



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:50 AM UTC

PDB ID : 8PFC / pdb_00008pfc
Title : Crystal structure of binary complex between Aster yellows witches'-broom phytoplasma effector SAP05 and the zinc finger domain of SPL5 from Arabidopsis thaliana
Authors : Huang, W.; Liu, Q.; Maqbool, A.; Stevenson, C.E.M.; Lawson, D.M.; Kamoun, S.; Hogenhout, S.A.
Deposited on : 2023-06-15
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

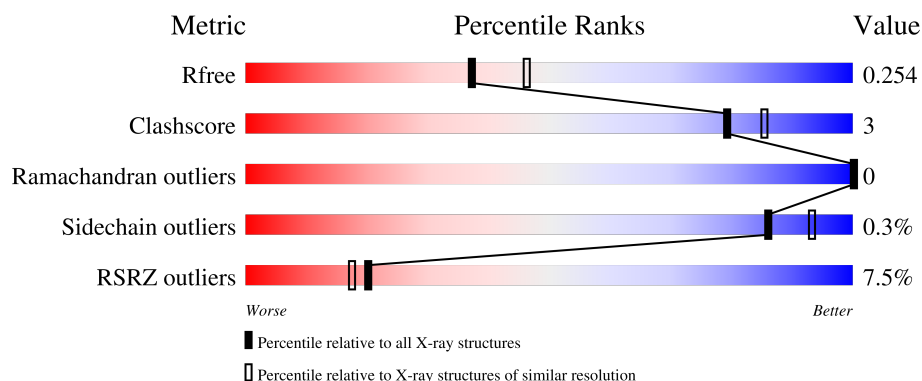
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	105	9% 85% 8% 8%
1	C	105	5% 87% 5% 9%
1	E	105	9% 84% 9% 8%
1	G	105	4% 84% 9% 8%
1	I	105	10% 85% 8% 8%

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Mol	Chain	Length	Quality of chain
1	K	105	
1	M	105	
1	O	105	
2	B	70	
2	D	70	
2	F	70	
2	H	70	
2	J	70	
2	L	70	
2	N	70	
2	P	70	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11073 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 Sequence-variable mosaic (SVM) signal sequence domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			801	519	130	149	3			
1	C	96	Total	C	N	O	S	0	0	0
			795	517	129	146	3			
1	E	97	Total	C	N	O	S	0	0	0
			798	518	130	147	3			
1	G	97	Total	C	N	O	S	0	0	0
			801	519	130	149	3			
1	I	97	Total	C	N	O	S	0	0	0
			793	514	129	147	3			
1	K	97	Total	C	N	O	S	0	0	0
			797	517	130	147	3			
1	M	97	Total	C	N	O	S	0	0	0
			801	519	130	149	3			
1	O	97	Total	C	N	O	S	0	0	0
			800	520	130	147	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP Q2NK94
A	32	PRO	-	expression tag	UNP Q2NK94
C	31	GLY	-	expression tag	UNP Q2NK94
C	32	PRO	-	expression tag	UNP Q2NK94
E	31	GLY	-	expression tag	UNP Q2NK94
E	32	PRO	-	expression tag	UNP Q2NK94
G	31	GLY	-	expression tag	UNP Q2NK94
G	32	PRO	-	expression tag	UNP Q2NK94
I	31	GLY	-	expression tag	UNP Q2NK94
I	32	PRO	-	expression tag	UNP Q2NK94
K	31	GLY	-	expression tag	UNP Q2NK94
K	32	PRO	-	expression tag	UNP Q2NK94

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Chain	Residue	Modelled	Actual	Comment	Reference
M	31	GLY	-	expression tag	UNP Q2NK94
M	32	PRO	-	expression tag	UNP Q2NK94
O	31	GLY	-	expression tag	UNP Q2NK94
O	32	PRO	-	expression tag	UNP Q2NK94

- Molecule 2 is a protein called Squamosa promoter-binding-like protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	67	Total	C	N	O	S	0	0	0
			549	333	115	95	6			
2	D	67	Total	C	N	O	S	0	0	0
			543	330	112	95	6			
2	F	67	Total	C	N	O	S	0	0	0
			545	331	115	93	6			
2	H	68	Total	C	N	O	S	0	0	0
			555	336	116	97	6			
2	J	66	Total	C	N	O	S	0	0	0
			531	321	110	94	6			
2	L	70	Total	C	N	O	S	0	0	0
			566	343	118	99	6			
2	N	66	Total	C	N	O	S	0	0	0
			532	324	108	94	6			
2	P	66	Total	C	N	O	S	0	0	0
			529	321	108	94	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	58	GLY	-	expression tag	UNP Q9S758
D	58	GLY	-	expression tag	UNP Q9S758
F	58	GLY	-	expression tag	UNP Q9S758
H	58	GLY	-	expression tag	UNP Q9S758
J	58	GLY	-	expression tag	UNP Q9S758
L	58	GLY	-	expression tag	UNP Q9S758
N	58	GLY	-	expression tag	UNP Q9S758
P	58	GLY	-	expression tag	UNP Q9S758

