



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2025 – 07:52 PM JST

PDB ID : 8X78
Title : Crystal Structure of N-Acyl Homoserine Lactone Lactonase from *Pseudomonas poae*
Authors : Li, X.H.; Su, D.
Deposited on : 2023-11-23
Resolution : 2.36 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

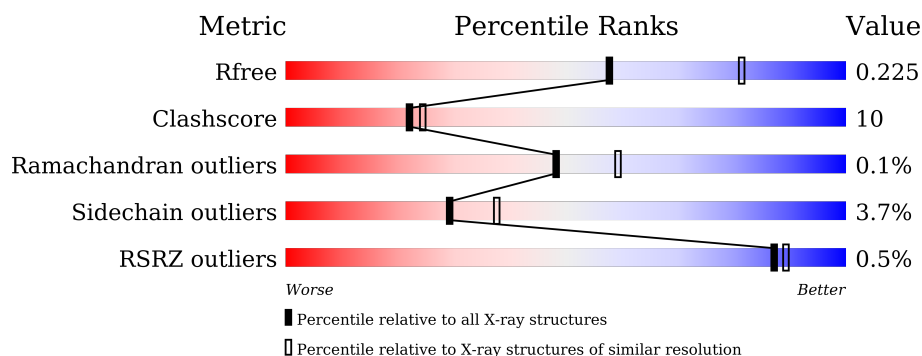
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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	306	<div> <div style="width: 80%;"></div> <div style="width: 14%;"></div> <div style="width: 6%;"></div> </div> <div>80% 14% • 6%</div>
1	B	306	<div> <div style="width: 79%;"></div> <div style="width: 14%;"></div> <div style="width: 6%;"></div> </div> <div>79% 14% • 6%</div>
1	C	306	<div> <div style="width: 76%;"></div> <div style="width: 17%;"></div> <div style="width: 6%;"></div> </div> <div>76% 17% • 6%</div>
1	D	306	<div> <div style="width: 78%;"></div> <div style="width: 15%;"></div> <div style="width: 6%;"></div> </div> <div>78% 15% • 6%</div>
1	E	306	<div> <div style="width: 78%;"></div> <div style="width: 15%;"></div> <div style="width: 6%;"></div> </div> <div>78% 15% • 6%</div>
1	F	306	<div> <div style="width: 80%;"></div> <div style="width: 15%;"></div> <div style="width: 5%;"></div> </div> <div>80% 15% 5%</div>

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Mol	Chain	Length	Quality of chain
1	G	306	<div><div></div><div>73%21%6%</div></div>
1	H	306	<div><div>3%</div><div></div><div>56%33%7%</div></div>
1	I	306	<div><div></div><div>66%26%7%</div></div>
1	J	306	<div><div></div><div>80%14%6%</div></div>
1	K	306	<div><div>%</div><div></div><div>68%22%6%</div></div>
1	L	306	<div><div></div><div>75%17%6%</div></div>

2 Entry composition

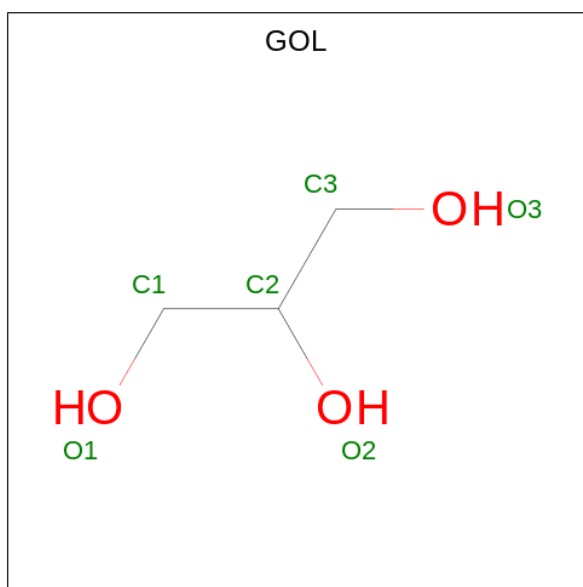
There are 4 unique types of molecules in this entry. The entry contains 28301 atoms, of which 104 are hydrogens and 0 are deuteriums.

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 Glyoxylase, beta-lactamase superfamily II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	287	Total	C	N	O	S	0	0	0
			2310	1467	399	434	10			
1	K	287	Total	C	N	O	S	0	0	0
			2306	1466	396	434	10			
1	G	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			
1	H	286	Total	C	N	O	S	0	0	0
			2298	1461	395	432	10			
1	I	285	Total	C	N	O	S	0	0	0
			2288	1455	391	432	10			
1	J	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			
1	F	291	Total	C	N	O	S	0	0	0
			2338	1483	403	442	10			
1	E	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			
1	A	289	Total	C	N	O	S	0	0	0
			2324	1477	401	436	10			
1	B	288	Total	C	N	O	S	0	0	0
			2314	1470	397	437	10			
1	C	287	Total	C	N	O	S	0	0	0
			2310	1467	399	434	10			
1	D	288	Total	C	N	O	S	0	0	0
			2317	1472	400	435	10			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	L	1	Total	C	H	O	0	0
			14	3	8	3		
2	K	1	Total	C	H	O	0	0
			14	3	8	3		
2	G	1	Total	C	H	O	0	0
			14	3	8	3		
2	H	1	Total	C	H	O	0	0
			14	3	8	3		
2	I	1	Total	C	H	O	0	0
			14	3	8	3		
2	J	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Inter-

est" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	2	Total 2	Zn 2	0	0
3	K	2	Total 2	Zn 2	0	0
3	G	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	J	2	Total 2	Zn 2	0	0
3	F	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	A	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0
3	C	2	Total 2	Zn 2	0	0
3	D	2	Total 2	Zn 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	13	Total 13	O 13	0	0
4	K	5	Total 5	O 5	0	0
4	G	4	Total 4	O 4	0	0
4	H	8	Total 8	O 8	0	0
4	I	14	Total 14	O 14	0	0
4	J	34	Total 34	O 34	0	0
4	F	37	Total 37	O 37	0	0

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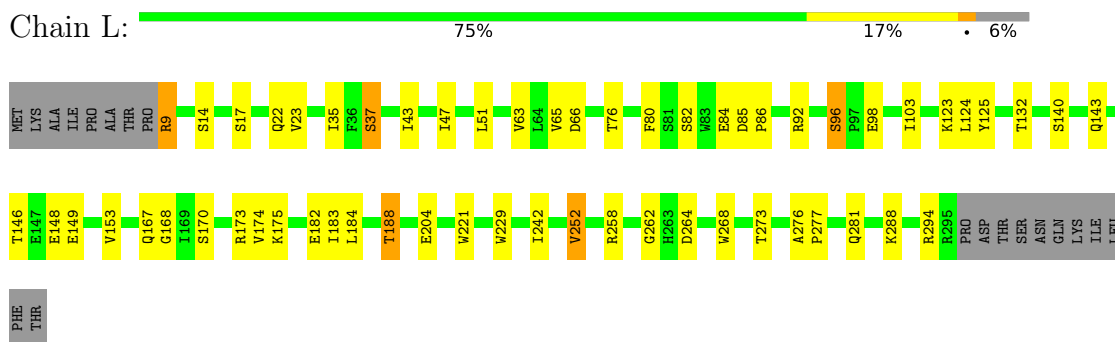
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	33	Total 33	O 33	0	0
4	A	56	Total 56	O 56	0	0
4	B	61	Total 61	O 61	0	0
4	C	37	Total 37	O 37	0	0
4	D	37	Total 37	O 37	0	0

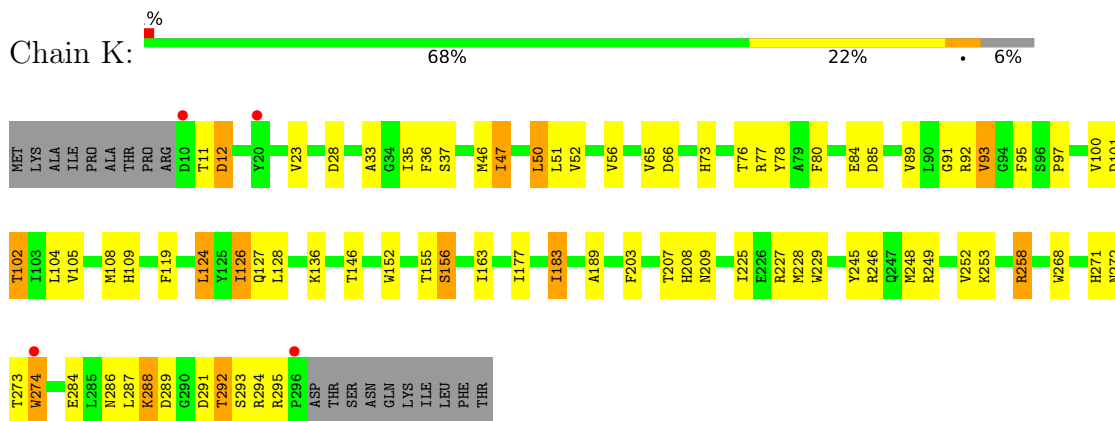
3 Residue-property plots [i](#)

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.

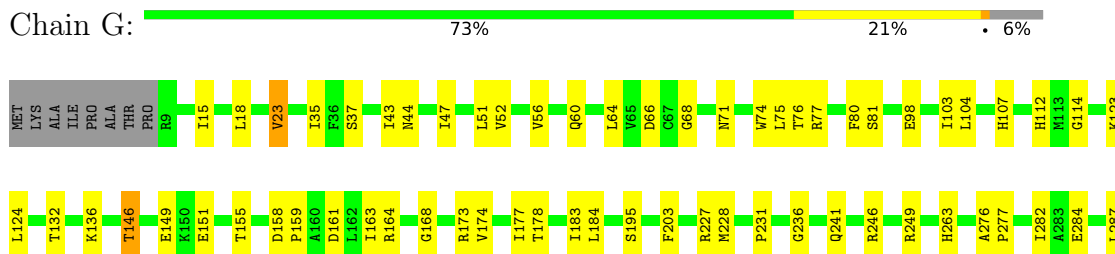
- Molecule 1: Glyoxylase, beta-lactamase superfamily II

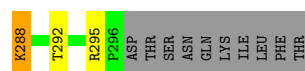


- Molecule 1: Glyoxylase, beta-lactamase superfamily II

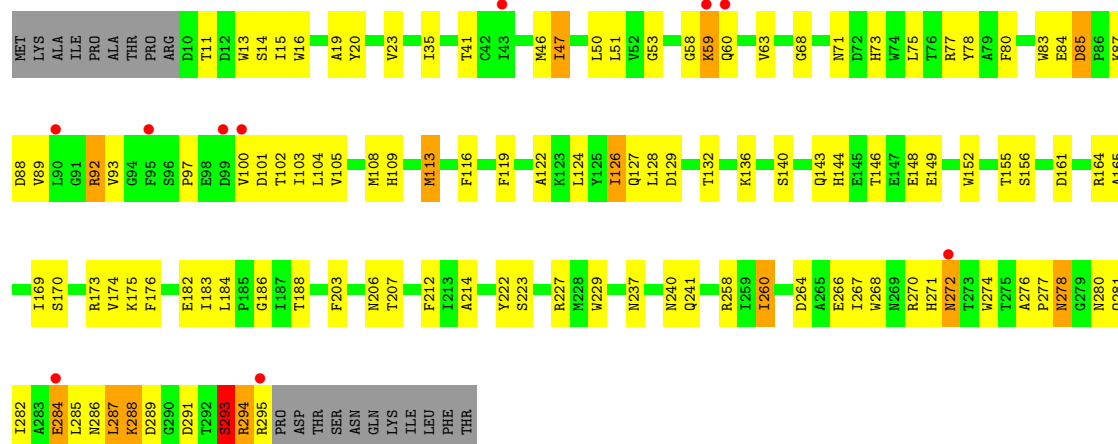


- Molecule 1: Glyoxylase, beta-lactamase superfamily II

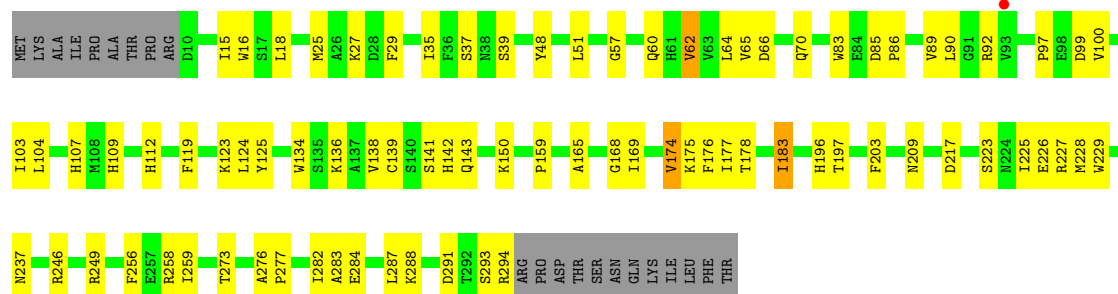




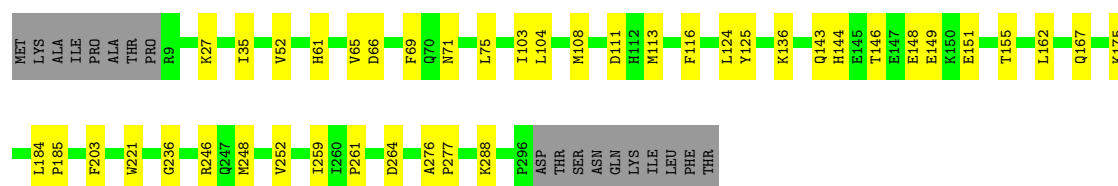
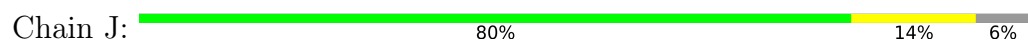
• Molecule 1: Glyoxylase, beta-lactamase superfamily II



