



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 10:39 PM UTC

PDB ID : 9RG3 / pdb\_00009rg3  
Title : Unspecific peroxygenase from *Psathyrella aberdarensis*, Grogu variant, in complex with anisole  
Authors : Fernandez-Garcia, A.; Sanz-Aparicio, J.  
Deposited on : 2025-06-05  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

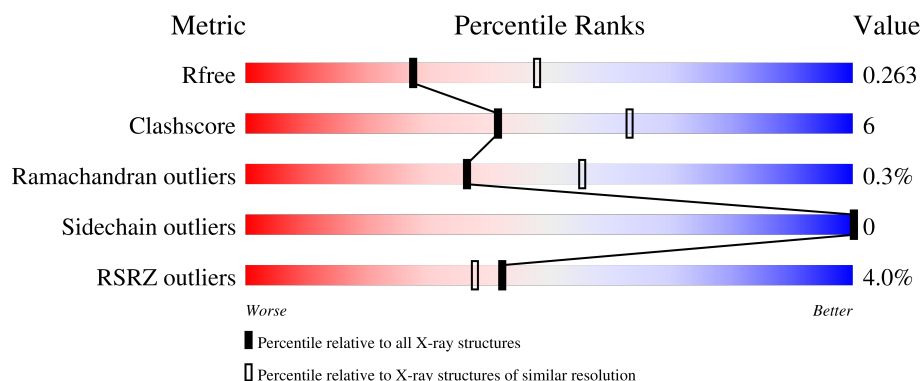
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	334	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>
1	B	334	<div> <div>5%</div> <div>91%</div> <div>9%</div> </div>
2	J	2	<div> <div>50%</div> <div>50%</div> </div>
2	M	2	<div> <div>100%</div> </div>
2	X	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	a	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	A	403	-	-	X	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 5686 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 Heme-thiolate peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2598	1659	437	495	7			
1	B	334	Total	C	N	O	S	0	1	0
			2593	1656	436	494	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	SER	engineered mutation	UNP A0A4Q2DF39
A	79	ILE	LEU	engineered mutation	UNP A0A4Q2DF39
A	252	LEU	ALA	engineered mutation	UNP A0A4Q2DF39
B	61	ALA	SER	engineered mutation	UNP A0A4Q2DF39
B	79	ILE	LEU	engineered mutation	UNP A0A4Q2DF39
B	252	LEU	ALA	engineered mutation	UNP A0A4Q2DF39

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	a	2	Total	C	N	O	0	0	0
			28	16	2	10			

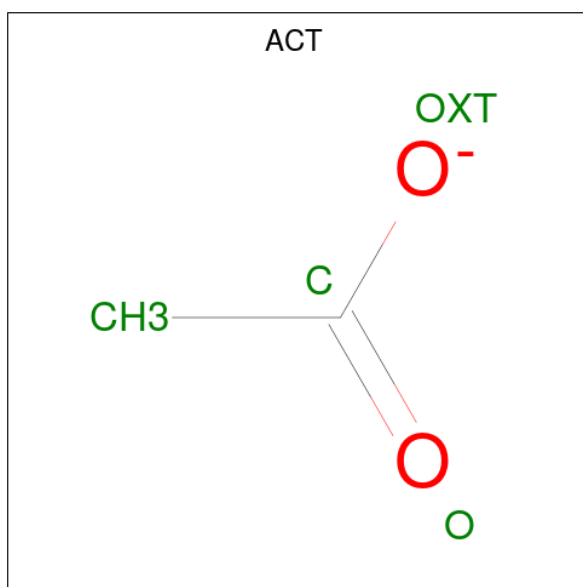


- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



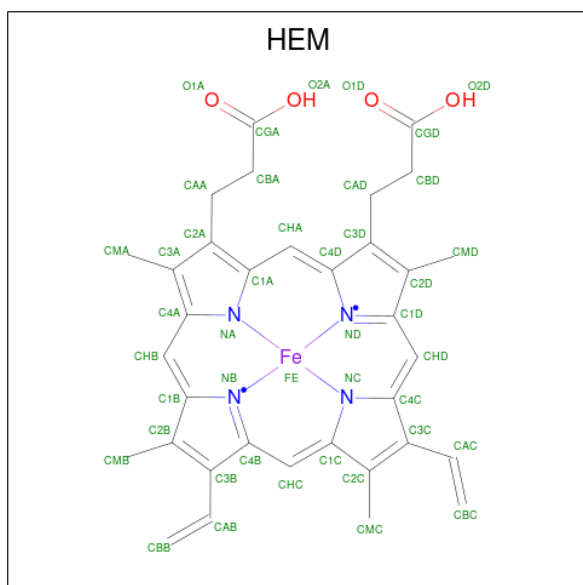
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

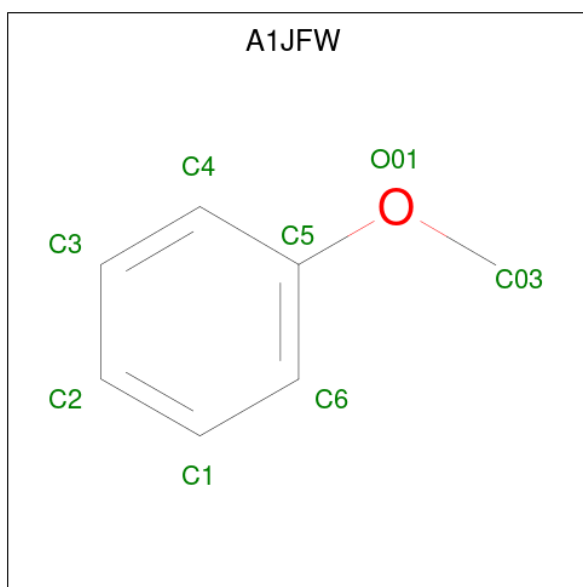
- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



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

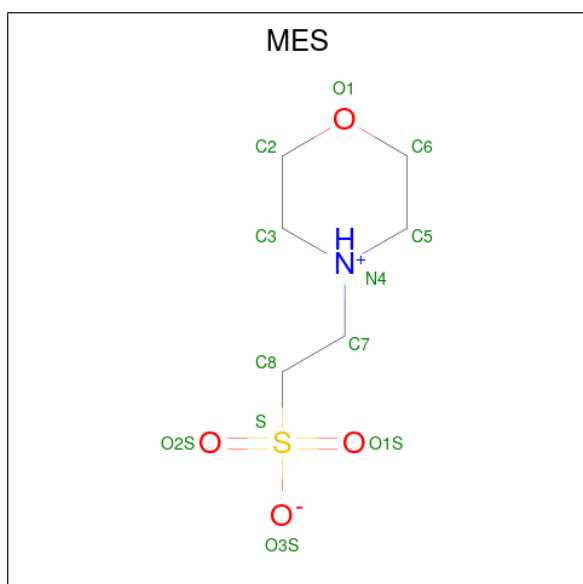
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).





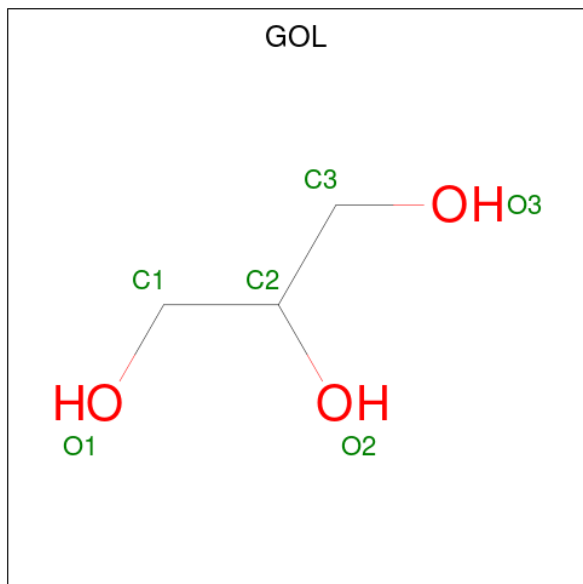
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	7	1		
6	B	1	Total	C	O	0	0
			8	7	1		
6	B	1	Total	C	O	0	0
			8	7	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	P	0	0
			5	4	1		

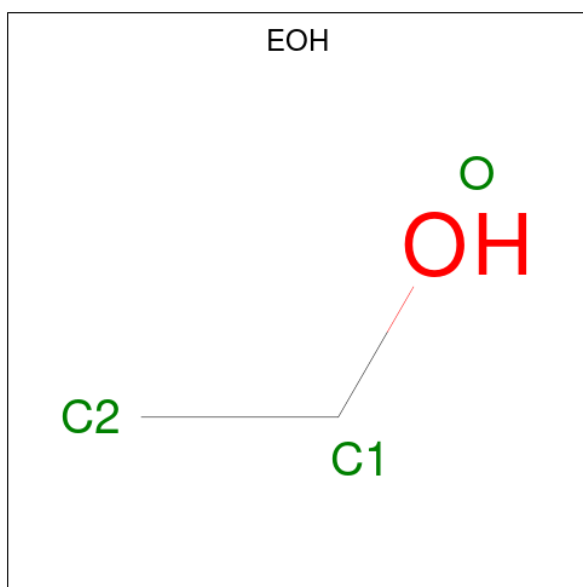
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	9	Total	Zn	0	0
			9	9		
11	B	7	Total	Zn	0	0
			7	7		

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Mg	0	0
			1	1		
12	B	1	Total	Mg	0	0
			1	1		

- Molecule 13 is ETHANOL (CCD ID: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			3	2	1		

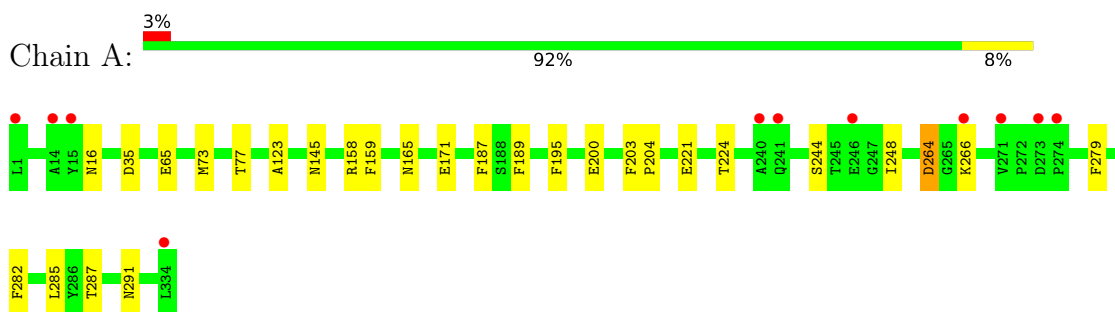
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	56	Total	O	0	0
			56	56		
14	B	74	Total	O	0	0
			74	74		

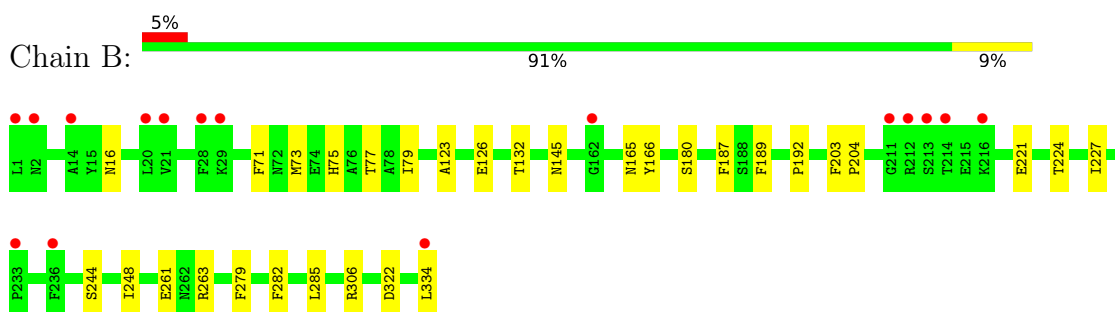
### 3 Residue-property plots

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

- Molecule 1: Heme-thiolate peroxidase



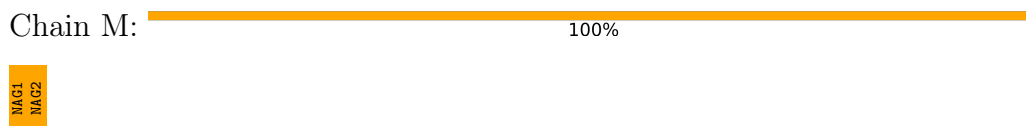
- Molecule 1: Heme-thiolate peroxidase



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



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



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

Chain X:  50% 50%

MAG1  
MAG2

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

Chain a:  50% 50%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.78Å 75.78Å 273.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.39 – 2.50 47.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.39-2.50) 99.9 (47.39-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.214 , 0.262 0.217 , 0.263	Depositor DCC
$R_{free}$ test set	1570 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, ACT, HEM, NAG, A1JFW, PO4, ZN, PEG, EOH, MES, GOL

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	0.55	0/2680	1.00	2/3655 (0.1%)
1	B	0.54	0/2672	0.97	0/3644
All	All	0.54	0/5352	0.99	2/7299 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	65	GLU	CB-CA-C	-5.09	102.66	110.81

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2461	28	0
1	B	2593	0	2455	33	0
2	J	28	0	25	2	0
2	M	28	0	25	3	0
2	X	28	0	25	4	0
2	a	28	0	25	4	0
3	A	28	0	26	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	5	0
4	A	4	0	3	2	0
4	B	4	0	3	1	0
5	A	43	0	30	3	0
5	B	43	0	30	5	0
6	A	8	0	0	1	0
6	B	16	0	0	0	0
7	A	24	0	26	0	0
7	B	12	0	13	0	0
8	A	12	0	16	0	0
8	B	12	0	16	1	0
9	A	7	0	10	0	0
10	A	5	0	0	0	0
11	A	9	0	0	0	0
11	B	7	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	B	3	0	6	0	0
14	A	56	0	0	5	1
14	B	74	0	0	6	1
All	All	5686	0	5208	67	1

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 6.

The worst 5 of 67 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:HD21	2:M:1:NAG:C1	1.14	1.60
1:B:145:ASN:HD21	2:a:1:NAG:C1	1.40	1.35
1:A:165:ASN:ND2	2:J:1:NAG:C1	1.97	1.28
1:A:291:ASN:HD21	3:A:402:NAG:C1	1.51	1.24
1:A:145:ASN:ND2	2:M:1:NAG:C1	1.99	1.22

All (1) 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)
14:A:541:HOH:O	14:B:517:HOH:O[6_564]	2.10	0.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/334 (100%)	323 (97%)	10 (3%)	1 (0%)	36	55
1	B	333/334 (100%)	319 (96%)	13 (4%)	1 (0%)	36	55
All	All	667/668 (100%)	642 (96%)	23 (3%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	ALA
1	A	123	ALA

### 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	276/274 (101%)	276 (100%)	0	100	100
1	B	275/274 (100%)	275 (100%)	0	100	100
All	All	551/548 (100%)	551 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	312	ASN
1	B	16	ASN

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	165	ASN
1	A	312	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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	J	1	2	14,14,15	0.35	0	17,19,21	2.23	4 (23%)
2	NAG	J	2	2	14,14,15	0.32	0	17,19,21	0.96	0
2	NAG	M	1	2	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
2	NAG	M	2	2	14,14,15	0.28	0	17,19,21	1.16	2 (11%)
2	NAG	X	1	2	14,14,15	0.41	0	17,19,21	2.49	3 (17%)
2	NAG	X	2	2	14,14,15	0.35	0	17,19,21	0.57	0
2	NAG	a	1	2	14,14,15	0.39	0	17,19,21	0.97	1 (5%)
2	NAG	a	2	2	14,14,15	0.30	0	17,19,21	0.93	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	2	-	4/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	1/6/23/26	0/1/1/1
2	NAG	X	1	2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	3/6/23/26	0/1/1/1
2	NAG	a	1	2	-	1/6/23/26	0/1/1/1
2	NAG	a	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1	NAG	O5-C1-C2	8.70	124.75	111.29
2	J	1	NAG	O5-C1-C2	6.94	122.03	111.29
2	J	1	NAG	C1-O5-C5	4.31	117.96	112.19
2	X	1	NAG	C1-O5-C5	3.57	116.97	112.19
2	X	1	NAG	C1-C2-N2	3.13	115.36	110.43

