



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 11:07 PM UTC

PDB ID : 9RG1 / pdb\_00009rg1  
Title : Unspecific peroxygenase from *Psathyrella aberdarensis*, Grogu variant, in complex with alpha-ionone  
Authors : Fernandez-Garcia, A.; Sanz-Aparicio, J.  
Deposited on : 2025-06-05  
Resolution : 1.85 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

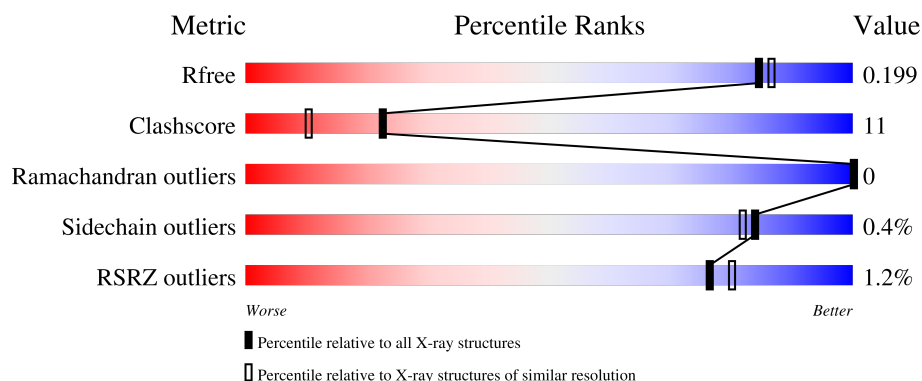
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 style="width: 94%;"></div> <div style="width: 6%;"></div> </div>
1	B	334	<div> <div style="width: 90%;"></div> <div style="width: 10%;"></div> </div>
2	G	3	<div> <div style="width: 33%;"></div> <div style="width: 67%;"></div> </div>
2	U	3	<div> <div style="width: 33%;"></div> <div style="width: 33%;"></div> <div style="width: 33%;"></div> </div>
3	H	2	<div> <div style="width: 50%;"></div> <div style="width: 50%;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	f	2	 100%

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
13	GOL	B	406	-	-	X	-
3	NAG	H	2	-	-	X	-
5	MES	A	409	-	-	X	-
7	A1IUB	B	404	-	-	X	-
9	EOH	B	408	-	-	X	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 6373 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.

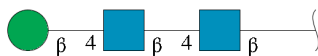
- Molecule 1 is a protein called Heme-thiolate peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	2	0
			2601	1661	439	494	7			
1	B	334	Total	C	N	O	S	0	2	0
			2597	1659	436	495	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 beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

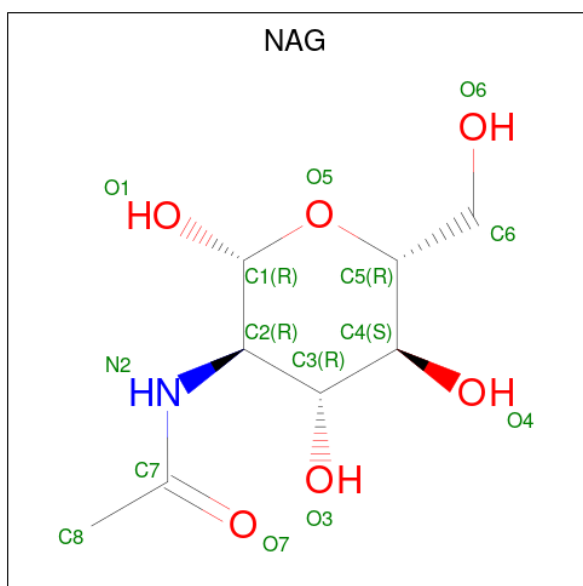
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





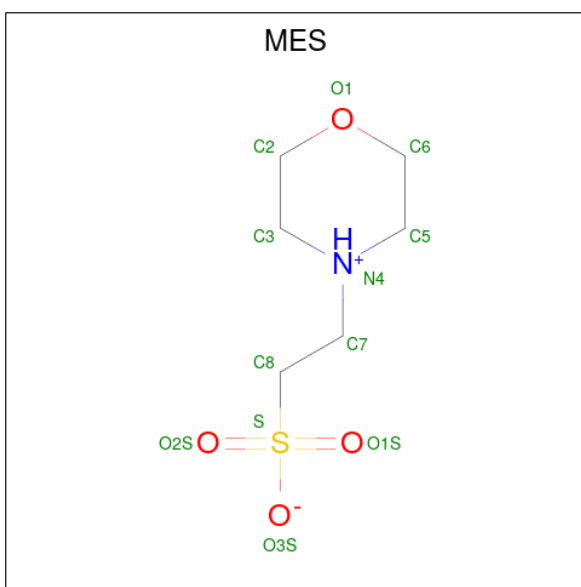
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	f	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



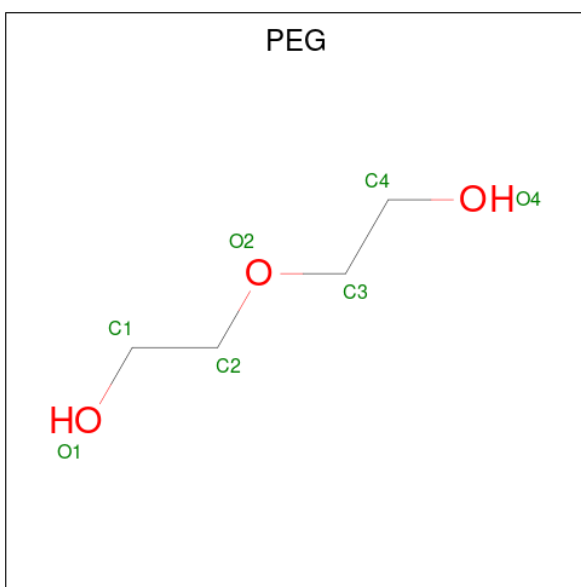
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



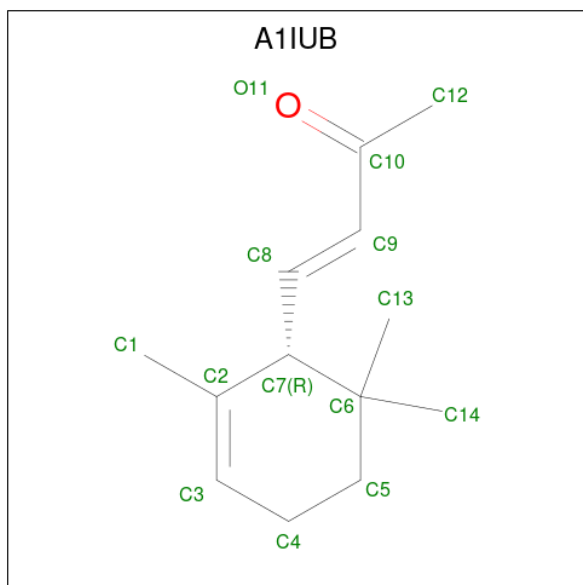
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 7 is alpha-ionone (CCD ID: A1IUB) (formula:  $C_{13}H_{20}O$ ) (labeled as "Ligand of Interest" by depositor).



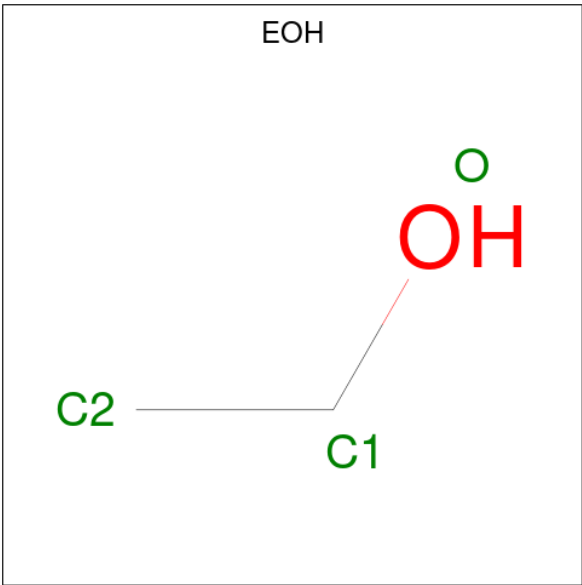
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			14	13	1		
7	B	1	Total	C	O	0	0
			14	13	1		
7	B	1	Total	C	O	0	0
			14	13	1		

- Molecule 8 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
8	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
8	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 9 is ETHANOL (CCD ID: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



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

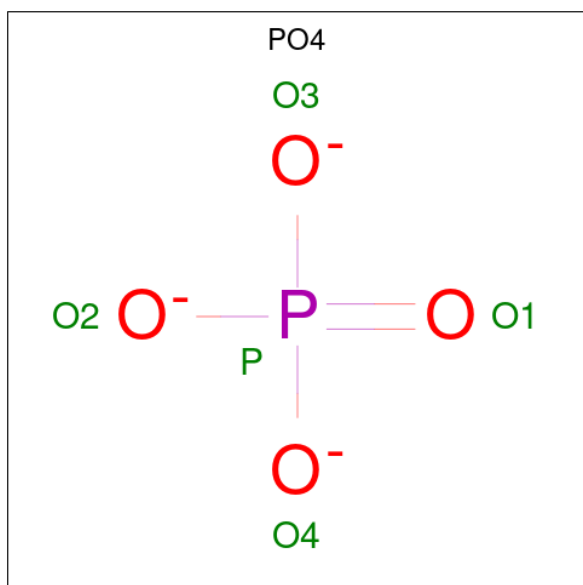
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	8	Total	Zn	0	0
			8	8		
10	B	6	Total	Zn	0	0
			6	6		

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	357	Total	O	0	0
			357	357		
14	B	415	Total	O	0	0
			415	415		

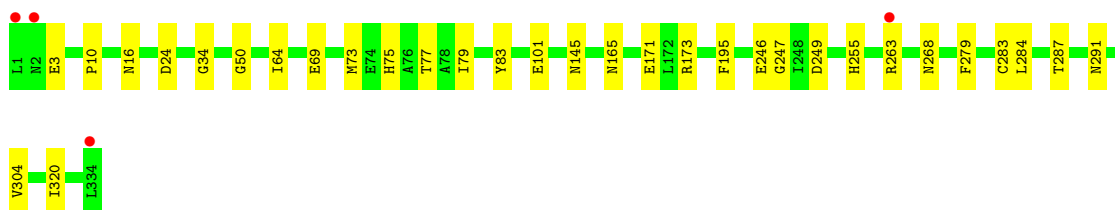
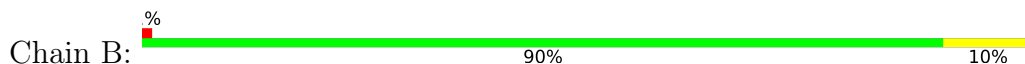
### 3 Residue-property plots

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



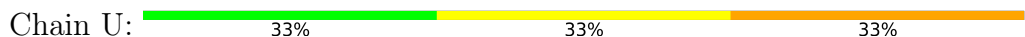
- Molecule 1: Heme-thiolate peroxidase



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



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



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



MAG1  
MAG2

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

Chain f:

100%

MAG1  
MAG2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.59Å 76.59Å 271.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 1.85 47.52 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.52-1.85) 99.9 (47.52-1.85)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.161 , 0.191 0.171 , 0.199	Depositor DCC
$R_{free}$ test set	3895 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: HEM, NAG, A1IUB, EOH, PEG, PO4, MES, MG, ZN, BMA, 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	0.51	0/2683	0.88	1/3658 (0.0%)
1	B	0.51	0/2679	0.87	0/3654
All	All	0.51	0/5362	0.88	1/7312 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLU	CB-CA-C	-5.72	101.12	110.85

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	2601	0	2464	36	0
1	B	2597	0	2458	55	0
2	G	39	0	34	3	0
2	U	39	0	34	4	0
3	H	28	0	25	17	0
3	f	28	0	25	4	0
4	A	28	0	26	8	0
4	B	14	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	24	0	26	21	0
5	B	12	0	13	0	0
6	A	14	0	20	1	0
7	A	14	0	0	0	0
7	B	28	0	0	9	0
8	A	43	0	30	4	0
8	B	43	0	30	3	0
9	A	3	0	6	1	0
9	B	3	0	6	3	0
10	A	8	0	0	0	1
10	B	6	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	10	0	0	1	0
12	B	5	0	0	0	0
13	B	12	0	16	6	0
14	A	357	0	0	10	0
14	B	415	0	0	19	1
All	All	6373	0	5226	114	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 11.

The worst 5 of 114 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:16:ASN:HD21	4:A:402:NAG:C1	1.01	1.57
1:A:291:ASN:HD21	4:A:401:NAG:C1	0.93	1.55
1:B:165:ASN:HD21	2:U:1:NAG:C1	0.92	1.53
1:B:145:ASN:ND2	3:f:1:NAG:C1	1.71	1.53
1:B:16:ASN:ND2	4:B:401:NAG:C1	1.72	1.53

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)
10:A:410:ZN:ZN	14:B:510:HOH:O[6_444]	1.33	0.87

## 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%)	11 (3%)	0	100	100
1	B	334/334 (100%)	321 (96%)	13 (4%)	0	100	100
All	All	668/668 (100%)	644 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	275 (100%)	1 (0%)	84	82
1	B	276/274 (101%)	275 (100%)	1 (0%)	84	82
All	All	552/548 (101%)	550 (100%)	2 (0%)	84	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ARG
1	B	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN

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Mol	Chain	Res	Type
1	B	33	GLN
1	B	234	GLN
1	B	165	ASN
1	A	234	GLN

### 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 ⓘ

10 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	G	1	2	14,14,15	0.37	0	17,19,21	0.76	0
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	1.12	2 (11%)
2	BMA	G	3	2	11,11,12	0.52	0	15,15,17	0.58	0
3	NAG	H	1	3,1	14,14,15	0.37	0	17,19,21	0.81	0
3	NAG	H	2	3	14,14,15	0.42	0	17,19,21	0.90	1 (5%)
2	NAG	U	1	2	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
2	NAG	U	2	2	14,14,15	0.35	0	17,19,21	0.54	0
2	BMA	U	3	2	11,11,12	0.60	0	15,15,17	0.92	1 (6%)
3	NAG	f	1	3	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
3	NAG	f	2	3	14,14,15	0.29	0	17,19,21	0.78	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
2	NAG	U	1	2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	BMA	U	3	2	-	0/2/19/22	0/1/1/1
3	NAG	f	1	3	-	0/6/23/26	0/1/1/1
3	NAG	f	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C1-C2-N2	2.95	115.08	110.43
2	U	3	BMA	C1-O5-C5	2.87	116.04	112.19
2	G	2	NAG	C1-C2-N2	2.65	114.61	110.43
2	U	1	NAG	O5-C1-C2	2.55	115.24	111.29
3	f	1	NAG	O4-C4-C3	-2.37	104.79	110.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

