wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 07:52 am BST

PDB ID	:	9RFY / pdb_00009rfy
Title	:	Unspecific peroxygenase from Psathyrella aberdarensis, Grogu variant
Authors	:	Fernandez-Garcia, A.; Sanz-Aparicio, J.
Deposited on	:	2025-06-05
Resolution	:	2.55 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

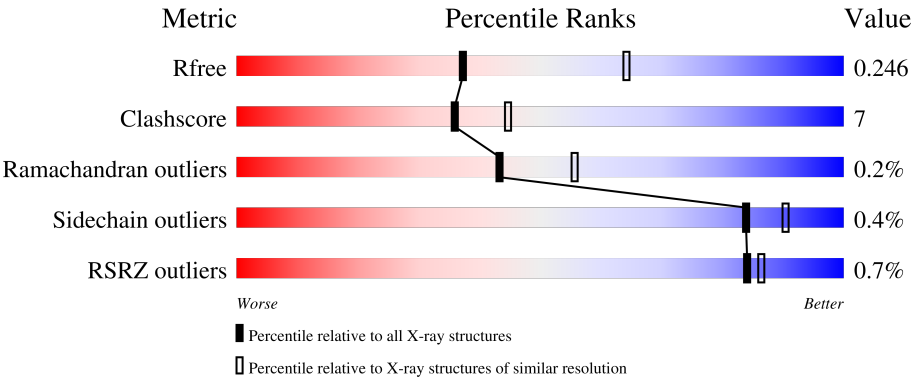
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 89% 11%
1	B	334	% 89% 10%
2	C	7	71% 29%
3	D	2	50% 50%
3	E	2	50% 50%

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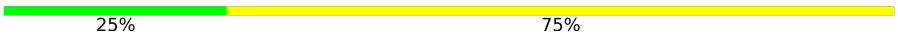
Mol	Chain	Length	Quality of chain
3	G	2	
4	F	4	

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
8	NAG	B	403	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 5776 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.

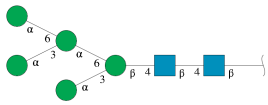
- Molecule 1 is a protein called Heme-thiolate peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2593	1656	436	494	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 alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



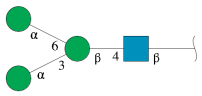
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



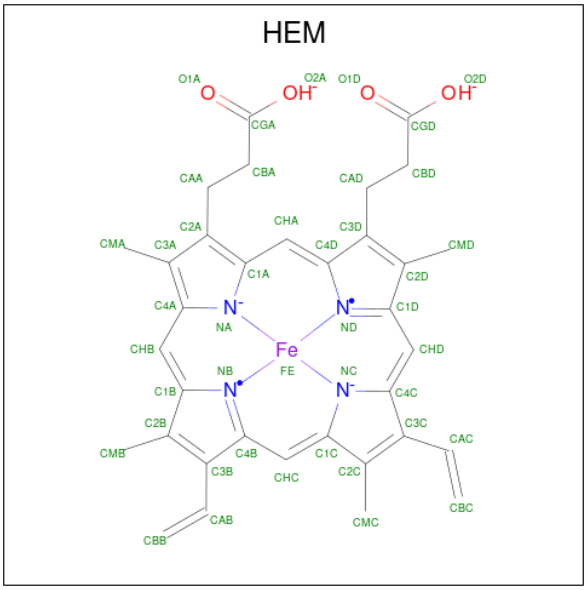
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0
3	E	2	Total C N O 28 16 2 10	0	0	0
3	G	2	Total C N O 28 16 2 10	0	0	0

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



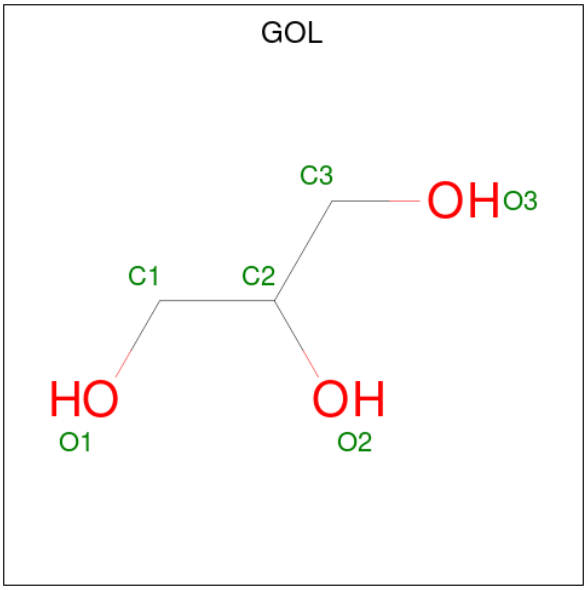
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	4	Total C N O 47 26 1 20	0	0	0

- 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).



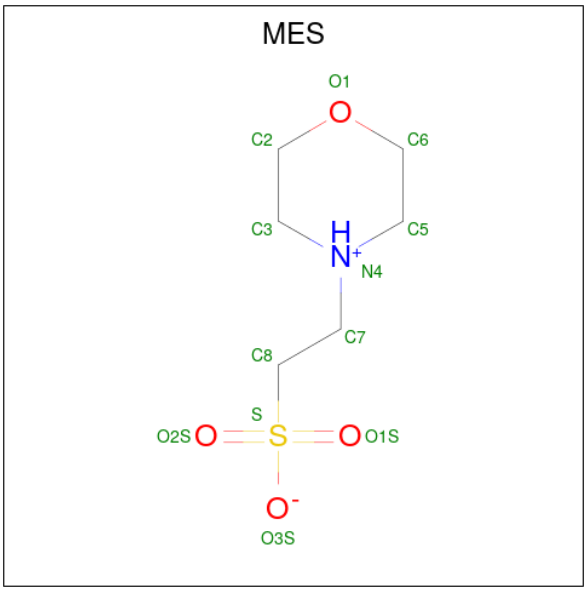
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



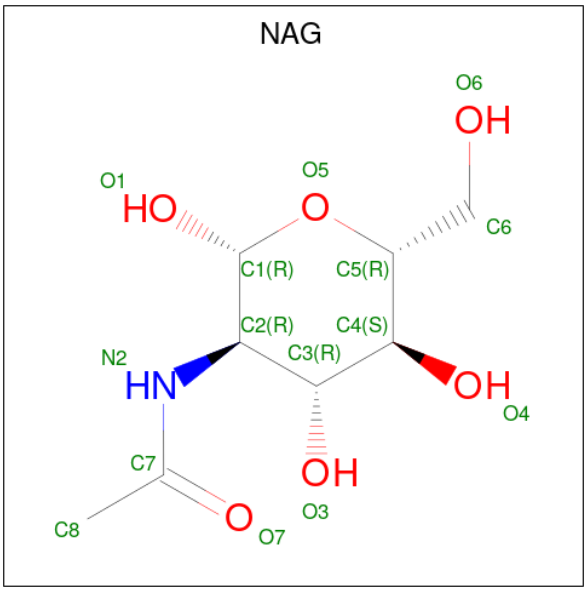
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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



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

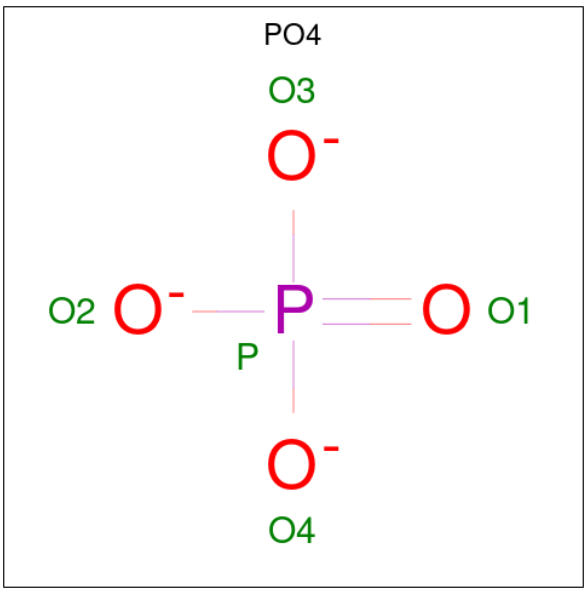
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- 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 8 8	0	0
10	B	6	Total Zn 6 6	0	0

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

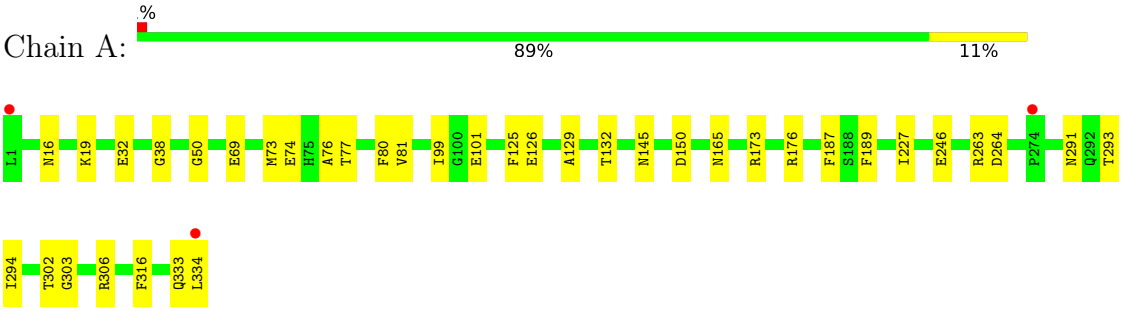
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	69	Total O 69 69	0	0
12	B	66	Total O 66 66	0	0

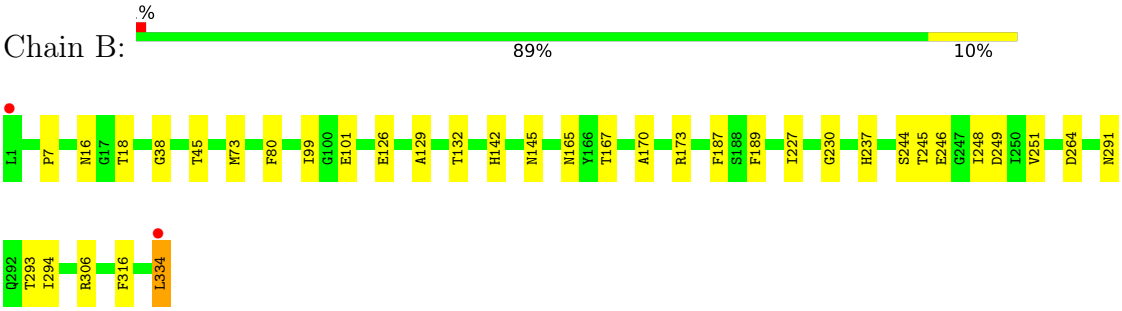
3 Residue-property plots (i)

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

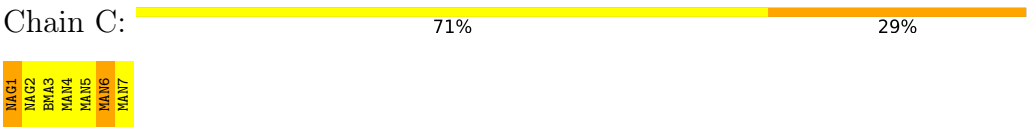
• Molecule 1: Heme-thiolate peroxidase



• Molecule 1: Heme-thiolate peroxidase



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



• Molecule 3: 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

Chain E:





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

Chain G:





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

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	76.68Å 76.68Å 273.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.71 – 2.55 47.71 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.71-2.55) 99.8 (47.71-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.191 , 0.247 0.194 , 0.246	Depositor DCC
R_{free} test set	1442 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5776	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, GOL, MES, HEM, NAG, MG, MAN, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.61	0/2672	1.10	2/3644 (0.1%)
1	B	0.60	0/2672	1.06	1/3644 (0.0%)
All	All	0.60	0/5344	1.08	3/7288 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	ASP	CA-CB-CG	11.92	124.52	112.60
1	B	264	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	150	ASP	CA-CB-CG	5.22	117.82	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	ARG	Sidechain

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	2593	0	2453	35	0
1	B	2593	0	2452	38	0
2	C	83	0	70	5	0
3	D	28	0	25	3	0
3	E	28	0	25	4	0
3	G	28	0	25	4	0
4	F	47	0	40	4	0
5	A	43	0	30	1	0
5	B	43	0	30	5	0
6	A	12	0	16	0	0
6	B	6	0	8	1	0
7	A	24	0	26	2	0
7	B	36	0	39	2	0
8	A	28	0	26	6	0
8	B	28	0	26	12	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	8	0	0	1	0
10	B	6	0	0	0	0
11	B	5	0	0	0	0
12	A	69	0	0	8	0
12	B	66	0	0	2	0
All	All	5776	0	5291	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 80 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:165:ASN:HD21	3:D:1:NAG:C1	1.08	1.60
1:B:145:ASN:HD21	8:B:403:NAG:C1	1.15	1.57
1:B:291:ASN:HD21	3:G:1:NAG:C1	1.14	1.57
1:B:16:ASN:ND2	8:B:401:NAG:C1	1.67	1.56
1:B:165:ASN:HD21	3:E:1:NAG:C1	1.05	1.56

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/334 (100%)	317 (95%)	16 (5%)	0	100	100
1	B	333/334 (100%)	320 (96%)	12 (4%)	1 (0%)	36	45
All	All	666/668 (100%)	637 (96%)	28 (4%)	1 (0%)	43	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	244	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/274 (100%)	274 (100%)	1 (0%)	84	90
1	B	275/274 (100%)	274 (100%)	1 (0%)	84	90
All	All	550/548 (100%)	548 (100%)	2 (0%)	84	90

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

Mol	Chain	Res	Type
1	A	263	ARG
1	B	334	LEU

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	291	ASN
1	B	165	ASN
1	B	33	GLN
1	A	291	ASN
1	B	145	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	1	2	14,14,15	0.50	0	17,19,21	0.74	1 (5%)
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	1.04	1 (5%)
2	BMA	C	3	2	11,11,12	0.92	1 (9%)	15,15,17	0.82	1 (6%)
2	MAN	C	4	2	11,11,12	1.18	2 (18%)	15,15,17	1.30	2 (13%)
2	MAN	C	5	2	11,11,12	1.04	1 (9%)	15,15,17	0.92	0
2	MAN	C	6	2	11,11,12	0.97	1 (9%)	15,15,17	1.19	1 (6%)
2	MAN	C	7	2	11,11,12	1.09	1 (9%)	15,15,17	1.04	1 (6%)
3	NAG	D	1	3	14,14,15	0.44	0	17,19,21	0.94	1 (5%)
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.94	1 (5%)
3	NAG	E	1	3	14,14,15	0.45	0	17,19,21	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.90	0
4	NAG	F	1	4	14,14,15	0.40	0	17,19,21	0.67	0
4	BMA	F	2	4	11,11,12	1.07	1 (9%)	15,15,17	1.50	2 (13%)
4	MAN	F	3	4	11,11,12	0.77	0	15,15,17	0.91	0
4	MAN	F	4	4	11,11,12	1.34	2 (18%)	15,15,17	1.05	1 (6%)
3	NAG	G	1	3	14,14,15	0.81	0	17,19,21	1.19	3 (17%)
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	1.60	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	BMA	F	2	4	-	0/2/19/22	0/1/1/1
4	MAN	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	MAN	O5-C5	3.10	1.49	1.43
4	F	2	BMA	O5-C5	3.00	1.49	1.43
2	C	6	MAN	O5-C5	2.97	1.49	1.43
2	C	7	MAN	O5-C5	2.69	1.48	1.43
2	C	4	MAN	C2-C3	2.65	1.56	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	2	NAG	C2-N2-C7	5.11	130.18	122.90
4	F	2	BMA	C1-O5-C5	4.22	117.91	112.19
2	C	4	MAN	C1-O5-C5	3.29	116.64	112.19
3	G	1	NAG	C1-C2-N2	2.85	115.36	110.49
2	C	2	NAG	C2-N2-C7	2.80	126.89	122.90

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	G	2	NAG	C3-C2-N2-C7
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2

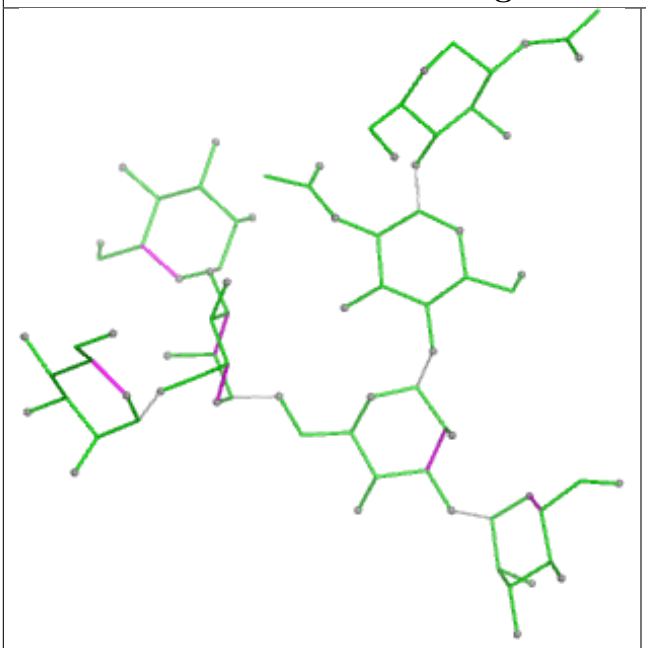
There are no ring outliers.