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	a	2	NAG	O5-C5-C6-O6

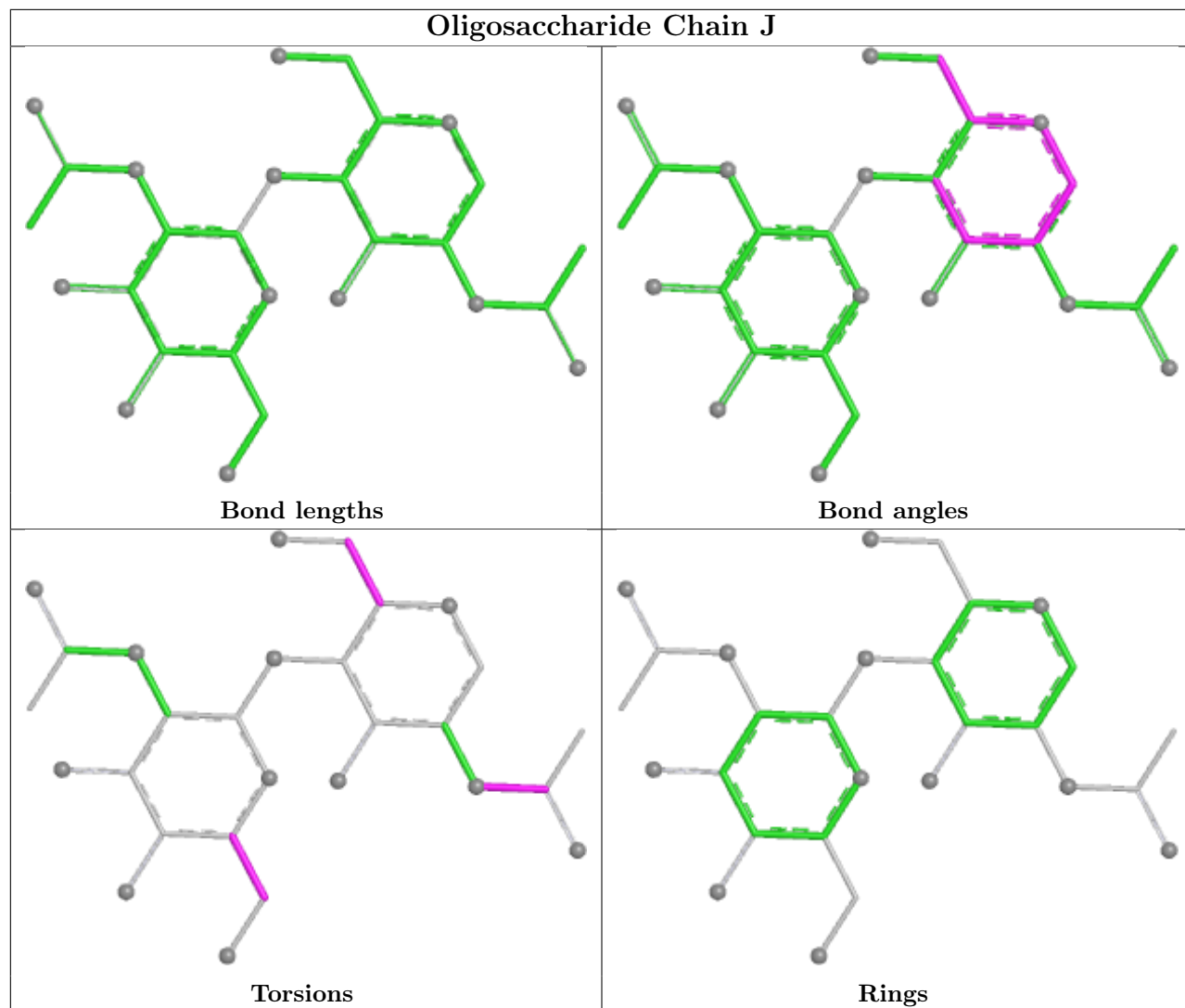
There are no ring outliers.

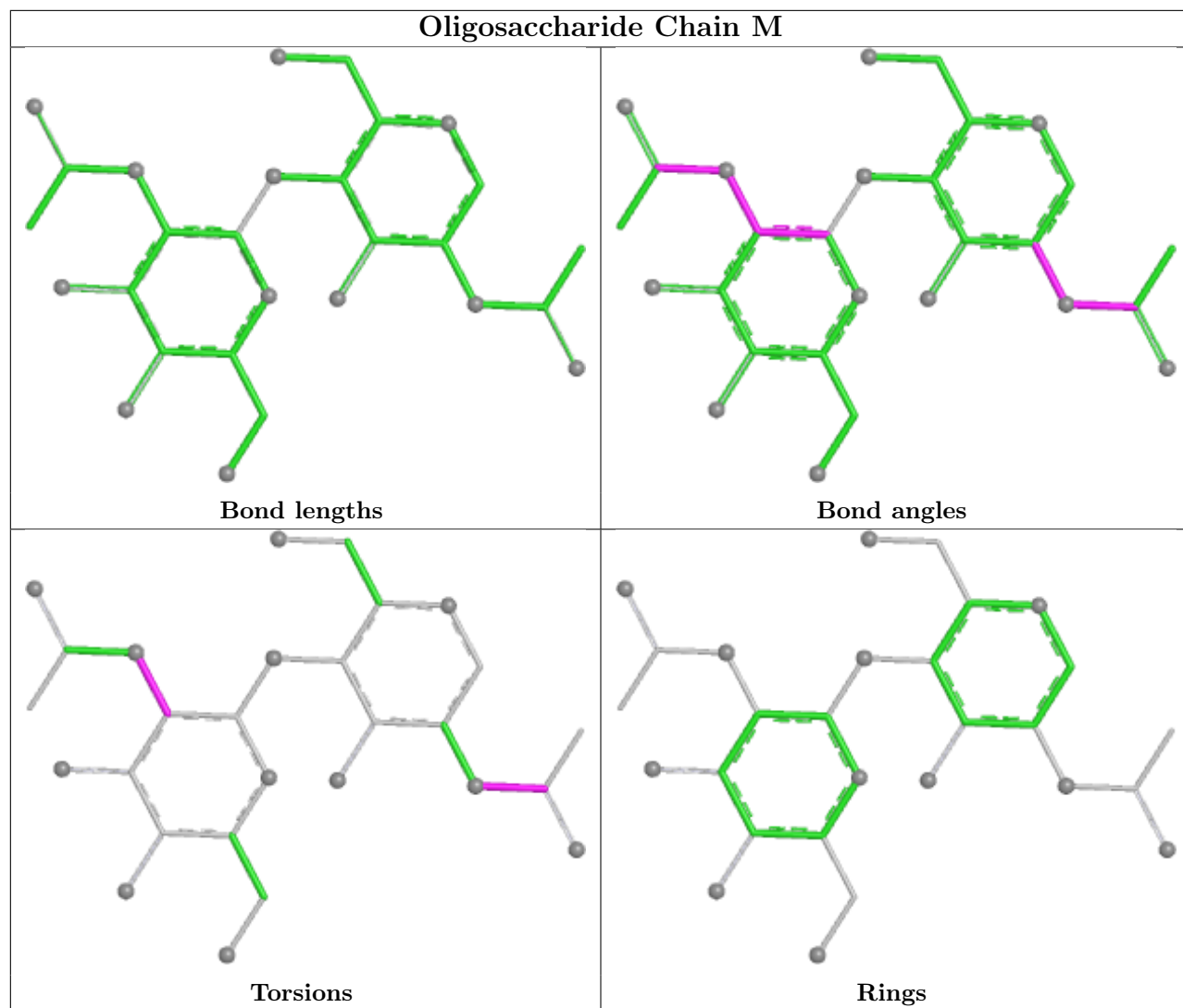
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	NAG	2	0
2	J	1	NAG	2	0
2	X	1	NAG	4	0
2	M	2	NAG	1	0
2	a	1	NAG	4	0

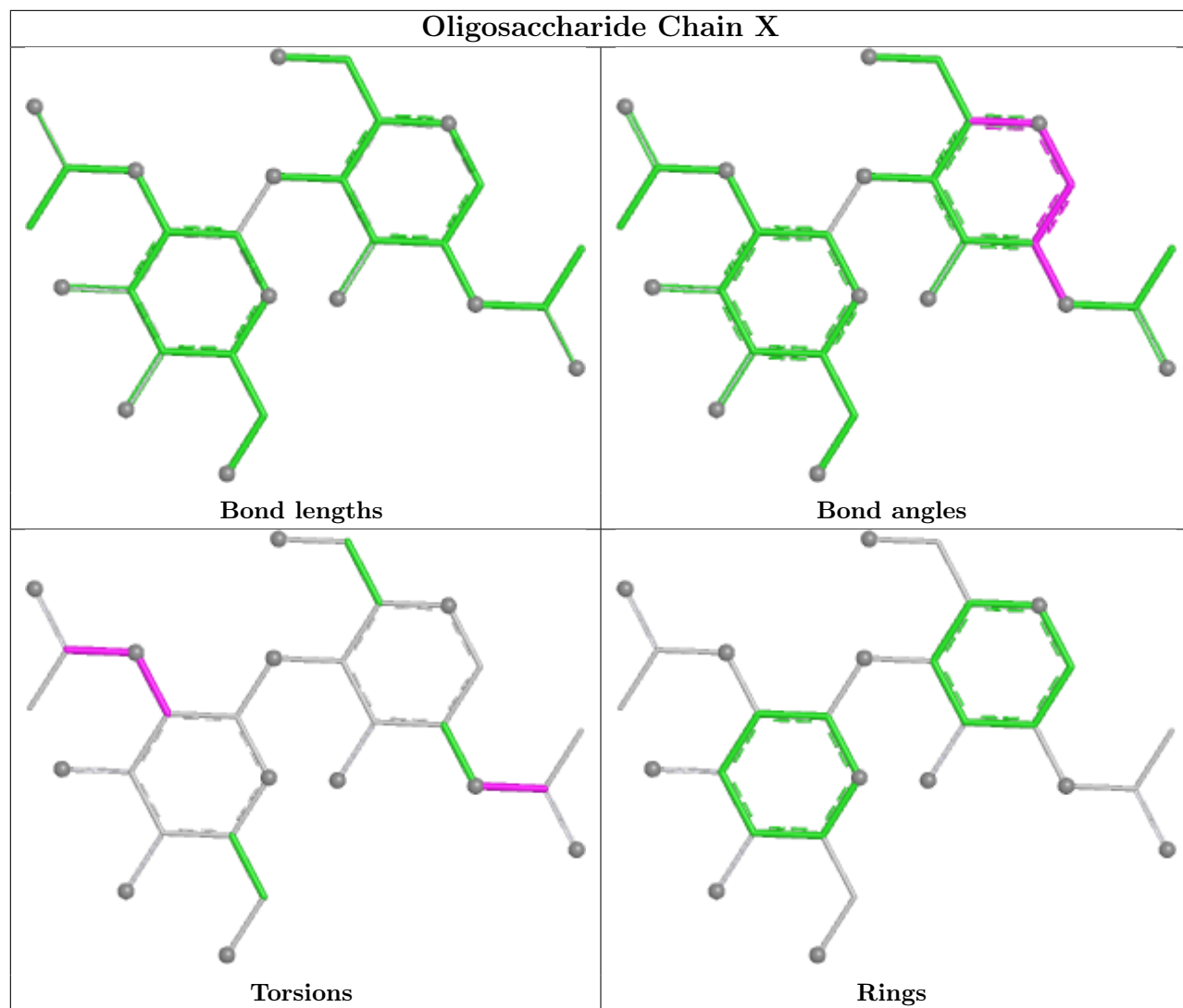
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

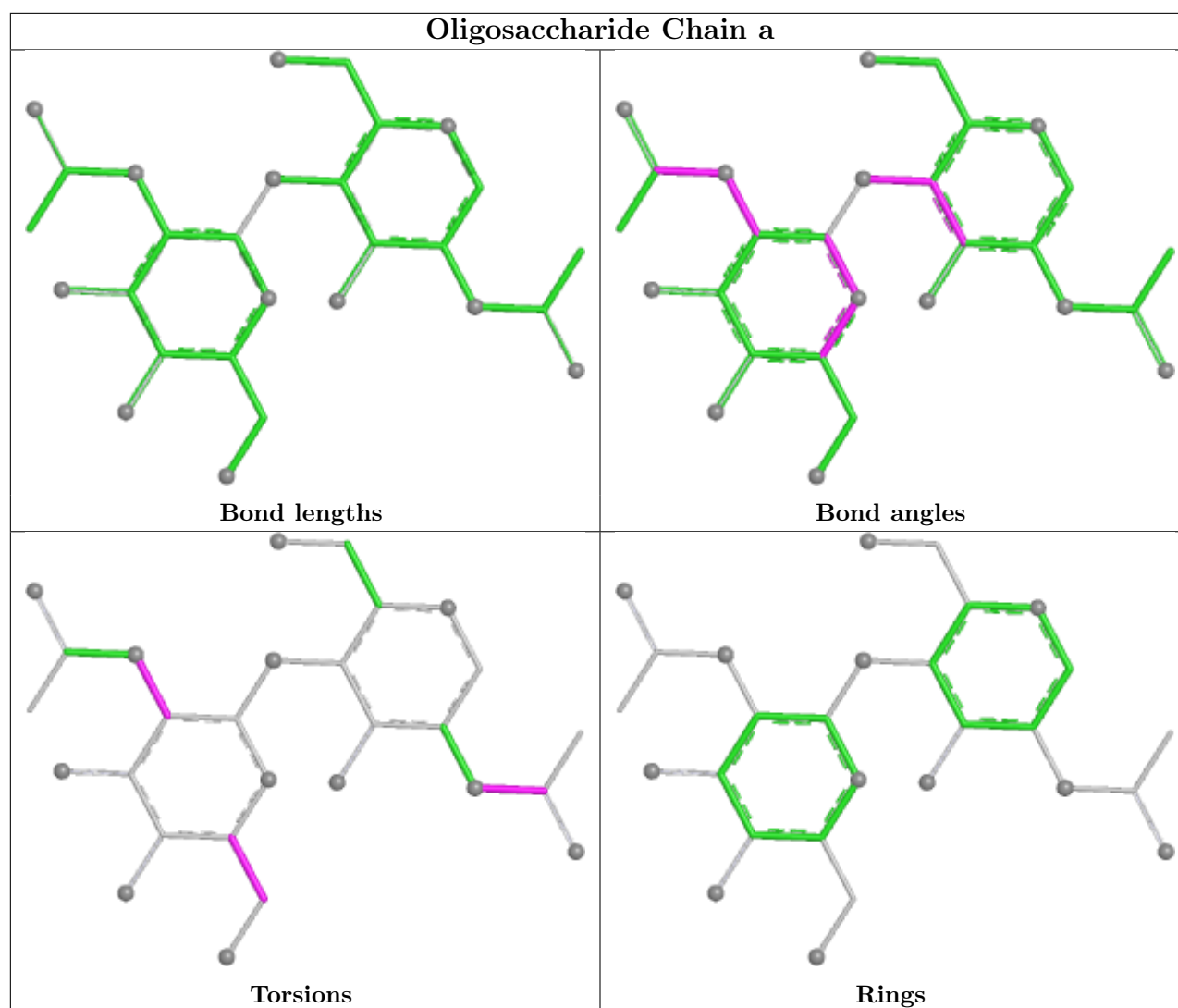
bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 18 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	A1JFW	A	405	-	8,8,8	0.63	0	9,9,9	0.67	0
8	GOL	A	407	-	5,5,5	0.19	0	5,5,5	0.43	0
3	NAG	B	401	-	14,14,15	0.39	0	17,19,21	1.02	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	A	403	-	3,3,3	1.01	0	3,3,3	0.85	0
7	MES	B	403	-	12,12,12	0.83	0	15,16,16	0.62	0
5	HEM	A	404	12,1	50,50,50	1.62	7 (14%)	67,82,82	1.58	18 (26%)
8	GOL	B	405	-	5,5,5	0.16	0	5,5,5	0.42	0
7	MES	A	409	-	12,12,12	0.86	0	15,16,16	0.60	0
5	HEM	B	402	12,1	50,50,50	1.52	11 (22%)	67,82,82	1.92	17 (25%)
9	PEG	A	410	-	6,6,6	0.18	0	5,5,5	0.09	0
8	GOL	A	408	-	5,5,5	0.12	0	5,5,5	0.33	0
7	MES	A	406	-	12,12,12	0.76	0	15,16,16	0.83	0
6	A1JFW	B	404	-	8,8,8	0.87	1 (12%)	9,9,9	0.98	0
4	ACT	B	406	-	3,3,3	0.93	0	3,3,3	0.96	0
6	A1JFW	B	407	-	8,8,8	0.70	0	9,9,9	0.61	0
8	GOL	B	408	-	5,5,5	0.15	0	5,5,5	0.42	0
3	NAG	A	401	-	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
3	NAG	A	402	-	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
10	PO4	A	411	-	4,4,4	0.88	0	6,6,6	0.55	0
13	EOH	B	409	-	2,2,2	0.08	0	1,1,1	0.09	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
6	A1JFW	A	405	-	-	2/2/2/2	0/1/1/1
8	GOL	B	405	-	-	0/4/4/4	-
8	GOL	A	407	-	-	1/4/4/4	-
8	GOL	A	408	-	-	0/4/4/4	-
7	MES	A	406	-	-	0/6/14/14	0/1/1/1
3	NAG	A	401	-	-	2/6/23/26	0/1/1/1
3	NAG	A	402	-	-	1/6/23/26	0/1/1/1
3	NAG	B	401	-	-	1/6/23/26	0/1/1/1
6	A1JFW	B	404	-	-	2/2/2/2	0/1/1/1
5	HEM	B	402	12,1	-	5/14/54/54	-
7	MES	A	409	-	-	3/6/14/14	0/1/1/1
6	A1JFW	B	407	-	-	2/2/2/2	0/1/1/1
7	MES	B	403	-	-	0/6/14/14	0/1/1/1
9	PEG	A	410	-	-	0/4/4/4	-
5	HEM	A	404	12,1	-	4/14/54/54	-
8	GOL	B	408	-	-	0/4/4/4	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	HEM	FE-NB	5.84	2.12	1.94
5	B	402	HEM	FE-NC	4.10	2.08	1.95
5	A	404	HEM	C1B-NB	-3.88	1.33	1.40
5	B	402	HEM	C4B-NB	-3.30	1.32	1.38
5	A	404	HEM	C4B-NB	-3.09	1.32	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	HEM	CHC-C4B-NB	5.89	130.76	124.42
5	B	402	HEM	C3B-C4B-NB	-5.03	105.86	109.47
5	B	402	HEM	C1B-NB-C4B	4.51	110.55	105.21
5	B	402	HEM	CHB-C1B-NB	4.30	129.69	124.37
5	B	402	HEM	CHA-C4D-ND	3.94	129.24	124.37