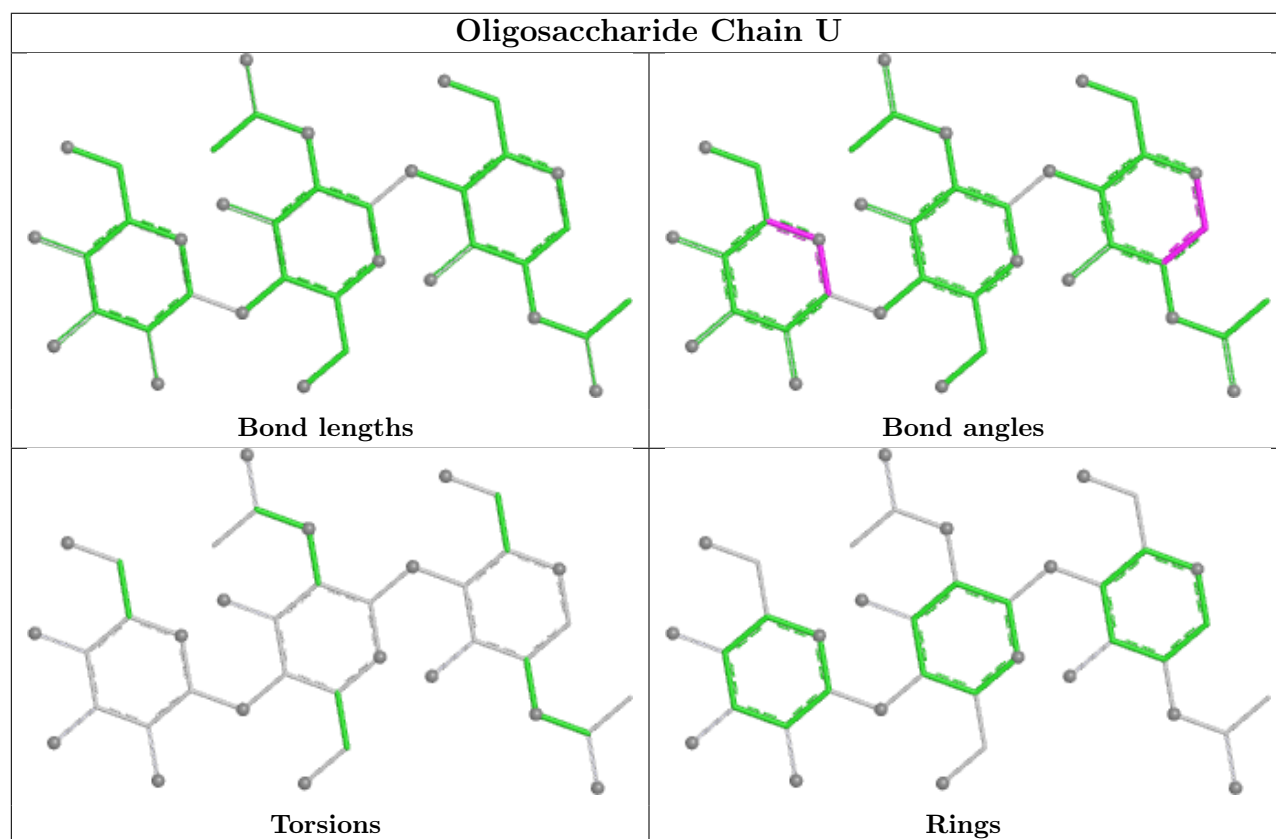
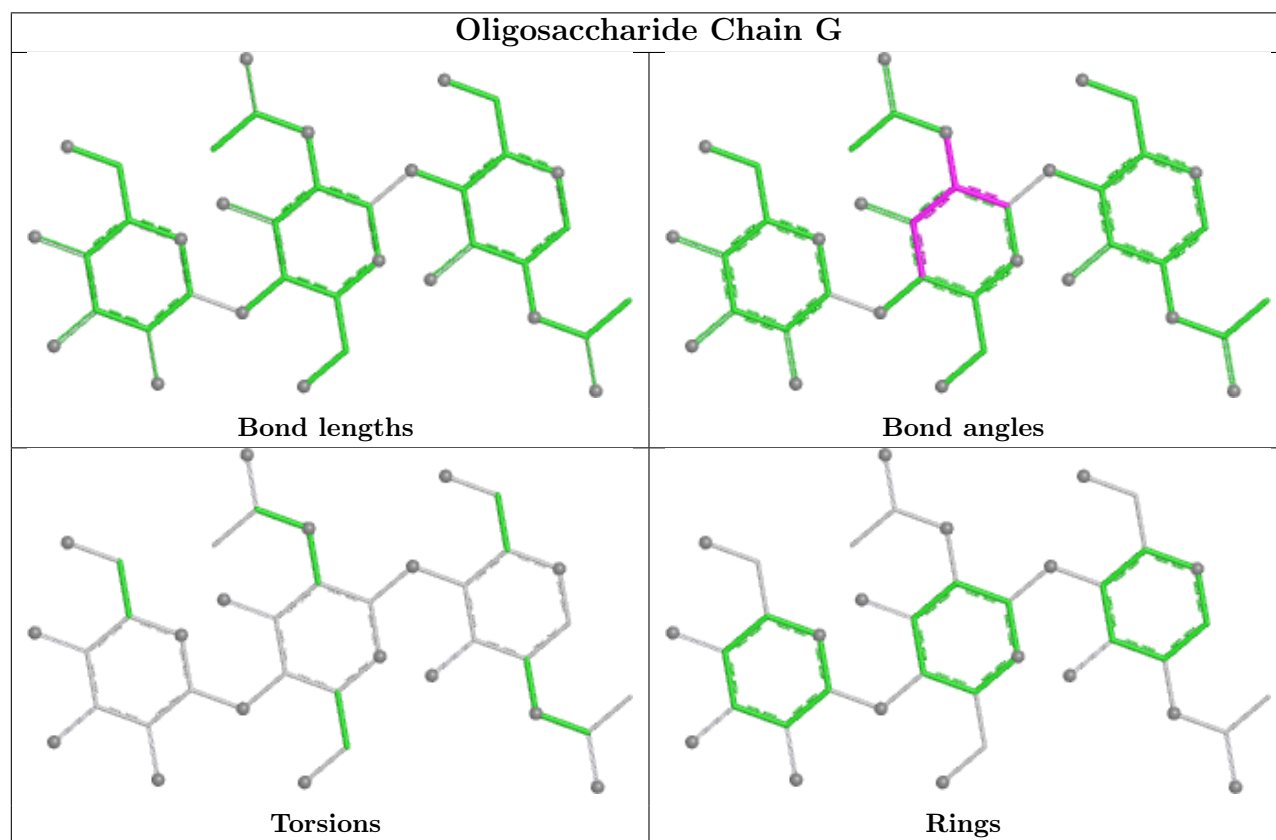
Mol	Chain	Res	Type	Atoms
3	f	2	NAG	C1-C2-N2-C7
3	f	2	NAG	C8-C7-N2-C2
3	f	2	NAG	O7-C7-N2-C2

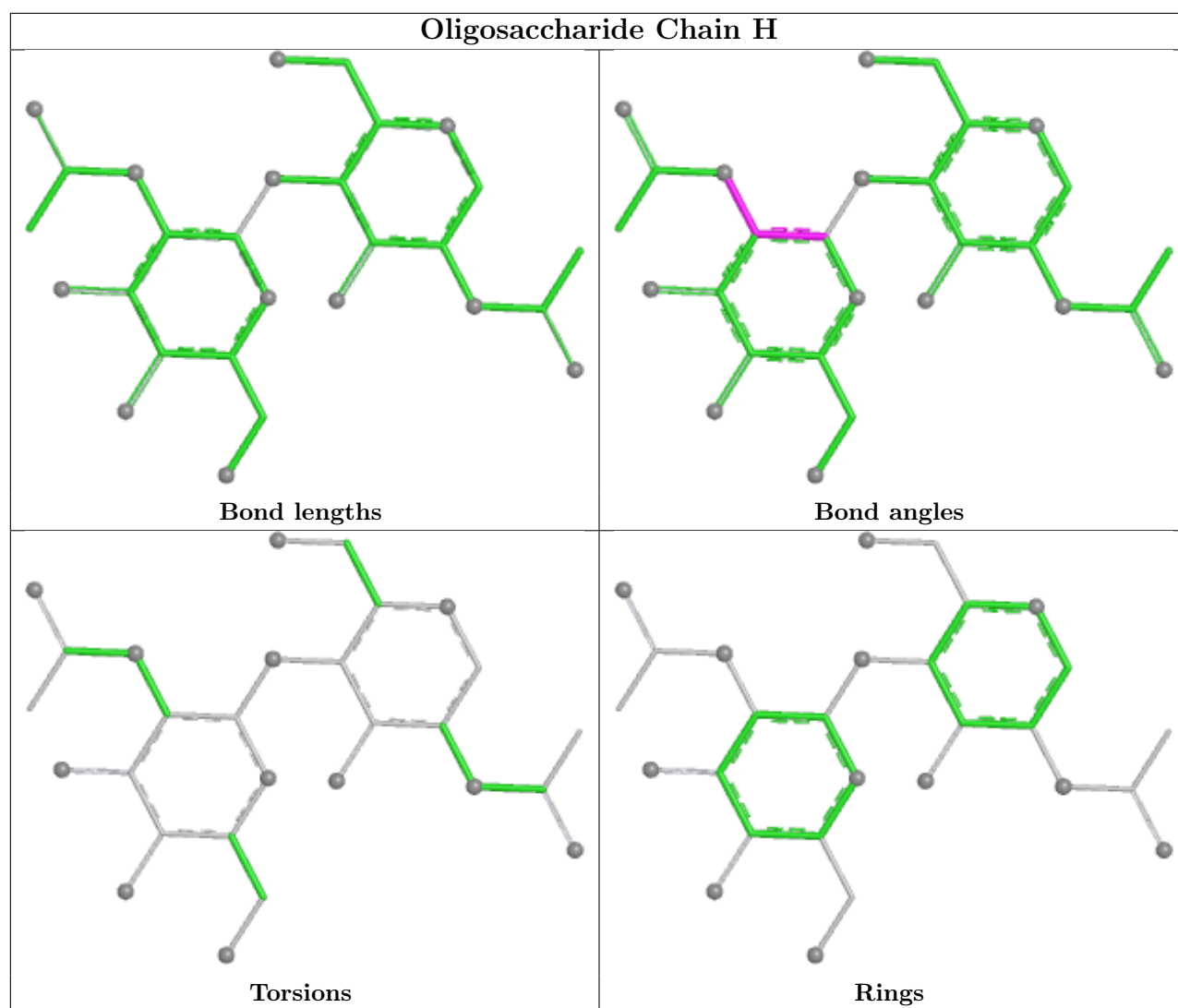
There are no ring outliers.

6 monomers are involved in 28 short contacts:

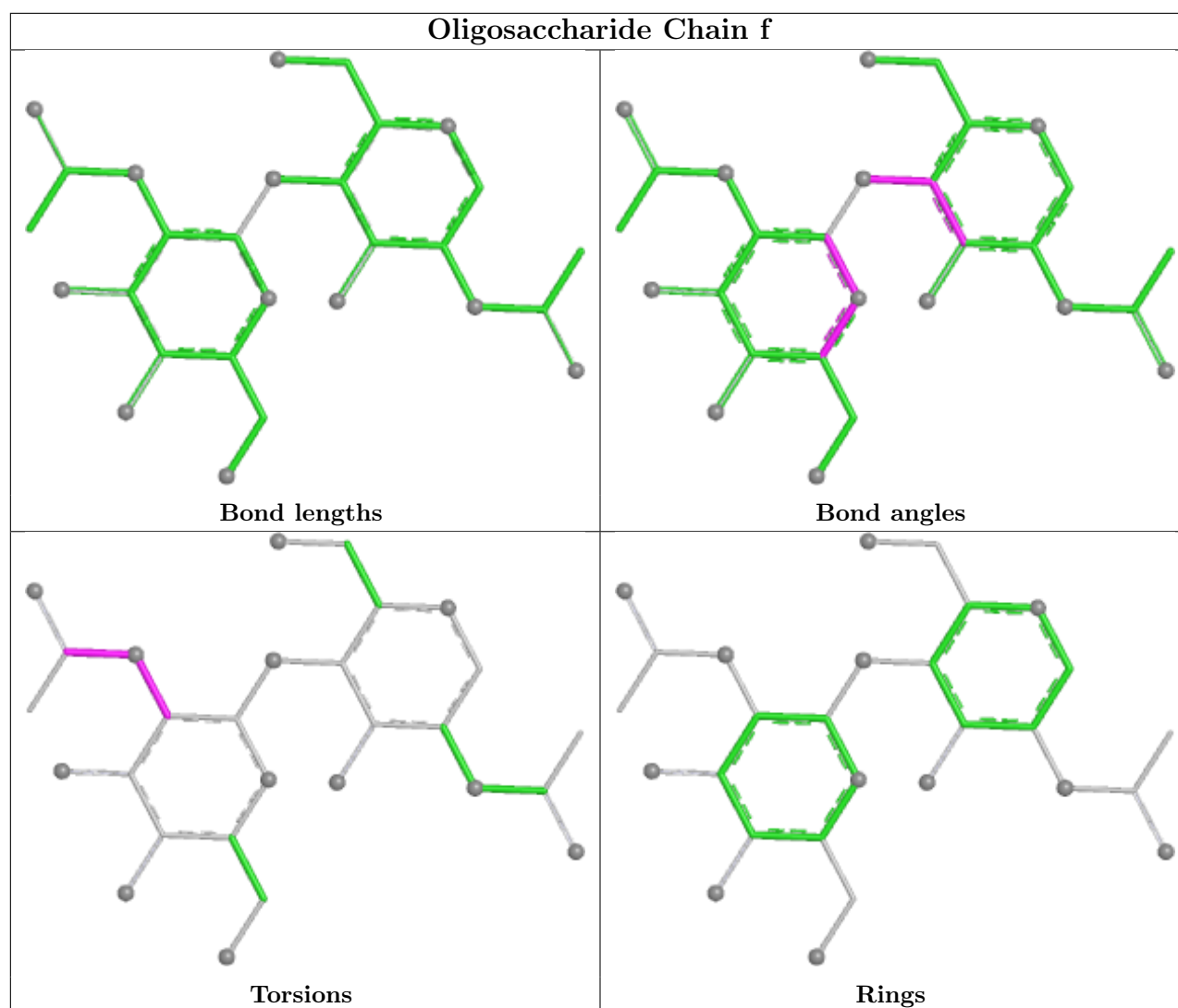
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	3	0
3	f	1	NAG	4	0
3	H	1	NAG	1	0
3	H	2	NAG	16	0
3	f	2	NAG	2	0
2	U	1	NAG	4	0

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 36 ligands modelled in this entry, 16 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	$\# Z  > 2$
4	NAG	B	401	-	14,14,15	0.29	0	17,19,21	0.68	0
7	A1IUB	B	404	-	13,14,14	1.07	1 (7%)	15,20,20	1.29	2 (13%)
12	PO4	A	420	-	4,4,4	0.64	0	6,6,6	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	PO4	A	419	-	4,4,4	1.10	1 (25%)	6,6,6	0.50	0
4	NAG	A	401	-	14,14,15	0.34	0	17,19,21	1.34	3 (17%)
7	A1IUB	B	403	-	13,14,14	0.76	1 (7%)	15,20,20	1.02	2 (13%)
12	PO4	B	416	-	4,4,4	1.08	1 (25%)	6,6,6	0.58	0
8	HEM	A	406	14,1,11	50,50,50	1.49	6 (12%)	67,82,82	1.54	11 (16%)
9	EOH	A	407	-	2,2,2	0.11	0	1,1,1	0.15	0
5	MES	A	409	-	12,12,12	0.71	0	15,16,16	0.70	0
5	MES	B	402	-	12,12,12	0.77	0	15,16,16	0.77	1 (6%)
8	HEM	B	407	14,1,11	50,50,50	1.42	7 (14%)	67,82,82	1.59	13 (19%)
6	PEG	A	408	-	6,6,6	0.25	0	5,5,5	0.15	0
5	MES	A	403	-	12,12,12	0.80	0	15,16,16	1.01	1 (6%)
7	A1IUB	A	405	-	13,14,14	0.50	0	15,20,20	1.05	2 (13%)
13	GOL	B	406	-	5,5,5	0.18	0	5,5,5	0.51	0
4	NAG	A	402	-	14,14,15	0.39	0	17,19,21	0.90	0
13	GOL	B	405	-	5,5,5	0.13	0	5,5,5	0.27	0
9	EOH	B	408	-	2,2,2	0.10	0	1,1,1	0.11	0
6	PEG	A	404	-	6,6,6	0.34	0	5,5,5	0.19	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
4	NAG	B	401	-	-	0/6/23/26	0/1/1/1
5	MES	B	402	-	-	0/6/14/14	0/1/1/1
4	NAG	A	402	-	-	2/6/23/26	0/1/1/1
7	A1IUB	B	404	-	-	1/5/22/22	0/1/1/1
13	GOL	B	405	-	-	0/4/4/4	-
8	HEM	B	407	14,1,11	-	3/14/54/54	-
4	NAG	A	401	-	-	0/6/23/26	0/1/1/1
7	A1IUB	B	403	-	-	0/5/22/22	0/1/1/1
6	PEG	A	408	-	-	0/4/4/4	-
7	A1IUB	A	405	-	-	0/5/22/22	0/1/1/1
8	HEM	A	406	14,1,11	-	2/14/54/54	-
13	GOL	B	406	-	-	0/4/4/4	-
6	PEG	A	404	-	-	1/4/4/4	-
5	MES	A	403	-	-	0/6/14/14	0/1/1/1
5	MES	A	409	-	-	5/6/14/14	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	406	HEM	FE-NB	4.19	2.07	1.94
8	A	406	HEM	C1B-NB	-4.19	1.33	1.40
8	A	406	HEM	FE-NC	3.85	2.07	1.95
8	B	407	HEM	C1B-NB	-3.75	1.33	1.40
8	B	407	HEM	FE-NC	3.72	2.07	1.95

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	407	HEM	CHC-C4B-NB	4.05	128.78	124.42
8	A	406	HEM	C1B-NB-C4B	3.64	109.52	105.21
8	A	406	HEM	CHC-C4B-NB	3.54	128.24	124.42
4	A	401	NAG	O5-C1-C2	3.42	116.59	111.29
8	B	407	HEM	C1B-NB-C4B	3.30	109.11	105.21

