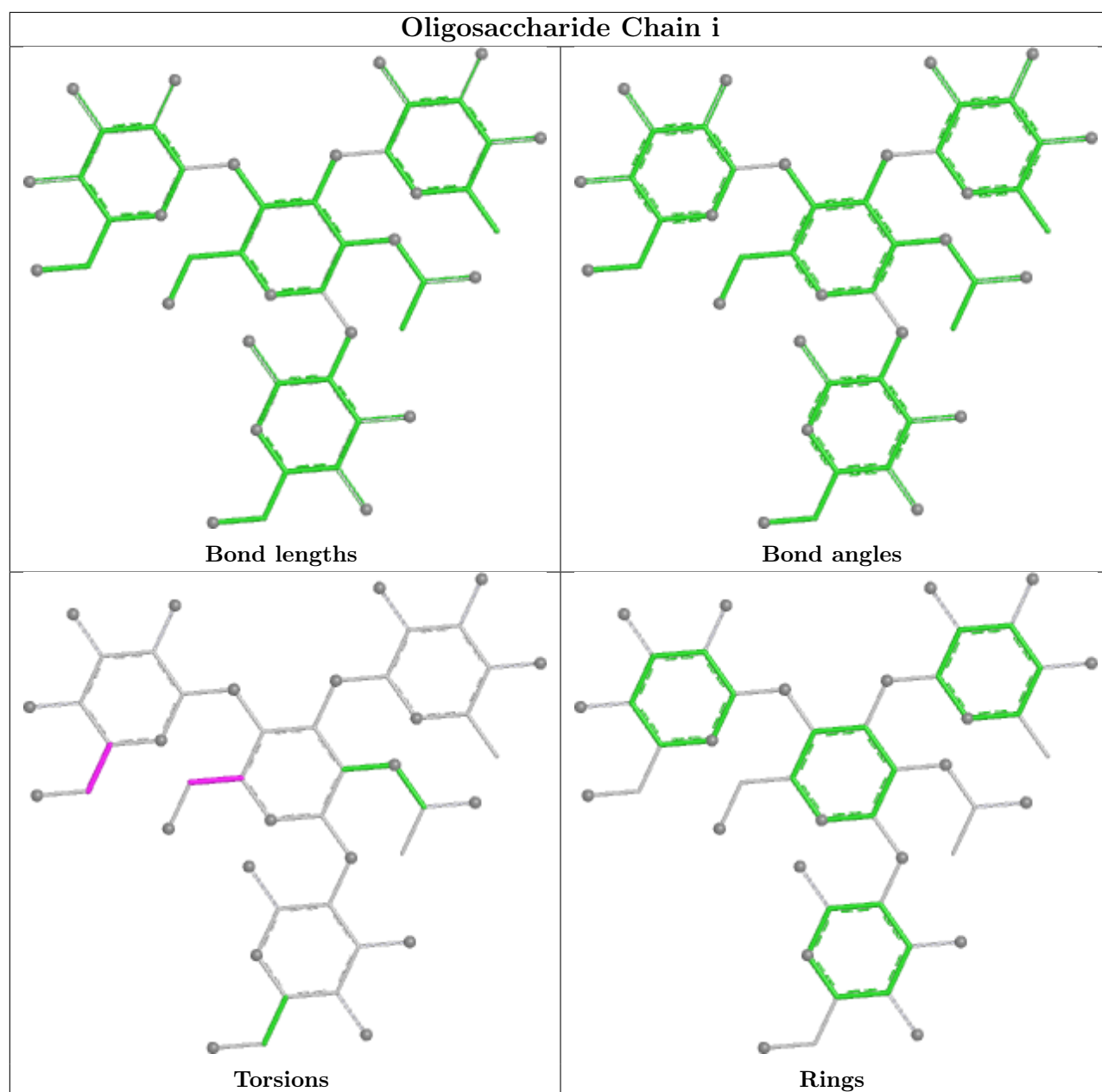


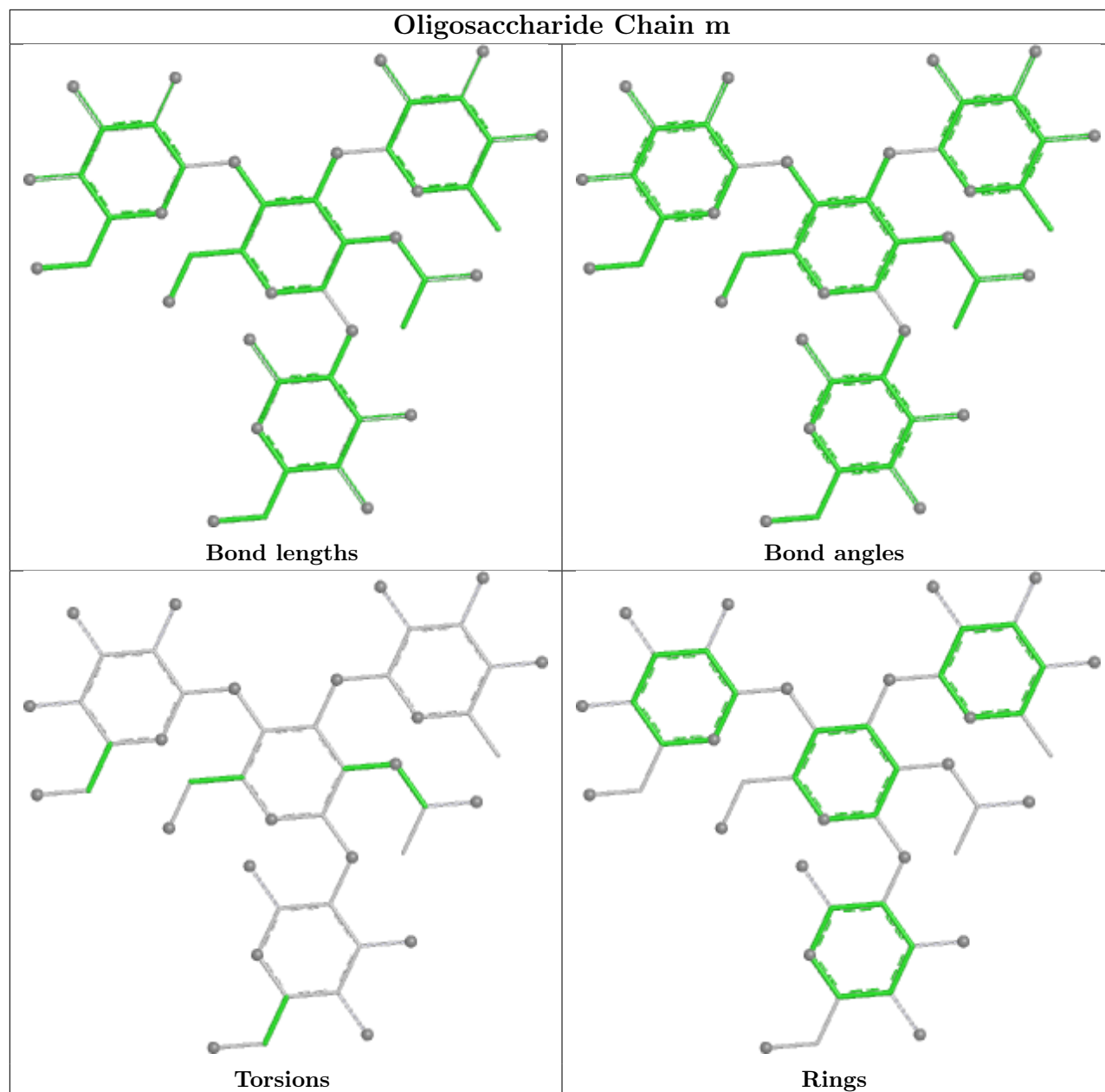


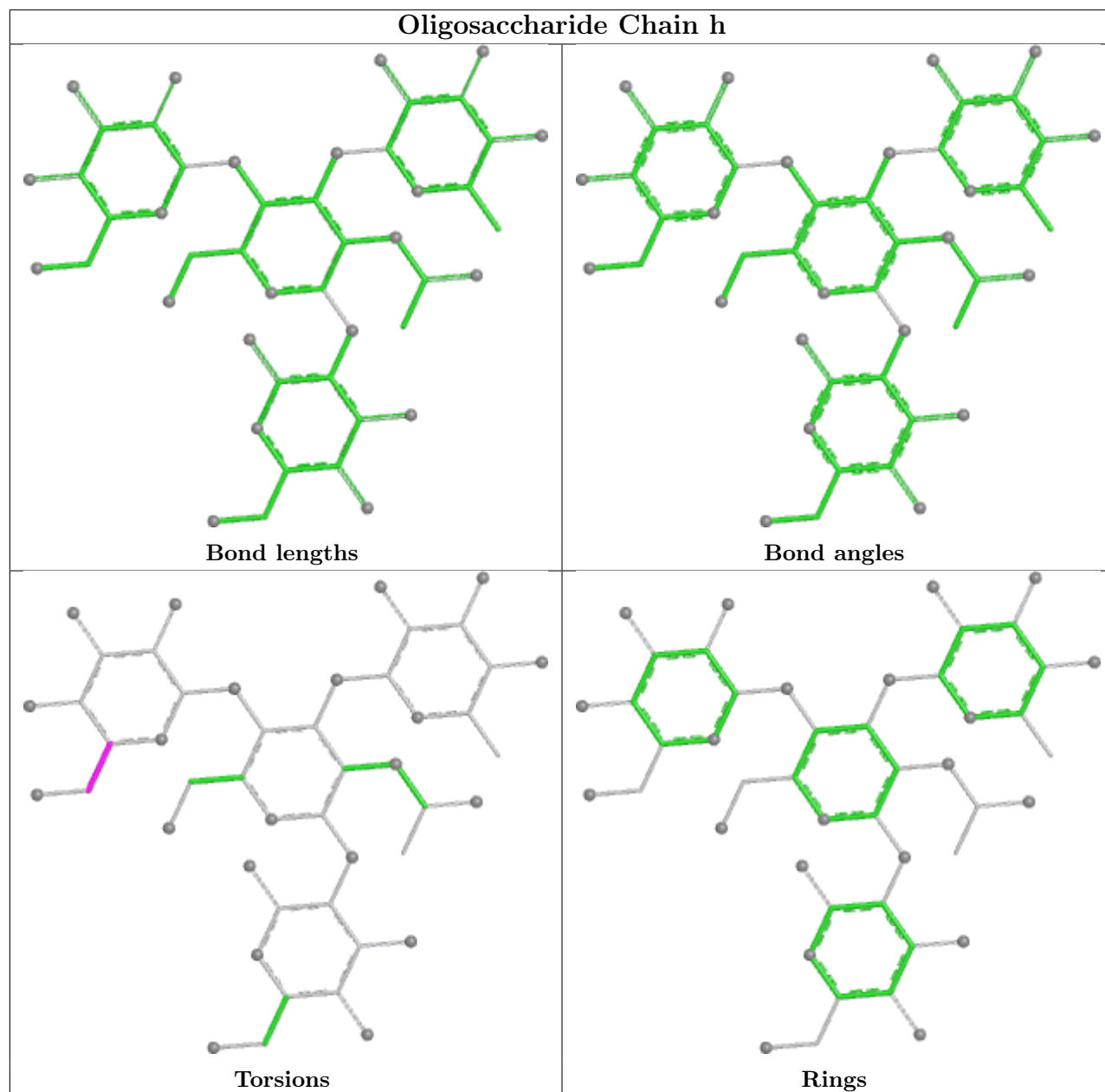


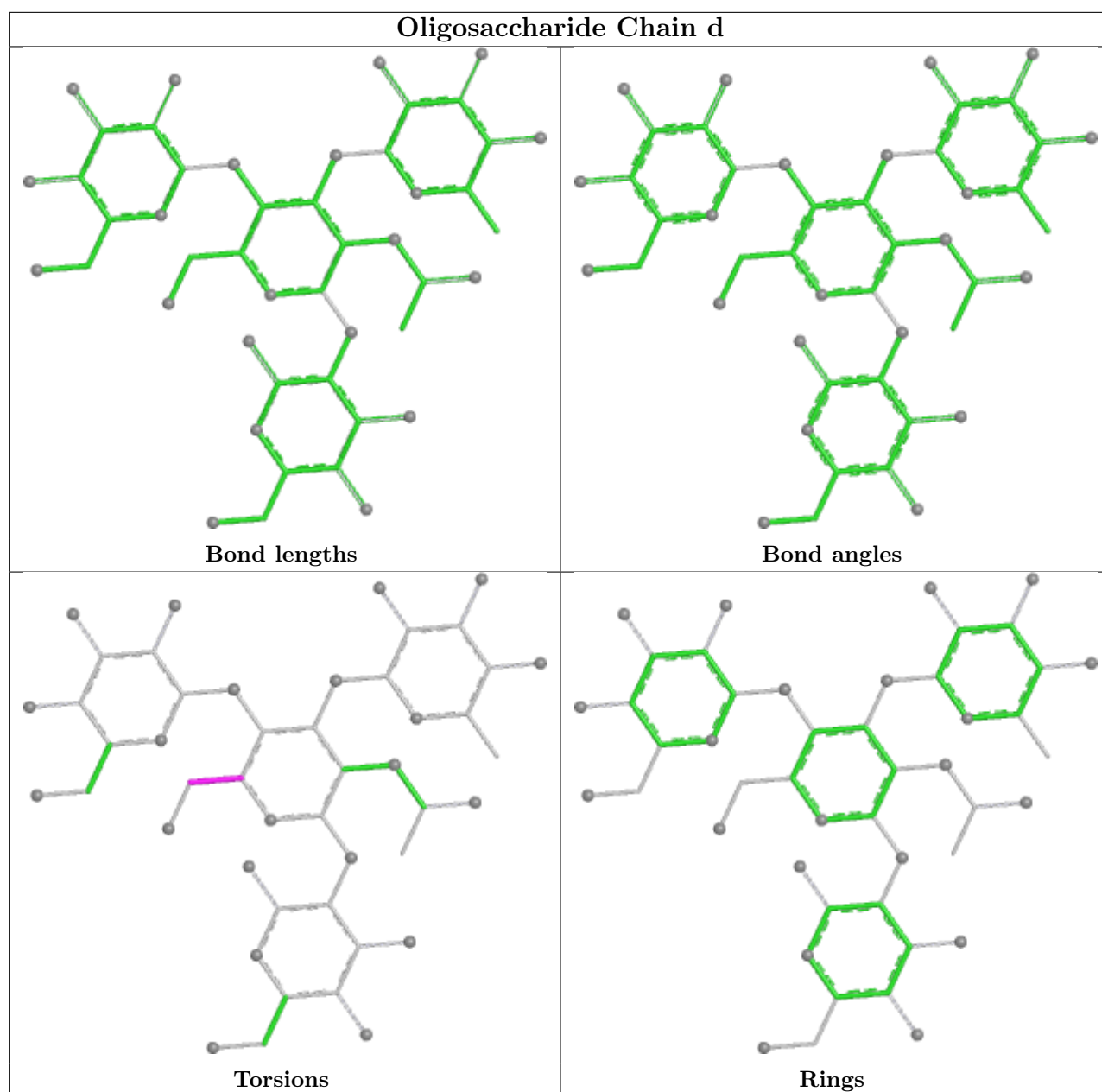


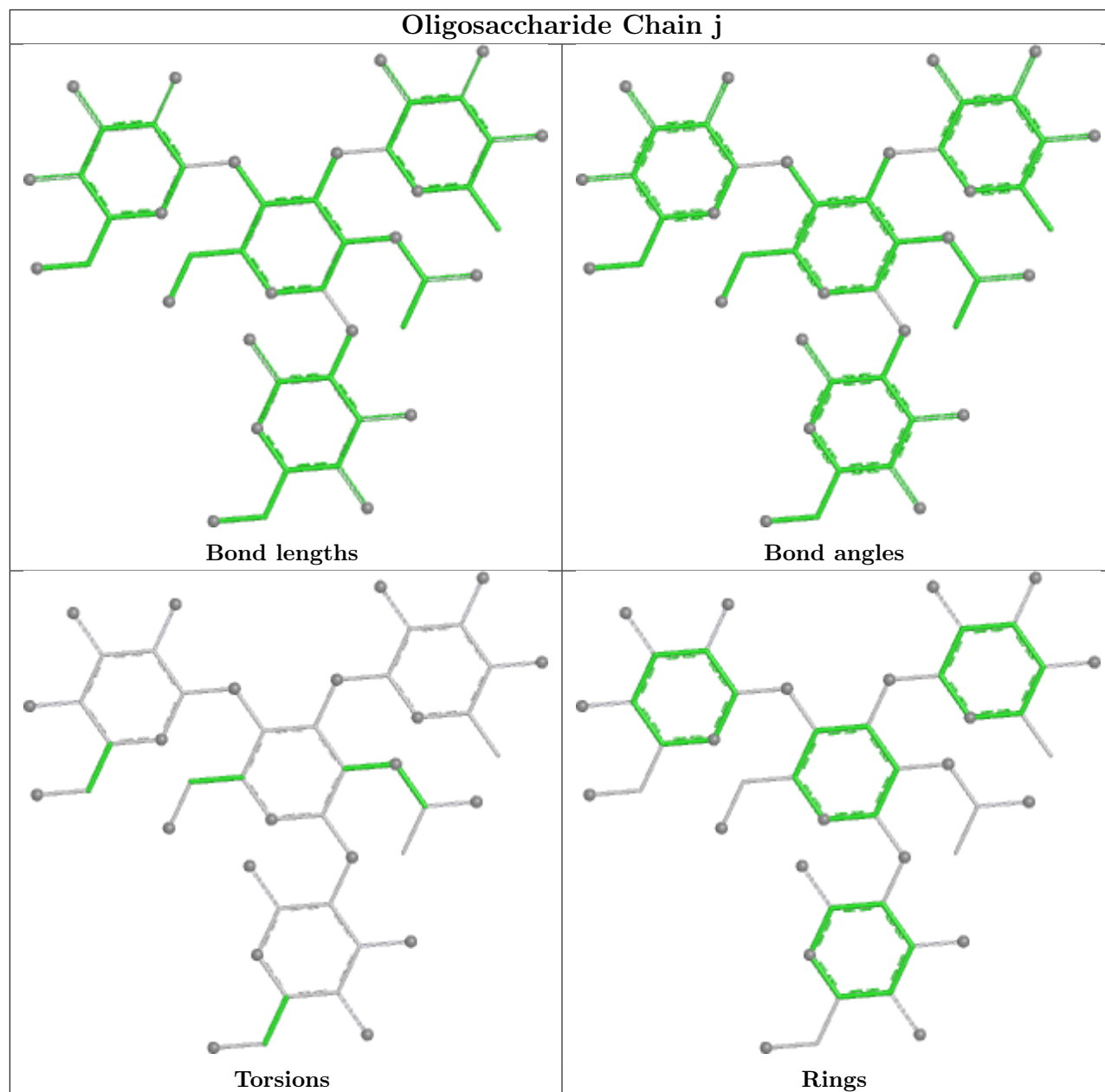




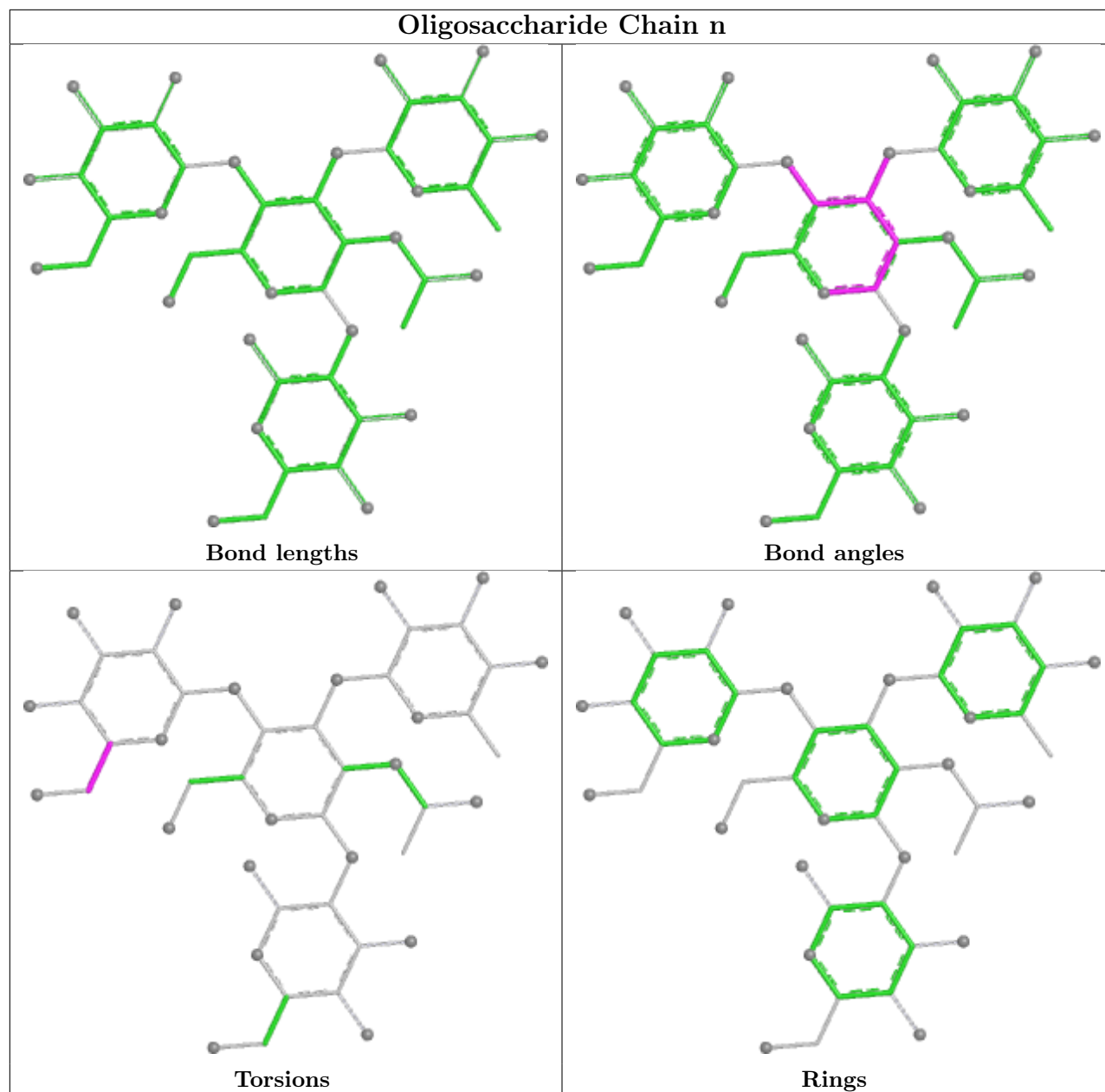


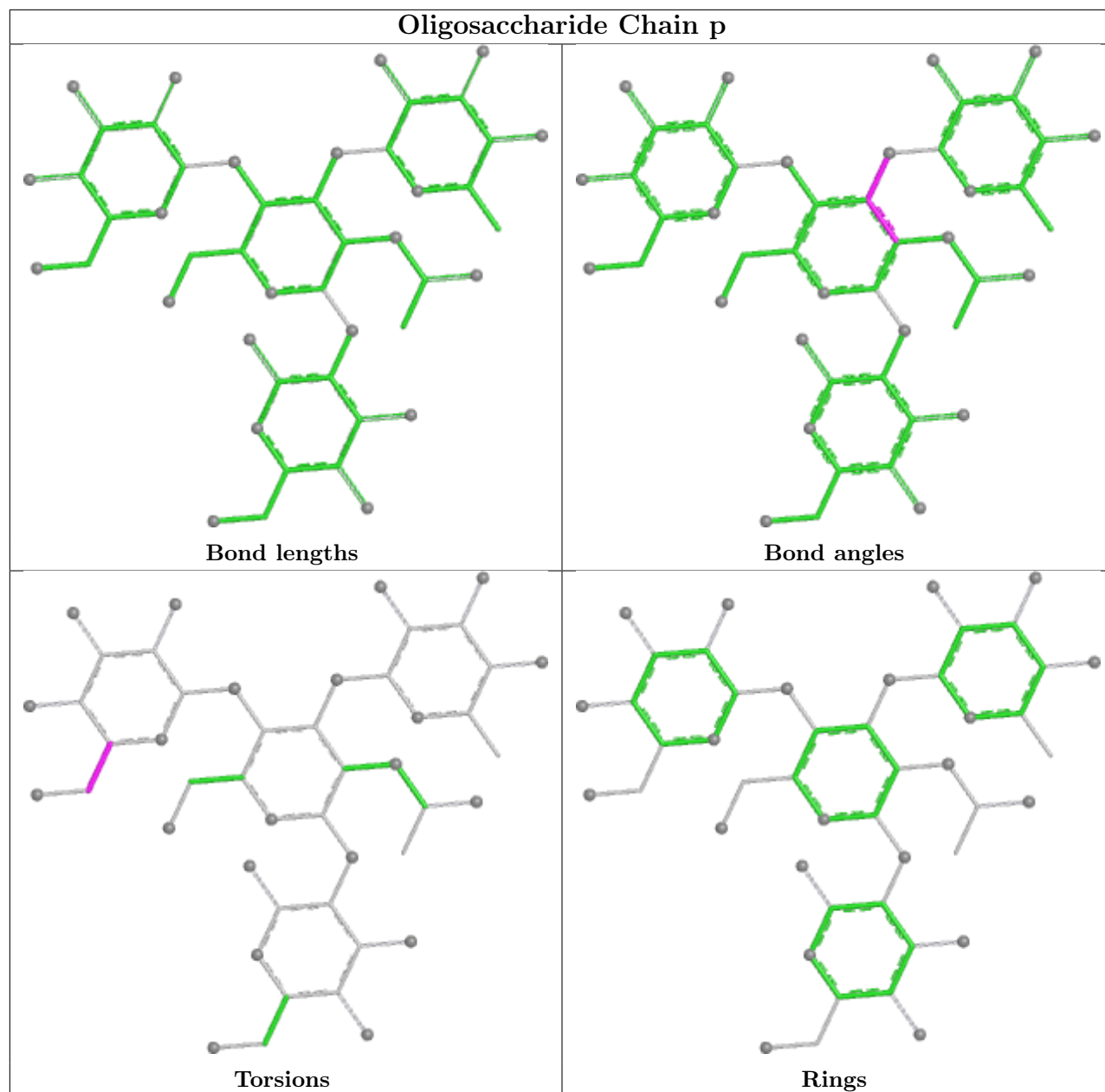


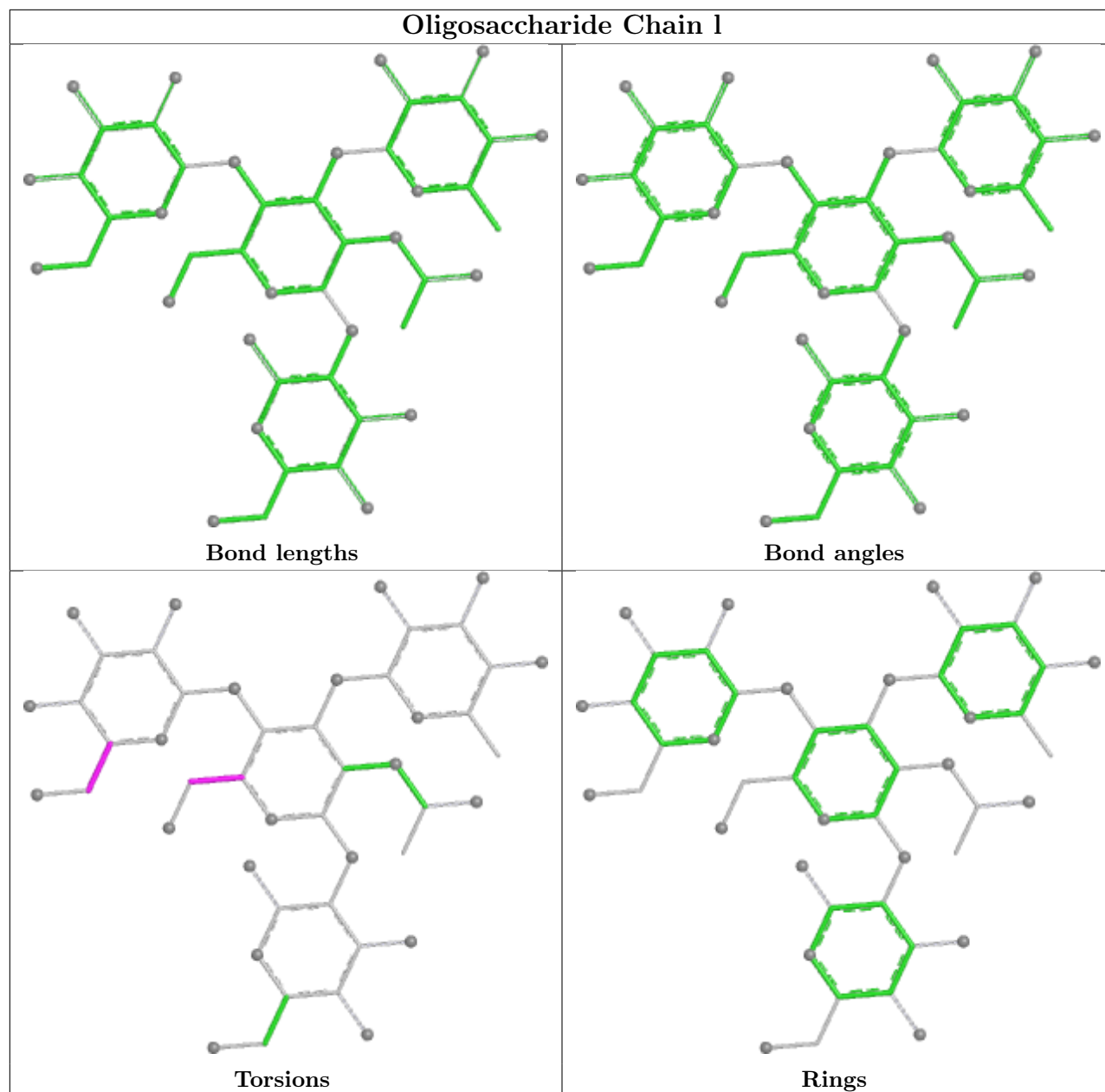


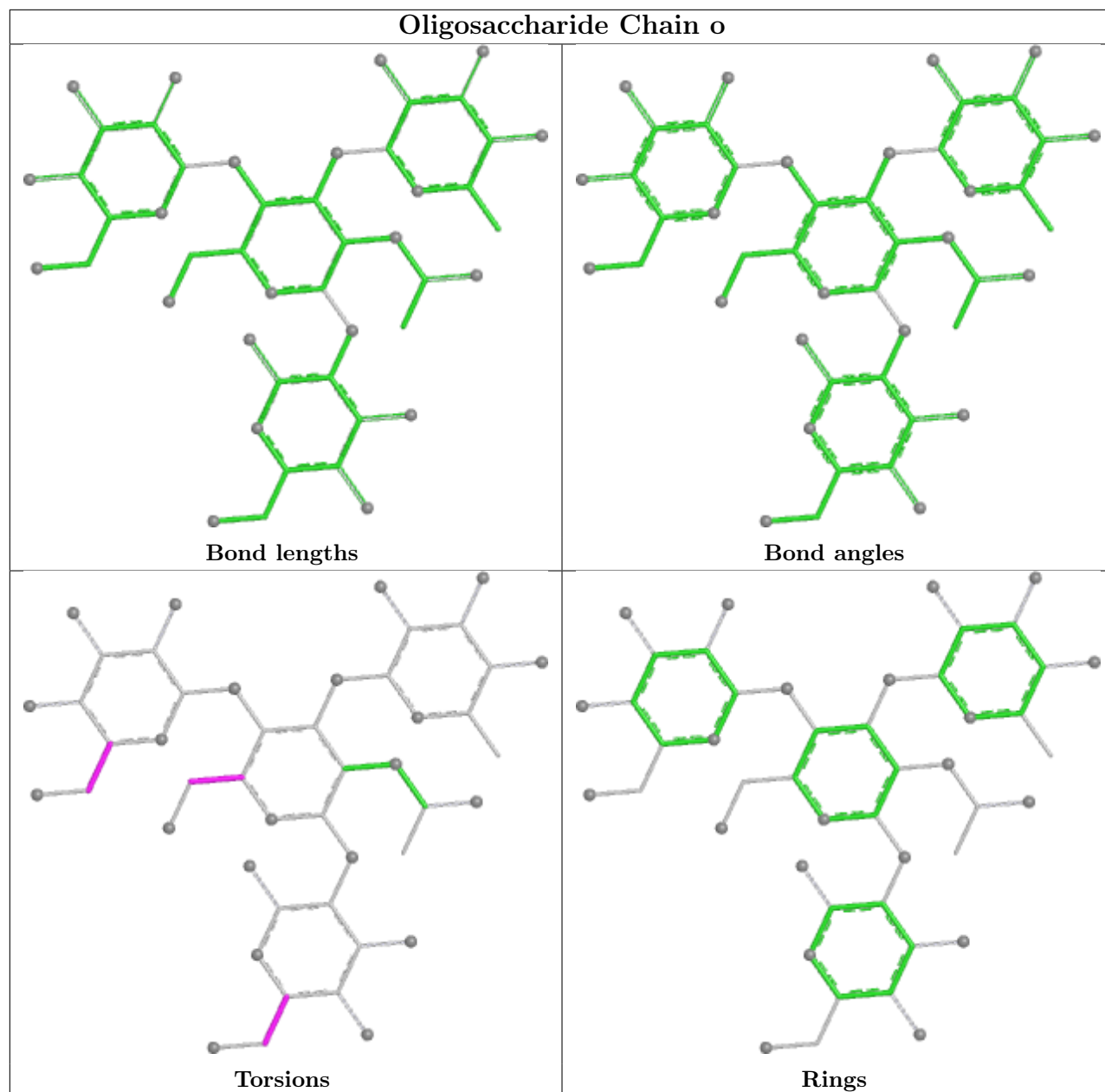


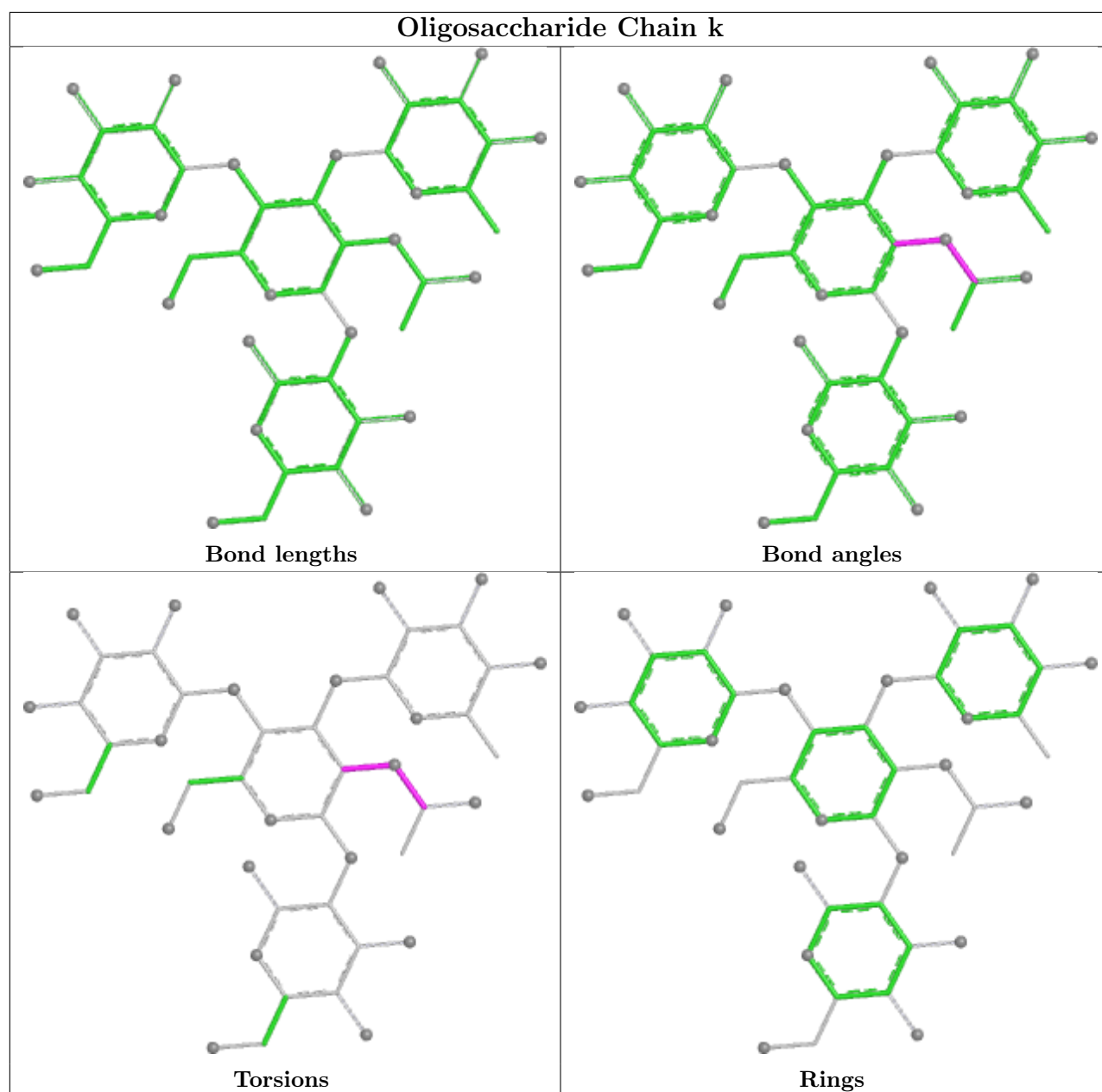


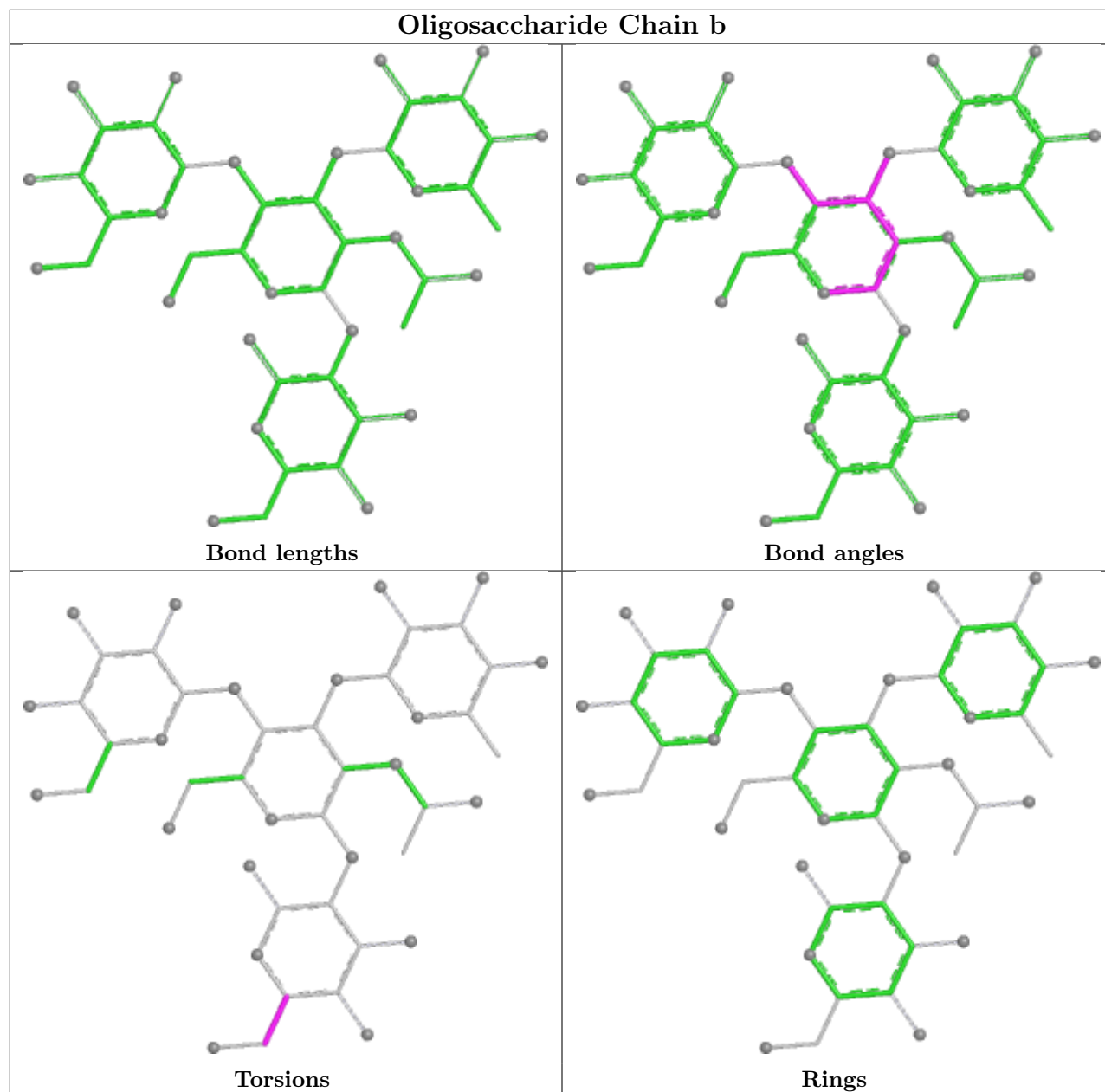


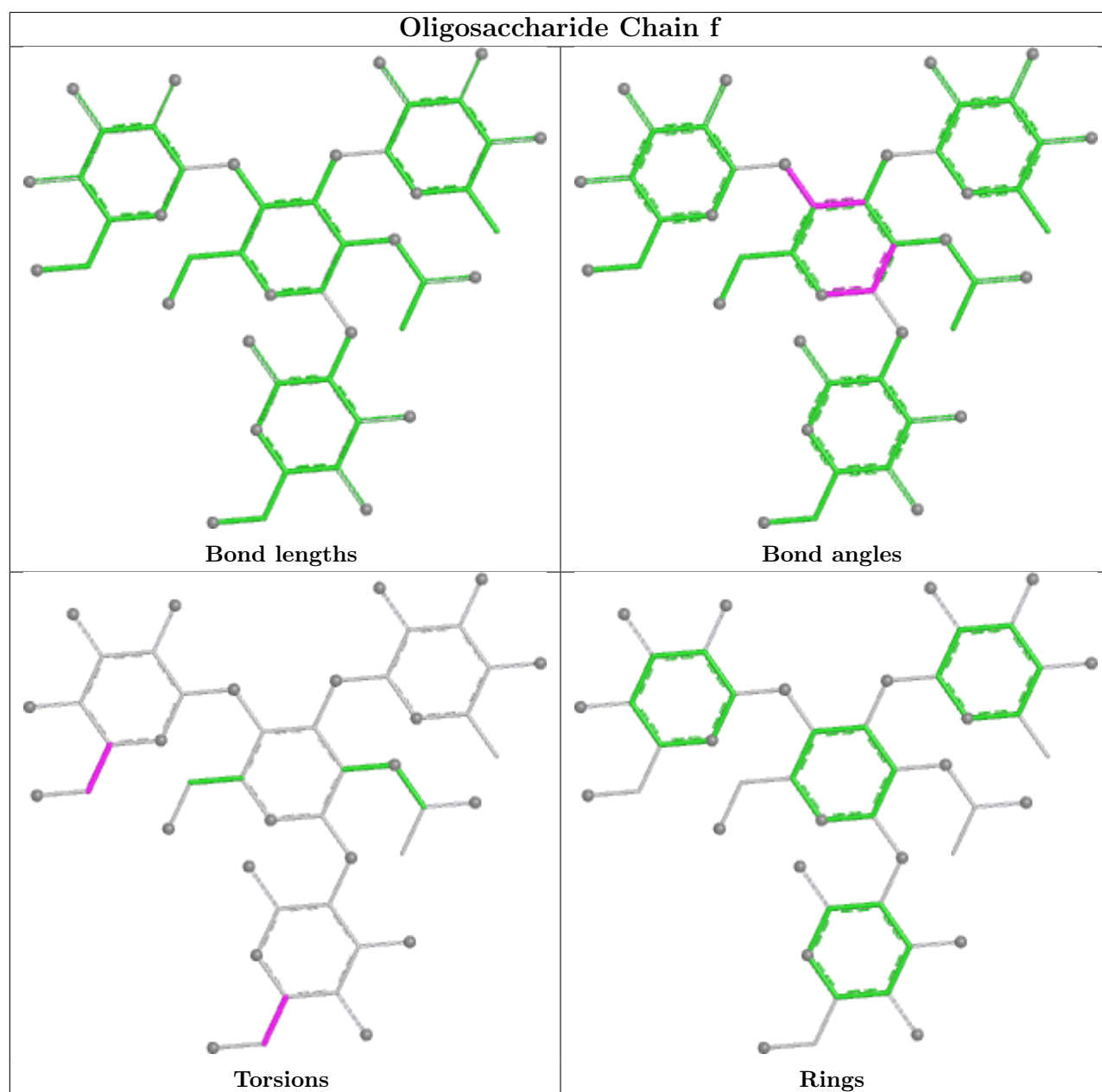












## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	233/264 (88%)	0.24	4 (1%) 69 65	26, 44, 62, 77	0
1	B	234/264 (88%)	0.17	5 (2%) 63 59	25, 42, 60, 78	1 (0%)
1	C	234/264 (88%)	0.28	11 (4%) 36 32	28, 42, 59, 92	0
1	D	233/264 (88%)	0.21	5 (2%) 63 59	25, 38, 57, 68	0
1	E	234/264 (88%)	0.11	3 (1%) 75 71	21, 39, 58, 80	0
1	F	234/264 (88%)	0.33	7 (2%) 52 48	23, 43, 61, 78	0
1	G	232/264 (87%)	-0.15	3 (1%) 75 71	23, 31, 48, 70	0
1	H	232/264 (87%)	-0.14	1 (0%) 88 86	22, 31, 48, 68	0
1	I	232/264 (87%)	0.20	5 (2%) 62 58	26, 40, 58, 71	0
1	J	232/264 (87%)	-0.01	2 (0%) 81 78	22, 34, 53, 77	0
1	K	234/264 (88%)	1.01	41 (17%) 4 3	32, 61, 88, 98	0
1	L	234/264 (88%)	0.60	14 (5%) 27 24	29, 50, 68, 73	0
1	M	232/264 (87%)	-0.12	2 (0%) 81 78	22, 29, 48, 69	0
1	N	233/264 (88%)	-0.13	3 (1%) 75 71	23, 29, 46, 68	0
1	O	234/264 (88%)	0.08	7 (2%) 52 48	22, 39, 55, 68	0
1	P	232/264 (87%)	0.37	6 (2%) 57 52	19, 46, 65, 71	1 (0%)
All	All	3729/4224 (88%)	0.19	119 (3%) 50 46	19, 39, 64, 98	2 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1	ALA	5.5
1	K	249	VAL	4.8
1	K	130	ALA	4.6
1	I	249	VAL	4.4
1	K	48	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	L	249	VAL	4.0
1	O	2	GLN	4.0
1	P	1	ALA	3.8
1	D	249	VAL	3.7
1	N	1	ALA	3.6
1	K	143	LEU	3.6
1	L	62	SER	3.6
1	C	130	ALA	3.6
1	C	1	ALA	3.5
1	K	104	GLY	3.5
1	L	1	ALA	3.5
1	M	1	ALA	3.4
1	K	1	ALA	3.4
1	C	44	SER	3.4
1	B	130	ALA	3.3
1	F	1	ALA	3.3
1	K	82	SER	3.3
1	K	230	ASP	3.3
1	K	102	HIS	3.2
1	K	129	ALA	3.2
1	A	1	ALA	3.2
1	F	249	VAL	3.2
1	E	129	ALA	3.1
1	B	131	SER	3.1
1	K	105	PHE	3.1
1	K	22	GLY	3.1
1	K	43	VAL	3.1
1	L	250	ALA	3.1
1	L	61	ASP	3.1
1	O	82	SER	3.0
1	K	248	ASN	3.0
1	L	84	ILE	3.0
1	O	1	ALA	3.0
1	P	206	SER	2.9
1	K	47	ALA	2.9
1	D	1	ALA	2.9
1	K	142	TYR	2.9
1	K	106	LEU	2.8
1	N	250	ALA	2.8
1	K	85	ALA	2.8
1	I	2	GLN	2.8
1	K	147	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	45	SER	2.8
1	K	131	SER	2.8
1	L	87	GLY	2.7
1	K	132	SER	2.7
1	L	228	GLY	2.7
1	F	130	ALA	2.7
1	A	163	ARG	2.7
1	K	146	ASP	2.6
1	G	147	TYR	2.6
1	B	2	GLN	2.6
