



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 02:00 AM UTC

PDB ID : 9RG5 / pdb_00009rg5
Title : Unspecific peroxygenase from *Psathyrella aberdarensis*, Grogue variant, in complex with veratryl alcohol
Authors : Fernandez-Garcia, A.; Sanz-Aparicio, J.
Deposited on : 2025-06-05
Resolution : 1.90 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

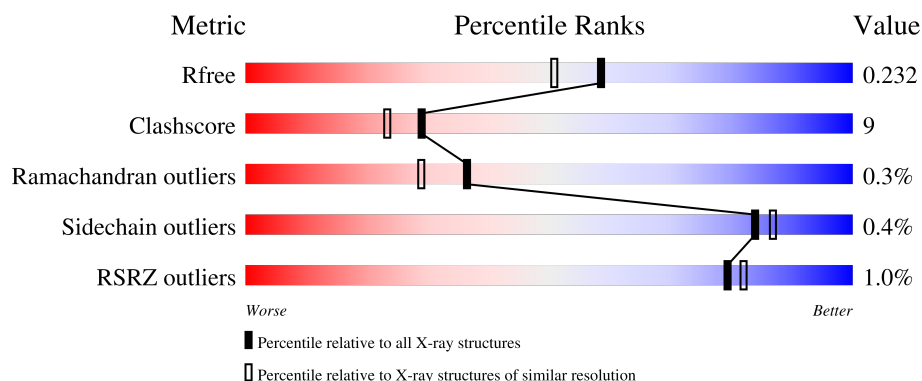
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



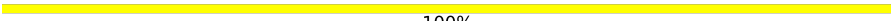
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 91%, green 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 91% 9% </div> </div>
1	B	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 91%, green 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 1% 91% 9% </div> </div>
2	J	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>
2	K	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, orange 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>
2	T	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, yellow 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	U	3	 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
12	GOL	A	420	-	-	X	-
12	GOL	B	405	-	-	X	-
4	NAG	A	402	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 6339 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
			2604	1662	440	495	7			
1	B	334	Total	C	N	O	S	0	1	0
			2594	1655	437	496	6			

There are 6 discrepancies between the modelled and reference sequences:

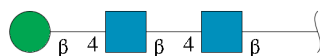
Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	SER	engineered mutation	UNP A0A4Q2DF39
A	79	ILE	LEU	engineered mutation	UNP A0A4Q2DF39
A	252	LEU	ALA	engineered mutation	UNP A0A4Q2DF39
B	61	ALA	SER	engineered mutation	UNP A0A4Q2DF39
B	79	ILE	LEU	engineered mutation	UNP A0A4Q2DF39
B	252	LEU	ALA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

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



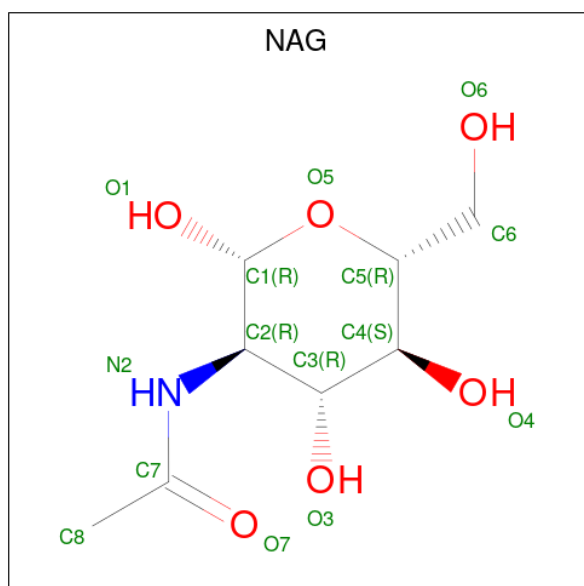
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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.



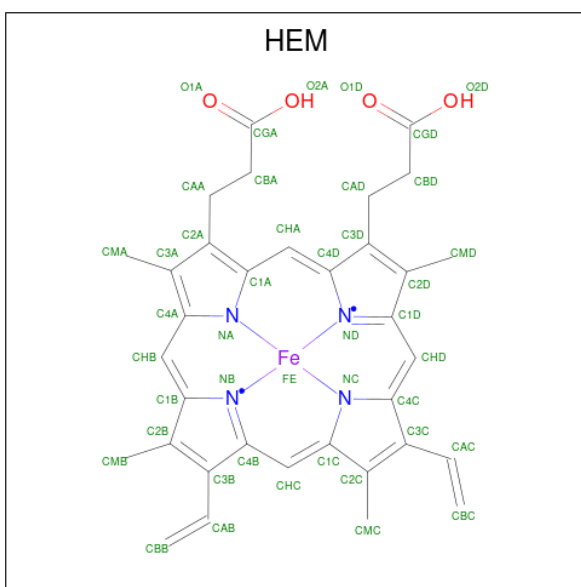
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



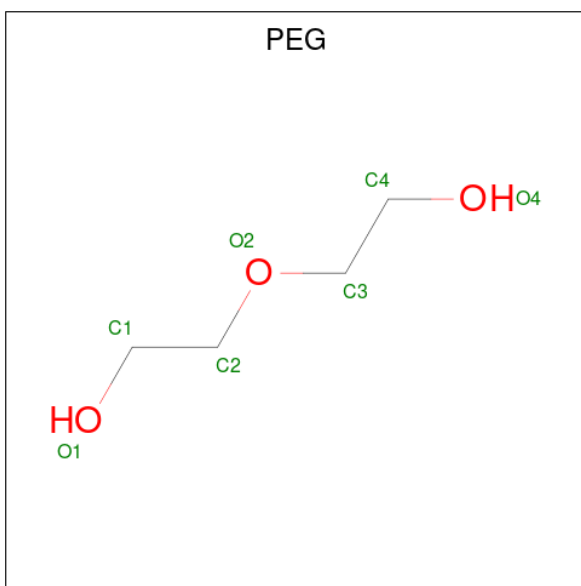
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- 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 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

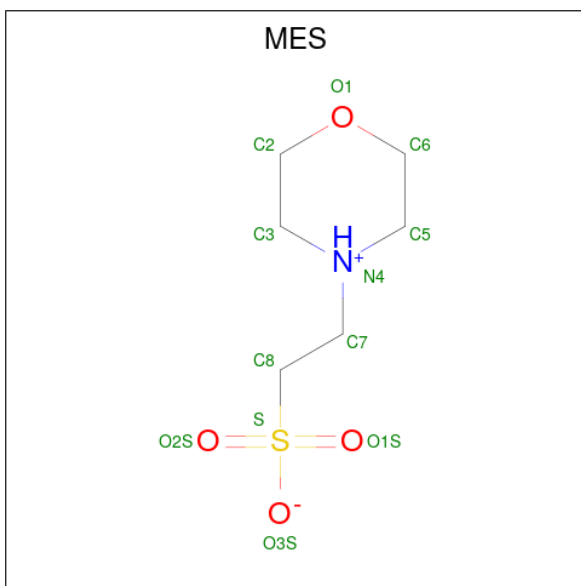
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

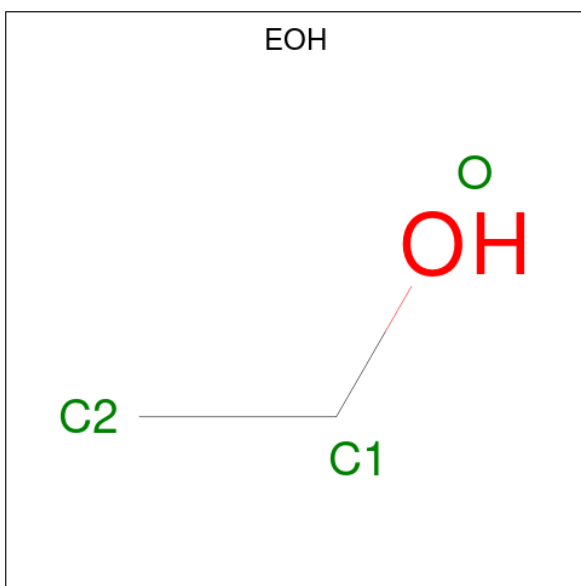
- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:

$C_6H_{13}NO_4S$).



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		

- Molecule 8 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



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

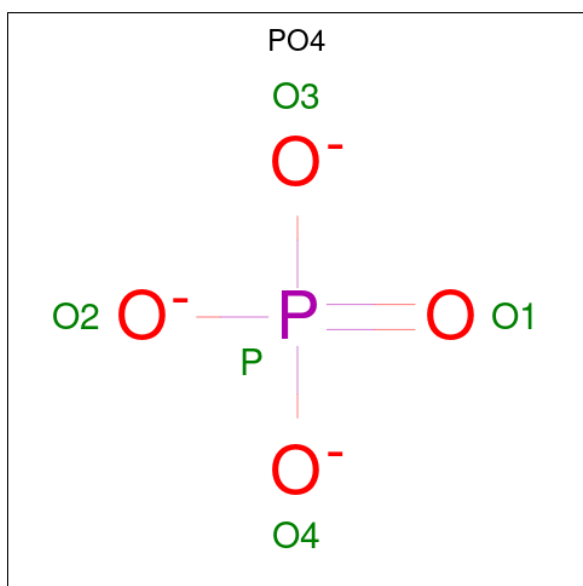
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	9	Total Zn 9 9	0	0
9	B	6	Total Zn 6 6	0	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

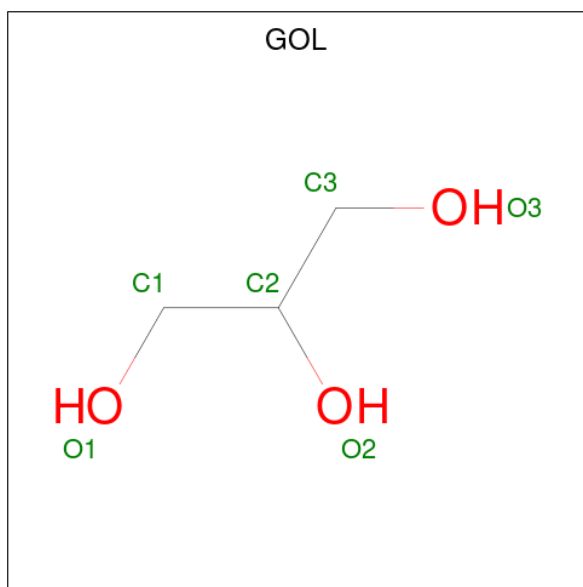
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Mg 1 1	0	0
10	B	1	Total Mg 1 1	0	0

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



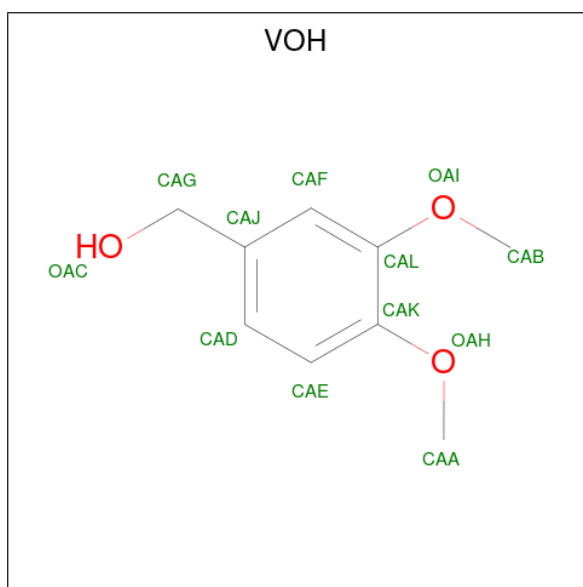
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	P	0	0
			5	4	1		
11	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 13 is Veratryl alcohol (CCD ID: VOH) (formula: $C_9H_{12}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			12	9	3		

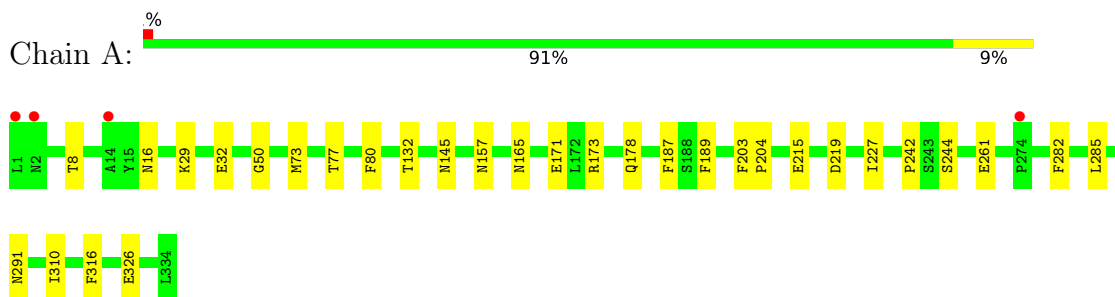
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	375	Total	O	0	0
			375	375		
14	B	383	Total	O	0	0
			383	383		

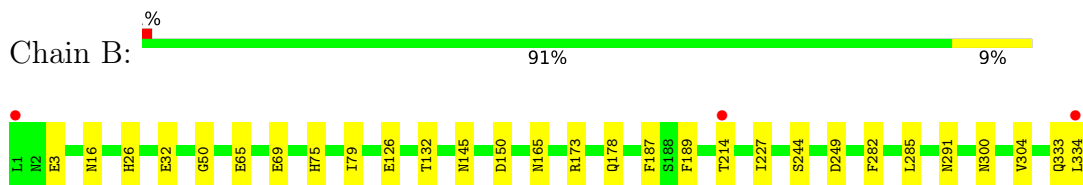
3 Residue-property plots [i](#)

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



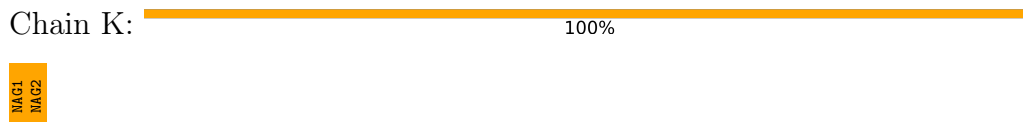
- Molecule 1: Heme-thiolate peroxidase



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



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



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





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

Chain U:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	76.84Å 76.84Å 272.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.52 – 1.90 45.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.52-1.90) 99.8 (45.52-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.174 , 0.220 0.182 , 0.232	Depositor DCC
R_{free} test set	3712 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6339	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.57	0/2683	0.93	0/3658
1	B	0.55	0/2670	0.92	0/3642
All	All	0.56	0/5353	0.92	0/7300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2464	44	0
1	B	2594	0	2447	43	0
2	J	28	0	25	4	0
2	K	28	0	25	4	0
2	T	28	0	25	2	0
3	U	39	0	34	4	0
4	A	28	0	26	12	0
4	B	28	0	26	8	0
5	A	43	0	30	3	0
5	B	43	0	30	1	0
6	A	7	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	24	0	26	1	0
7	B	12	0	13	0	0
8	A	6	0	12	0	0
9	A	9	0	0	0	0
9	B	6	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	5	0	0	0	0
11	B	5	0	0	0	0
12	A	6	0	8	4	0
12	B	24	0	32	4	0
13	B	12	0	0	1	0
14	A	375	0	0	19	1
14	B	383	0	0	23	1
All	All	6339	0	5233	94	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 9.