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	409	MES	C8-C7-N4-C3
5	A	409	MES	C7-C8-S-O1S
5	A	409	MES	C7-C8-S-O3S
7	B	404	A1IUB	C7-C8-C9-C10
4	A	402	NAG	C8-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 59 short contacts:

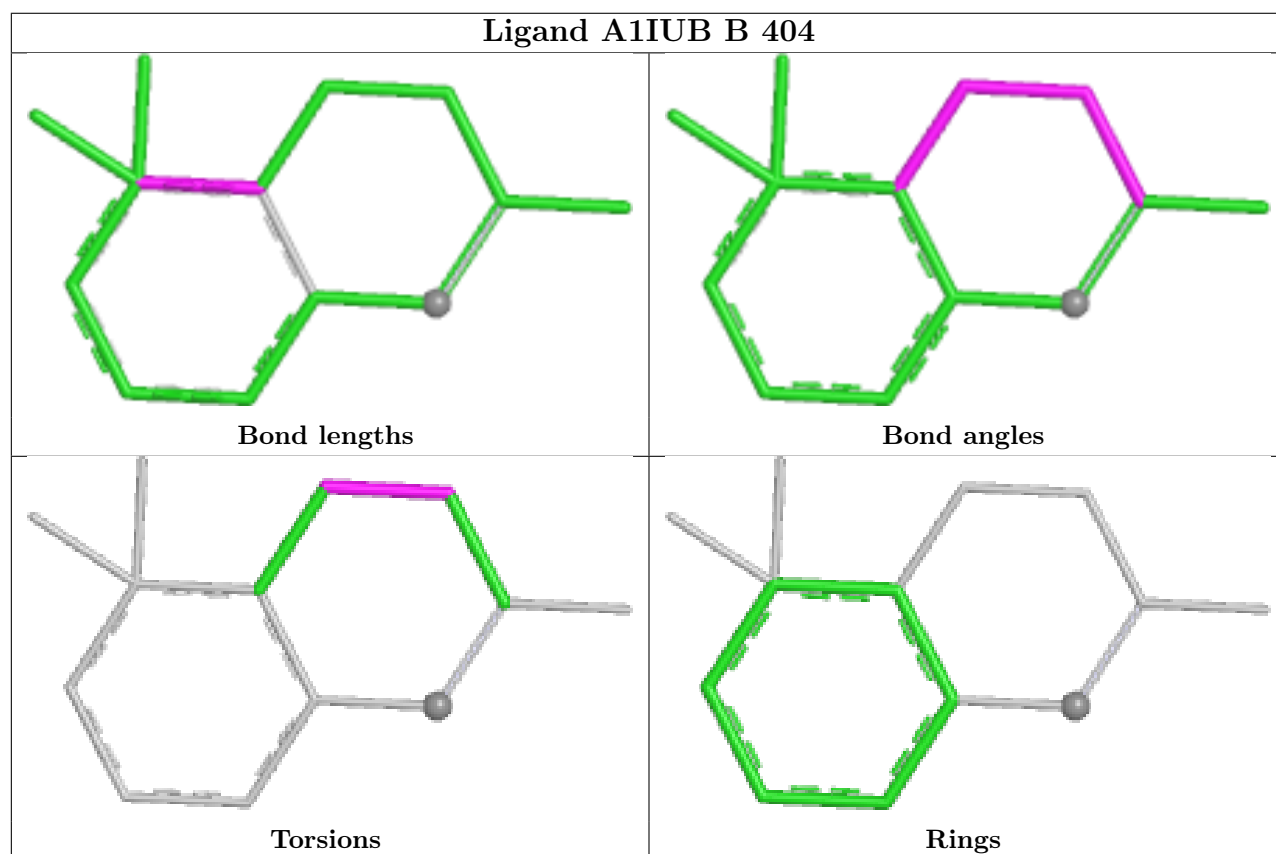
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	NAG	2	0
7	B	404	A1IUB	7	0
12	A	420	PO4	1	0
4	A	401	NAG	4	0
7	B	403	A1IUB	4	0
8	A	406	HEM	4	0
9	A	407	EOH	1	0
5	A	409	MES	21	0
8	B	407	HEM	3	0
13	B	406	GOL	6	0
4	A	402	NAG	4	0

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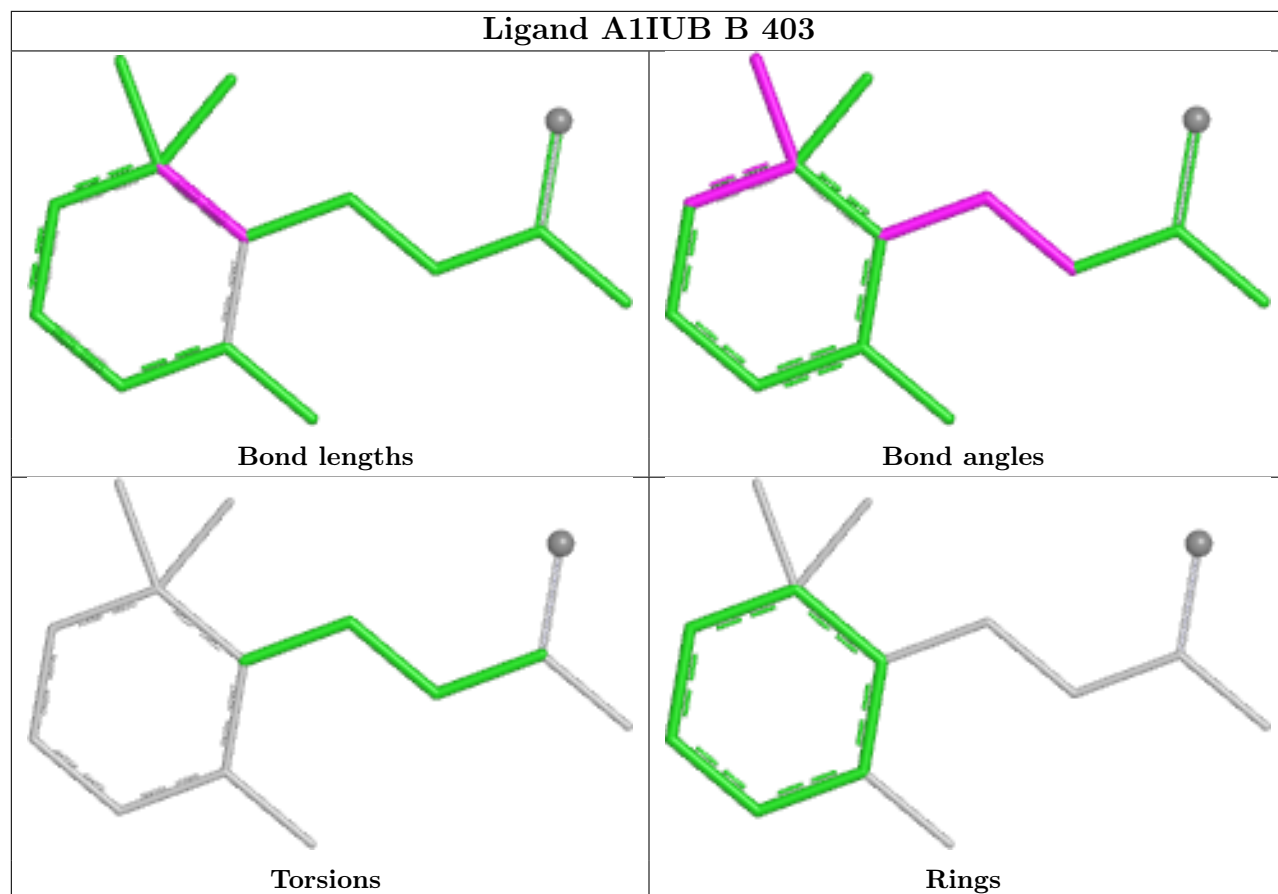
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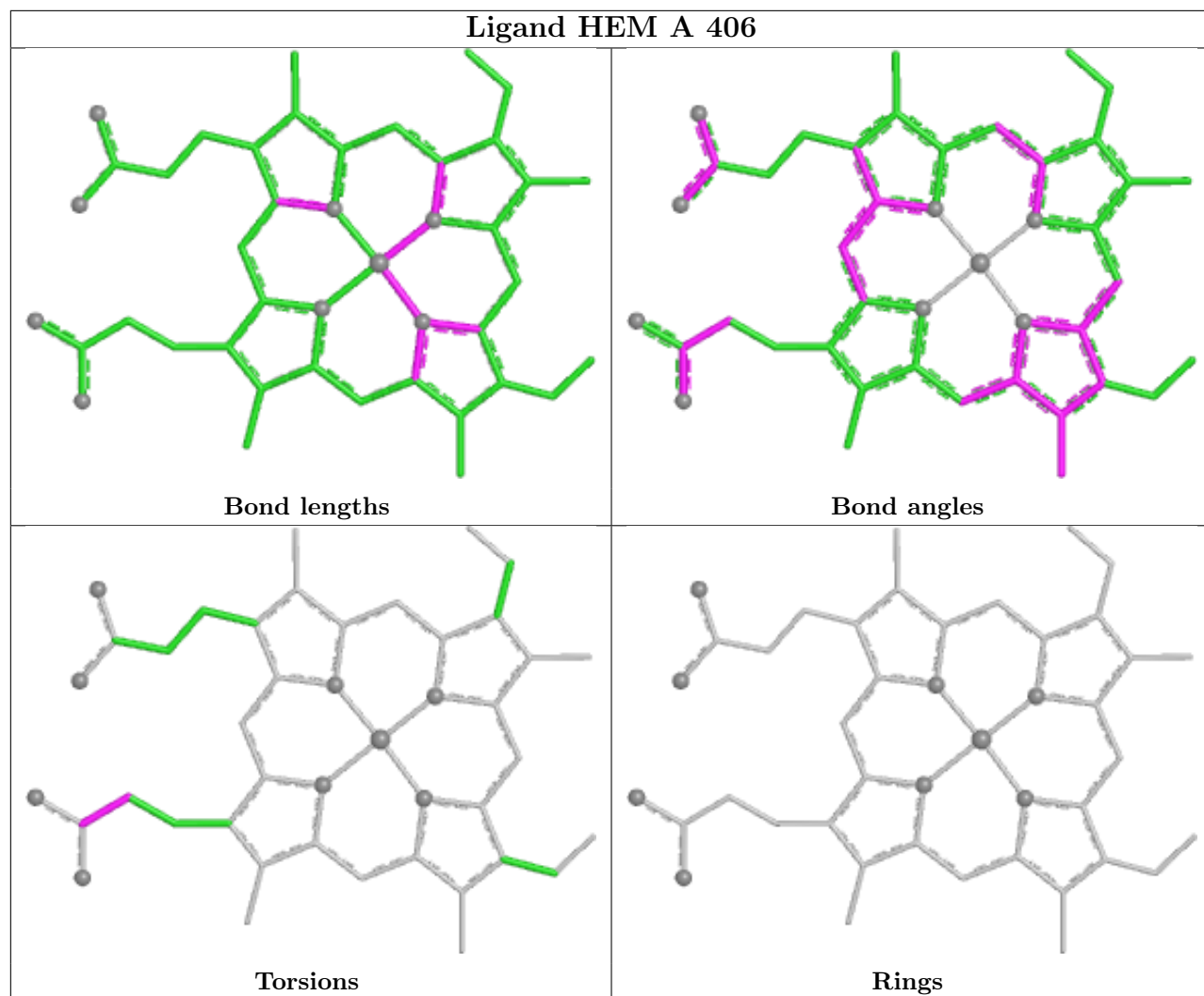
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	408	EOH	3	0
6	A	404	PEG	1	0

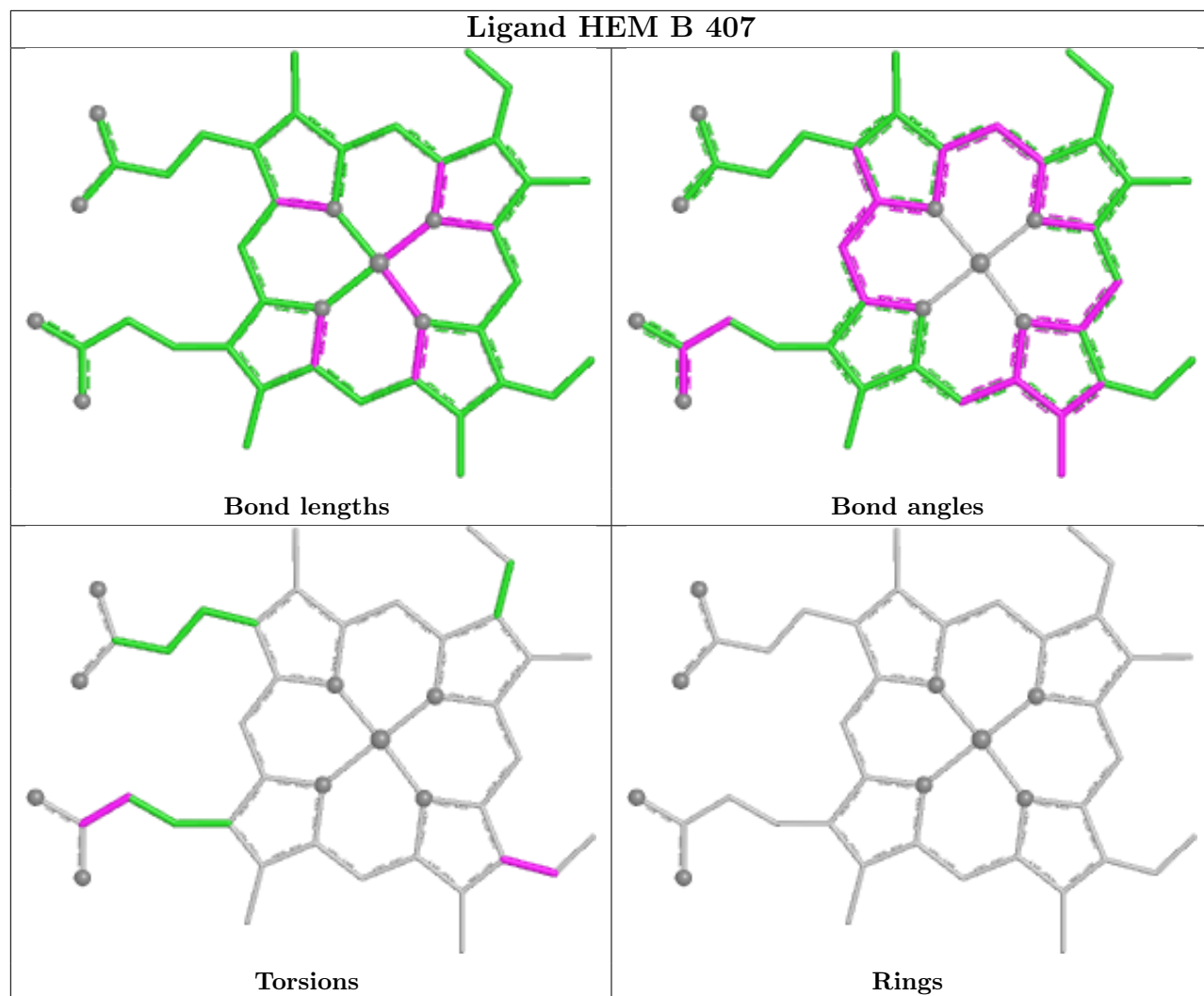
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