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAG	C1-C2-N2-C7
6	A	405	A1JFW	C4-C5-O01-C03
6	B	407	A1JFW	C6-C5-O01-C03
6	A	405	A1JFW	C6-C5-O01-C03
6	B	407	A1JFW	C4-C5-O01-C03

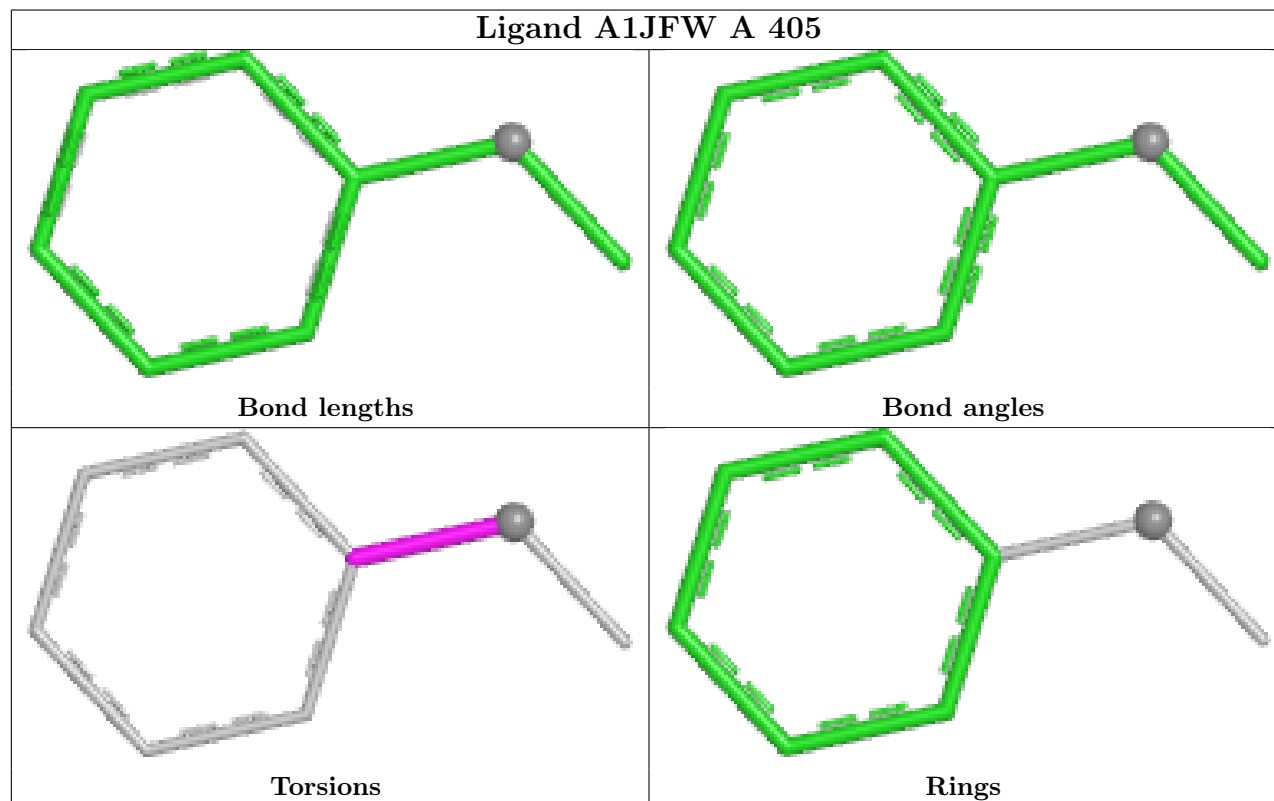
There are no ring outliers.

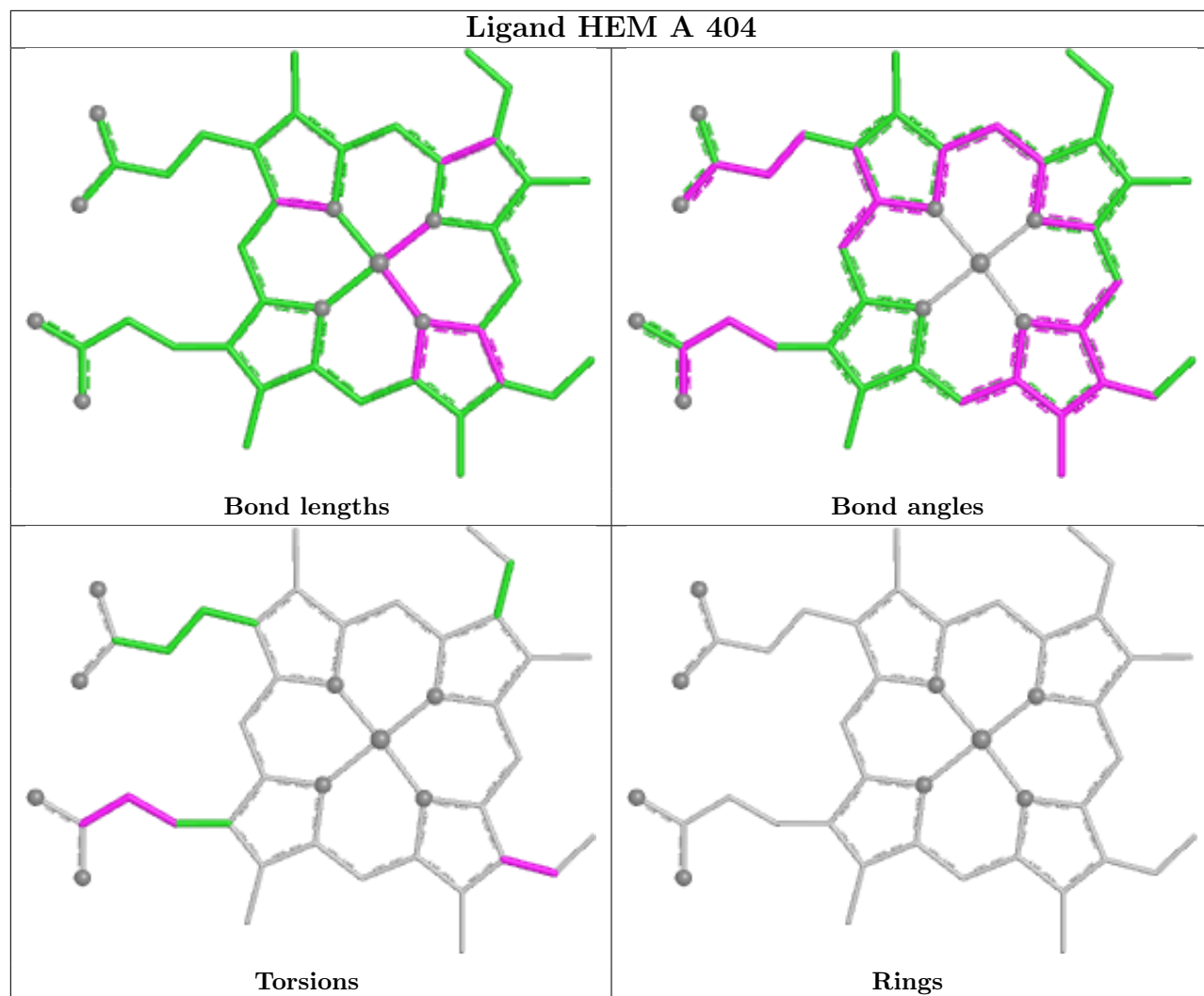
9 monomers are involved in 25 short contacts:

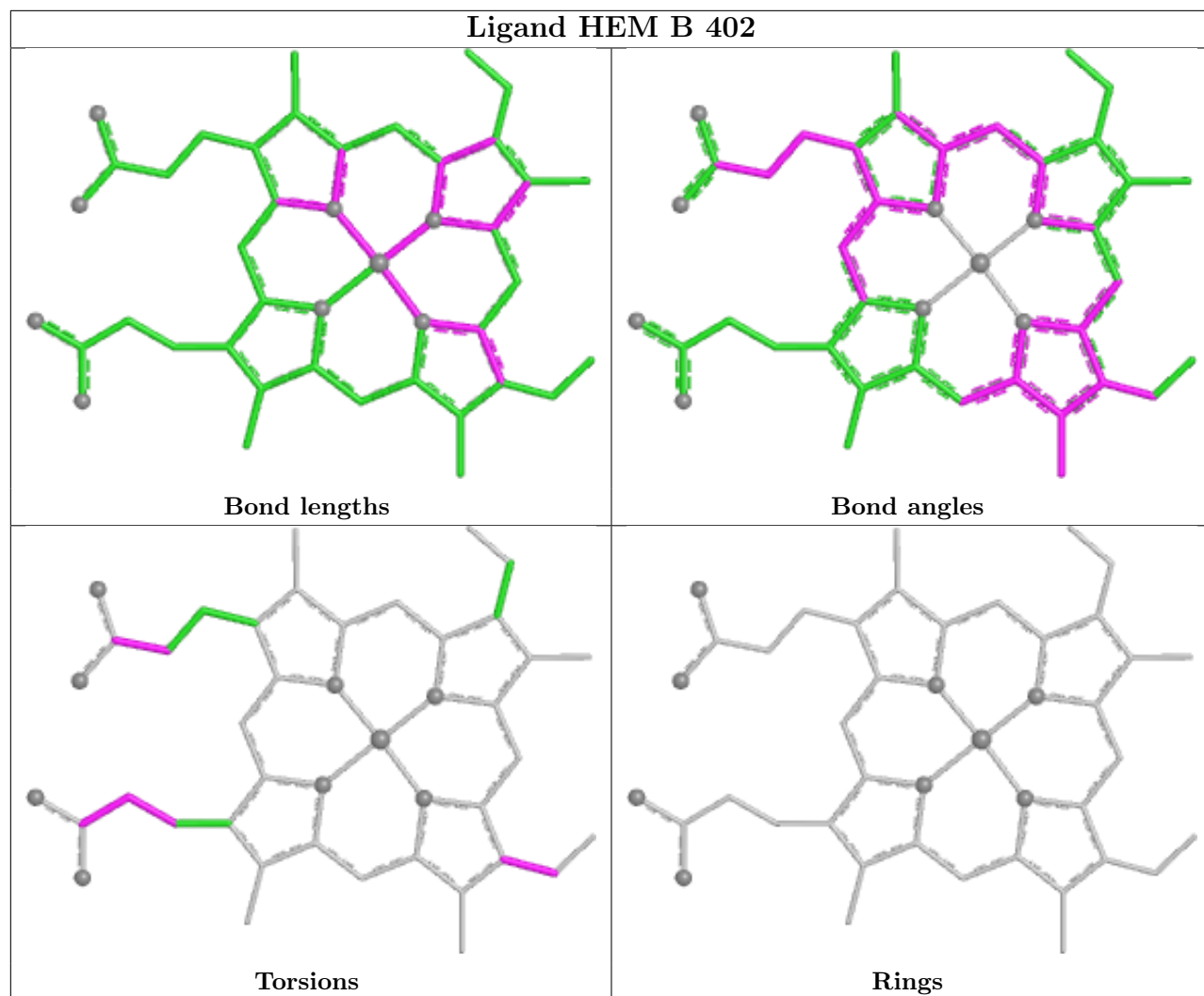
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	405	A1JFW	1	0
3	B	401	NAG	5	0
4	A	403	ACT	2	0
5	A	404	HEM	3	0
5	B	402	HEM	5	0
4	B	406	ACT	1	0
8	B	408	GOL	1	0
3	A	401	NAG	3	0
3	A	402	NAG	5	0

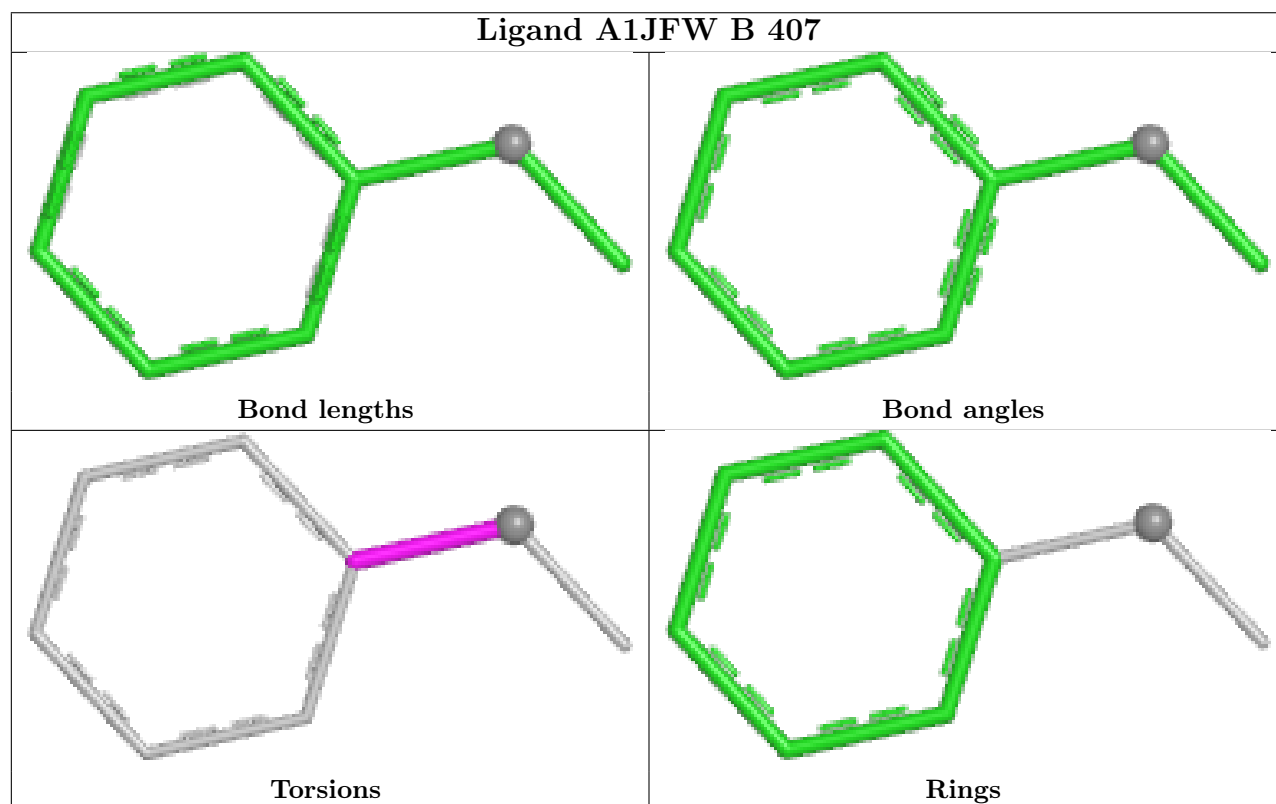
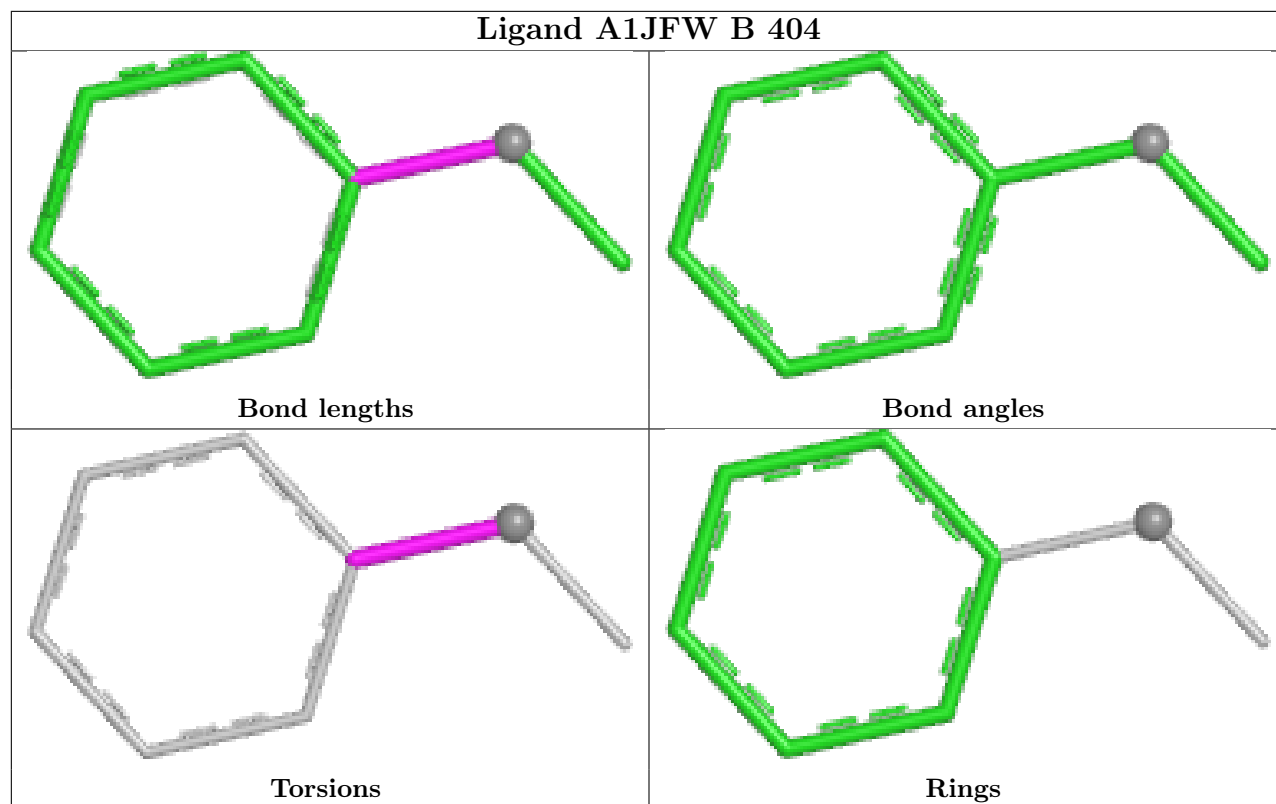
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/334 (100%)	0.29	11 (3%) 49 45	29, 50, 81, 119	2 (0%)
1	B	334/334 (100%)	0.51	16 (4%) 35 31	32, 56, 89, 123	1 (0%)
All	All	668/668 (100%)	0.40	27 (4%) 42 38	29, 53, 87, 123	3 (0%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	LEU	3.6
1	A	274	PRO	3.5
1	B	334	LEU	3.4
1	A	1	LEU	3.3
1	B	233	PRO	3.2