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	1	Total Zn 1 1	0	0
3	F	2	Total Zn 2 2	0	0
3	H	3	Total Zn 3 3	0	0
3	J	2	Total Zn 2 2	0	0
3	L	3	Total Zn 3 3	0	0
3	N	2	Total Zn 2 2	0	0
3	P	2	Total Zn 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	27	Total O 27 27	0	0
4	C	12	Total O 12 12	0	0
4	D	18	Total O 18 18	0	0
4	E	14	Total O 14 14	0	0
4	F	27	Total O 27 27	0	0
4	G	20	Total O 20 20	0	0
4	H	35	Total O 35 35	0	0
4	I	14	Total O 14 14	0	0
4	J	13	Total O 13 13	0	0

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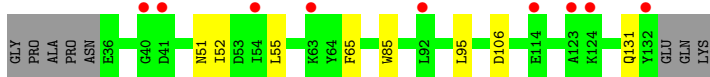
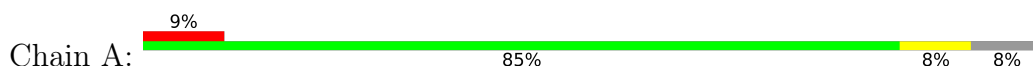
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	16	Total 16	O 16	0	0
4	L	33	Total 33	O 33	0	0
4	M	17	Total 17	O 17	0	0
4	N	21	Total 21	O 21	0	0
4	O	21	Total 21	O 21	0	0
4	P	11	Total 11	O 11	0	0

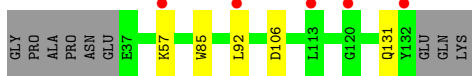
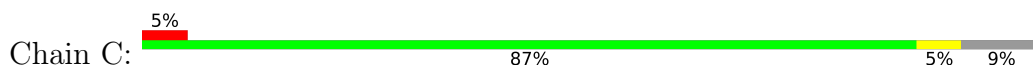
3 Residue-property plots [i](#)

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.

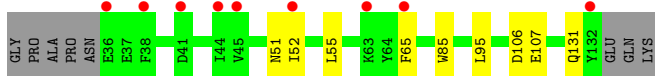
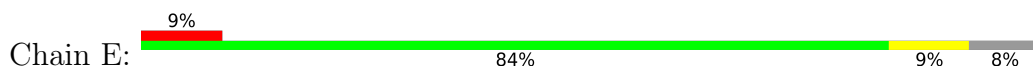
- Molecule 1: Sequence-variable mosaic (SVM) signal sequence domain-containing protein



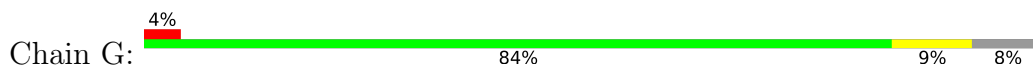
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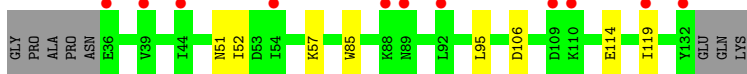
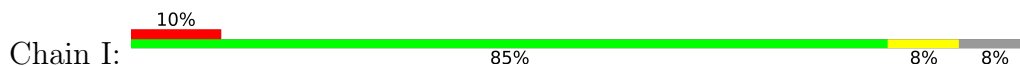
- Molecule 1: Sequence-variable mosaic (SVM) signal sequence domain-containing protein



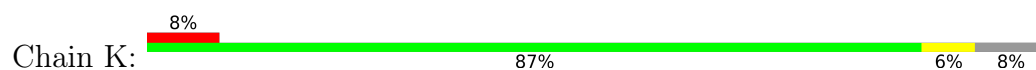
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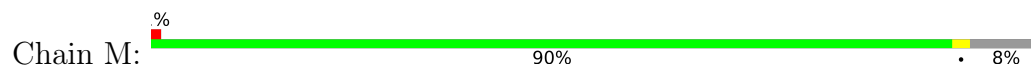
- Molecule 1: Sequence-variable mosaic (SVM) signal sequence domain-containing protein