1	M	248	ASN	2.6
1	C	249	VAL	2.6
1	K	148	GLY	2.6
1	K	228	GLY	2.5
1	A	249	VAL	2.5
1	J	249	VAL	2.5
1	H	1	ALA	2.5
1	J	1	ALA	2.5
1	C	146	ASP	2.5
1	P	231	LYS	2.5
1	A	130	ALA	2.5
1	K	101	TYR	2.4
1	K	227	THR	2.4
1	K	99	ILE	2.4
1	G	113	ASN	2.4
1	N	249	VAL	2.4
1	K	84	ILE	2.4
1	L	148	GLY	2.4
1	K	45	SER	2.3
1	K	113	ASN	2.3
1	L	226	SER	2.3
1	F	229	GLN	2.3
1	G	1	ALA	2.3
1	B	14[A]	ASN	2.3
1	P	233	ARG	2.3
1	K	83	ARG	2.3
1	D	7	SER	2.3
1	F	206	SER	2.3
1	E	249	VAL	2.3
1	P	43	VAL	2.3
1	I	13	PRO	2.3
1	K	144	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	44	SER	2.2
1	K	226	SER	2.2
1	O	61	ASP	2.2
1	C	43	VAL	2.2
1	C	38	SER	2.2
1	K	26	SER	2.2
1	I	145	PRO	2.2
1	O	249	VAL	2.2
1	C	199	GLY	2.2
1	F	217	GLU	2.2
1	O	129	ALA	2.2
1	K	107	GLY	2.2
1	C	129	ALA	2.1
1	D	28	ASN	2.1
1	K	151	ASN	2.1
1	L	104	GLY	2.1
1	C	231	LYS	2.1
1	L	130	ALA	2.1
1	F	86	ASP	2.1
1	D	250	ALA	2.0
1	K	14	ASN	2.0
1	P	62	SER	2.0
1	K	79	PRO	2.0
1	K	150	PRO	2.0
1	K	109	PHE	2.0
1	L	143	LEU	2.0
1	E	61	ASP	2.0
1	L	230	ASP	2.0
1	B	61	ASP	2.0
1	O	53	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	a	1	12/12	-	-	49,54,58,59	0
2	NAG	a	2	14/15	-	-	49,53,63,64	0
2	FUC	a	3	10/11	-	-	57,62,63,64	0
2	GAL	a	4	11/12	-	-	53,56,66,75	0
2	MAN	e	1	12/12	-	-	43,52,55,56	0
2	NAG	e	2	14/15	-	-	47,54,61,65	0
2	FUC	e	3	10/11	-	-	50,53,57,63	0
2	GAL	e	4	11/12	-	-	47,53,58,63	0
2	MAN	c	1	12/12	-	-	36,42,55,56	0
2	NAG	c	2	14/15	-	-	35,41,53,57	0
2	FUC	c	3	10/11	-	-	55,58,63,66	0
2	GAL	c	4	11/12	-	-	45,52,62,66	0
2	MAN	g	1	12/12	-	-	24,31,41,50	0
2	NAG	g	2	14/15	-	-	31,39,43,51	0
2	FUC	g	3	10/11	-	-	61,73,88,105	0
2	GAL	g	4	11/12	-	-	33,42,47,55	0
2	MAN	i	1	12/12	-	-	39,45,56,60	0
2	NAG	i	2	14/15	-	-	41,49,54,54	0
2	FUC	i	3	10/11	-	-	45,55,58,63	0
2	GAL	i	4	11/12	-	-	58,61,68,74	0
2	MAN	m	1	12/12	-	-	27,32,43,45	0
2	NAG	m	2	14/15	-	-	25,37,46,49	0
2	FUC	m	3	10/11	-	-	39,50,54,58	0
2	GAL	m	4	11/12	-	-	36,46,51,54	0
2	MAN	h	1	12/12	-	-	28,33,41,43	0
2	NAG	h	2	14/15	-	-	28,37,41,46	0
2	FUC	h	3	10/11	-	-	37,40,41,41	0
2	GAL	h	4	11/12	-	-	43,50,52,57	0
2	MAN	d	1	12/12	-	-	42,48,52,55	0
2	NAG	d	2	14/15	-	-	29,34,41,41	0
2	FUC	d	3	10/11	-	-	34,40,47,53	0
2	GAL	d	4	11/12	-	-	36,46,52,59	0
2	MAN	j	1	12/12	-	-	30,36,43,45	0
2	NAG	j	2	14/15	-	-	23,32,42,42	0
2	FUC	j	3	10/11	-	-	38,42,52,56	0
2	GAL	j	4	11/12	-	-	39,43,48,60	0
2	MAN	n	1	12/12	-	-	26,36,44,52	0
2	NAG	n	2	14/15	-	-	22,33,42,43	0
2	FUC	n	3	10/11	-	-	38,47,53,60	0
2	GAL	n	4	11/12	-	-	40,48,58,75	0
2	MAN	p	1	12/12	-	-	55,60,65,65	0
2	NAG	p	2	14/15	-	-	49,53,65,67	0
2	FUC	p	3	10/11	-	-	49,52,56,63	0