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	J	1	14/15	-	-	61,75,80,84	0
2	NAG	J	2	14/15	-	-	82,95,109,109	0
2	NAG	M	1	14/15	-	-	53,65,78,92	0
2	NAG	M	2	14/15	-	-	64,89,98,102	0
2	NAG	X	1	14/15	-	-	59,69,81,93	0

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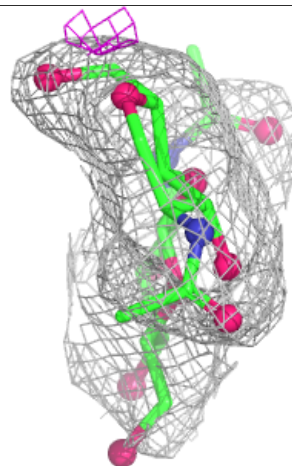
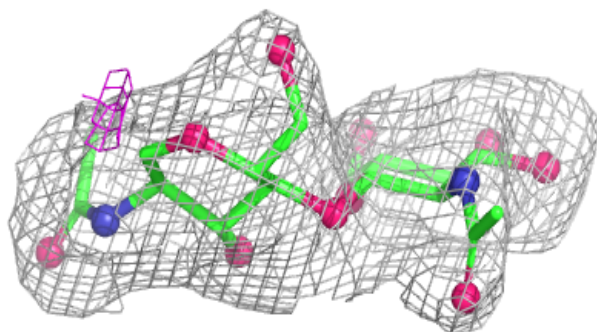
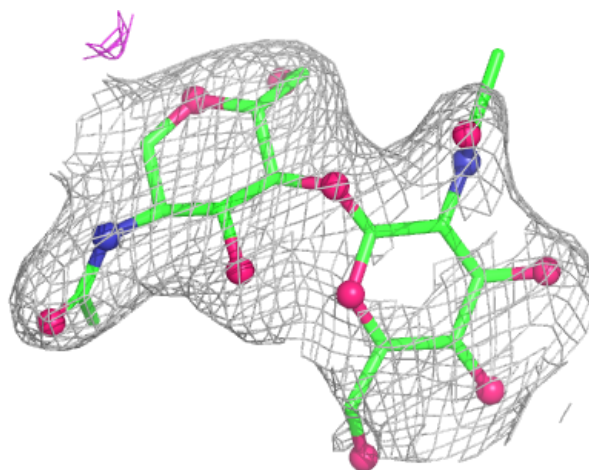
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	X	2	14/15	-	-	89,105,112,113	0
2	NAG	a	1	14/15	-	-	69,76,85,89	0
2	NAG	a	2	14/15	-	-	79,92,104,107	0

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.

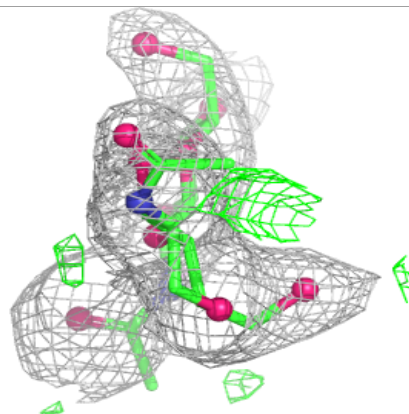
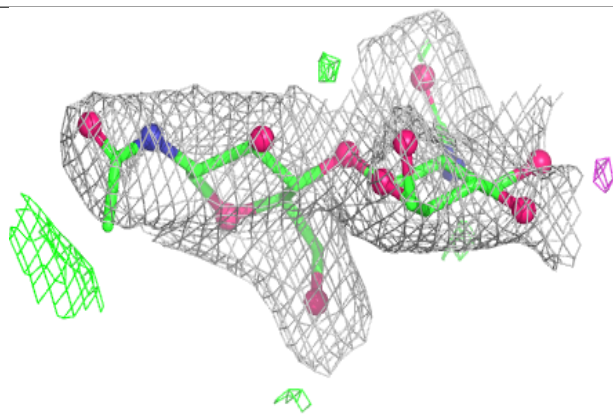
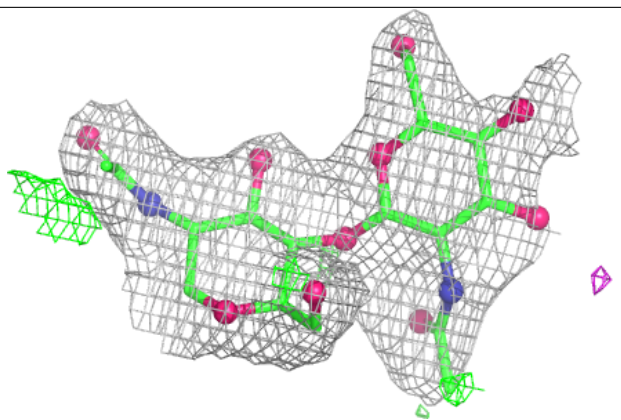
#### Electron density around Chain J:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

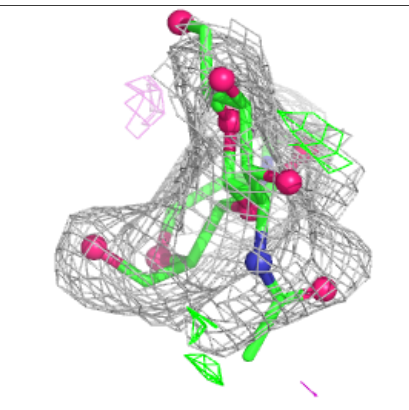
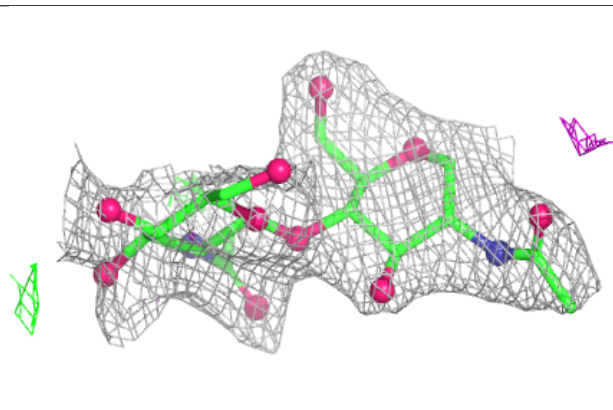
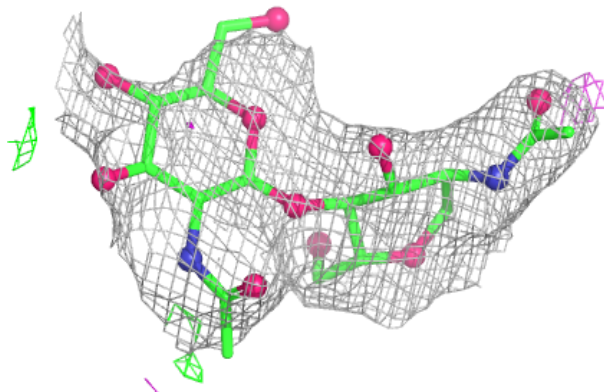


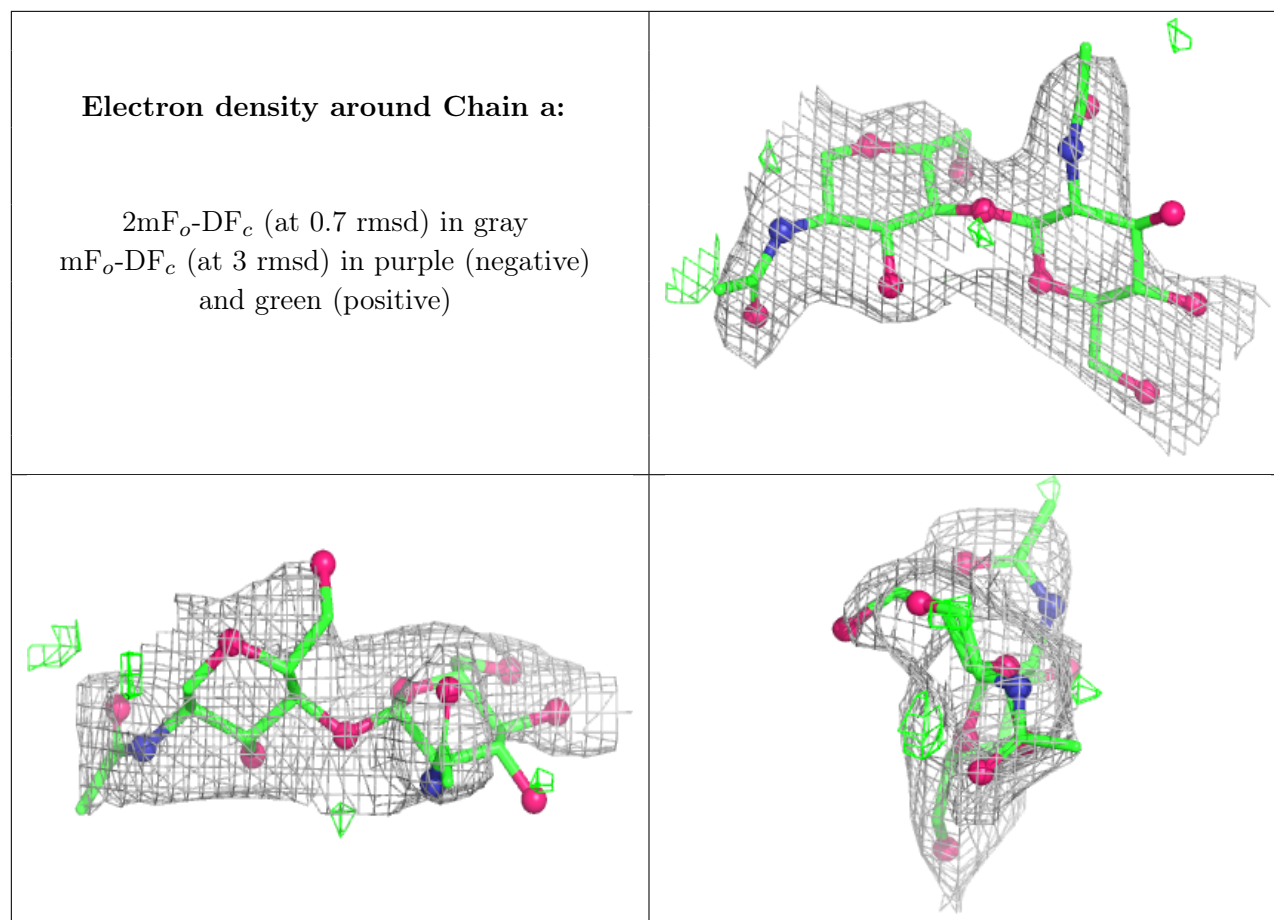
**Electron density around Chain M:**

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

**Electron density around Chain X:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	EOH	B	409	3/3	0.42	0.30	76,76,77,78	0
3	NAG	A	402	14/15	0.60	0.16	82,112,116,116	0
8	GOL	A	407	6/6	0.66	0.16	64,73,74,75	0
8	GOL	B	405	6/6	0.67	0.22	65,75,78,81	0
3	NAG	A	401	14/15	0.72	0.17	93,105,110,112	0
7	MES	A	409	12/12	0.73	0.20	86,97,102,105	0
9	PEG	A	410	7/7	0.74	0.14	77,85,87,89	0
6	A1JFW	B	404	8/8	0.77	0.27	63,73,79,81	0
8	GOL	B	408	6/6	0.77	0.16	76,87,89,89	0
6	A1JFW	A	405	8/8	0.79	0.27	61,81,91,93	0
10	PO4	A	411	5/5	0.79	0.15	77,79,82,95	0
8	GOL	A	408	6/6	0.79	0.13	68,72,75,76	0

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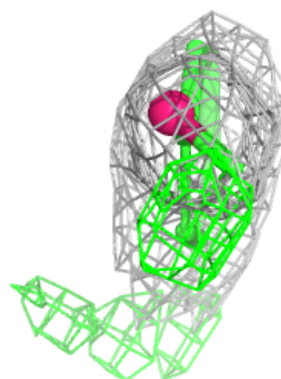
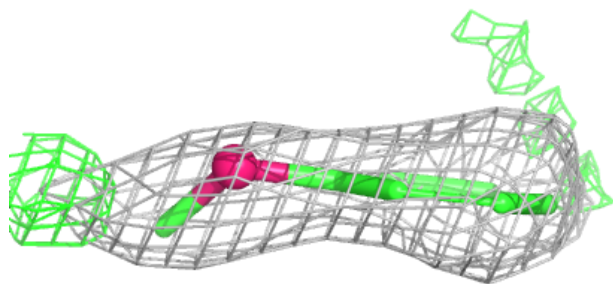
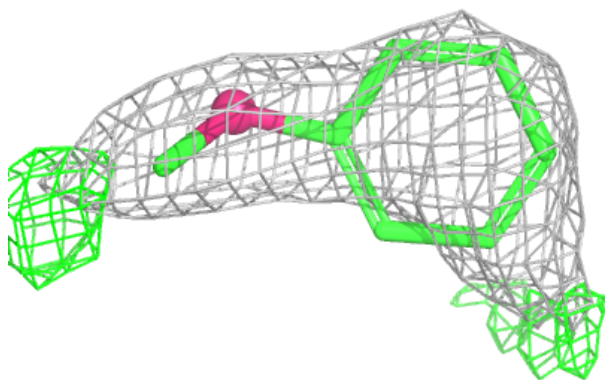
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACT	A	403	4/4	0.83	0.20	54,57,58,66	0
3	NAG	B	401	14/15	0.84	0.12	70,84,89,90	0
4	ACT	B	406	4/4	0.85	0.15	66,69,70,72	0
6	A1JFW	B	407	8/8	0.87	0.27	90,96,103,106	0
7	MES	B	403	12/12	0.90	0.16	49,74,87,90	0
7	MES	A	406	12/12	0.90	0.18	45,62,87,89	0
11	ZN	A	412	1/1	0.93	0.07	95,95,95,95	0
11	ZN	B	411	1/1	0.94	0.10	95,95,95,95	0
11	ZN	A	420	1/1	0.96	0.05	87,87,87,87	0
5	HEM	B	402	43/43	0.96	0.09	32,39,50,56	0
11	ZN	B	416	1/1	0.96	0.05	90,90,90,90	0
11	ZN	A	417	1/1	0.96	0.05	57,57,57,57	0
5	HEM	A	404	43/43	0.98	0.07	31,40,45,46	0
11	ZN	A	416	1/1	0.98	0.07	53,53,53,53	0
11	ZN	B	410	1/1	0.98	0.04	66,66,66,66	0
11	ZN	A	419	1/1	0.99	0.03	66,66,66,66	0
11	ZN	B	412	1/1	0.99	0.03	62,62,62,62	0
11	ZN	B	413	1/1	0.99	0.04	81,81,81,81	0
11	ZN	B	414	1/1	0.99	0.05	45,45,45,45	0
11	ZN	B	415	1/1	0.99	0.03	74,74,74,74	0
11	ZN	A	413	1/1	0.99	0.02	66,66,66,66	0
11	ZN	A	418	1/1	0.99	0.02	67,67,67,67	0
11	ZN	A	415	1/1	1.00	0.02	54,54,54,54	0
12	MG	A	421	1/1	1.00	0.02	24,24,24,24	0
12	MG	B	417	1/1	1.00	0.06	30,30,30,30	0
11	ZN	A	414	1/1	1.00	0.02	53,53,53,53	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.