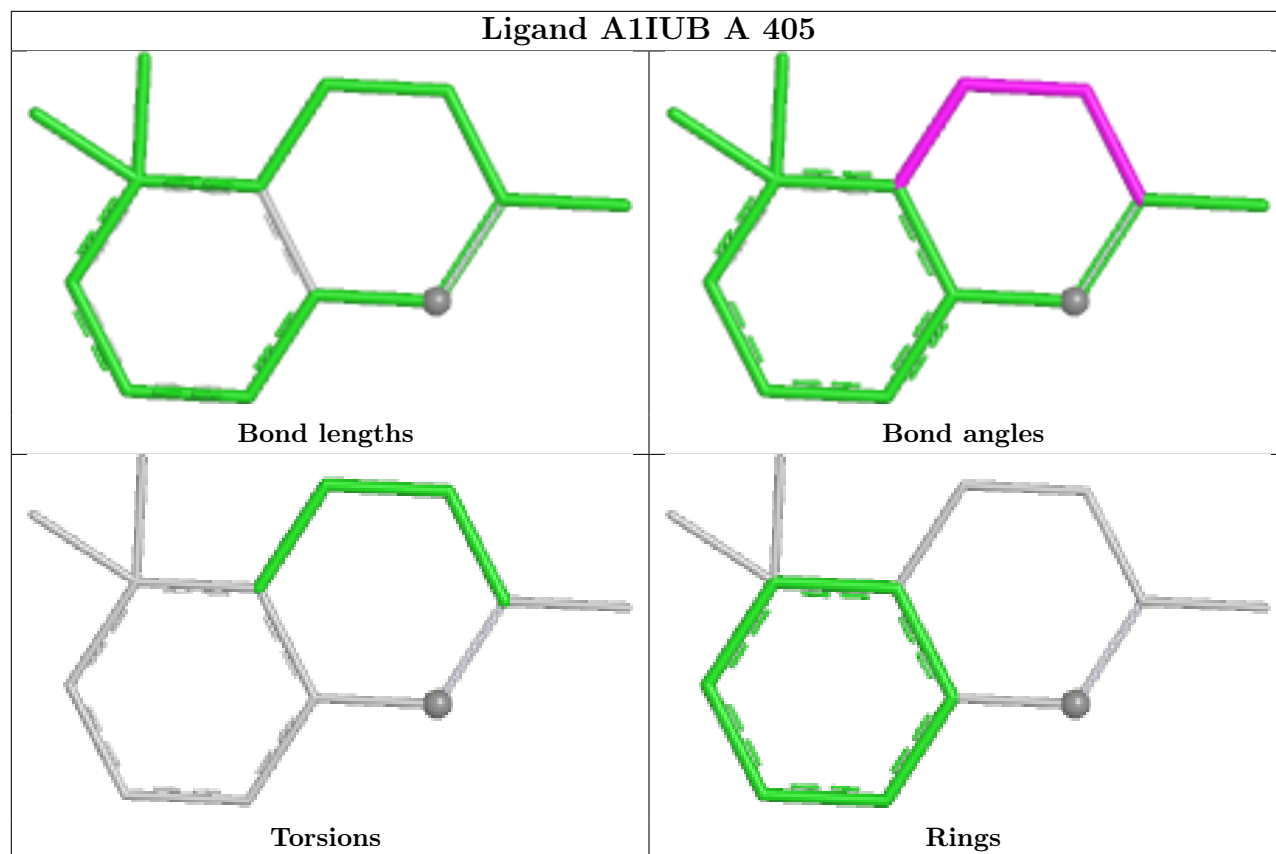


## Ligand A1IUB B 403









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.12	4 (1%) 76 80	16, 28, 42, 98	2 (0%)
1	B	334/334 (100%)	-0.00	4 (1%) 76 80	15, 30, 44, 95	2 (0%)
All	All	668/668 (100%)	-0.06	8 (1%) 76 80	15, 29, 44, 98	4 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	LEU	7.7
1	A	1	LEU	5.9
1	B	2	ASN	3.1
1	B	263	ARG	3.0
1	A	334	LEU	2.7

### 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	G	1	14/15	-	-	33,35,38,43	0
2	NAG	G	2	14/15	-	-	51,57,64,65	0
2	BMA	G	3	11/12	-	-	59,61,66,67	0
2	NAG	U	1	14/15	-	-	35,37,41,44	0
2	NAG	U	2	14/15	-	-	49,55,59,61	0

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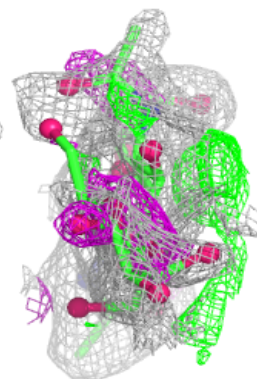
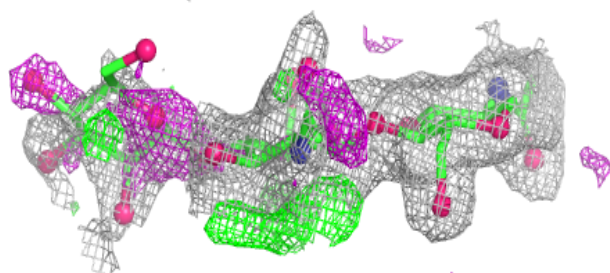
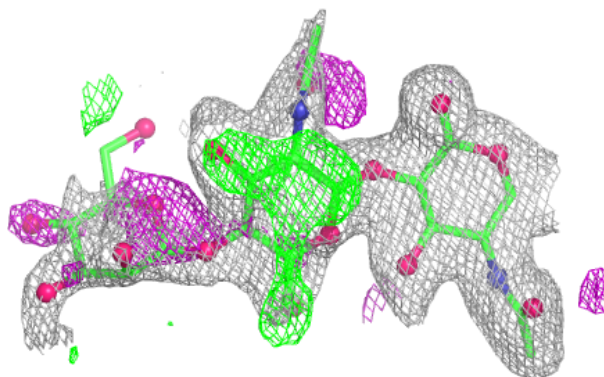
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	U	3	11/12	-	-	60,63,66,66	0
3	NAG	H	1	14/15	-	-	40,44,50,53	0
3	NAG	H	2	14/15	-	-	49,53,55,57	0
3	NAG	f	1	14/15	-	-	39,42,48,48	0
3	NAG	f	2	14/15	-	-	54,57,62,62	0

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.

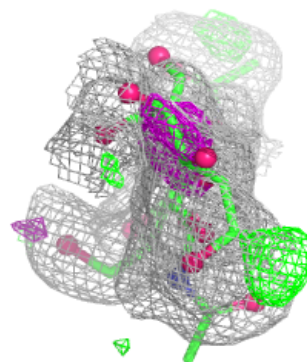
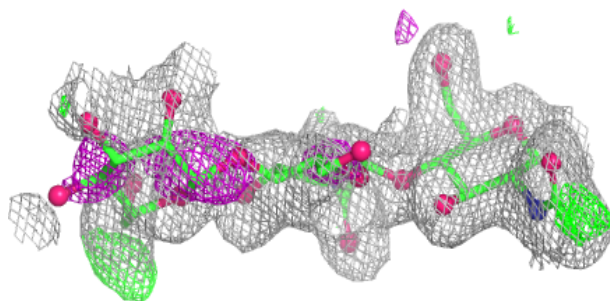
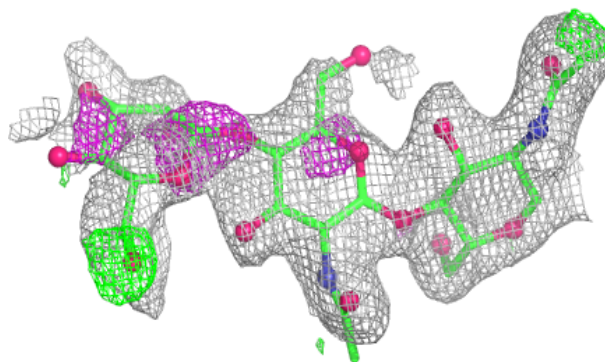
#### Electron density around Chain G:

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)



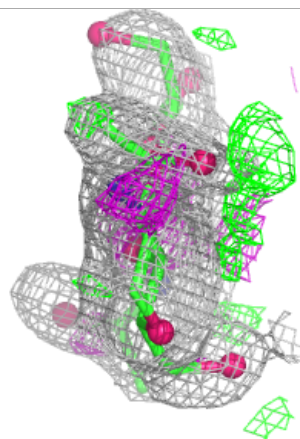
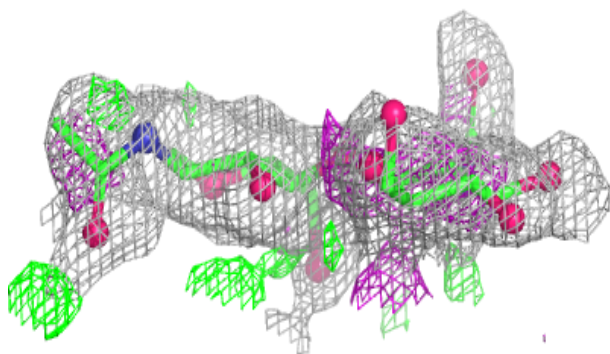
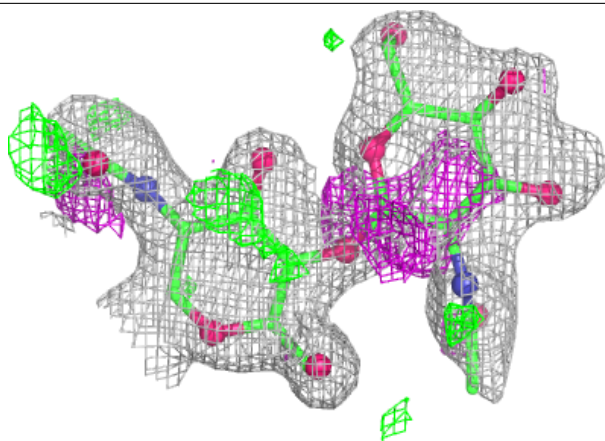
**Electron density around Chain U:**

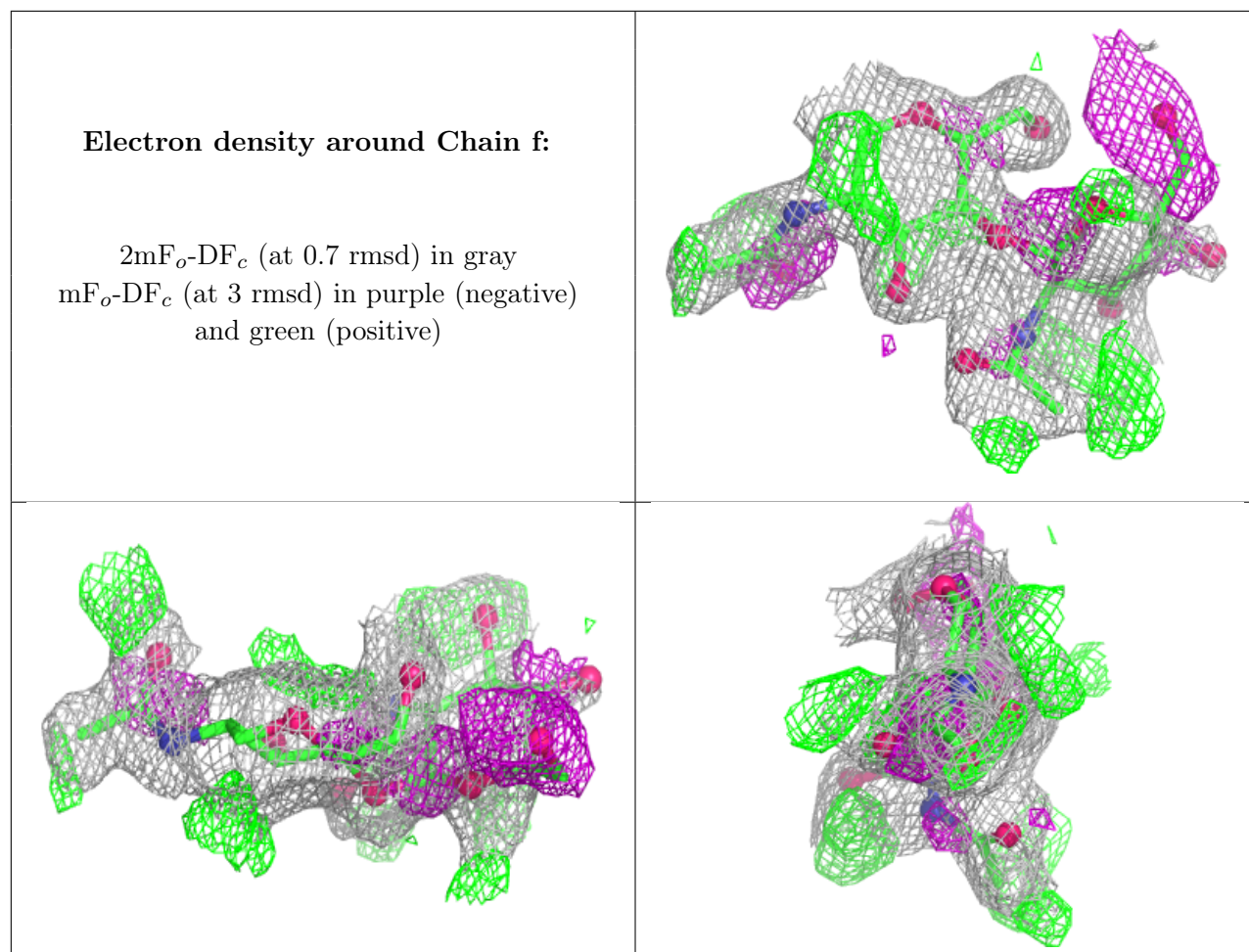
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	402	14/15	0.48	0.20	51,57,62,63	0
6	PEG	A	408	7/7	0.53	0.19	42,46,48,48	0
7	A1IUB	A	405	14/14	0.55	0.26	42,48,49,52	0
12	PO4	A	420	5/5	0.60	0.14	48,52,55,56	5
7	A1IUB	B	404	14/14	0.62	0.27	41,45,49,50	0
7	A1IUB	B	403	14/14	0.66	0.23	42,48,50,52	0
4	NAG	A	401	14/15	0.67	0.15	56,59,61,64	0
12	PO4	B	416	5/5	0.70	0.12	47,50,53,54	5
5	MES	A	409	12/12	0.71	0.17	40,43,44,47	0
13	GOL	B	405	6/6	0.72	0.16	38,42,44,45	0
12	PO4	A	419	5/5	0.73	0.14	47,50,52,55	5

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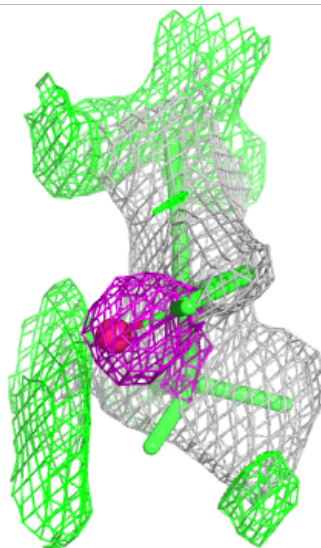
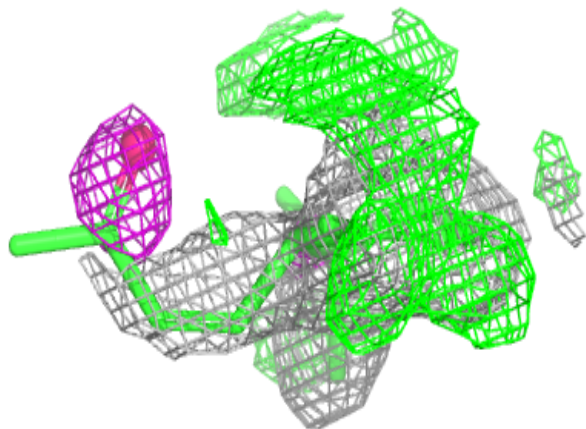
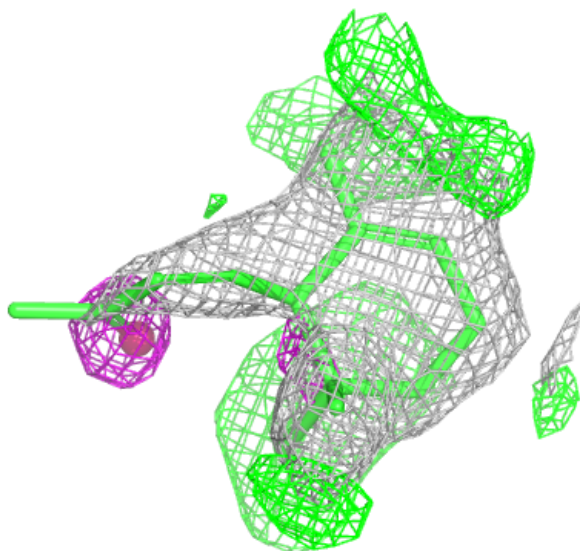
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	A	404	7/7	0.76	0.19	40,42,44,45	0
9	EOH	B	408	3/3	0.79	0.23	39,39,40,40	0
10	ZN	B	410	1/1	0.83	0.10	51,51,51,51	0
9	EOH	A	407	3/3	0.84	0.18	41,41,43,44	0
13	GOL	B	406	6/6	0.85	0.11	37,39,43,44	0
4	NAG	B	401	14/15	0.91	0.09	33,38,41,46	0
10	ZN	B	414	1/1	0.92	0.22	56,56,56,56	0
10	ZN	B	412	1/1	0.93	0.08	53,53,53,53	0
5	MES	B	402	12/12	0.94	0.13	25,34,41,41	12
5	MES	A	403	12/12	0.94	0.13	23,33,39,40	12
10	ZN	B	413	1/1	0.96	0.20	50,50,50,50	0
10	ZN	B	411	1/1	0.96	0.07	42,42,42,42	0
11	MG	B	415	1/1	0.96	0.18	5,5,5,5	0
10	ZN	A	410	1/1	0.96	0.06	48,48,48,48	0
10	ZN	B	409	1/1	0.97	0.05	37,37,37,37	0
10	ZN	A	413	1/1	0.97	0.05	36,36,36,36	0
10	ZN	A	414	1/1	0.97	0.05	43,43,43,43	0
10	ZN	A	417	1/1	0.97	0.04	34,34,34,34	0
8	HEM	A	406	43/43	0.98	0.07	20,22,25,30	0
8	HEM	B	407	43/43	0.98	0.06	20,23,25,29	0
10	ZN	A	411	1/1	0.99	0.02	31,31,31,31	0
10	ZN	A	412	1/1	0.99	0.03	34,34,34,34	0
10	ZN	A	415	1/1	0.99	0.11	43,43,43,43	0
11	MG	A	418	1/1	0.99	0.17	2,2,2,2	0
10	ZN	A	416	1/1	0.99	0.06	41,41,41,41	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.