• Molecule 1: Glyoxylase, beta-lactamase superfamily II

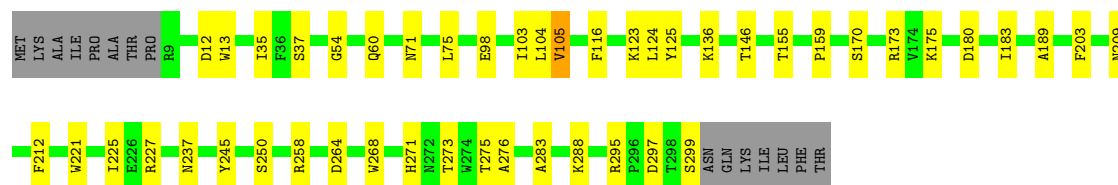


• Molecule 1: Glyoxylase, beta-lactamase superfamily II



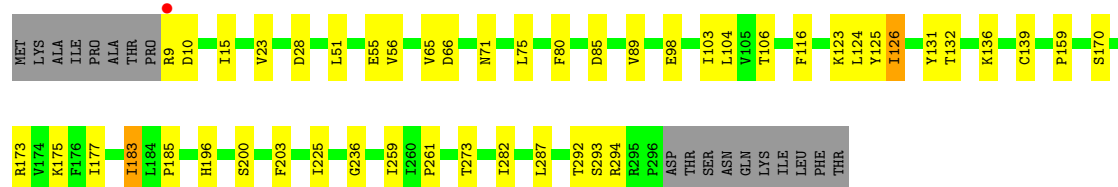
• Molecule 1: Glyoxylase, beta-lactamase superfamily II





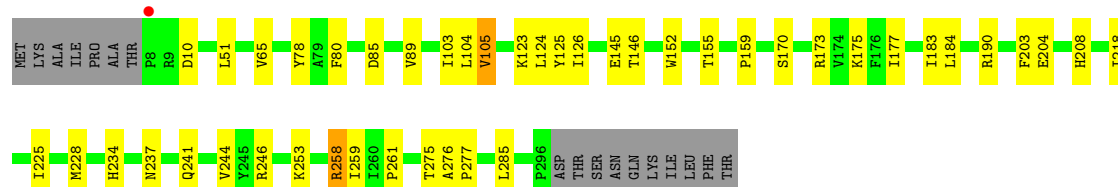
- Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain E: 78% 15% • 6%



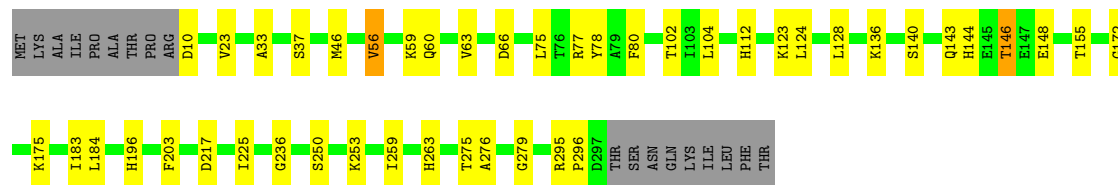
- Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain A: 80% 14% • 6%



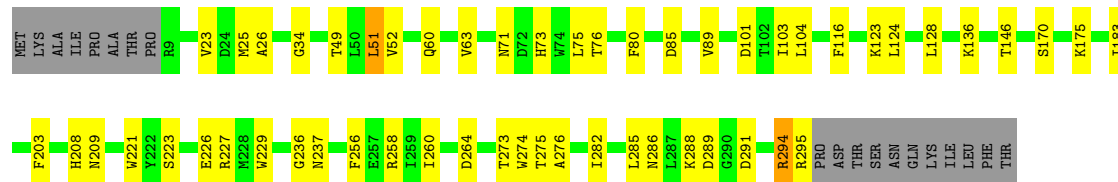
- Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain B: 79% 14% • 6%



- Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain C: 76% 17% • 6%



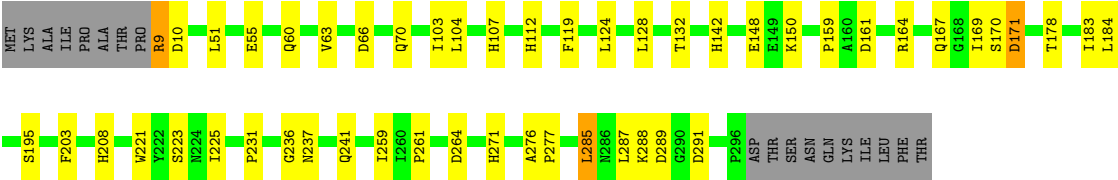
- Molecule 1: Glyoxylase, beta-lactamase superfamily II

Chain D:

78%

15%

6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.59Å 87.67Å 159.24Å 90.00° 115.79° 90.00°	Depositor
Resolution (Å)	39.96 – 2.36 39.96 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.96-2.36) 99.6 (39.96-2.36)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.168 , 0.223 0.172 , 0.225	Depositor DCC
R_{free} test set	143685 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28301	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3175e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/2396	0.67	0/3258
1	B	0.48	0/2385	0.67	0/3244
1	C	0.46	0/2380	0.64	0/3235
1	D	0.49	0/2388	0.64	0/3247
1	E	0.45	0/2388	0.63	0/3247
1	F	0.47	0/2409	0.66	0/3276
1	G	0.39	0/2388	0.60	0/3247
1	H	0.40	0/2368	0.57	0/3220
1	I	0.43	0/2358	0.62	0/3207
1	J	0.49	0/2388	0.65	0/3247
1	K	0.47	0/2377	0.66	0/3233
1	L	0.43	0/2380	0.61	0/3235
All	All	0.46	0/28605	0.63	0/38896

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 [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	2324	0	2166	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2314	0	2149	42	0
1	C	2310	0	2151	41	0
1	D	2317	0	2158	36	0
1	E	2317	0	2158	37	0
1	F	2338	0	2174	27	0
1	G	2317	0	2158	40	0
1	H	2298	0	2135	101	0
1	I	2288	0	2125	80	0
1	J	2317	0	2158	37	0
1	K	2306	0	2145	94	0
1	L	2310	0	2151	60	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
2	C	6	8	8	1	0
2	D	6	8	8	0	0
2	E	6	8	8	0	0
2	F	12	16	16	0	0
2	G	6	8	8	0	0
2	H	6	8	8	0	0
2	I	6	8	7	0	0
2	J	6	8	8	0	0
2	K	6	8	7	0	0
2	L	6	8	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	56	0	0	1	0
4	B	61	0	0	0	0
4	C	37	0	0	1	0
4	D	37	0	0	1	0
4	E	33	0	0	1	0
4	F	37	0	0	1	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	8	0	0	2	0
4	I	14	0	0	0	0
4	J	34	0	0	0	0
4	K	5	0	0	0	0
4	L	13	0	0	1	0
All	All	28197	104	25930	563	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 10.

The worst 5 of 563 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:E:123:LYS:HD3	1:E:175:LYS:HE2	1.31	1.12
1:I:57:GLY:HA2	1:C:295:ARG:HE	1.08	1.06
1:L:143:GLN:NE2	1:K:246:ARG:HD3	1.74	1.02
1:L:96:SER:HB2	1:L:98:GLU:OE1	1.64	0.96
1:H:100:VAL:HG23	1:H:122:ALA:HB2	1.49	0.93

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	287/306 (94%)	278 (97%)	9 (3%)	0	100	100
1	B	286/306 (94%)	273 (96%)	13 (4%)	0	100	100
1	C	285/306 (93%)	272 (95%)	13 (5%)	0	100	100
1	D	286/306 (94%)	275 (96%)	11 (4%)	0	100	100
1	E	286/306 (94%)	276 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	289/306 (94%)	278 (96%)	11 (4%)	0	100	100
1	G	286/306 (94%)	274 (96%)	12 (4%)	0	100	100
1	H	284/306 (93%)	261 (92%)	22 (8%)	1 (0%)	30	34
1	I	283/306 (92%)	271 (96%)	12 (4%)	0	100	100
1	J	286/306 (94%)	277 (97%)	9 (3%)	0	100	100
1	K	285/306 (93%)	264 (93%)	20 (7%)	1 (0%)	30	34
1	L	285/306 (93%)	274 (96%)	11 (4%)	0	100	100
All	All	3428/3672 (93%)	3273 (96%)	153 (4%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	289	ASP
1	H	293	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	246/261 (94%)	240 (98%)	6 (2%)	44	55
1	B	245/261 (94%)	240 (98%)	5 (2%)	50	63
1	C	244/261 (94%)	235 (96%)	9 (4%)	29	38
1	D	245/261 (94%)	238 (97%)	7 (3%)	37	48
1	E	245/261 (94%)	242 (99%)	3 (1%)	67	80
1	F	248/261 (95%)	239 (96%)	9 (4%)	30	39
1	G	245/261 (94%)	230 (94%)	15 (6%)	15	17
1	H	242/261 (93%)	220 (91%)	22 (9%)	7	7
1	I	242/261 (93%)	234 (97%)	8 (3%)	33	42
1	J	245/261 (94%)	243 (99%)	2 (1%)	79	88
1	K	244/261 (94%)	228 (93%)	16 (7%)	14	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	244/261 (94%)	236 (97%)	8 (3%)	33	42
All	All	2935/3132 (94%)	2825 (96%)	110 (4%)	29	38

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	287	LEU
1	F	60	GLN
1	D	287	LEU
1	C	183	ILE
1	H	293	SER

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	D	112	HIS
1	J	143	GLN
1	I	143	GLN
1	H	278	ASN
1	I	196	HIS

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 24 are monoatomic - leaving 13 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	$\# Z > 2$
2	GOL	C	401	-	5,5,5	0.51	0	5,5,5	1.29	0
2	GOL	F	402	-	5,5,5	0.87	0	5,5,5	1.13	0
2	GOL	E	401	-	5,5,5	0.99	0	5,5,5	1.09	0
2	GOL	L	401	-	5,5,5	0.75	0	5,5,5	0.93	0
2	GOL	K	401	3	5,5,5	1.12	1 (20%)	5,5,5	0.79	0
2	GOL	F	401	-	5,5,5	0.96	0	5,5,5	1.16	0
2	GOL	G	401	-	5,5,5	0.97	0	5,5,5	0.66	0
2	GOL	D	401	-	5,5,5	1.05	0	5,5,5	1.10	0
2	GOL	I	401	-	5,5,5	1.12	0	5,5,5	1.44	1 (20%)
2	GOL	B	401	-	5,5,5	0.89	0	5,5,5	1.15	1 (20%)
2	GOL	J	401	-	5,5,5	1.10	0	5,5,5	1.07	0
2	GOL	H	403	-	5,5,5	0.56	0	5,5,5	0.32	0
2	GOL	A	401	-	5,5,5	1.06	0	5,5,5	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	F	402	-	-	4/4/4/4	-
2	GOL	E	401	-	-	4/4/4/4	-
2	GOL	L	401	-	-	2/4/4/4	-
2	GOL	K	401	3	-	3/4/4/4	-
2	GOL	F	401	-	-	4/4/4/4	-
2	GOL	G	401	-	-	3/4/4/4	-
2	GOL	D	401	-	-	4/4/4/4	-
2	GOL	I	401	-	-	0/4/4/4	-
2	GOL	B	401	-	-	4/4/4/4	-
2	GOL	J	401	-	-	3/4/4/4	-
2	GOL	H	403	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	GOL	C3-C2	2.16	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	GOL	C3-C2-C1	-2.38	102.45	111.70
2	B	401	GOL	C3-C2-C1	-2.03	103.81	111.70

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	401	GOL	O1-C1-C2-O2
2	G	401	GOL	O1-C1-C2-C3
2	J	401	GOL	C1-C2-C3-O3
2	F	401	GOL	C1-C2-C3-O3
2	F	402	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	GOL	1	0

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 ⓘ

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	289/306 (94%)	-0.61	1 (0%) 90 91	30, 42, 57, 92	0
1	B	288/306 (94%)	-0.63	0 100 100	31, 43, 63, 117	0
1	C	287/306 (93%)	-0.43	0 100 100	34, 49, 68, 90	0
1	D	288/306 (94%)	-0.31	0 100 100	35, 52, 76, 110	0
1	E	288/306 (94%)	-0.44	1 (0%) 90 91	33, 50, 73, 100	0
1	F	291/306 (95%)	-0.53	0 100 100	32, 46, 67, 100	0
1	G	288/306 (94%)	-0.13	0 100 100	41, 67, 95, 119	0
1	H	286/306 (93%)	0.25	10 (3%) 47 53	30, 75, 108, 126	0
1	I	285/306 (93%)	0.01	1 (0%) 89 90	42, 67, 91, 113	0
1	J	288/306 (94%)	-0.49	0 100 100	32, 45, 69, 98	0
1	K	287/306 (93%)	0.12	4 (1%) 73 77	40, 76, 109, 142	0
1	L	287/306 (93%)	-0.12	0 100 100	39, 64, 93, 116	0
All	All	3452/3672 (94%)	-0.28	17 (0%) 87 89	30, 54, 93, 142	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	99	ASP	6.8
1	H	272	ASN	4.3
1	H	284	GLU	4.3
1	H	295	ARG	3.7
1	E	9	ARG	3.5

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 [i](#)

There are no monosaccharides in this entry.