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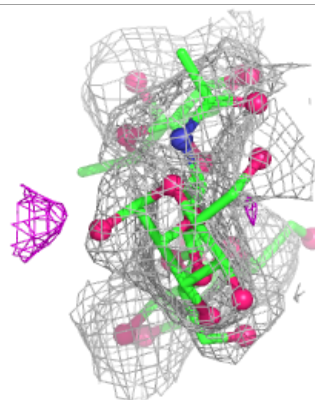
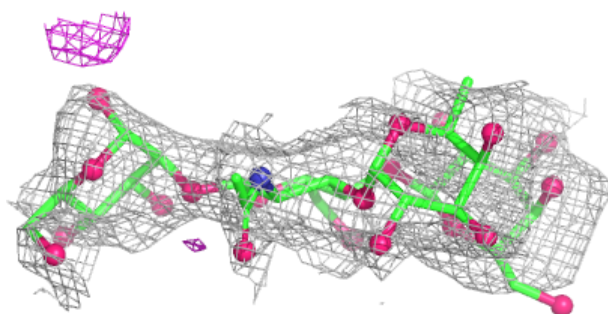
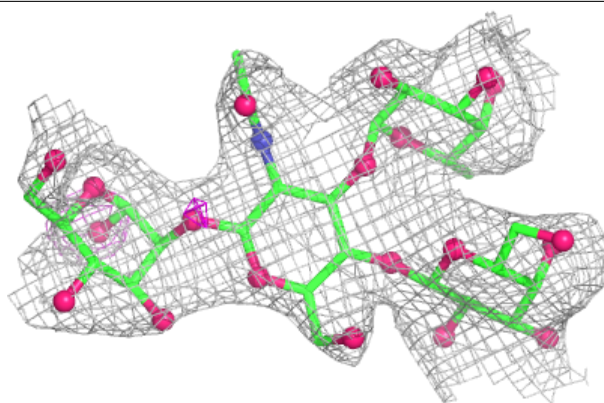
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GAL	p	4	11/12	-	-	54,58,72,77	0
2	MAN	l	1	12/12	-	-	51,61,65,71	0
2	NAG	l	2	14/15	-	-	61,62,65,68	0
2	FUC	l	3	10/11	-	-	63,68,73,78	0
2	GAL	l	4	11/12	-	-	66,72,79,79	0
2	MAN	o	1	12/12	-	-	43,46,53,54	0
2	NAG	o	2	14/15	-	-	47,52,57,60	0
2	FUC	o	3	10/11	-	-	45,51,57,64	0
2	GAL	o	4	11/12	-	-	50,57,68,76	0
2	MAN	k	1	12/12	-	-	78,82,83,85	0
2	NAG	k	2	14/15	-	-	68,85,100,103	0
2	FUC	k	3	10/11	-	-	97,98,102,103	0
2	GAL	k	4	11/12	-	-	97,100,105,106	0
2	MAN	b	1	12/12	-	-	44,51,60,71	0
2	NAG	b	2	14/15	-	-	42,53,64,83	0
2	FUC	b	3	10/11	-	-	47,54,61,62	0
2	GAL	b	4	11/12	-	-	91,91,97,101	0
2	MAN	f	1	12/12	-	-	47,49,51,51	0
2	NAG	f	2	14/15	-	-	48,51,58,59	0
2	FUC	f	3	10/11	-	-	44,48,51,54	0
2	GAL	f	4	11/12	-	-	49,53,61,65	0

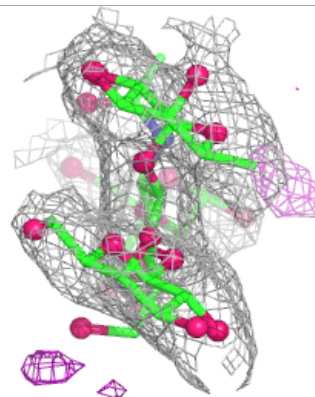
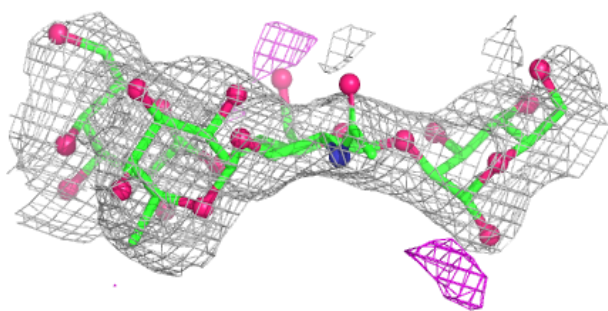
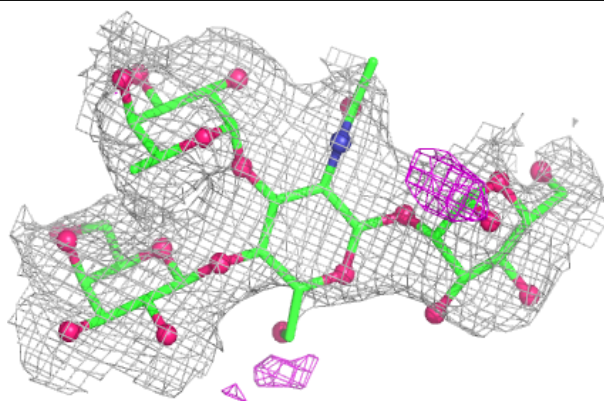
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain a:**

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

**Electron density around Chain e:**

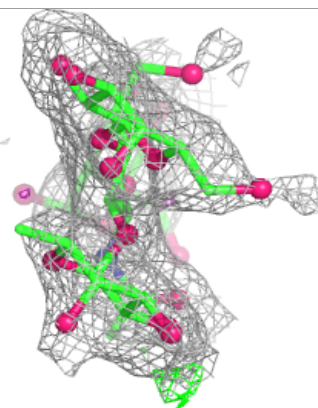
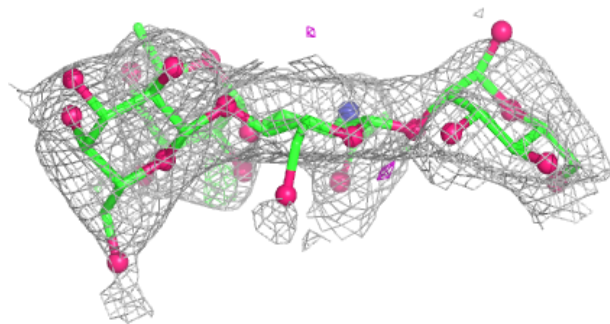
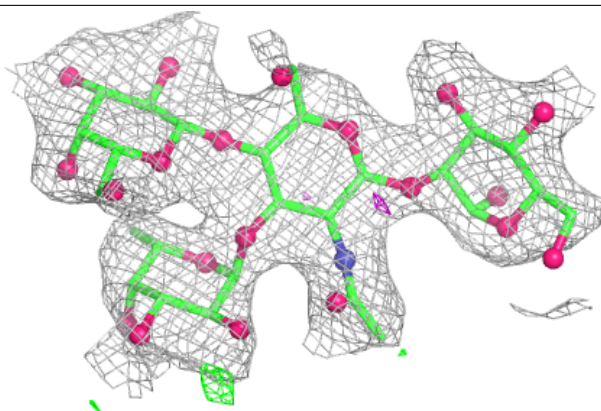
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain c:**

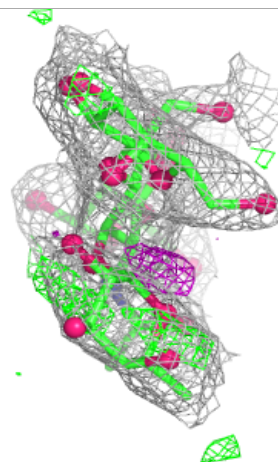
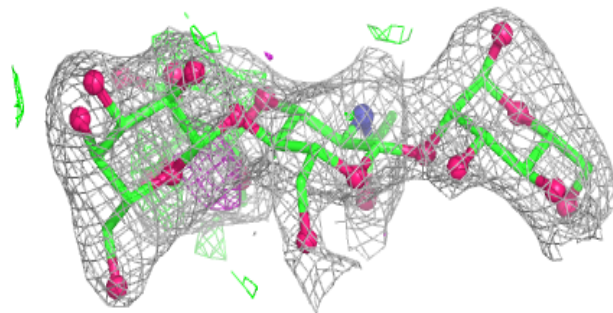
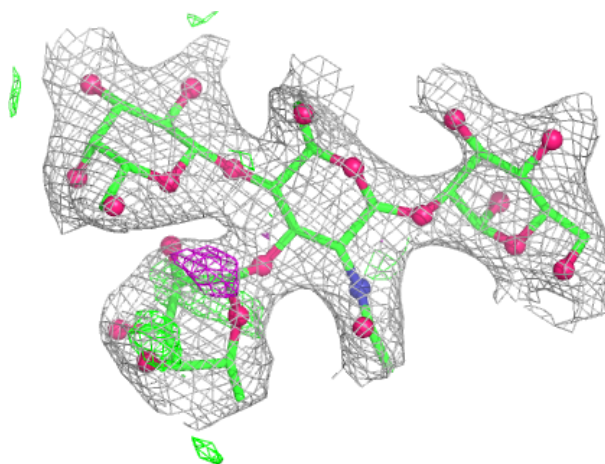
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





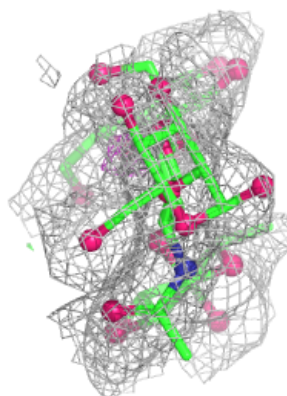
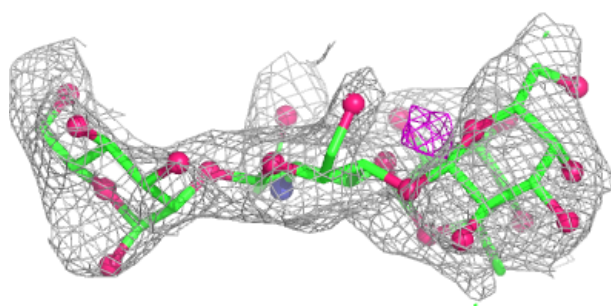
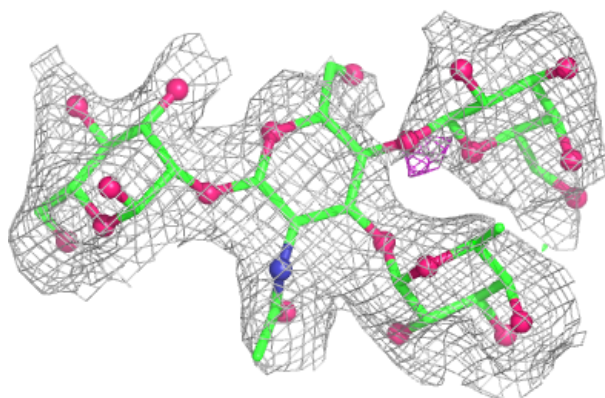
**Electron density around Chain g:**

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

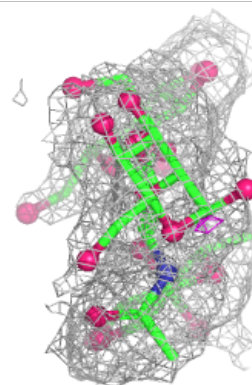
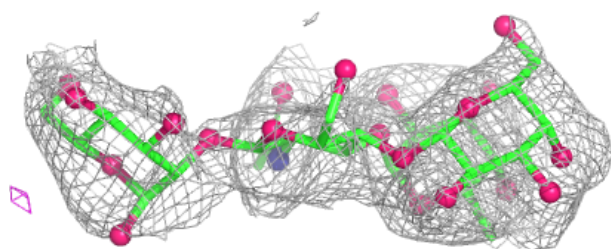
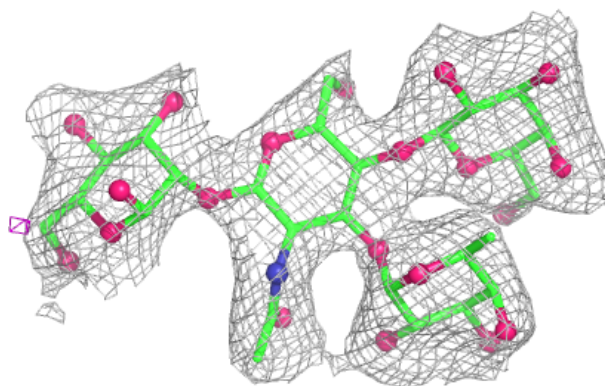


**Electron density around Chain i:**

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

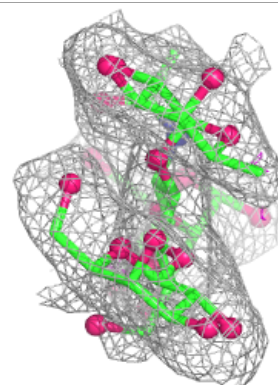
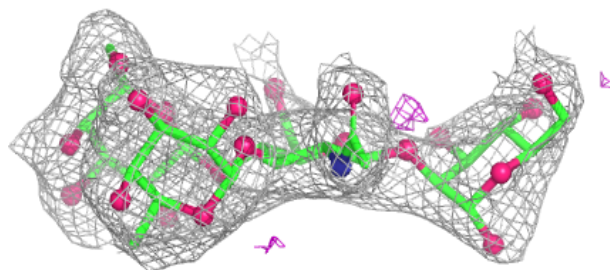
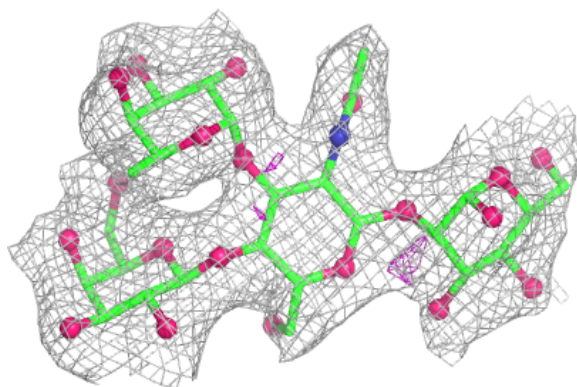
**Electron density around Chain m:**

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

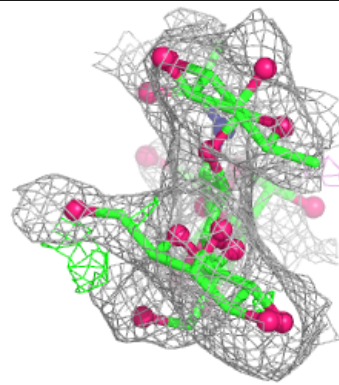
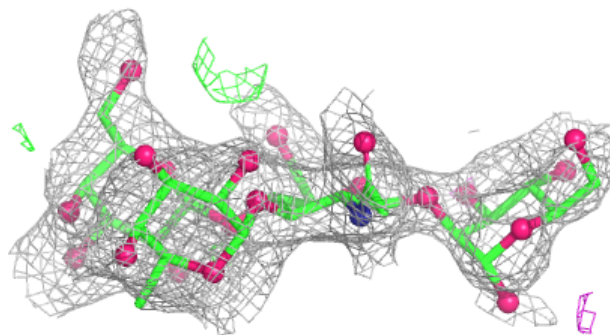
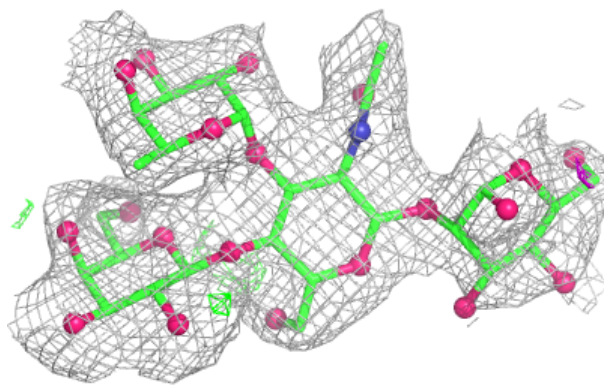


**Electron density around Chain h:**

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

**Electron density around Chain d:**

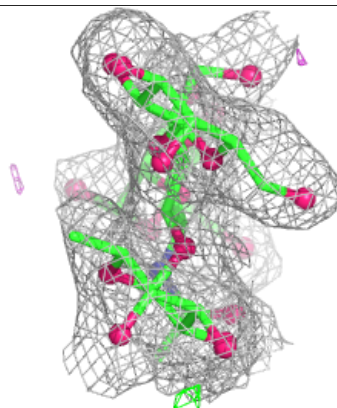
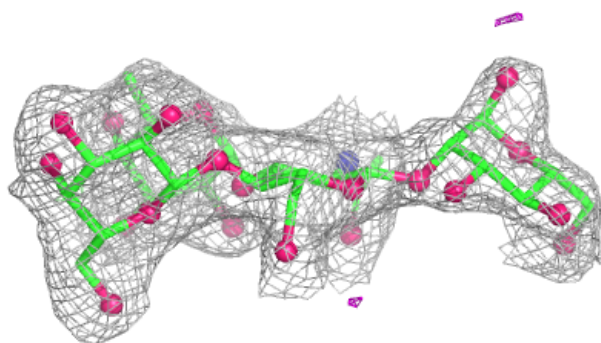
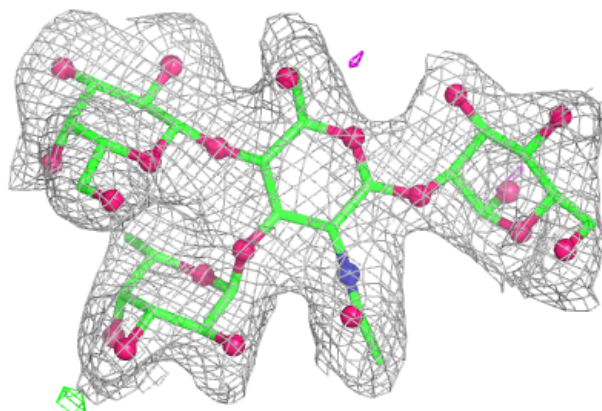
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



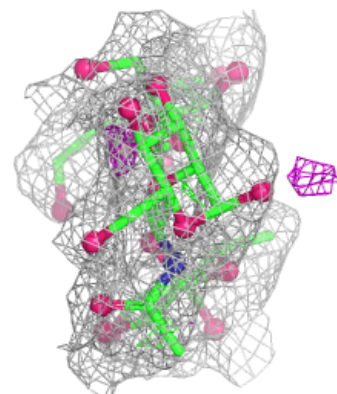
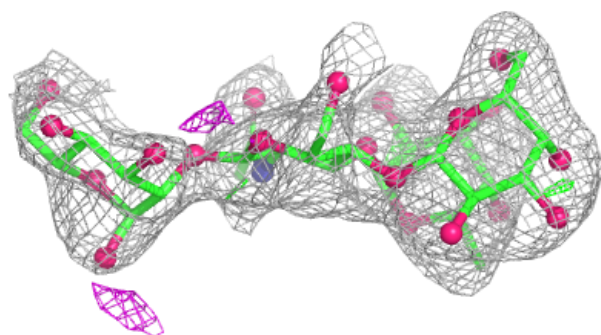
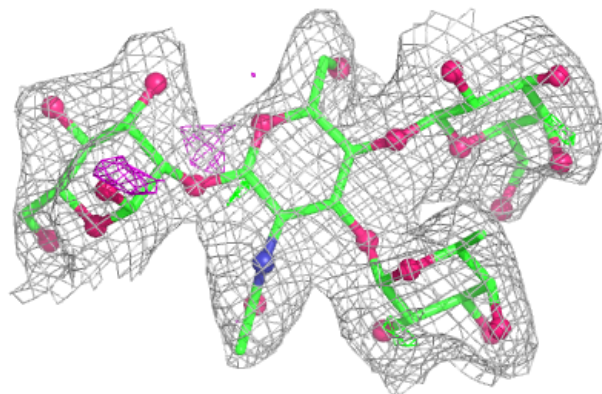


**Electron density around Chain j:**

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

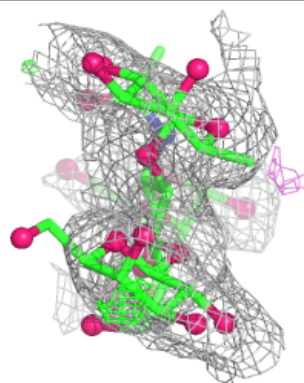
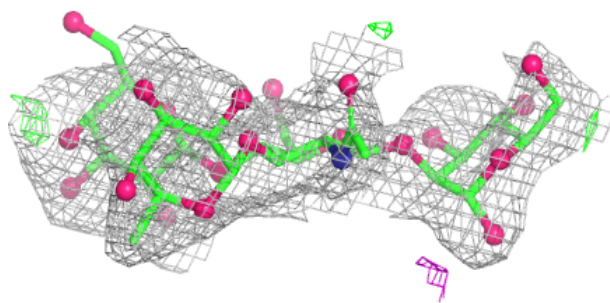
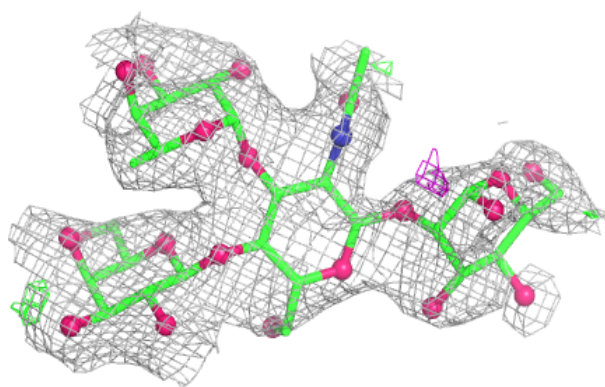
**Electron density around Chain n:**