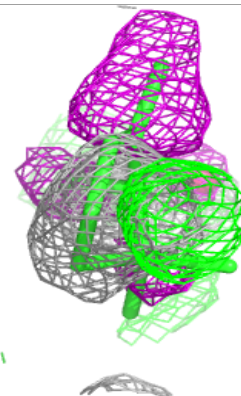
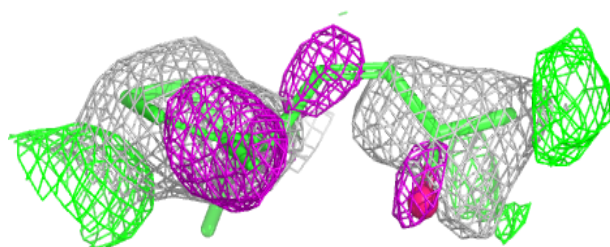
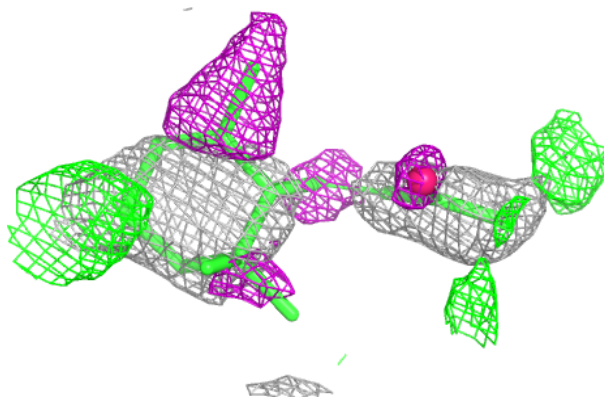
**Electron density around A1IUB A 405:**

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

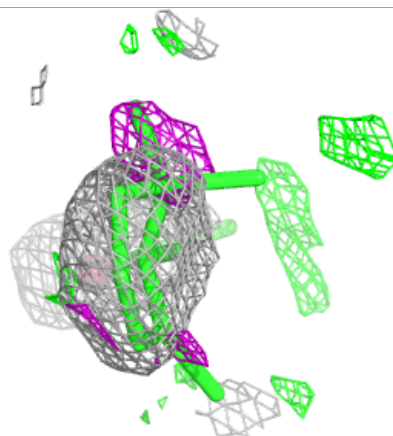
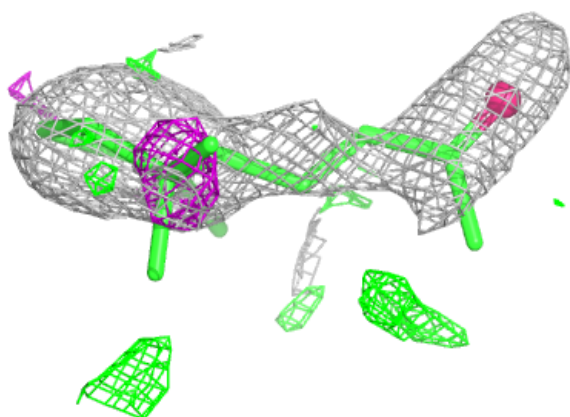
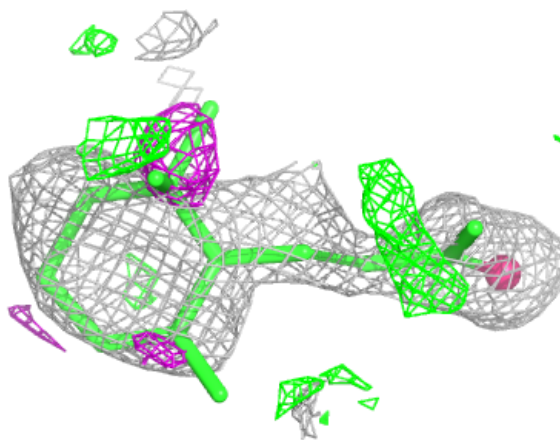


**Electron density around A1IUB B 404:**

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

**Electron density around A1IUB B 403:**

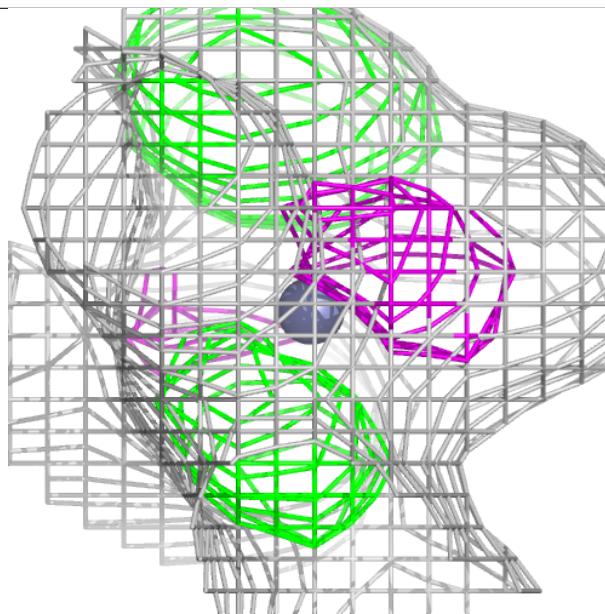
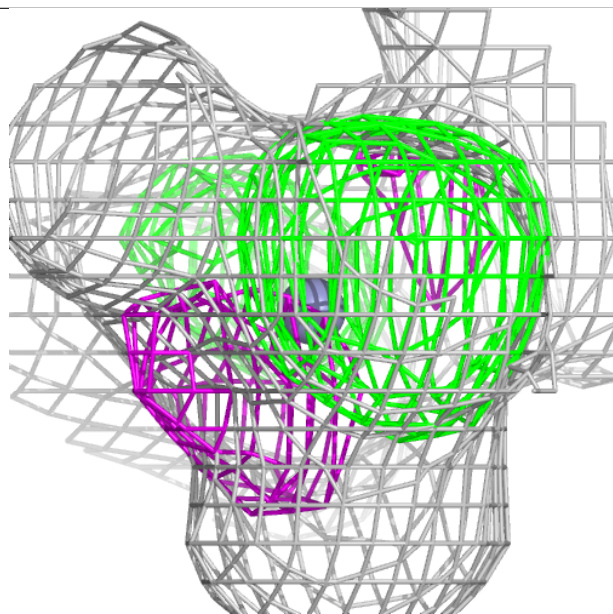
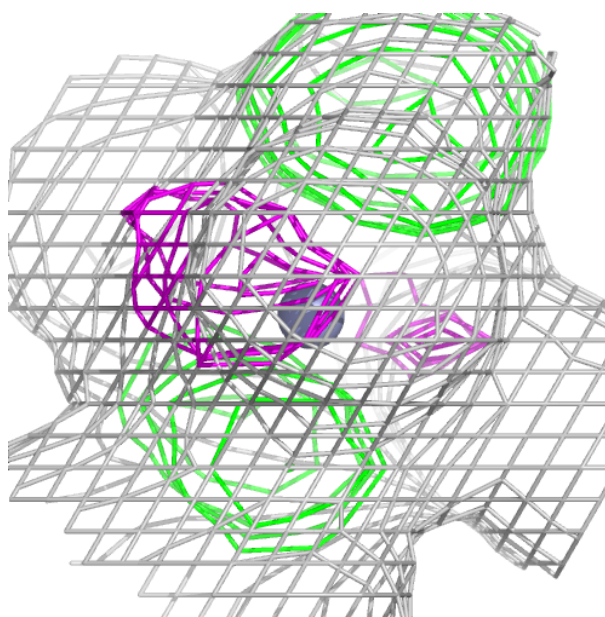
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





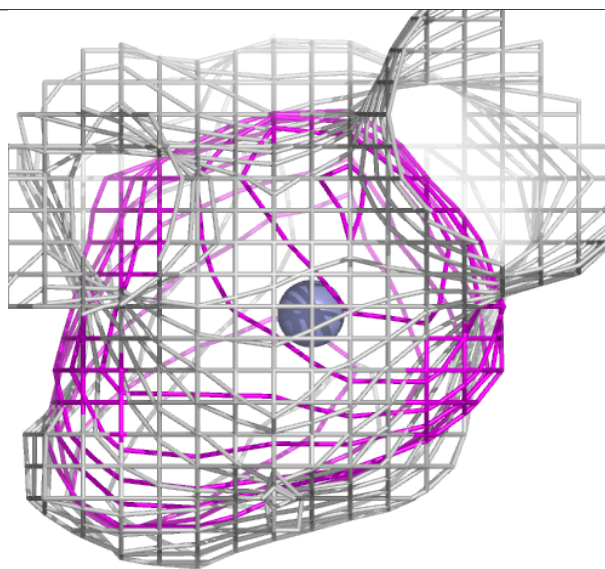
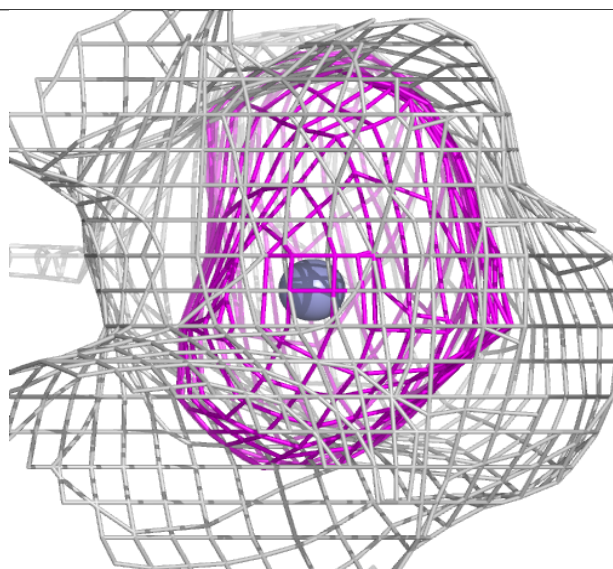
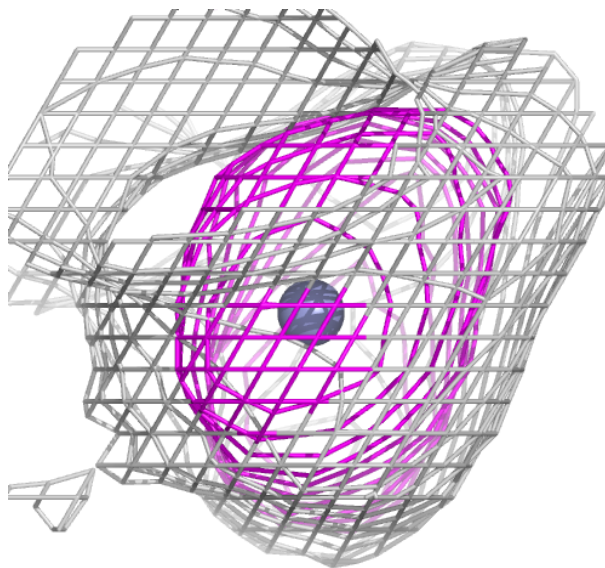
**Electron density around ZN B 410:**

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



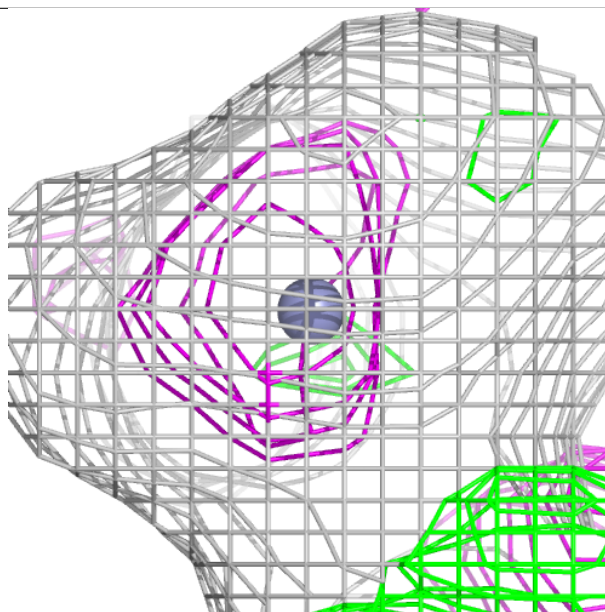
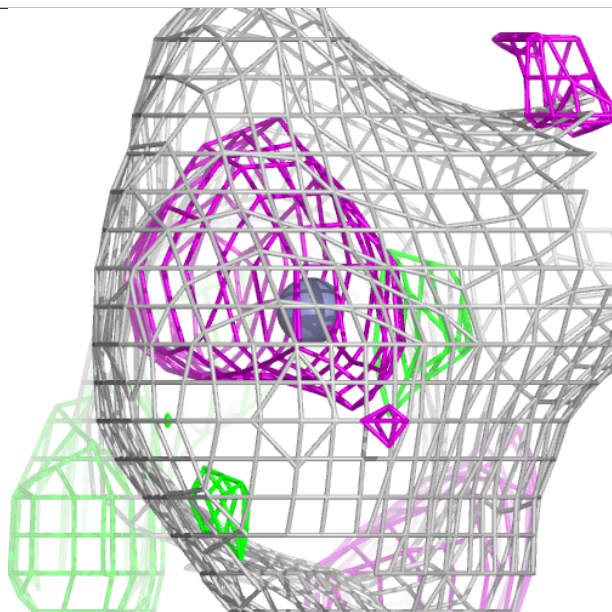
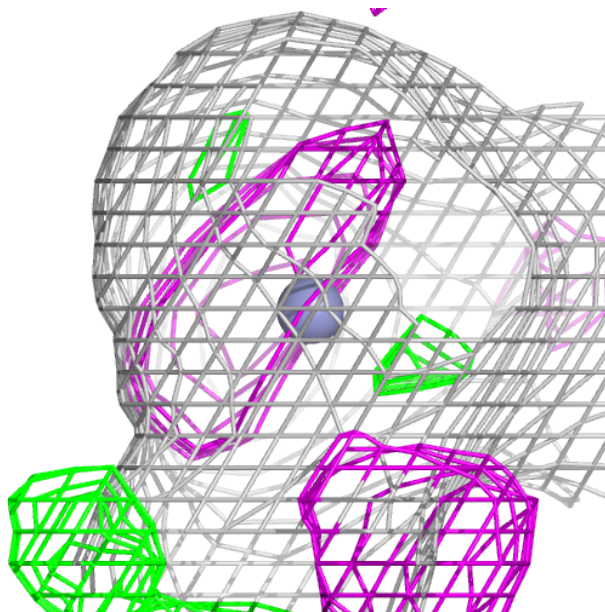
**Electron density around ZN B 414:**