6 monomers are involved in 20 short contacts:

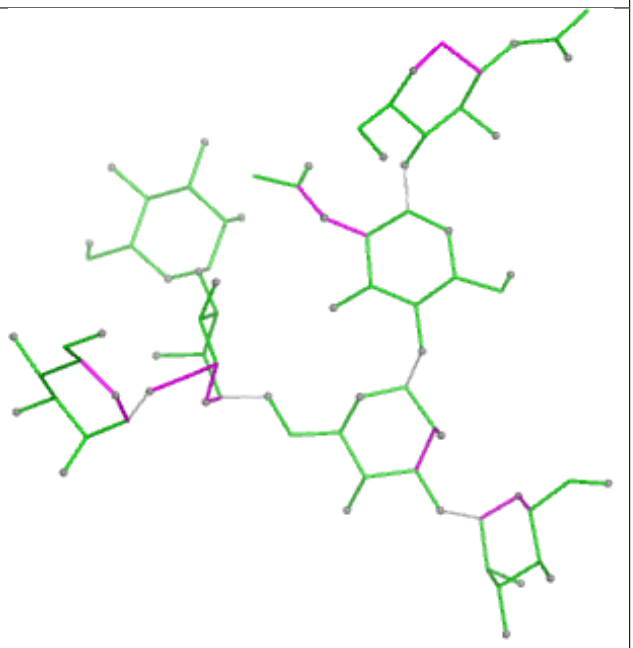
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	3	0
2	C	6	MAN	1	0
3	G	1	NAG	4	0
4	F	1	NAG	4	0
3	E	1	NAG	4	0
2	C	1	NAG	4	0