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

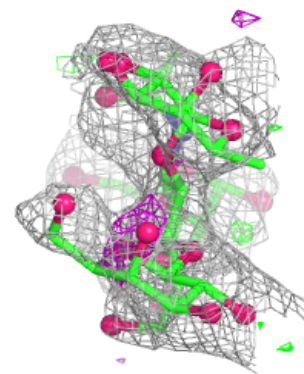
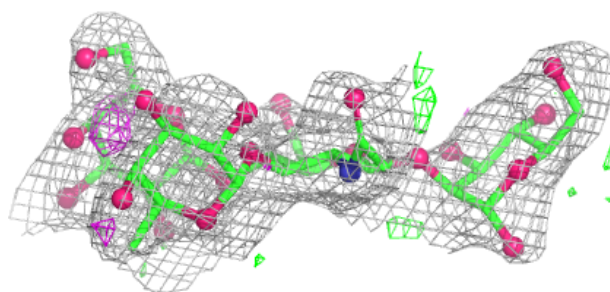
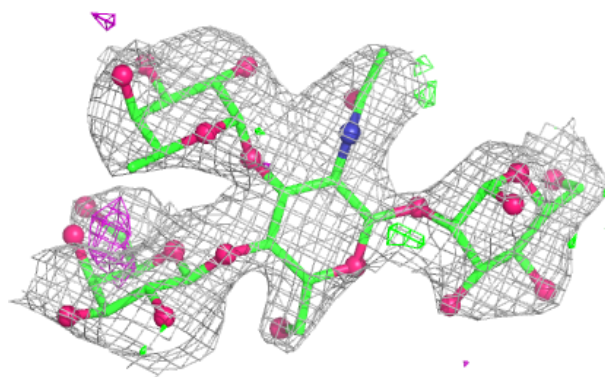


**Electron density around Chain p:**

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

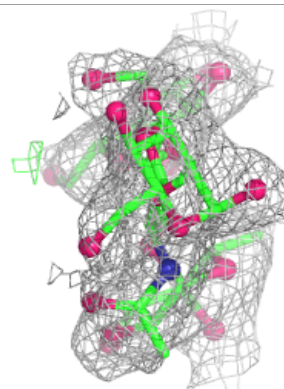
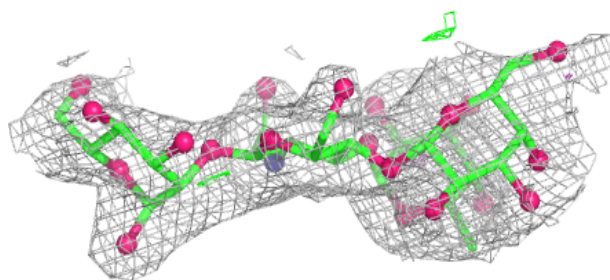
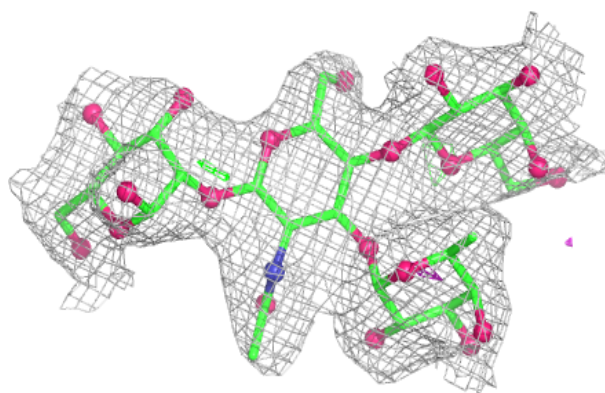
**Electron density around Chain l:**

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

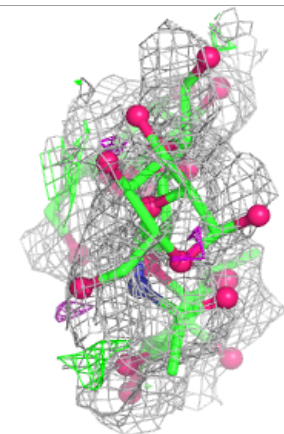
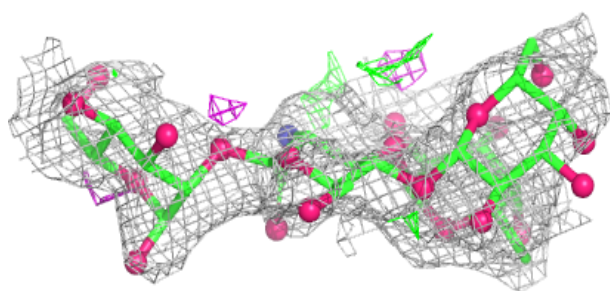
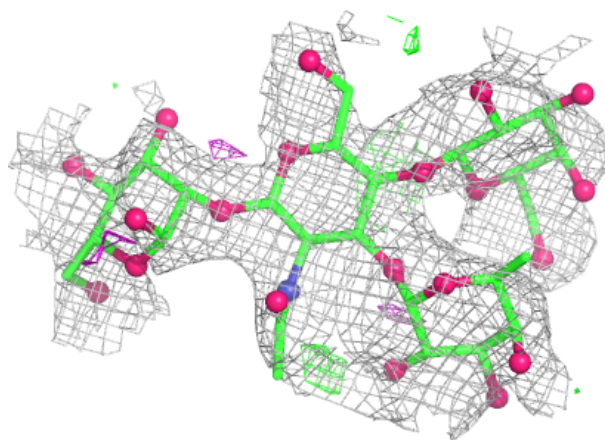


**Electron density around Chain o:**

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

**Electron density around Chain k:**

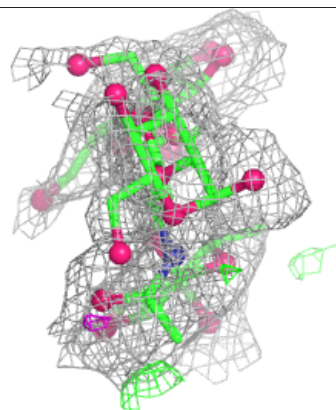
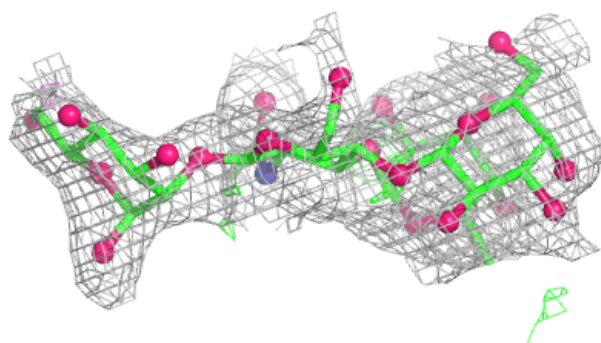
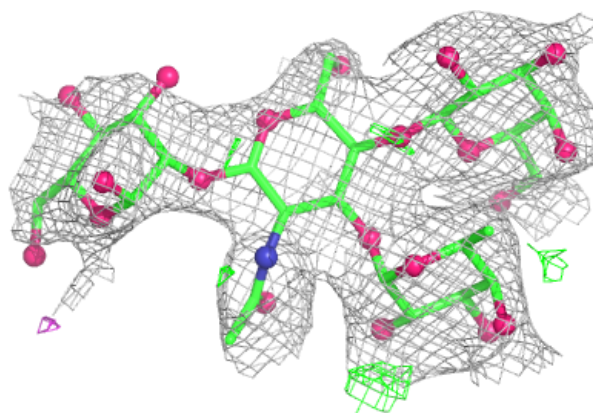
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



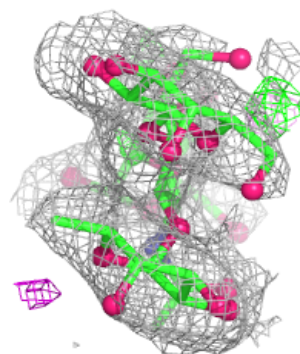
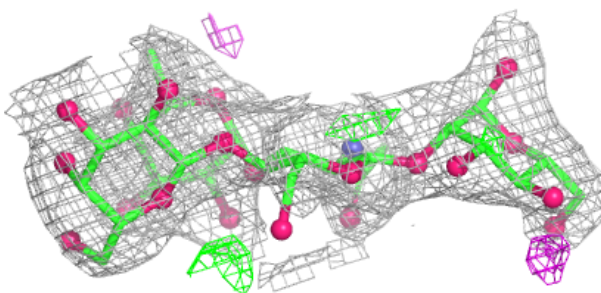
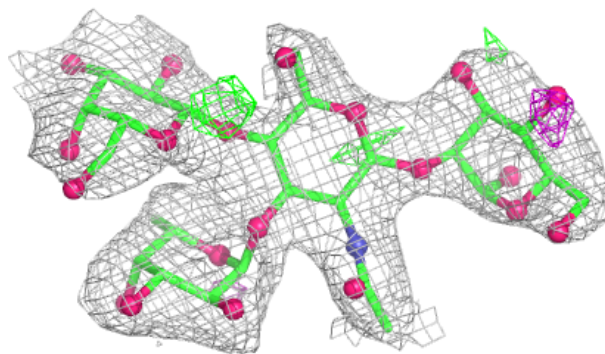


**Electron density around Chain b:**

$2mF_o-DF_c$  (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)



## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

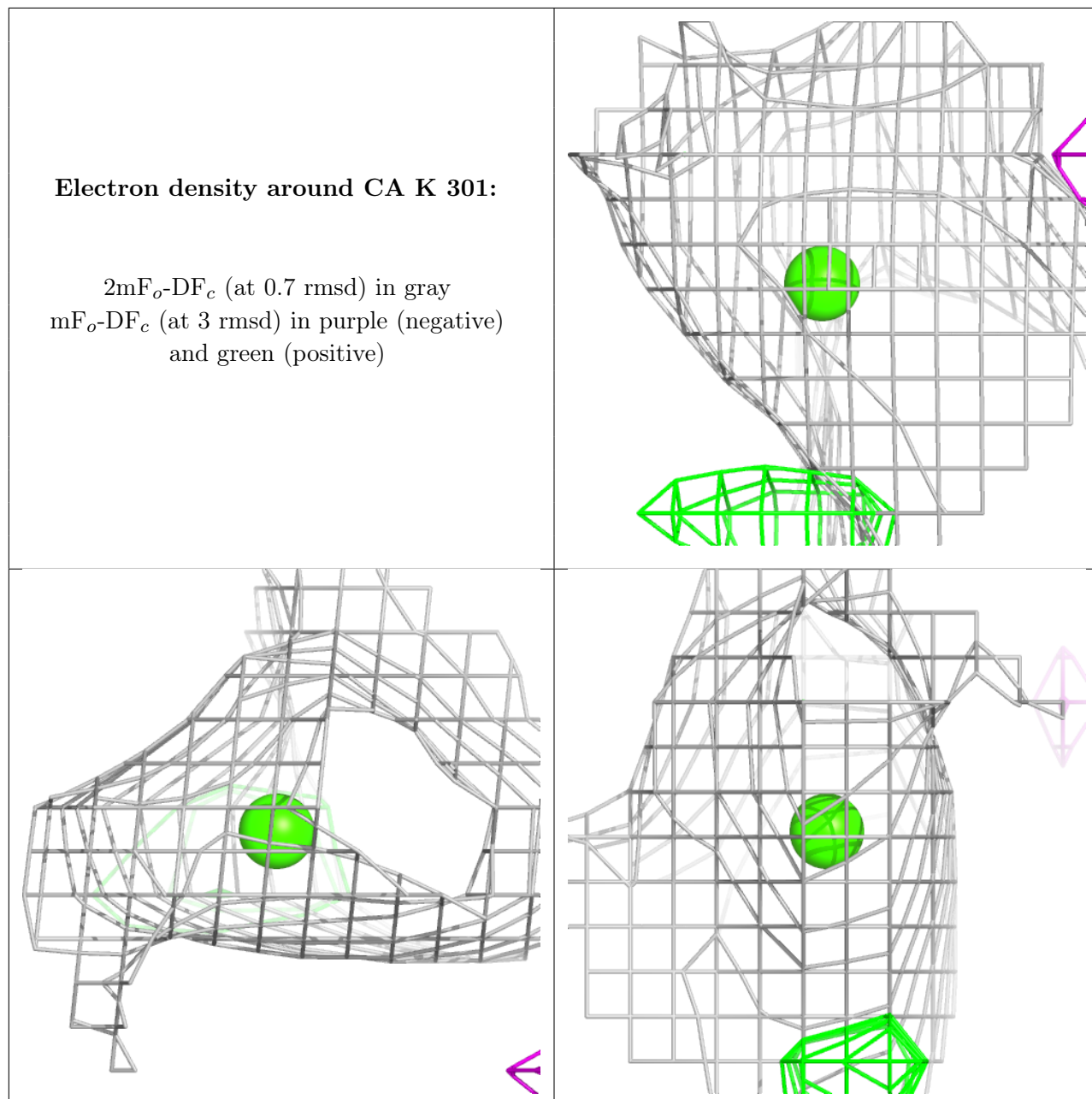
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	K	301	1/1	0.90	0.09	70,70,70,70	0
3	CA	O	301	1/1	0.91	0.09	43,43,43,43	0
3	CA	H	301	1/1	0.93	0.10	24,24,24,24	0
3	CA	E	301	1/1	0.95	0.12	37,37,37,37	0
3	CA	B	301	1/1	0.96	0.10	45,45,45,45	0
3	CA	F	301	1/1	0.96	0.07	42,42,42,42	0
3	CA	M	301	1/1	0.96	0.07	23,23,23,23	0
4	MN	K	302	1/1	0.96	0.06	68,68,68,68	0
3	CA	J	301	1/1	0.97	0.09	26,26,26,26	0
3	CA	P	301	1/1	0.97	0.09	51,51,51,51	0
3	CA	L	301	1/1	0.97	0.05	46,46,46,46	0
4	MN	A	302	1/1	0.97	0.04	48,48,48,48	0
4	MN	C	302	1/1	0.97	0.04	42,42,42,42	0
4	MN	G	302	1/1	0.97	0.06	32,32,32,32	0
3	CA	G	301	1/1	0.97	0.10	22,22,22,22	0
3	CA	D	301	1/1	0.98	0.12	26,26,26,26	0
3	CA	I	301	1/1	0.98	0.11	32,32,32,32	0
3	CA	C	301	1/1	0.98	0.09	38,38,38,38	0
4	MN	M	302	1/1	0.98	0.08	33,33,33,33	0
3	CA	A	301	1/1	0.98	0.04	27,27,27,27	0
4	MN	I	302	1/1	0.99	0.03	35,35,35,35	0
3	CA	N	301	1/1	0.99	0.10	21,21,21,21	0
4	MN	H	302	1/1	0.99	0.02	27,27,27,27	0
4	MN	J	302	1/1	0.99	0.04	33,33,33,33	0
4	MN	P	302	1/1	0.99	0.02	46,46,46,46	0
4	MN	L	302	1/1	0.99	0.03	52,52,52,52	0
4	MN	O	302	1/1	0.99	0.02	45,45,45,45	0
4	MN	B	302	1/1	0.99	0.04	42,42,42,42	0
4	MN	F	302	1/1	0.99	0.02	40,40,40,40	0
4	MN	N	302	1/1	0.99	0.06	27,27,27,27	0
4	MN	E	302	1/1	0.99	0.03	42,42,42,42	0
4	MN	D	302	1/1	1.00	0.04	35,35,35,35	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.



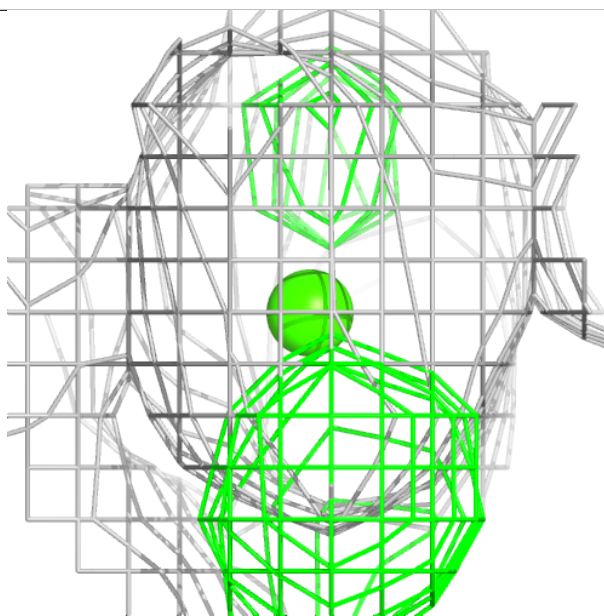
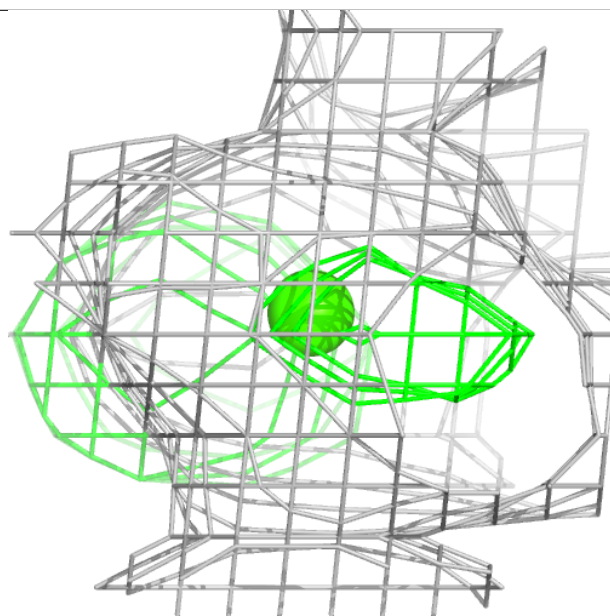
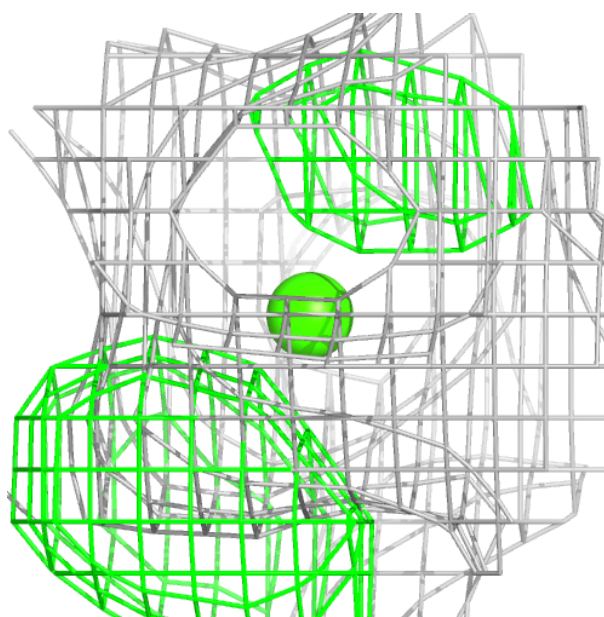
**Electron density around CA K 301:**

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



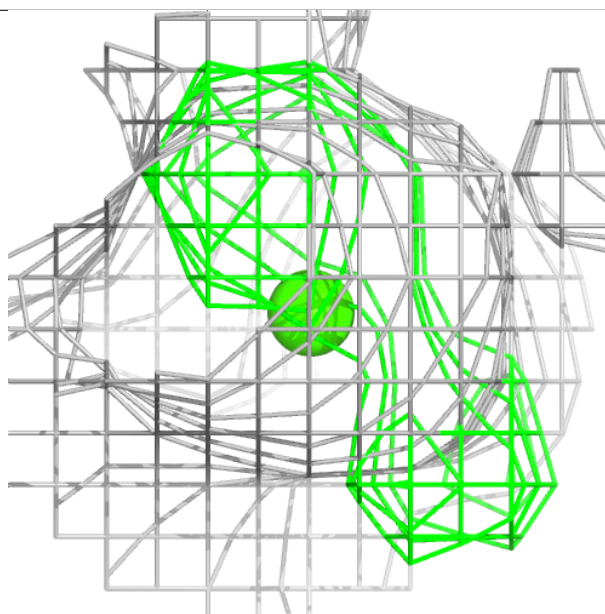
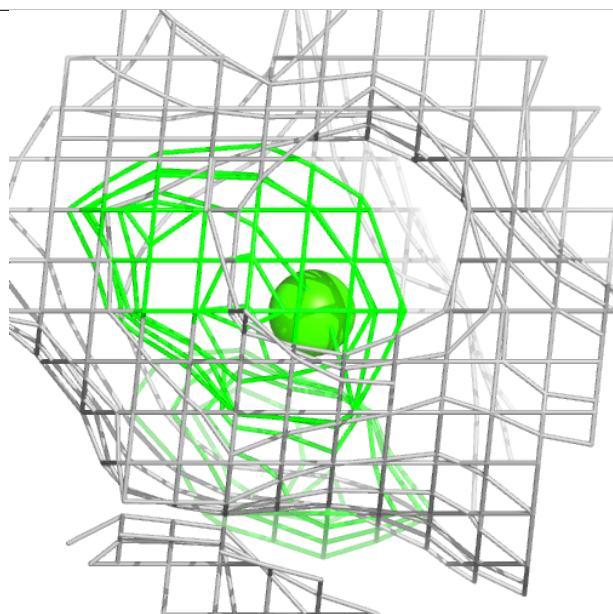
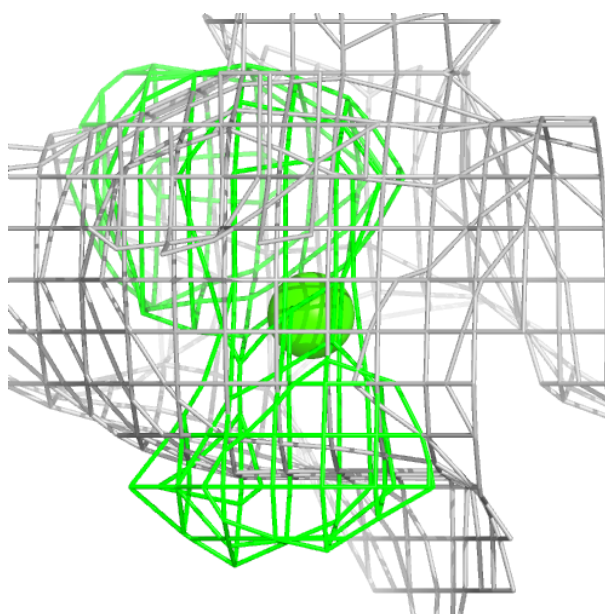
**Electron density around CA O 301:**

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



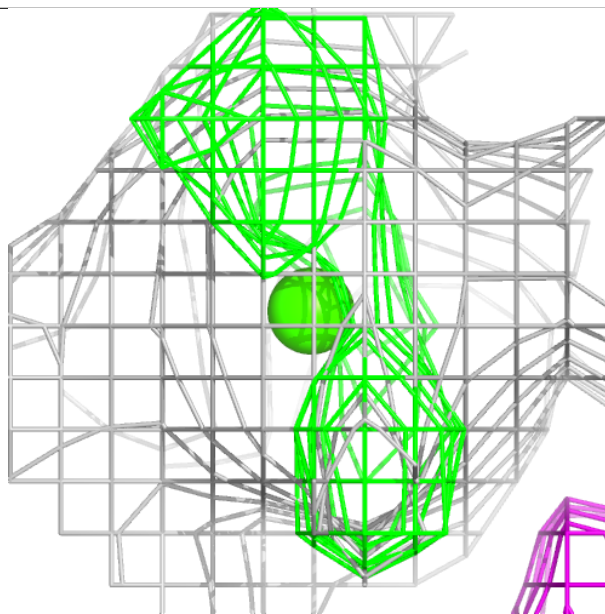
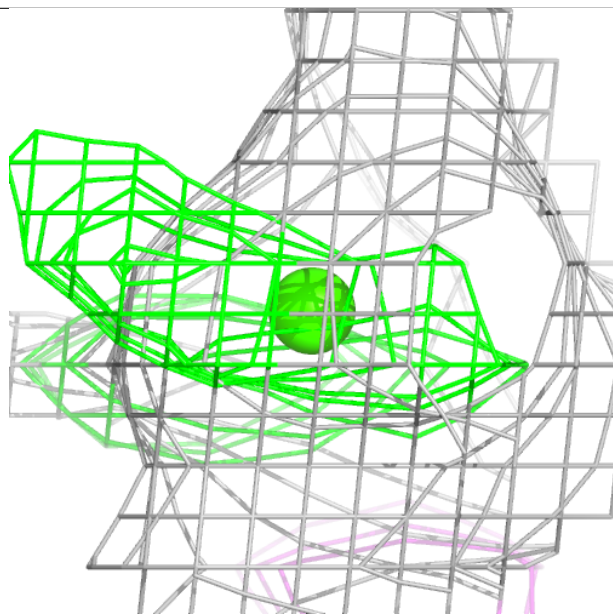
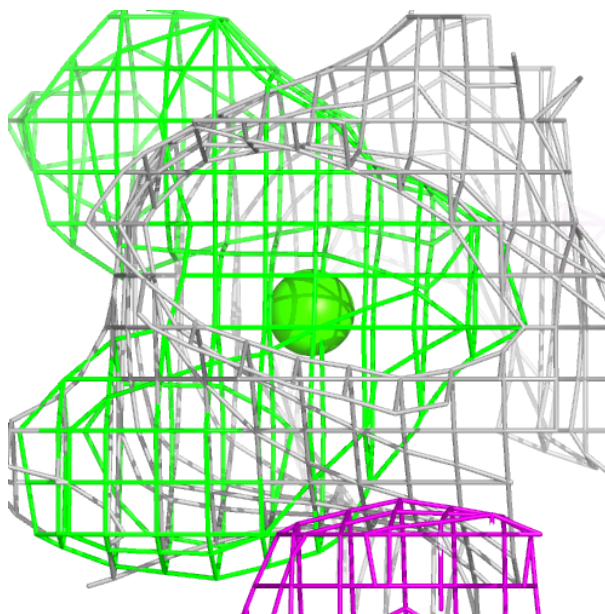
**Electron density around CA H 301:**