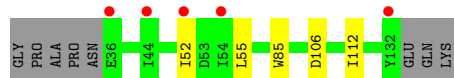
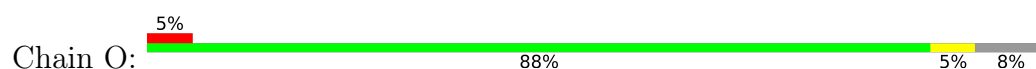
- Molecule 1: Sequence-variable mosaic (SVM) signal sequence domain-containing protein



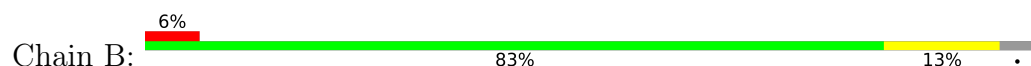
- Molecule 1: Sequence-variable mosaic (SVM) signal sequence domain-containing protein



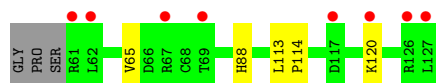
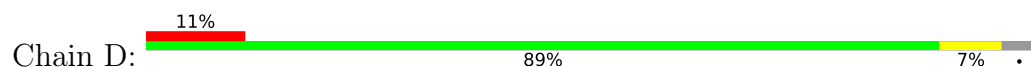
- Molecule 1: Sequence-variable mosaic (SVM) signal sequence domain-containing protein



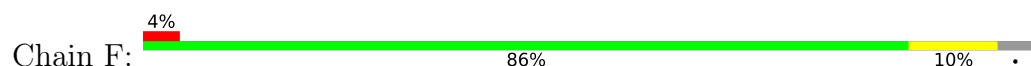
- Molecule 2: Squamosa promoter-binding-like protein 5



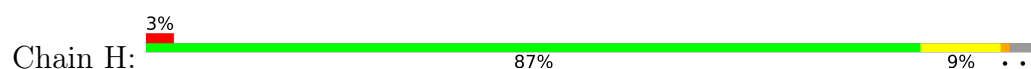
- Molecule 2: Squamosa promoter-binding-like protein 5



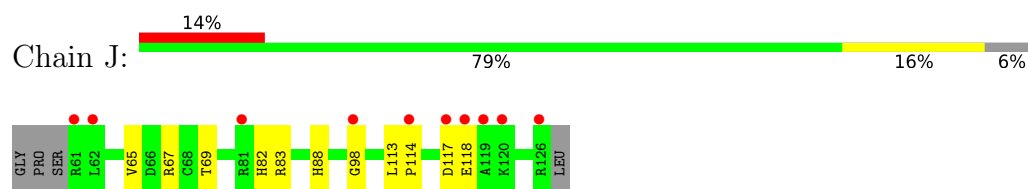
- Molecule 2: Squamosa promoter-binding-like protein 5



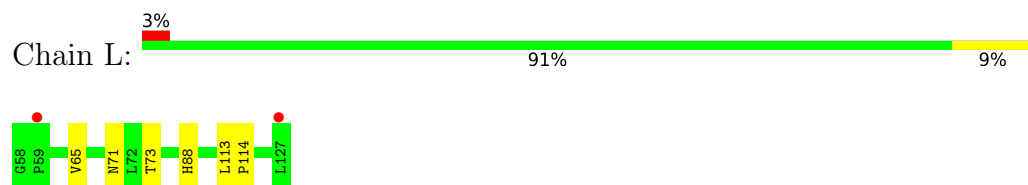
- Molecule 2: Squamosa promoter-binding-like protein 5



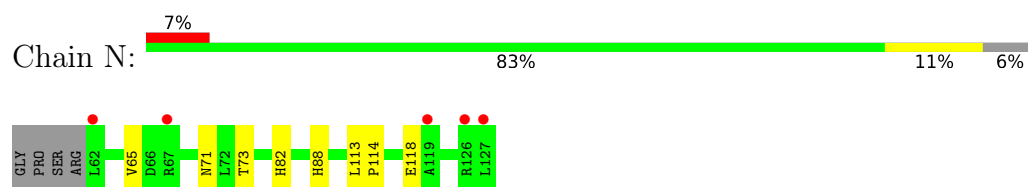
- Molecule 2: Squamosa promoter-binding-like protein 5



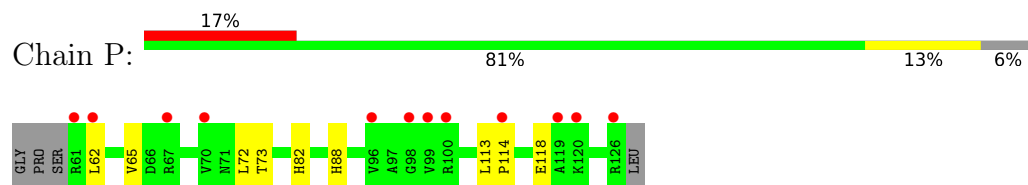
- Molecule 2: Squamosa promoter-binding-like protein 5