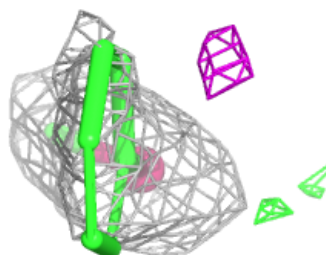
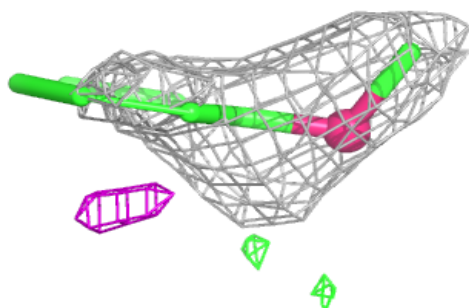
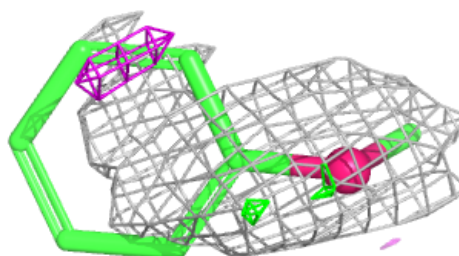


**Electron density around A1JFW B 404:**

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

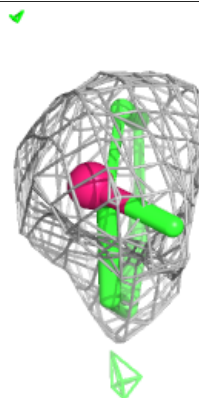
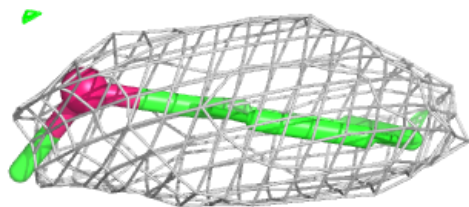
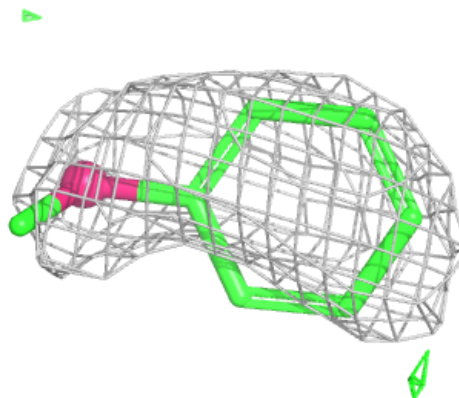
**Electron density around A1JFW A 405:**

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and green (positive)



**Electron density around A1JFW B 407:**

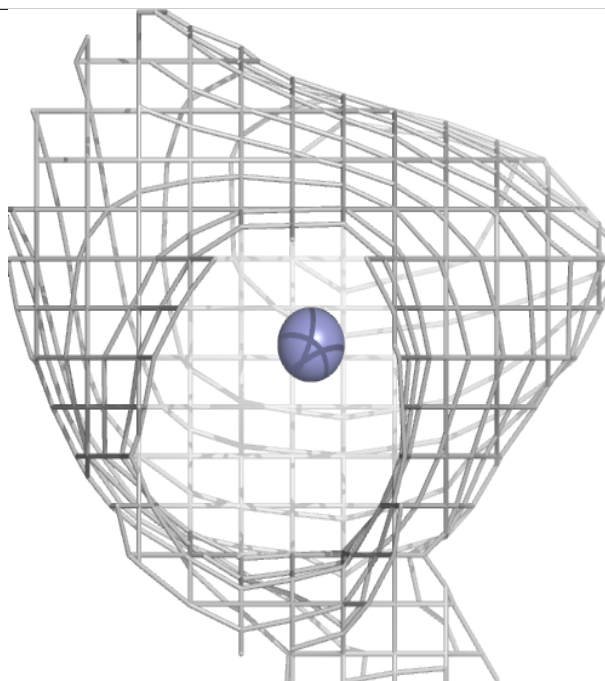
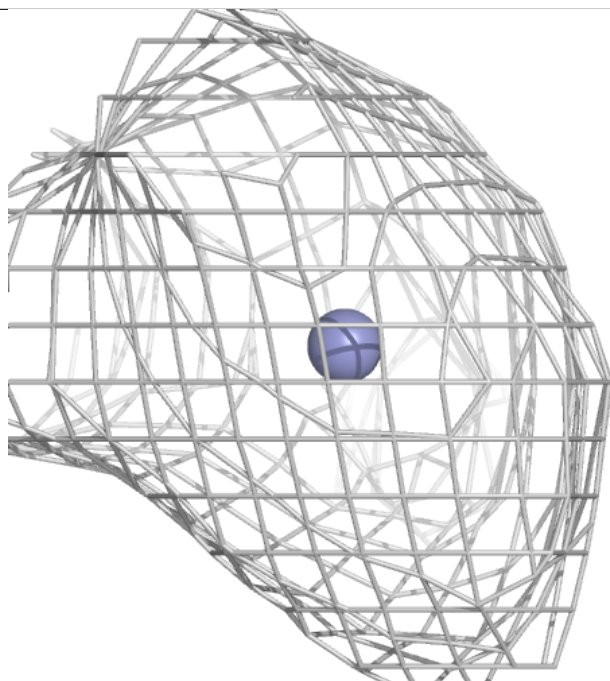
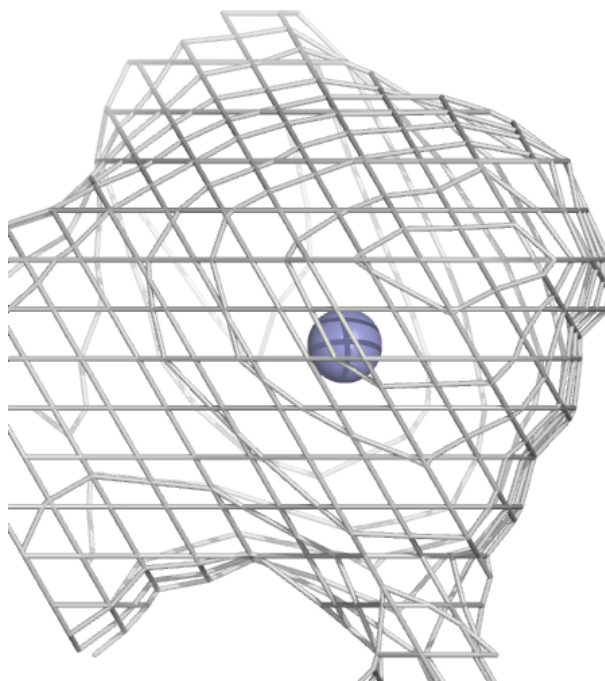
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





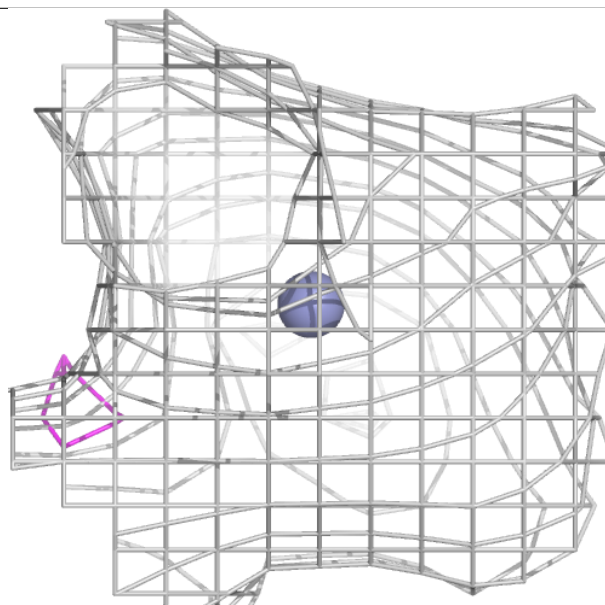
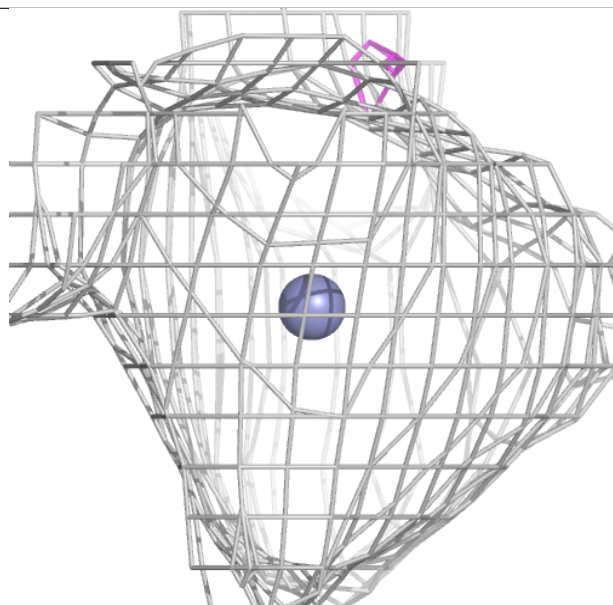
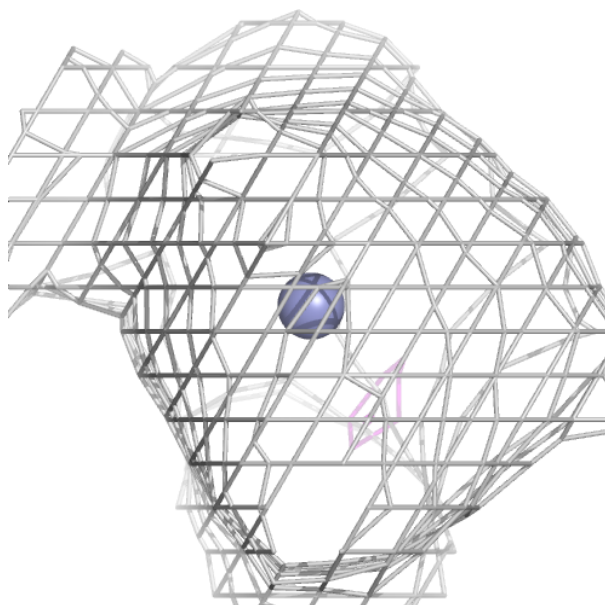
**Electron density around ZN A 412:**

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



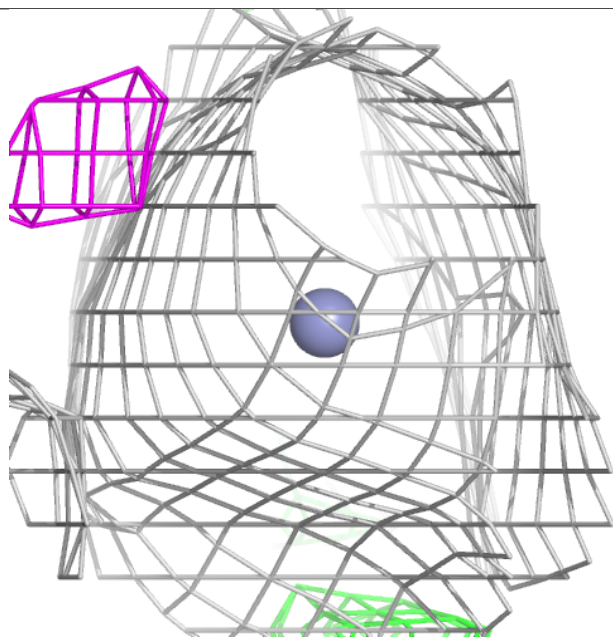
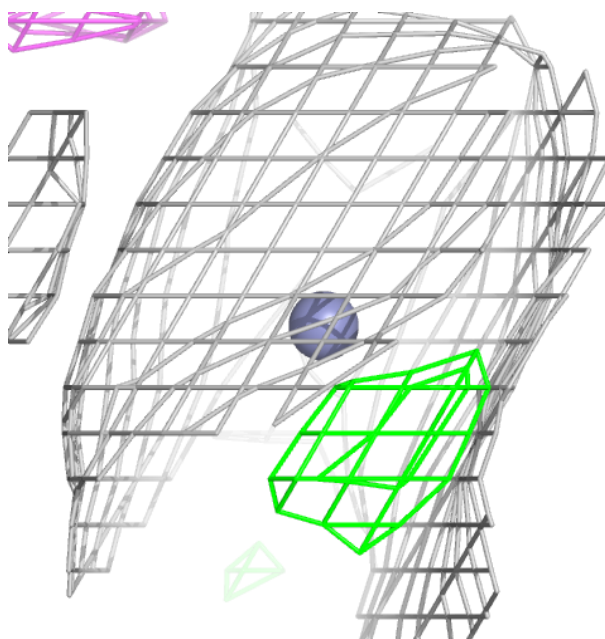
**Electron density around ZN B 411:**

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



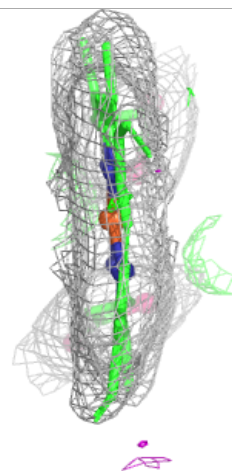
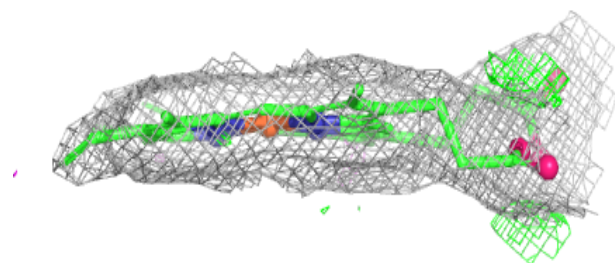
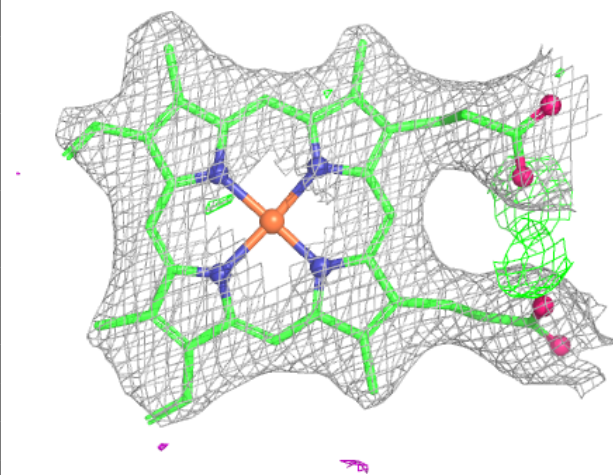
**Electron density around ZN A 420:**

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



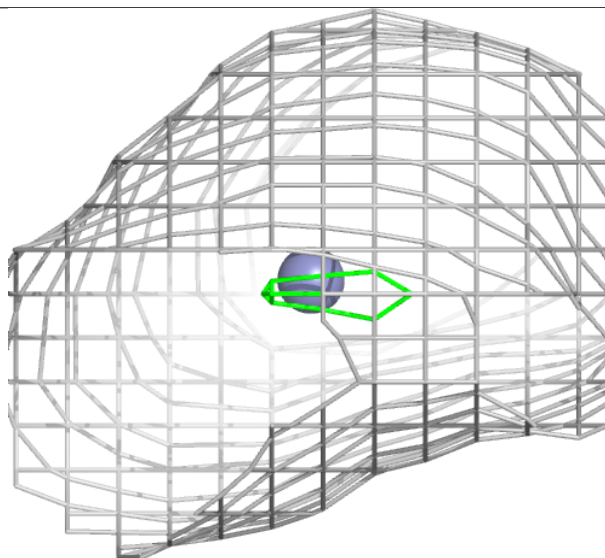
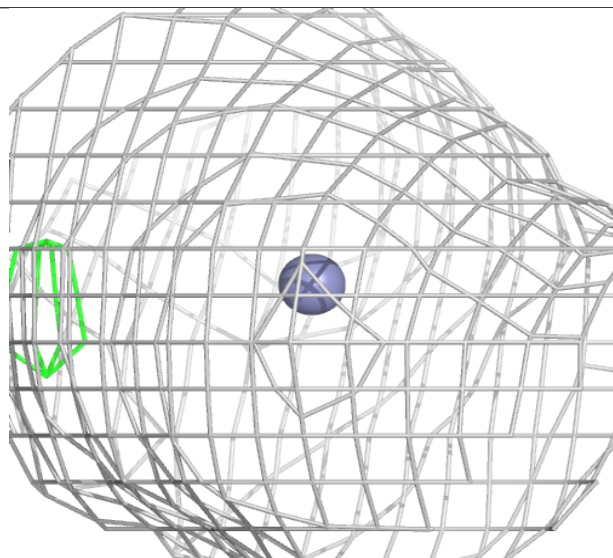
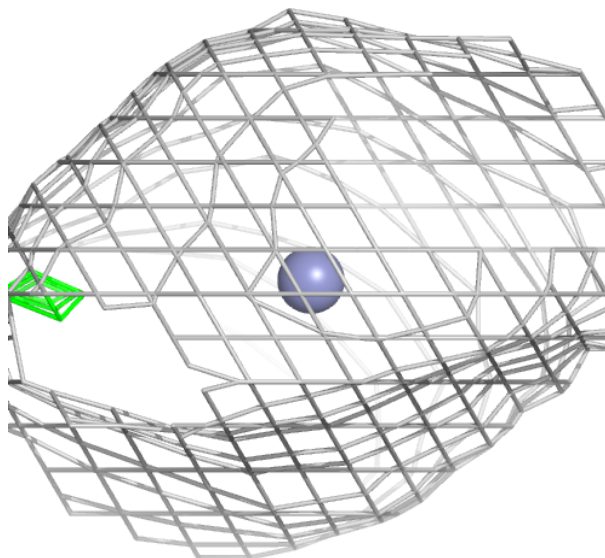
**Electron density around HEM B 402:**