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



**Electron density around ZN B 412:**

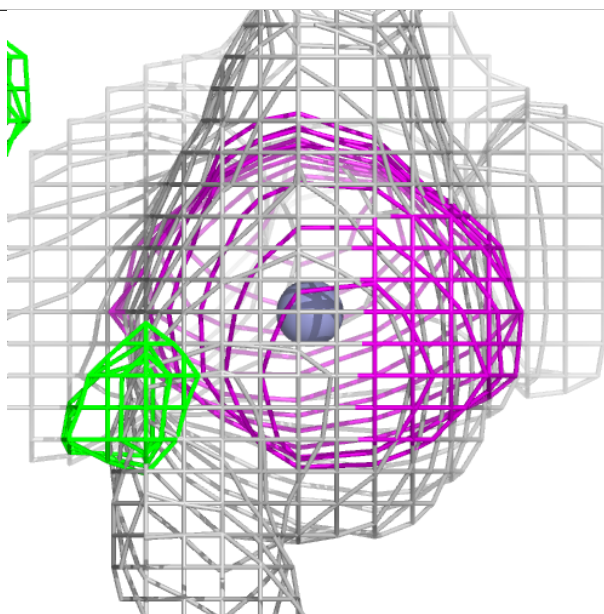
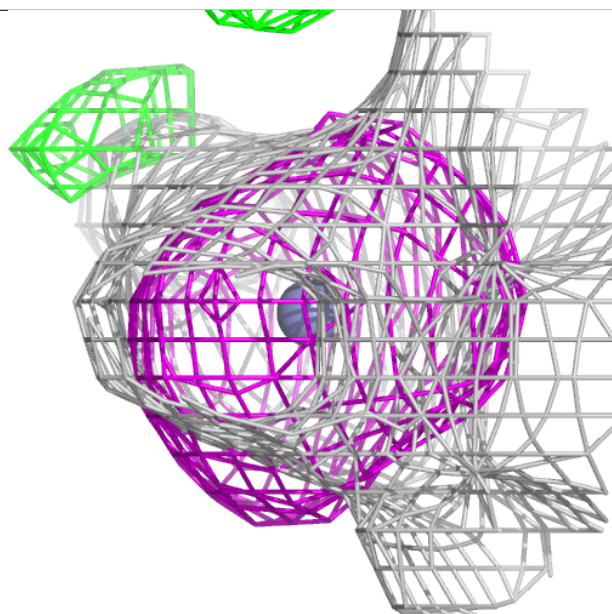
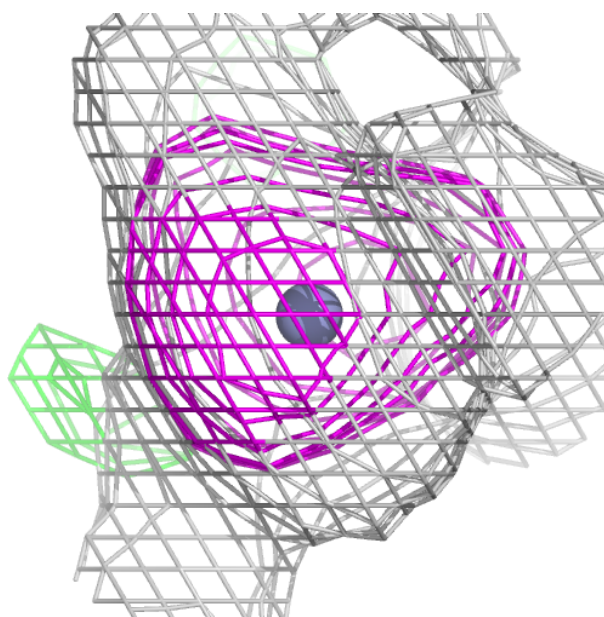
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





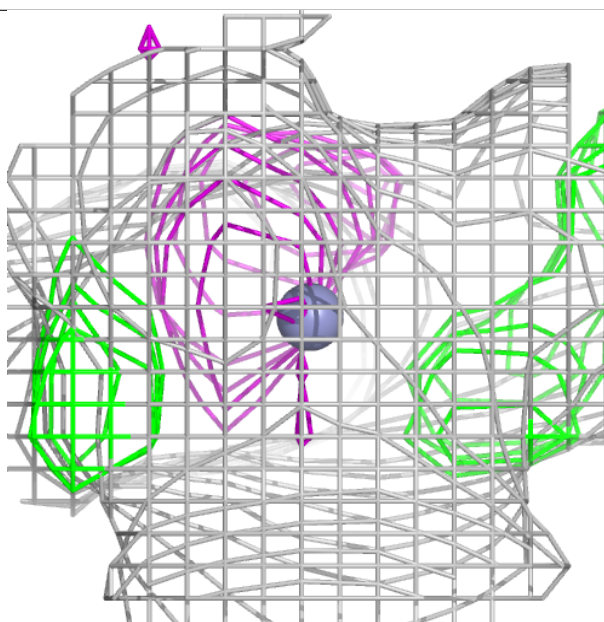
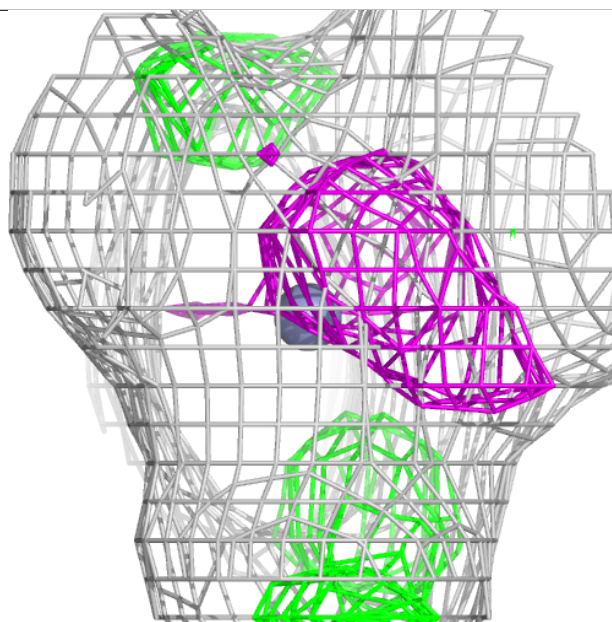
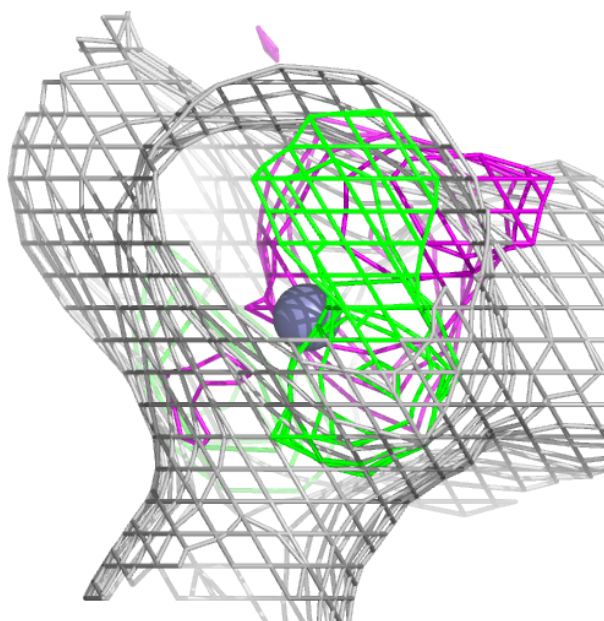
**Electron density around ZN B 413:**

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



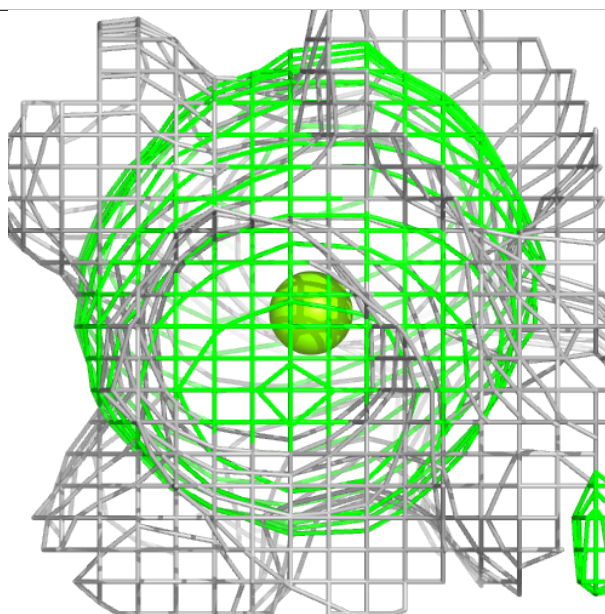
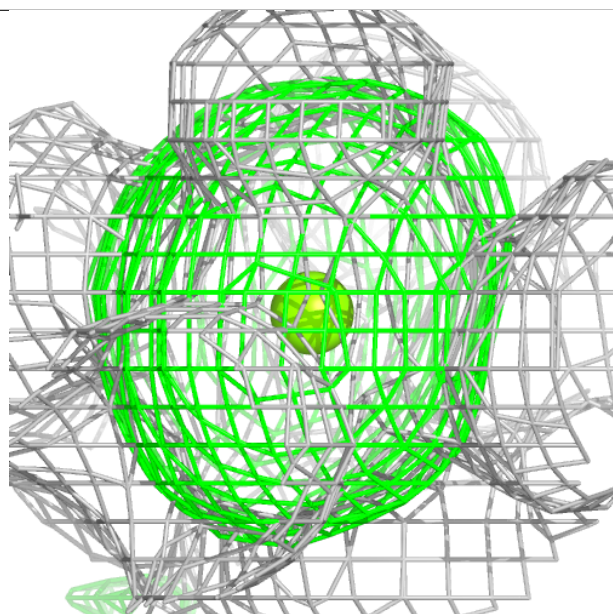
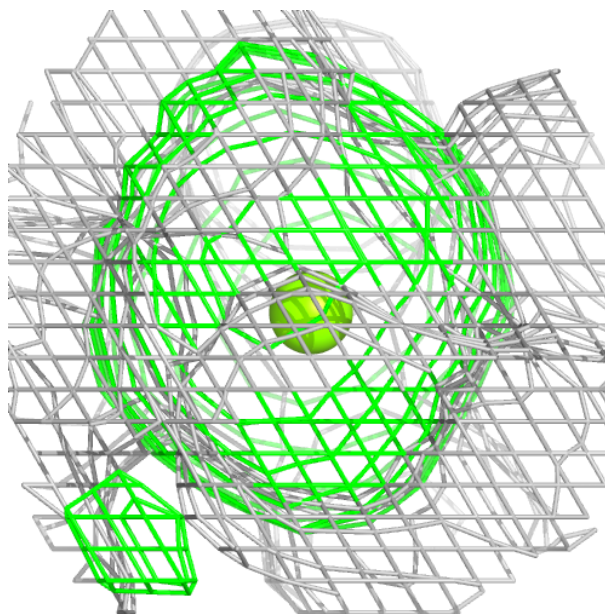
**Electron density around ZN B 411:**

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



**Electron density around MG B 415:**

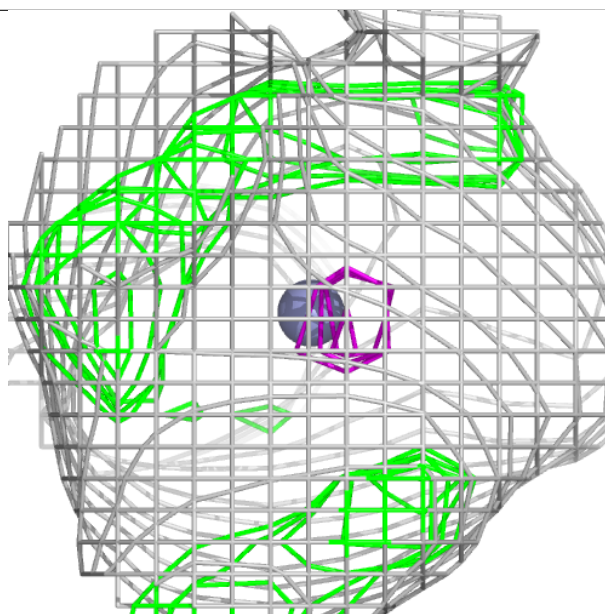
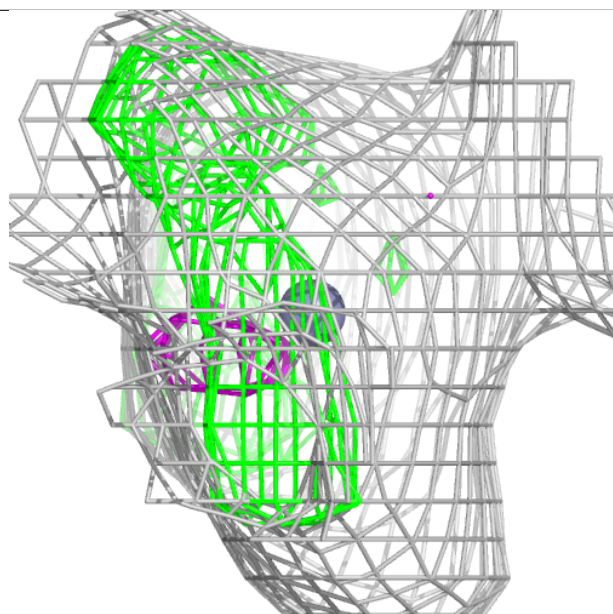
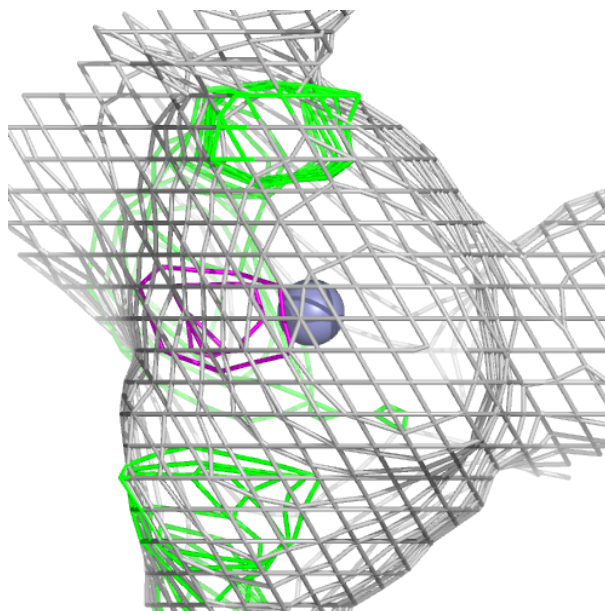
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





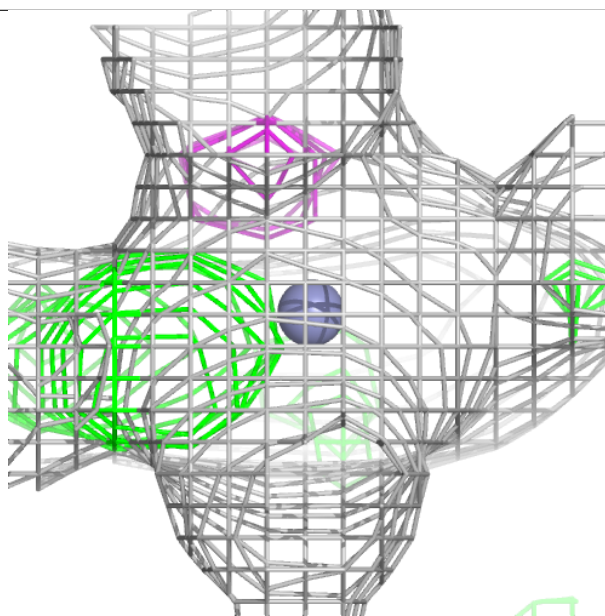
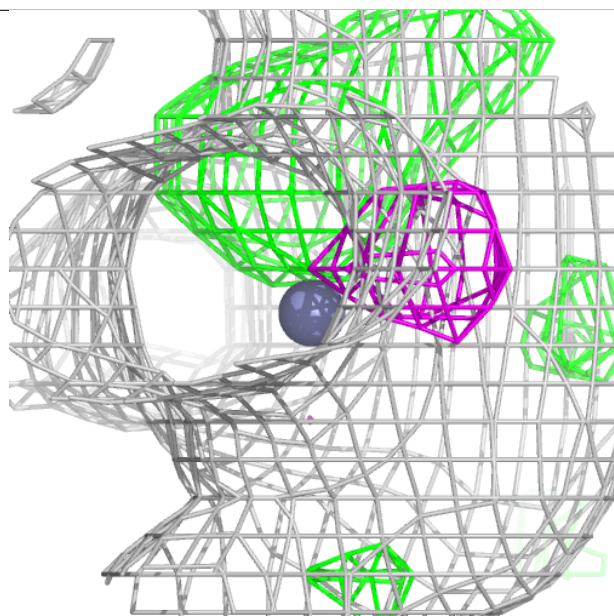
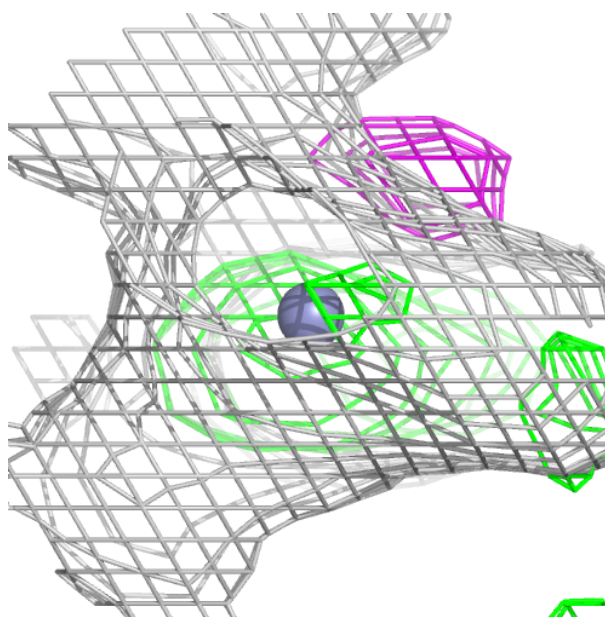
**Electron density around ZN A 410:**