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



**Electron density around CA E 301:**

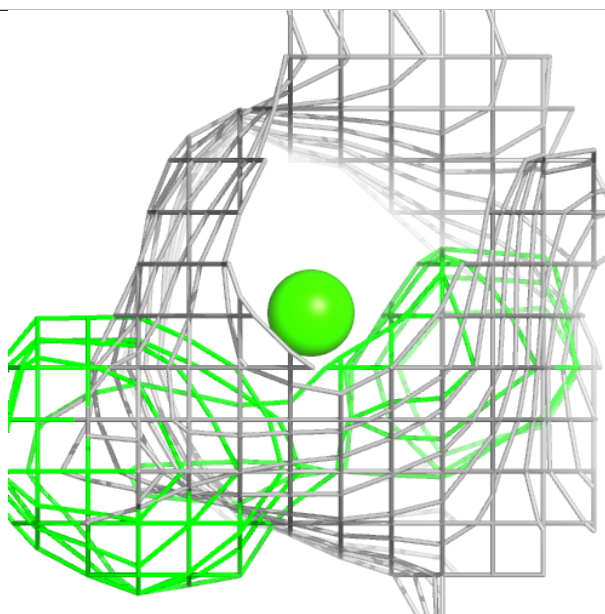
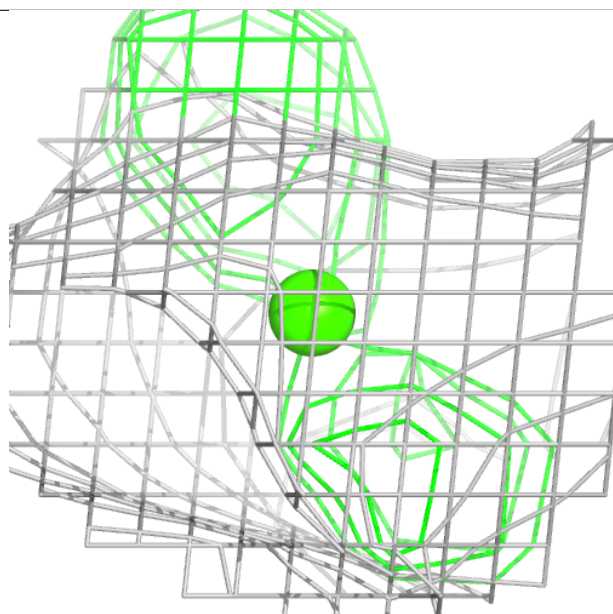
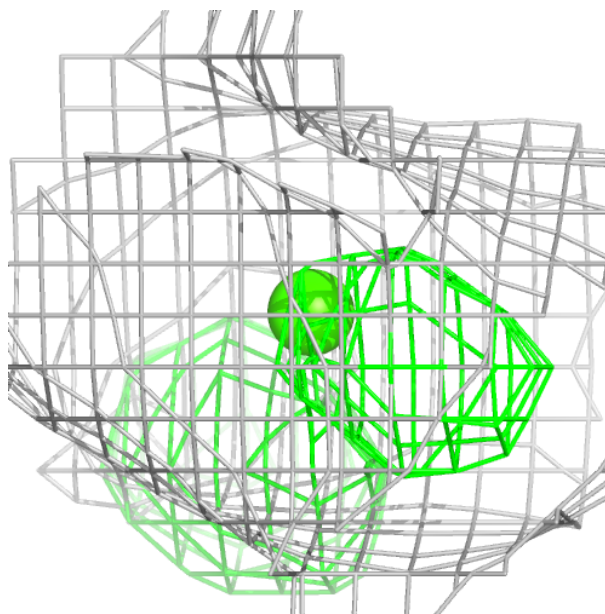
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





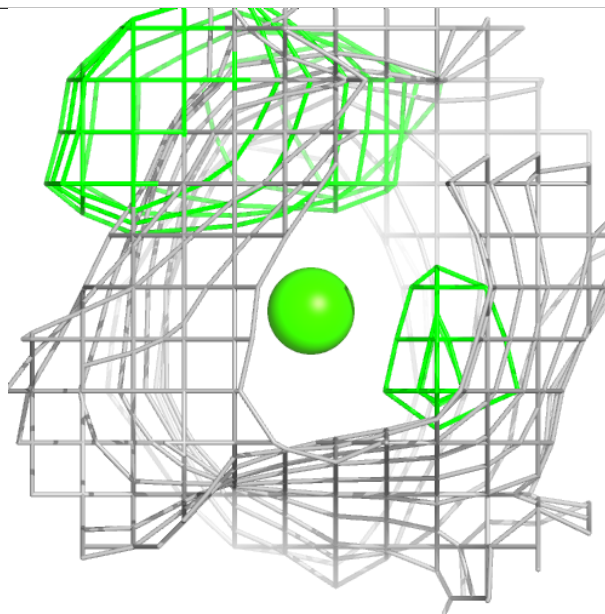
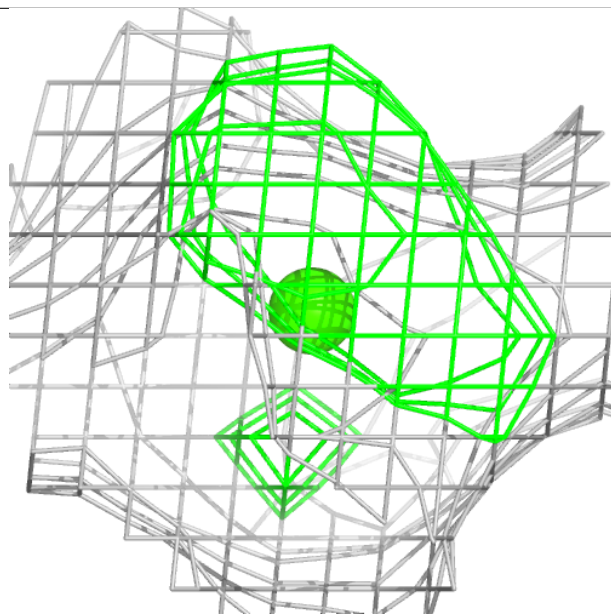
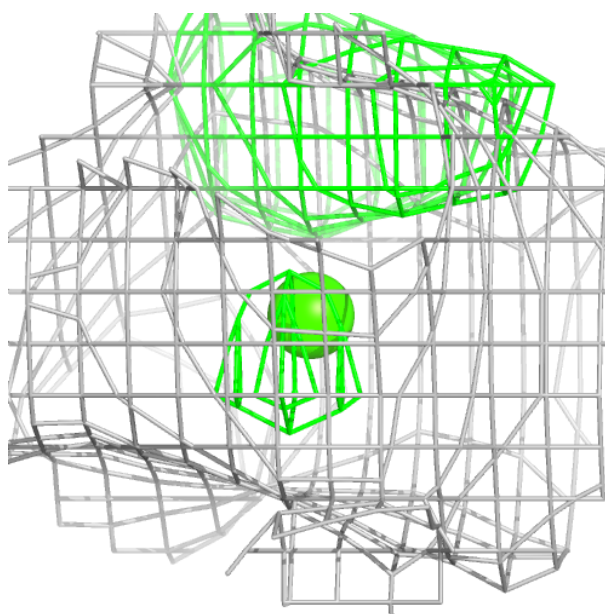
**Electron density around CA B 301:**

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



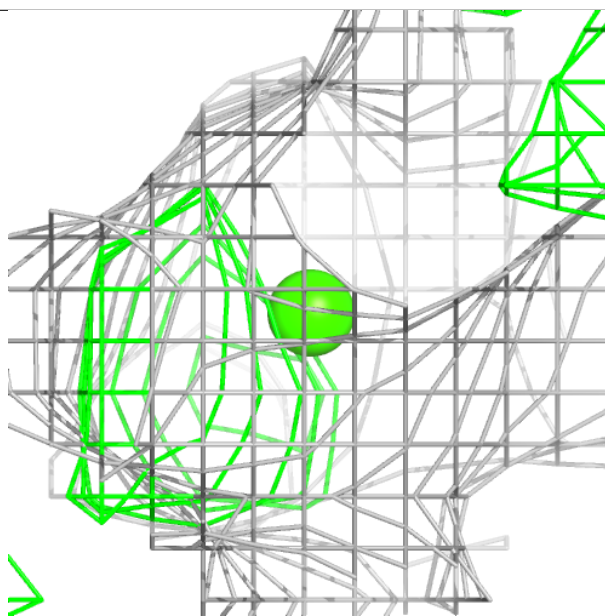
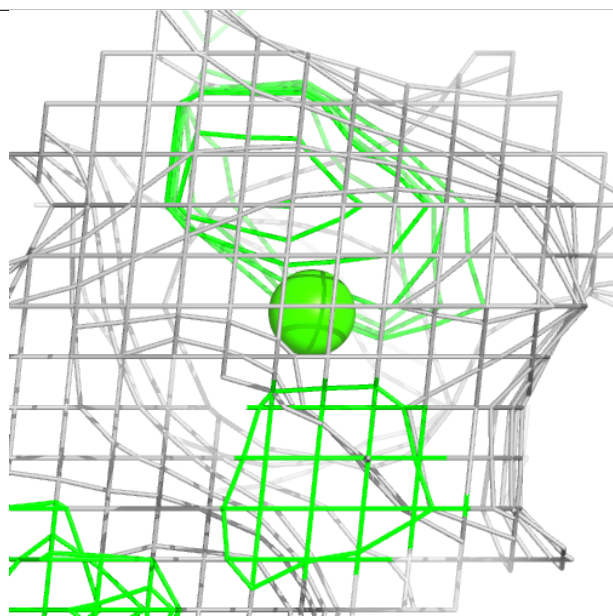
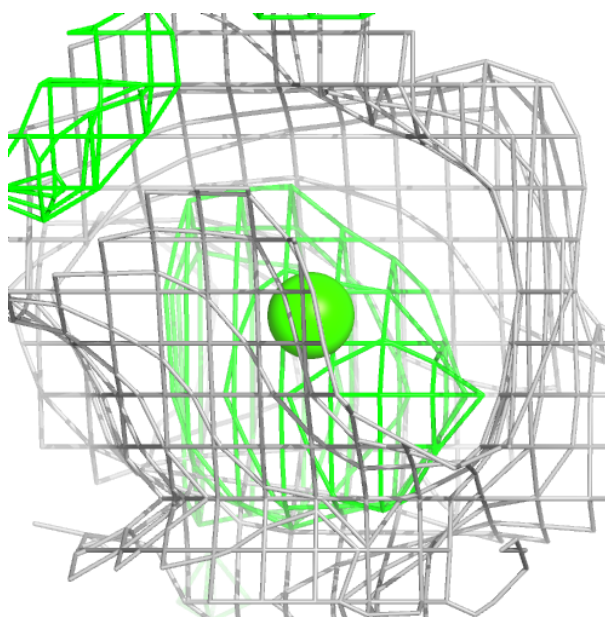
**Electron density around CA F 301:**

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



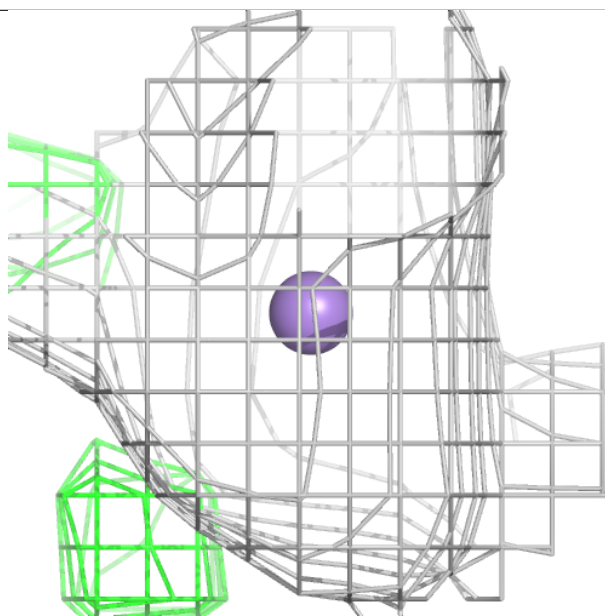
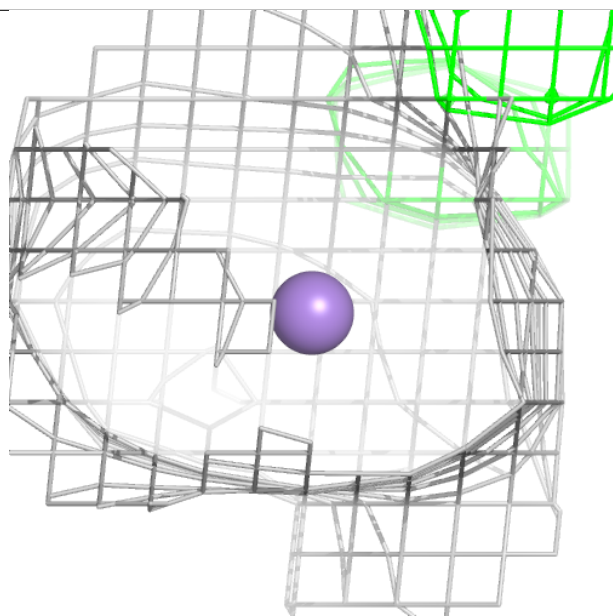
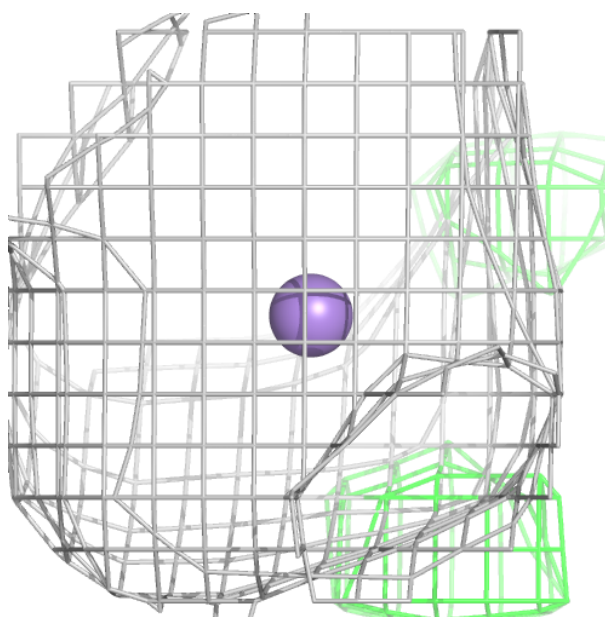
**Electron density around CA M 301:**

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



**Electron density around MN K 302:**

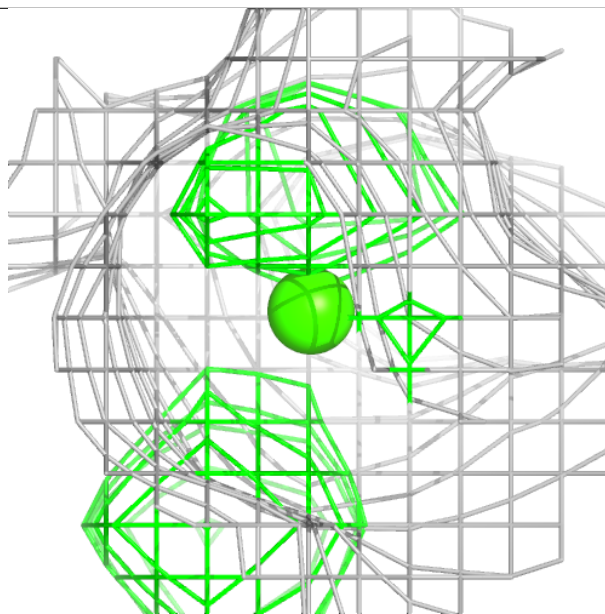
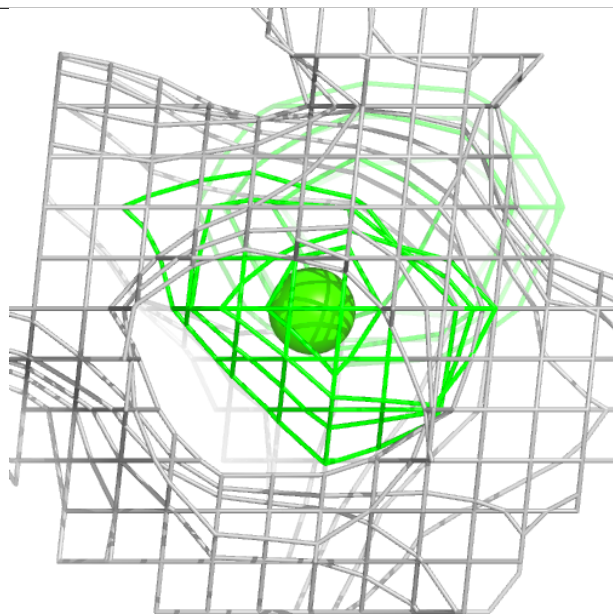
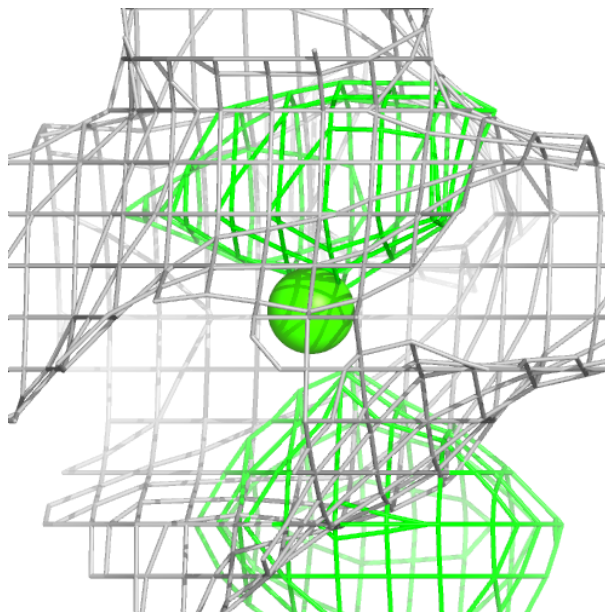
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





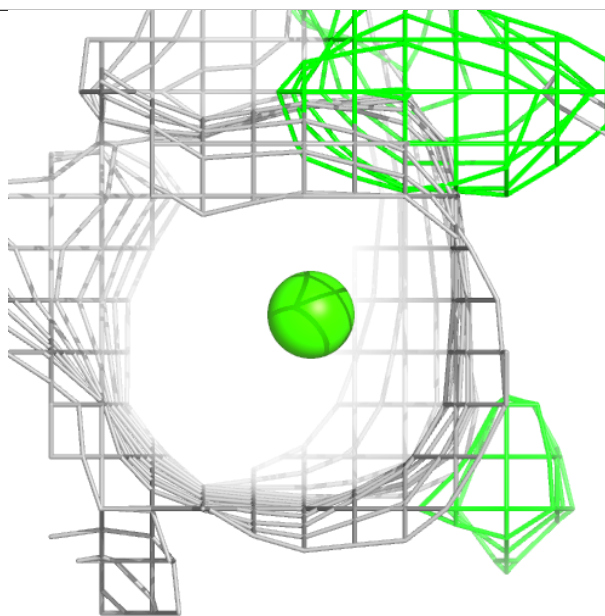
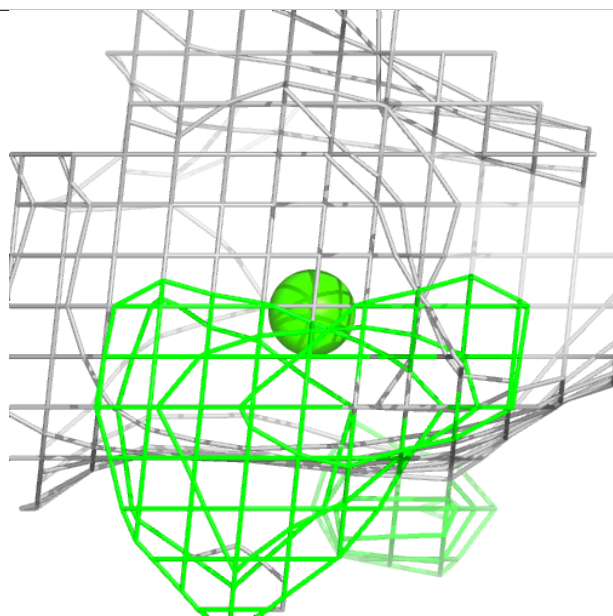
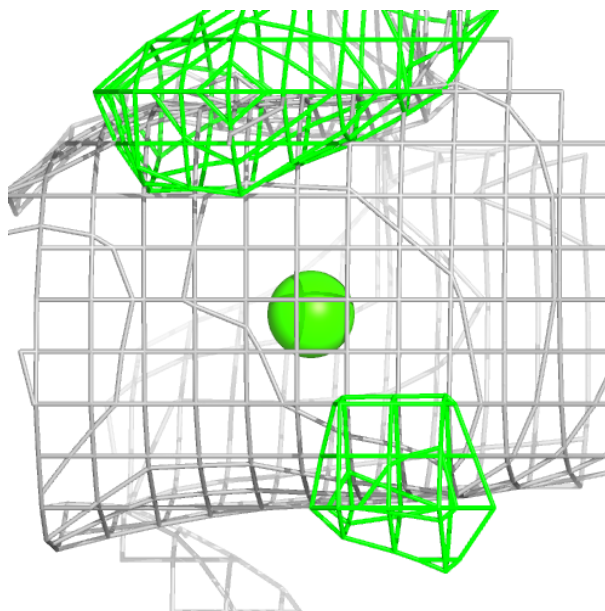
**Electron density around CA J 301:**

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



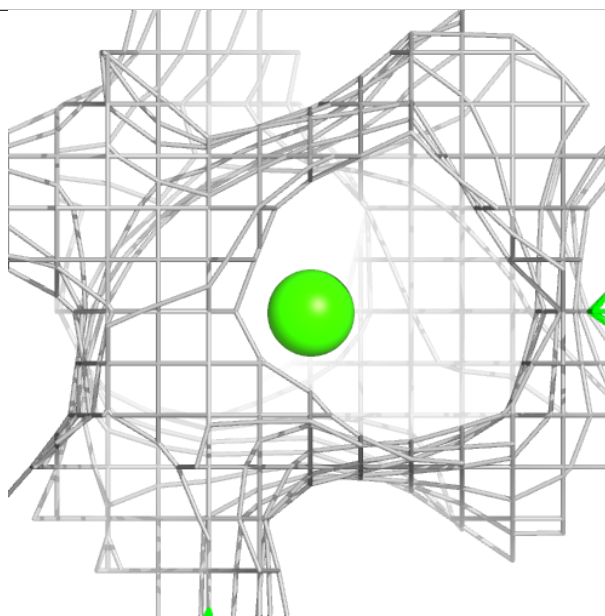
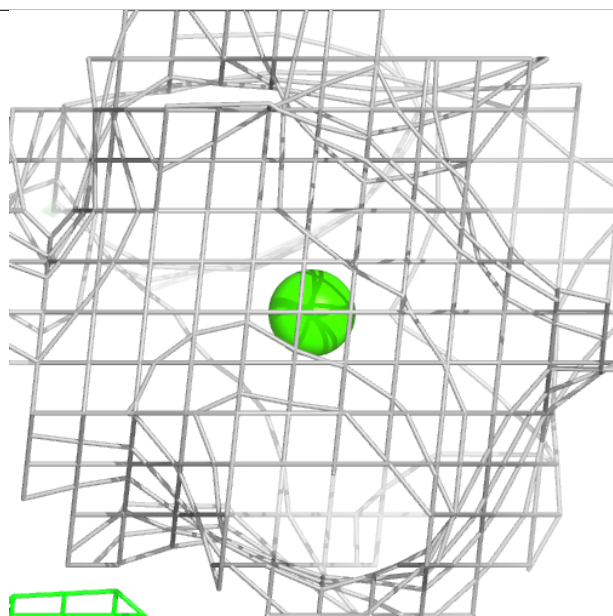
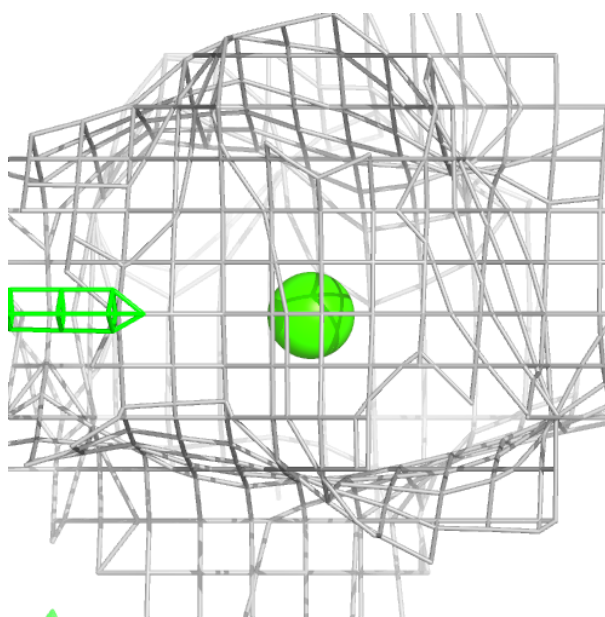
**Electron density around CA P 301:**