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

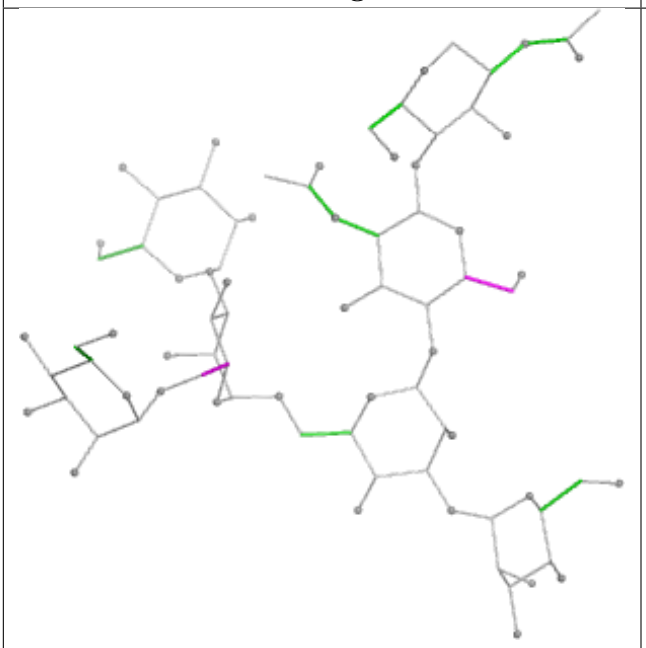
Oligosaccharide Chain C



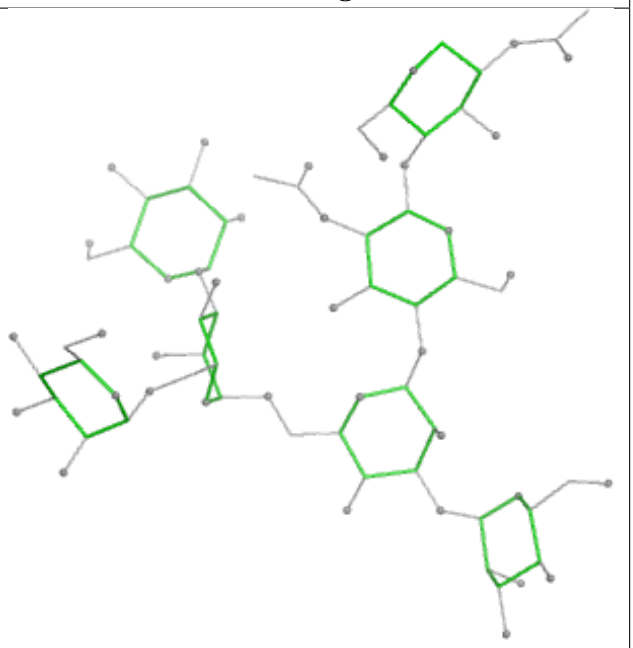
Bond lengths



Bond angles

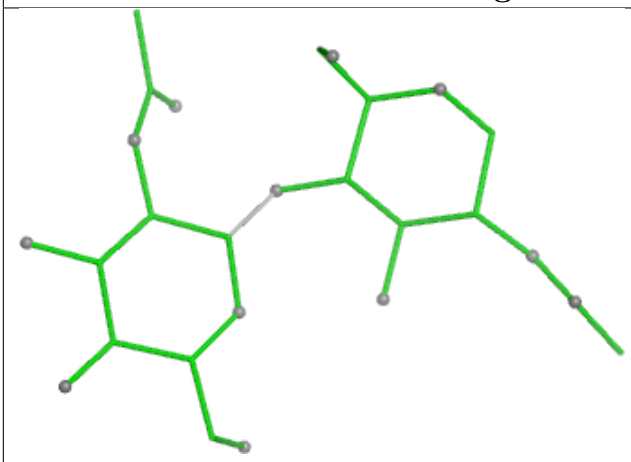


Torsions

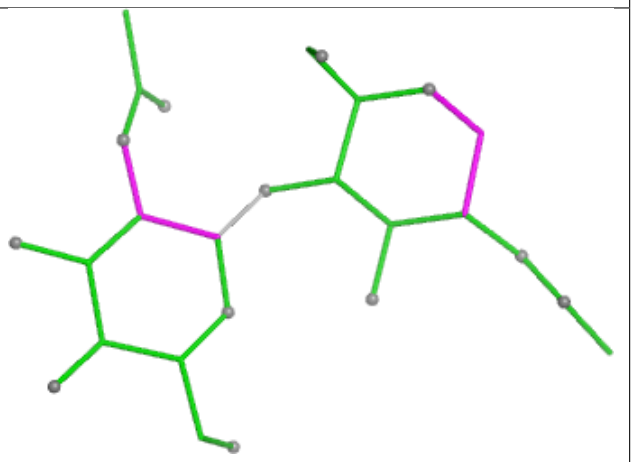


Rings

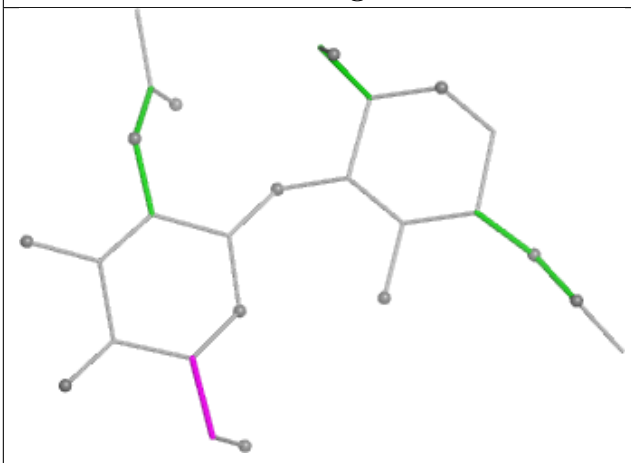
Oligosaccharide Chain D



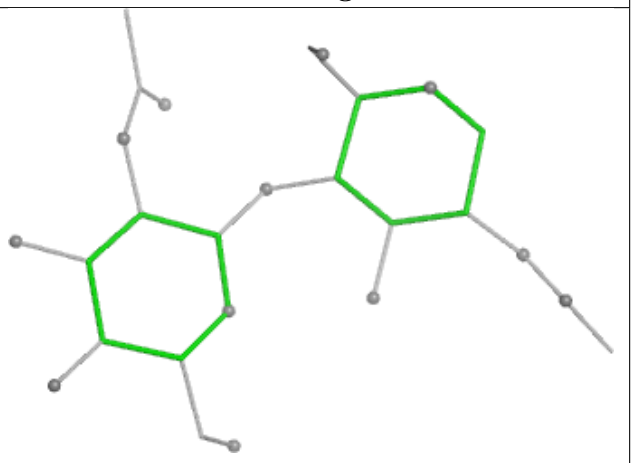
Bond lengths



Bond angles

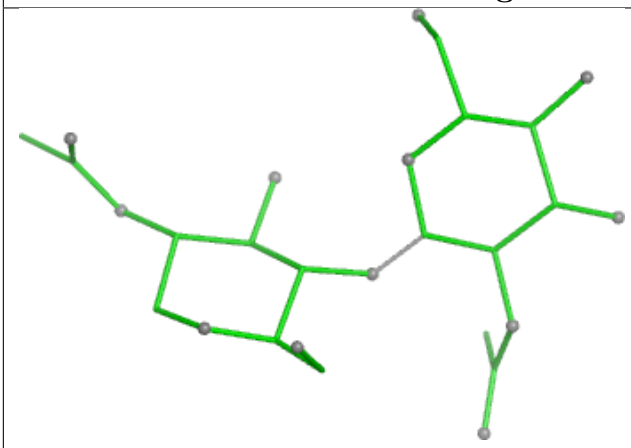


Torsions

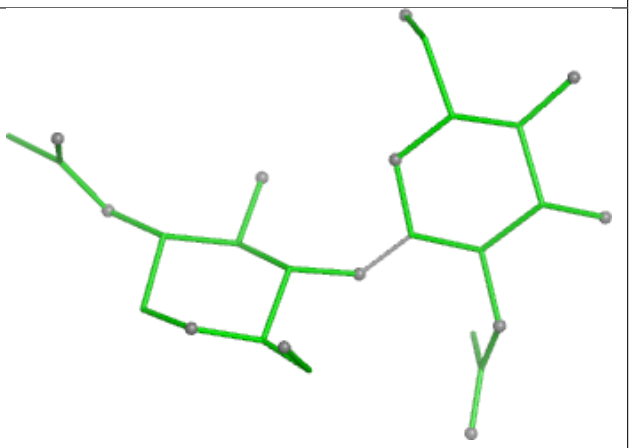


Rings

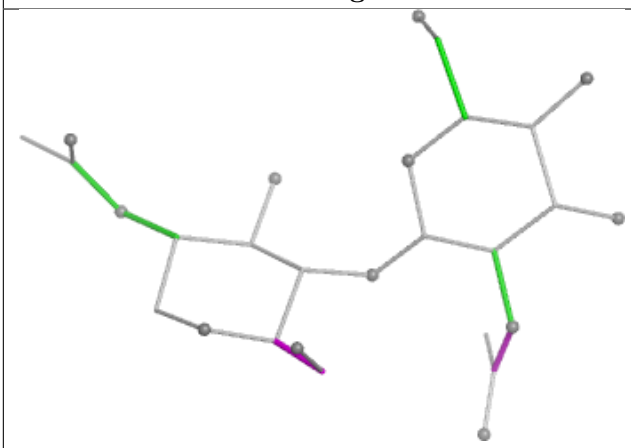
Oligosaccharide Chain E



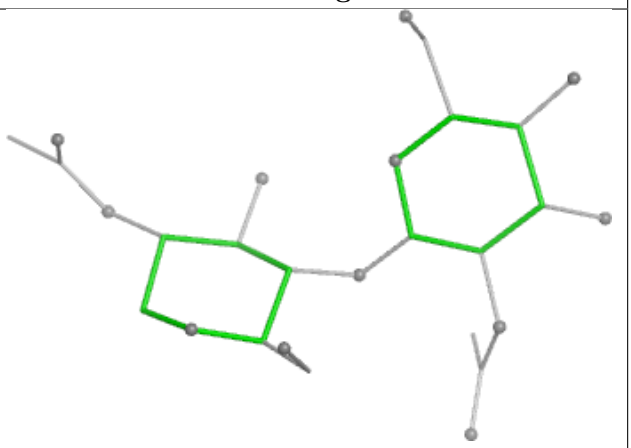
Bond lengths



Bond angles

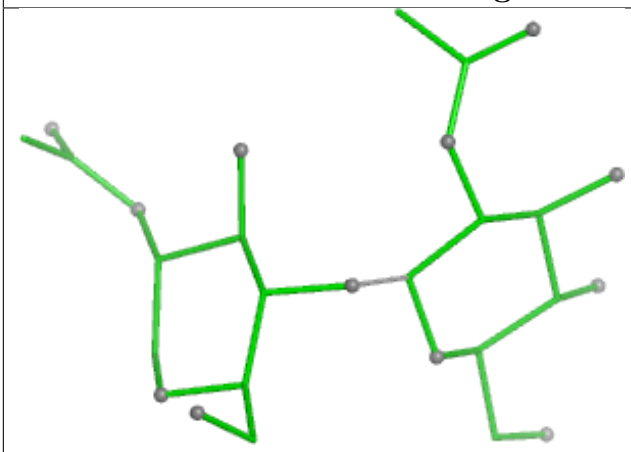


Torsions

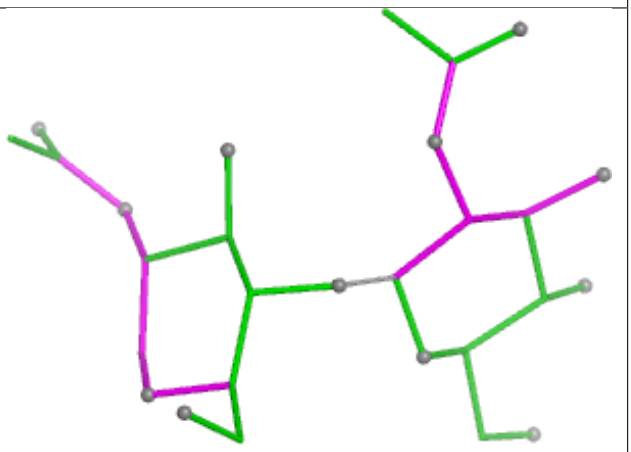


Rings

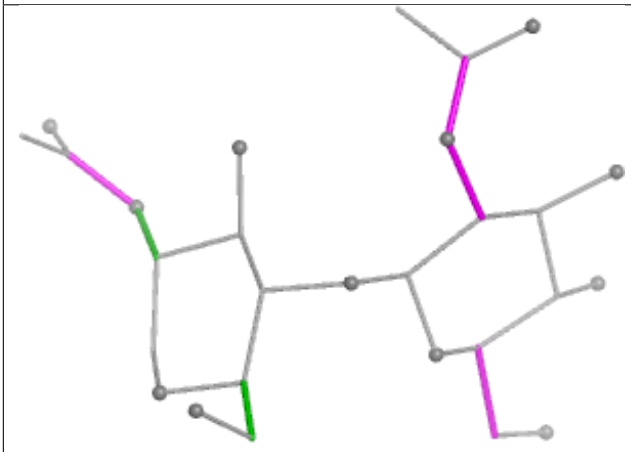
Oligosaccharide Chain G



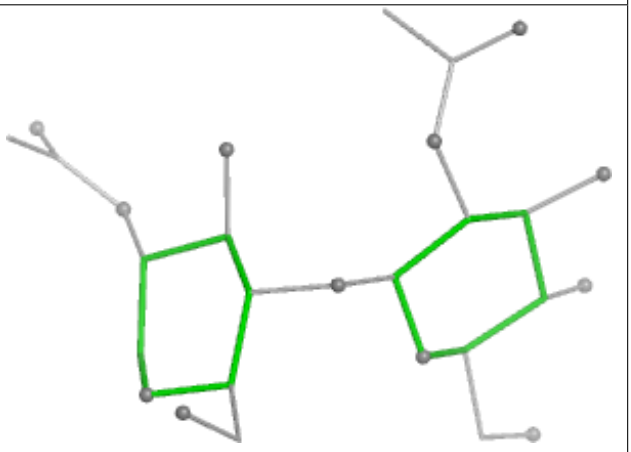
Bond lengths



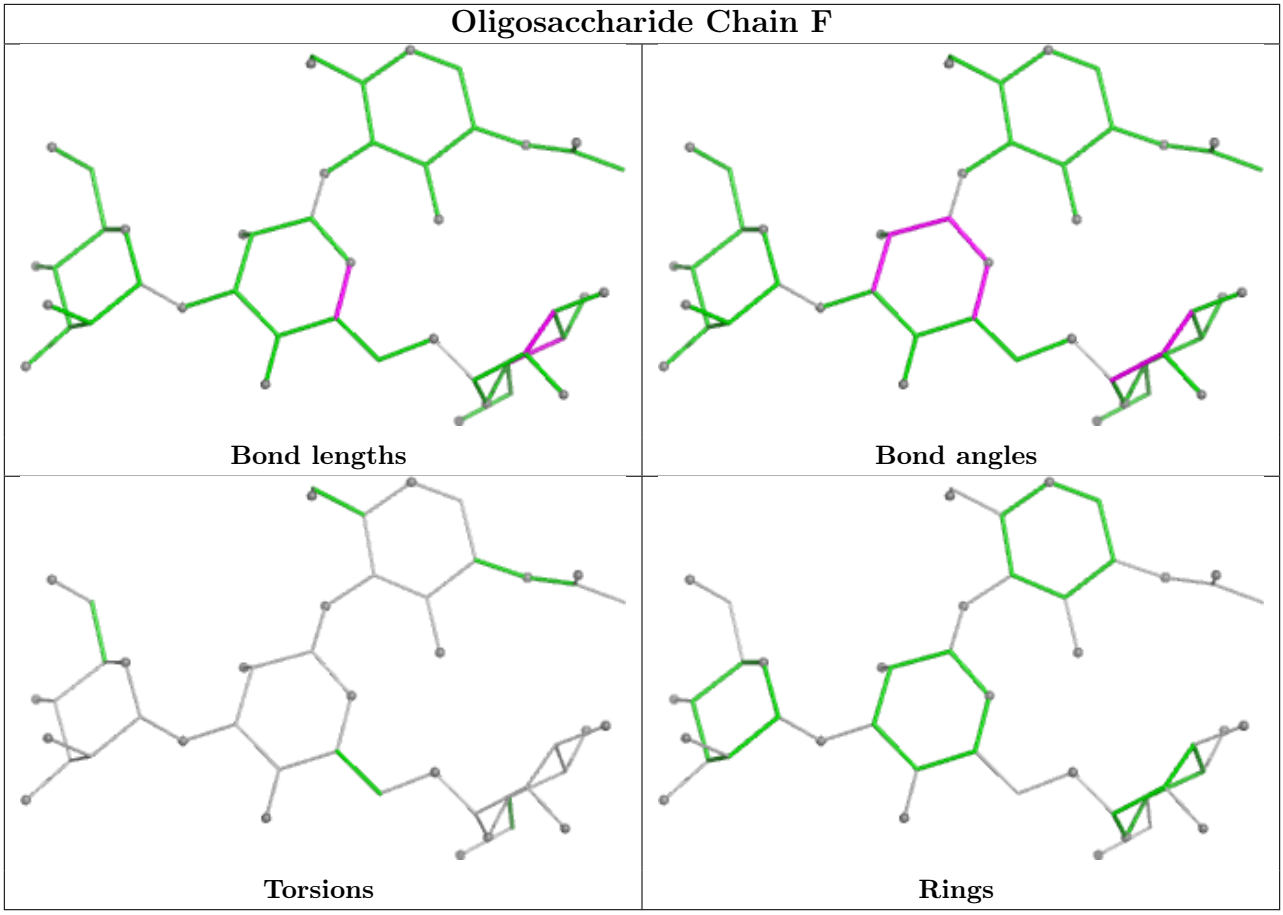
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 16 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
8	NAG	A	404	-	14,14,15	0.38	0	17,19,21	1.36	3 (17%)
8	NAG	B	403	-	14,14,15	0.35	0	17,19,21	1.43	3 (17%)
7	MES	A	405	-	12,12,12	1.29	1 (8%)	14,16,16	0.54	0
5	HEM	A	401	1,9	50,50,50	1.64	14 (28%)	66,82,82	1.67	15 (22%)
11	PO4	B	408	-	4,4,4	2.29	1 (25%)	6,6,6	0.73	0
7	MES	A	403	-	12,12,12	0.91	0	14,16,16	1.27	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MES	B	405	-	12,12,12	1.21	2 (16%)	14,16,16	0.62	0
8	NAG	A	406	-	14,14,15	0.37	0	17,19,21	0.84	0
6	GOL	A	407	-	5,5,5	0.38	0	5,5,5	0.46	0
5	HEM	B	402	1,9	50,50,50	1.66	12 (24%)	66,82,82	2.02	22 (33%)
7	MES	B	406	-	12,12,12	1.43	1 (8%)	14,16,16	1.27	2 (14%)
6	GOL	A	402	-	5,5,5	0.19	0	5,5,5	0.26	0
6	GOL	B	407	-	5,5,5	0.30	0	5,5,5	0.33	0
7	MES	B	404	-	12,12,12	0.92	0	14,16,16	1.34	2 (14%)
8	NAG	B	401	-	14,14,15	0.50	0	17,19,21	2.15	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
8	NAG	A	404	-	-	0/6/23/26	0/1/1/1
8	NAG	B	403	-	-	2/6/23/26	0/1/1/1
7	MES	A	405	-	-	3/6/14/14	0/1/1/1
5	HEM	A	401	1,9	-	4/14/54/54	-
7	MES	A	403	-	-	1/6/14/14	0/1/1/1
7	MES	B	405	-	-	2/6/14/14	0/1/1/1
8	NAG	A	406	-	-	3/6/23/26	0/1/1/1
6	GOL	A	407	-	-	2/4/4/4	-
5	HEM	B	402	1,9	-	3/14/54/54	-
7	MES	B	406	-	-	0/6/14/14	0/1/1/1
6	GOL	A	402	-	-	0/4/4/4	-
6	GOL	B	407	-	-	1/4/4/4	-
7	MES	B	404	-	-	1/6/14/14	0/1/1/1
8	NAG	B	401	-	-	0/6/23/26	0/1/1/1

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401	HEM	FE-NB	4.07	2.07	1.94
11	B	408	PO4	P-O1	4.01	1.60	1.50
5	A	401	HEM	C1B-NB	-3.72	1.33	1.40
5	B	402	HEM	C1B-NB	-3.56	1.34	1.40
5	B	402	HEM	C4D-ND	-3.22	1.34	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	401	NAG	O5-C1-C2	8.07	124.02	111.29
5	B	402	HEM	CHD-C4C-NC	5.25	130.12	124.44
5	B	402	HEM	C1B-NB-C4B	5.11	110.35	105.07
5	B	402	HEM	CHB-C1B-NB	4.38	129.77	124.37
5	B	402	HEM	C4C-NC-C1C	4.38	109.63	105.35

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	407	GOL	O1-C1-C2-C3
7	A	403	MES	C8-C7-N4-C5
7	B	405	MES	C8-C7-N4-C5
8	B	403	NAG	C8-C7-N2-C2
8	B	403	NAG	O7-C7-N2-C2

There are no ring outliers.

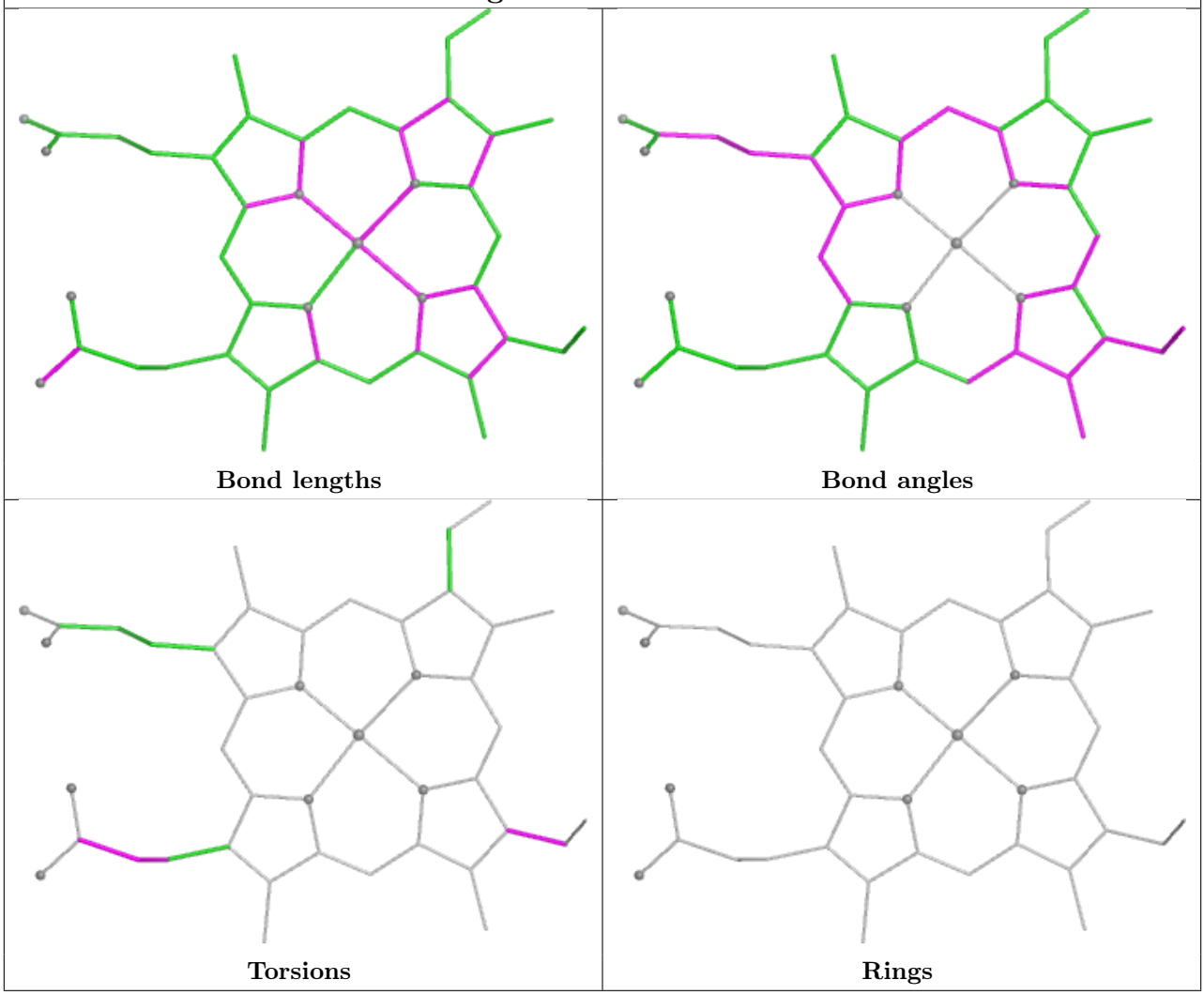
9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	404	NAG	3	0
8	B	403	NAG	8	0
7	A	405	MES	2	0
5	A	401	HEM	1	0
7	B	405	MES	2	0
8	A	406	NAG	3	0
5	B	402	HEM	5	0
6	B	407	GOL	1	0
8	B	401	NAG	4	0

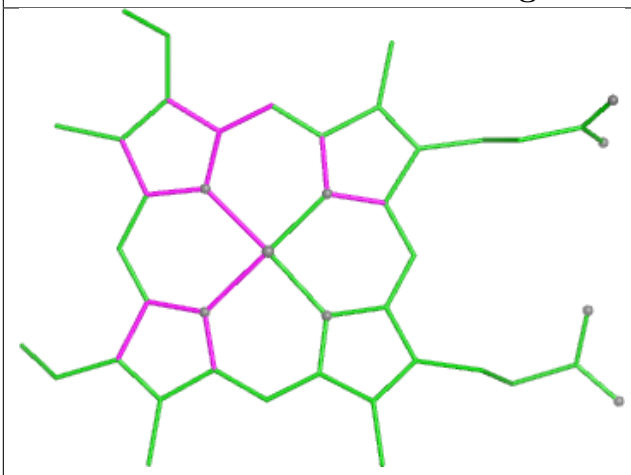
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

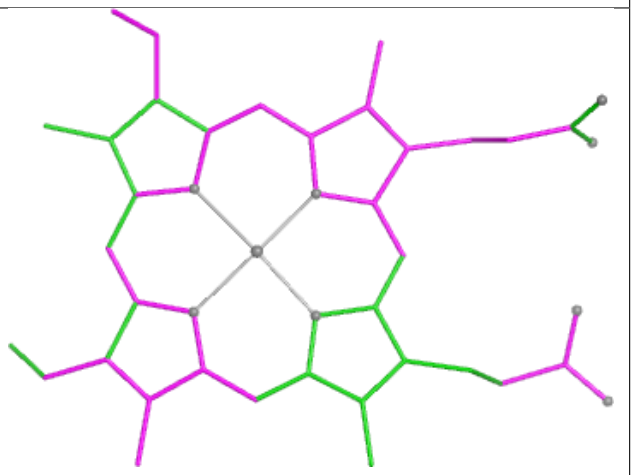
Ligand HEM A 401



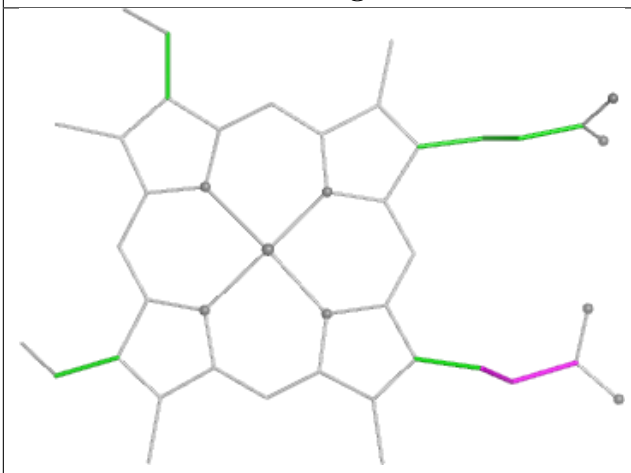
Ligand HEM B 402



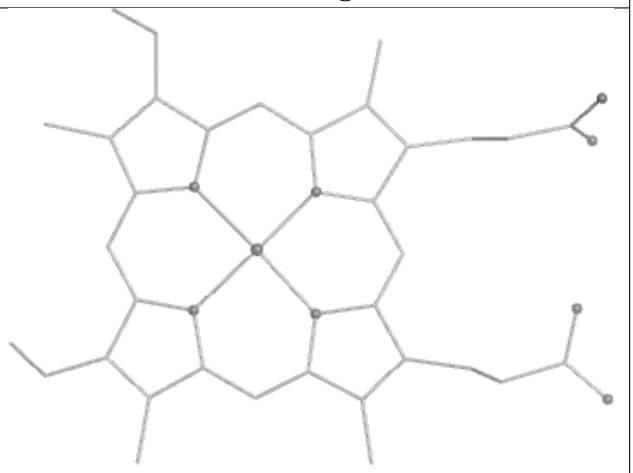
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/334 (100%)	0.02	3 (0%)	81	83	34, 51, 79, 131	1 (0%)
1	B	334/334 (100%)	-0.03	2 (0%)	85	88	33, 53, 73, 100	1 (0%)
All	All	668/668 (100%)	-0.01	5 (0%)	84	86	33, 53, 75, 131	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LEU	6.0
1	B	1	LEU	5.1
1	A	334	LEU	4.1
1	A	274	PRO	3.1
1	B	334	LEU	3.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	2	14/15	0.32	0.17	76,87,95,97	0
3	NAG	E	2	14/15	0.48	0.17	95,112,124,124	0
3	NAG	G	1	14/15	0.58	0.18	56,79,92,94	0
2	MAN	C	5	11/12	0.61	0.13	65,70,73,81	0

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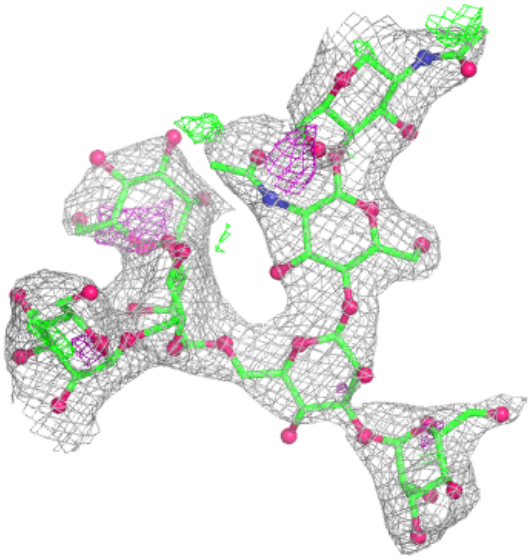
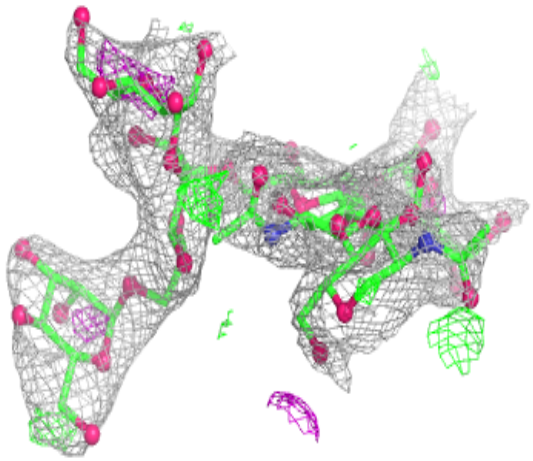
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	2	14/15	0.68	0.14	89,104,119,127	0
4	MAN	F	4	11/12	0.70	0.14	68,76,80,85	0
2	MAN	C	6	11/12	0.78	0.12	66,69,75,79	0
2	NAG	C	2	14/15	0.78	0.14	70,90,96,97	0
4	BMA	F	2	11/12	0.80	0.13	56,66,76,78	0
4	NAG	F	1	14/15	0.82	0.14	80,91,102,104	0
4	MAN	F	3	11/12	0.83	0.12	58,66,73,74	0
2	NAG	C	1	14/15	0.83	0.16	58,74,86,88	0
2	BMA	C	3	11/12	0.85	0.12	77,97,108,112	0
2	MAN	C	7	11/12	0.85	0.11	56,66,79,80	0
2	MAN	C	4	11/12	0.87	0.10	54,66,70,73	0
3	NAG	D	1	14/15	0.92	0.09	48,59,69,83	0
3	NAG	E	1	14/15	0.93	0.08	55,66,73,80	0