The worst 5 of 94 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:B:165:ASN:HD21	3:U:1:NAG:C1	1.01	1.62
1:A:291:ASN:HD21	4:A:401:NAG:C1	0.92	1.57
1:B:16:ASN:HD21	4:B:401:NAG:C1	1.15	1.56
1:B:145:ASN:ND2	2:T:1:NAG:C1	1.69	1.53
1:A:165:ASN:HD21	2:J:1:NAG:C1	1.21	1.52

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:755:HOH:O	14:B:524:HOH:O[5_555]	2.12	0.08

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%)	320 (96%)	13 (4%)	1 (0%)	36	29
1	B	333/334 (100%)	320 (96%)	12 (4%)	1 (0%)	36	29
All	All	667/668 (100%)	640 (96%)	25 (4%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	SER
1	B	244	SER

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	87
1	B	275/274 (100%)	274 (100%)	1 (0%)	84	87
All	All	551/548 (100%)	549 (100%)	2 (0%)	84	87

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 10

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	165	ASN
1	B	291	ASN
1	B	292	GLN
1	A	241	GLN
1	A	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	J	1	2	14,14,15	0.43	0	17,19,21	0.98	1 (5%)
2	NAG	J	2	2	14,14,15	0.39	0	17,19,21	1.03	1 (5%)
2	NAG	K	1	2	14,14,15	0.34	0	17,19,21	1.02	1 (5%)
2	NAG	K	2	2	14,14,15	0.44	0	17,19,21	0.99	2 (11%)
2	NAG	T	1	2	14,14,15	0.42	0	17,19,21	0.84	0
2	NAG	T	2	2	14,14,15	0.35	0	17,19,21	0.49	0
3	NAG	U	1	3	14,14,15	0.35	0	17,19,21	0.80	0
3	NAG	U	2	3	14,14,15	0.35	0	17,19,21	1.25	2 (11%)
3	BMA	U	3	3	11,11,12	0.73	1 (9%)	15,15,17	0.85	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	J	1	2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
2	NAG	K	1	2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	BMA	U	3	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	3	BMA	O5-C5	2.20	1.47	1.43

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2	NAG	C1-C2-N2	4.02	116.77	110.43
2	K	1	NAG	O5-C1-C2	-3.30	106.19	111.29
2	J	2	NAG	C1-C2-N2	3.05	115.24	110.43
2	J	1	NAG	C2-N2-C7	2.78	126.62	122.90
3	U	3	BMA	C1-O5-C5	2.77	115.90	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

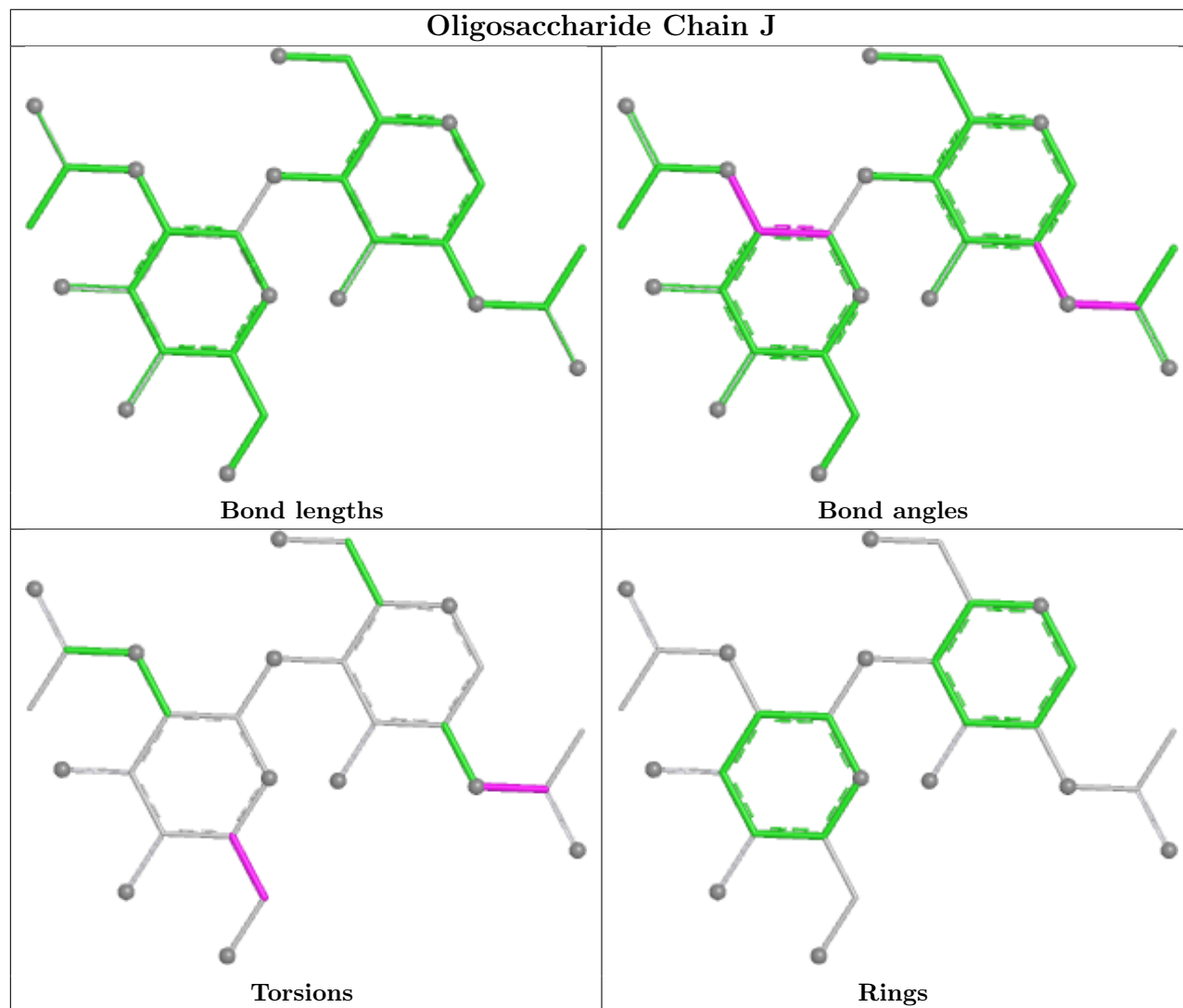
Mol	Chain	Res	Type	Atoms
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2

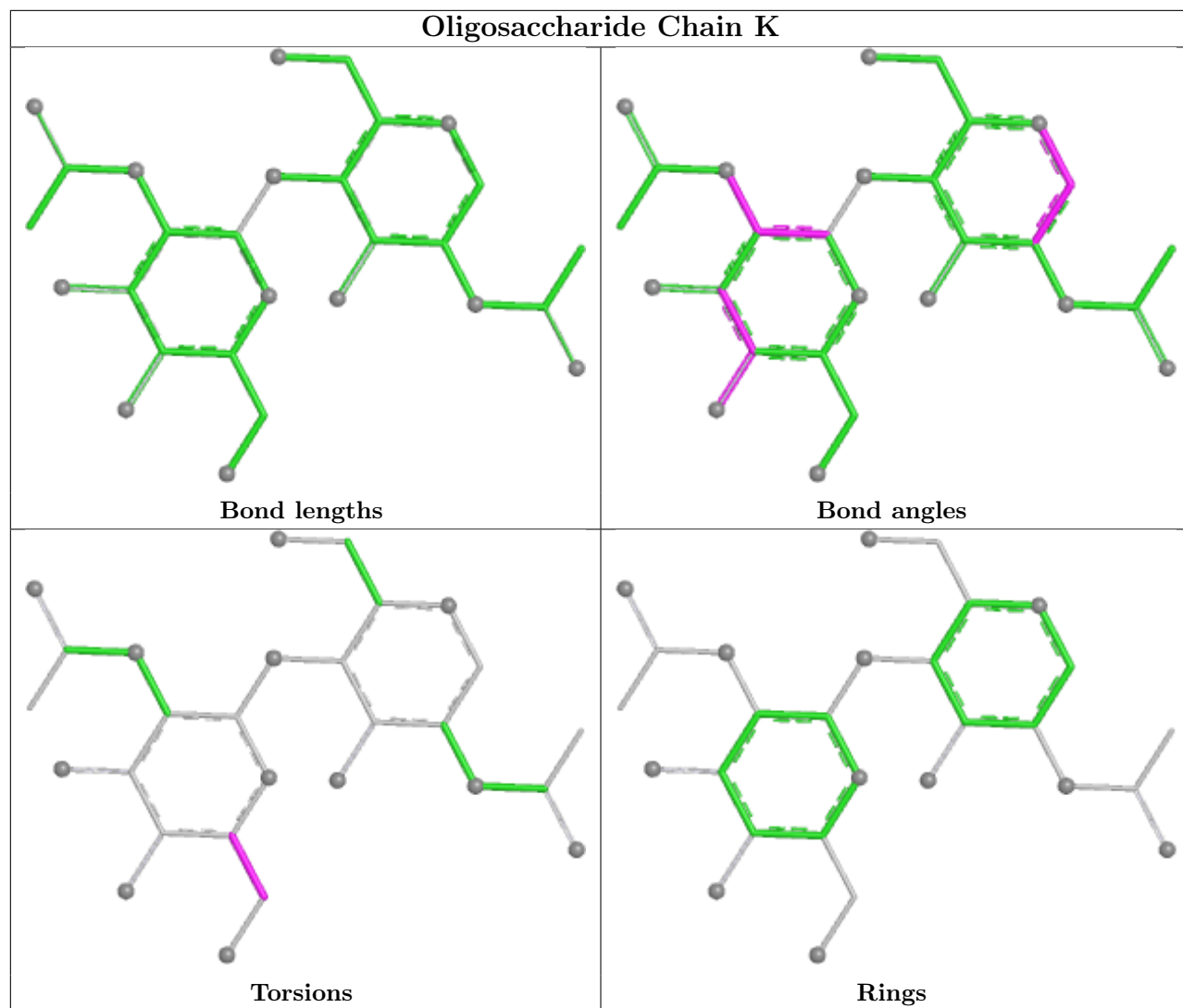
There are no ring outliers.

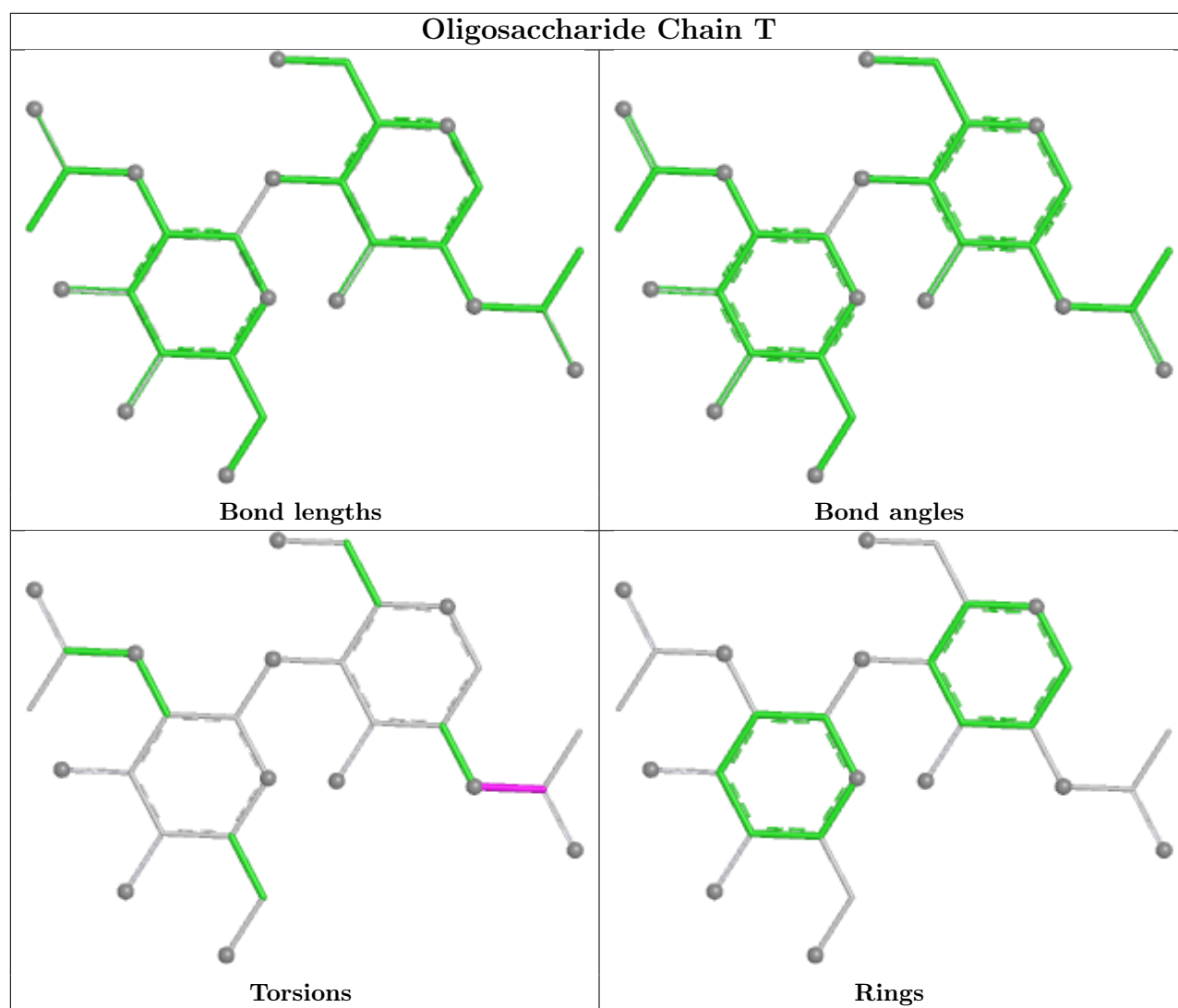
5 monomers are involved in 14 short contacts:

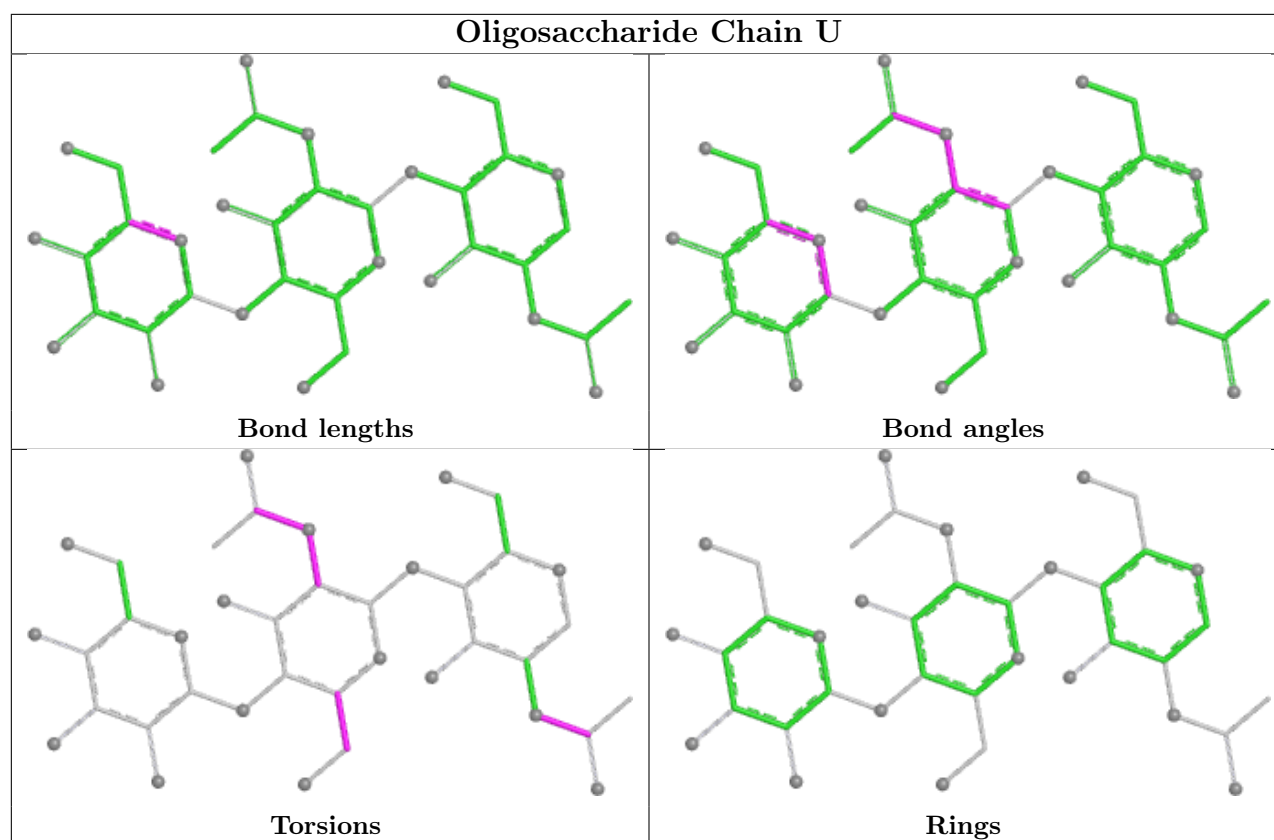
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	1	NAG	2	0
2	K	1	NAG	3	0
3	U	1	NAG	4	0
2	J	1	NAG	4	0
2	K	2	NAG	1	0