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



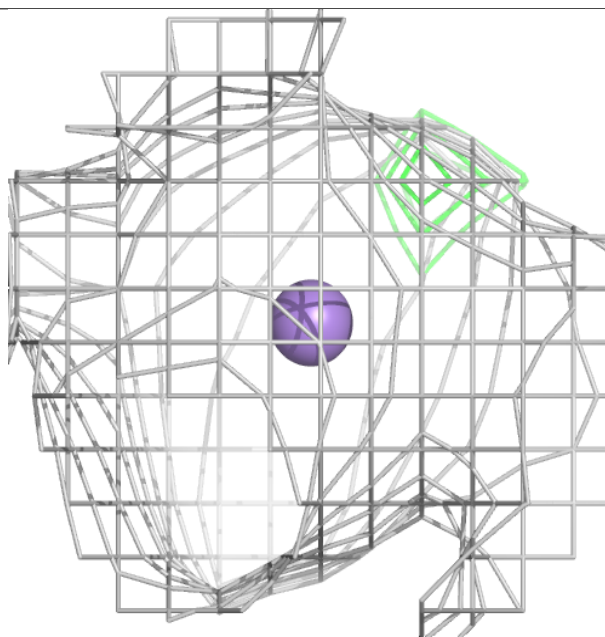
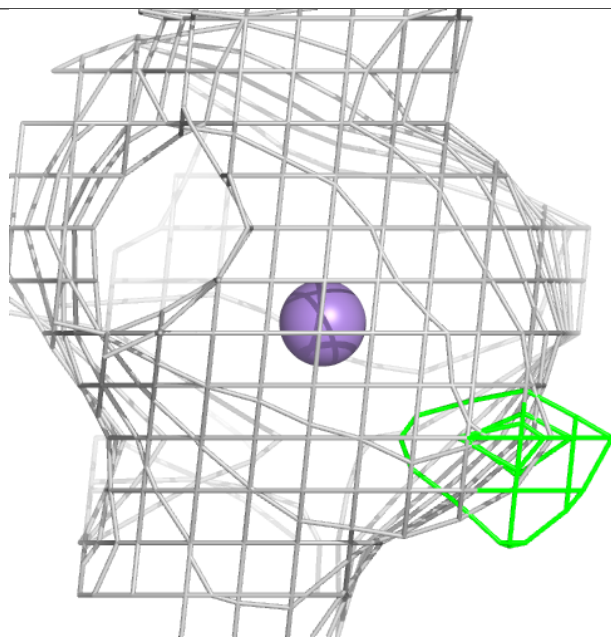
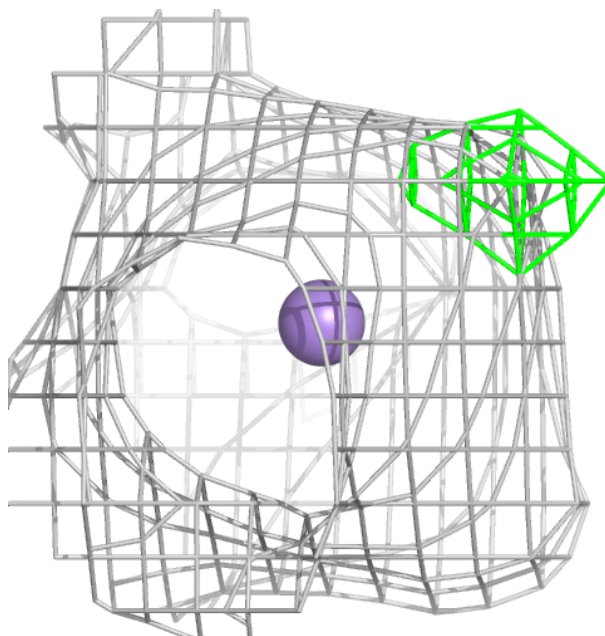
**Electron density around CA L 301:**

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



**Electron density around MN A 302:**

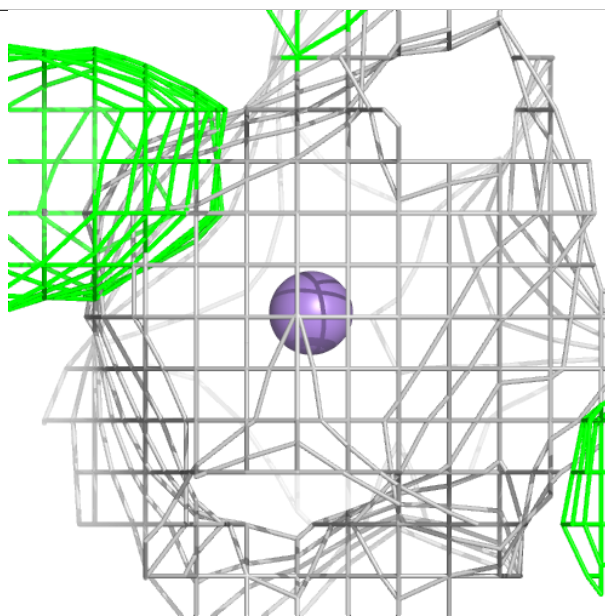
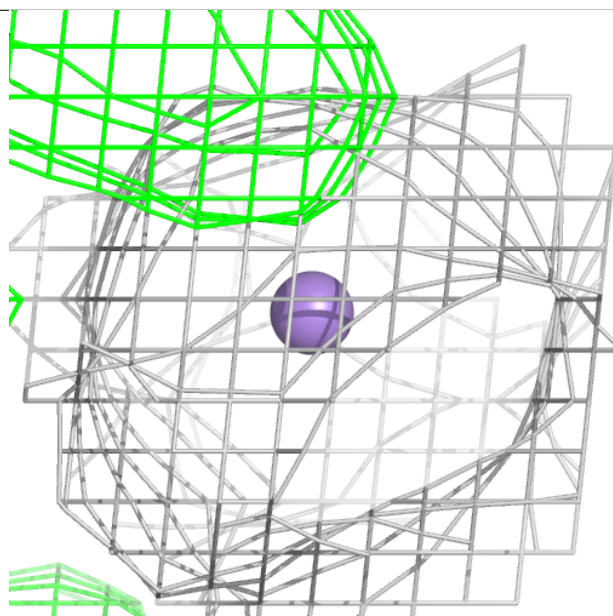
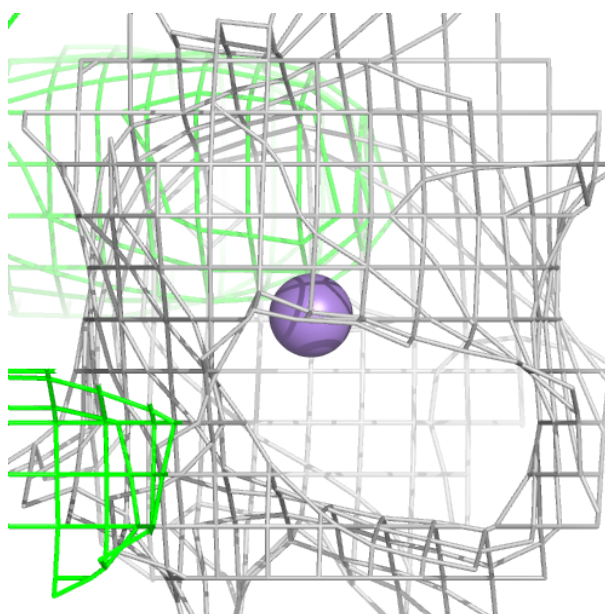
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





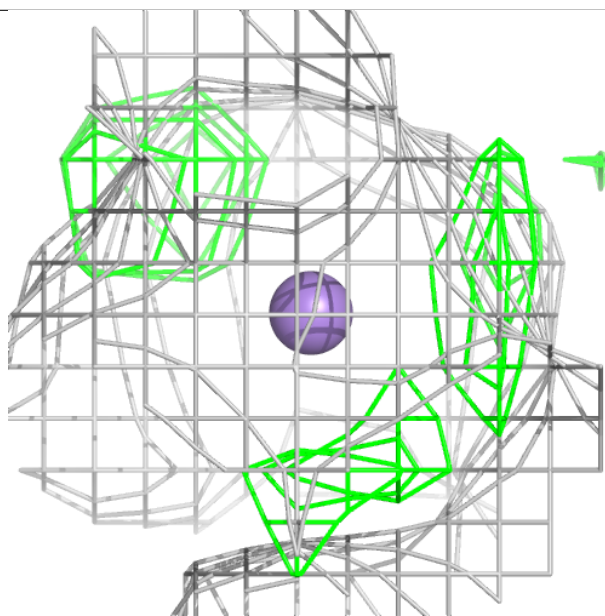
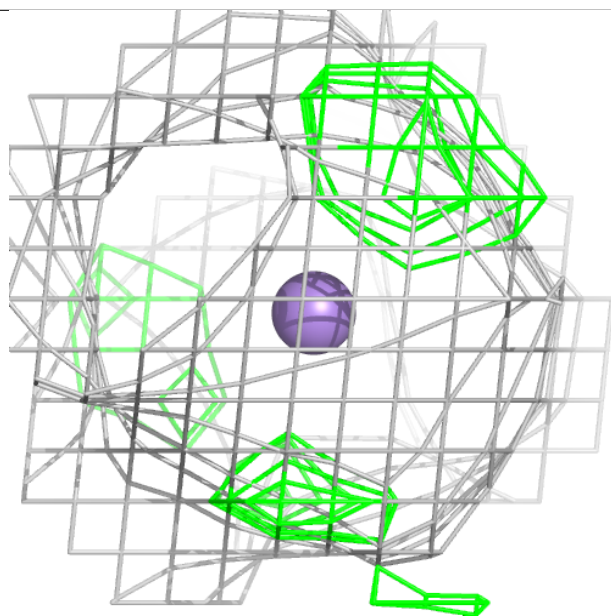
**Electron density around MN C 302:**

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



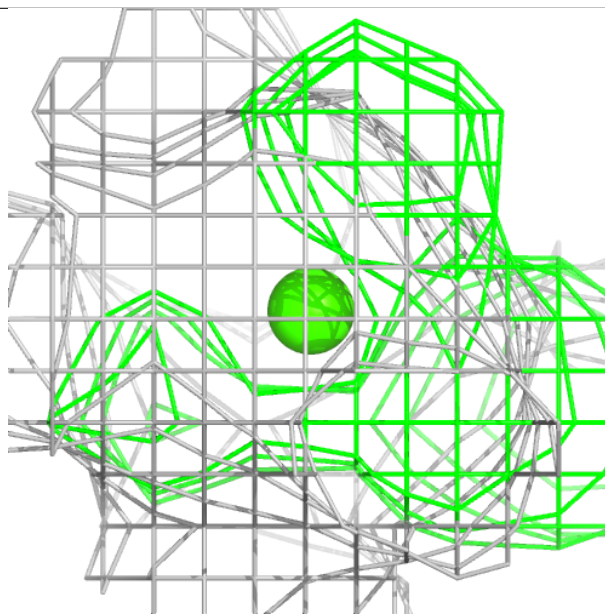
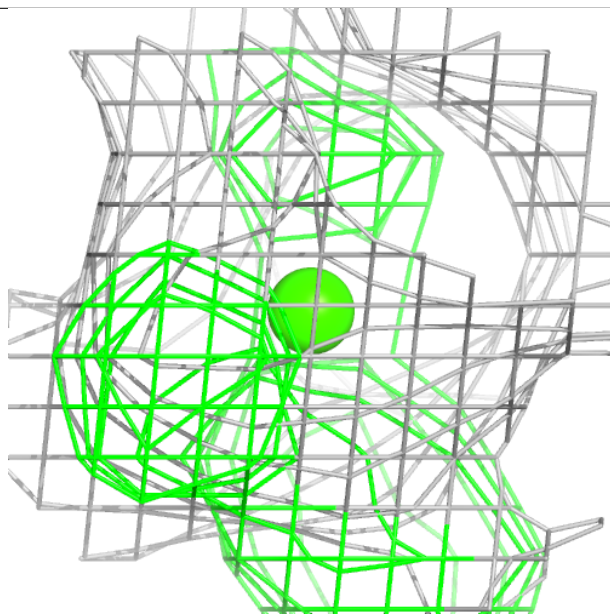
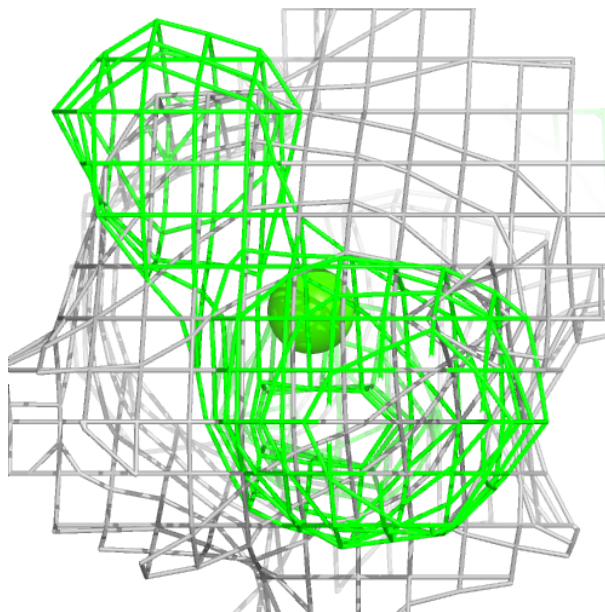
**Electron density around MN G 302:**

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



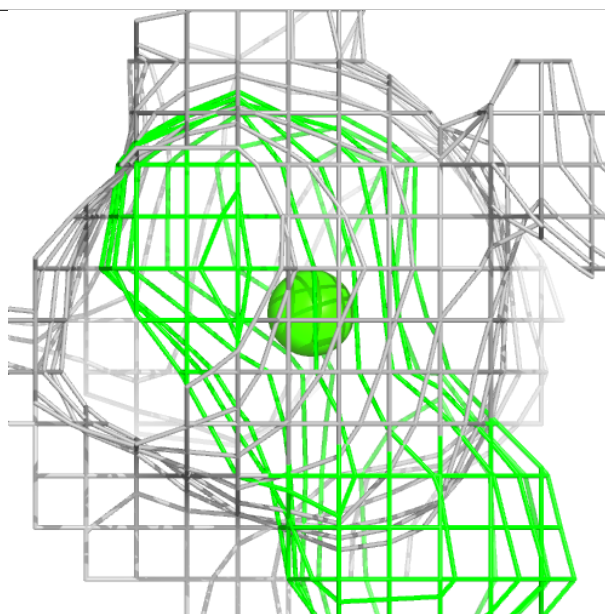
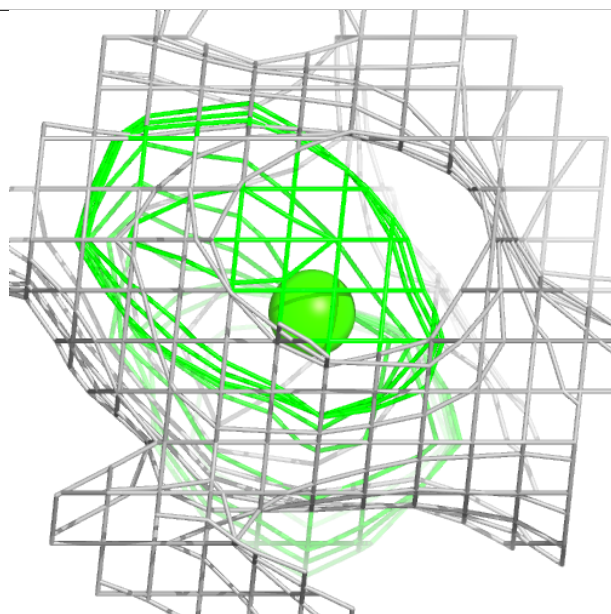
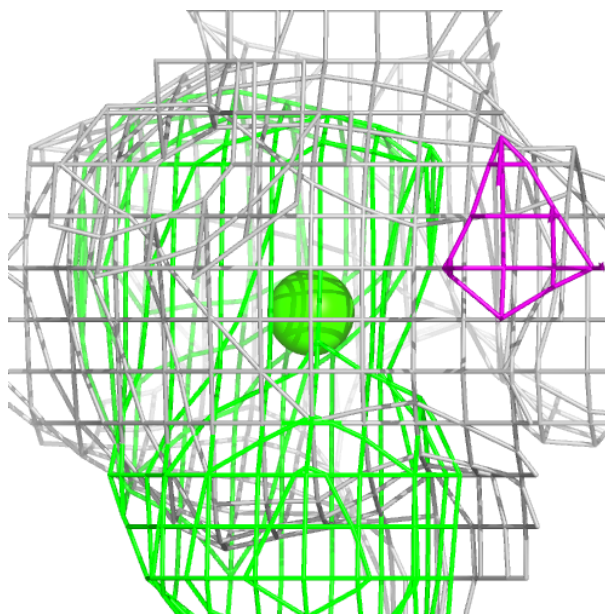
**Electron density around CA G 301:**

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



**Electron density around CA D 301:**

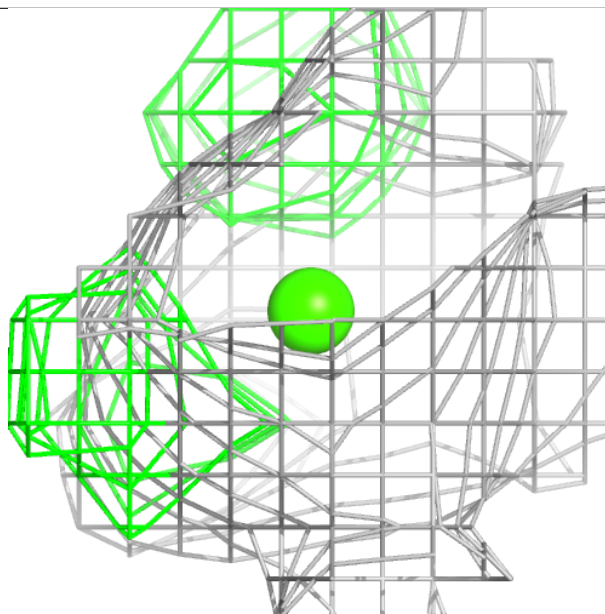
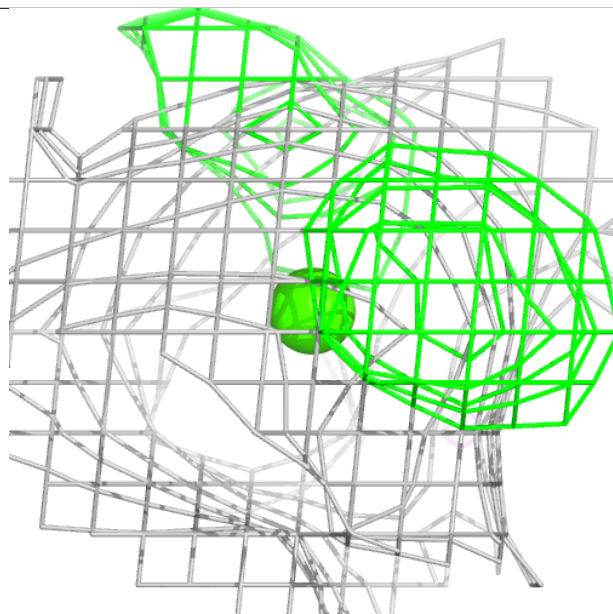
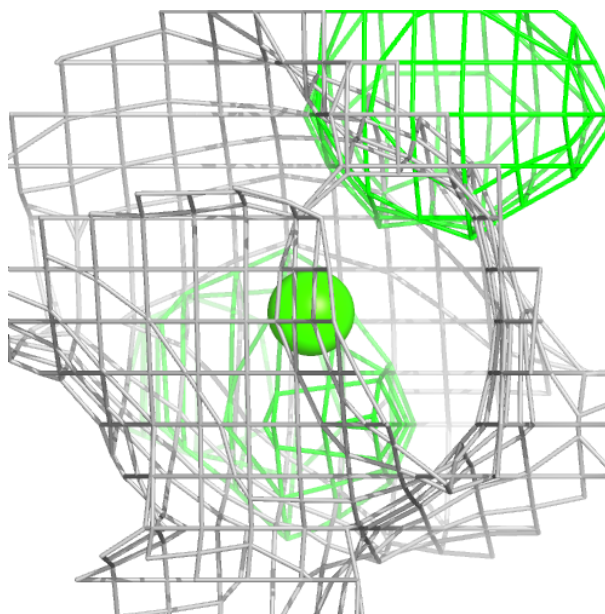
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





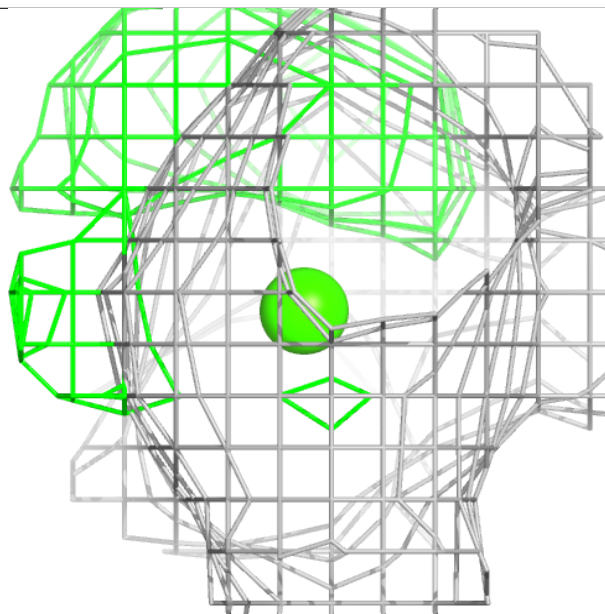
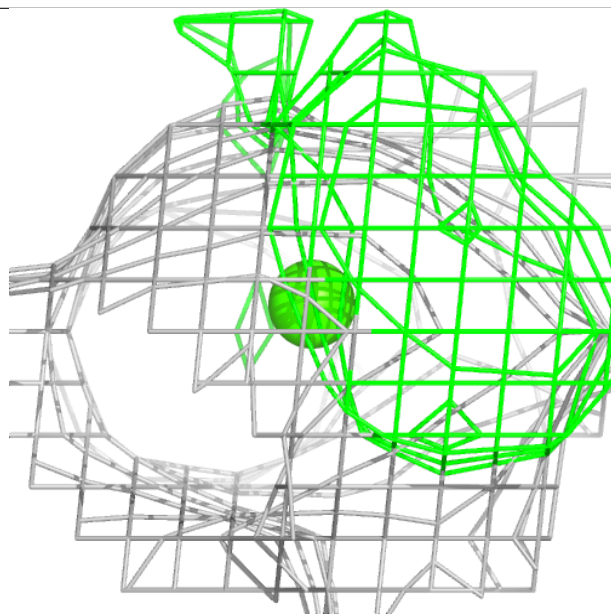
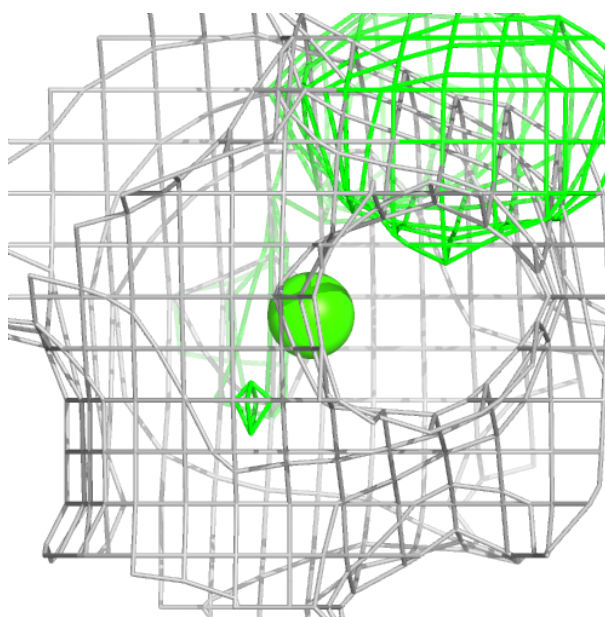
**Electron density around CA I 301:**