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



**Electron density around ZN B 409:**

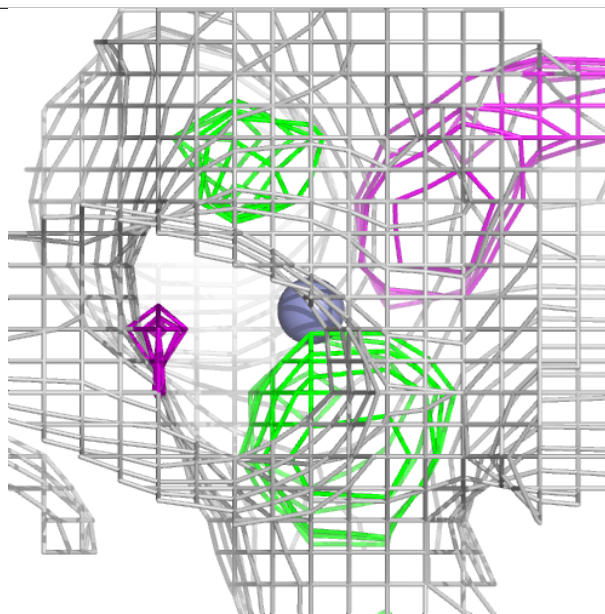
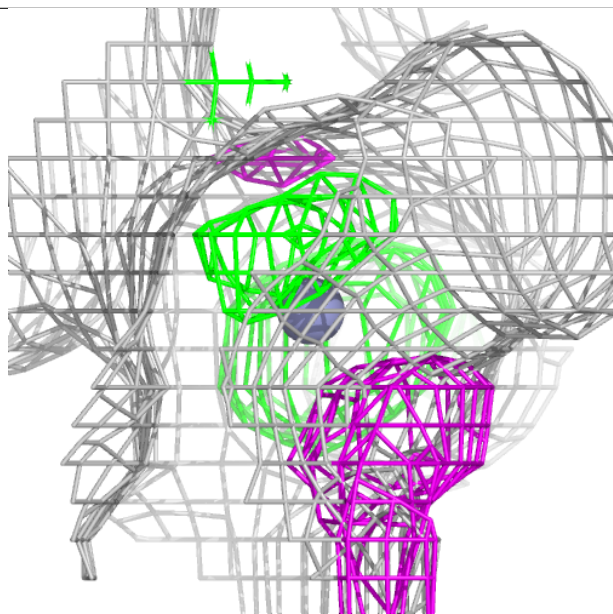
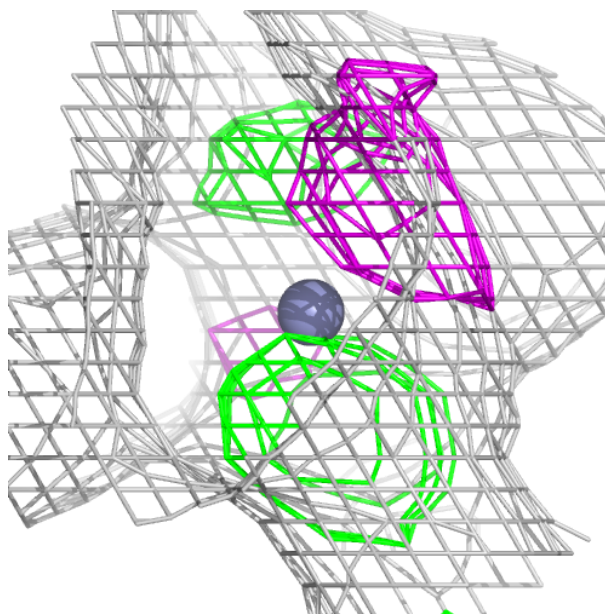
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





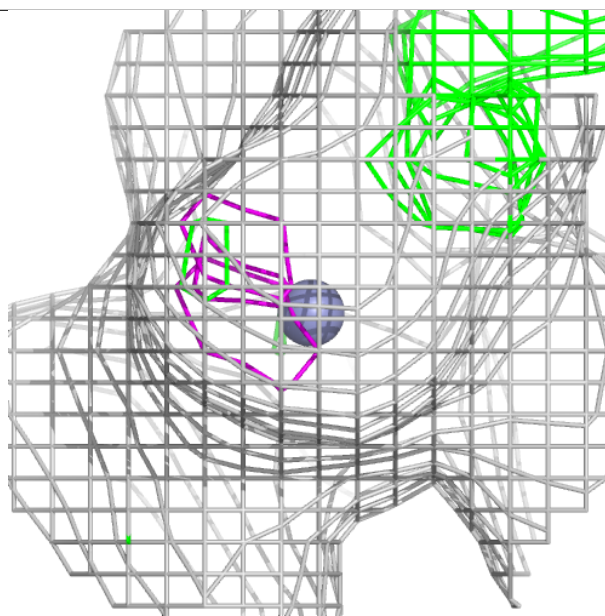
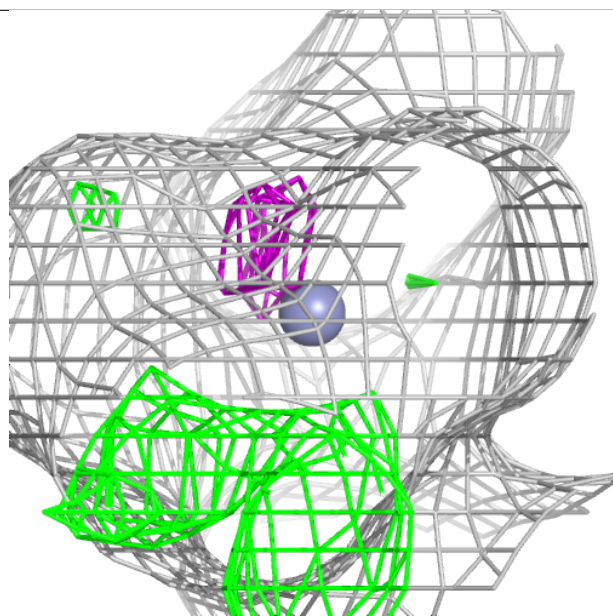
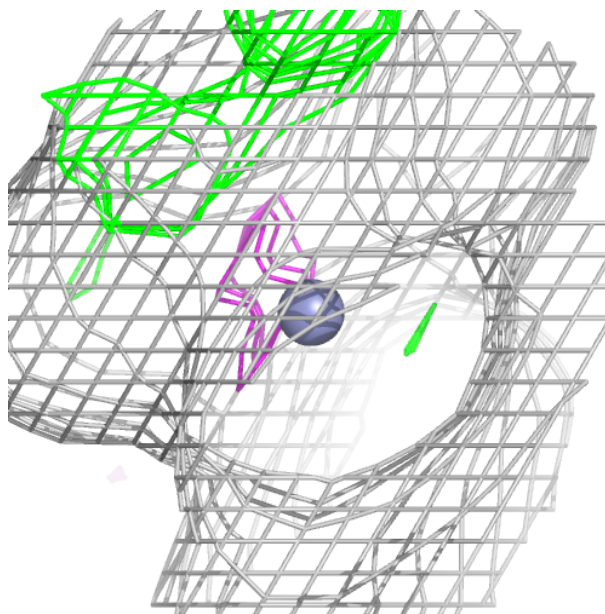
**Electron density around ZN A 413:**

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



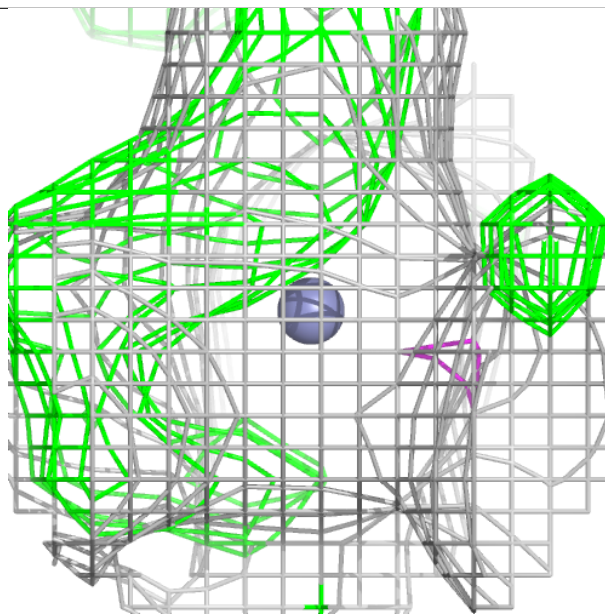
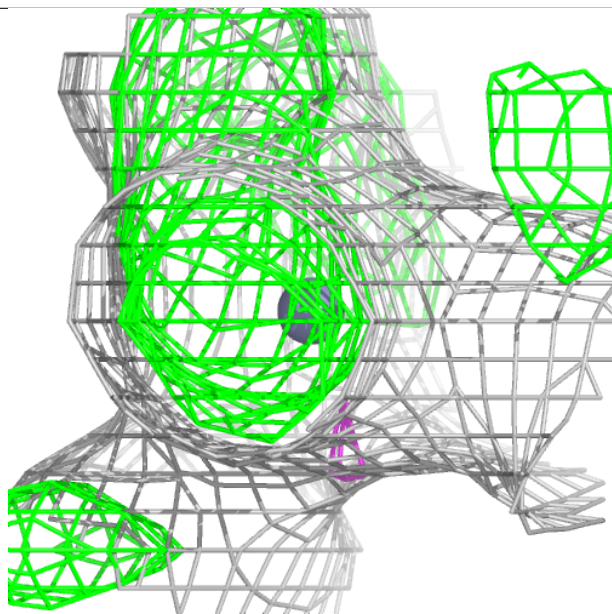
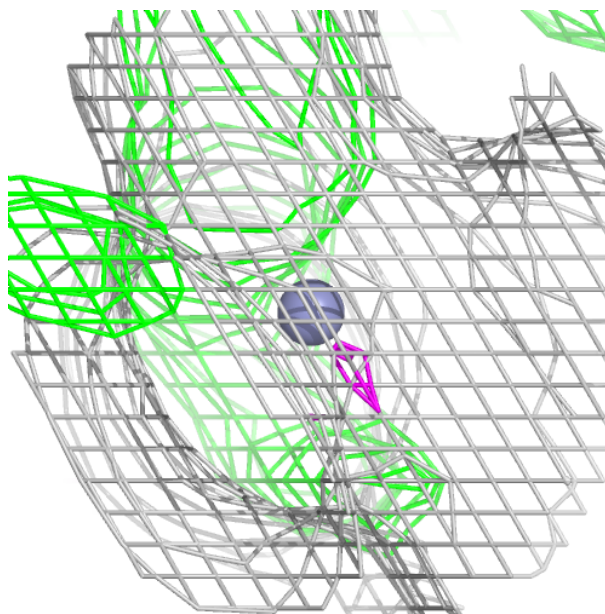
**Electron density around ZN A 414:**

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



**Electron density around ZN A 417:**

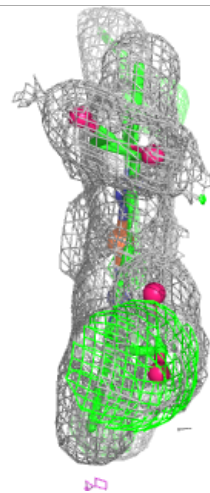
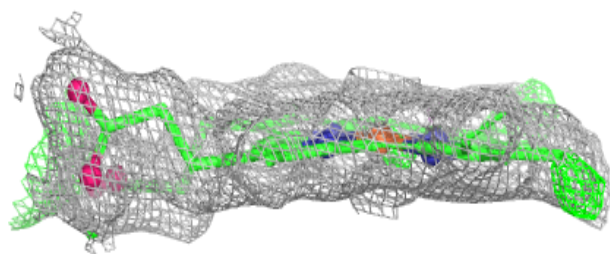
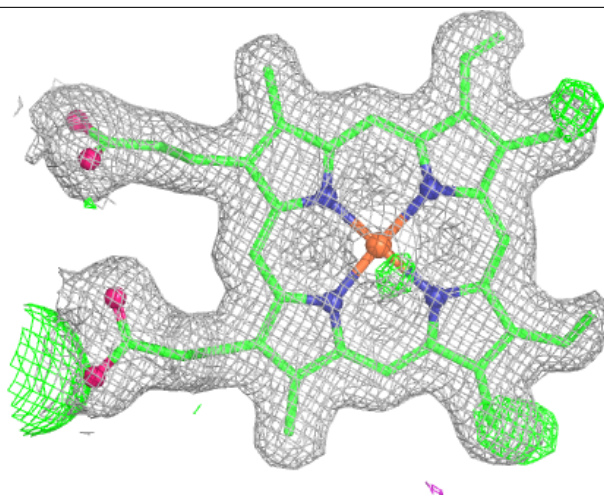
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





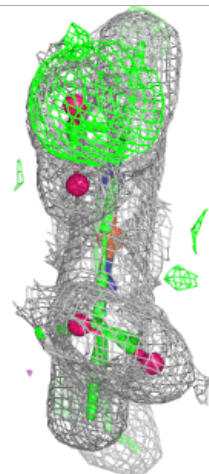
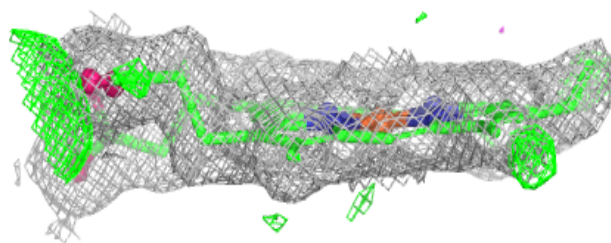
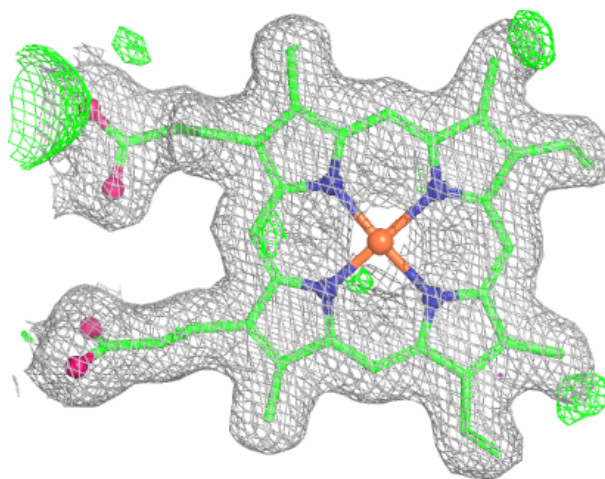
**Electron density around HEM A 406:**