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
2	GOL	H	403	6/6	0.25	0.29	30,30,30,30	0
2	GOL	E	401	6/6	0.80	0.15	47,68,78,85	0
2	GOL	L	401	6/6	0.82	0.13	61,74,85,91	0
2	GOL	B	401	6/6	0.82	0.16	48,62,74,81	0
2	GOL	F	402	6/6	0.83	0.12	53,76,88,95	0
2	GOL	G	401	6/6	0.83	0.14	53,73,89,89	0
2	GOL	J	401	6/6	0.83	0.12	42,55,73,76	0
2	GOL	C	401	6/6	0.83	0.13	49,67,82,93	0
2	GOL	F	401	6/6	0.85	0.12	44,66,77,79	0
3	ZN	K	403	1/1	0.86	0.10	76,76,76,76	0
2	GOL	A	401	6/6	0.87	0.12	47,64,80,83	0
2	GOL	I	401	6/6	0.87	0.11	58,77,94,97	0
2	GOL	D	401	6/6	0.90	0.11	47,70,84,86	0
2	GOL	K	401	6/6	0.90	0.14	64,85,102,102	0
3	ZN	H	402	1/1	0.91	0.08	69,69,69,69	0
3	ZN	J	403	1/1	0.91	0.08	57,57,57,57	0
3	ZN	D	403	1/1	0.93	0.08	56,56,56,56	0
3	ZN	L	403	1/1	0.94	0.26	30,30,30,30	0
3	ZN	F	404	1/1	0.94	0.07	56,56,56,56	0
3	ZN	C	403	1/1	0.94	0.08	54,54,54,54	0
3	ZN	I	403	1/1	0.94	0.09	72,72,72,72	0
3	ZN	I	402	1/1	0.96	0.04	60,60,60,60	0
3	ZN	G	403	1/1	0.98	0.04	65,65,65,65	0
3	ZN	E	403	1/1	0.98	0.06	54,54,54,54	0
3	ZN	H	401	1/1	0.98	0.05	66,66,66,66	0
3	ZN	K	402	1/1	0.98	0.04	66,66,66,66	0
3	ZN	E	402	1/1	0.99	0.02	45,45,45,45	0
3	ZN	G	402	1/1	0.99	0.05	58,58,58,58	0
3	ZN	A	402	1/1	0.99	0.02	42,42,42,42	0
3	ZN	A	403	1/1	0.99	0.03	52,52,52,52	0
3	ZN	B	402	1/1	0.99	0.02	37,37,37,37	0
3	ZN	C	402	1/1	0.99	0.02	48,48,48,48	0

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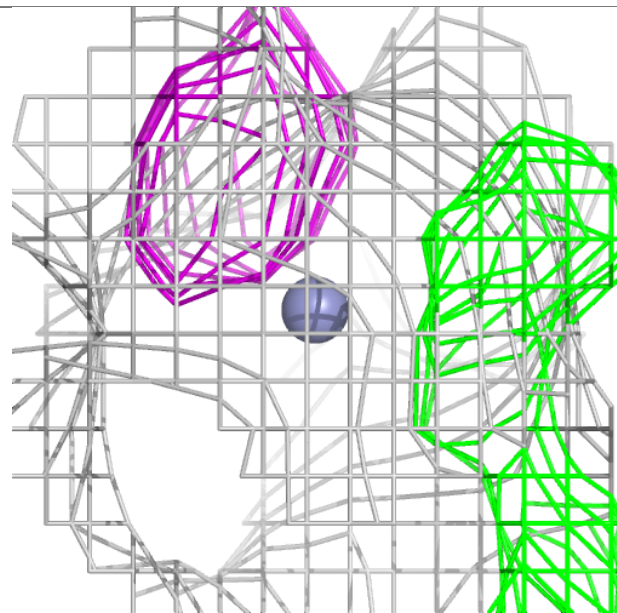
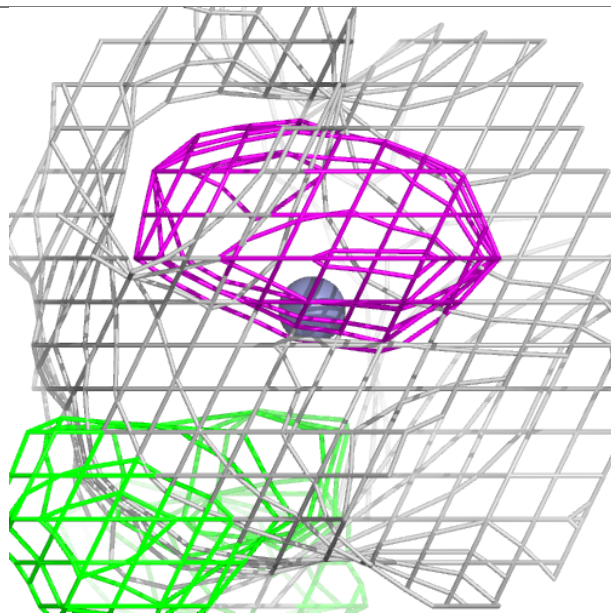
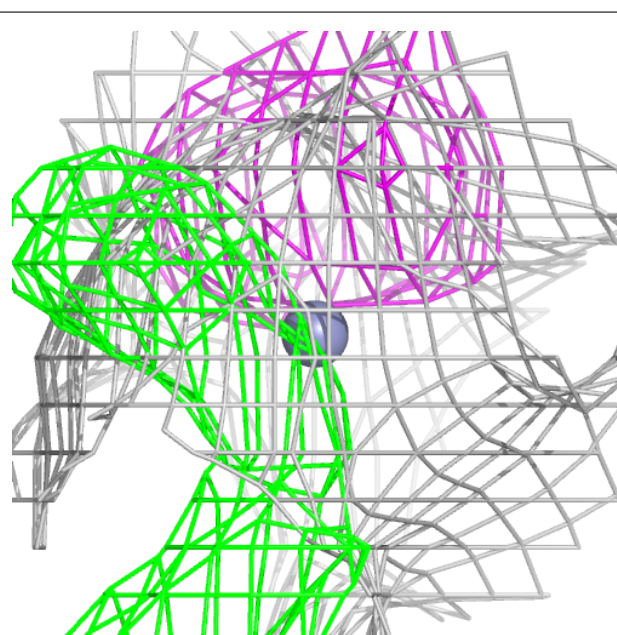
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	F	403	1/1	0.99	0.09	58,58,58,58	0
3	ZN	D	402	1/1	0.99	0.03	46,46,46,46	0
3	ZN	L	402	1/1	0.99	0.03	54,54,54,54	0
3	ZN	J	402	1/1	1.00	0.02	46,46,46,46	0
3	ZN	B	403	1/1	1.00	0.07	42,42,42,42	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.

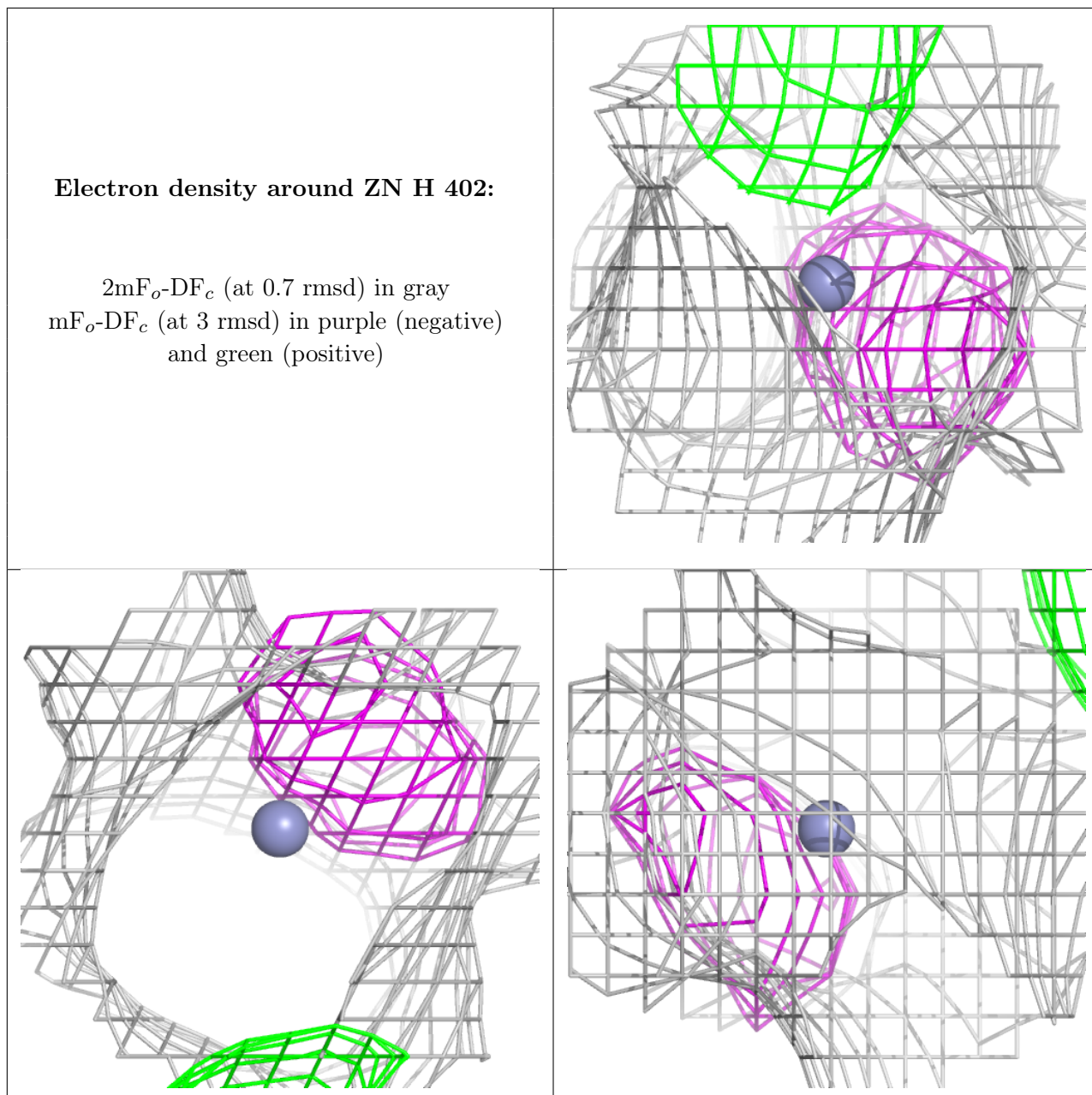
Electron density around ZN K 403:

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and green (positive)



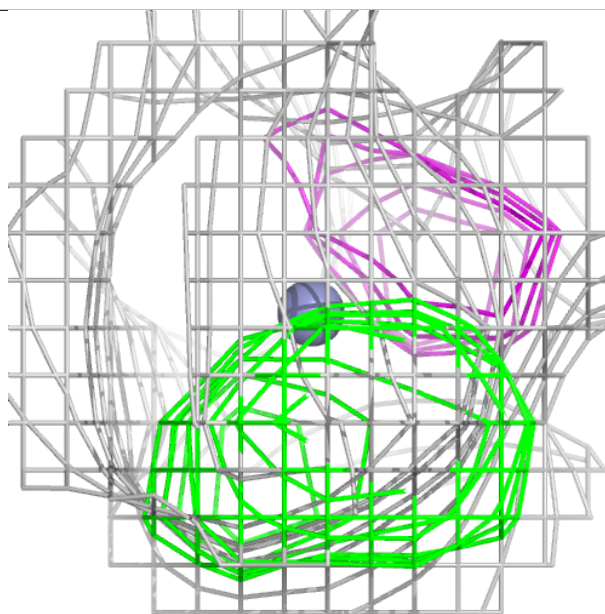
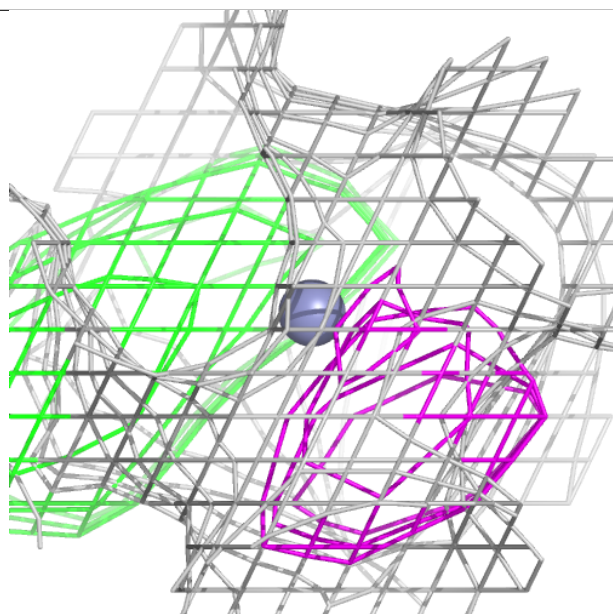
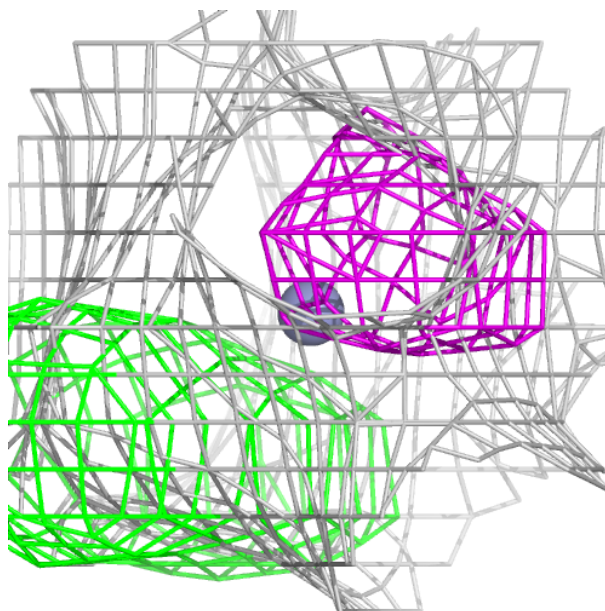
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and green (positive)



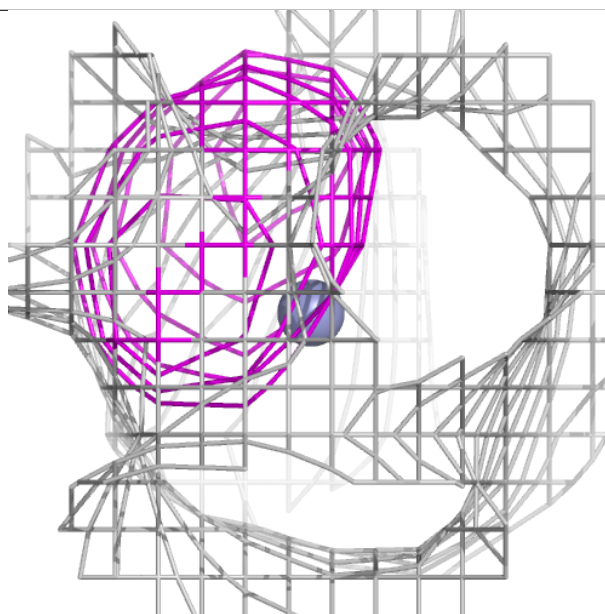
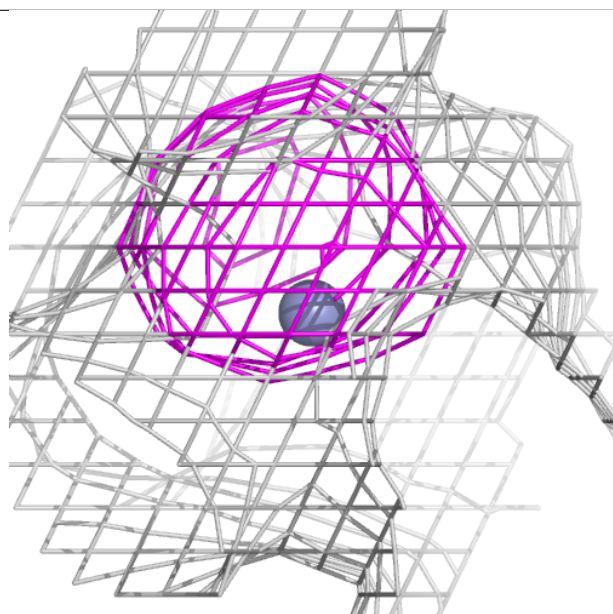
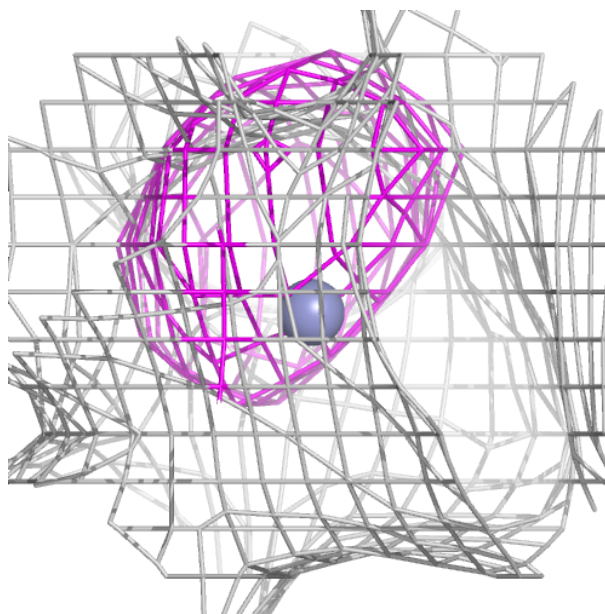
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and green (positive)