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



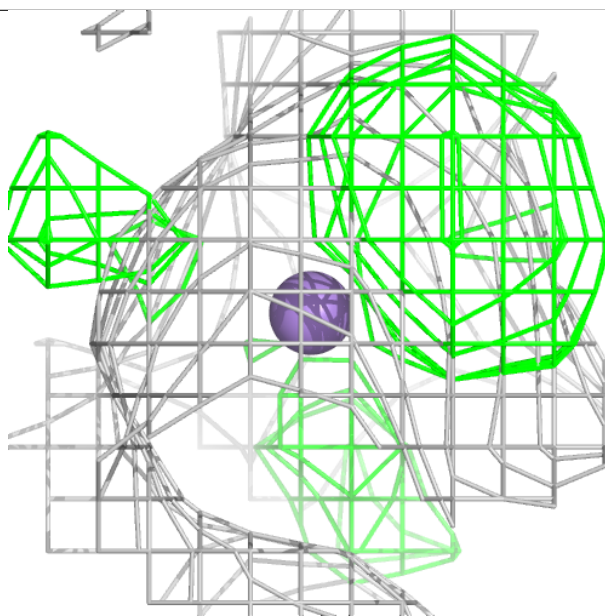
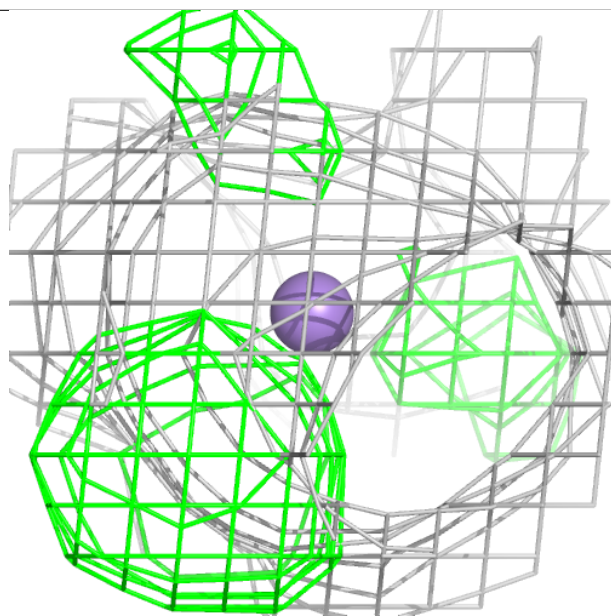
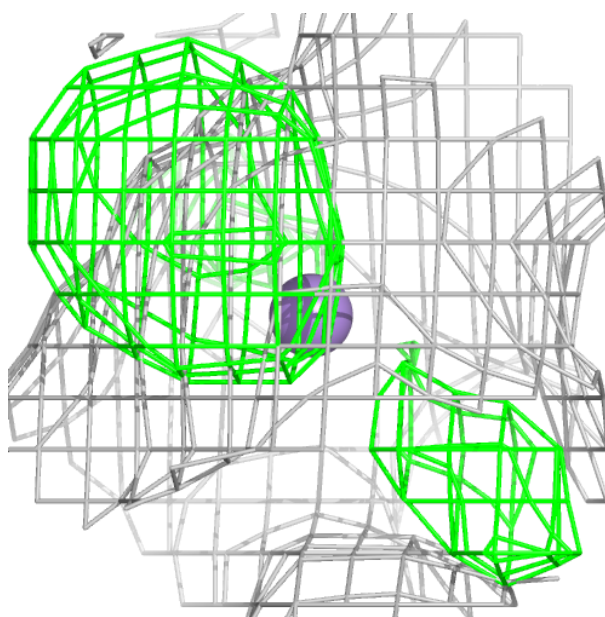
**Electron density around CA C 301:**

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



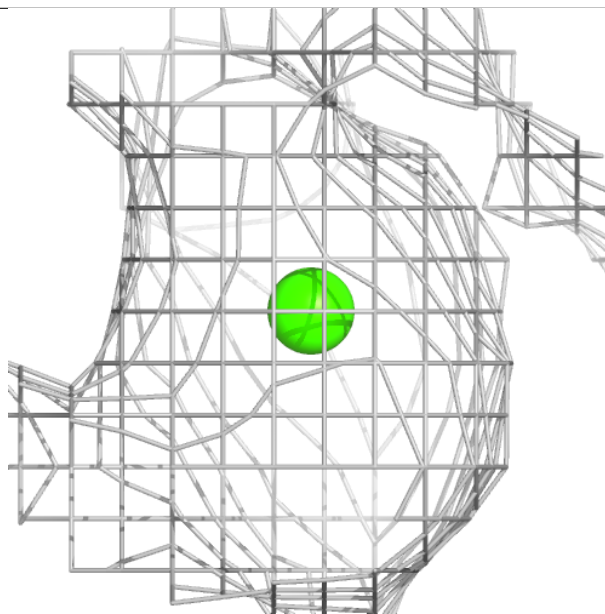
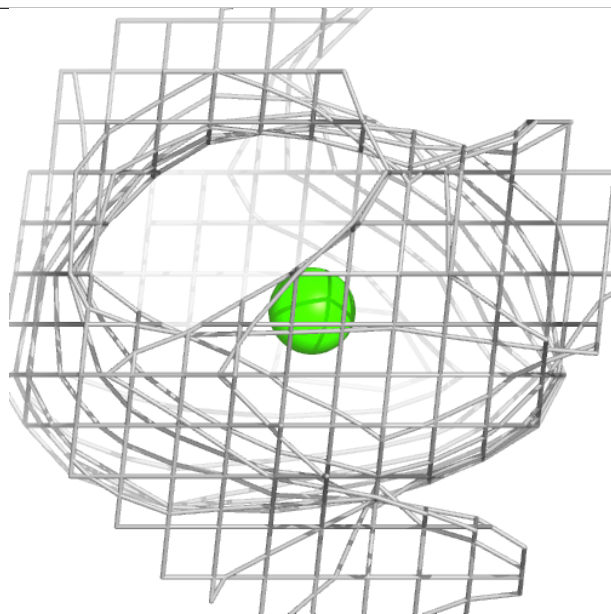
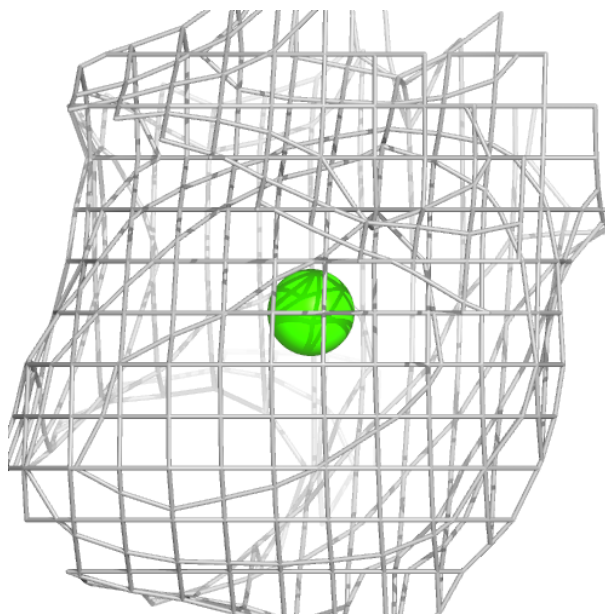
**Electron density around MN M 302:**

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



**Electron density around CA A 301:**

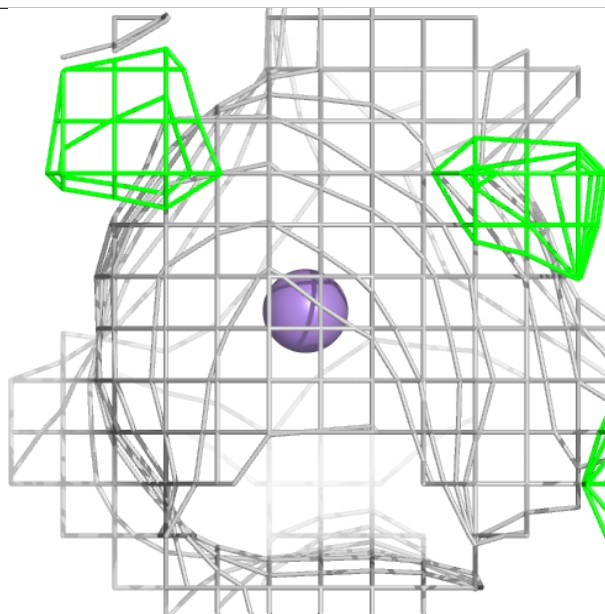
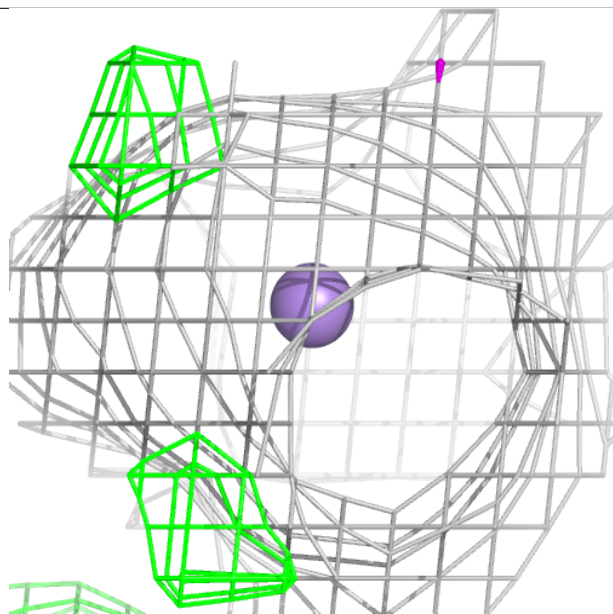
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





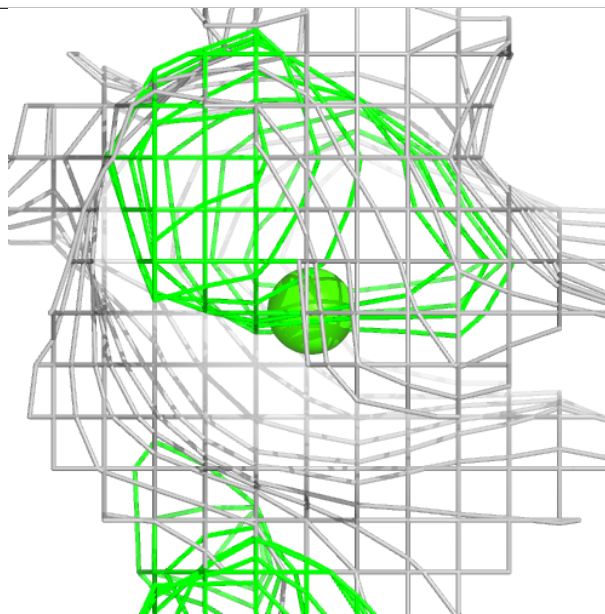
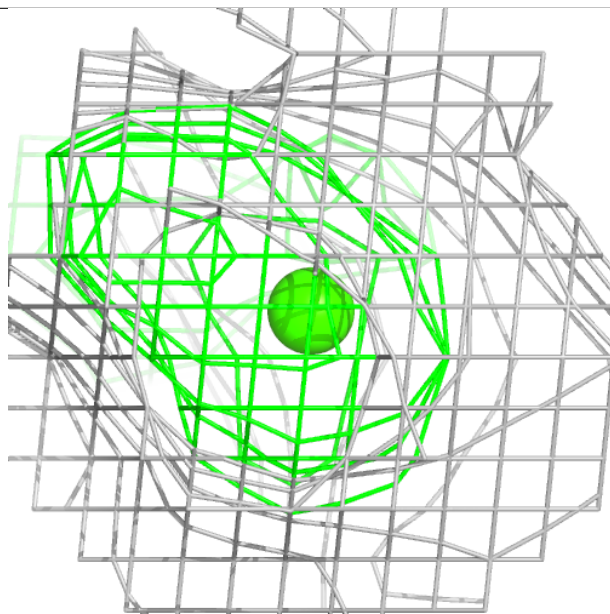
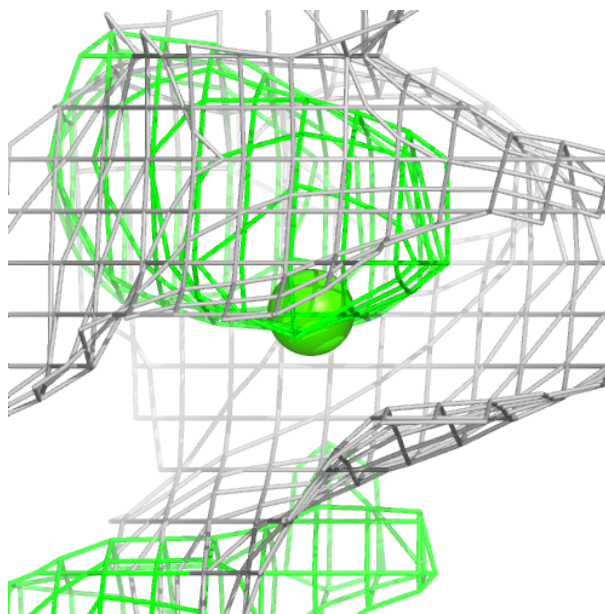
**Electron density around MN I 302:**

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



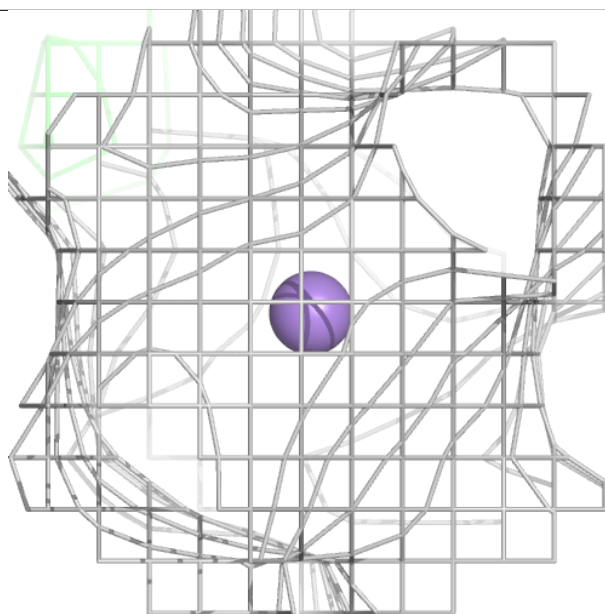
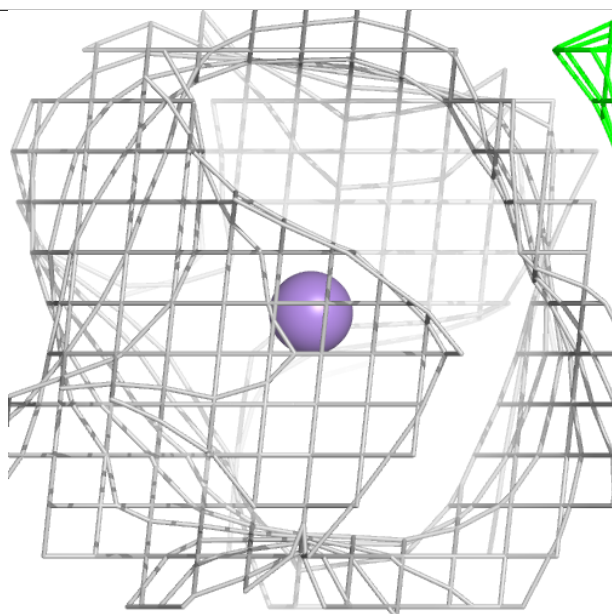
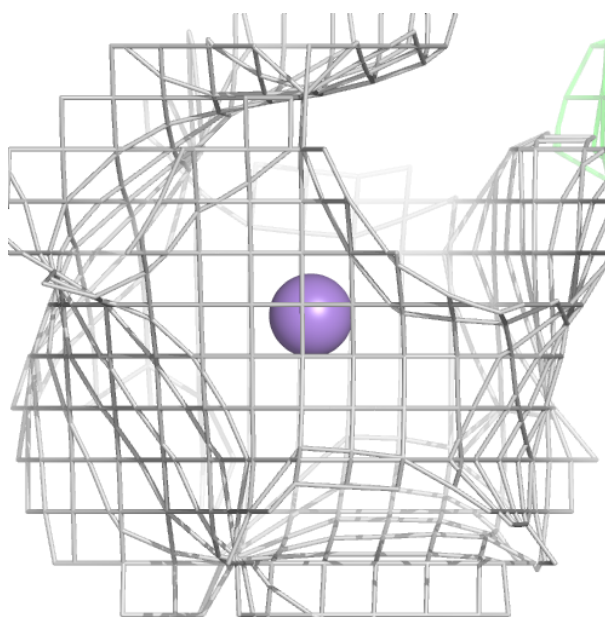
**Electron density around CA N 301:**

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



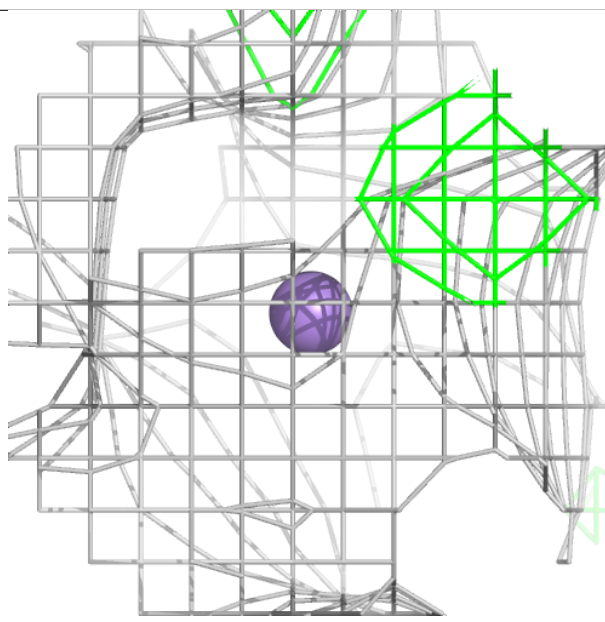
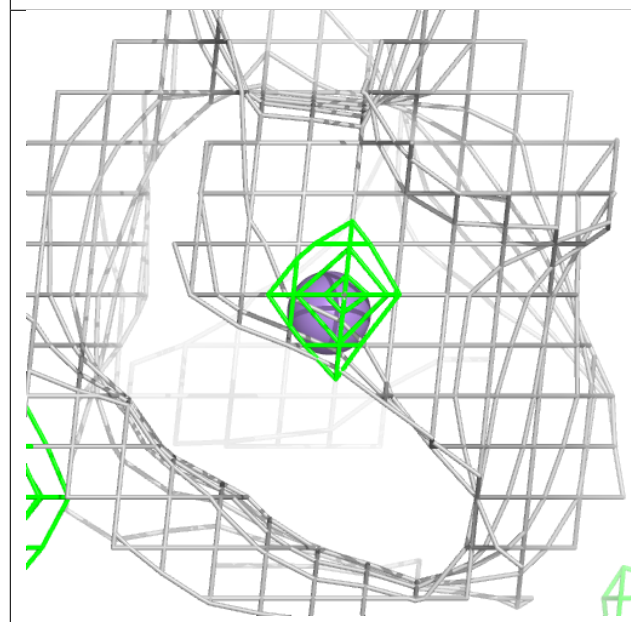
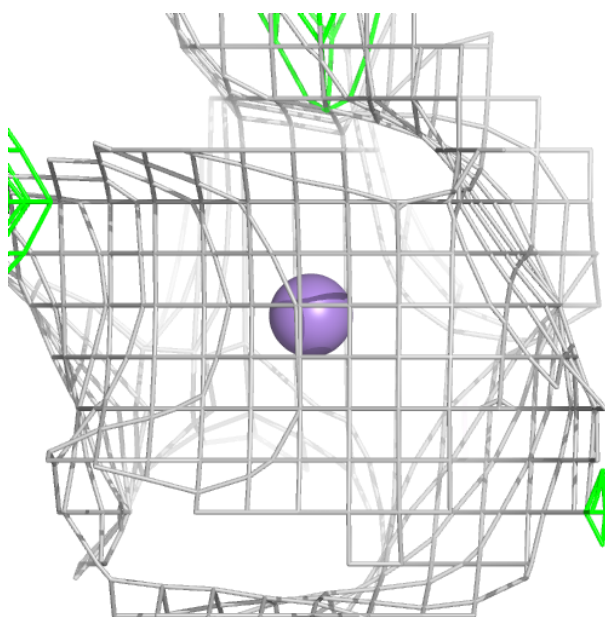
**Electron density around MN H 302:**

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



**Electron density around MN J 302:**

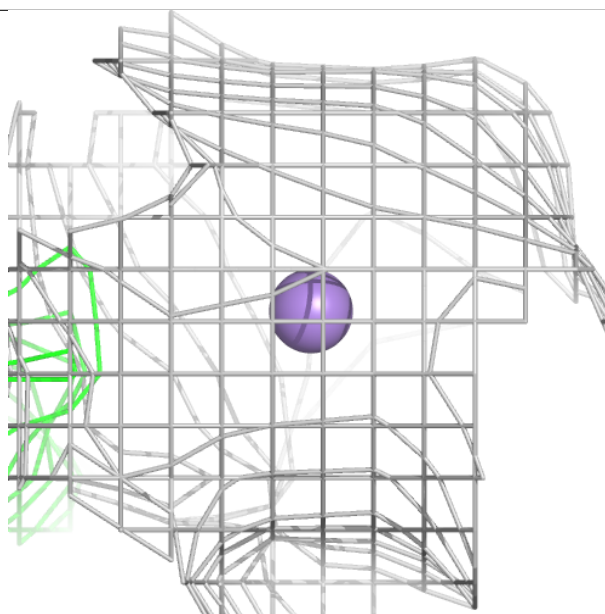
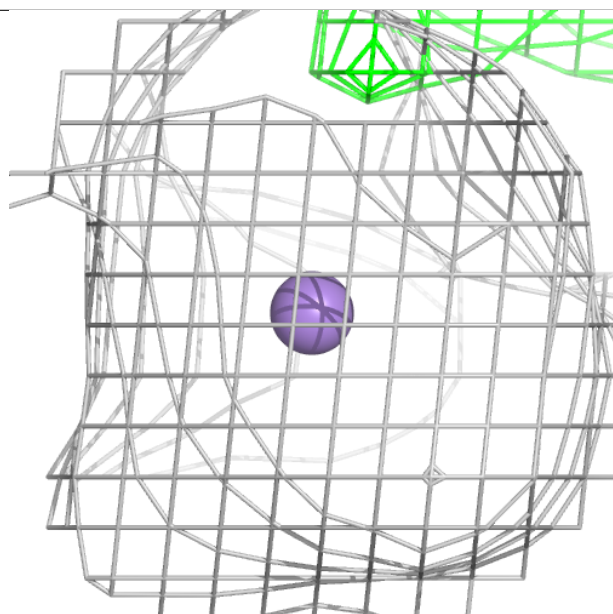
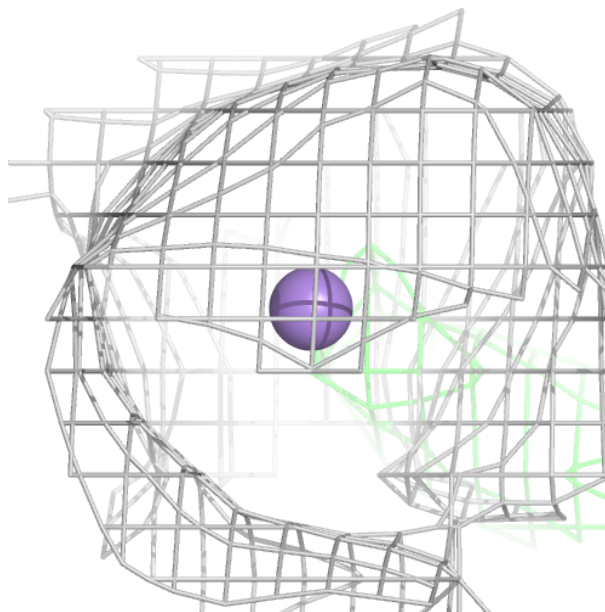
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