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



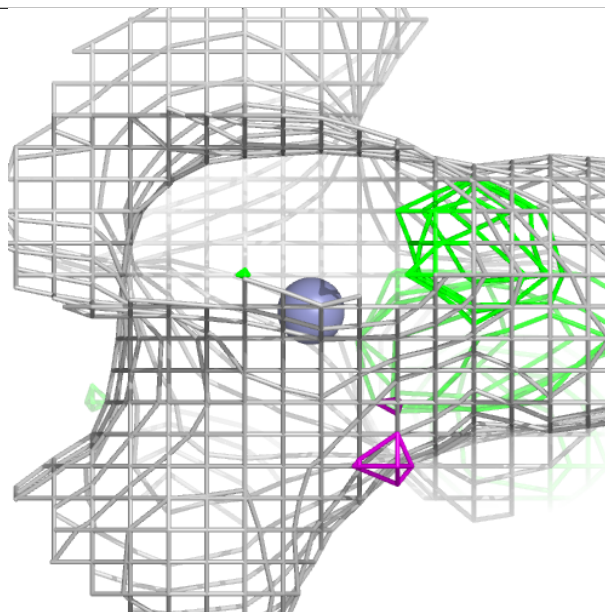
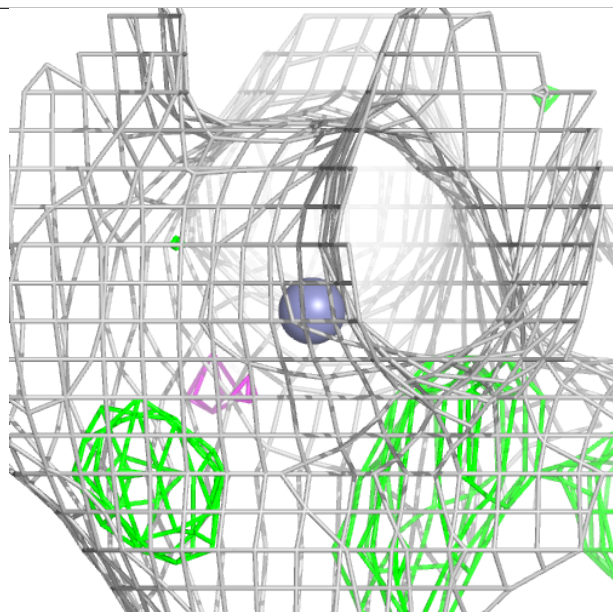
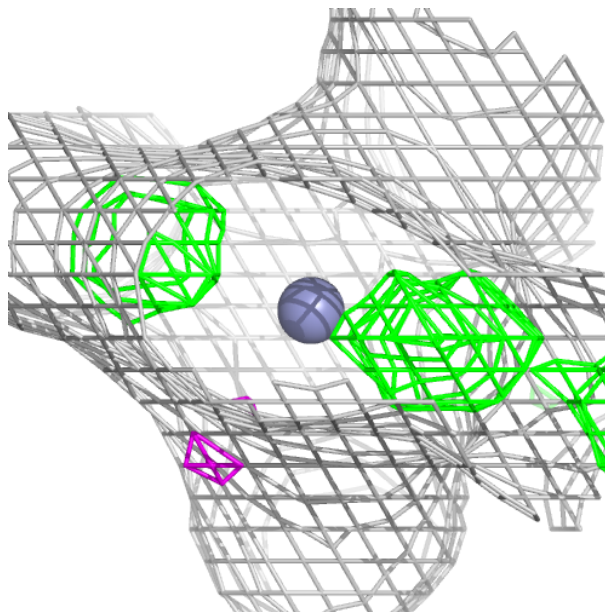
**Electron density around HEM B 407:**

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



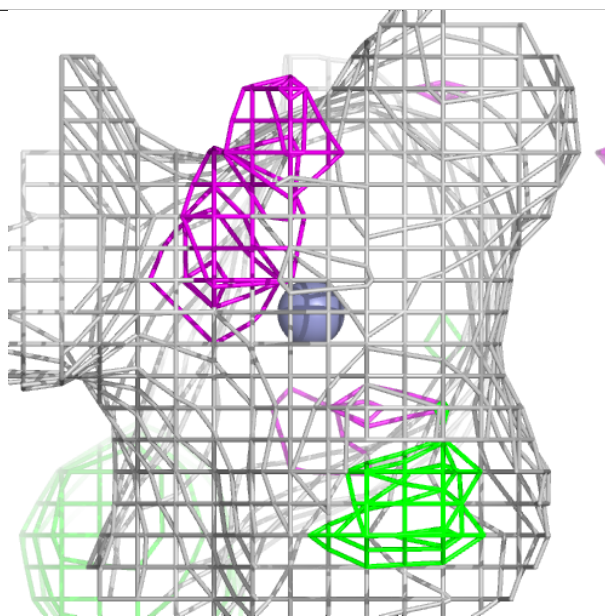
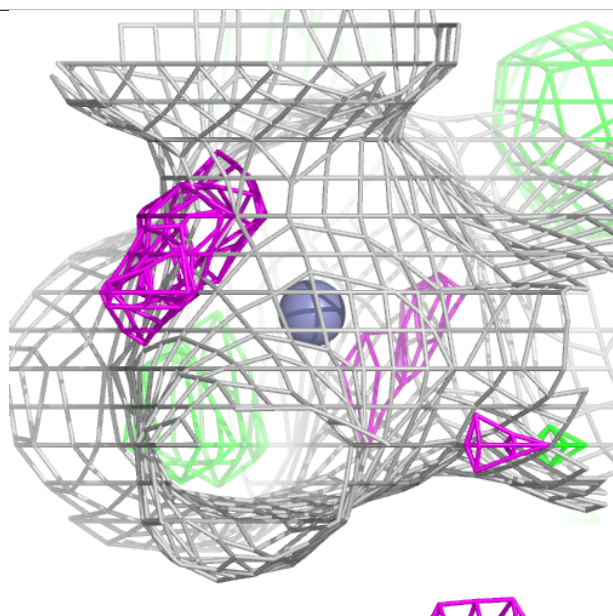
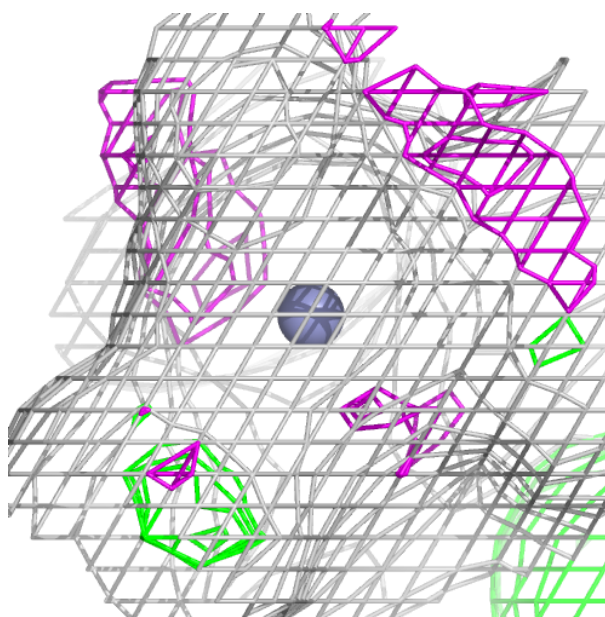
**Electron density around ZN A 411:**

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



**Electron density around ZN A 412:**

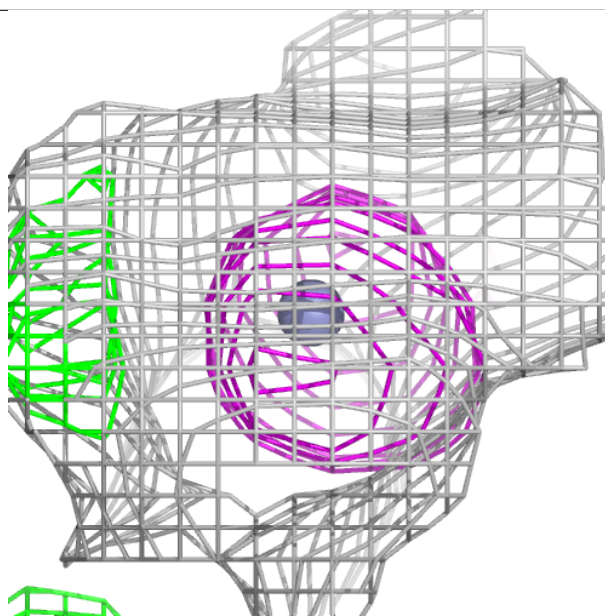
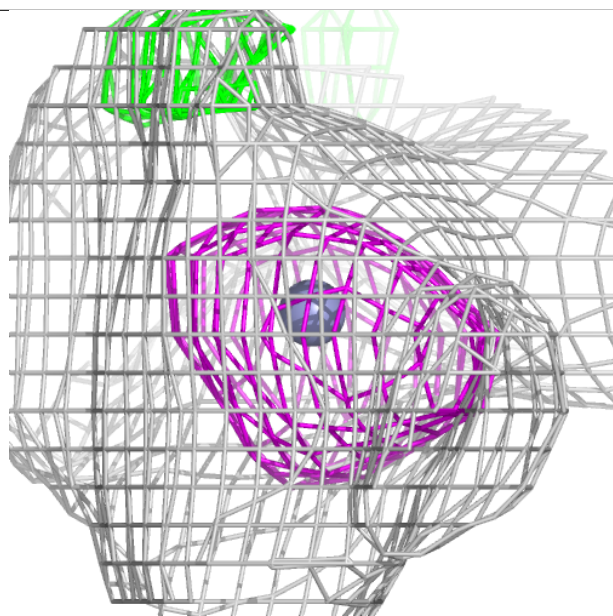
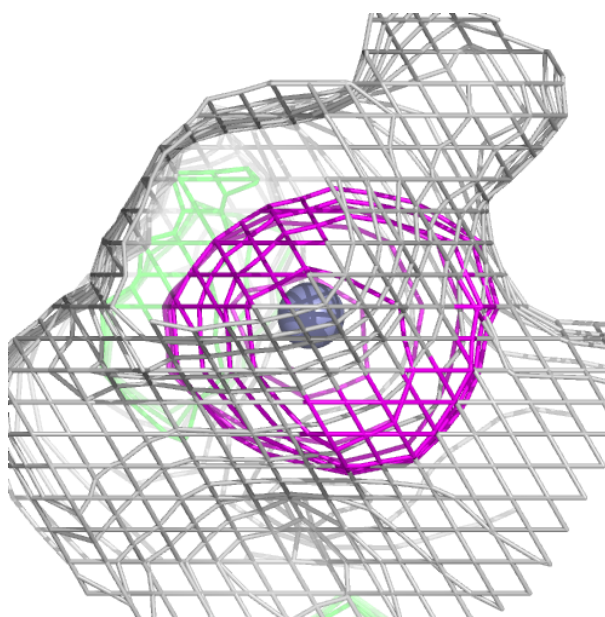
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ZN A 415:**

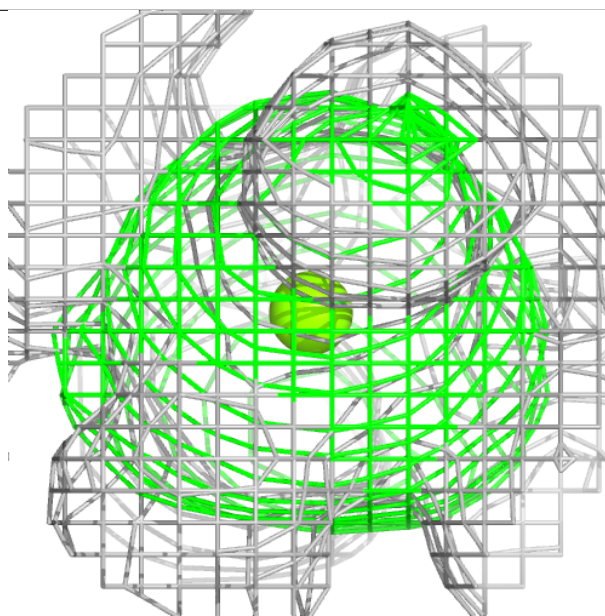
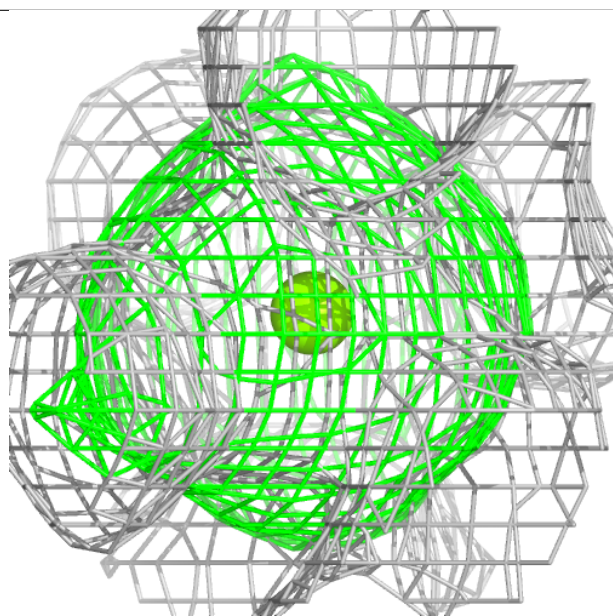
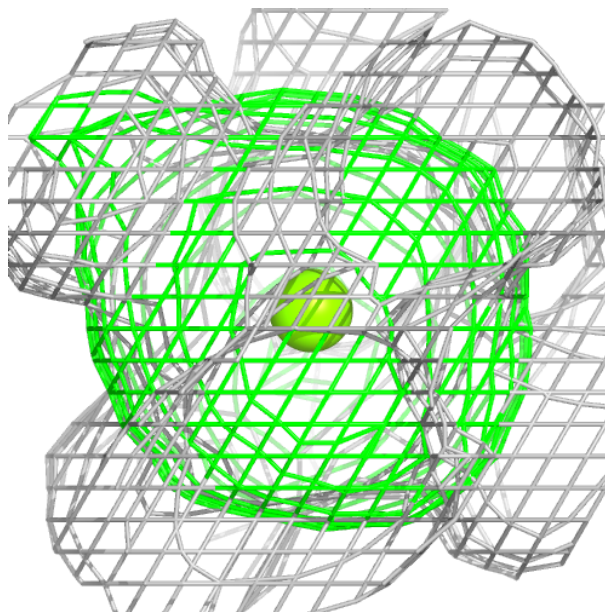
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





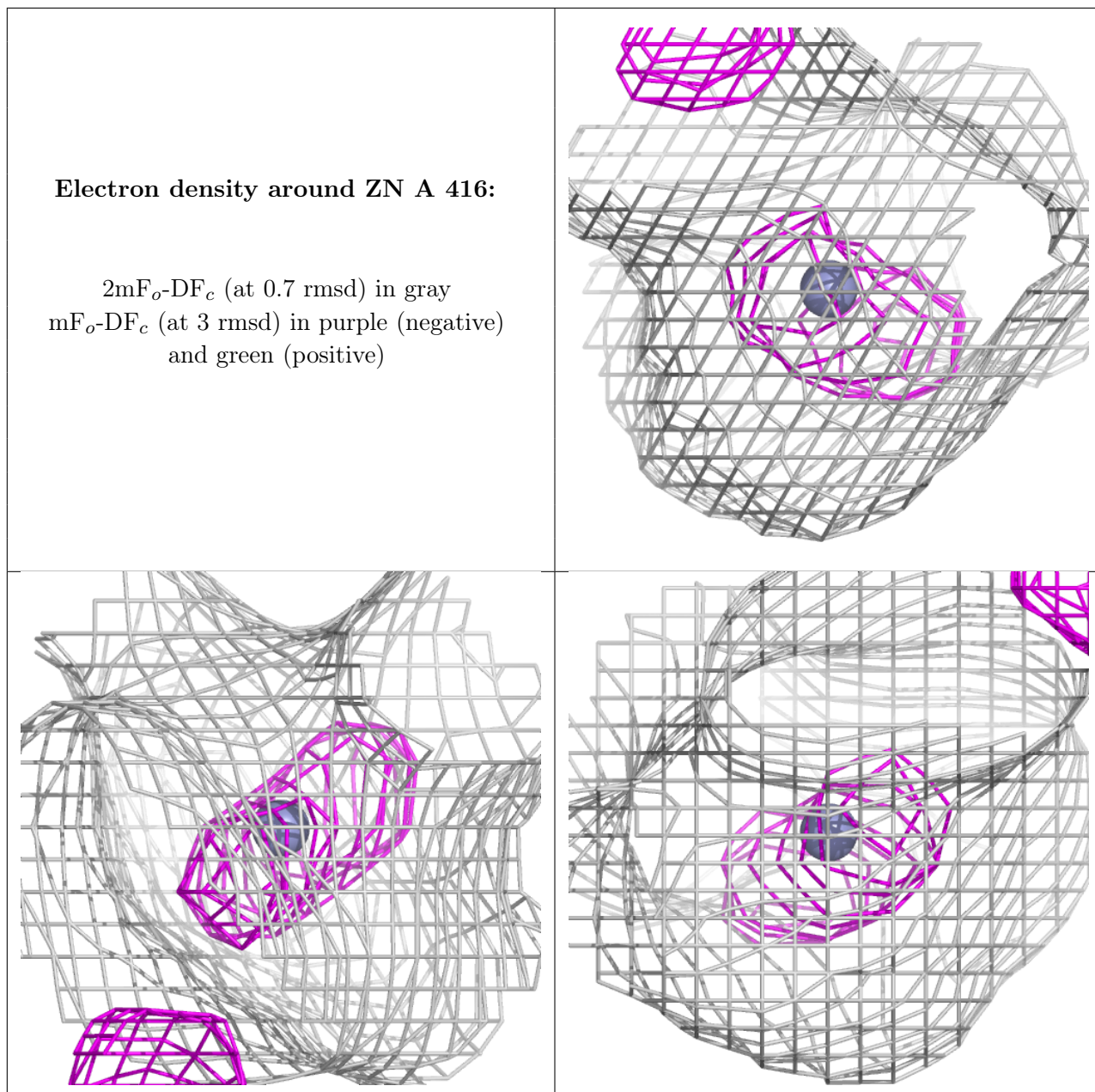
**Electron density around MG A 418:**

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



**Electron density around ZN A 416:**

$2mF_o-DF_c$  (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.