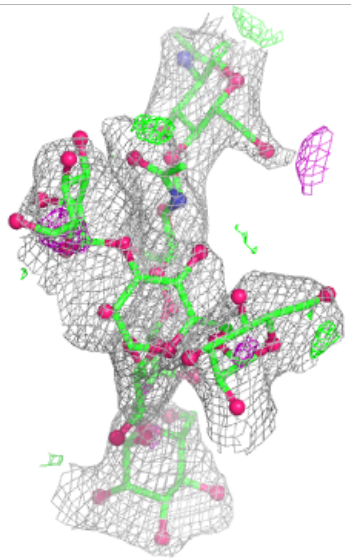
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

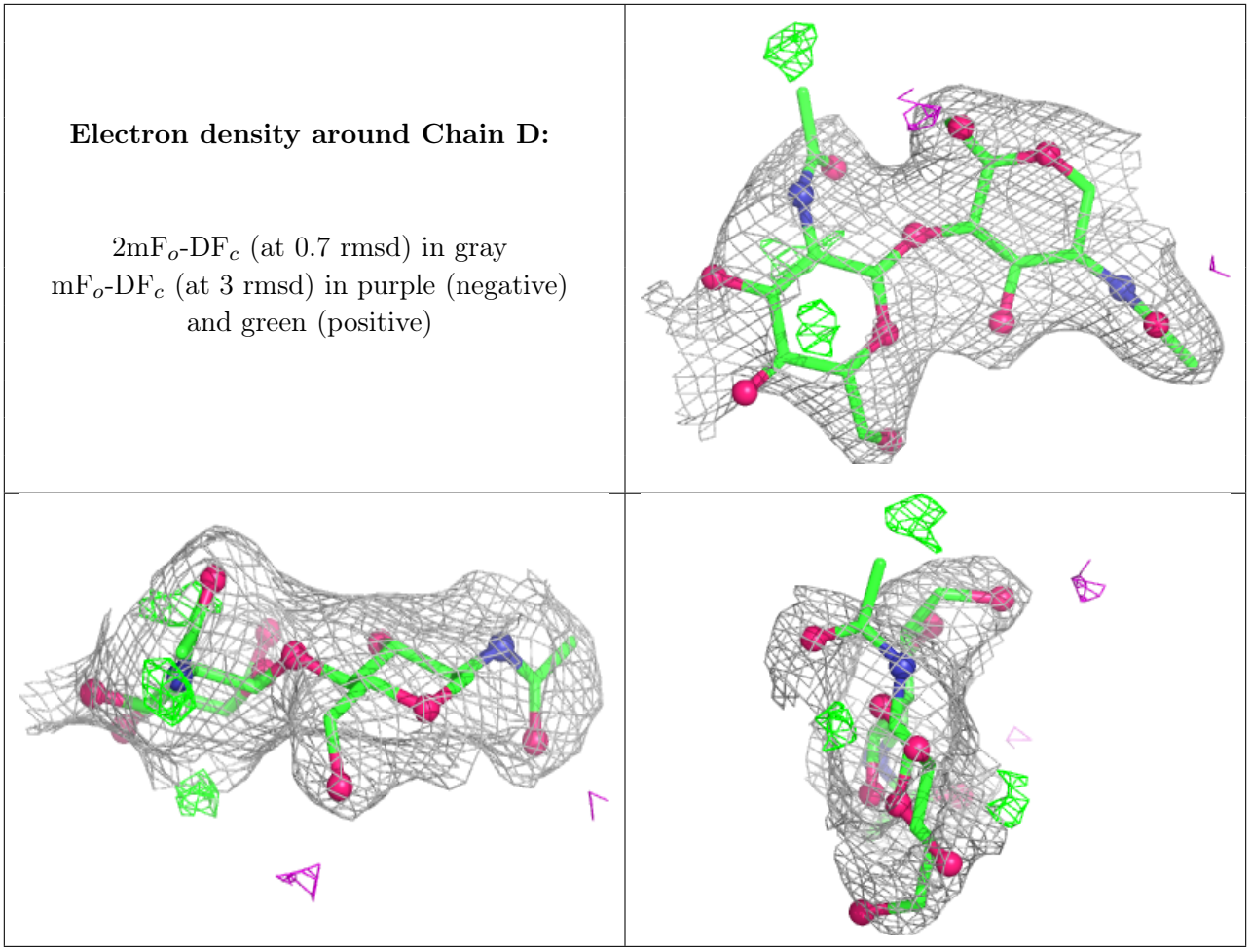






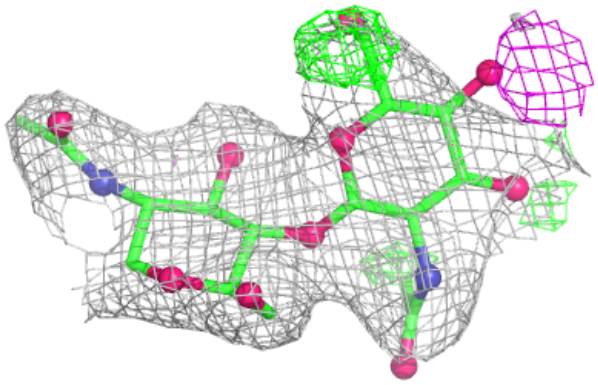
Electron density around Chain D:

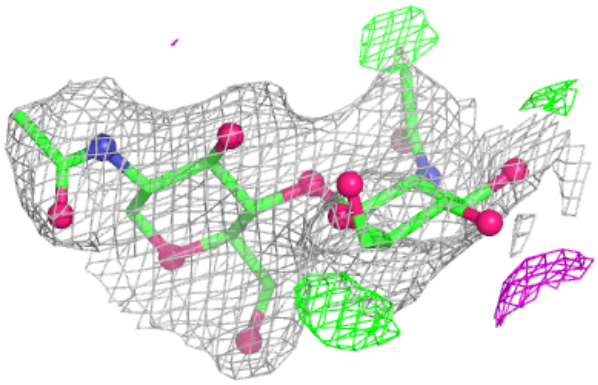
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

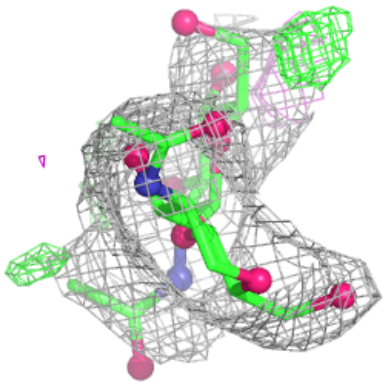


Electron density around Chain E:

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

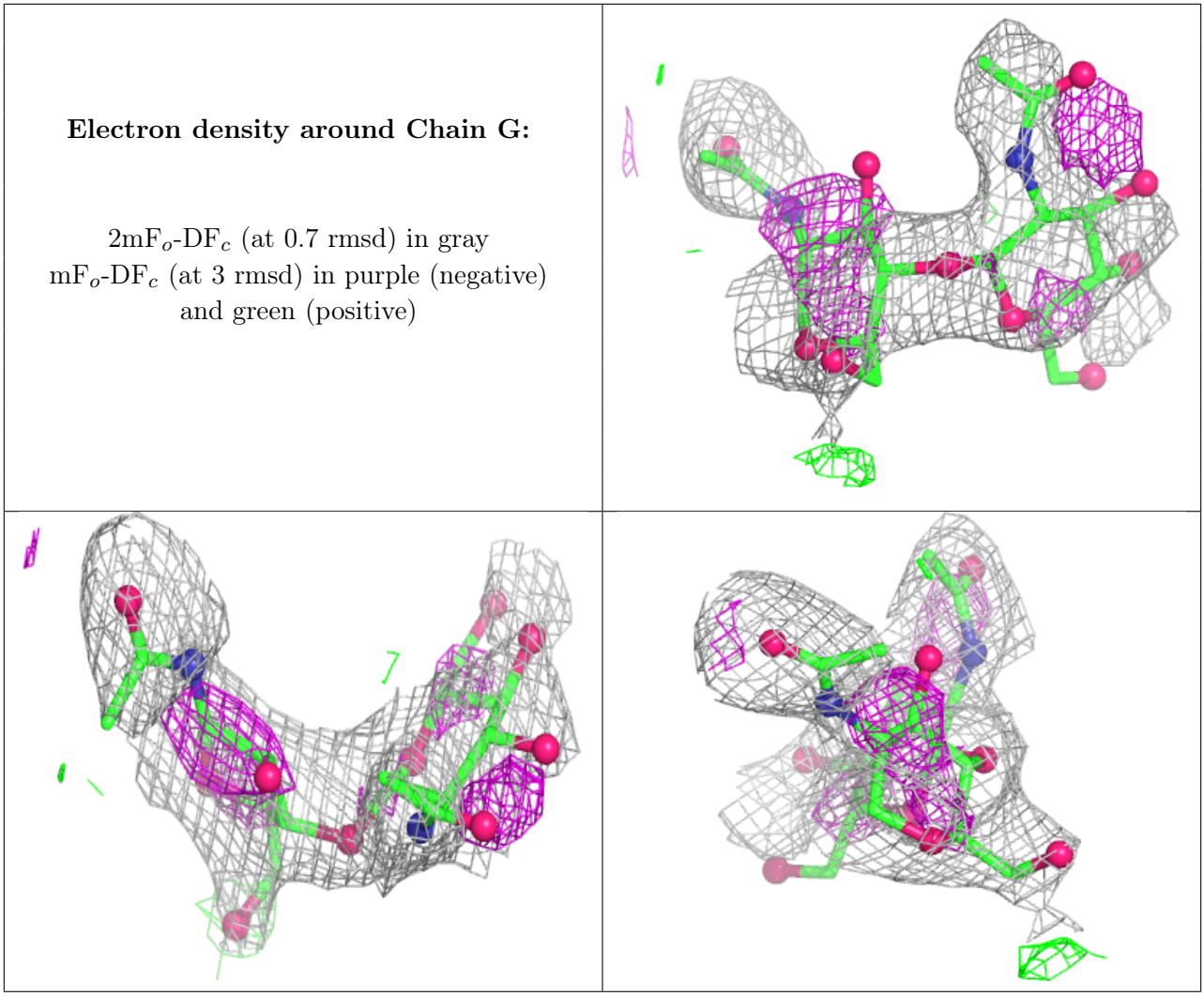






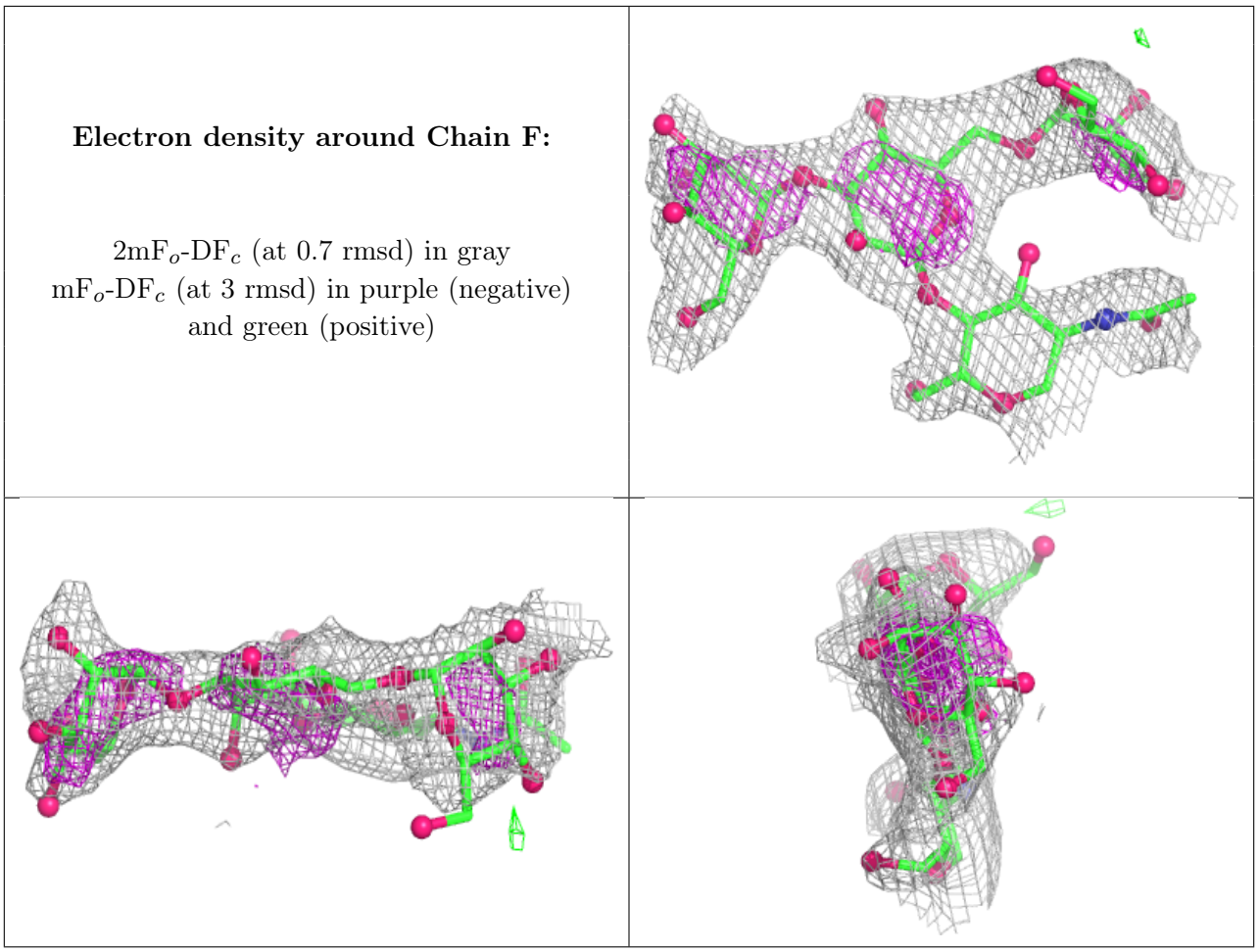
Electron density around Chain G:

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



Electron density around Chain F:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MES	B	406	12/12	0.30	0.22	62,67,75,78	0
8	NAG	A	406	14/15	0.62	0.18	67,82,93,94	0
7	MES	A	405	12/12	0.67	0.22	58,66,75,80	0
6	GOL	A	402	6/6	0.74	0.15	59,60,66,66	0
7	MES	B	405	12/12	0.75	0.20	58,62,70,72	0
6	GOL	B	407	6/6	0.77	0.15	47,59,64,65	0
8	NAG	A	404	14/15	0.79	0.13	61,76,94,96	0
6	GOL	A	407	6/6	0.79	0.12	47,55,58,59	0
11	PO4	B	408	5/5	0.81	0.12	55,57,60,81	0
10	ZN	A	415	1/1	0.83	0.10	70,70,70,70	0
8	NAG	B	403	14/15	0.87	0.15	75,88,98,104	0