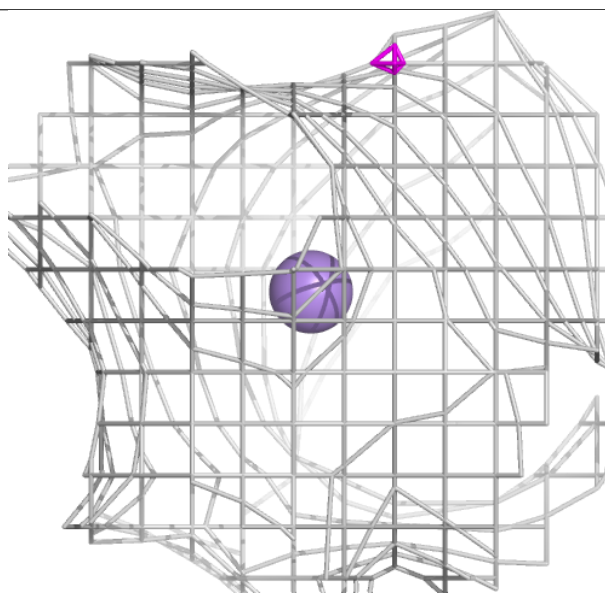
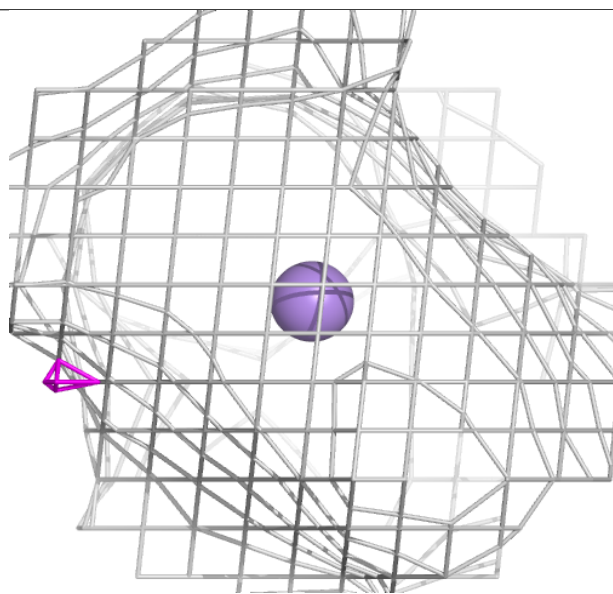
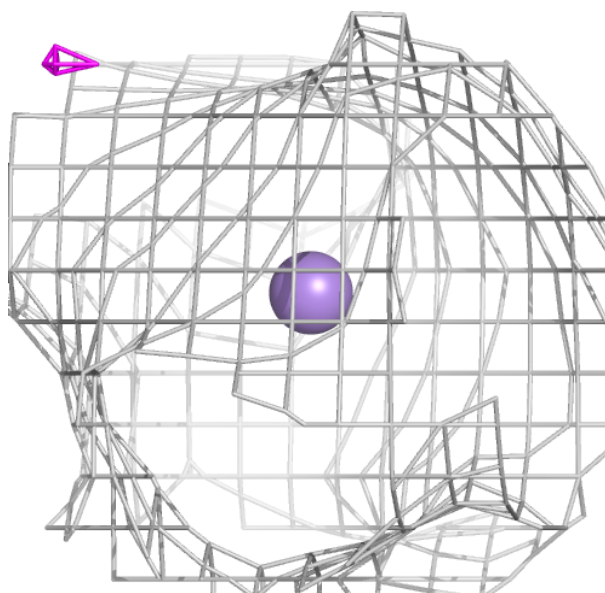
**Electron density around MN P 302:**

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



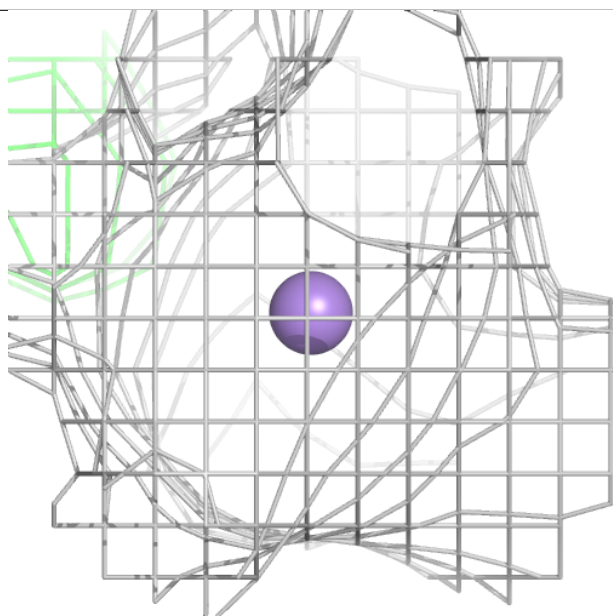
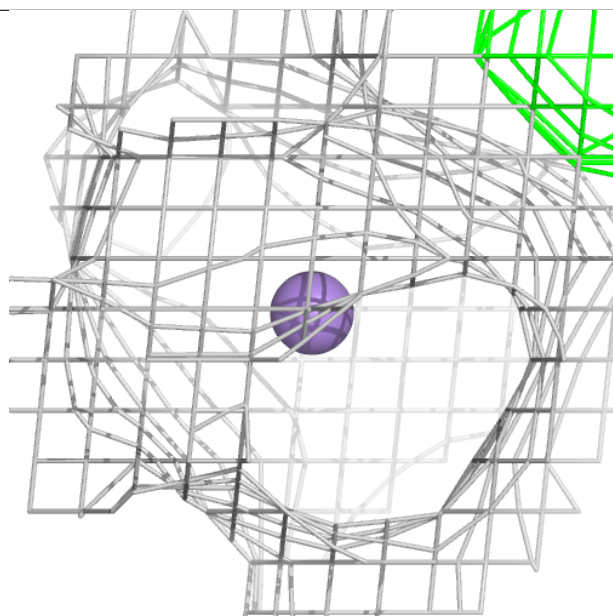
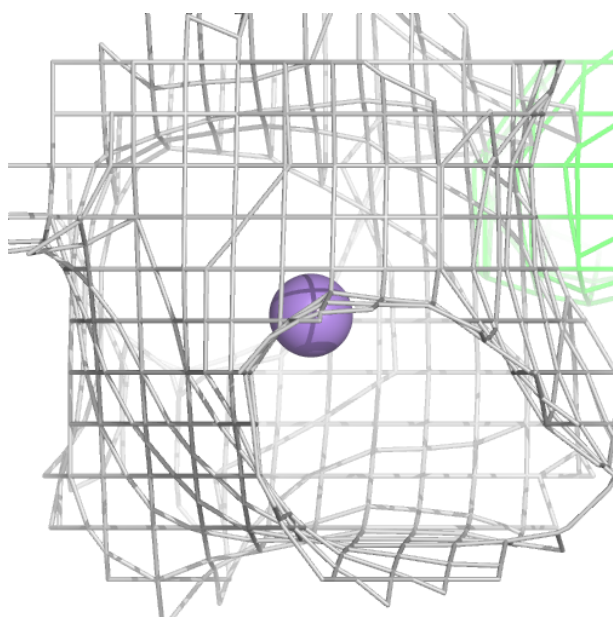
**Electron density around MN L 302:**

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



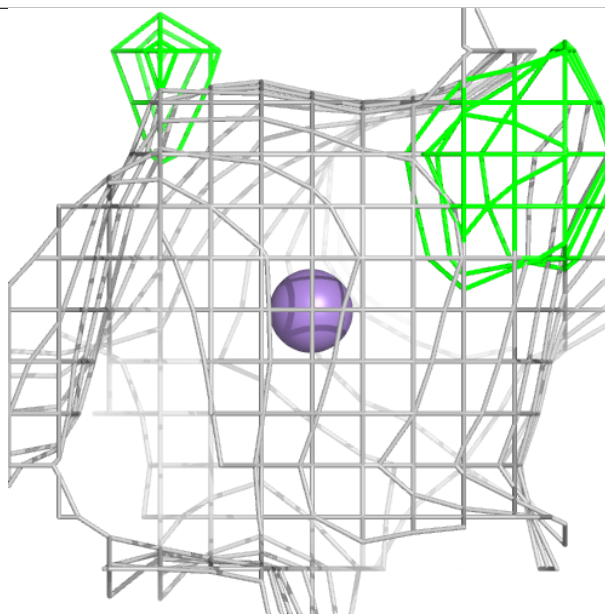
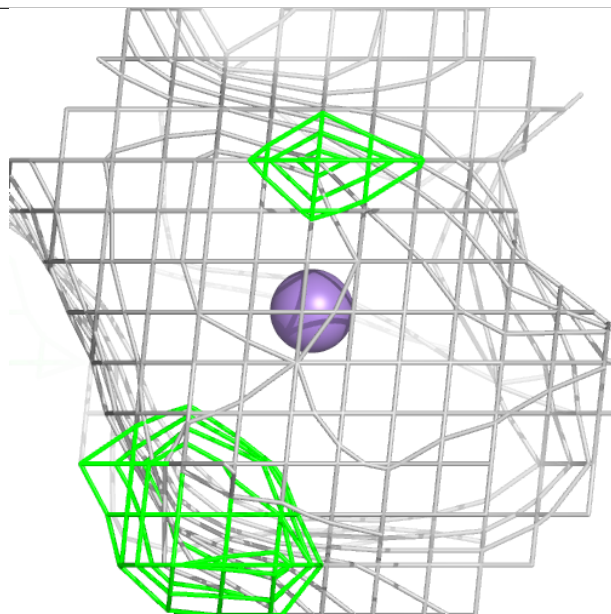
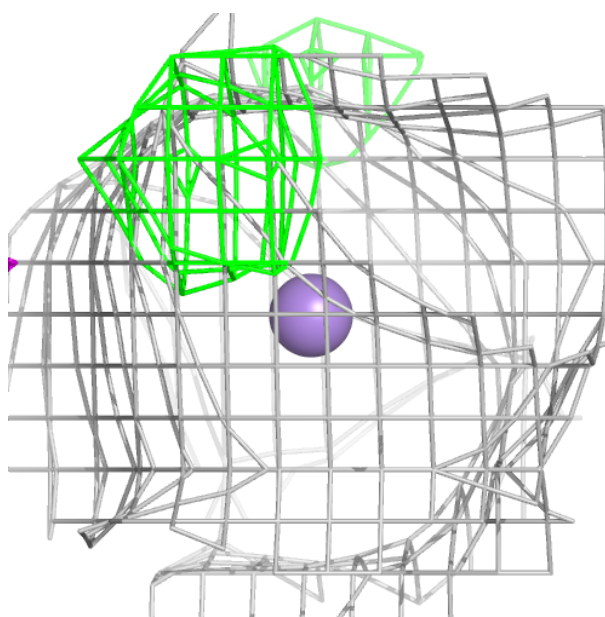
**Electron density around MN O 302:**

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



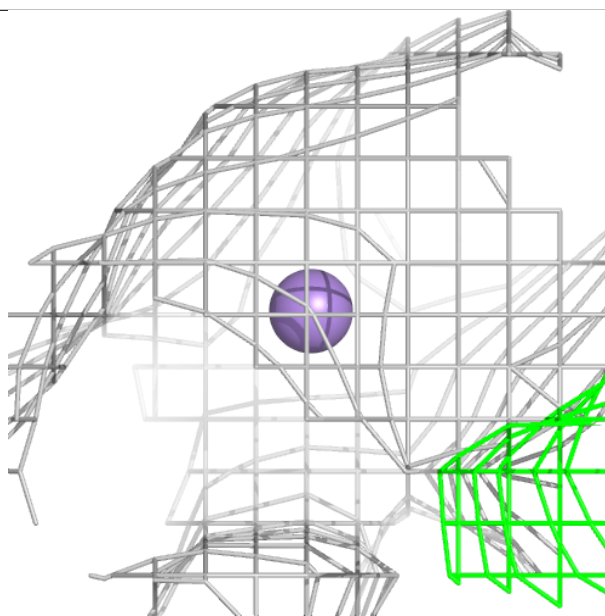
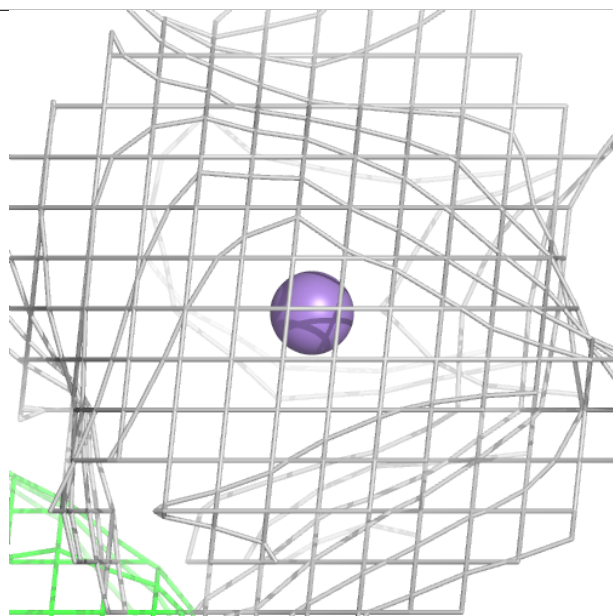
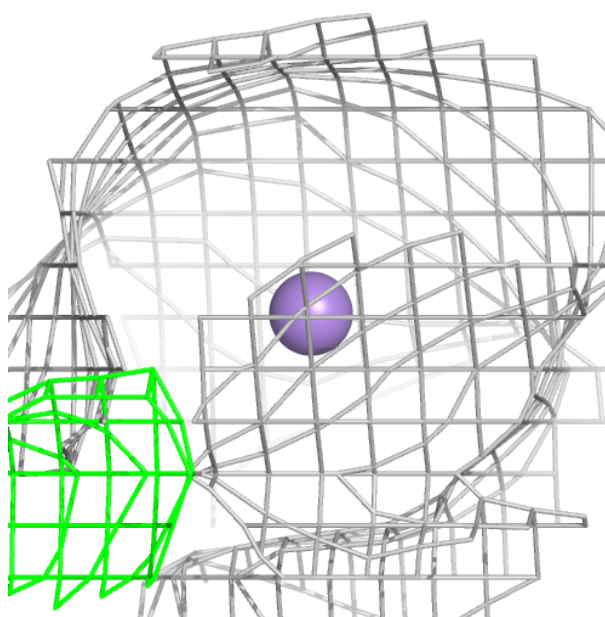
**Electron density around MN B 302:**

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



**Electron density around MN F 302:**

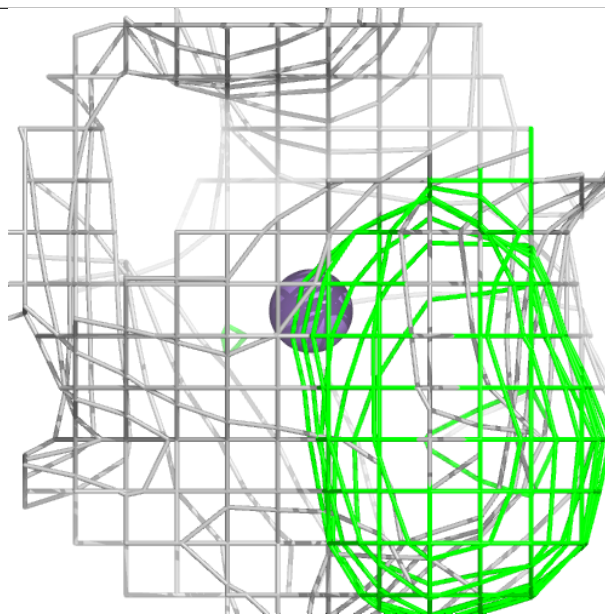
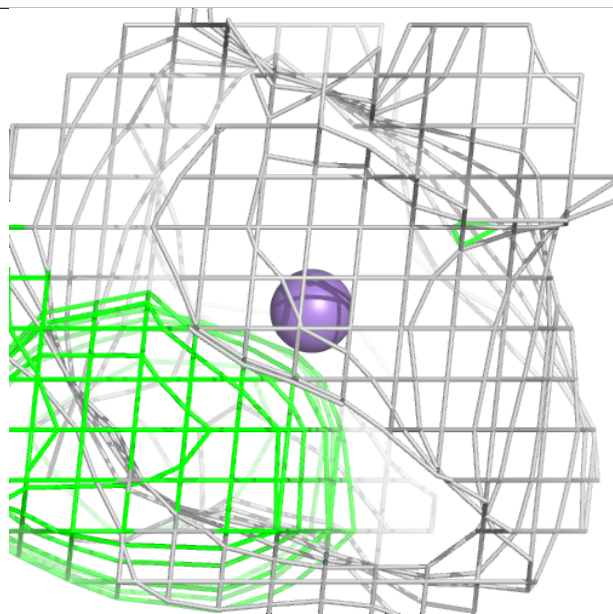
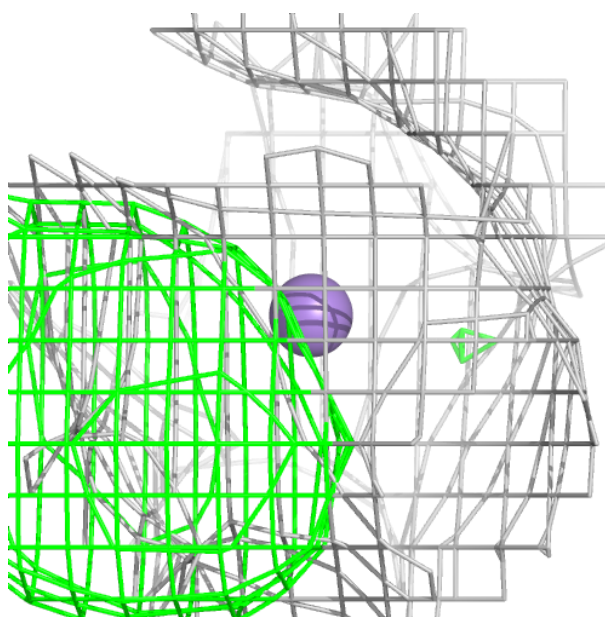
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





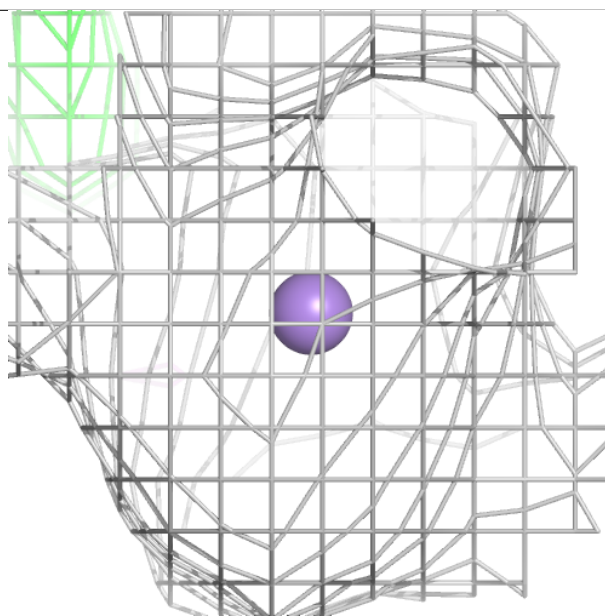
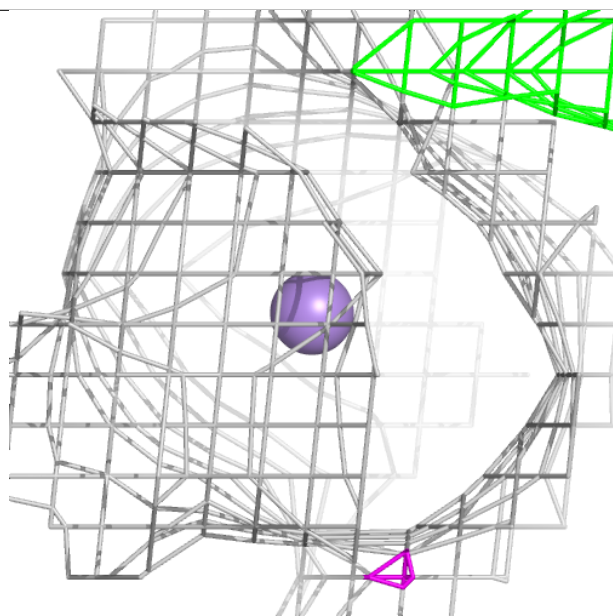
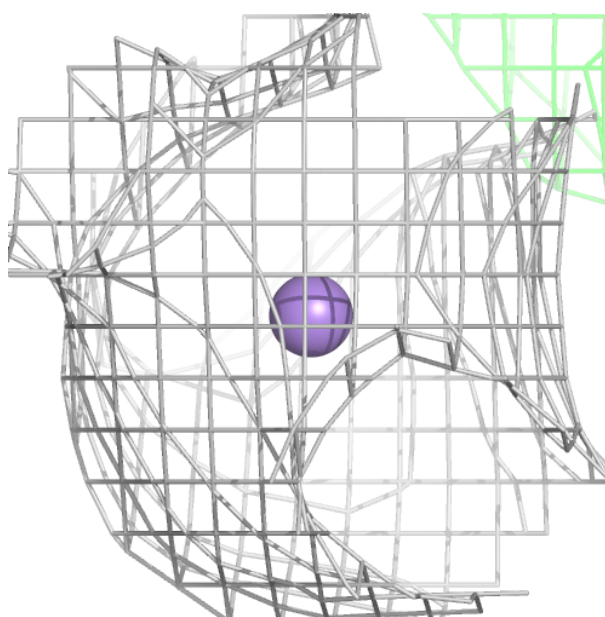
**Electron density around MN N 302:**

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



**Electron density around MN E 302:**

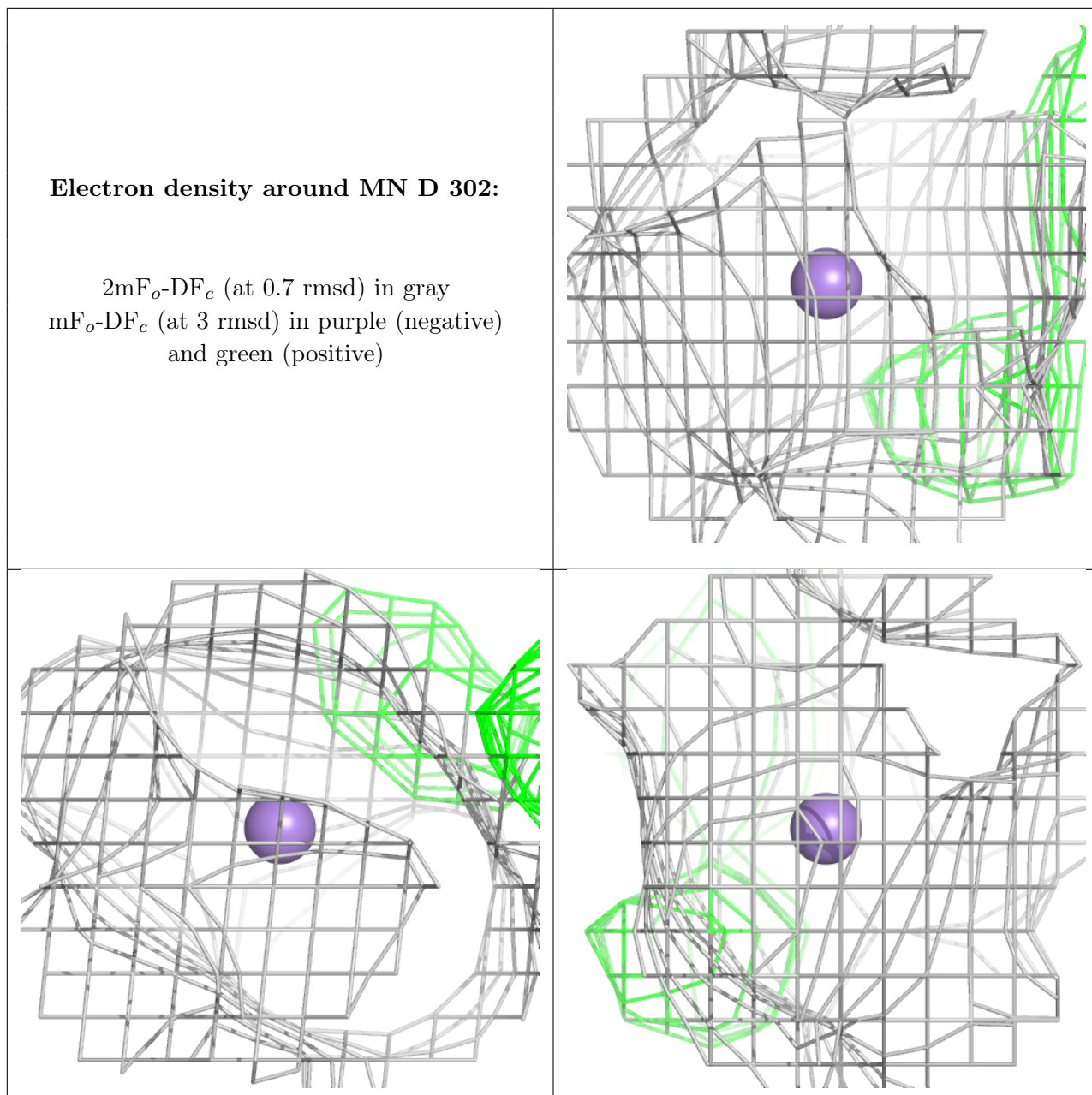
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN D 302:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.