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



**Electron density around ZN B 416:**

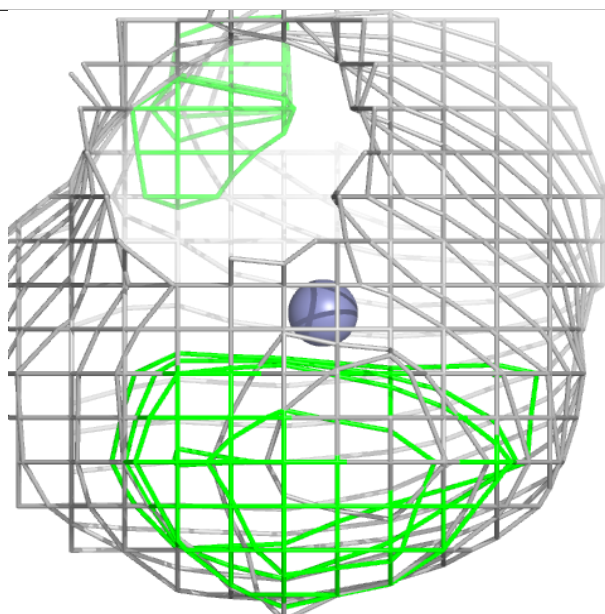
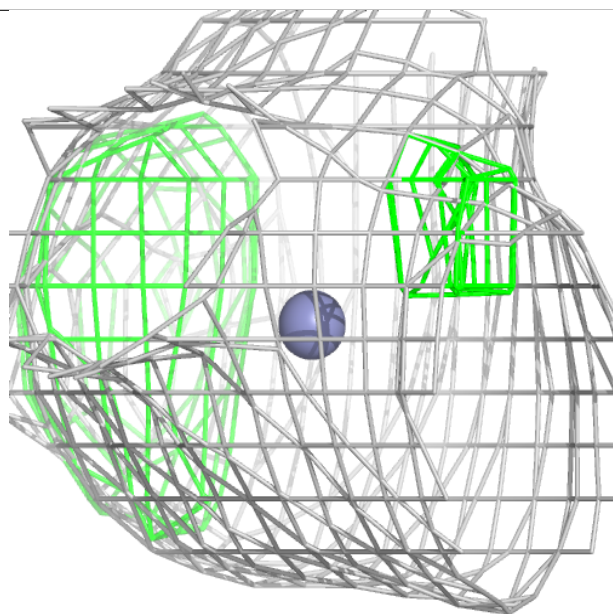
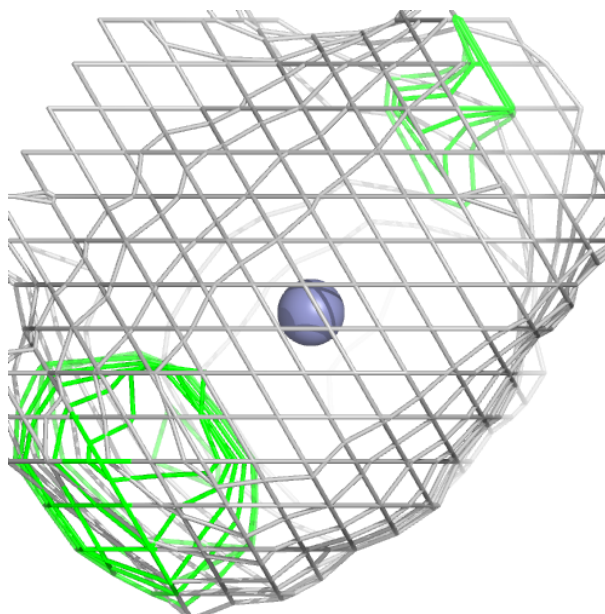
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





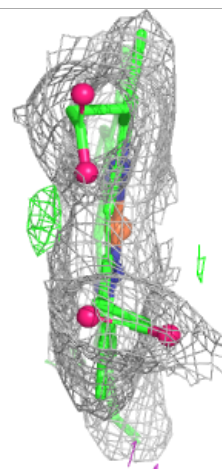
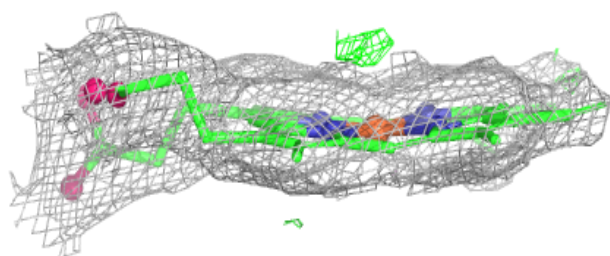
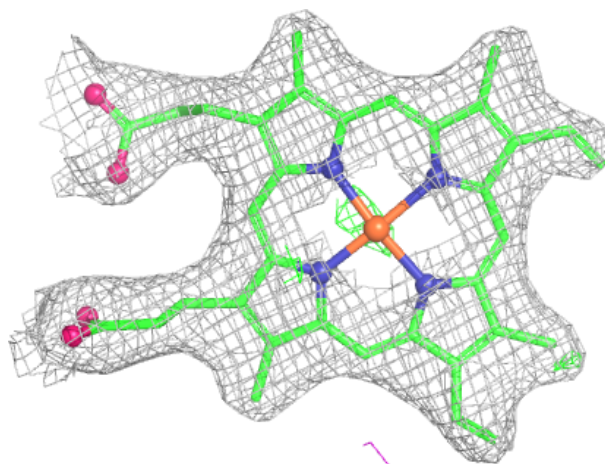
**Electron density around ZN A 417:**

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



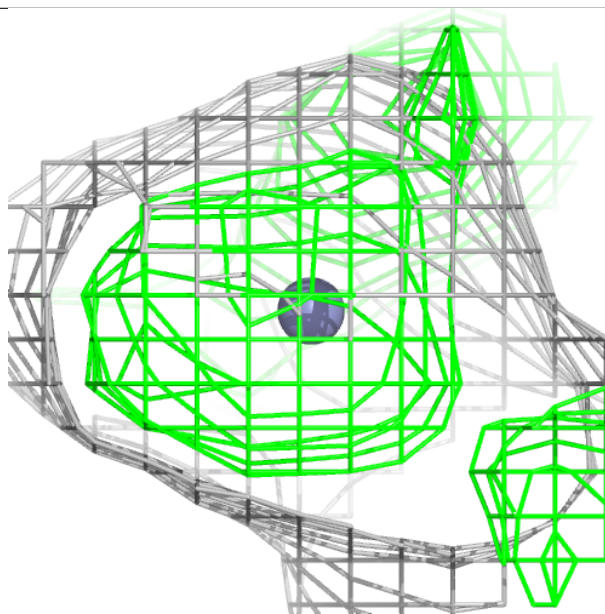
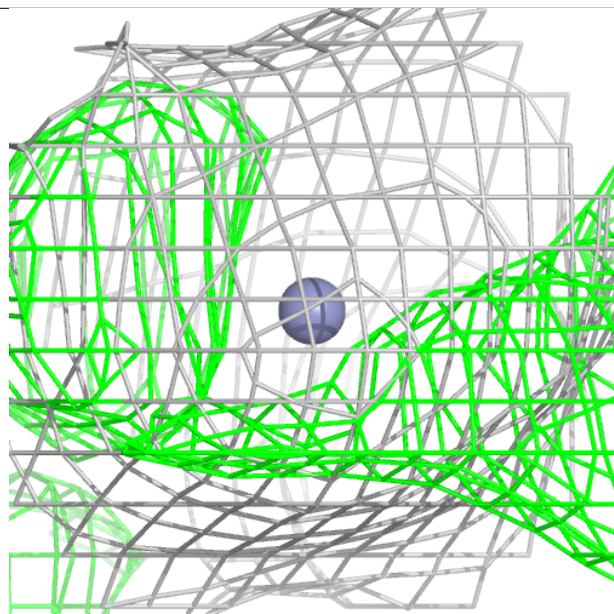
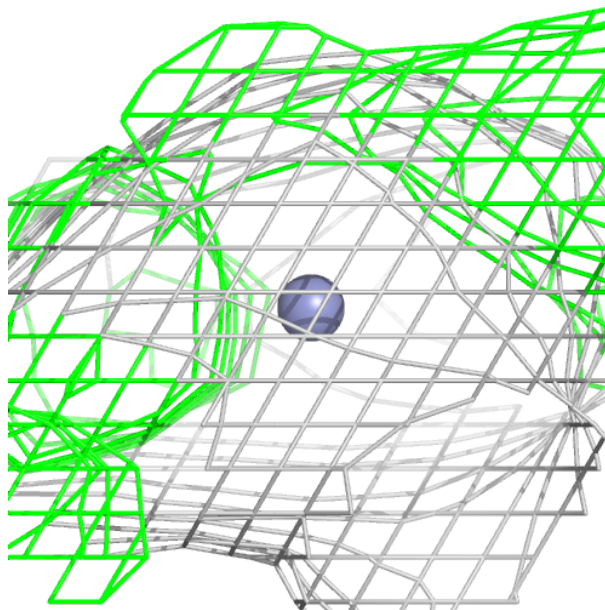
**Electron density around HEM A 404:**

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



**Electron density around ZN A 416:**

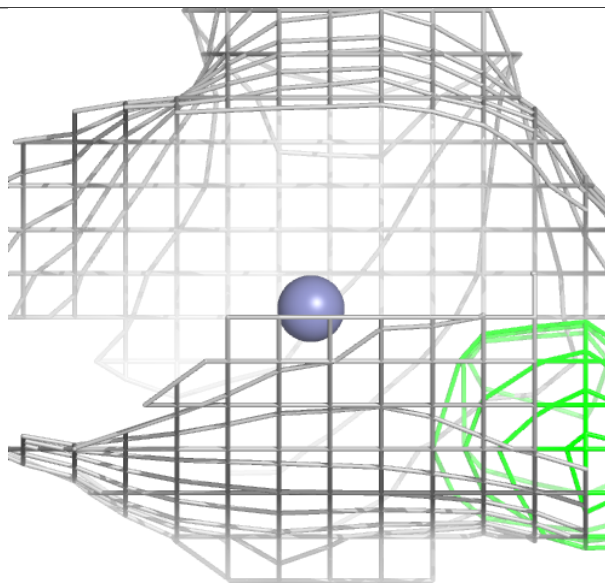
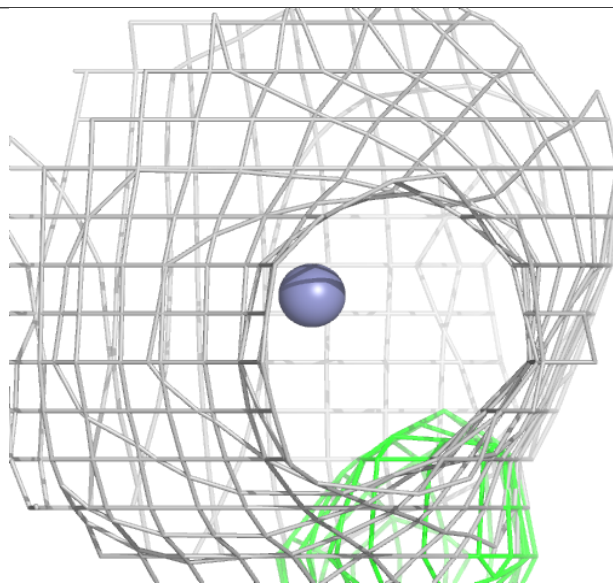
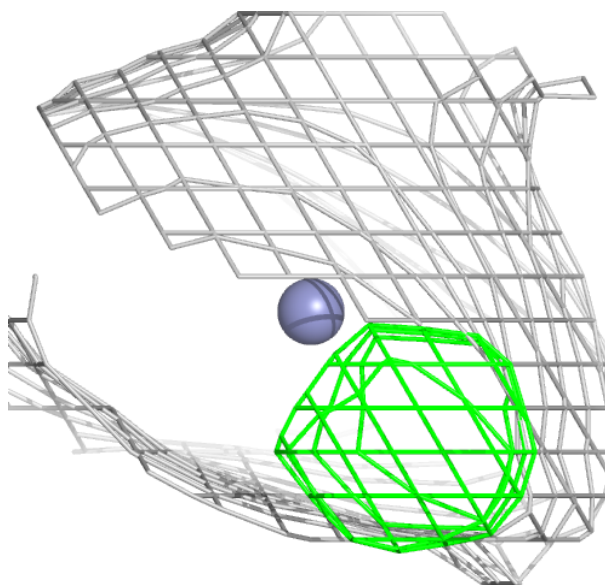
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





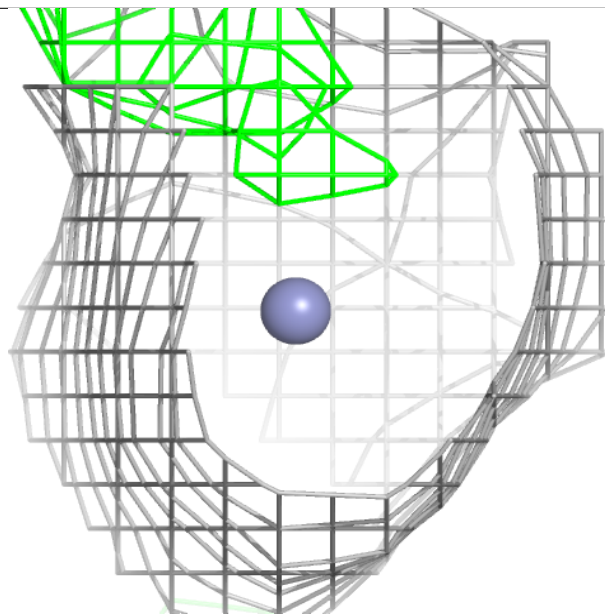
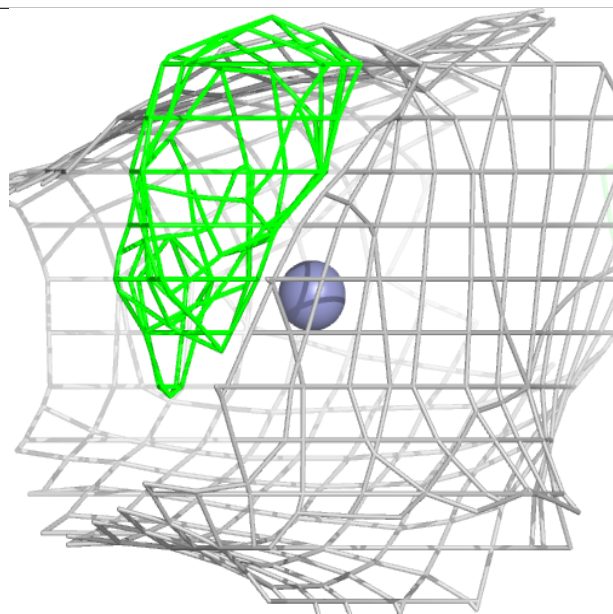
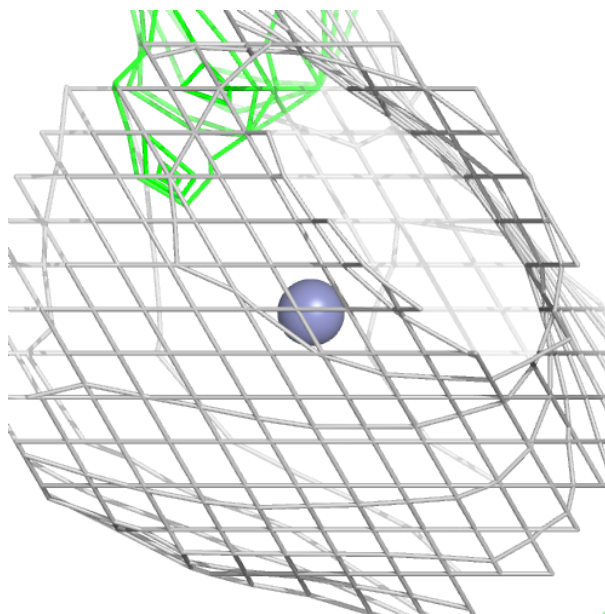
**Electron density around ZN B 410:**