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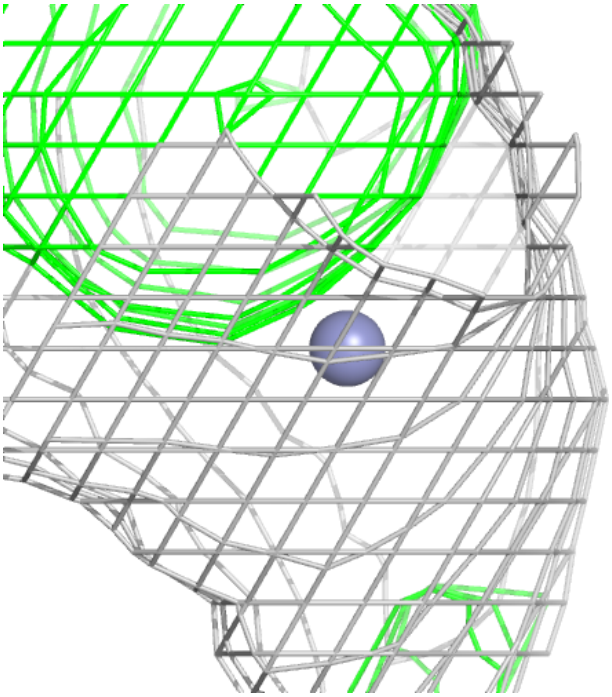
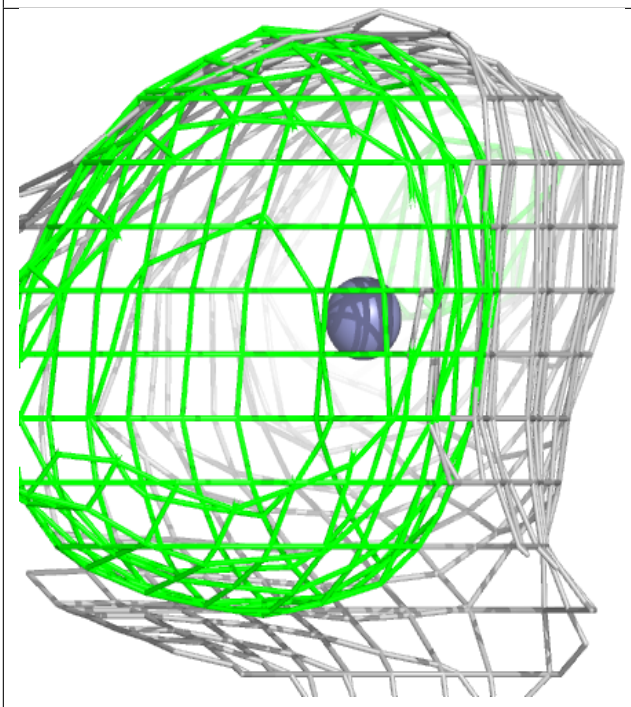
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	B	401	14/15	0.92	0.09	68,76,100,104	0
10	ZN	A	416	1/1	0.92	0.07	63,63,63,63	0
10	ZN	B	415	1/1	0.92	0.19	81,81,81,81	0
7	MES	A	403	12/12	0.92	0.13	44,52,64,64	0
7	MES	B	404	12/12	0.93	0.13	40,50,56,57	0
10	ZN	B	411	1/1	0.94	0.09	72,72,72,72	0
10	ZN	A	413	1/1	0.96	0.05	76,76,76,76	0
5	HEM	A	401	43/43	0.98	0.07	34,41,51,55	0
10	ZN	B	412	1/1	0.98	0.04	56,56,56,56	0
10	ZN	B	413	1/1	0.98	0.06	67,67,67,67	0
10	ZN	B	414	1/1	0.98	0.09	66,66,66,66	0
5	HEM	B	402	43/43	0.98	0.07	36,44,50,55	0
10	ZN	A	409	1/1	0.98	0.06	65,65,65,65	0
10	ZN	A	414	1/1	0.99	0.06	60,60,60,60	0
10	ZN	A	411	1/1	0.99	0.03	66,66,66,66	0
10	ZN	A	412	1/1	0.99	0.06	49,49,49,49	0
10	ZN	B	410	1/1	0.99	0.05	49,49,49,49	0
10	ZN	A	410	1/1	0.99	0.04	58,58,58,58	0
9	MG	B	409	1/1	1.00	0.04	34,34,34,34	0
9	MG	A	408	1/1	1.00	0.07	28,28,28,28	0

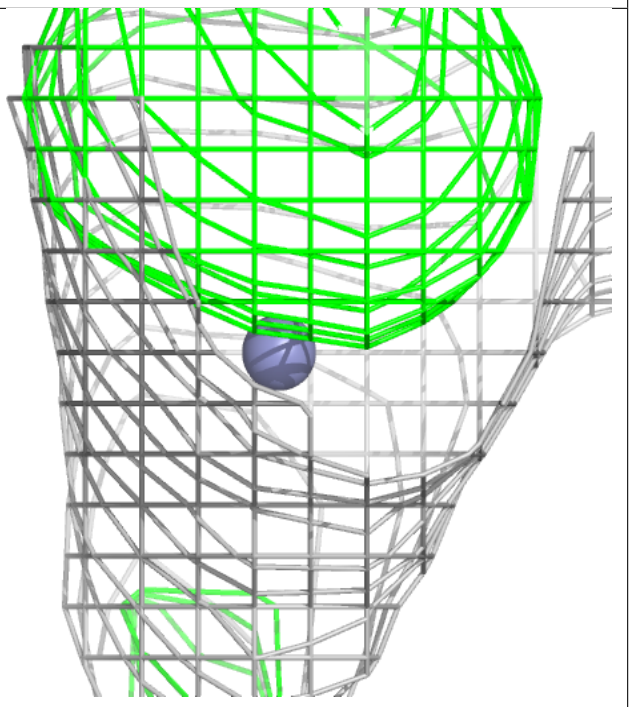
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

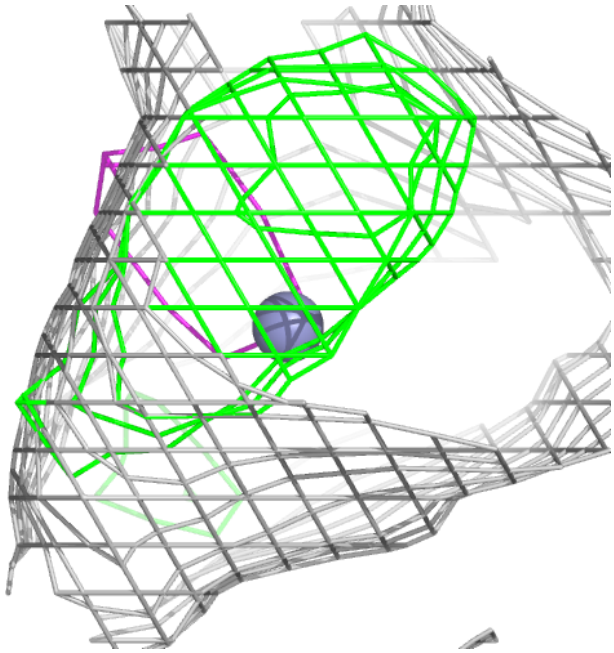


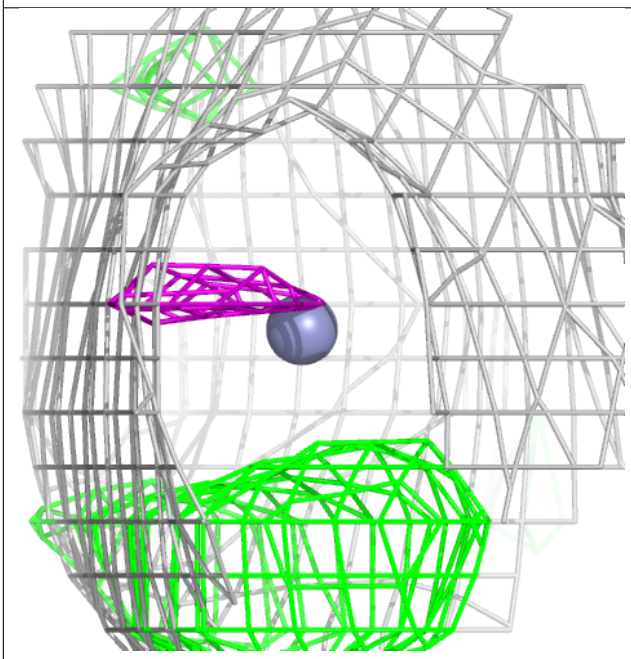


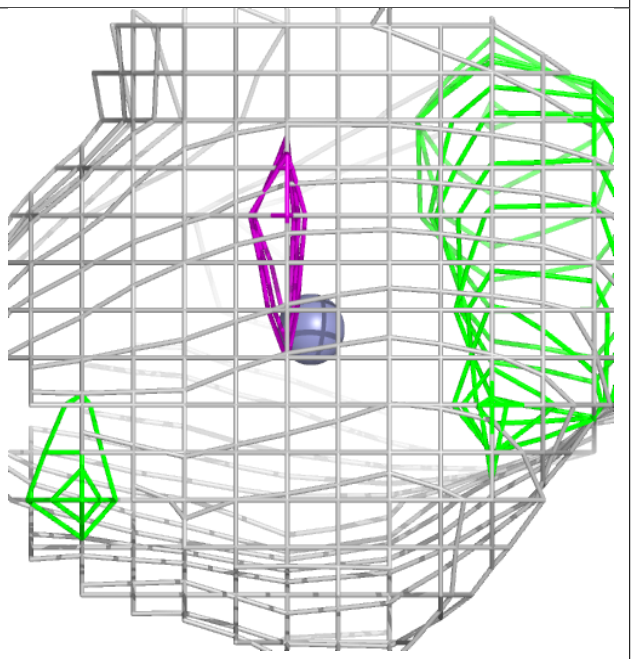


Electron density around ZN A 416:

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

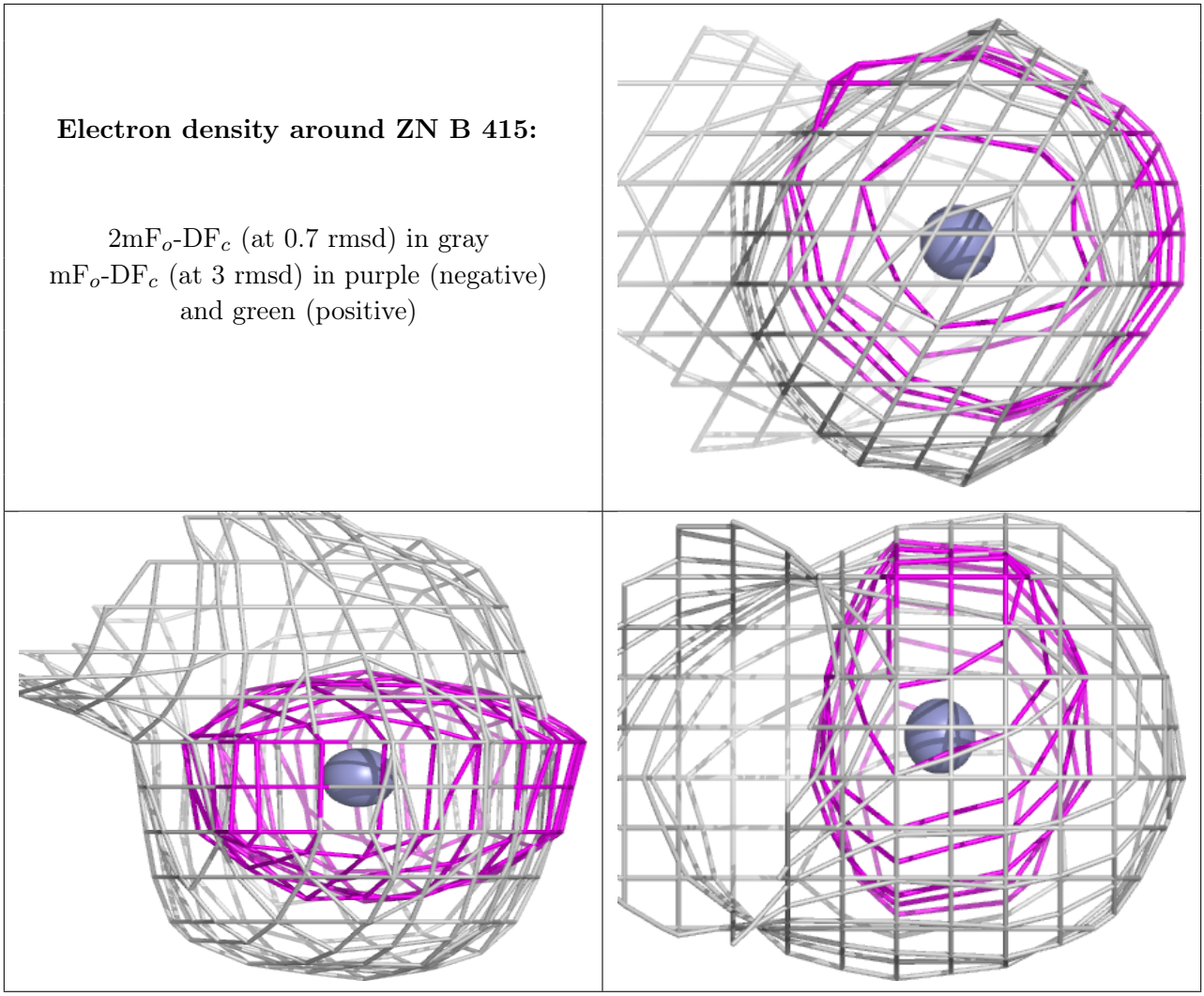






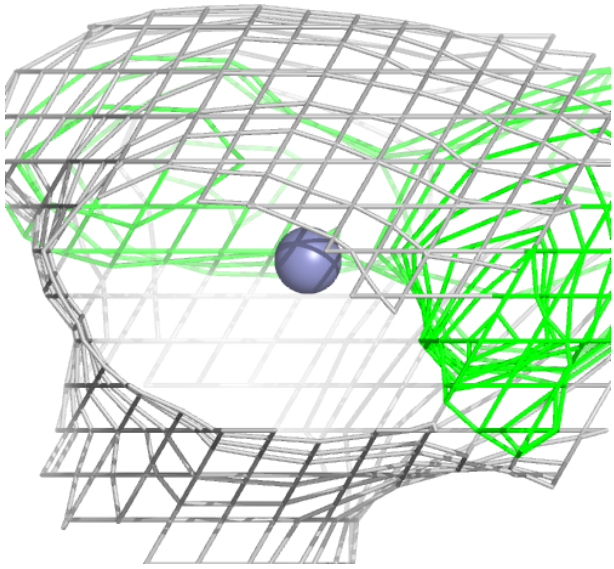
Electron density around ZN B 415:

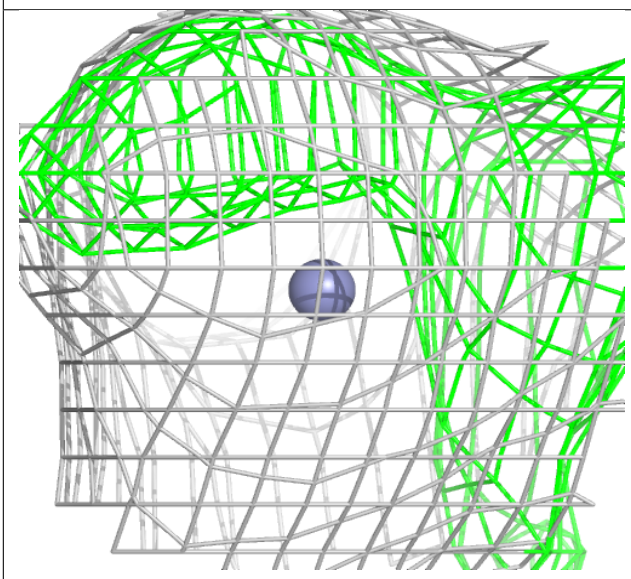
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

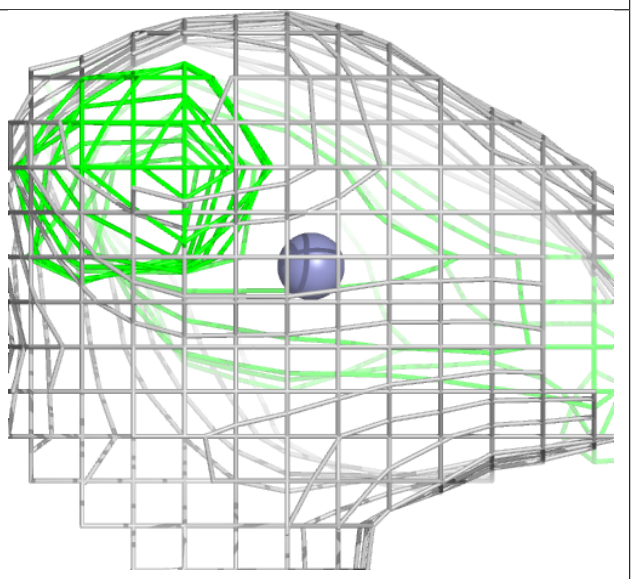


Electron density around ZN B 411:

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

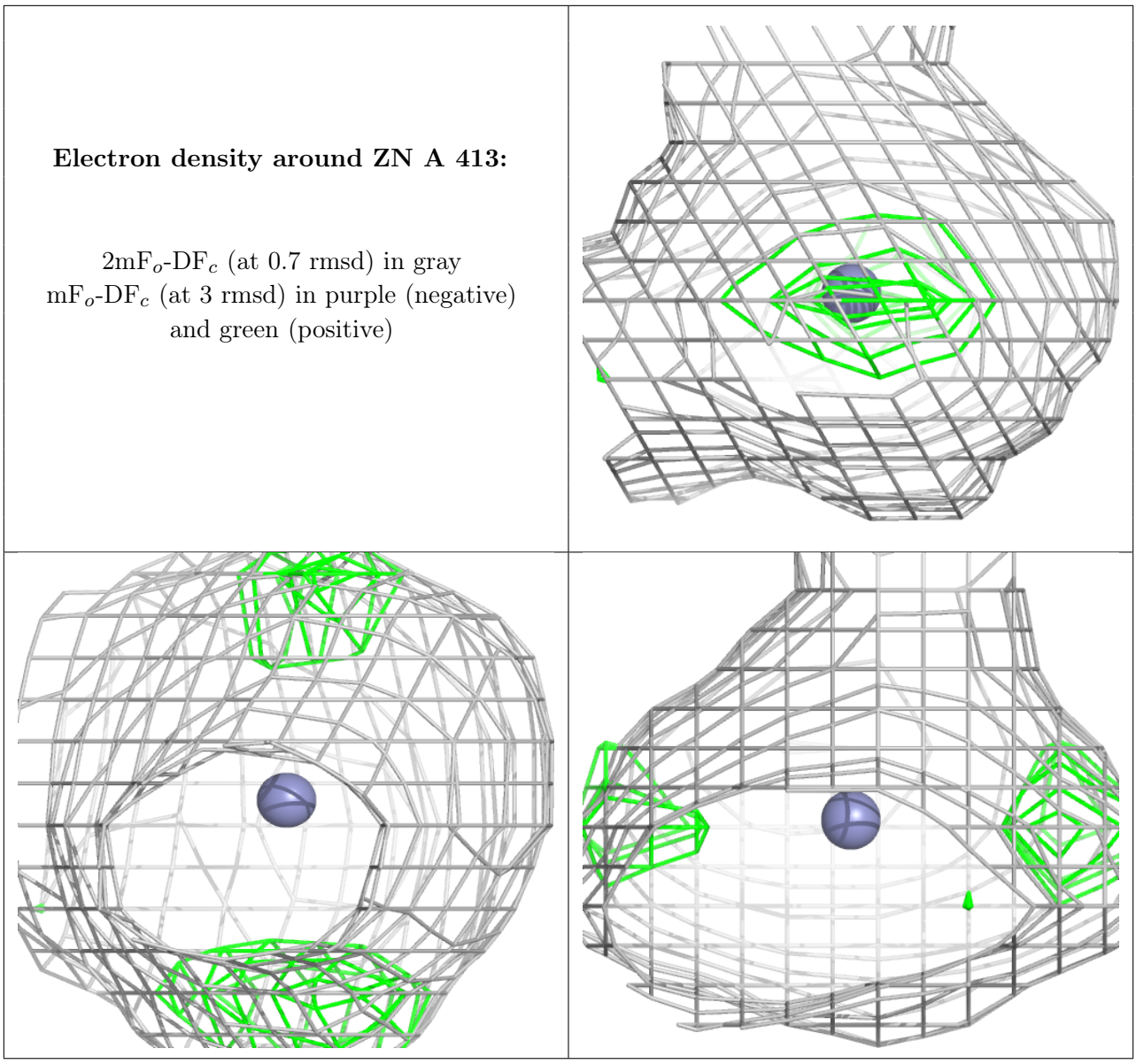






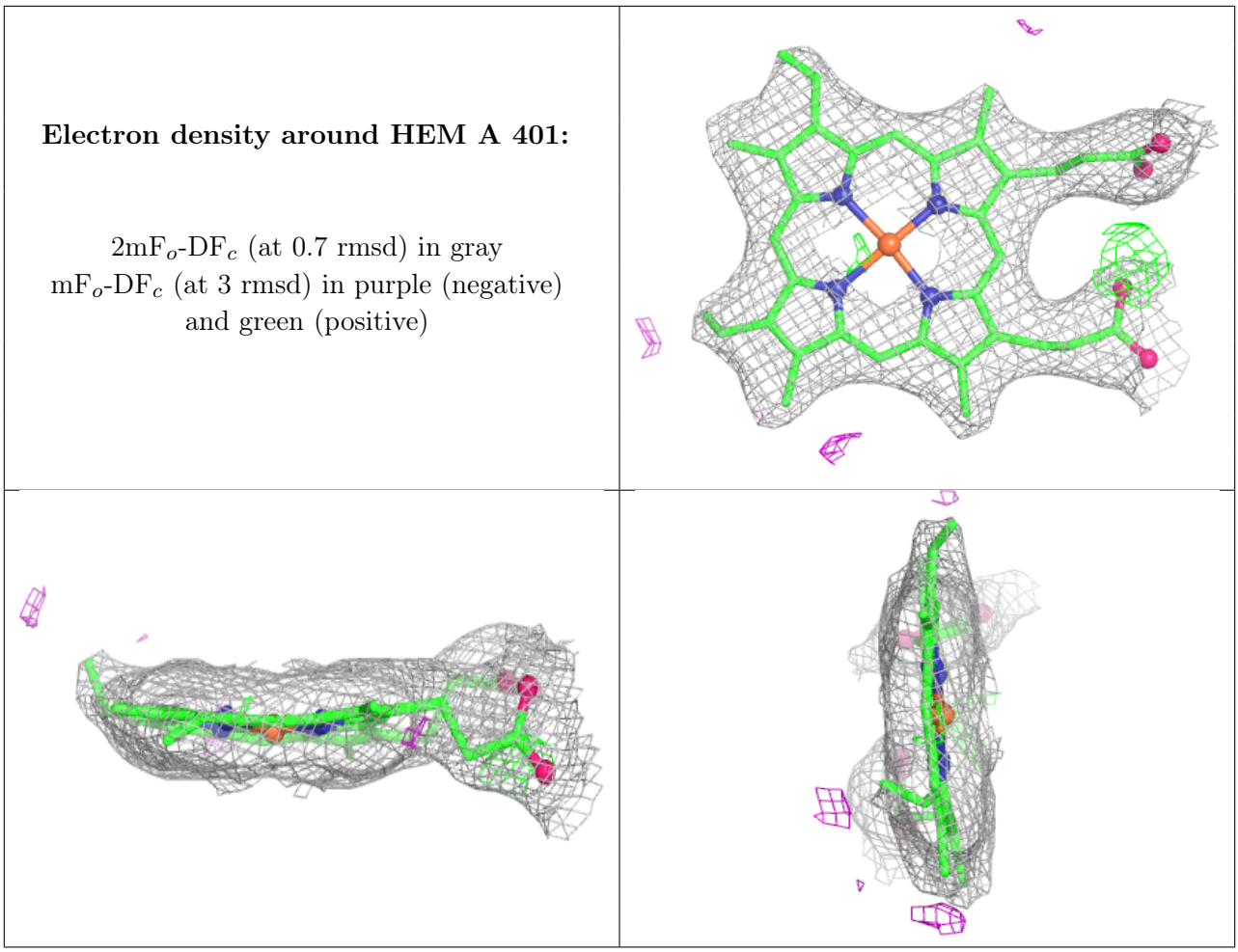
Electron density around ZN A 413:

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



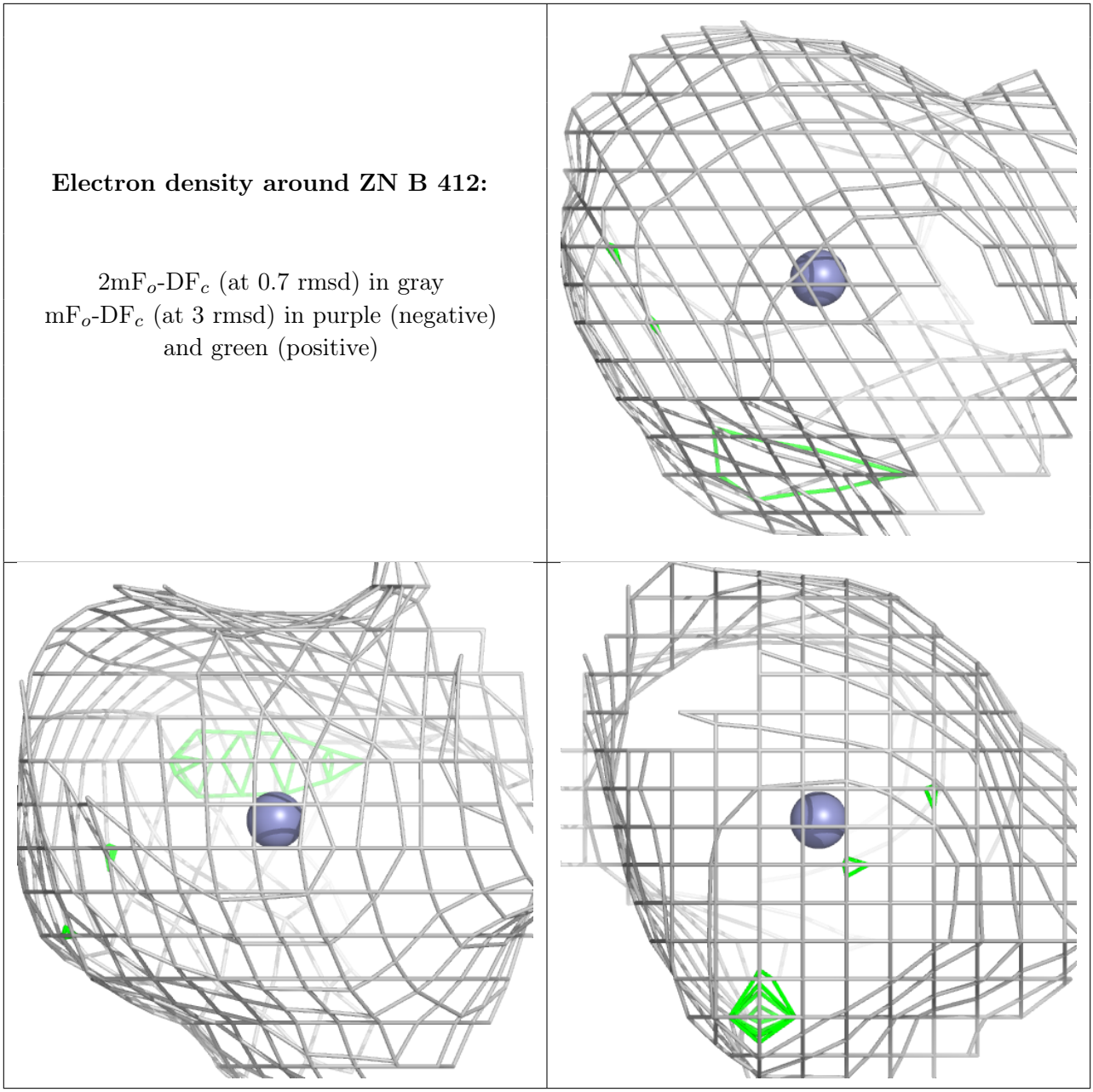
Electron density around HEM A 401:

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



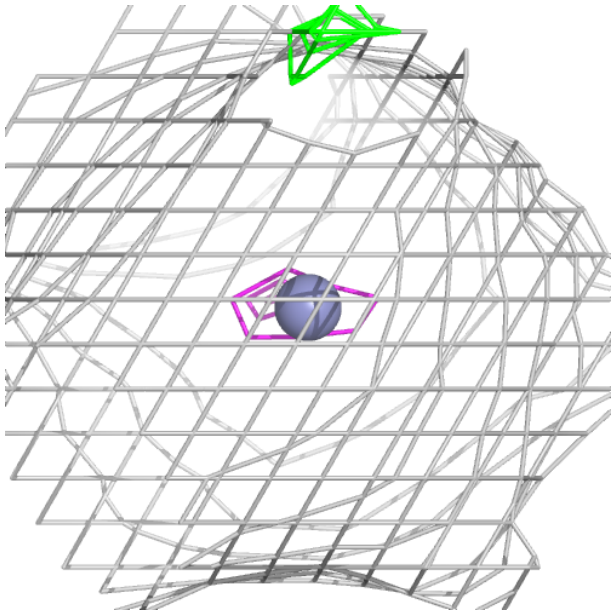
Electron density around ZN B 412:

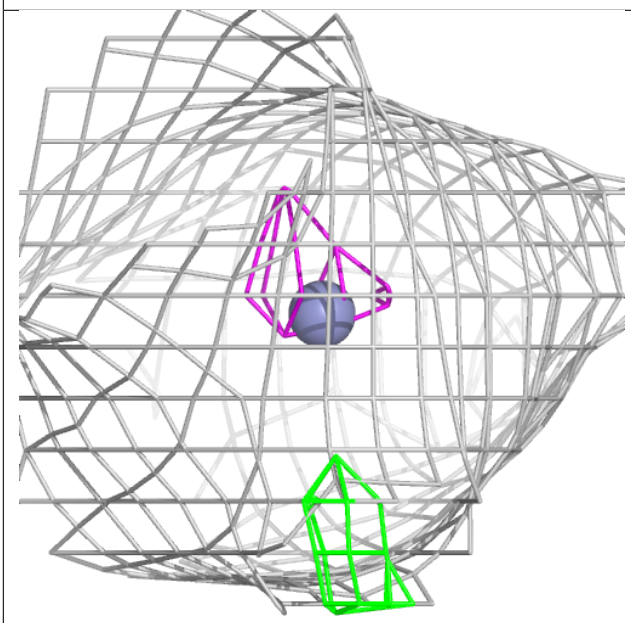
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

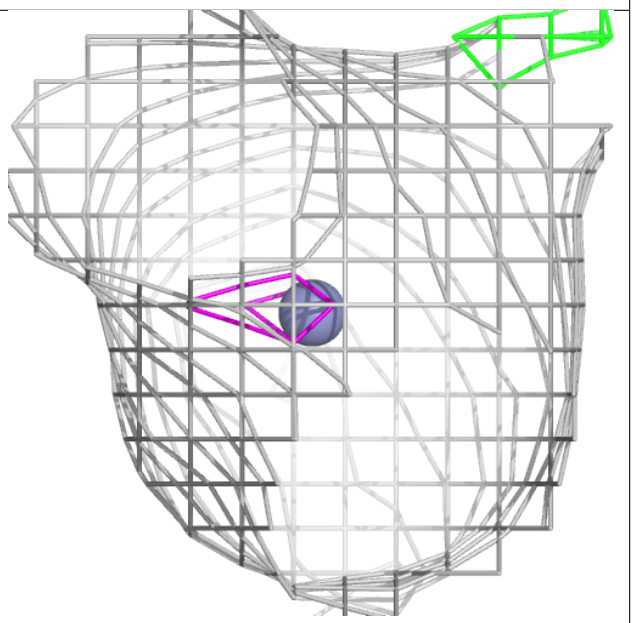


Electron density around ZN B 413:

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

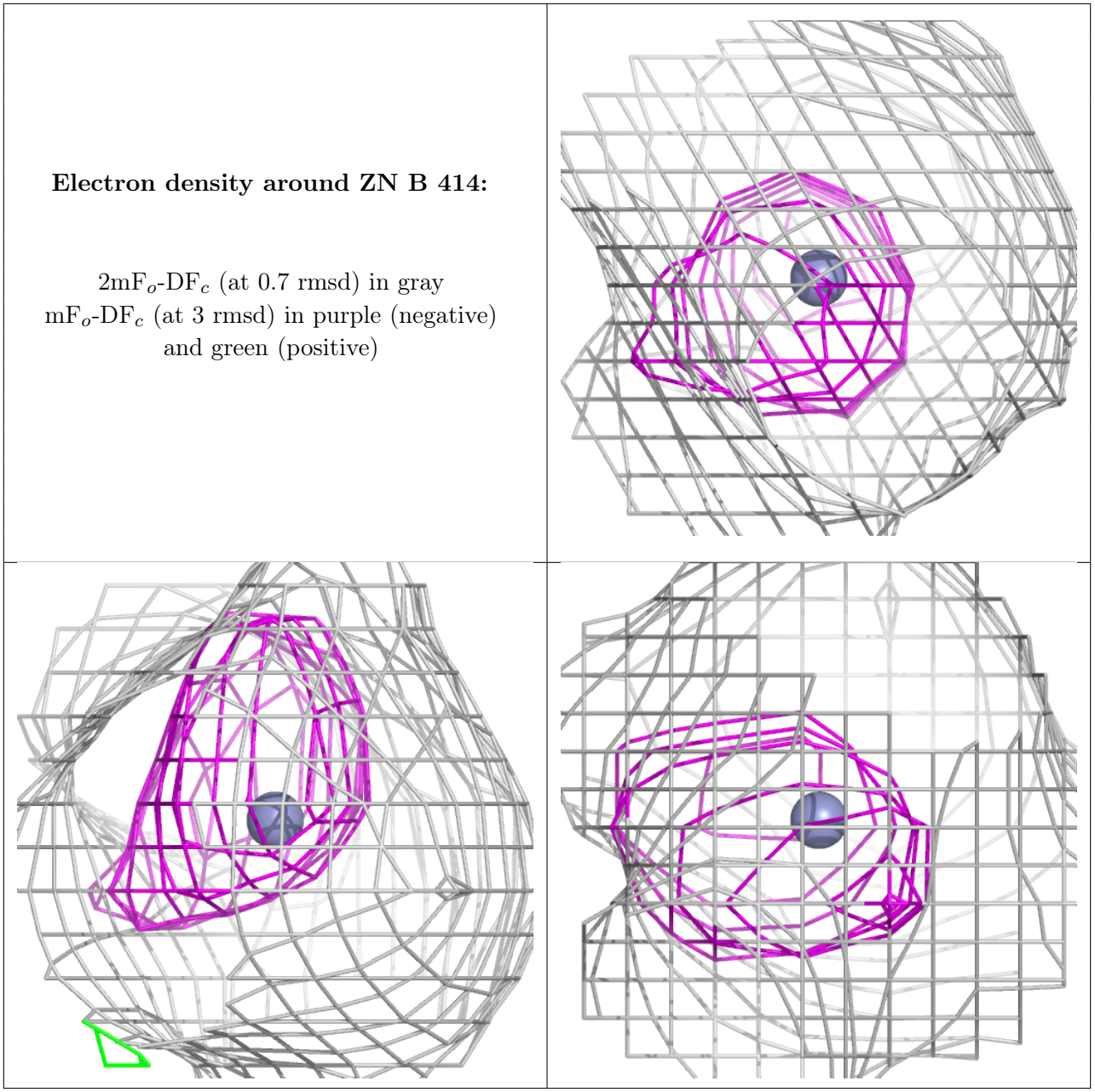






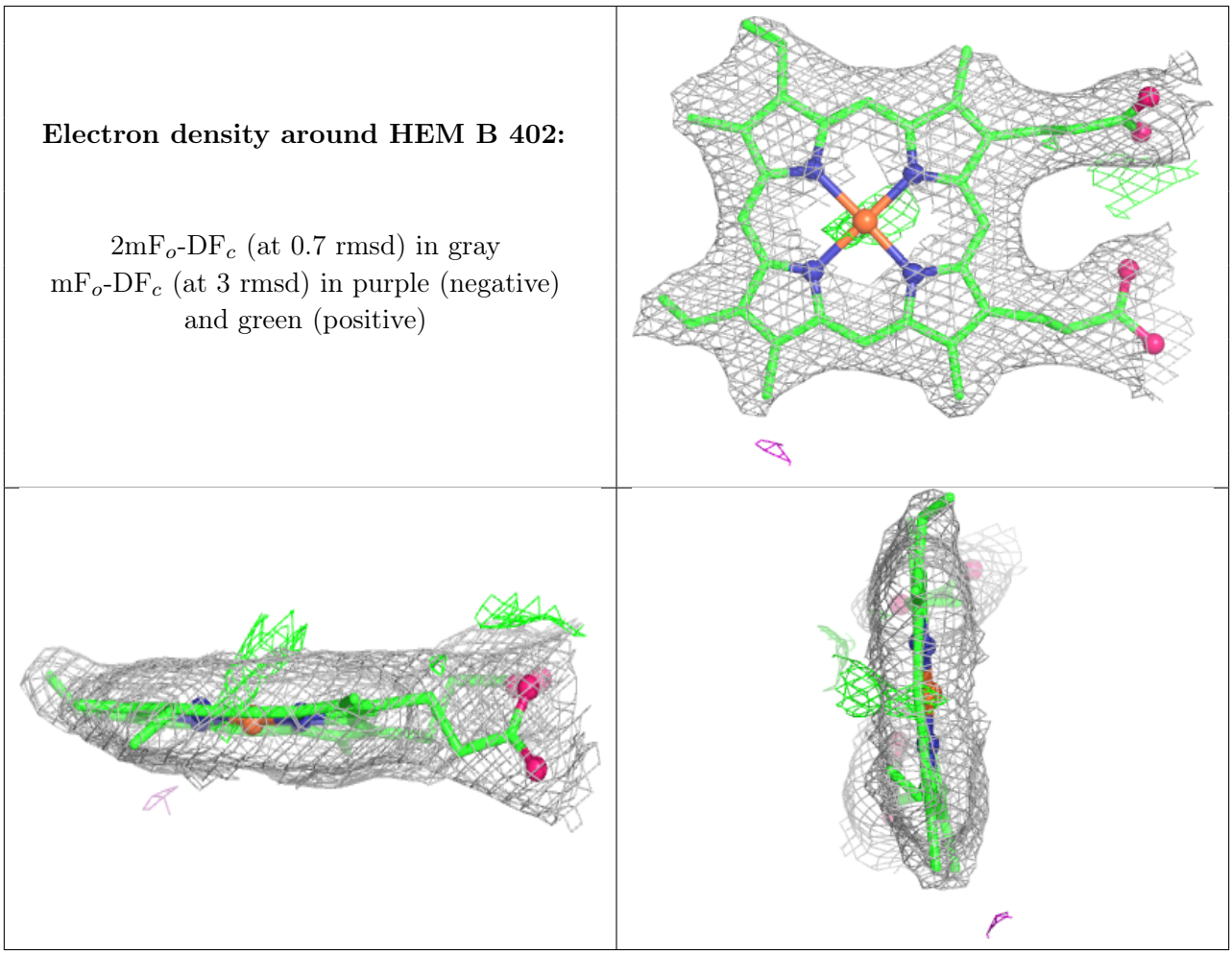
Electron density around ZN B 414:

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



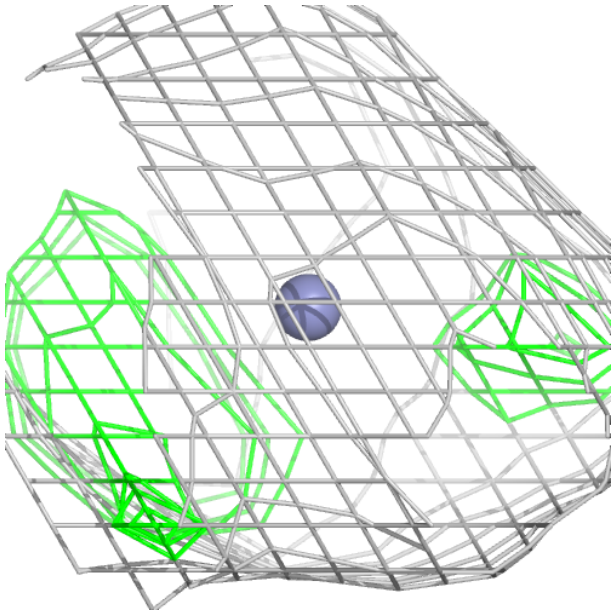
Electron density around HEM B 402:

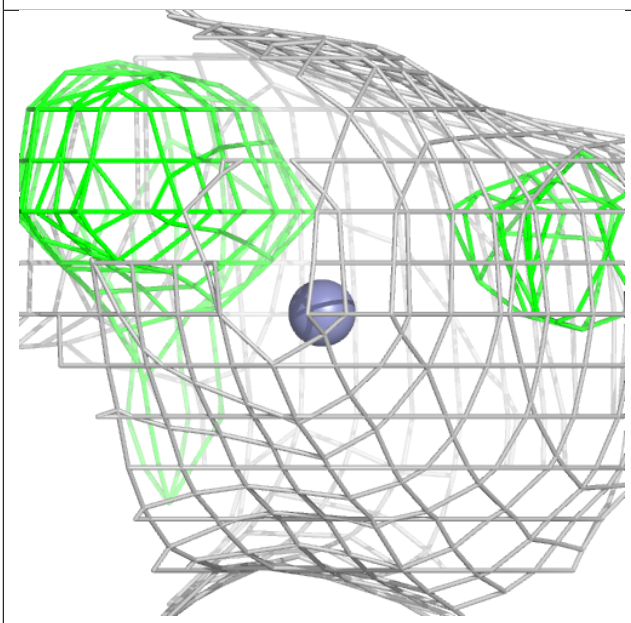
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

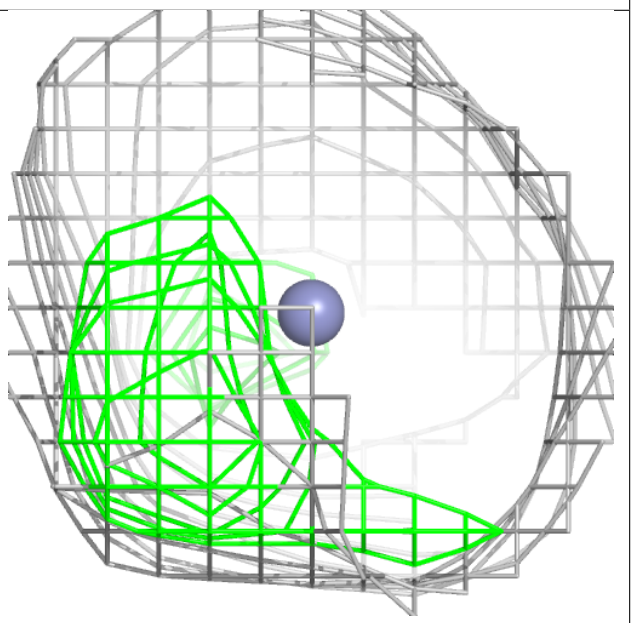


Electron density around ZN A 409:

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

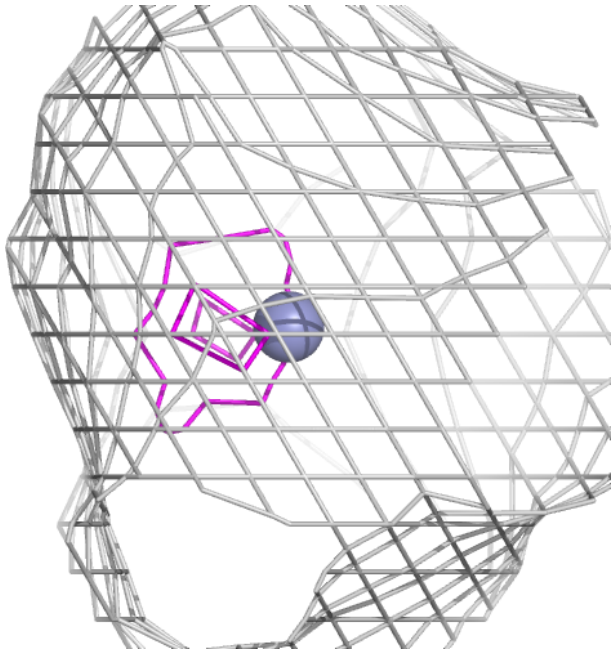


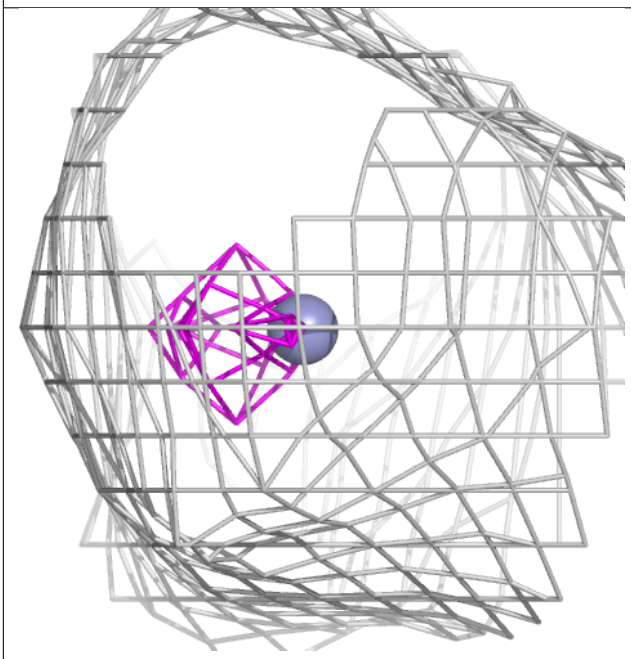


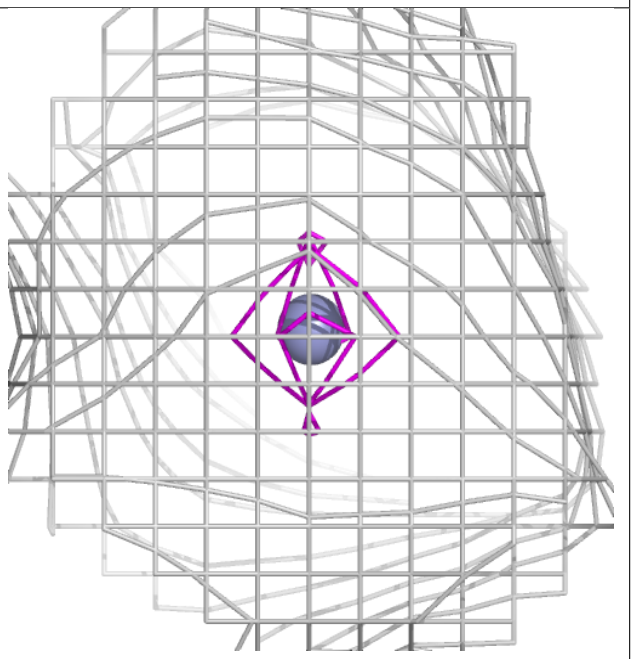


Electron density around ZN A 414:

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

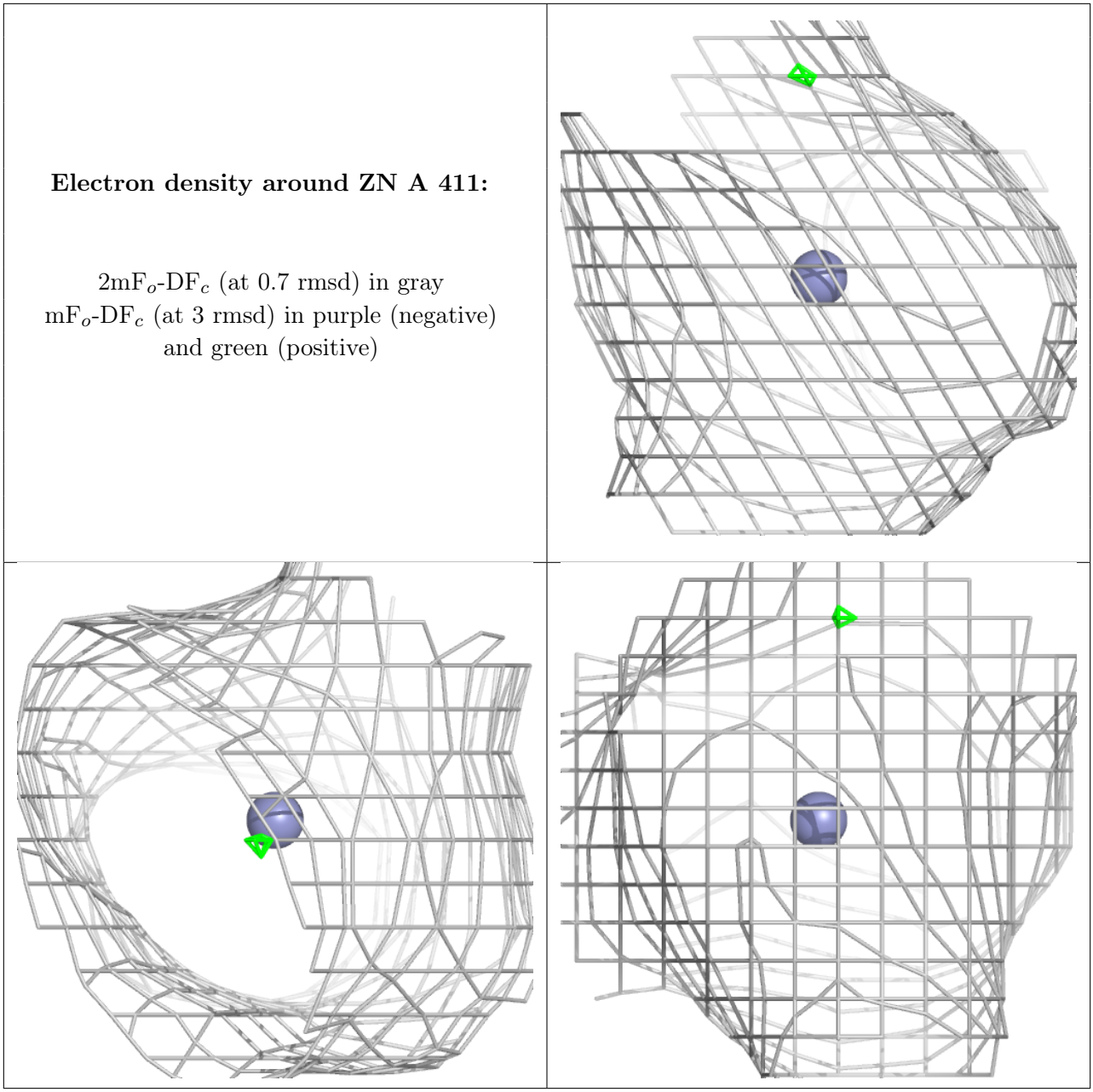






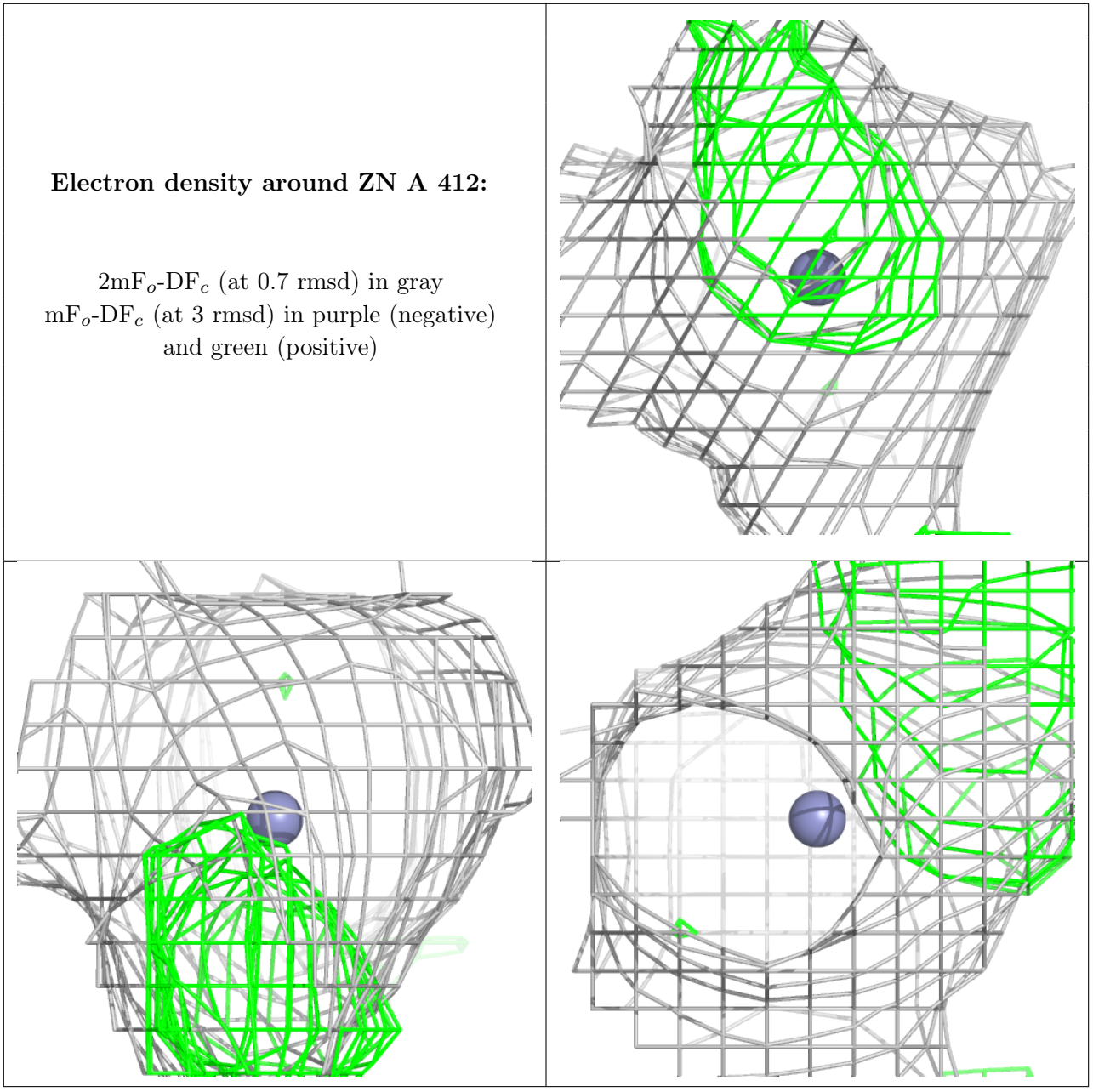
Electron density around ZN A 411:

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



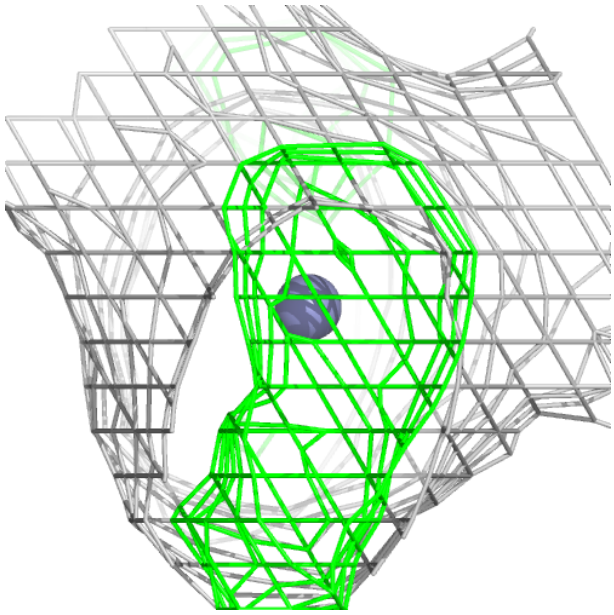
Electron density around ZN A 412:

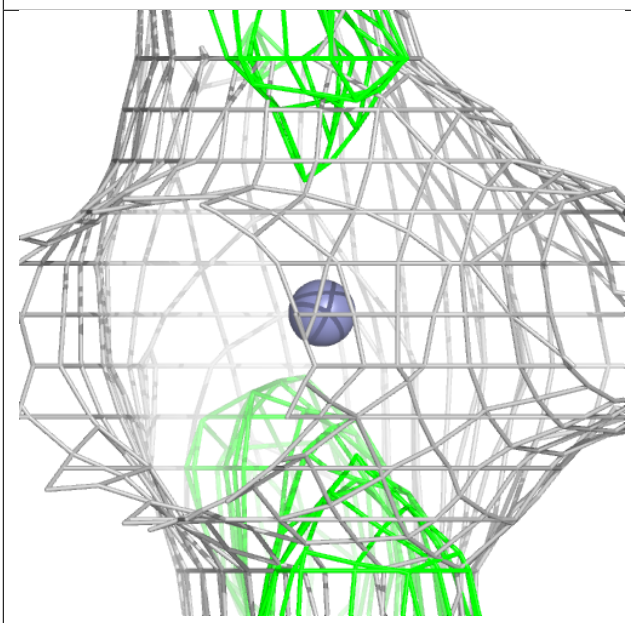
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

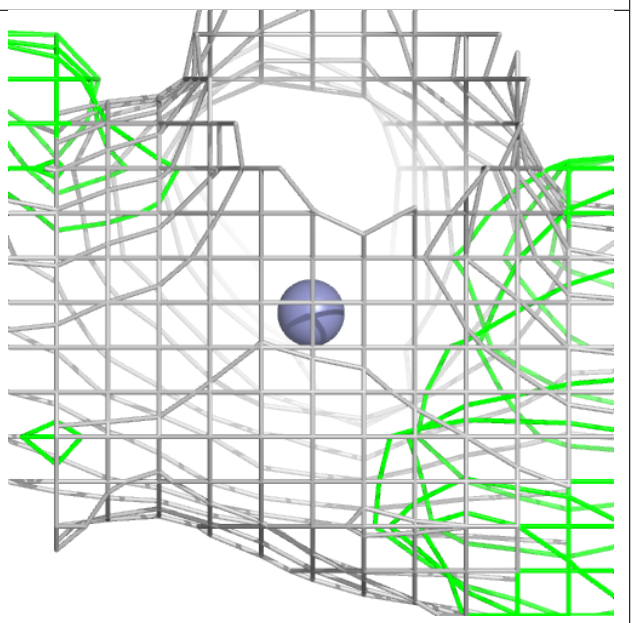


Electron density around ZN B 410:

$2mF_o$-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 410:

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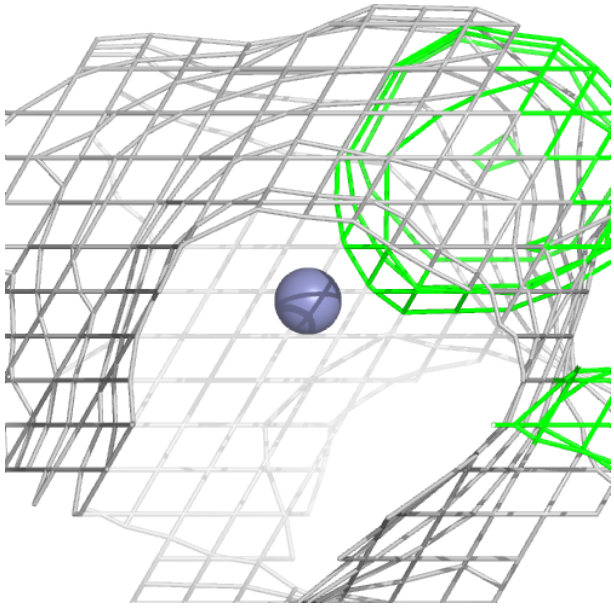
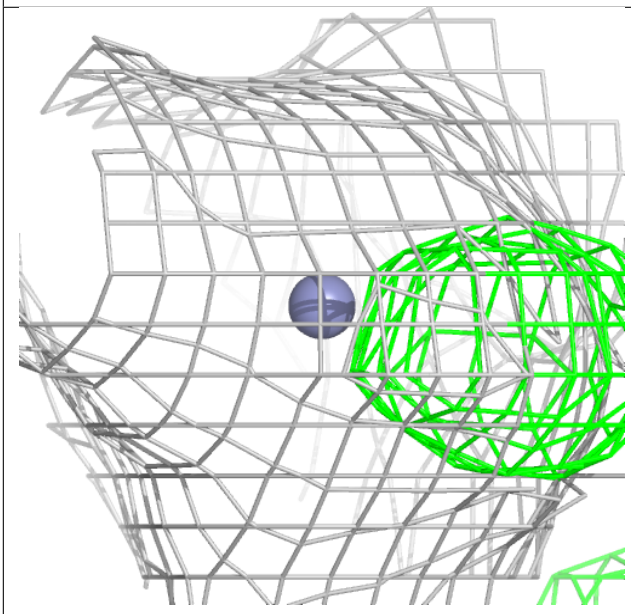
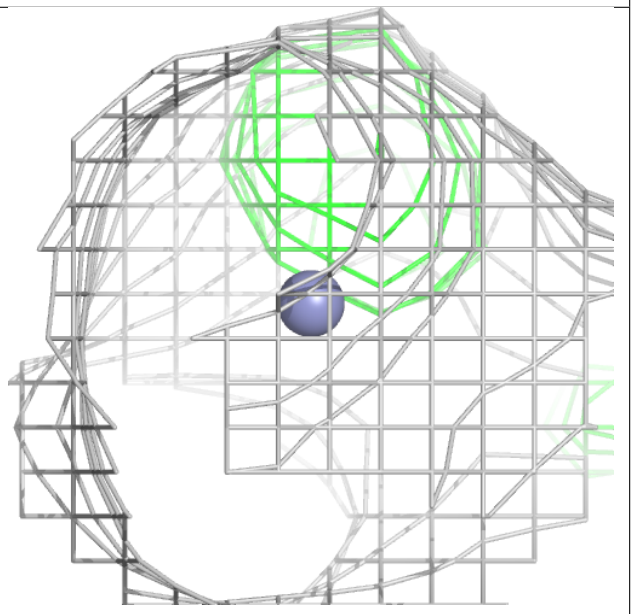
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

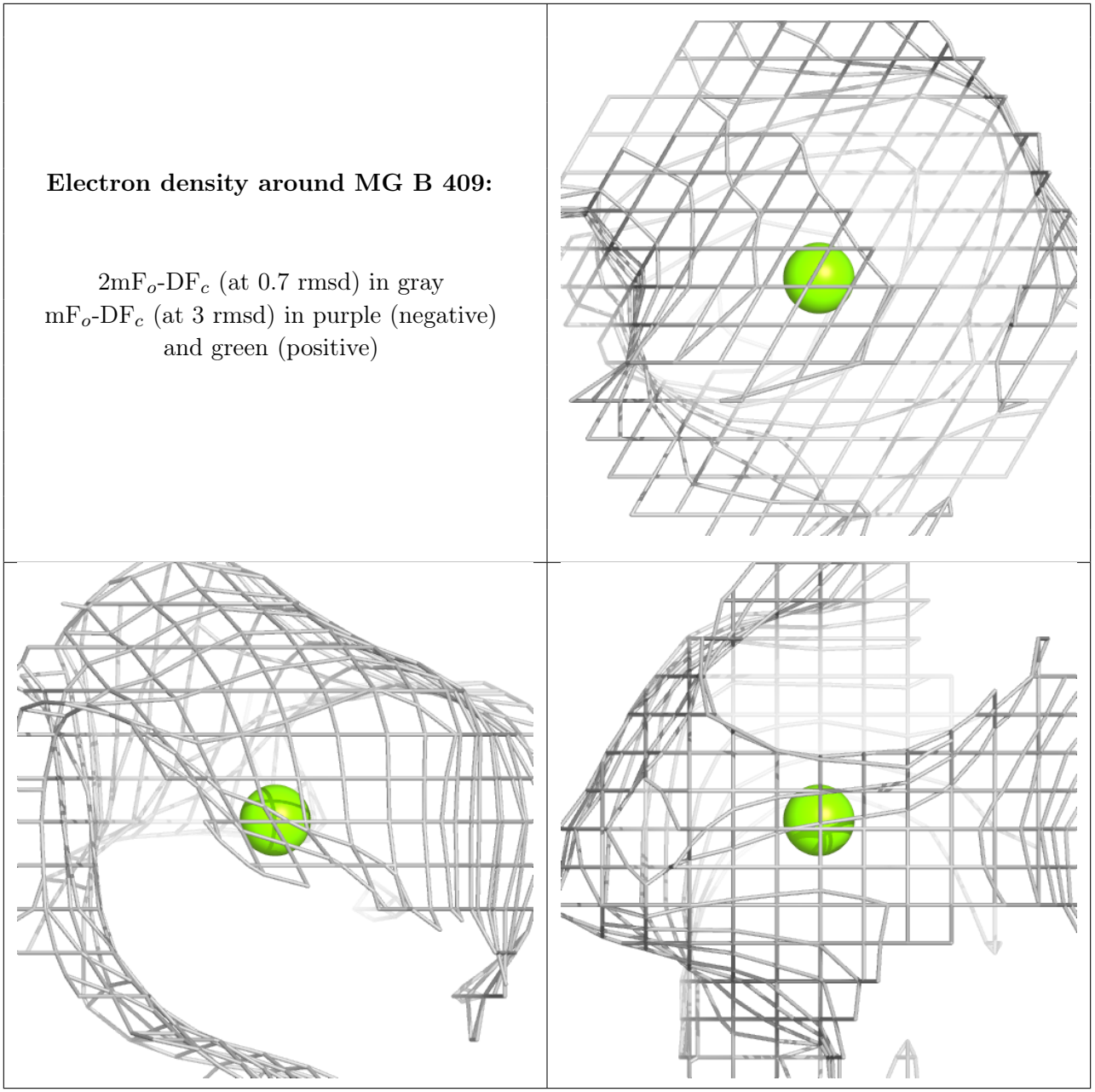






Electron density around MG B 409:

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



Electron density around MG A 408:

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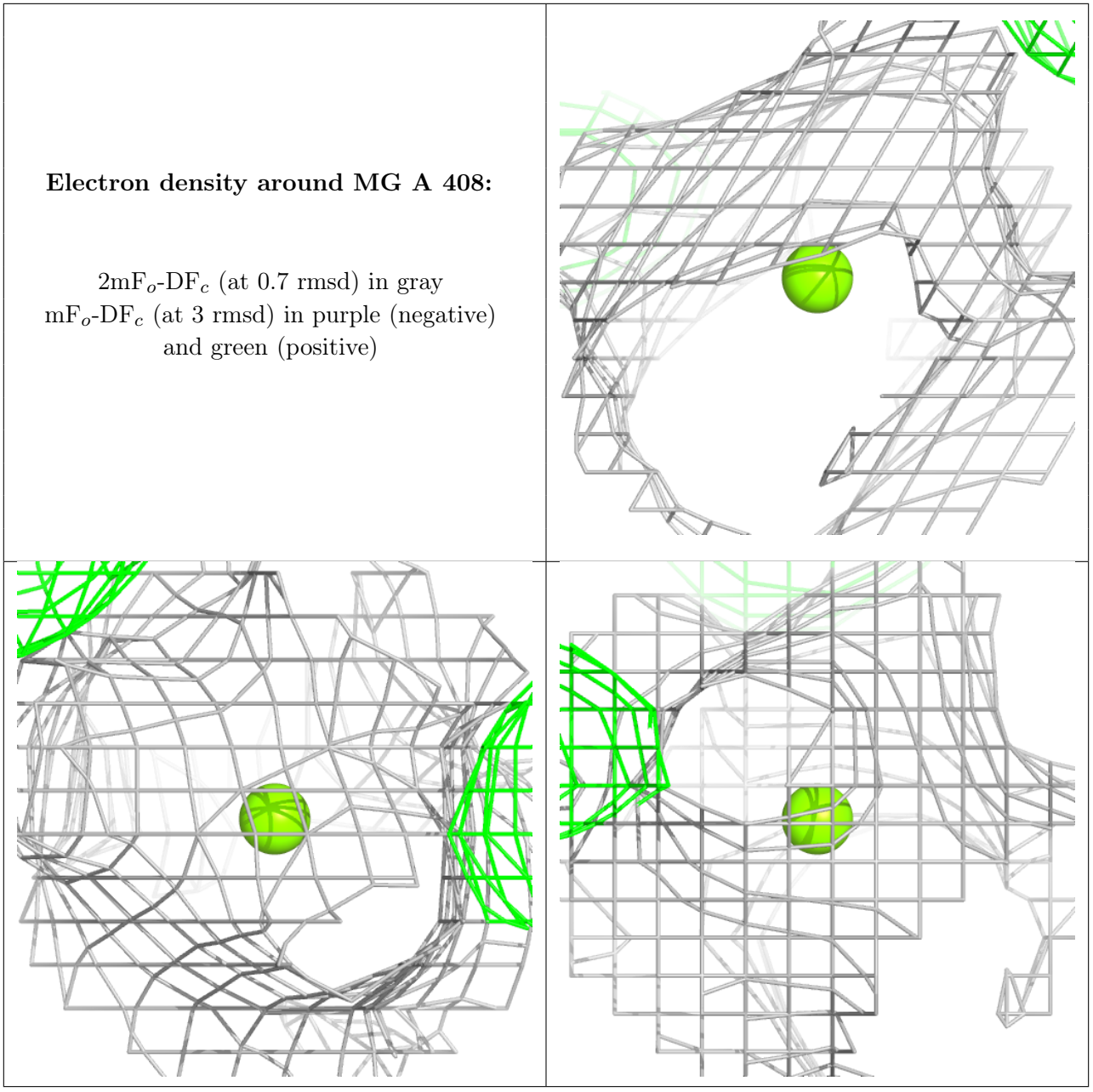
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.