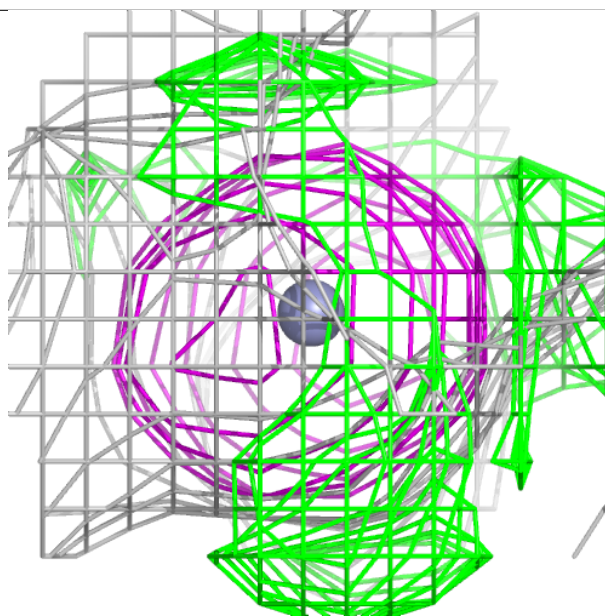
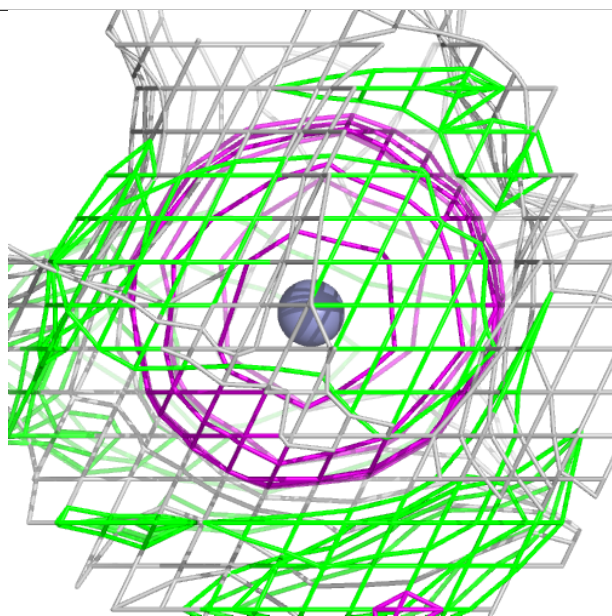
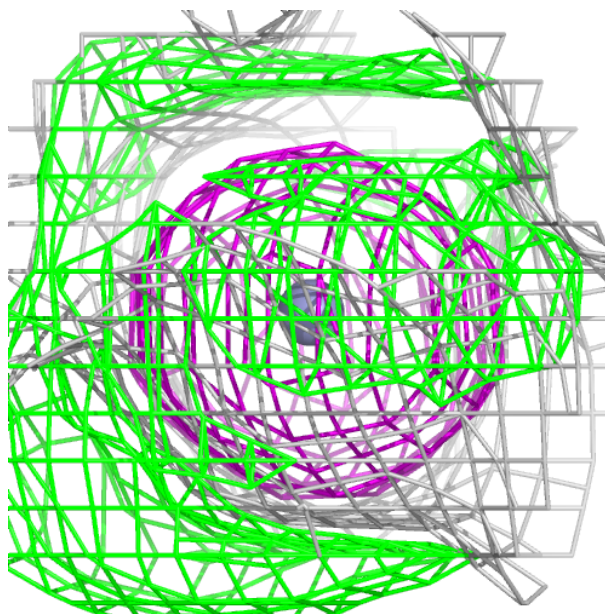
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and green (positive)



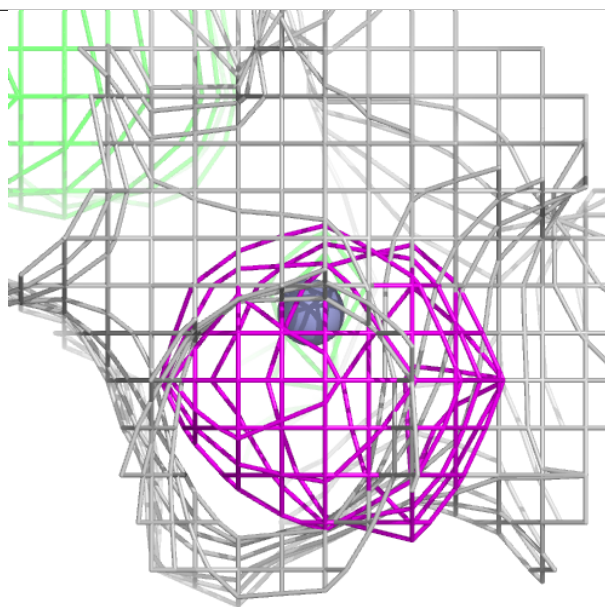
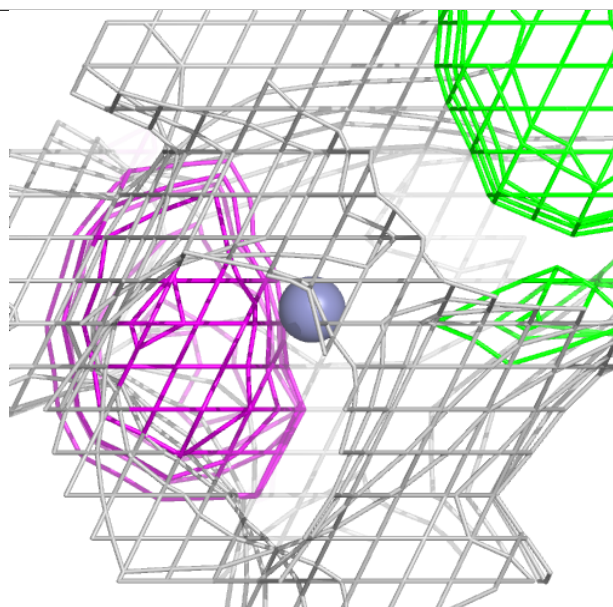
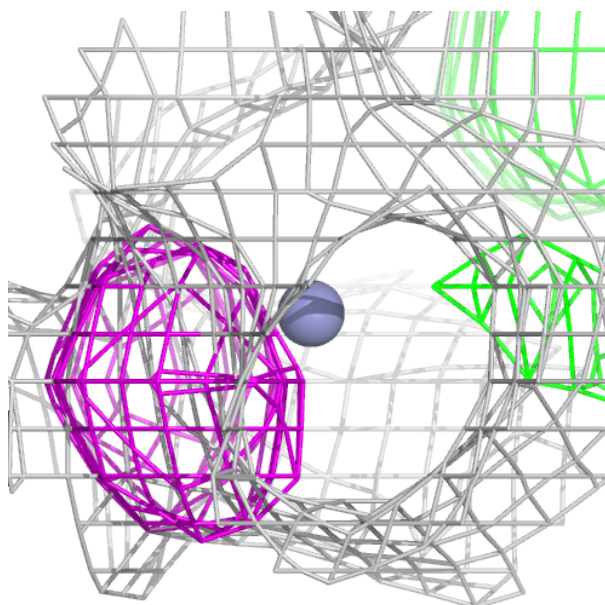
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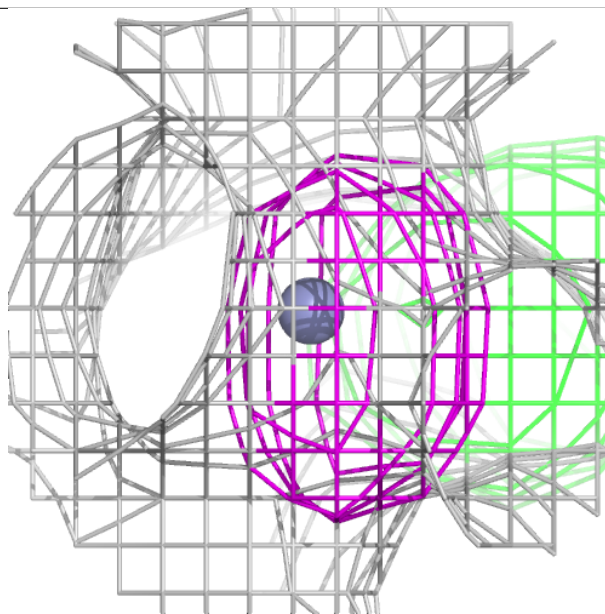
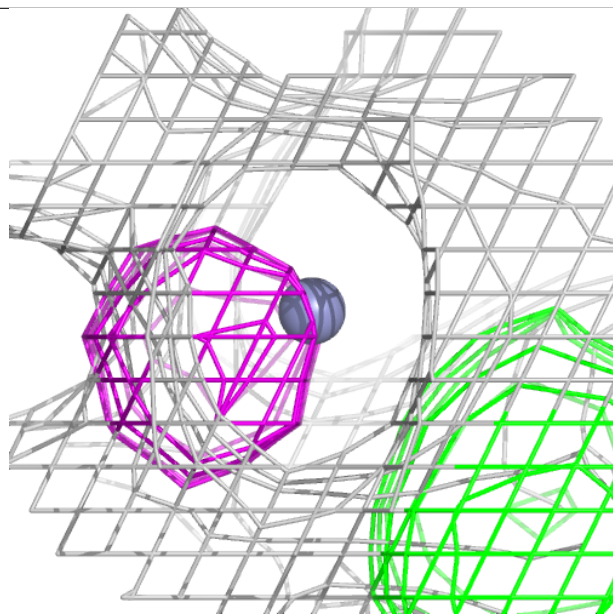
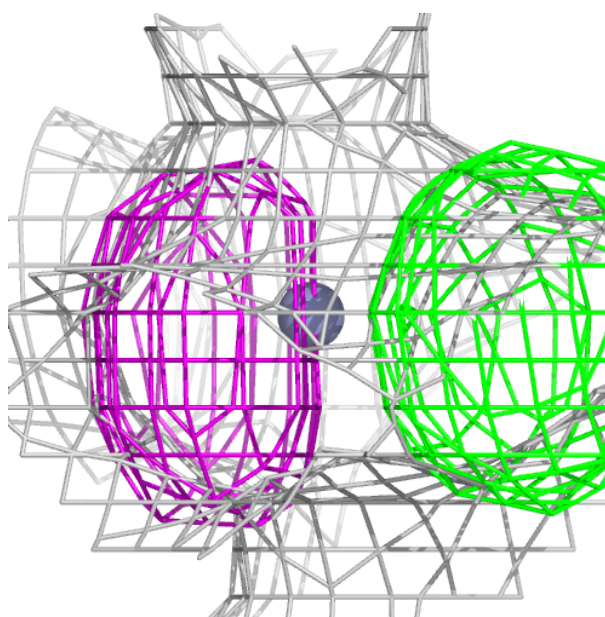
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and green (positive)