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



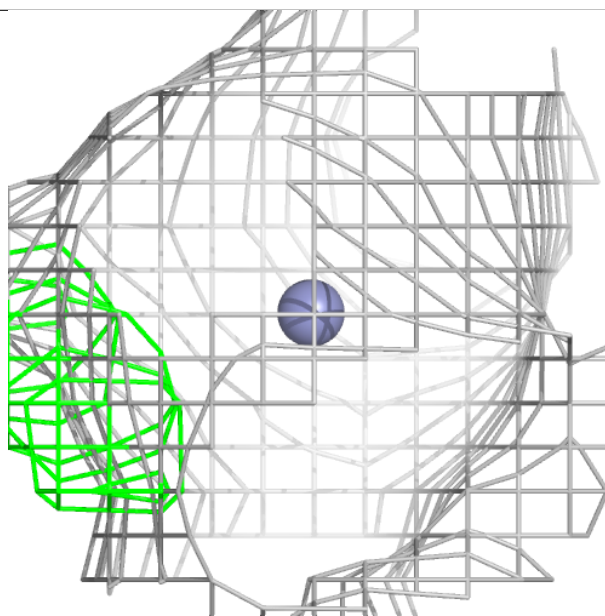
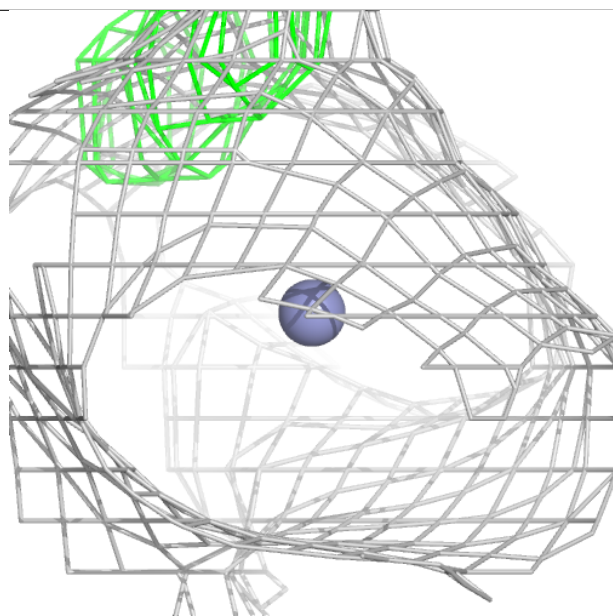
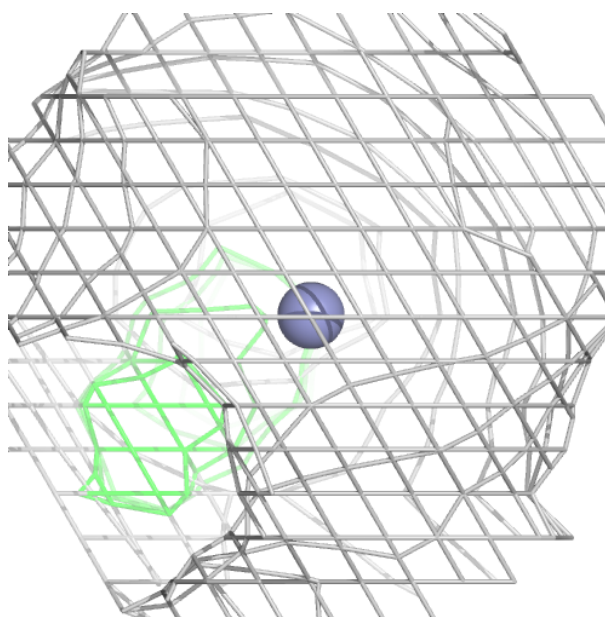
**Electron density around ZN A 419:**

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



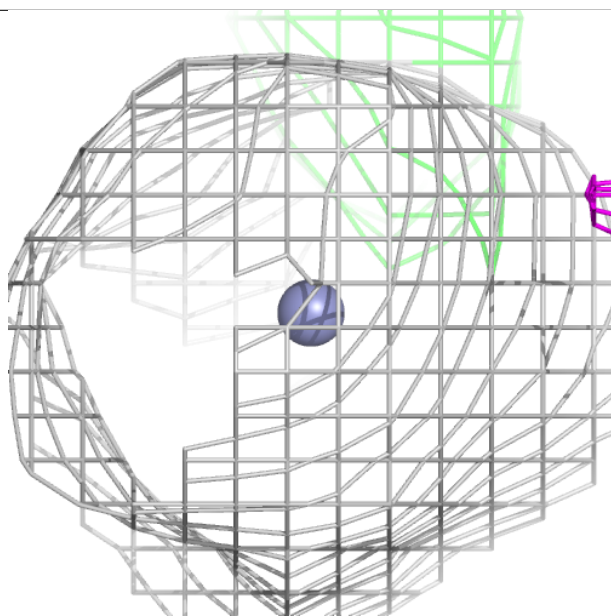
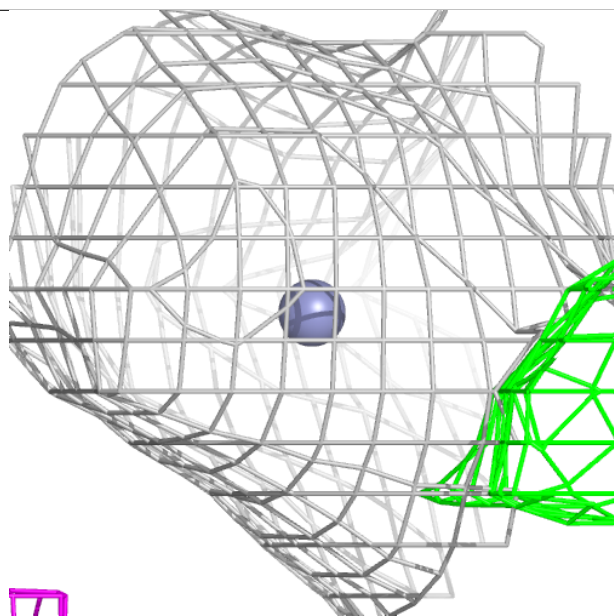
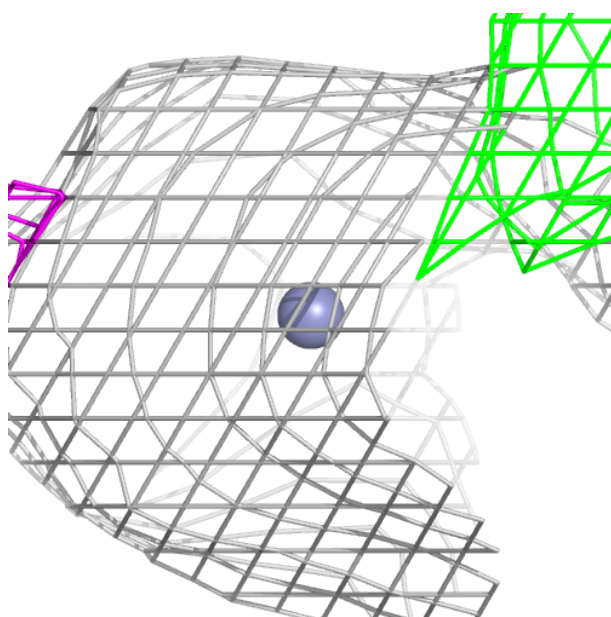
**Electron density around ZN B 412:**

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



**Electron density around ZN B 413:**

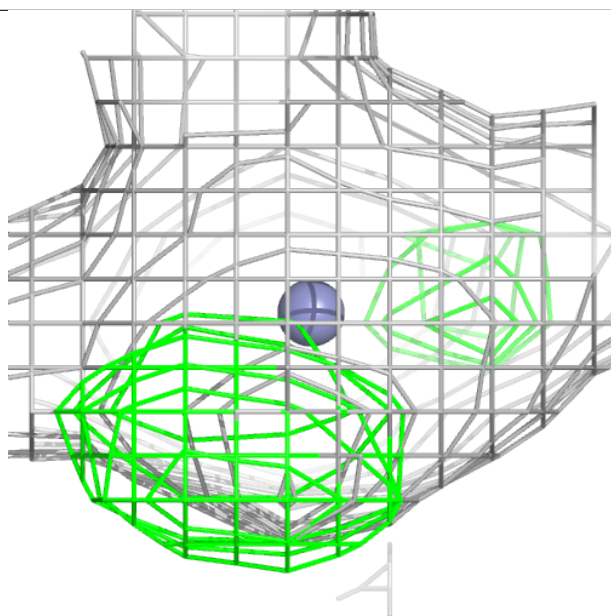
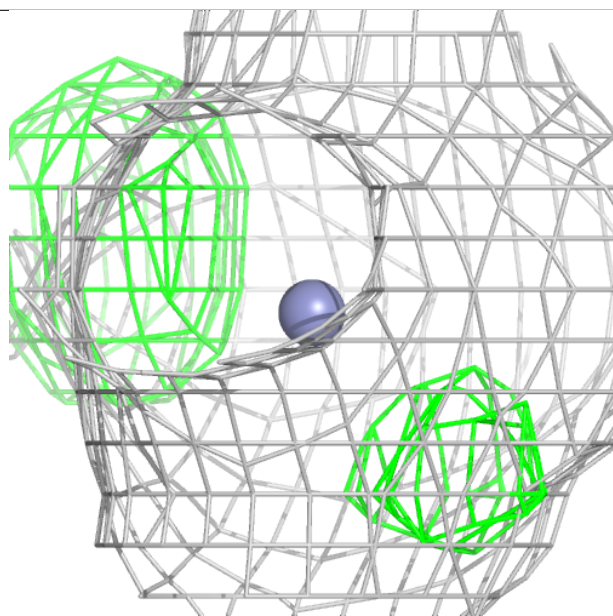
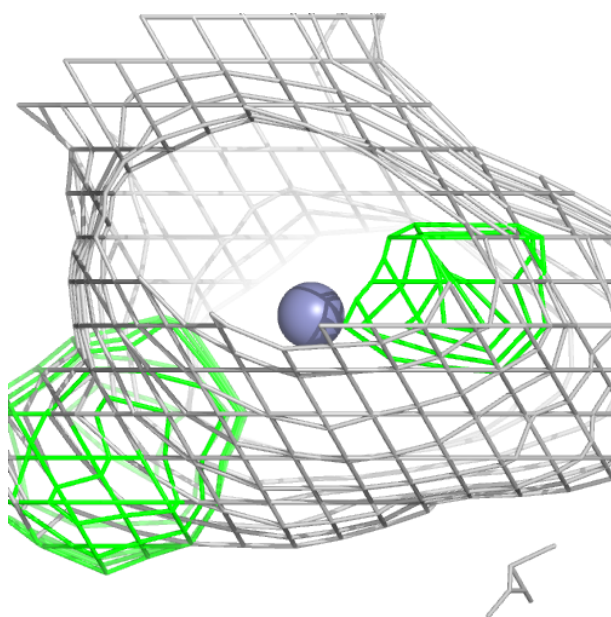
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





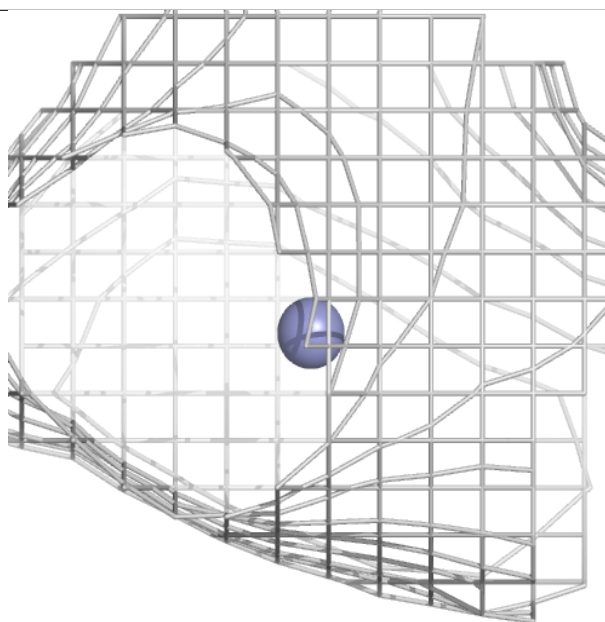
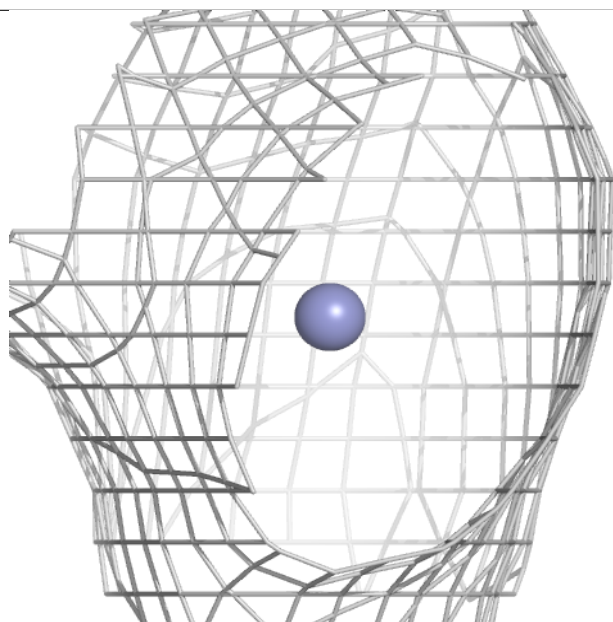
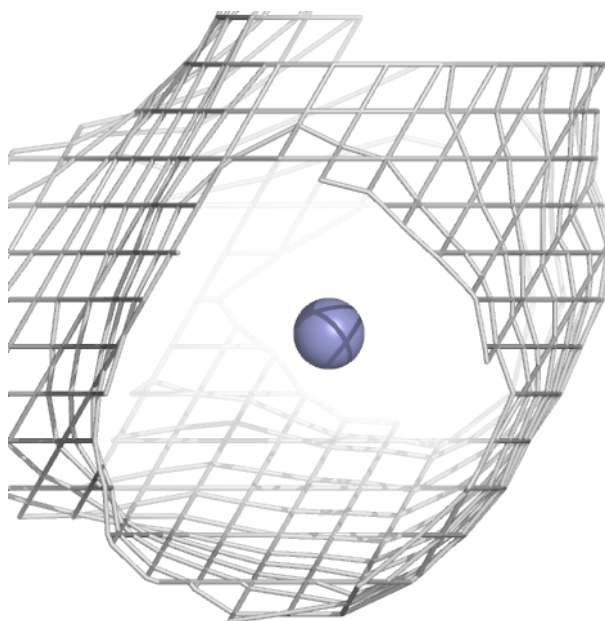
**Electron density around ZN B 414:**

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



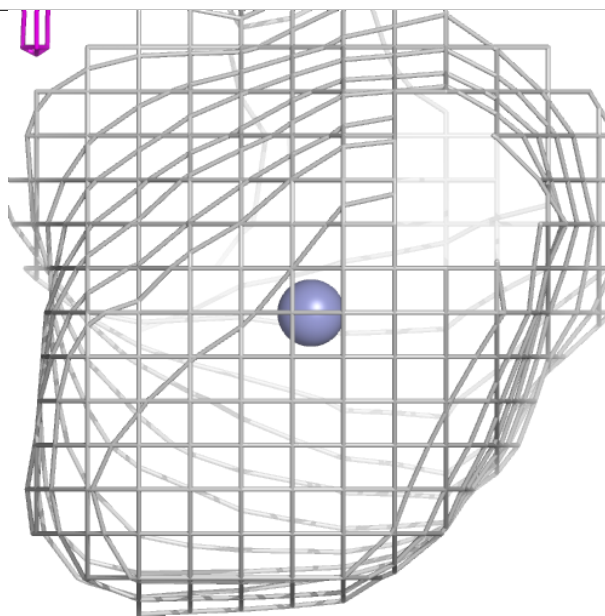
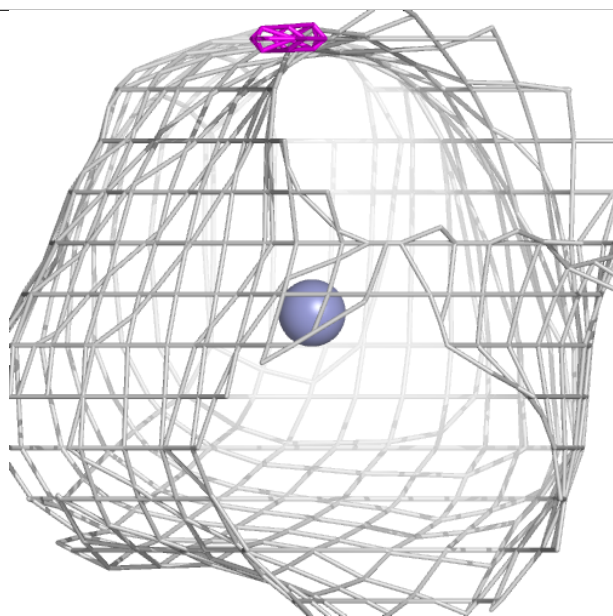
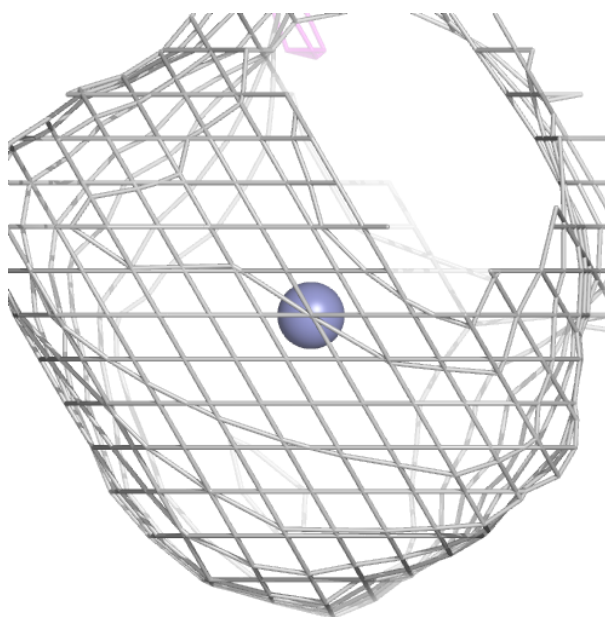
**Electron density around ZN B 415:**