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









5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 17 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
5	HEM	A	403	14,1,10	50,50,50	1.35	7 (14%)	67,82,82	1.57	18 (26%)
12	GOL	B	405	-	5,5,5	0.22	0	5,5,5	0.25	0
8	EOH	A	408	-	2,2,2	0.19	0	1,1,1	0.19	0
13	VOH	B	406	-	12,12,12	0.35	0	15,15,15	0.66	0
4	NAG	B	402	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	NAG	A	401	-	14,14,15	0.40	0	17,19,21	0.64	1 (5%)
12	GOL	A	420	-	5,5,5	0.13	0	5,5,5	0.32	0
4	NAG	A	402	-	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
7	MES	A	406	-	12,12,12	0.83	0	15,16,16	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	404	-	6,6,6	0.50	0	5,5,5	0.25	0
12	GOL	B	417	-	5,5,5	0.16	0	5,5,5	0.29	0
12	GOL	B	416	-	5,5,5	0.26	0	5,5,5	0.35	0
7	MES	B	403	-	12,12,12	0.88	0	15,16,16	1.34	1 (6%)
5	HEM	B	404	14,1,10	50,50,50	1.47	8 (16%)	67,82,82	1.67	18 (26%)
11	PO4	A	419	-	4,4,4	1.70	1 (25%)	6,6,6	0.54	0
11	PO4	B	414	-	4,4,4	1.54	1 (25%)	6,6,6	0.58	0
7	MES	A	405	-	12,12,12	0.78	0	15,16,16	0.45	0
4	NAG	B	401	-	14,14,15	0.46	0	17,19,21	1.19	3 (17%)
8	EOH	A	407	-	2,2,2	0.15	0	1,1,1	0.01	0
12	GOL	B	415	-	5,5,5	0.16	0	5,5,5	0.30	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
12	GOL	B	417	-	-	0/4/4/4	-
5	HEM	A	403	14,1,10	-	4/14/54/54	-
12	GOL	B	416	-	-	3/4/4/4	-
13	VOH	B	406	-	-	0/6/6/6	0/1/1/1
4	NAG	B	402	-	-	1/6/23/26	0/1/1/1
4	NAG	A	401	-	-	0/6/23/26	0/1/1/1
7	MES	B	403	-	-	0/6/14/14	0/1/1/1
5	HEM	B	404	14,1,10	-	3/14/54/54	-
12	GOL	B	405	-	-	1/4/4/4	-
12	GOL	A	420	-	-	4/4/4/4	-
7	MES	A	405	-	-	1/6/14/14	0/1/1/1
4	NAG	A	402	-	-	2/6/23/26	0/1/1/1
4	NAG	B	401	-	-	2/6/23/26	0/1/1/1
7	MES	A	406	-	-	1/6/14/14	0/1/1/1
12	GOL	B	415	-	-	0/4/4/4	-
6	PEG	A	404	-	-	3/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	HEM	C1B-NB	-4.36	1.32	1.40
5	B	404	HEM	FE-NB	3.42	2.05	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	HEM	C4D-ND	-3.39	1.34	1.40
5	A	403	HEM	C1B-NB	-3.35	1.34	1.40
11	A	419	PO4	P-O1	3.33	1.58	1.50

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	403	MES	O2S-S-C8	-4.49	99.94	106.73
5	B	404	HEM	CHC-C4B-NB	3.90	128.62	124.42
5	B	404	HEM	C1B-NB-C4B	3.85	109.77	105.21
5	A	403	HEM	CHD-C4C-NC	3.68	128.46	124.45
5	B	404	HEM	CHD-C4C-NC	3.58	128.35	124.45

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	405	MES	C8-C7-N4-C5
7	A	406	MES	C8-C7-N4-C5
12	B	416	GOL	O1-C1-C2-C3
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2

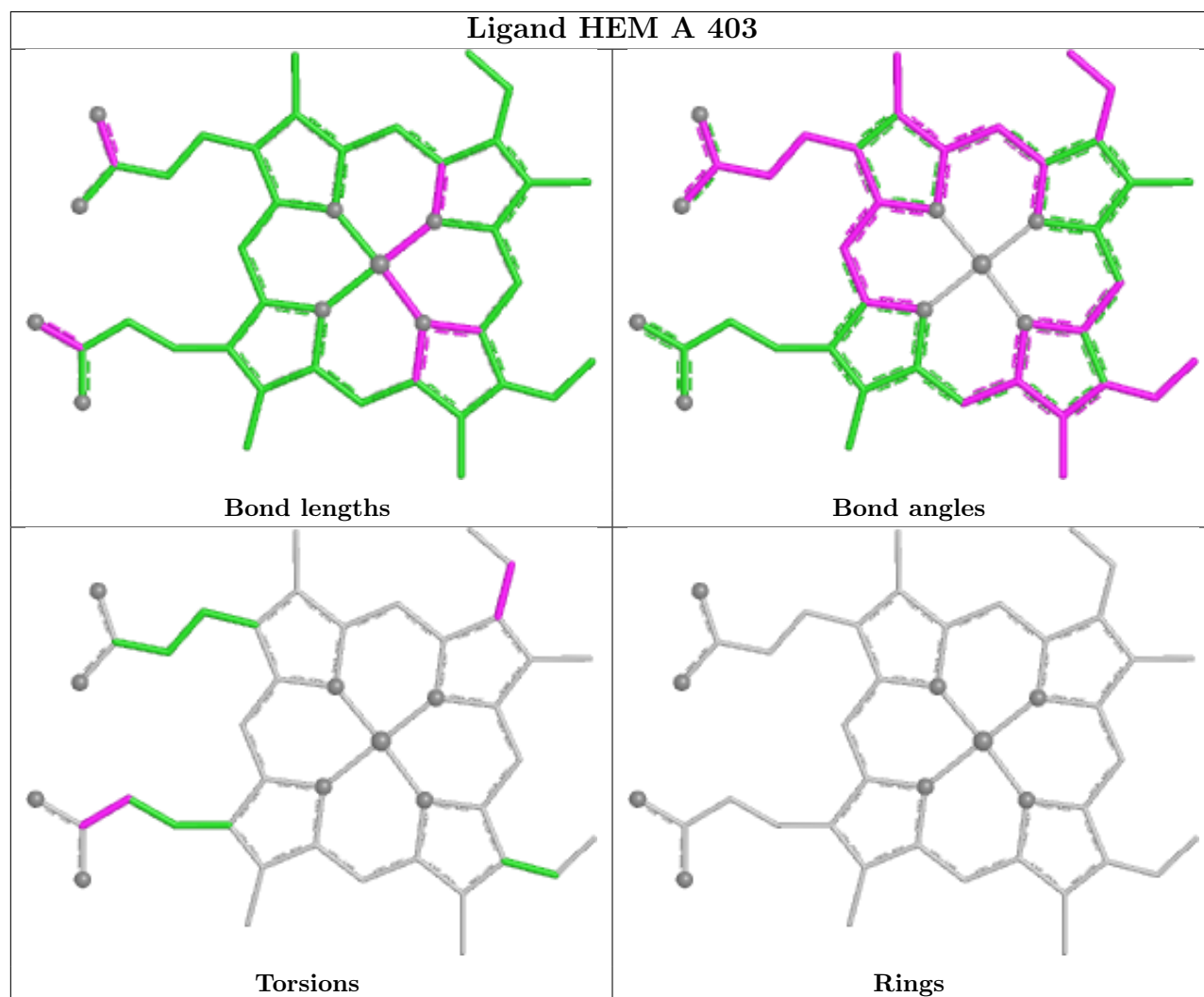
There are no ring outliers.

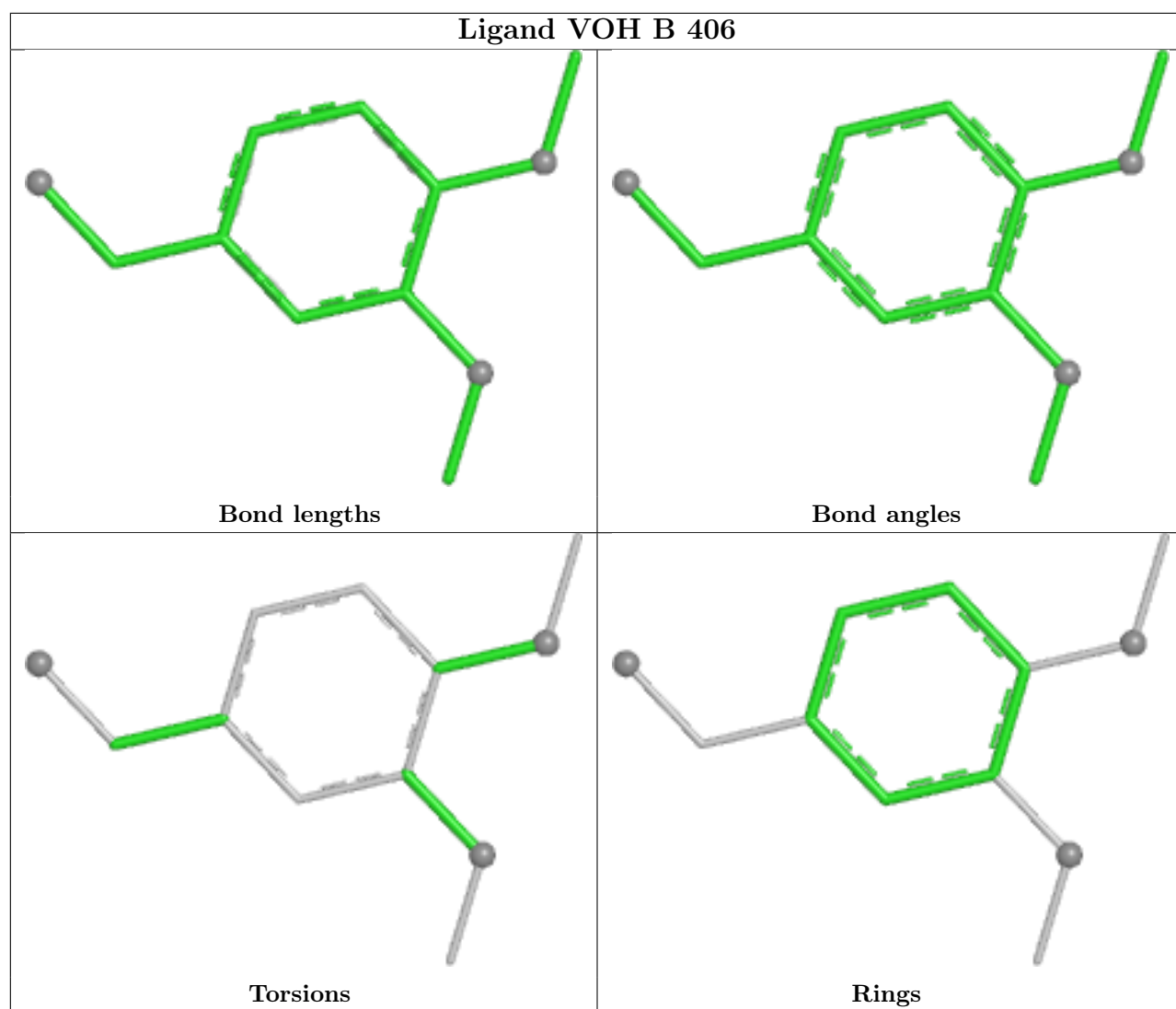
10 monomers are involved in 34 short contacts:

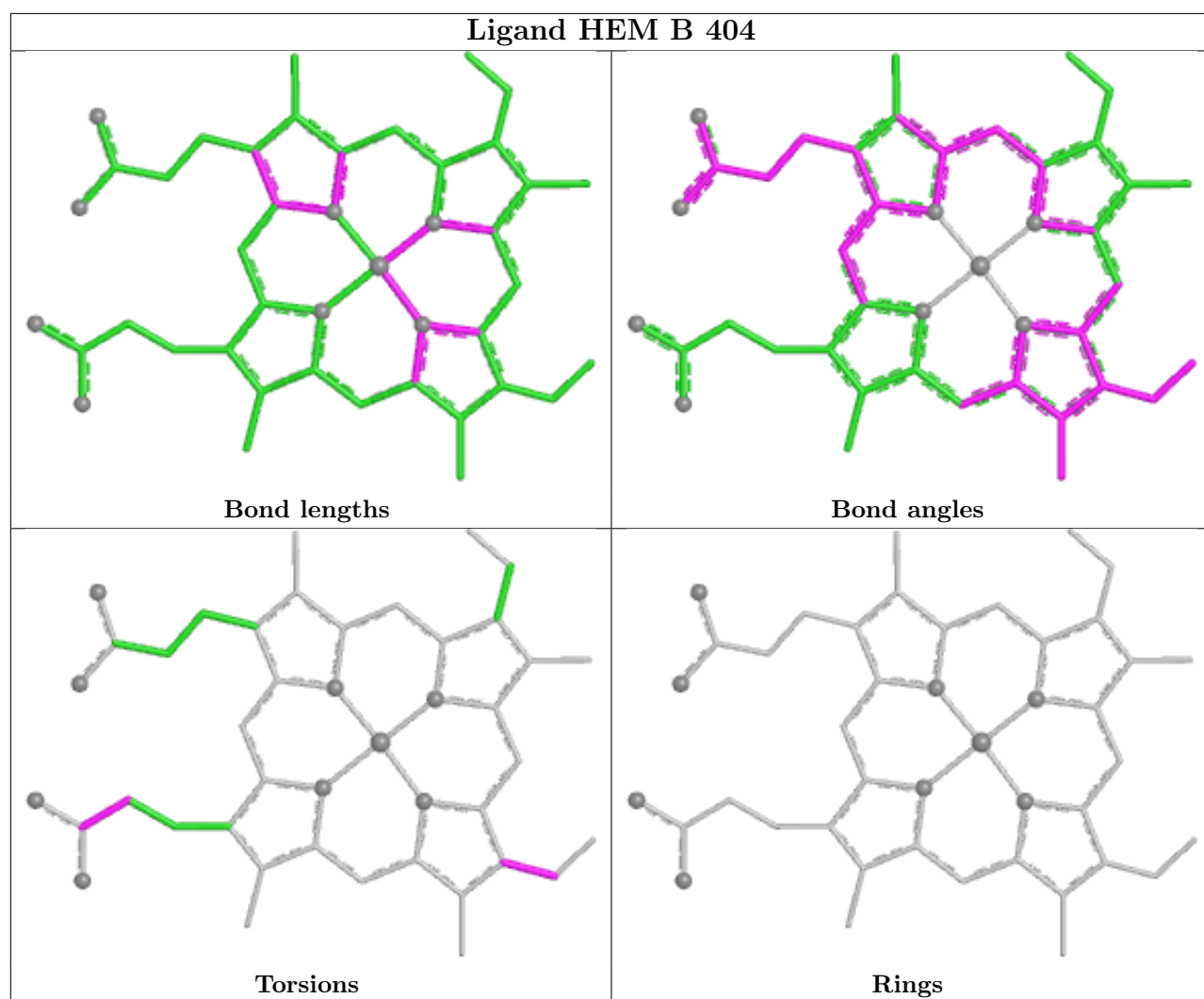
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	HEM	3	0
12	B	405	GOL	4	0
13	B	406	VOH	1	0
4	B	402	NAG	4	0
4	A	401	NAG	5	0
12	A	420	GOL	4	0
4	A	402	NAG	7	0
7	A	406	MES	1	0
5	B	404	HEM	1	0
4	B	401	NAG	4	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	0.09	4 (1%) 76 79	19, 39, 56, 108	2 (0%)
1	B	334/334 (100%)	0.11	3 (0%) 81 83	24, 41, 58, 94	1 (0%)
All	All	668/668 (100%)	0.10	7 (1%) 79 82	19, 40, 56, 108	3 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LEU	5.2
1	B	334	LEU	5.2
1	B	1	LEU	4.7
1	A	14	ALA	3.1
1	A	2	ASN	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, 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
2	NAG	J	1	14/15	-	-	43,46,52,57	0
2	NAG	J	2	14/15	-	-	60,64,78,84	0
2	NAG	K	1	14/15	-	-	46,51,56,58	0
2	NAG	K	2	14/15	-	-	54,67,70,71	0
2	NAG	T	1	14/15	-	-	48,56,64,66	0

Continued on next page...