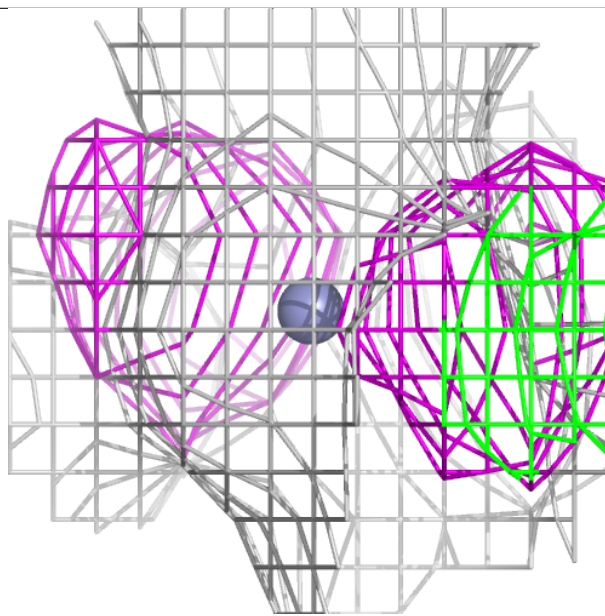
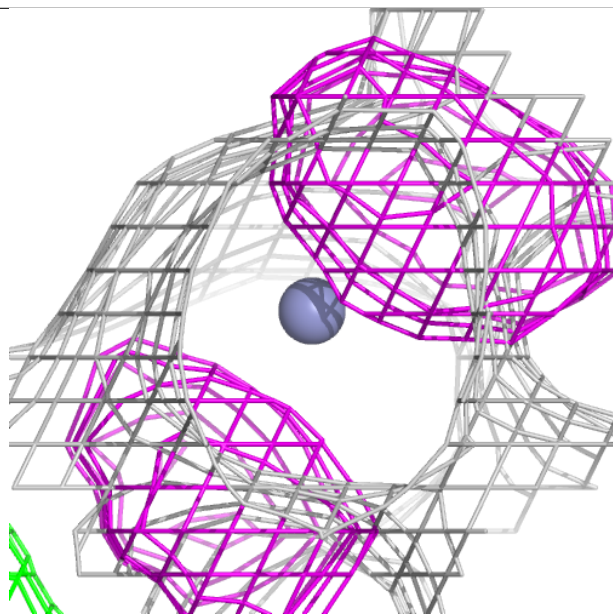
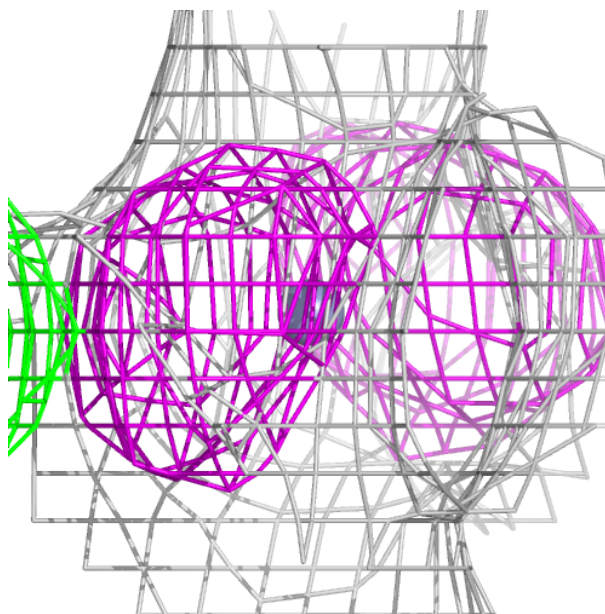
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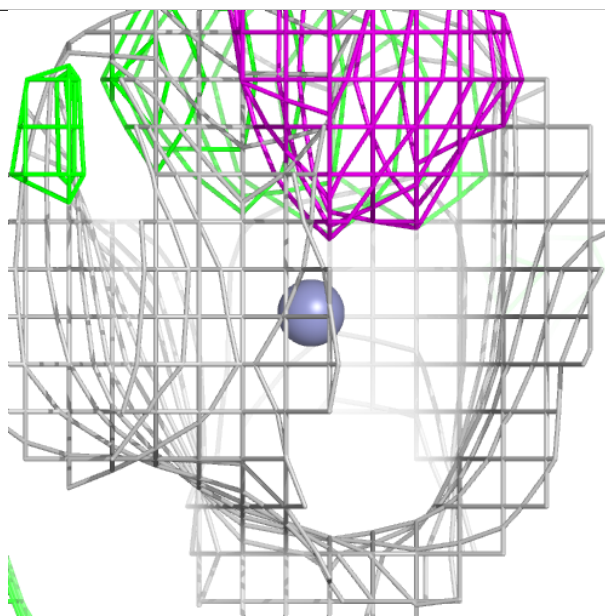
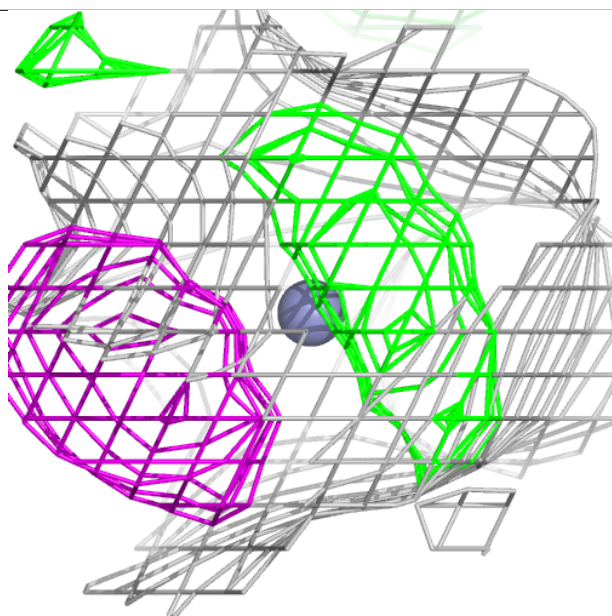
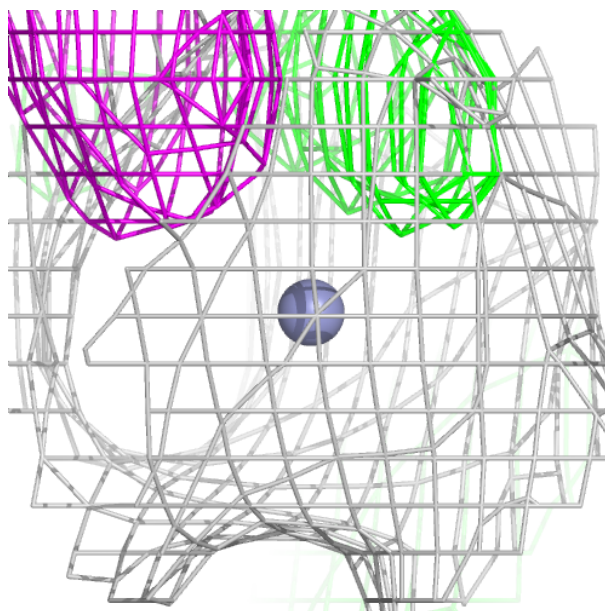
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and green (positive)