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



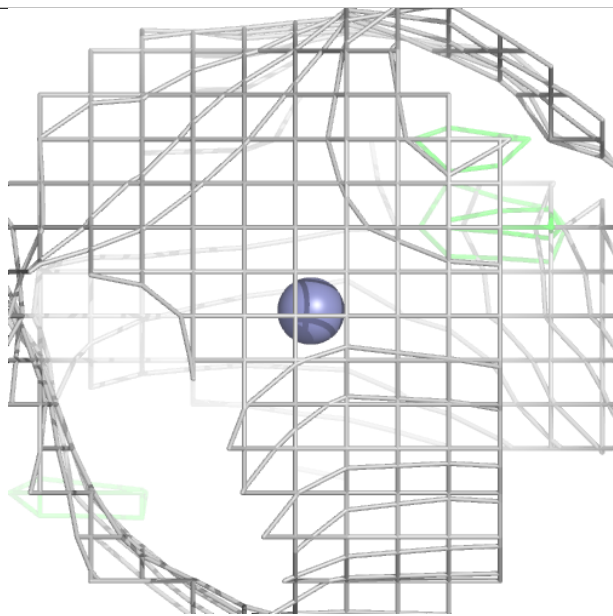
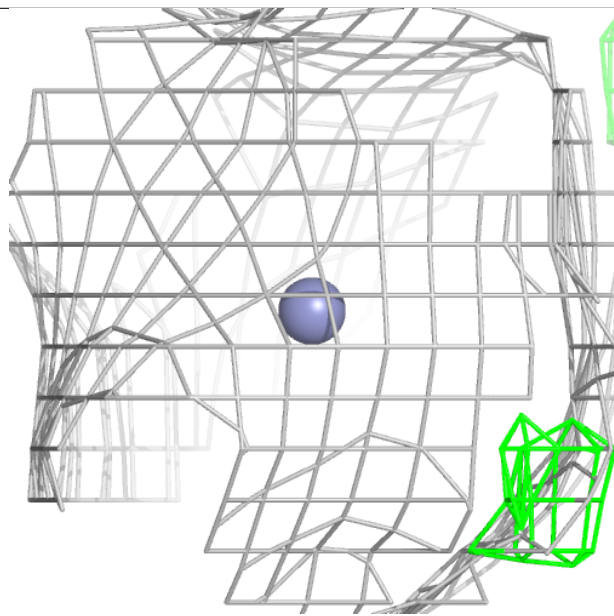
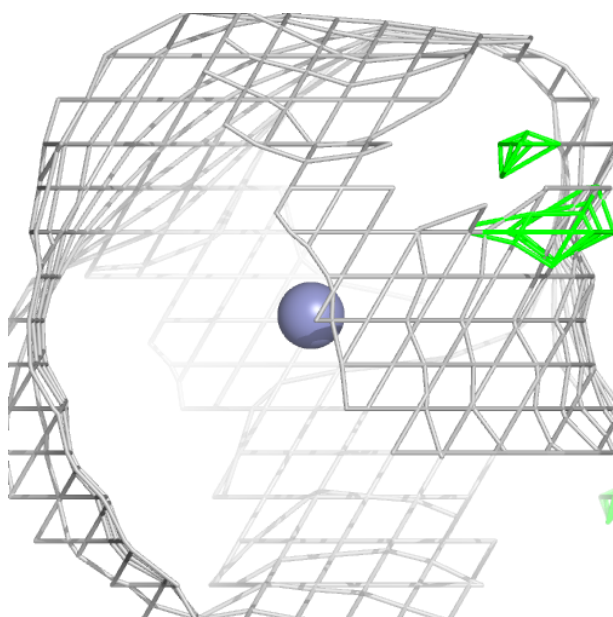
**Electron density around ZN A 413:**

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



**Electron density around ZN A 418:**

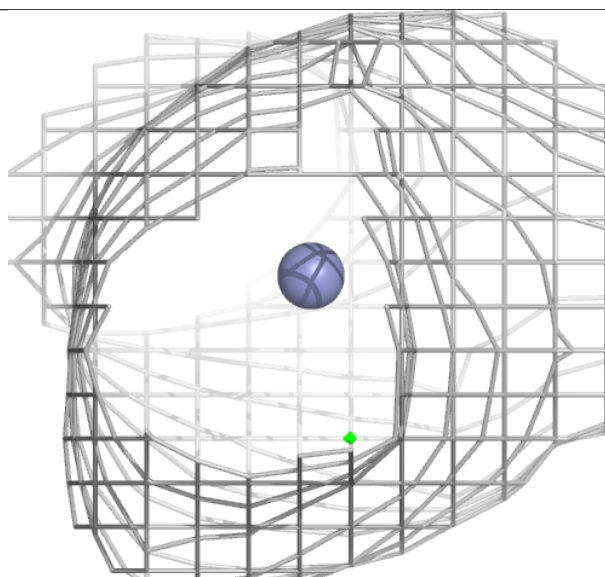
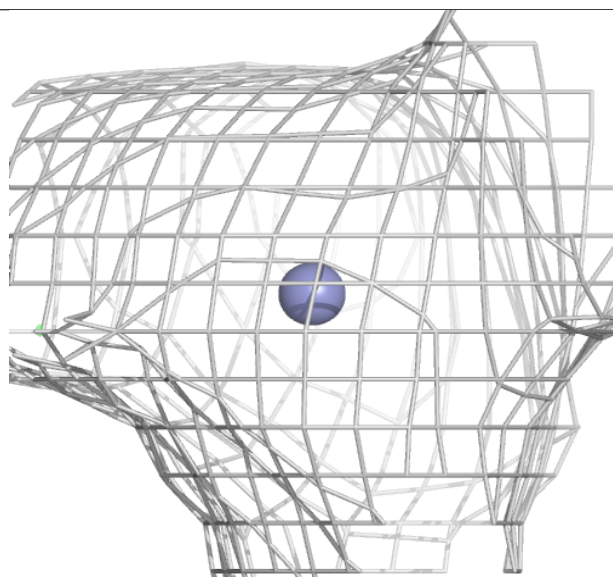
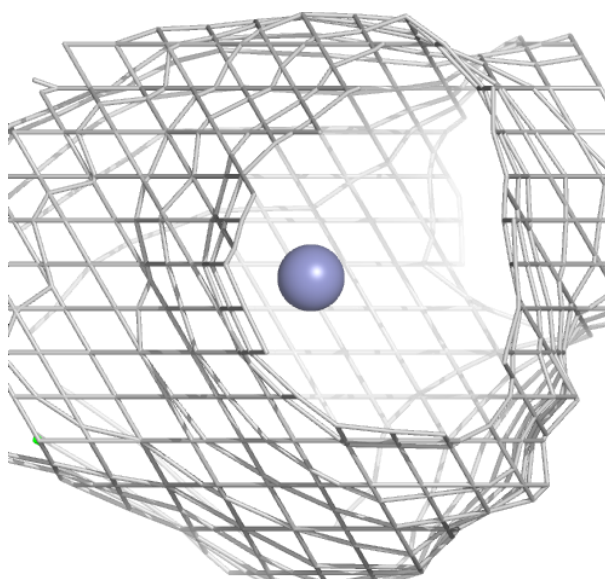
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





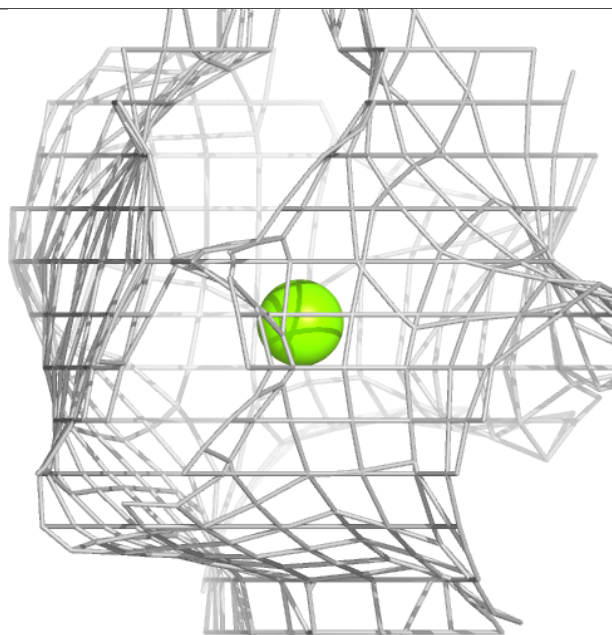
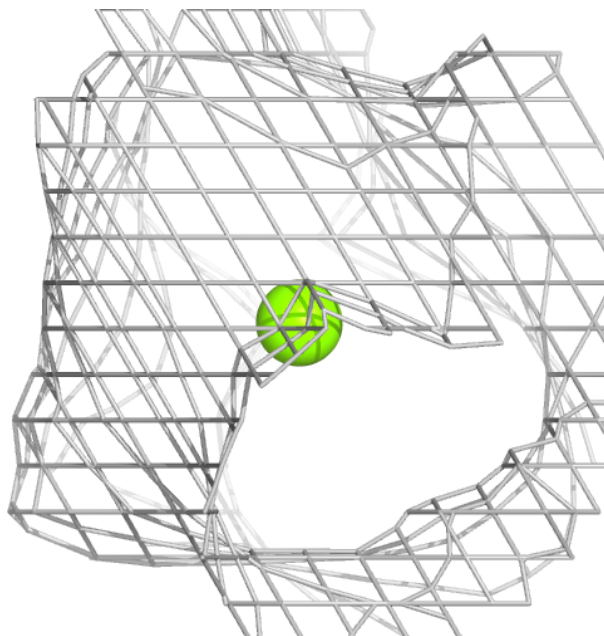
**Electron density around ZN A 415:**

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



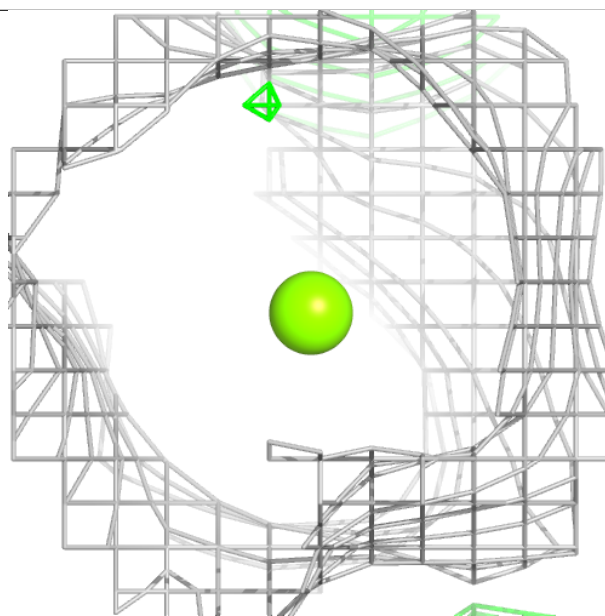
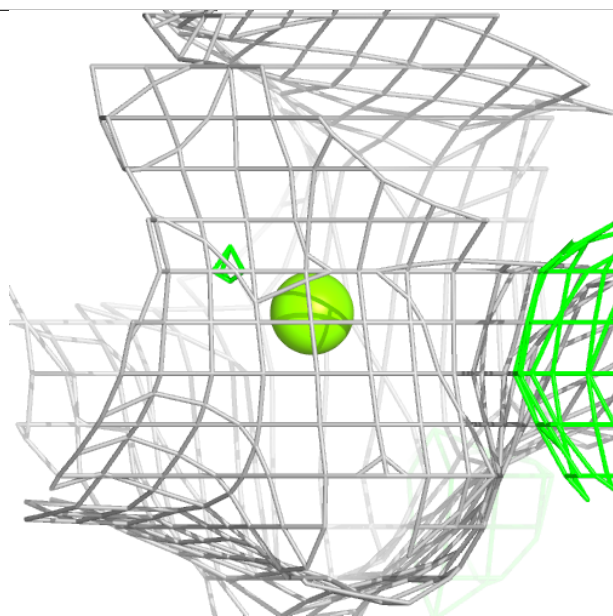
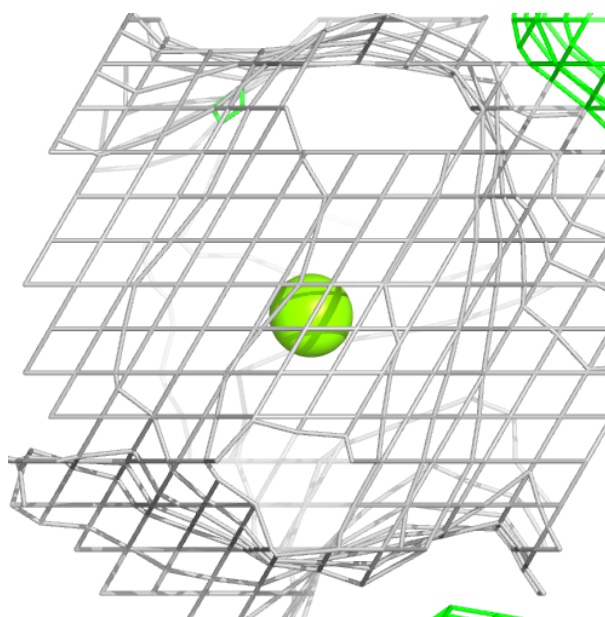
**Electron density around MG A 421:**

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



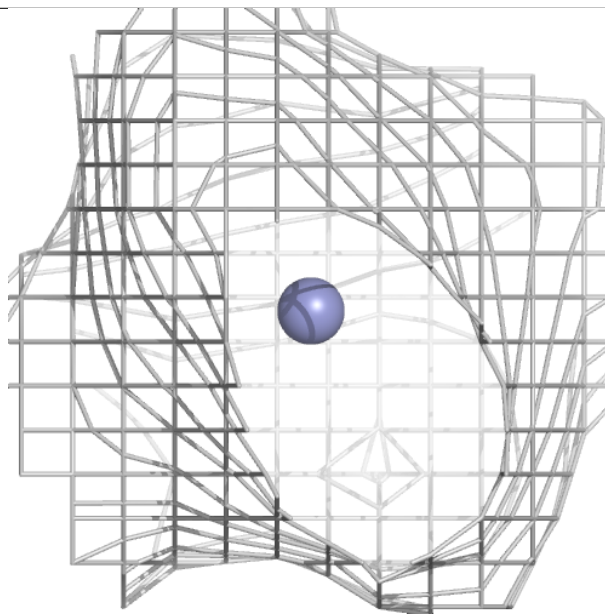
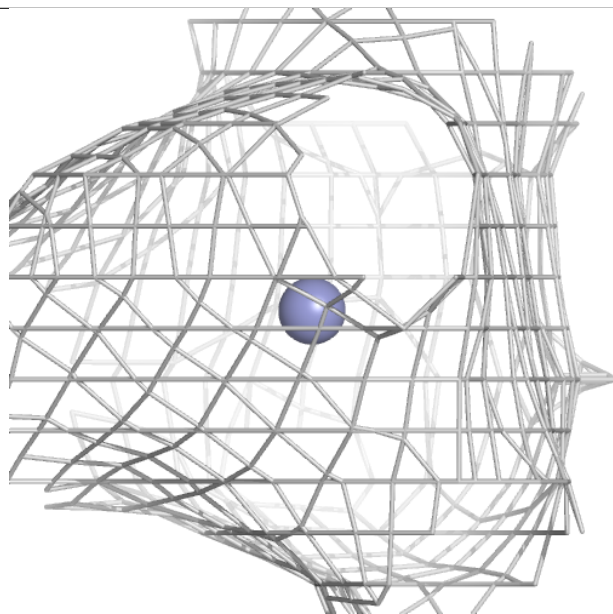
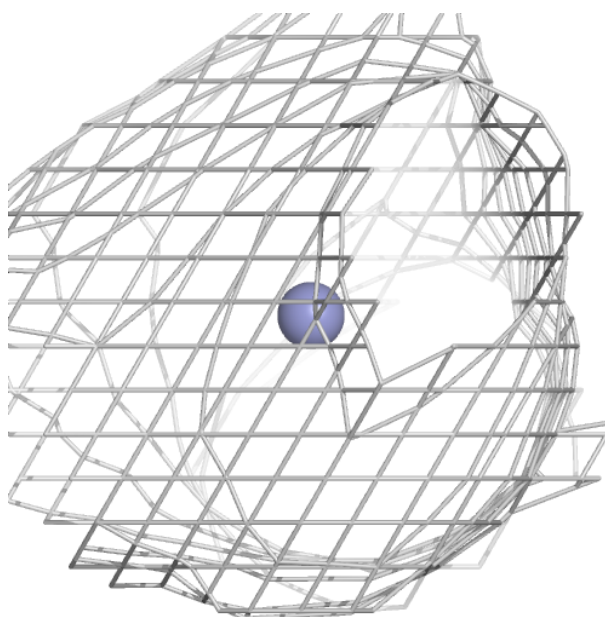
**Electron density around MG B 417:**

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



**Electron density around ZN A 414:**

$2mF_o-DF_c$  (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.