- Molecule 2: Squamosa promoter-binding-like protein 5



- Molecule 2: Squamosa promoter-binding-like protein 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.69Å 165.02Å 80.86Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	74.21 – 2.20 74.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (74.21-2.20) 100.0 (74.21-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.251 0.227 , 0.254	Depositor DCC
R_{free} test set	4855 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11073	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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 42.95 % 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 1.8938e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.98	0/820	1.23	0/1105
1	C	0.94	0/814	1.27	2/1097 (0.2%)
1	E	0.98	0/817	1.25	0/1101
1	G	0.99	0/820	1.29	2/1105 (0.2%)
1	I	0.99	0/812	1.31	1/1096 (0.1%)
1	K	0.99	0/816	1.26	0/1100
1	M	0.95	0/820	1.27	0/1105
1	O	0.98	0/819	1.28	0/1104
2	B	1.00	0/557	1.38	0/745
2	D	1.01	0/551	1.36	0/738
2	F	1.01	0/553	1.34	0/740
2	H	0.97	0/563	1.34	1/753 (0.1%)
2	J	1.05	1/539 (0.2%)	1.38	0/723
2	L	0.98	0/575	1.33	0/770
2	N	1.03	1/540 (0.2%)	1.35	1/724 (0.1%)
2	P	1.07	1/537 (0.2%)	1.41	2/720 (0.3%)
All	All	0.99	3/10953 (0.0%)	1.31	9/14726 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	82	HIS	CE1-NE2	6.12	1.38	1.32
2	N	82	HIS	CE1-NE2	5.37	1.38	1.32
2	J	82	HIS	CE1-NE2	5.12	1.37	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	104	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	G	104	ARG	NE-CZ-NH1	-5.47	116.03	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	118	GLU	CB-CA-C	-5.30	110.44	116.54
2	P	73	THR	CA-CB-OG1	-5.28	101.68	109.60
2	H	73	THR	CA-CB-OG1	-5.28	101.68	109.60
2	N	118	GLU	CB-CA-C	-5.28	110.47	116.54
1	C	131	GLN	CA-C-N	5.19	131.04	121.70
1	C	131	GLN	C-N-CA	5.19	131.04	121.70
1	I	51	ASN	CB-CA-C	5.10	119.04	109.86

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	801	0	771	4	0
1	C	795	0	774	2	0
1	E	798	0	769	6	0
1	G	801	0	771	5	0
1	I	793	0	756	5	0
1	K	797	0	767	4	0
1	M	801	0	771	1	0
1	O	800	0	776	4	0
2	B	549	0	536	7	0
2	D	543	0	525	3	0
2	F	545	0	532	4	0
2	H	555	0	541	5	0
2	J	531	0	503	8	0
2	L	566	0	551	3	0
2	N	532	0	512	3	0
2	P	529	0	503	3	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	H	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	2	0	0	0	0
3	L	3	0	0	0	0
3	N	2	0	0	0	0
3	P	2	0	0	0	0
4	A	18	0	0	0	0
4	B	27	0	0	0	0
4	C	12	0	0	0	0
4	D	18	0	0	0	0
4	E	14	0	0	0	0
4	F	27	0	0	1	0
4	G	20	0	0	0	0
4	H	35	0	0	0	0
4	I	14	0	0	0	0
4	J	13	0	0	0	0
4	K	16	0	0	0	0
4	L	33	0	0	0	0
4	M	17	0	0	0	0
4	N	21	0	0	0	0
4	O	21	0	0	0	0
4	P	11	0	0	0	0
All	All	11073	0	10358	57	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 3.