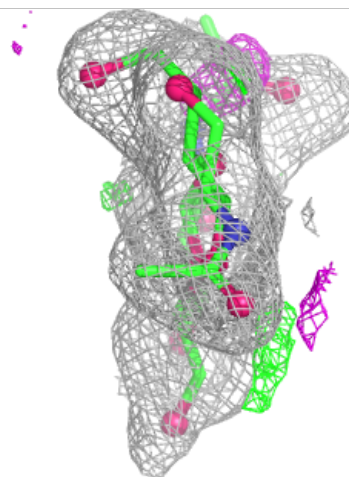
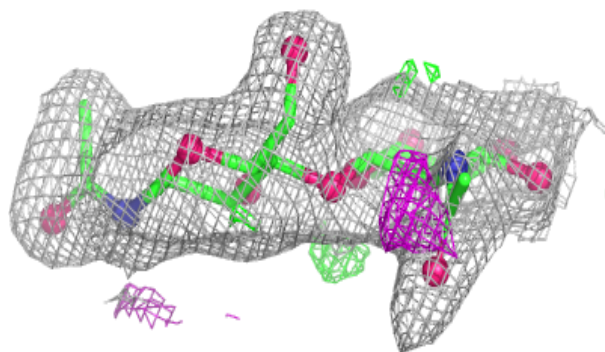
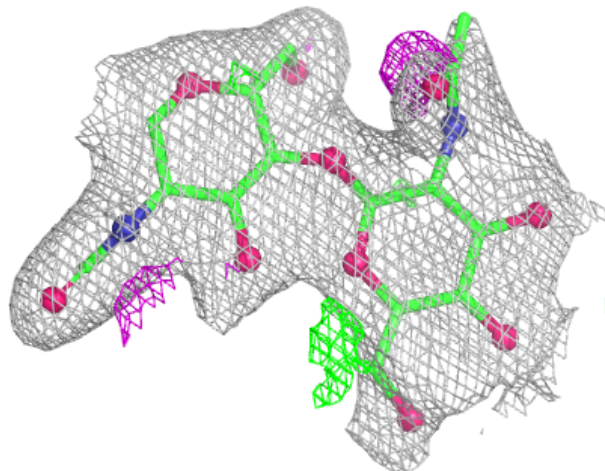
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	T	2	14/15	-	-	63,71,83,85	0
3	NAG	U	1	14/15	-	-	44,50,55,63	0
3	NAG	U	2	14/15	-	-	65,73,77,79	0
3	BMA	U	3	11/12	-	-	71,78,81,83	0

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

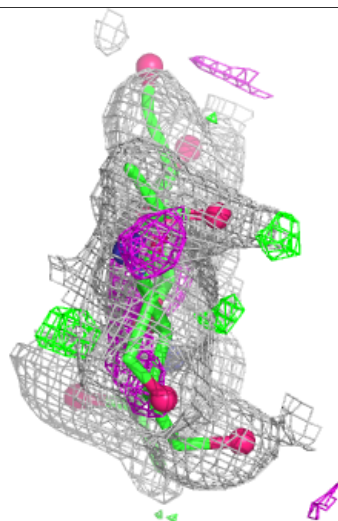
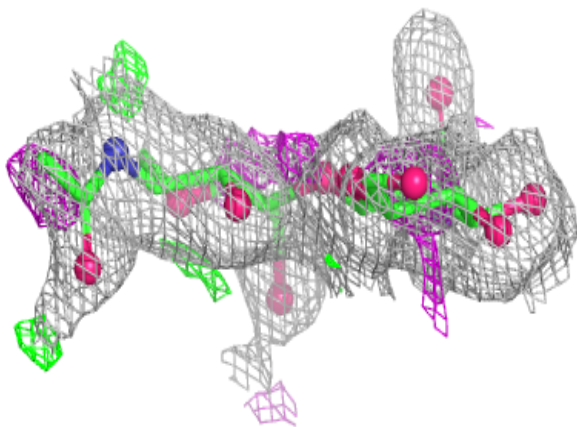
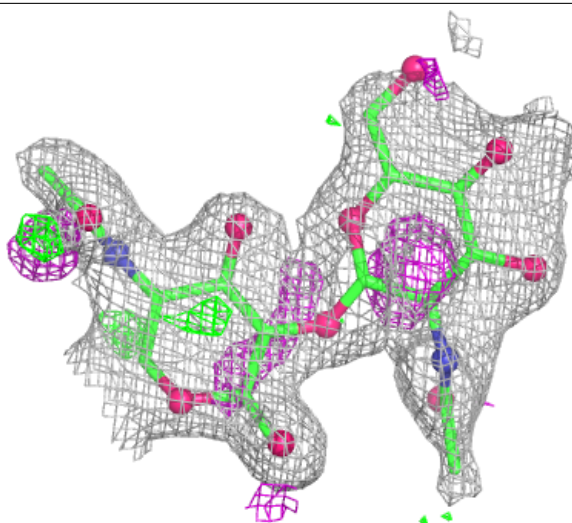
Electron density around Chain J:

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



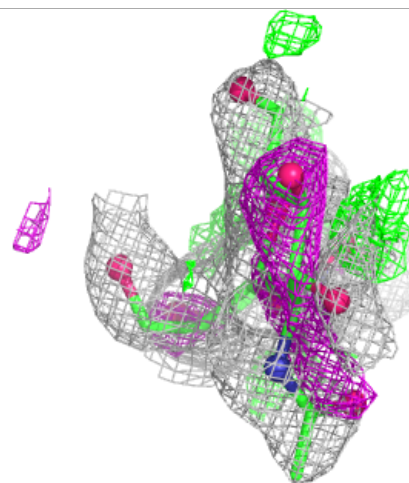
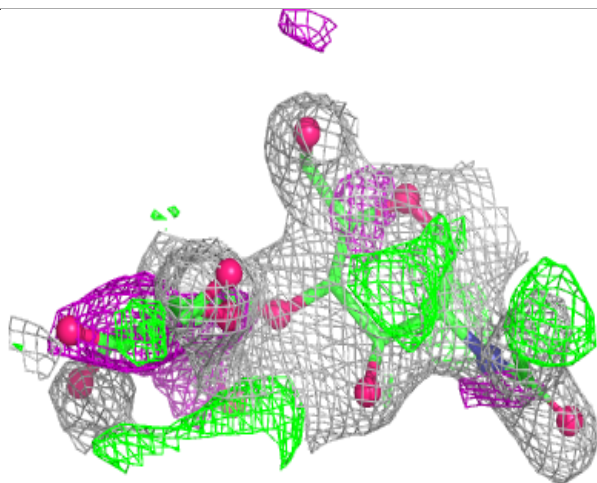
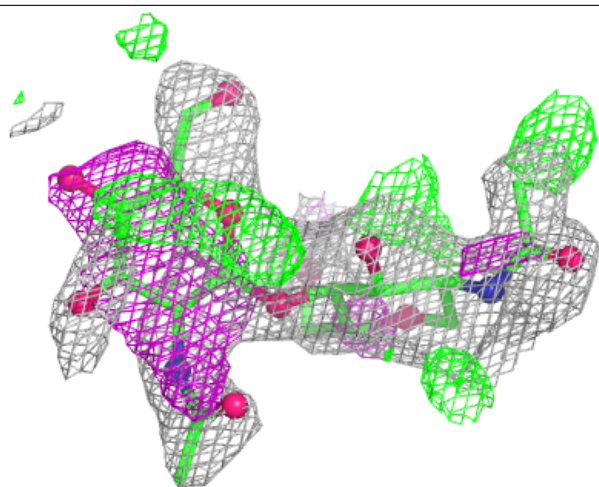
Electron density around Chain K:

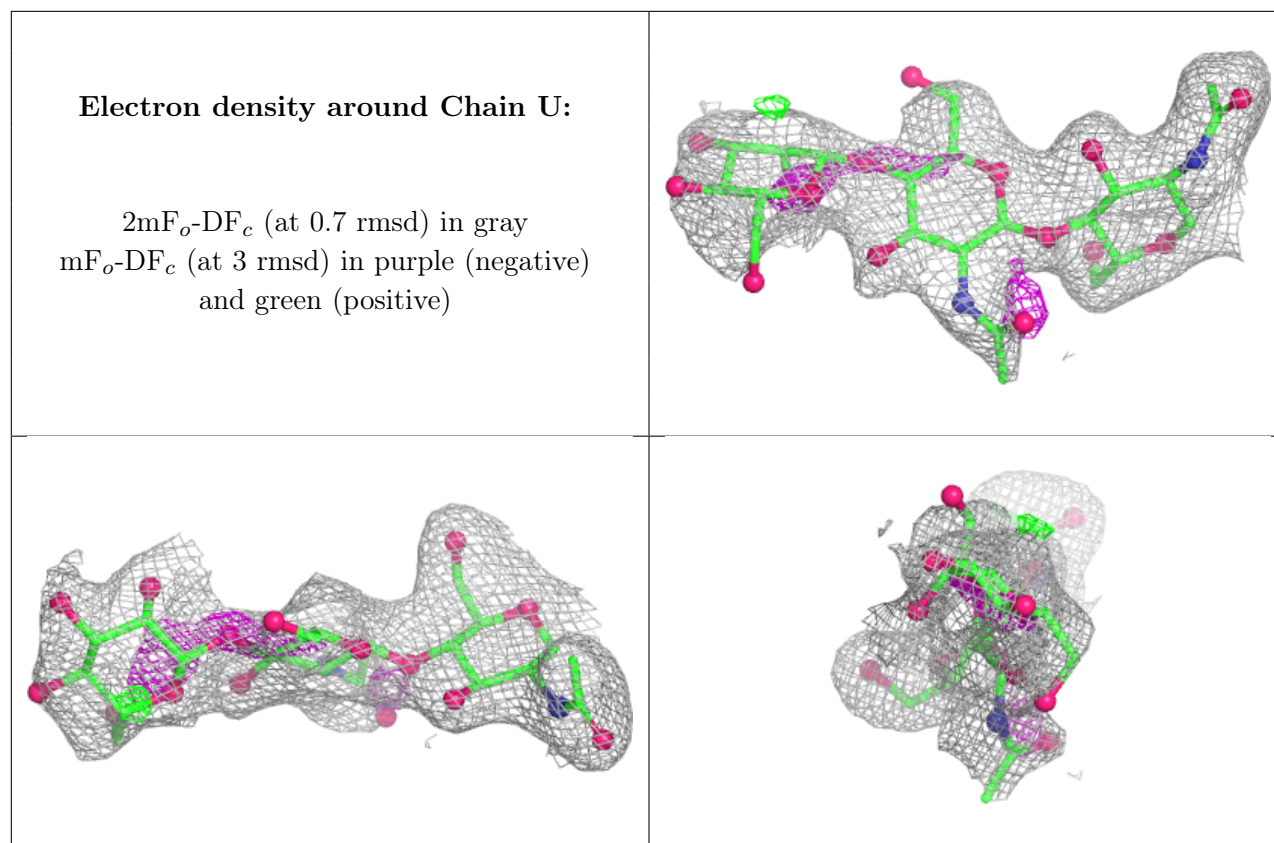
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain T:

$2mF_o-DF_c$ (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, 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
4	NAG	B	402	14/15	0.53	0.15	60,73,77,78	0
12	GOL	B	415	6/6	0.63	0.15	56,59,61,62	0
11	PO4	B	414	5/5	0.65	0.13	59,61,65,74	0
4	NAG	A	402	14/15	0.65	0.15	63,73,81,81	0
7	MES	A	406	12/12	0.66	0.24	43,53,60,63	12
4	NAG	A	401	14/15	0.68	0.15	68,74,80,88	0
12	GOL	B	416	6/6	0.72	0.16	57,61,63,65	0
12	GOL	A	420	6/6	0.74	0.14	54,54,57,58	0
12	GOL	B	417	6/6	0.75	0.14	51,57,59,60	0
8	EOH	A	407	3/3	0.76	0.17	55,55,55,57	0
11	PO4	A	419	5/5	0.79	0.12	64,66,74,80	0
12	GOL	B	405	6/6	0.82	0.13	44,47,51,51	0
4	NAG	B	401	14/15	0.82	0.12	51,56,62,62	0
8	EOH	A	408	3/3	0.83	0.17	54,54,57,59	0

Continued on next page...

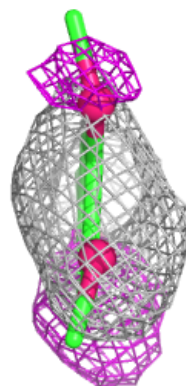
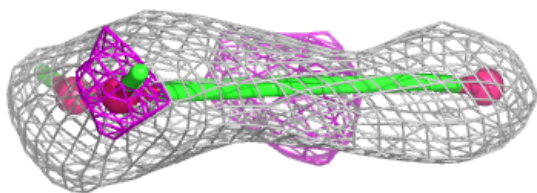
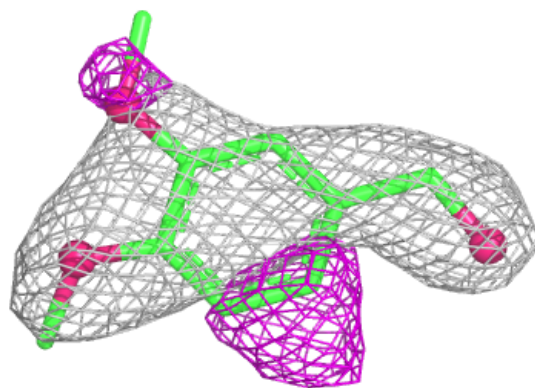
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	VOH	B	406	12/12	0.85	0.20	49,53,58,61	0
6	PEG	A	404	7/7	0.88	0.17	48,51,62,64	0
9	ZN	B	410	1/1	0.92	0.20	70,70,70,70	0
7	MES	B	403	12/12	0.93	0.14	31,44,52,55	12
9	ZN	B	411	1/1	0.93	0.15	77,77,77,77	0
9	ZN	A	415	1/1	0.94	0.07	54,54,54,54	0
9	ZN	A	416	1/1	0.94	0.29	75,75,75,75	0
9	ZN	A	409	1/1	0.96	0.06	55,55,55,55	0
9	ZN	B	408	1/1	0.96	0.05	71,71,71,71	0
7	MES	A	405	12/12	0.96	0.13	29,46,55,55	12
5	HEM	A	403	43/43	0.98	0.07	27,30,33,44	0
9	ZN	B	407	1/1	0.98	0.07	54,54,54,54	0
9	ZN	A	412	1/1	0.98	0.04	42,42,42,42	0
9	ZN	B	409	1/1	0.98	0.05	50,50,50,50	0
9	ZN	A	413	1/1	0.98	0.07	56,56,56,56	0
9	ZN	A	414	1/1	0.98	0.05	57,57,57,57	0
5	HEM	B	404	43/43	0.98	0.06	29,32,35,41	0
9	ZN	A	410	1/1	0.99	0.03	40,40,40,40	0
9	ZN	A	411	1/1	0.99	0.02	39,39,39,39	0
10	MG	A	418	1/1	0.99	0.16	12,12,12,12	0
10	MG	B	413	1/1	0.99	0.16	17,17,17,17	0
9	ZN	A	417	1/1	1.00	0.02	35,35,35,35	0
9	ZN	B	412	1/1	1.00	0.01	38,38,38,38	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.