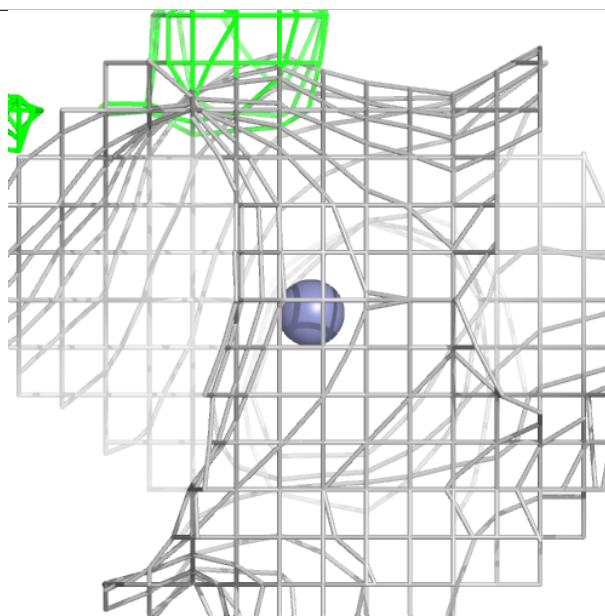
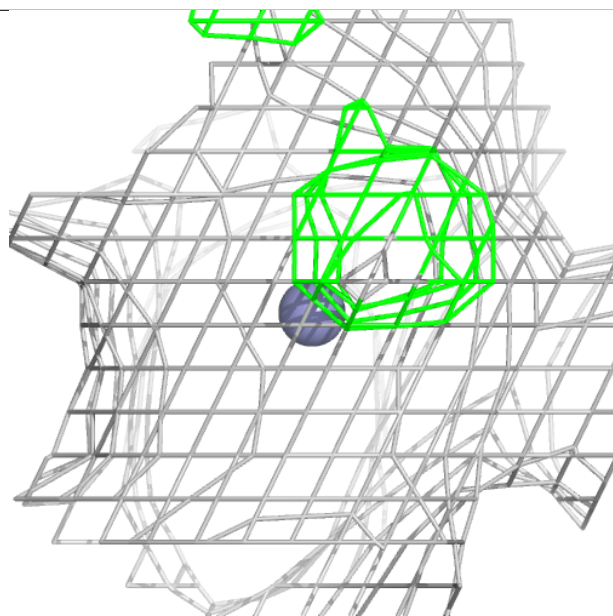
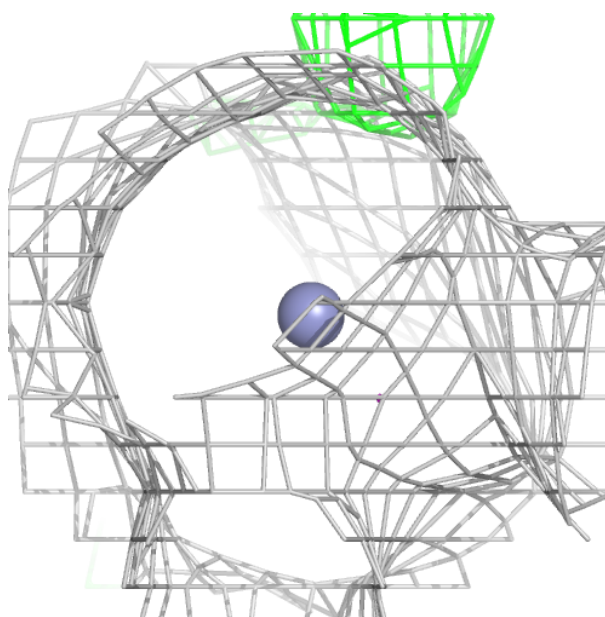
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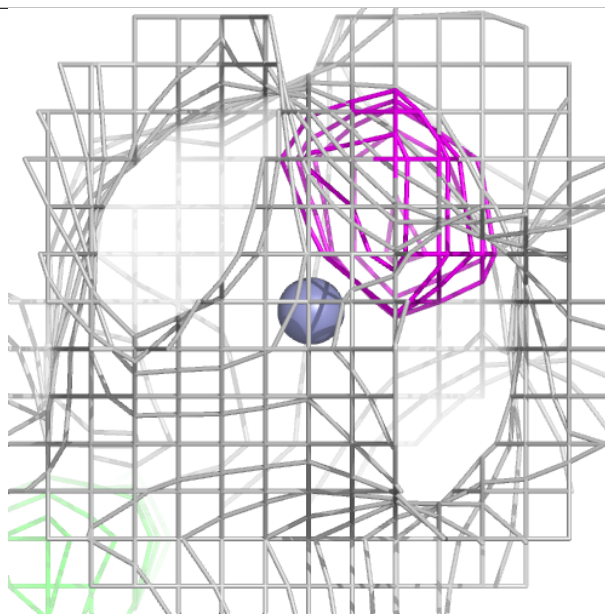
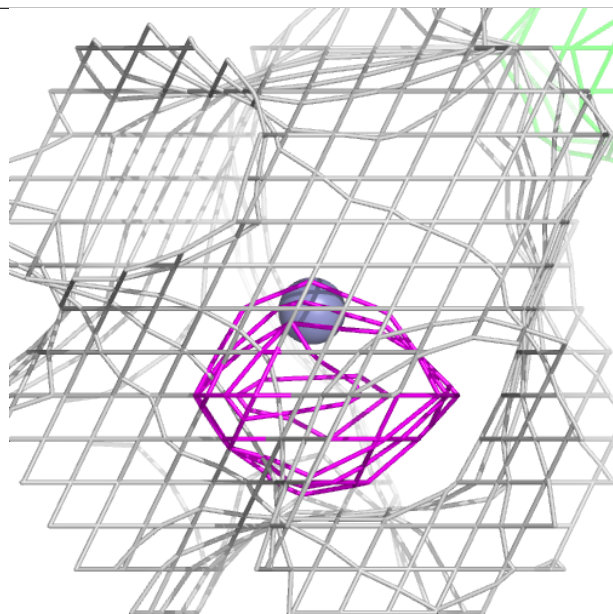
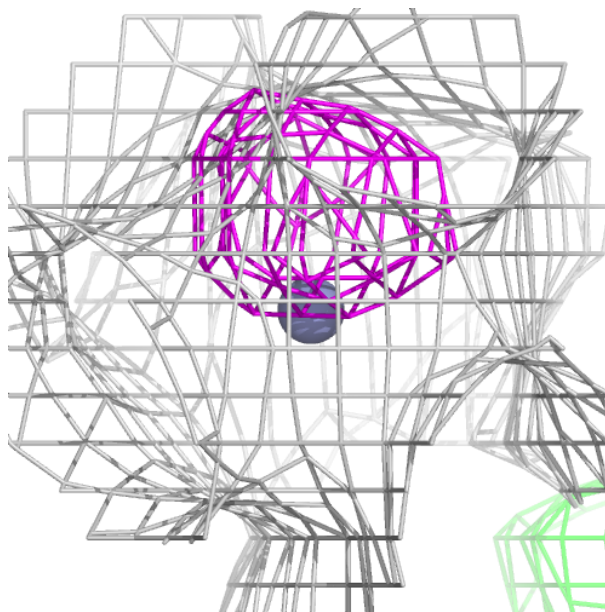
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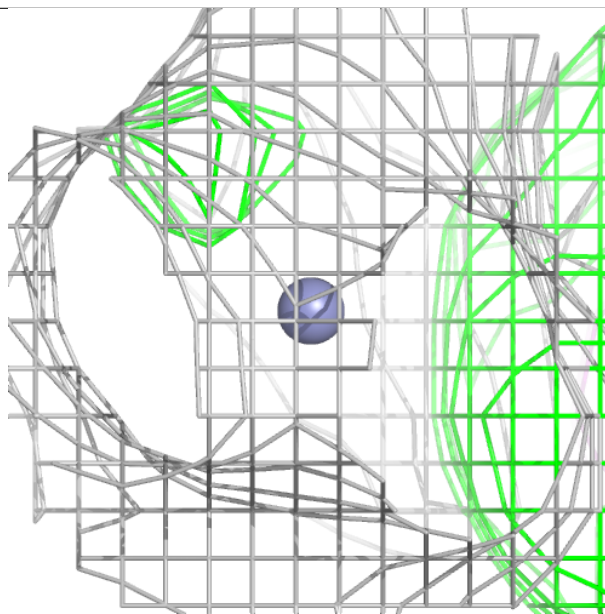
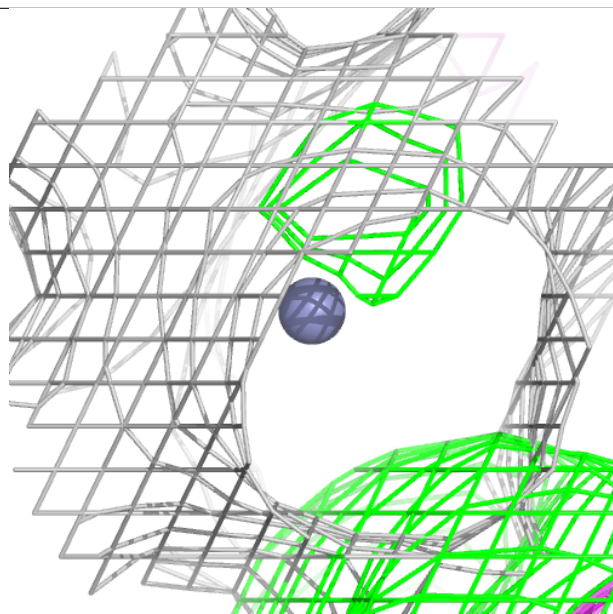
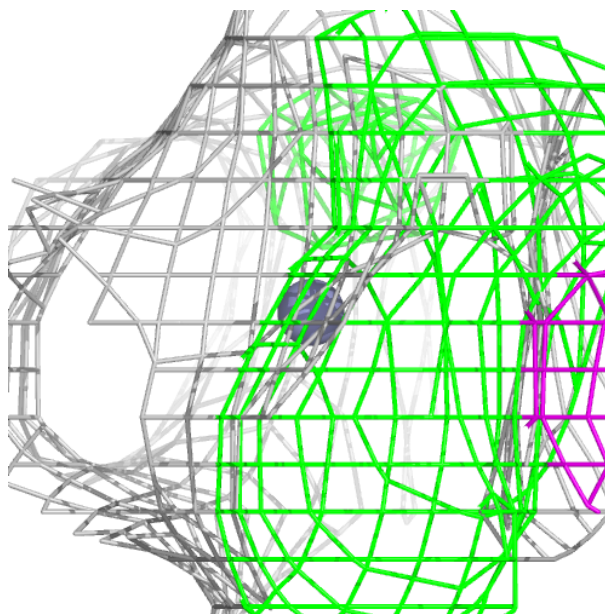
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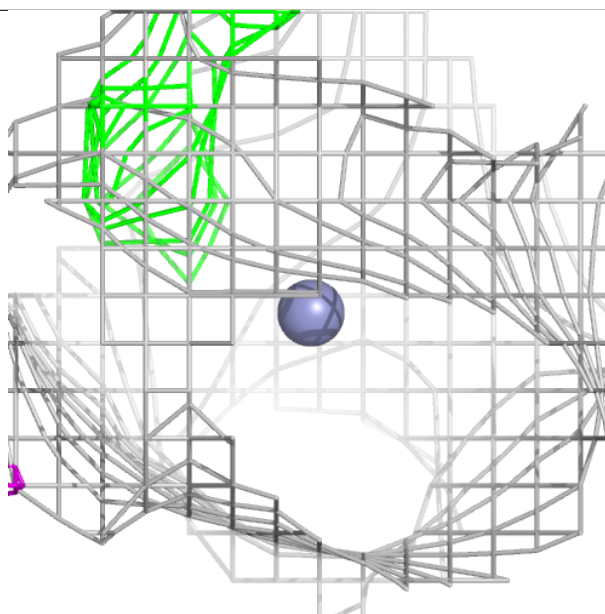
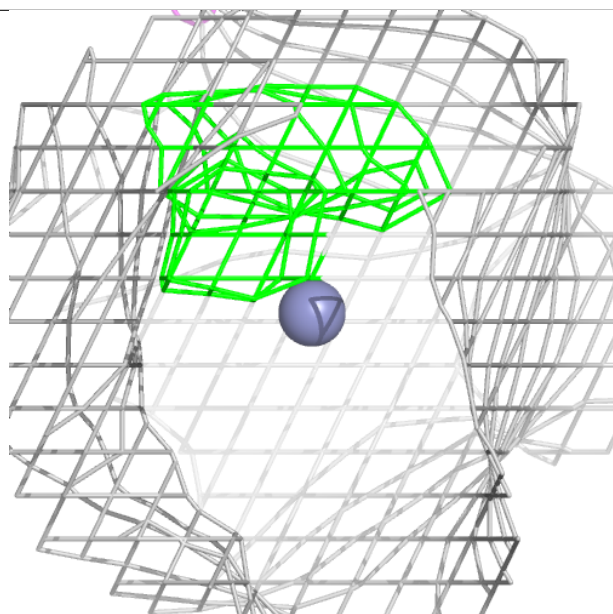
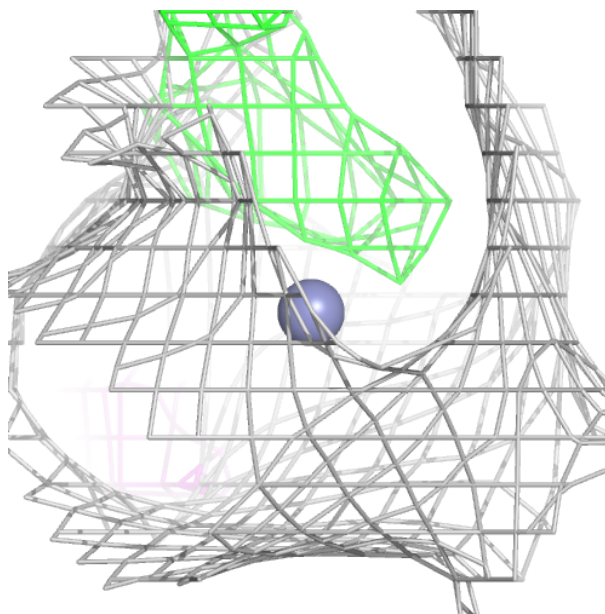
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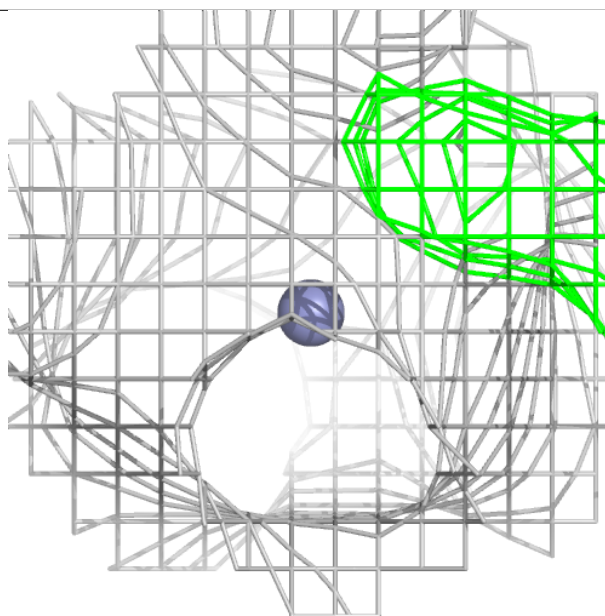
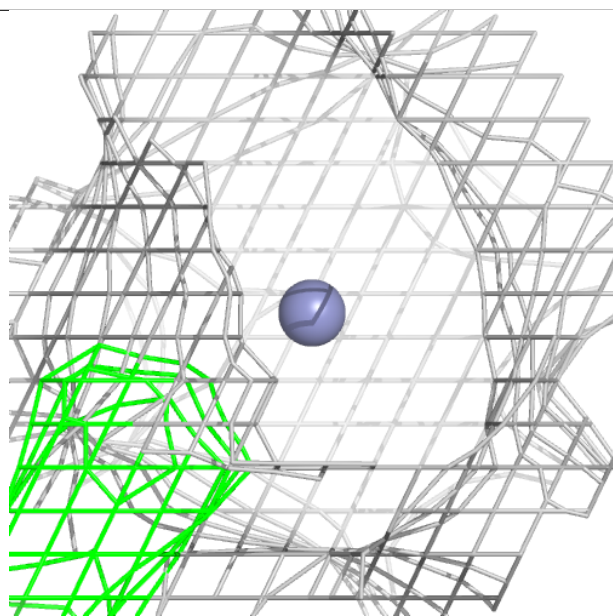
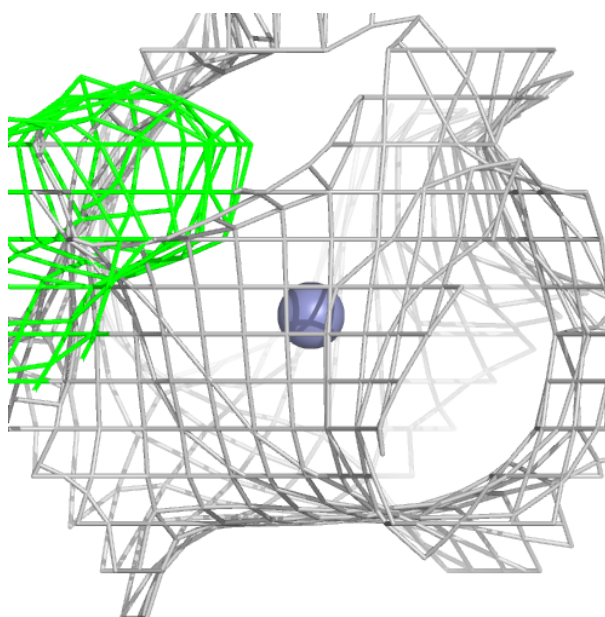
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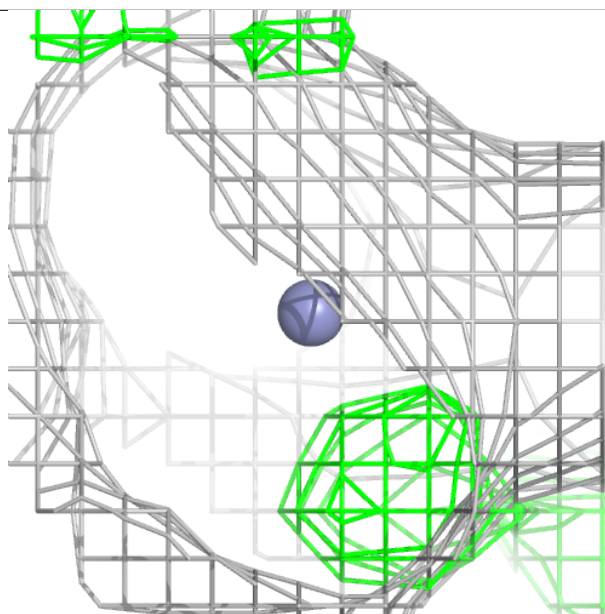
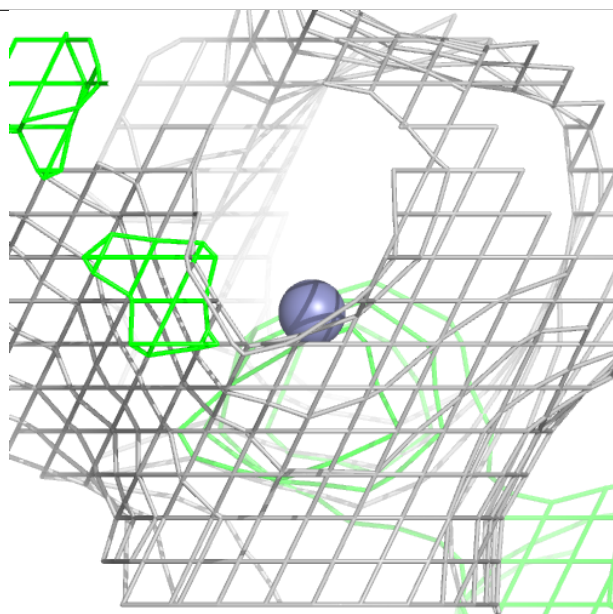
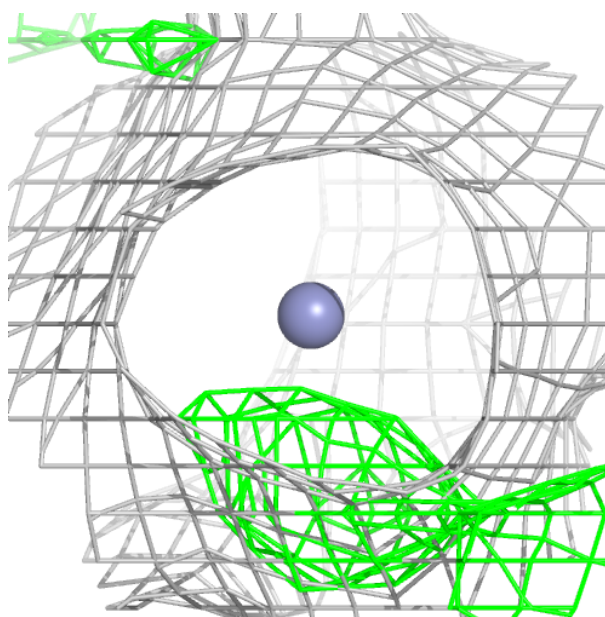
Electron density around ZN E 402:

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



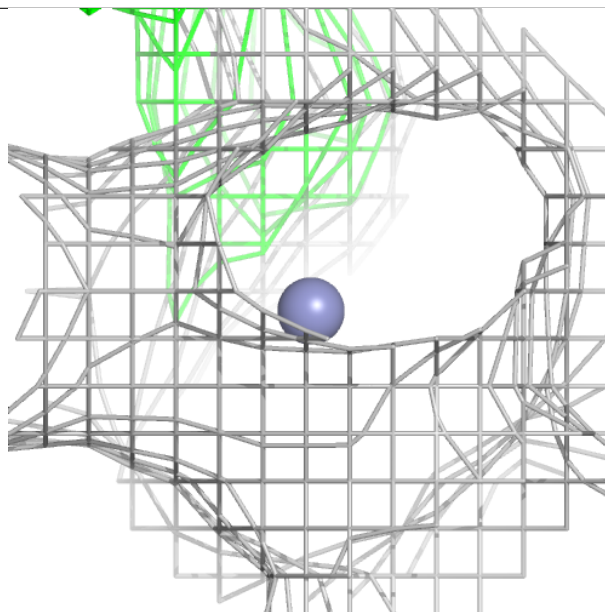
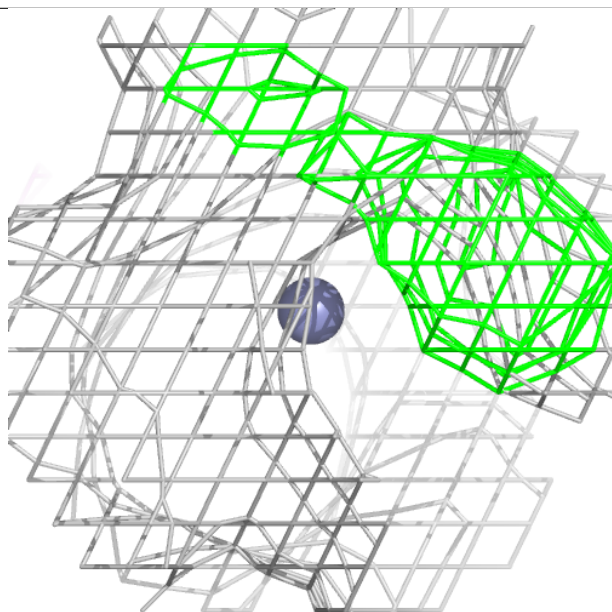
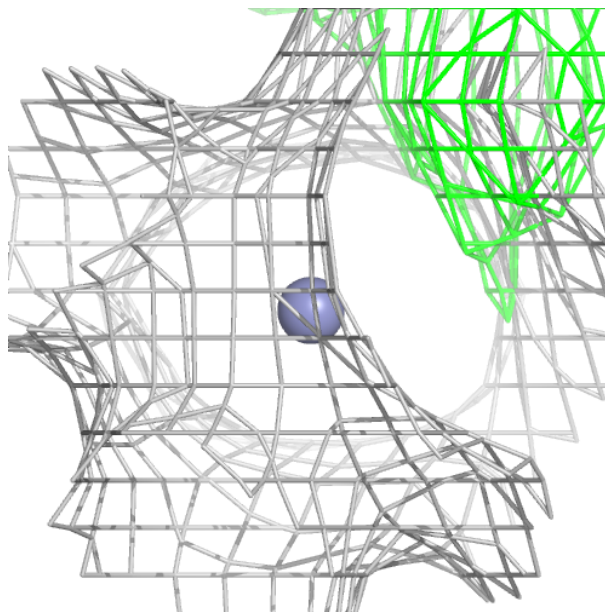
Electron density around ZN G 402:

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



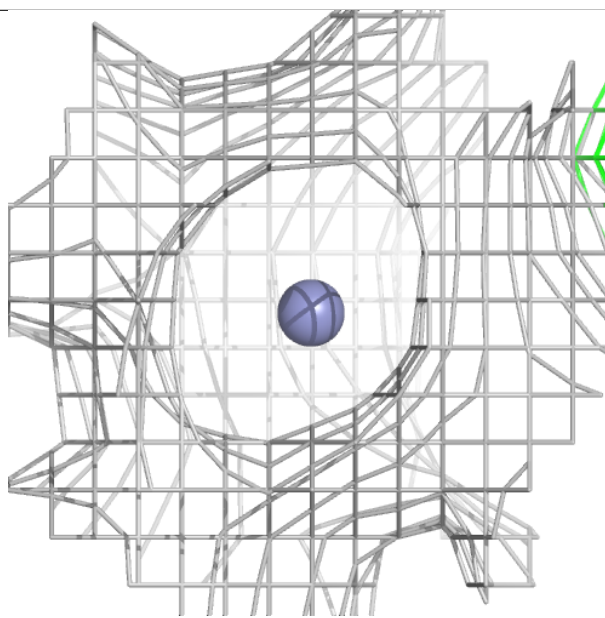
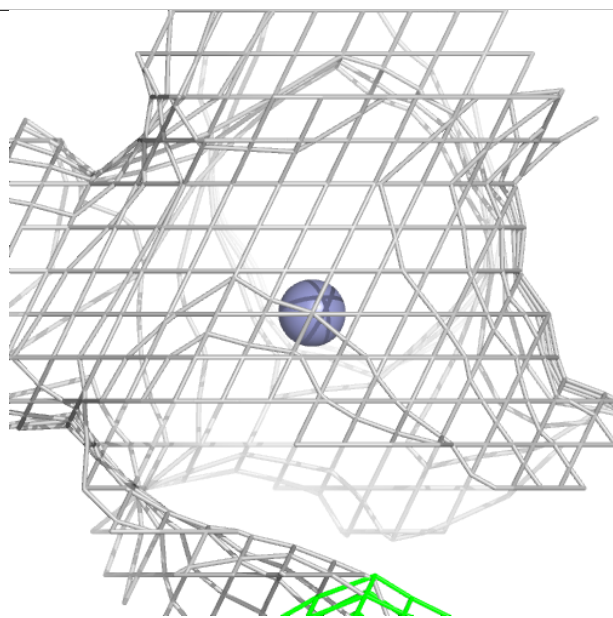
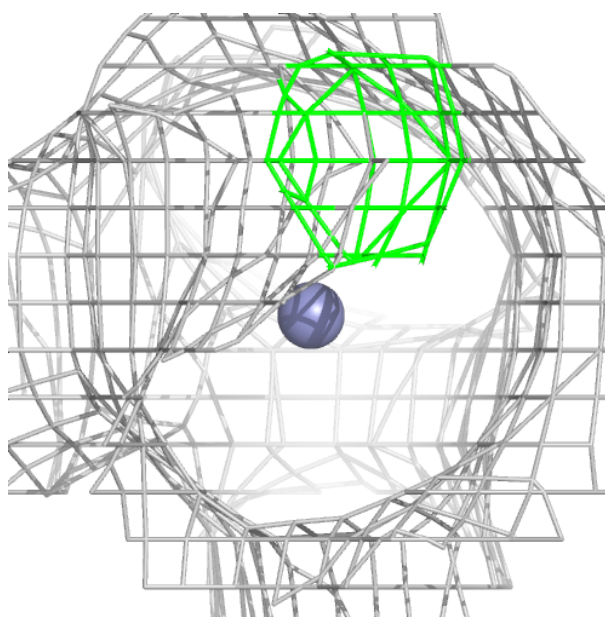
Electron density around ZN A 402:

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



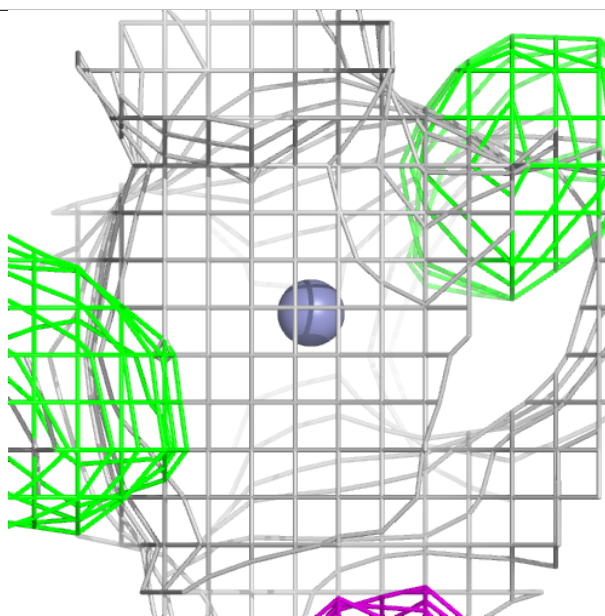
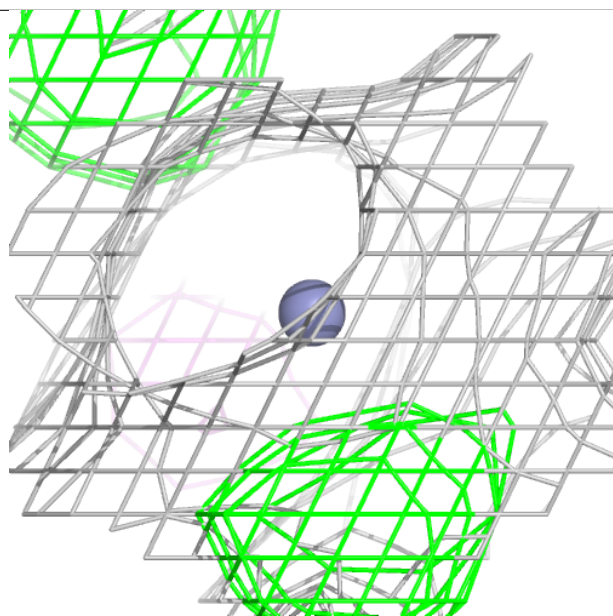
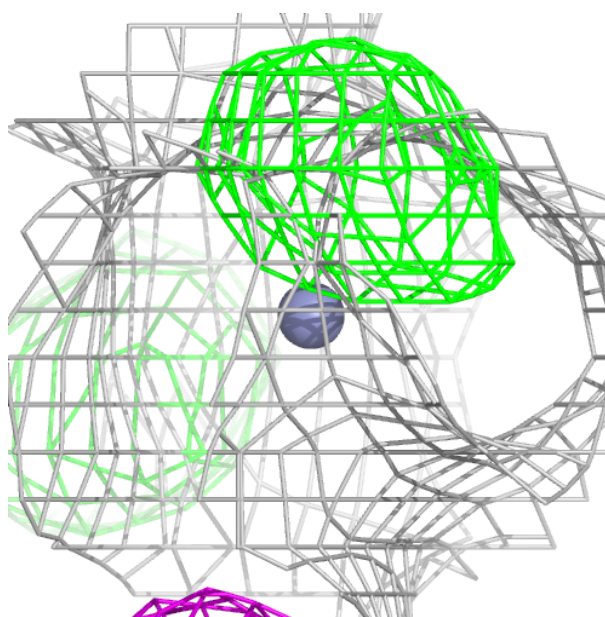
Electron density around ZN A 403:

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



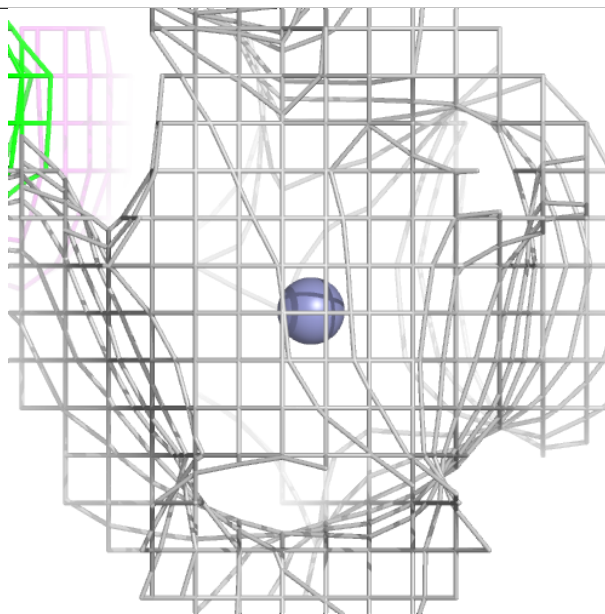
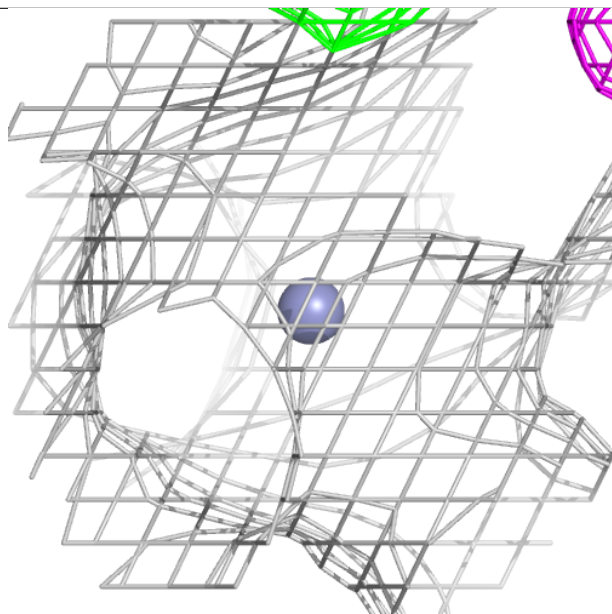
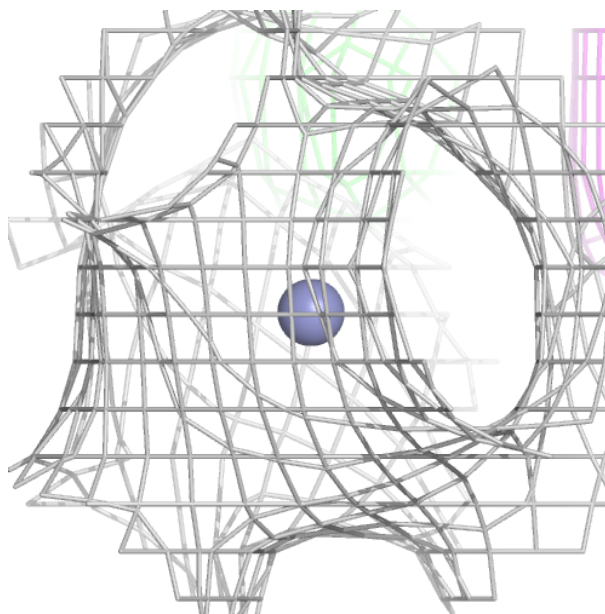
Electron density around ZN B 402:

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



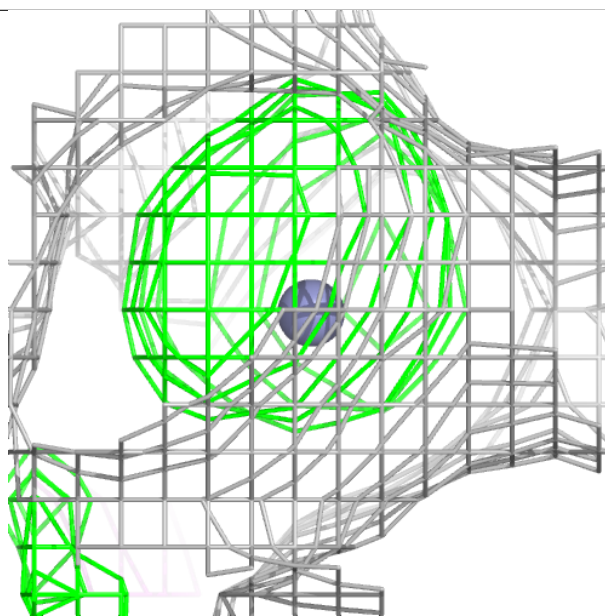
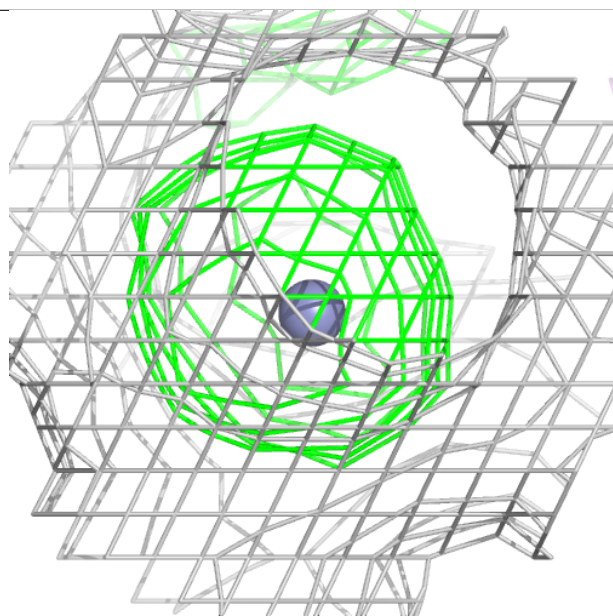
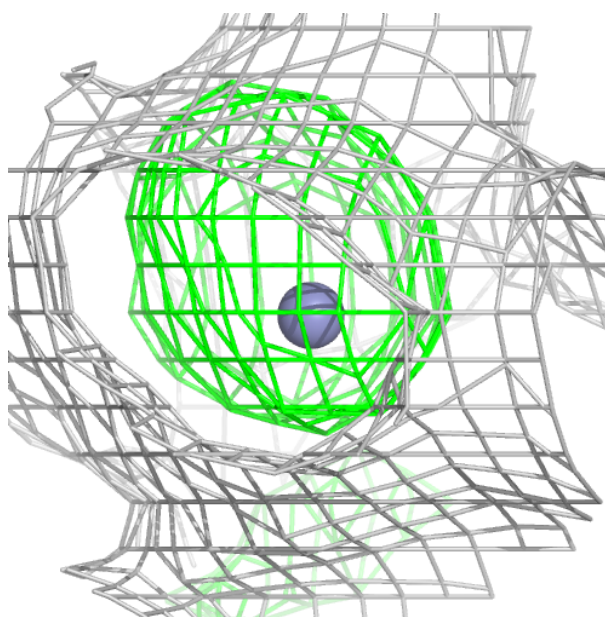
Electron density around ZN C 402:

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



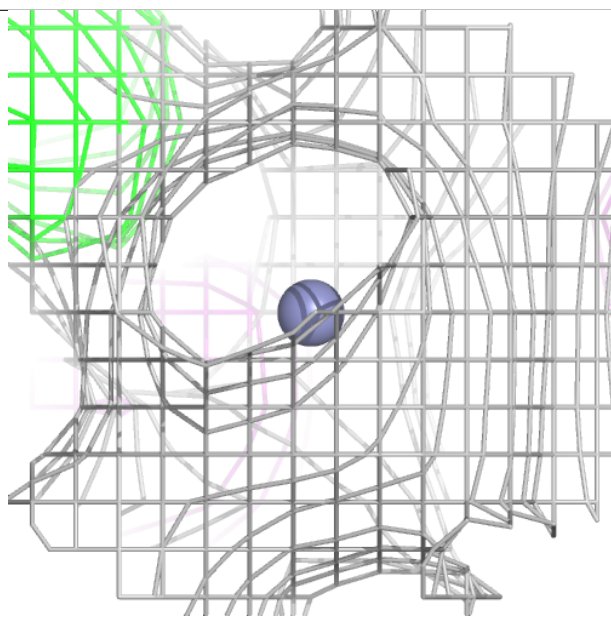
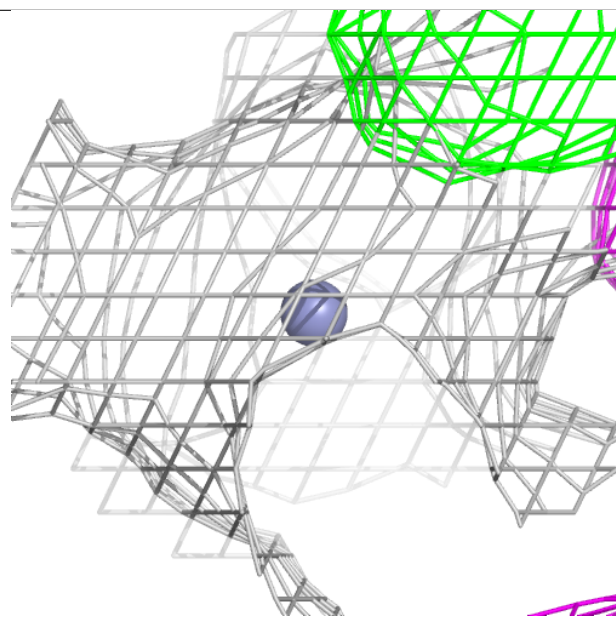
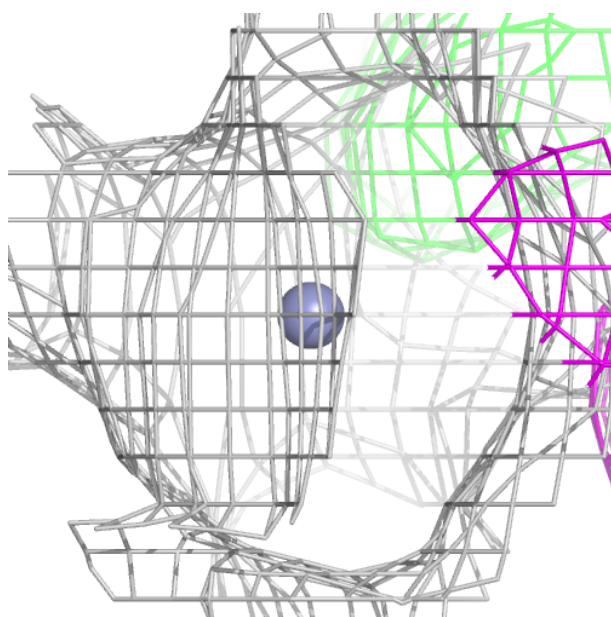
Electron density around ZN F 403:

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



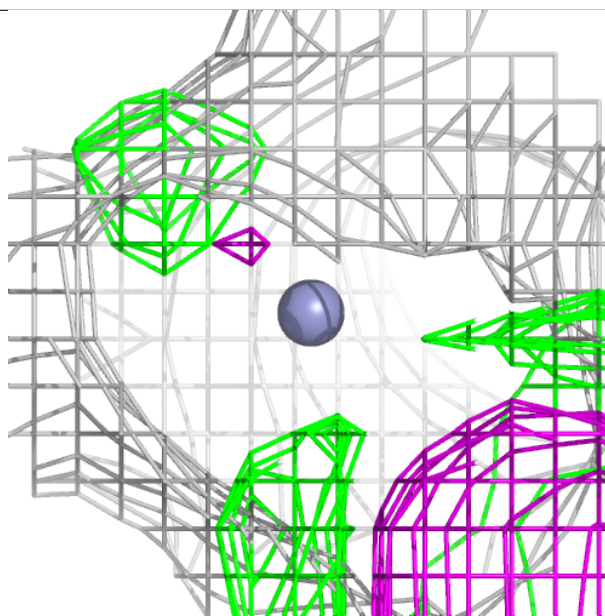
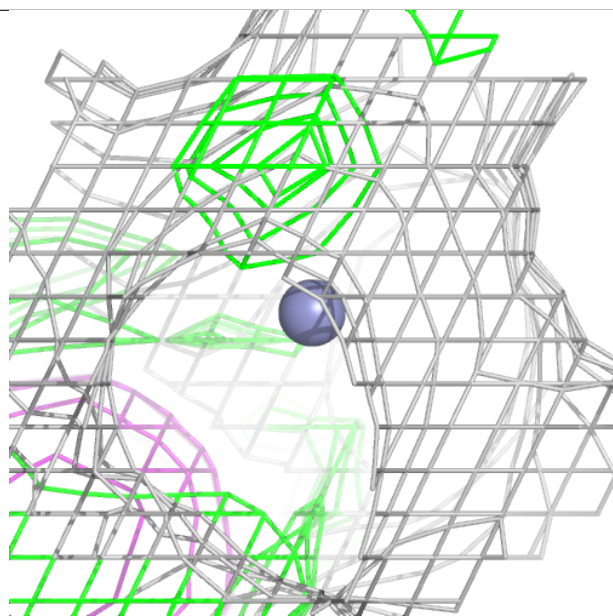
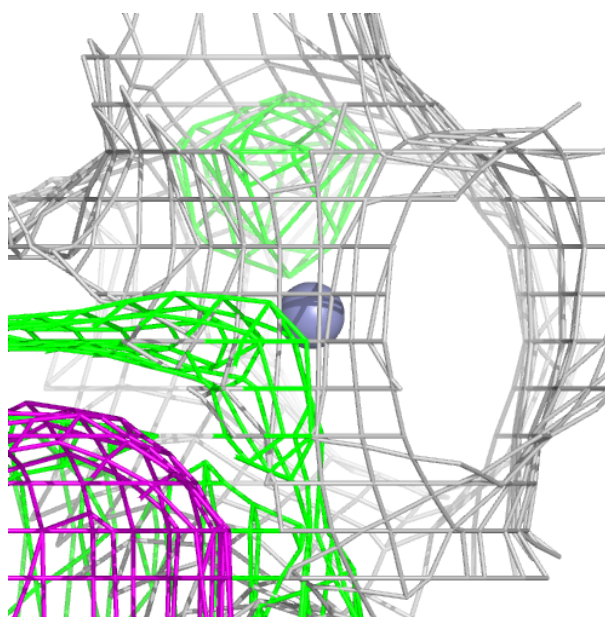
Electron density around ZN D 402:

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



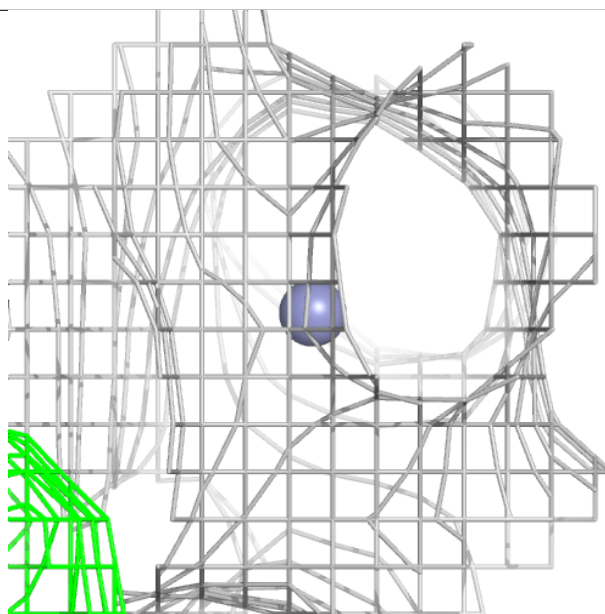
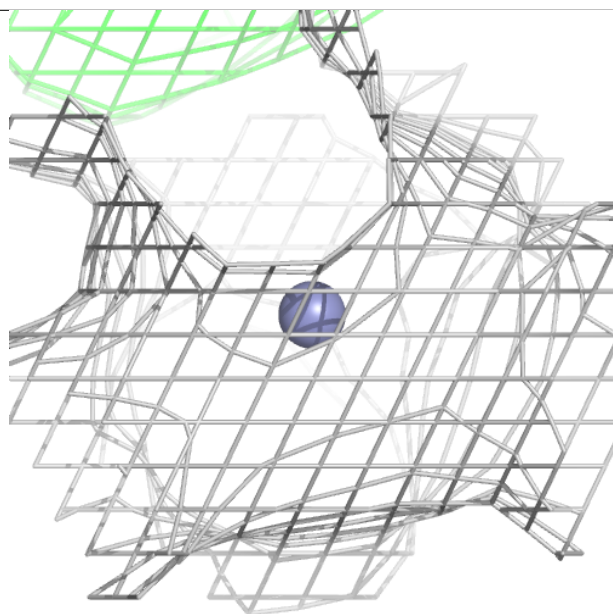
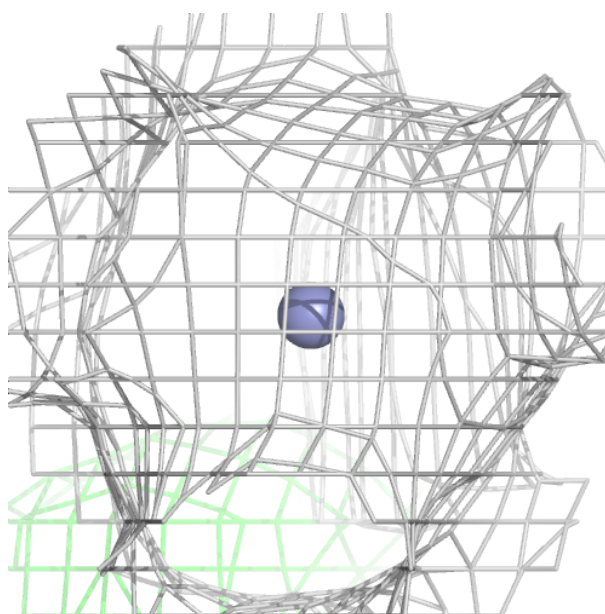
Electron density around ZN L 402:

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



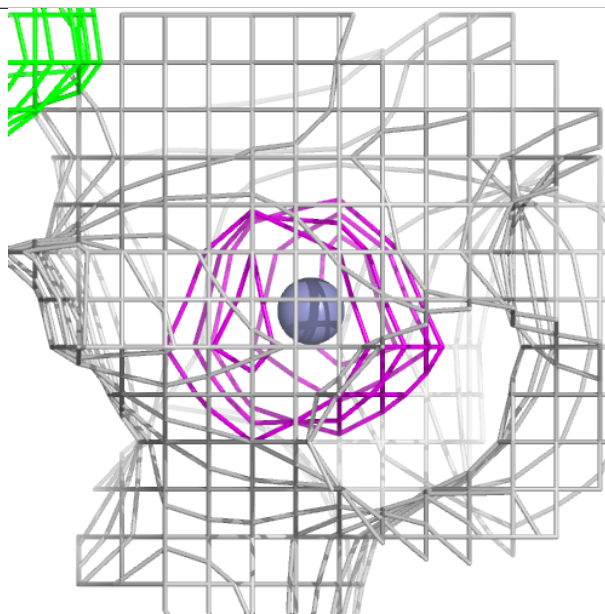
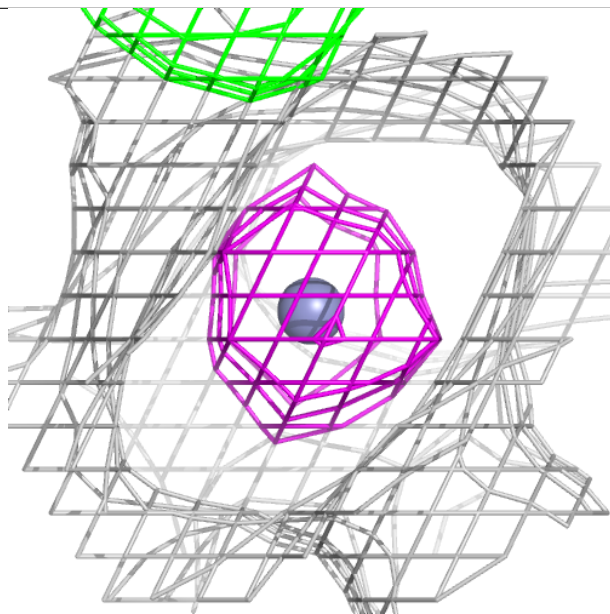
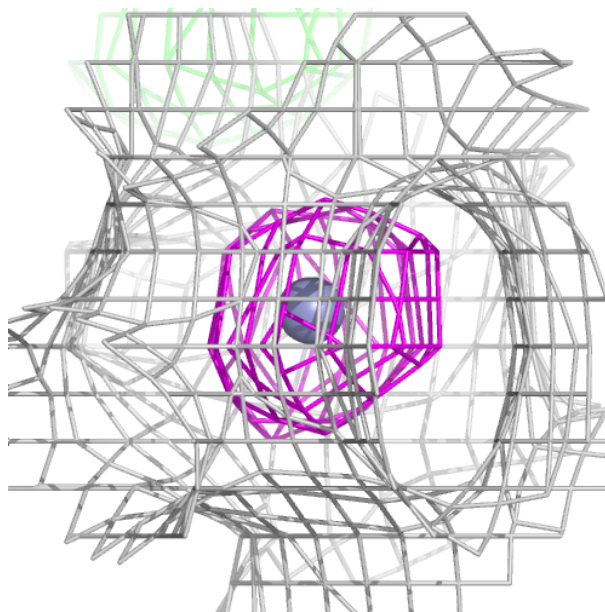
Electron density around ZN J 402:

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



Electron density around ZN B 403:

$2mF_o-DF_c$ (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.