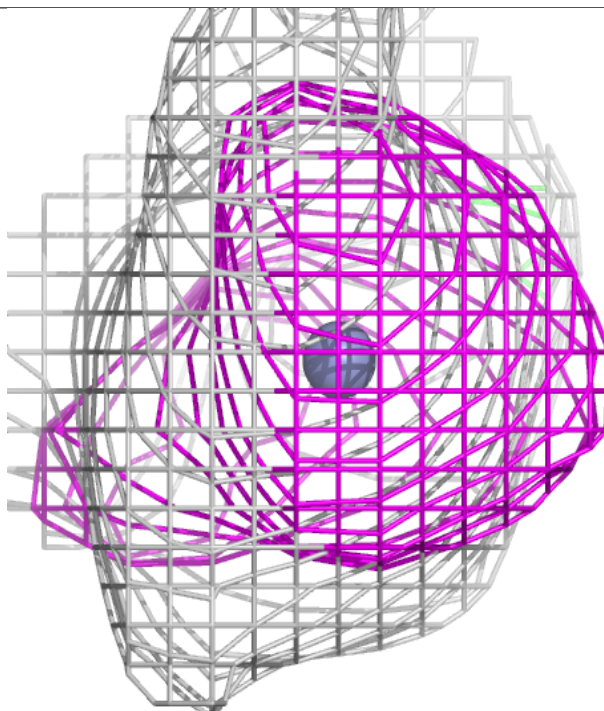
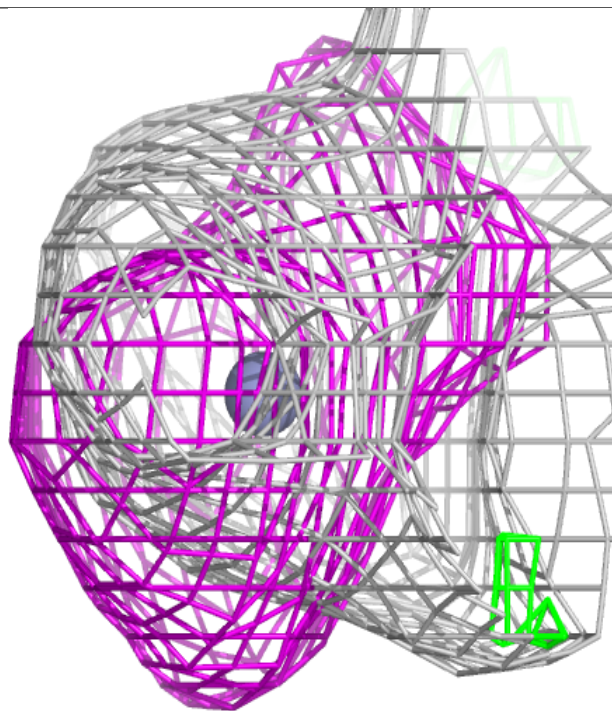
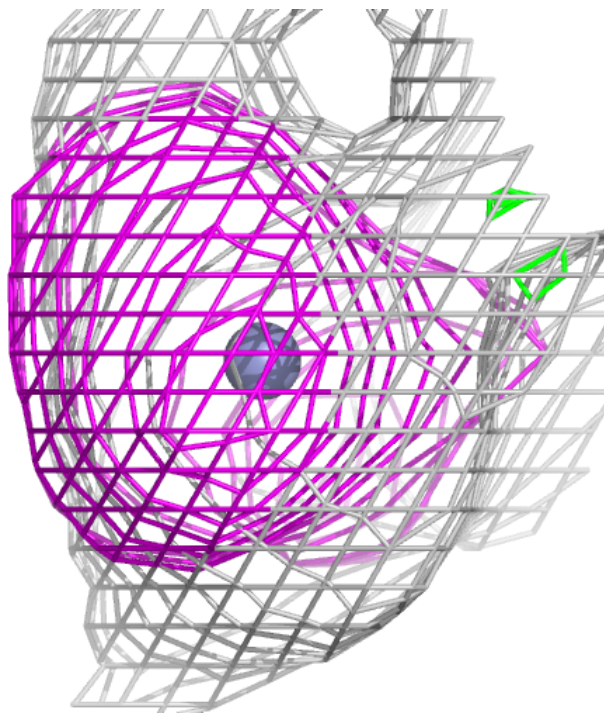
Electron density around VOH B 406:

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



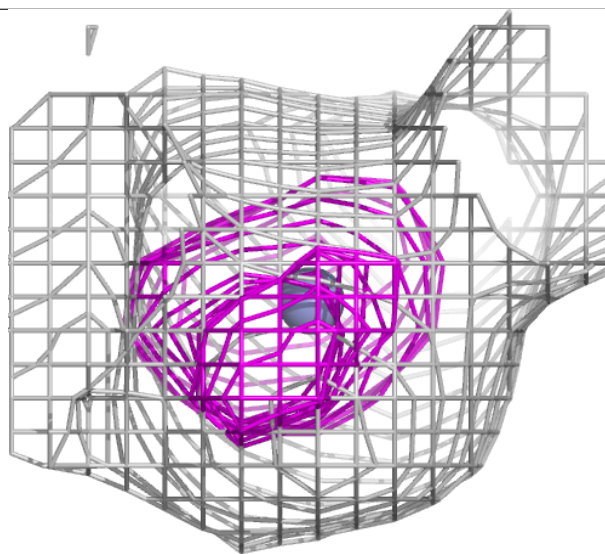
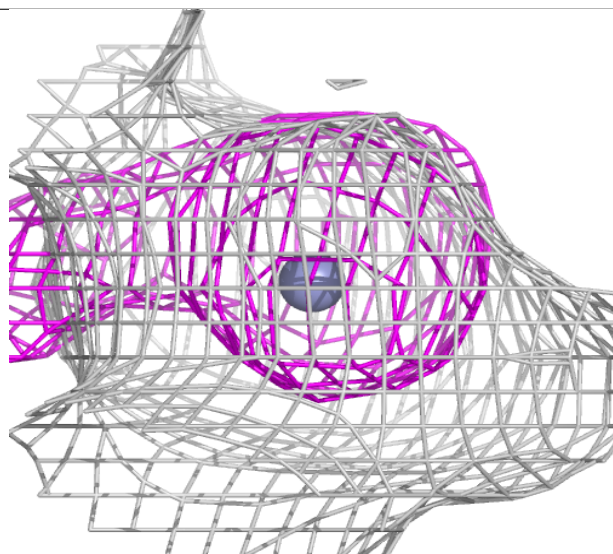
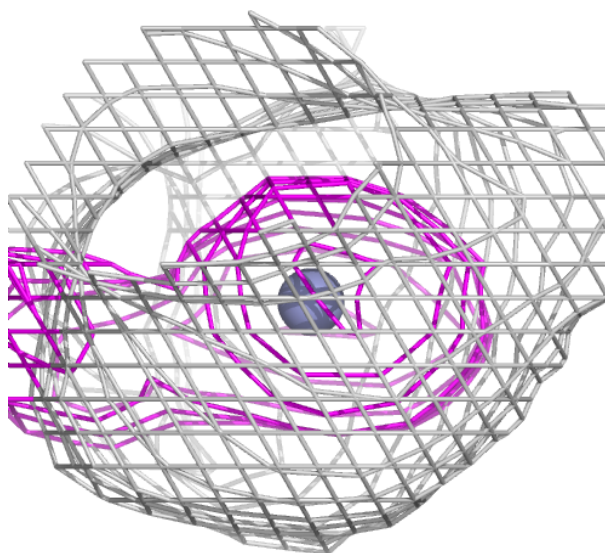
Electron density around ZN B 410:

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



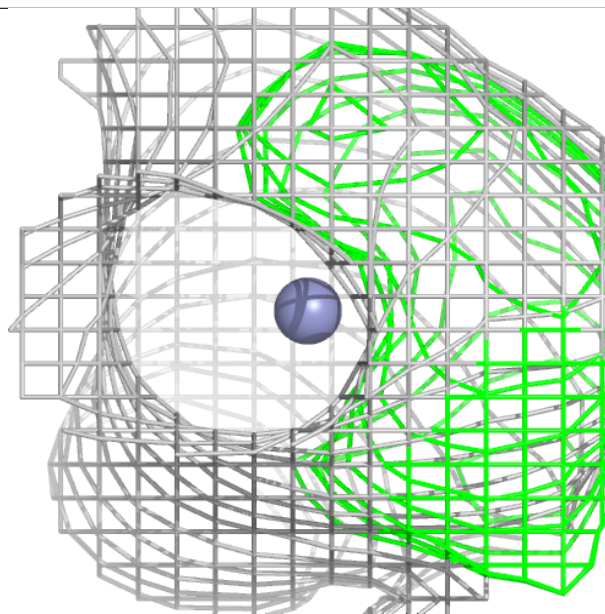
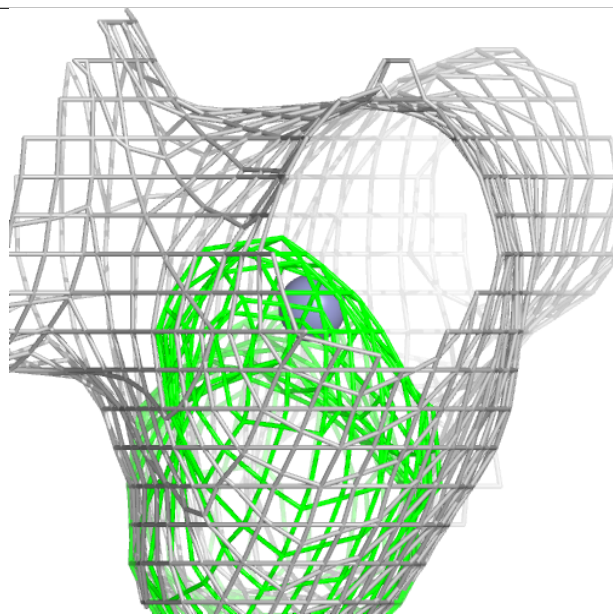
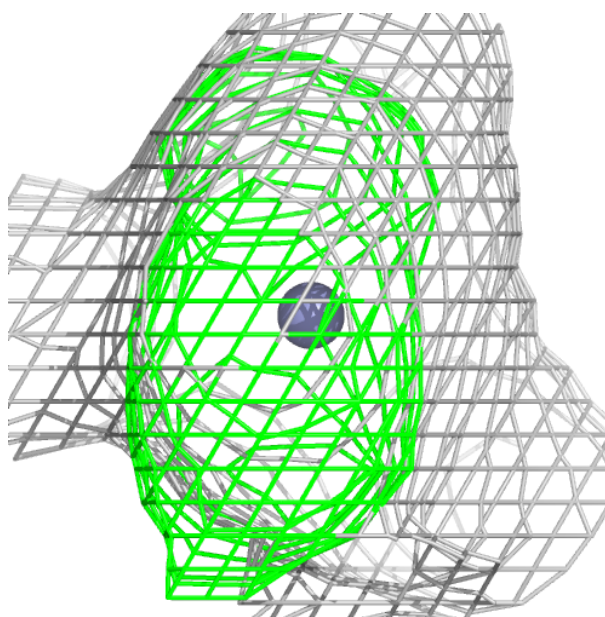
Electron density around ZN B 411:

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



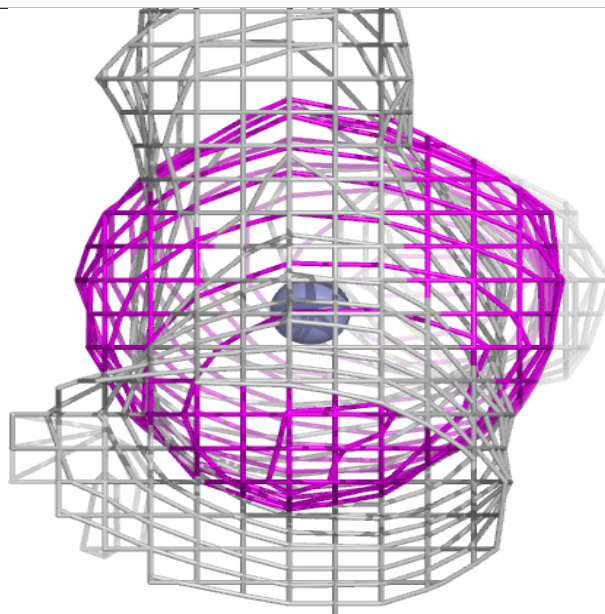
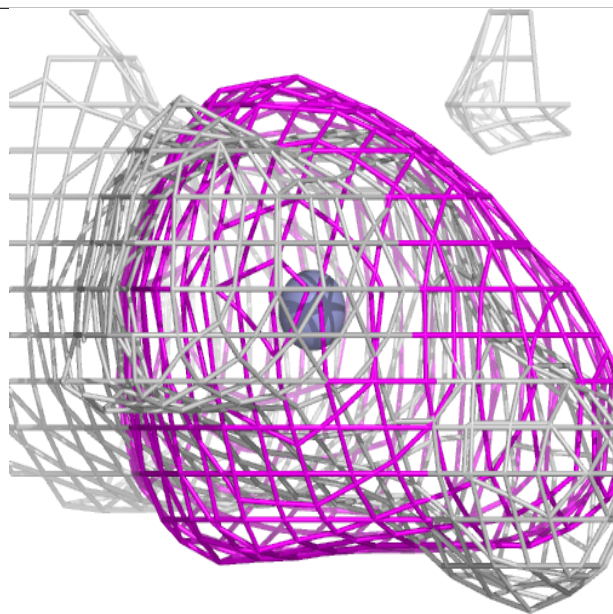
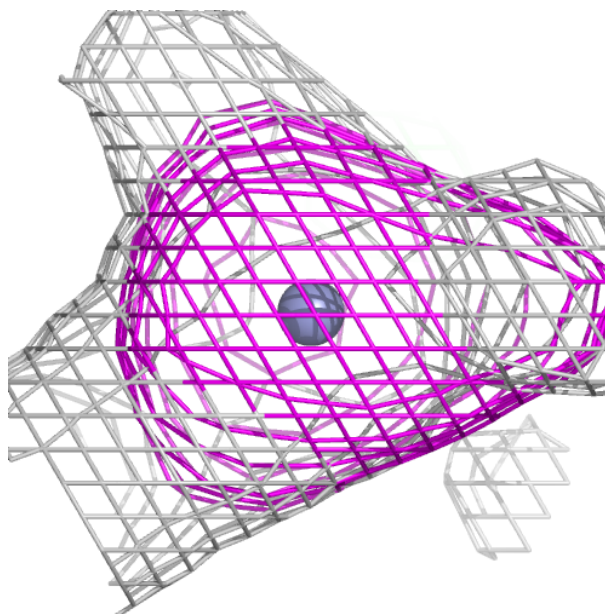
Electron density around ZN A 415:

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



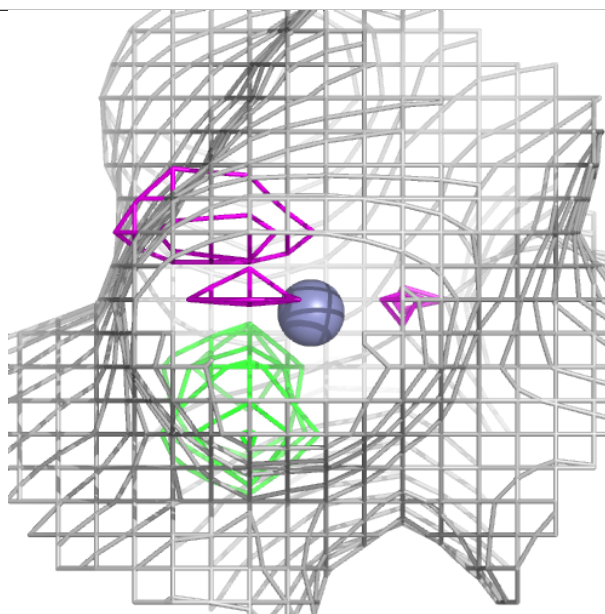
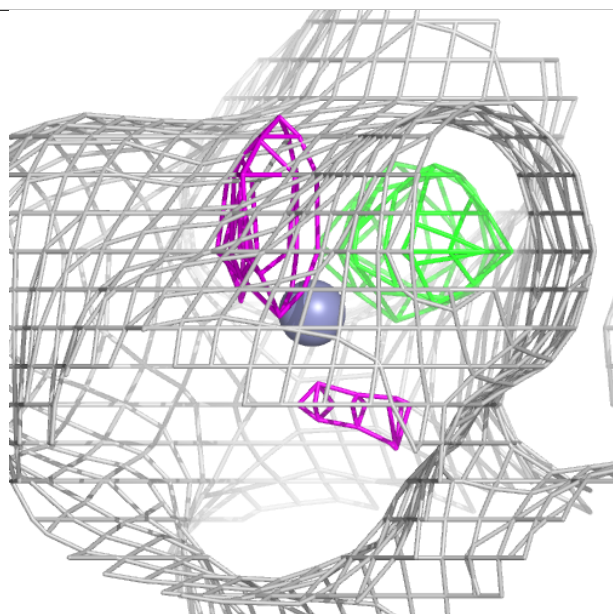
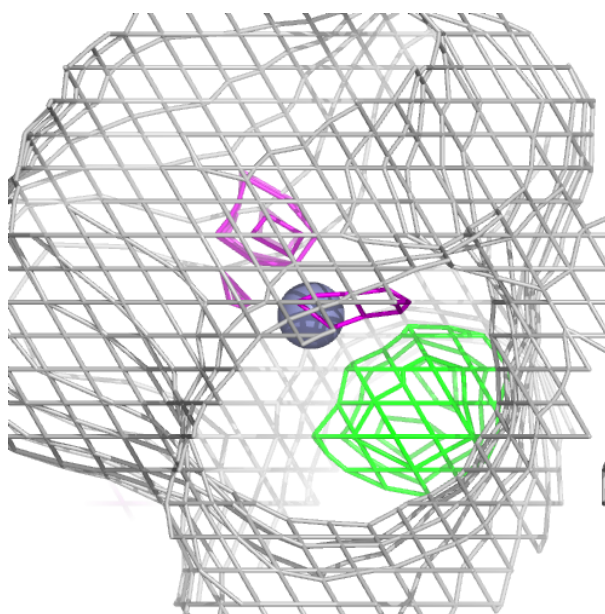
Electron density around ZN A 416:

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



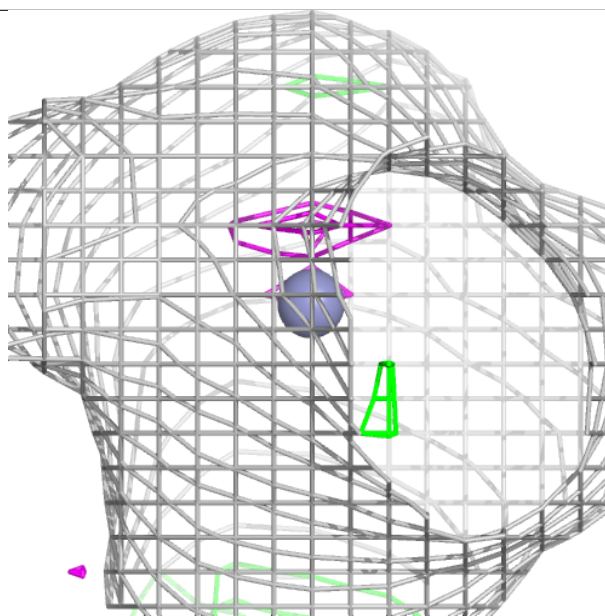
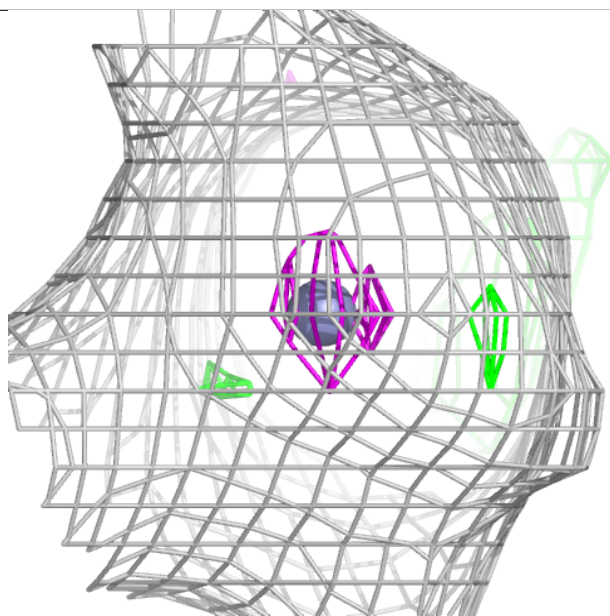
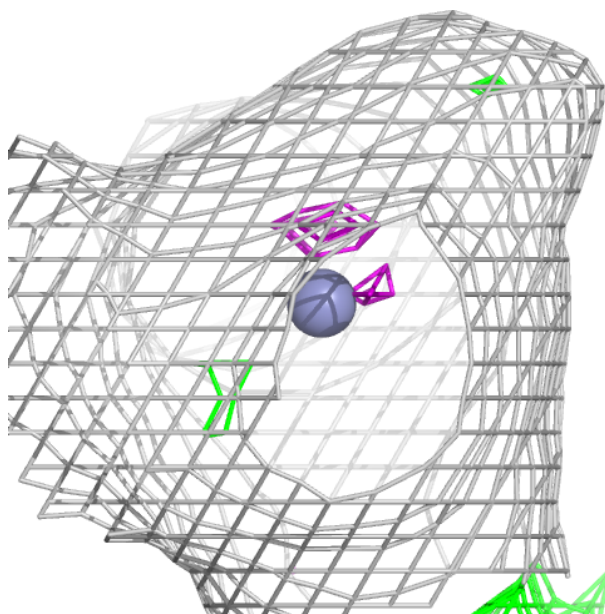
Electron density around ZN A 409:

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



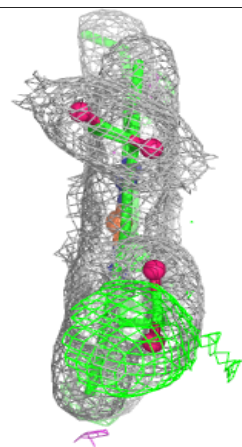
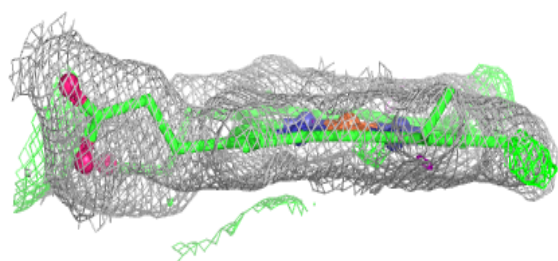
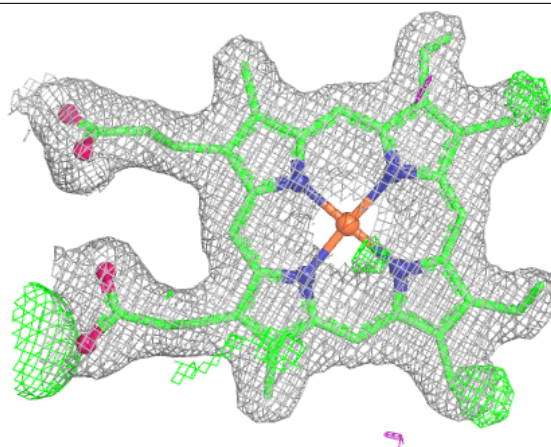
Electron density around ZN B 408:

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



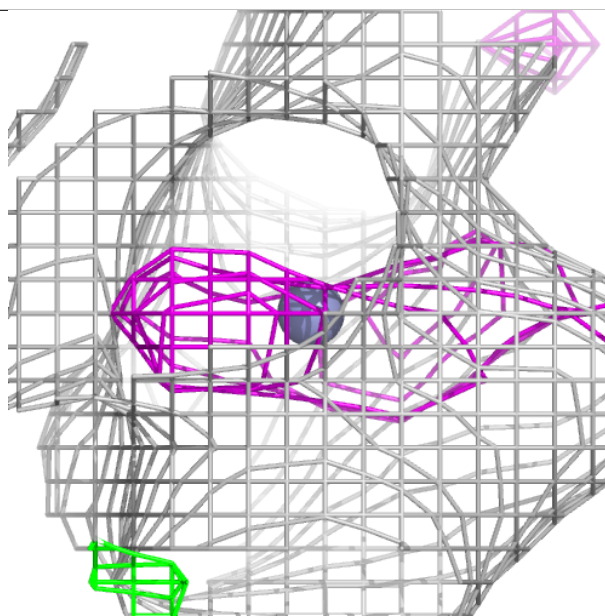
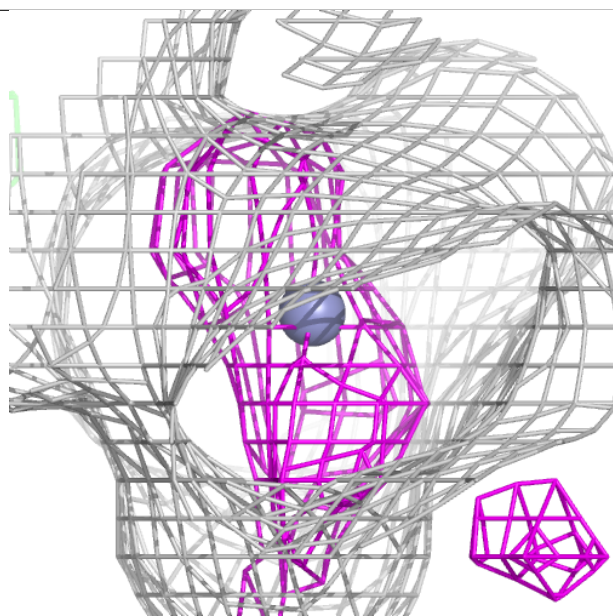
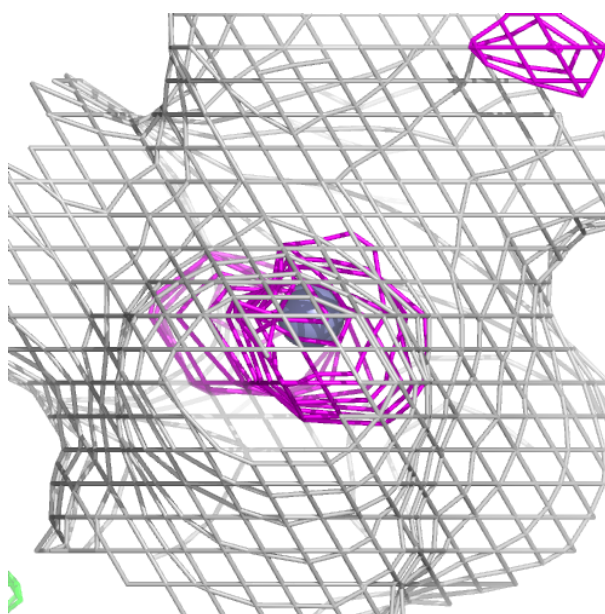
Electron density around HEM A 403:

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



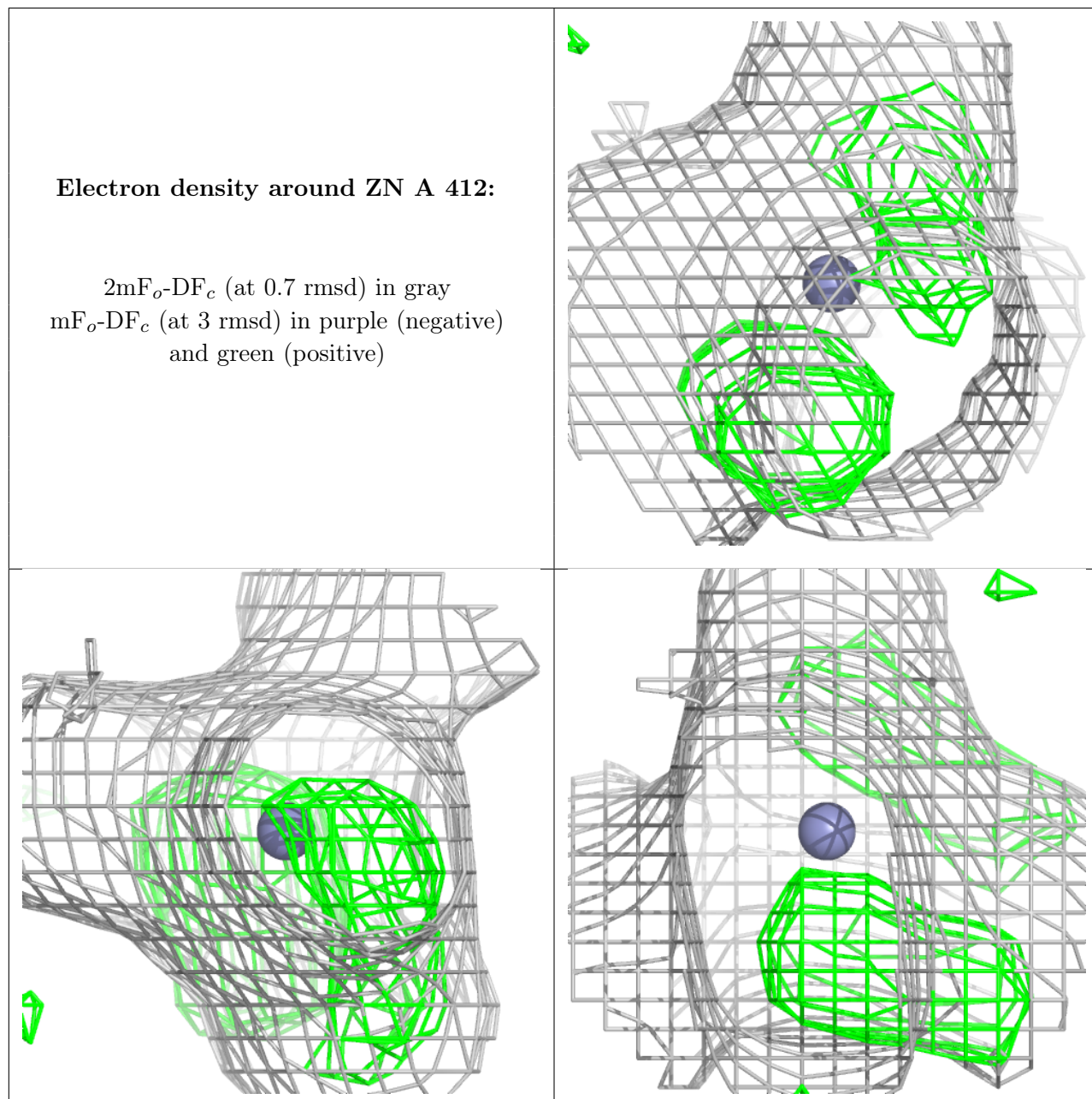
Electron density around ZN B 407:

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



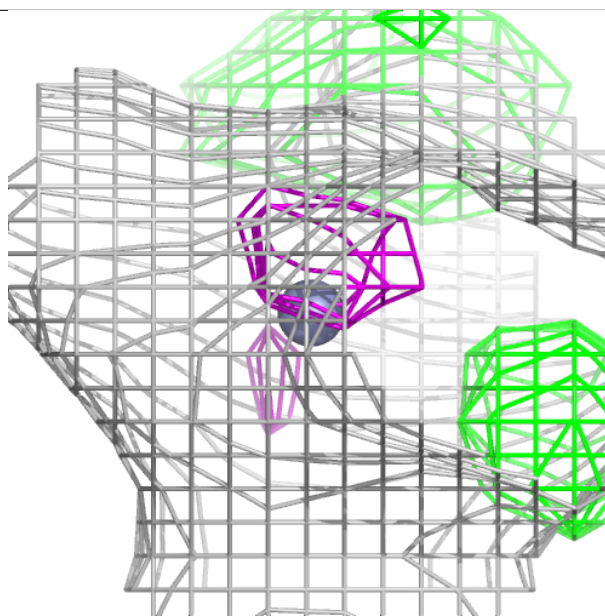
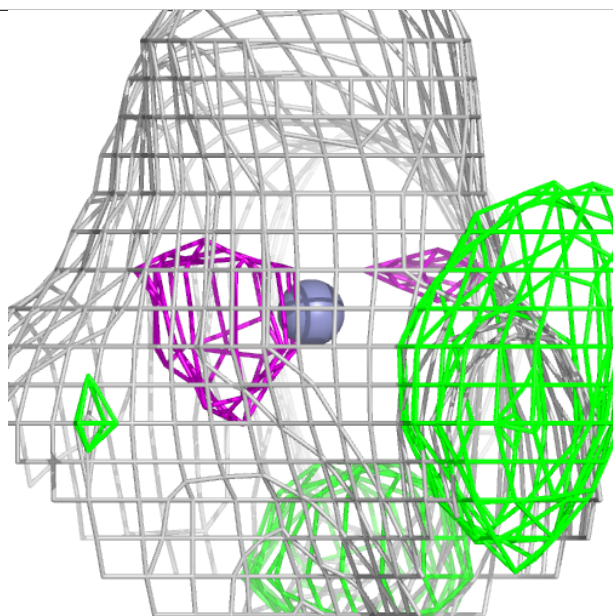
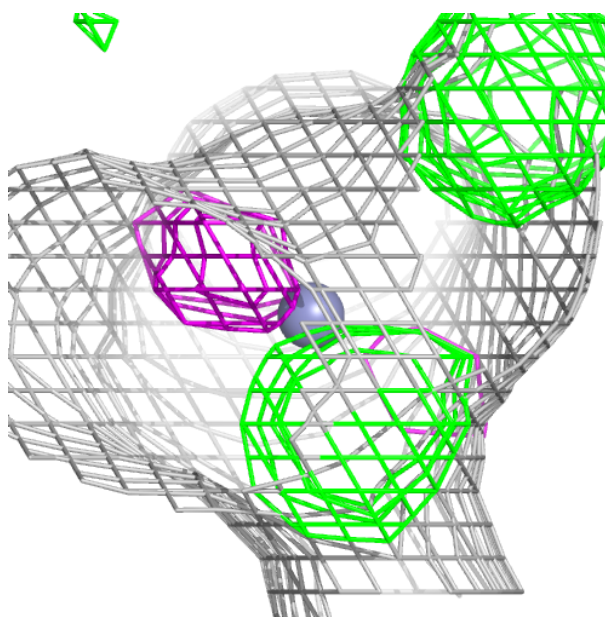
Electron density around ZN A 412:

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



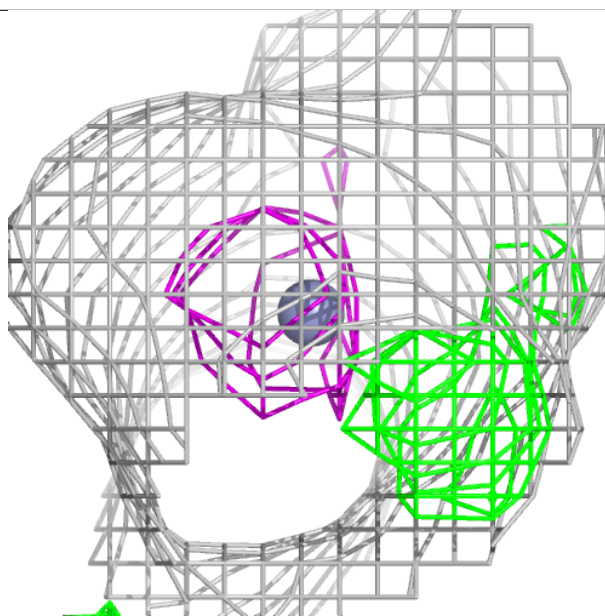
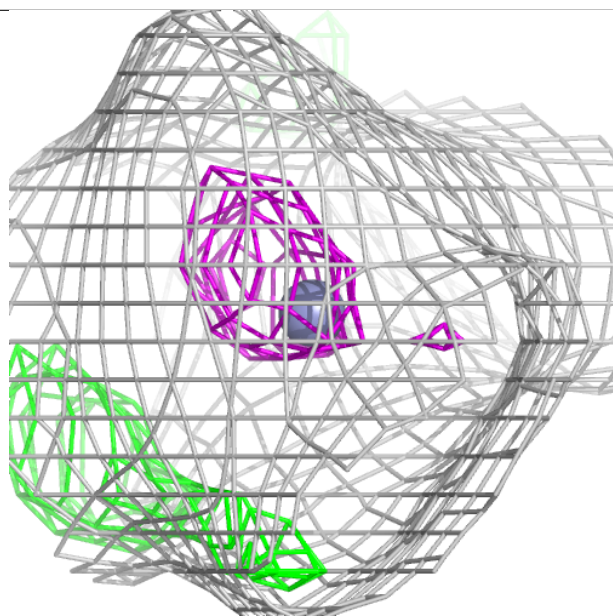
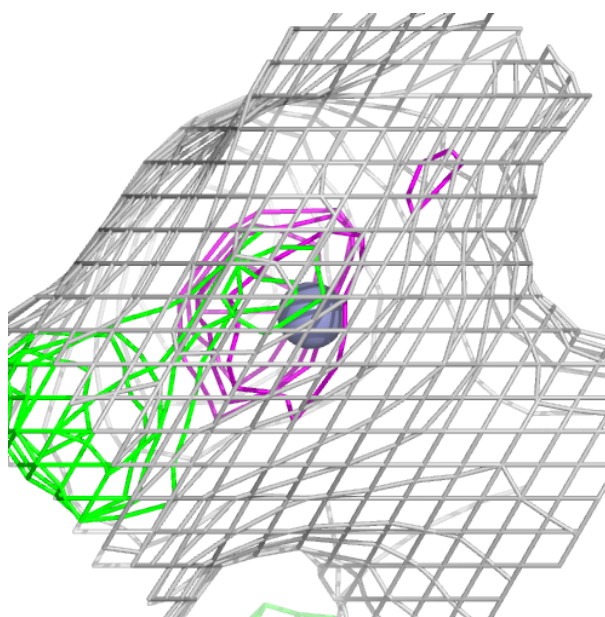
Electron density around ZN B 409:

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



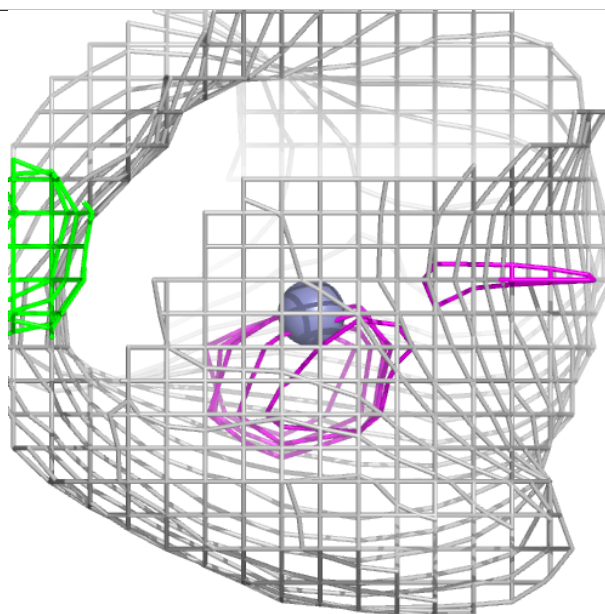
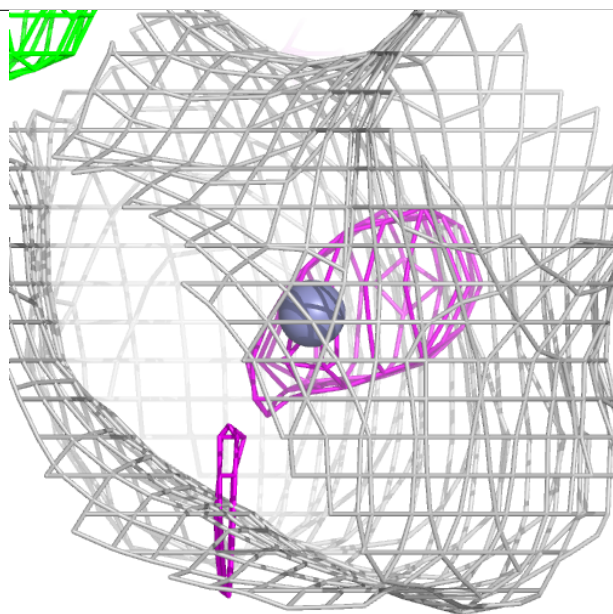
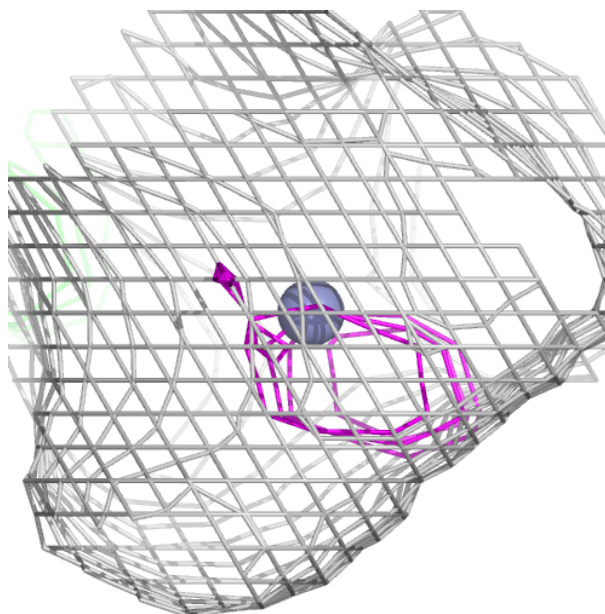
Electron density around ZN A 413:

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



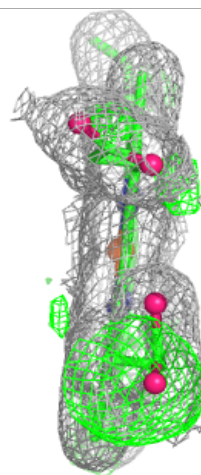
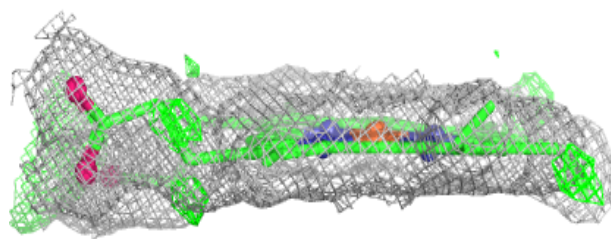
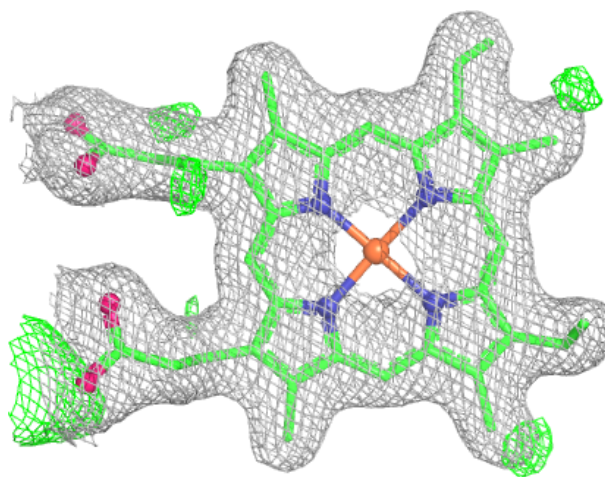
Electron density around ZN A 414:

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



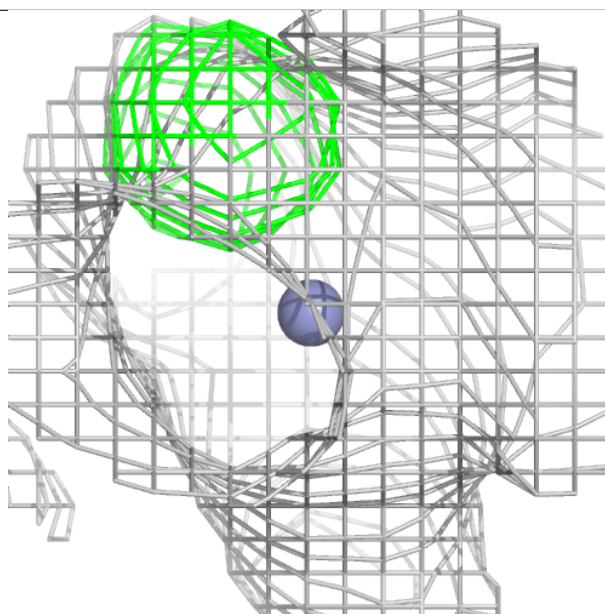
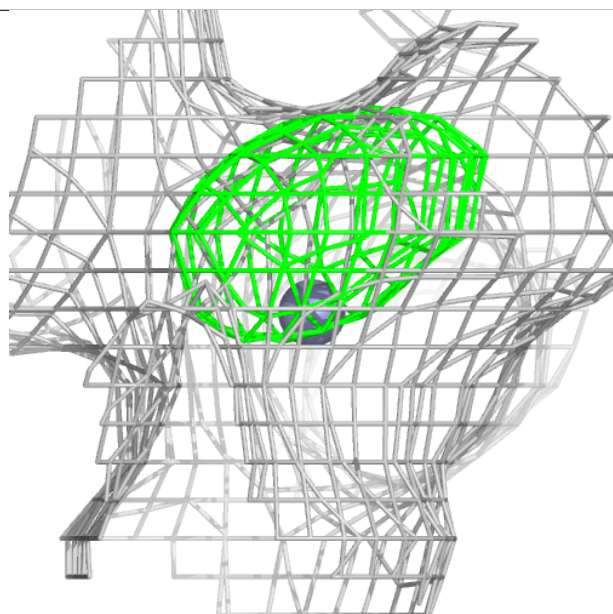
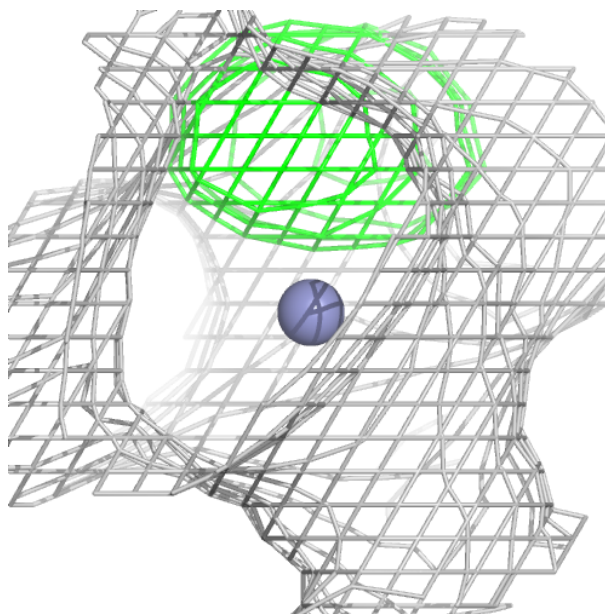
Electron density around HEM B 404:

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



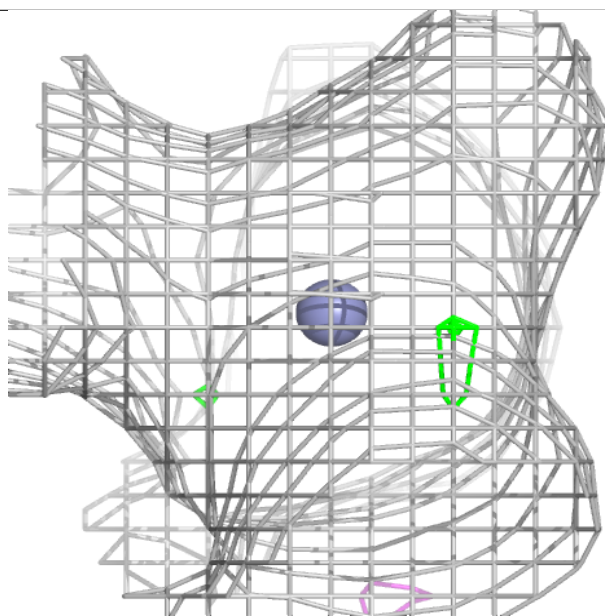
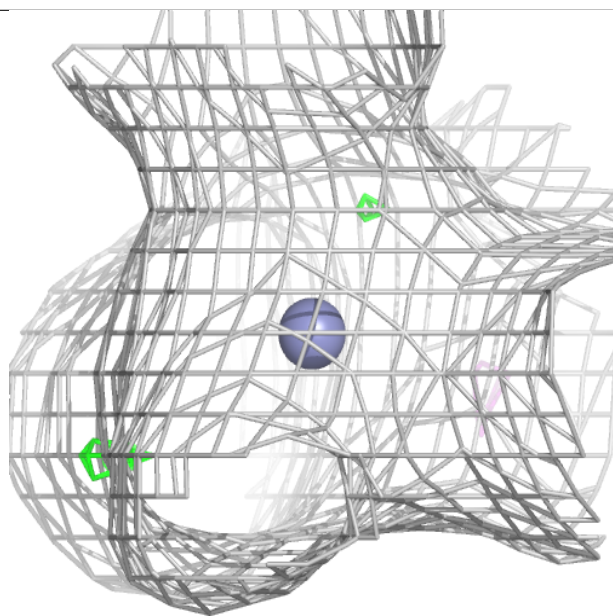
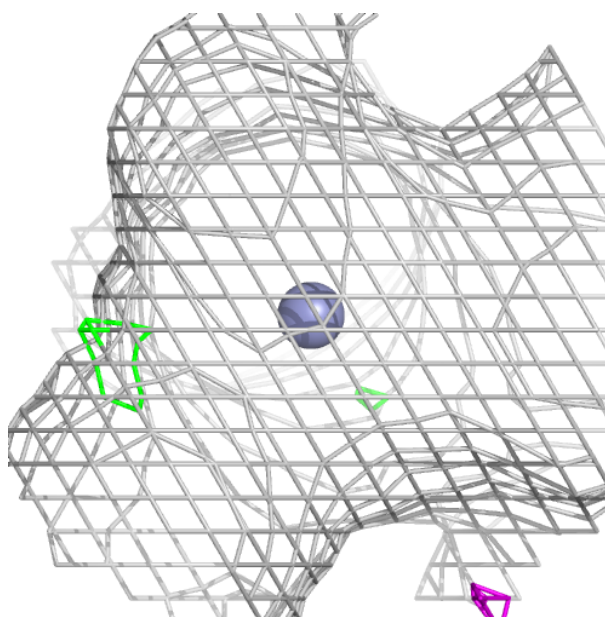
Electron density around ZN A 410:

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



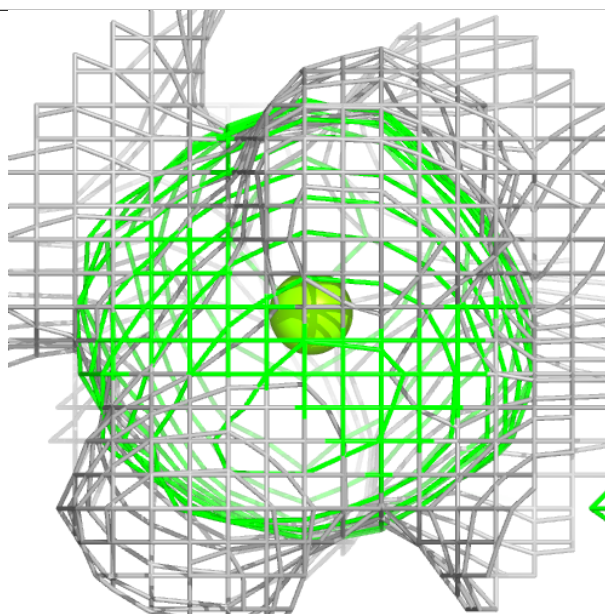
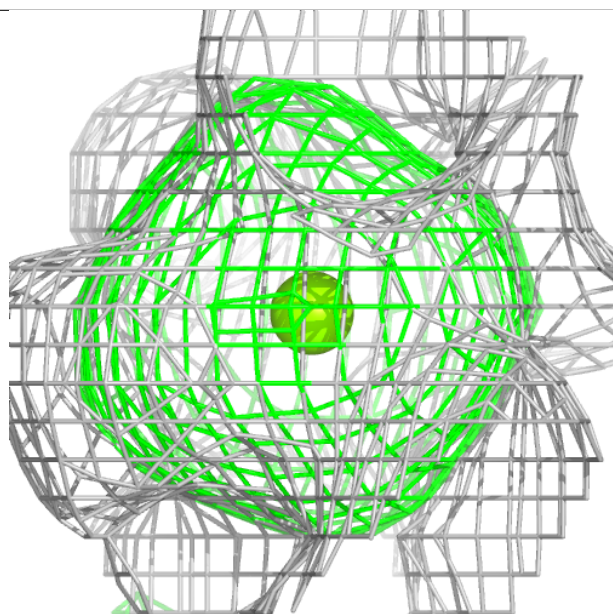
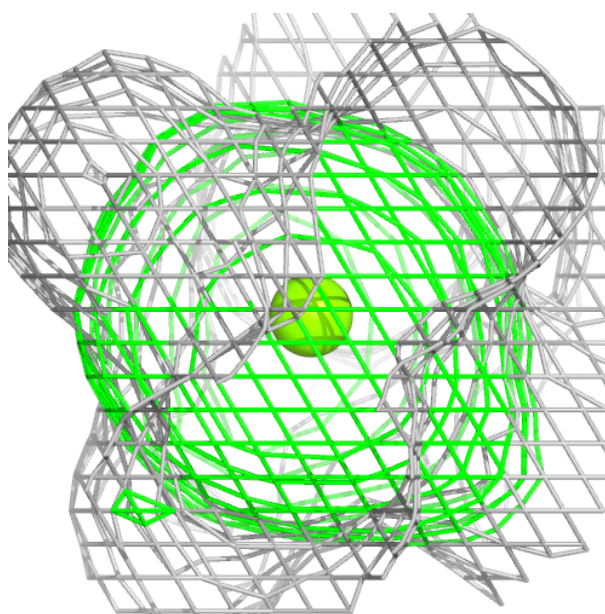
Electron density around ZN A 411:

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



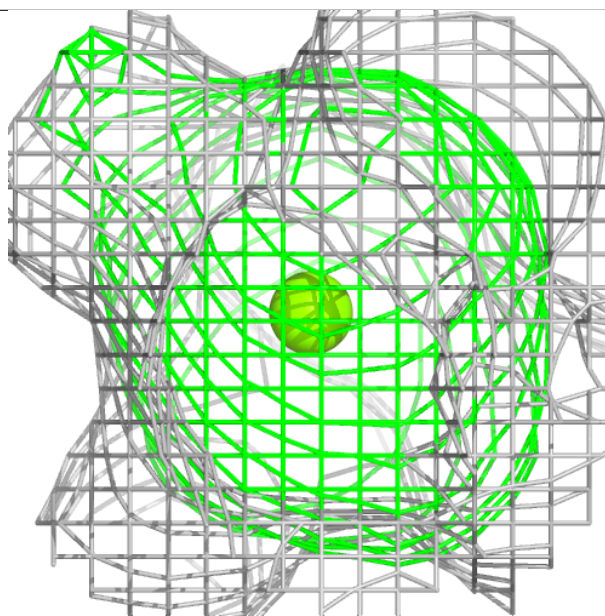
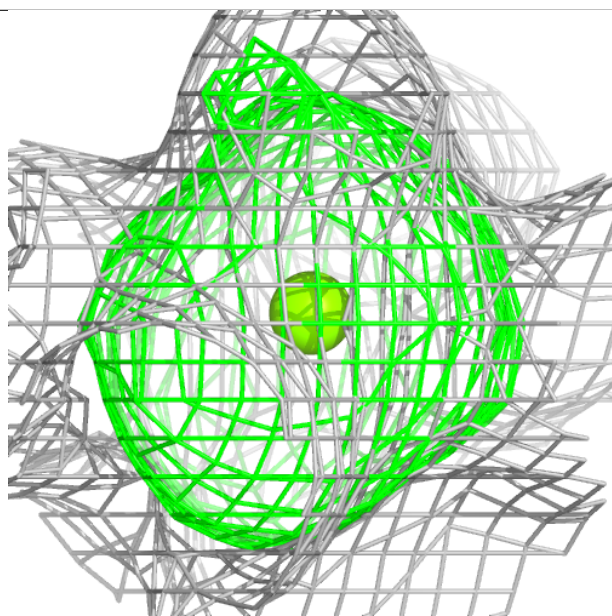
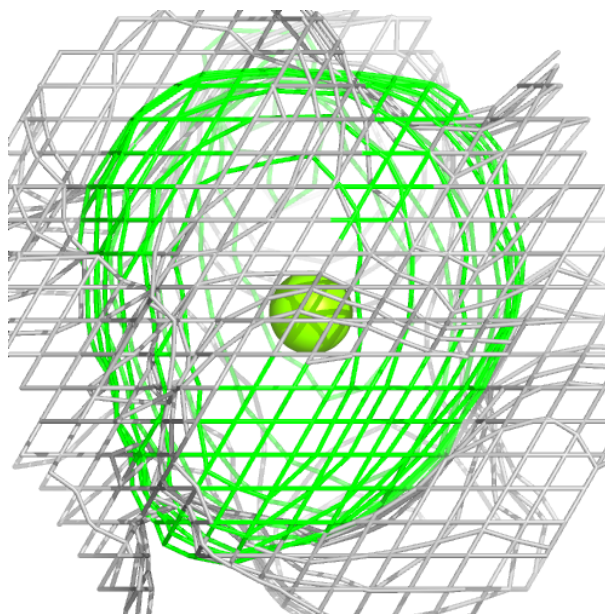
Electron density around MG A 418:

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



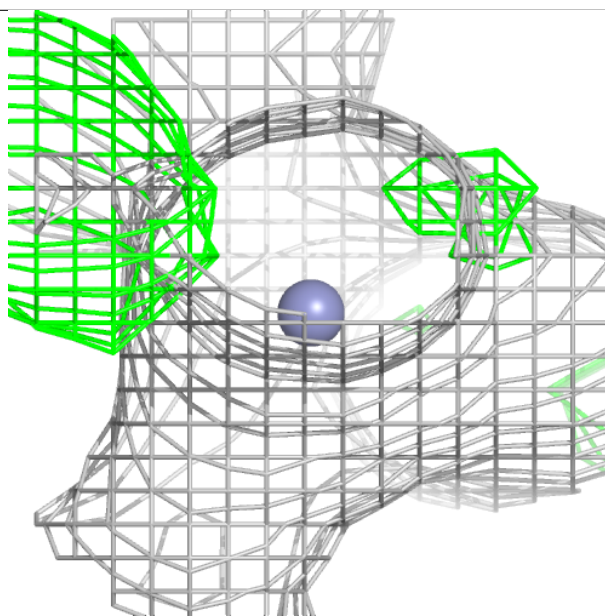
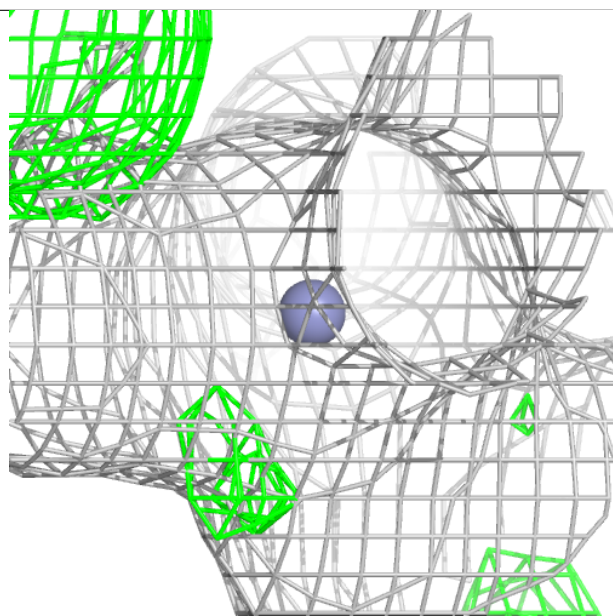
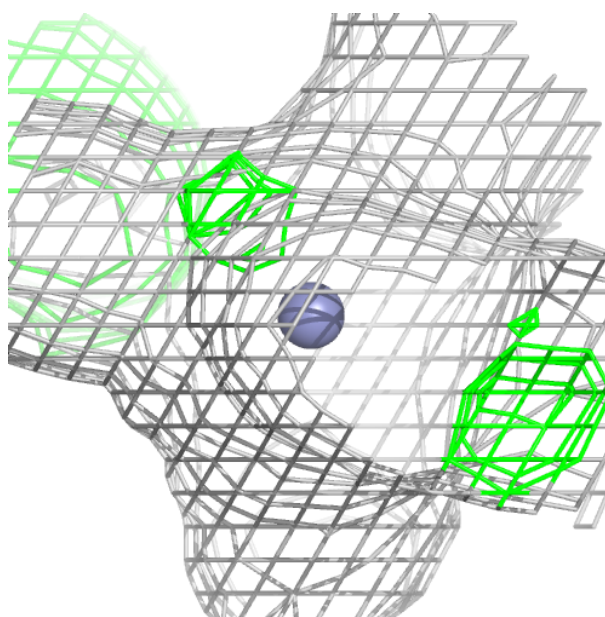
Electron density around MG B 413:

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



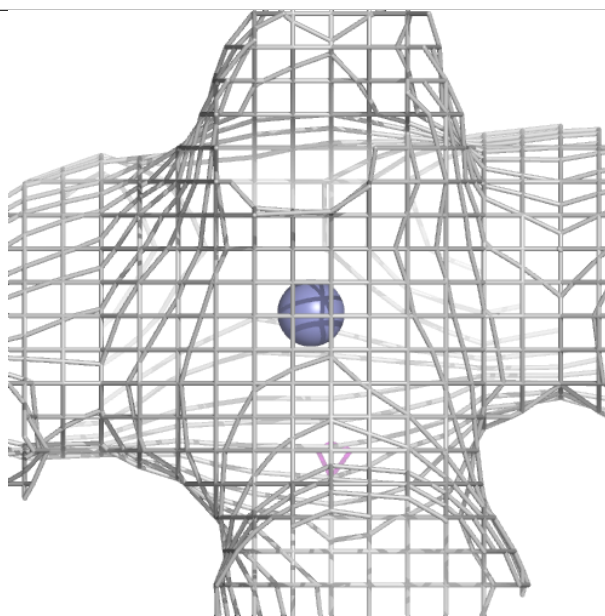
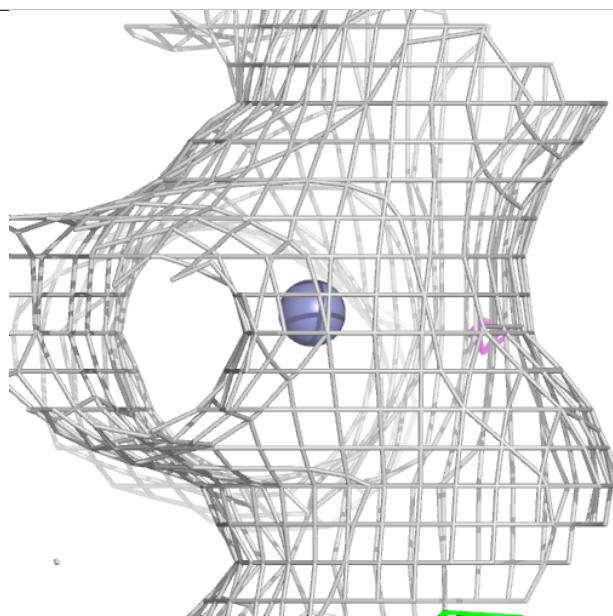
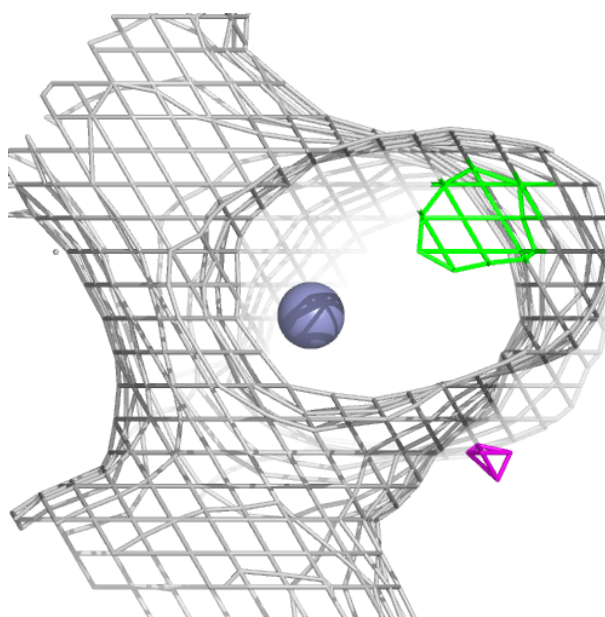
Electron density around ZN A 417:

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



Electron density around 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.