All (57) 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)
2:J:98:GLY:O	1:K:121:ASN:HA	1.61	1.01
2:B:107:CYS:SG	2:D:120:LYS:NZ	2.54	0.81
2:B:119:ALA:HB2	1:G:118:GLN:HE22	1.60	0.67
1:E:52:ILE:HD13	1:E:95:LEU:HB3	1.83	0.61
1:A:52:ILE:HD13	1:A:95:LEU:HB3	1.84	0.60
2:J:83:ARG:HD2	1:O:112:ILE:HD11	1.86	0.57
2:D:65:VAL:HG21	2:D:88:HIS:CG	2.42	0.55
2:N:65:VAL:HG21	2:N:88:HIS:CG	2.41	0.55
2:J:65:VAL:HG21	2:J:88:HIS:CG	2.42	0.55
2:P:65:VAL:HG21	2:P:88:HIS:CG	2.43	0.54
2:P:62:LEU:HD12	2:P:72:LEU:HB2	1.90	0.54
2:F:65:VAL:HG21	2:F:88:HIS:CG	2.44	0.53
1:I:85:TRP:CE2	1:I:106:ASP:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TRP:CE2	1:A:106:ASP:HB2	2.44	0.53
1:G:85:TRP:CE2	1:G:106:ASP:HB2	2.44	0.53
2:B:119:ALA:HB2	1:G:118:GLN:NE2	2.23	0.53
1:K:85:TRP:CE2	1:K:106:ASP:HB2	2.44	0.53
1:C:85:TRP:CE2	1:C:106:ASP:HB2	2.44	0.53
2:L:65:VAL:HG21	2:L:88:HIS:CG	2.43	0.52
1:M:85:TRP:CE2	1:M:106:ASP:HB2	2.45	0.52
1:O:85:TRP:CE2	1:O:106:ASP:HB2	2.43	0.52
2:B:65:VAL:HG21	2:B:88:HIS:CG	2.45	0.52
2:H:65:VAL:HG21	2:H:88:HIS:CG	2.43	0.52
2:H:126:ARG:CB	1:I:119:ILE:HG22	2.40	0.52
1:E:85:TRP:CE2	1:E:106:ASP:HB2	2.44	0.51
1:I:114:GLU:OE1	1:I:114:GLU:N	2.39	0.51
1:E:55:LEU:HD13	1:E:65:PHE:CE2	2.46	0.50
1:A:55:LEU:HD13	1:A:65:PHE:CE2	2.47	0.49
1:A:51:ASN:HA	1:A:131:GLN:HE21	1.76	0.49
1:G:51:ASN:HA	1:G:131:GLN:HE21	1.77	0.49
1:I:52:ILE:HD13	1:I:95:LEU:HD13	1.95	0.47
1:G:55:LEU:HD13	1:G:65:PHE:CE2	2.49	0.47
1:E:51:ASN:HA	1:E:131:GLN:HE21	1.79	0.47
1:K:55:LEU:HD13	1:K:65:PHE:CE2	2.49	0.46
1:E:107:GLU:HG3	2:J:69:THR:HB	1.96	0.46
1:C:92:LEU:H	1:C:92:LEU:CD1	2.28	0.46
2:J:113:LEU:N	2:J:114:PRO:CD	2.79	0.46
2:D:113:LEU:N	2:D:114:PRO:CD	2.79	0.45
2:J:67:ARG:HD2	1:K:40:GLY:O	2.16	0.45
2:P:113:LEU:N	2:P:114:PRO:CD	2.80	0.45
2:F:113:LEU:N	2:F:114:PRO:CD	2.80	0.45
2:N:113:LEU:N	2:N:114:PRO:CD	2.80	0.45
2:H:113:LEU:N	2:H:114:PRO:CD	2.80	0.44
2:B:113:LEU:N	2:B:114:PRO:CD	2.80	0.44
2:L:113:LEU:N	2:L:114:PRO:CD	2.81	0.43
2:F:66:ASP:HA	4:F:318:HOH:O	2.19	0.43
2:J:117:ASP:C	2:J:118:GLU:HG2	2.45	0.41
1:E:52:ILE:HD12	1:E:52:ILE:HA	1.95	0.41
1:O:52:ILE:HD12	1:O:55:LEU:HD12	2.01	0.41
2:F:71:ASN:OD1	2:F:73:THR:HB	2.21	0.41
2:B:71:ASN:OD1	2:B:73:THR:HB	2.21	0.41
2:L:71:ASN:OD1	2:L:73:THR:HB	2.20	0.41
2:B:100:ARG:HA	2:B:100:ARG:HD2	1.94	0.41
2:H:71:ASN:OD1	2:H:73:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:ARG:HB2	1:I:119:ILE:HG22	2.02	0.41
2:J:83:ARG:HD2	1:O:112:ILE:CD1	2.51	0.41
2:N:71:ASN:OD1	2:N:73:THR:HB	2.21	0.40

There are no symmetry-related clashes.

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	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
1	C	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
1	E	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
1	G	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
1	I	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
1	K	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
1	M	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
1	O	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
2	B	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
2	D	65/70 (93%)	65 (100%)	0	0	100	100
2	F	65/70 (93%)	65 (100%)	0	0	100	100
2	H	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
2	J	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
2	L	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
2	N	64/70 (91%)	64 (100%)	0	0	100	100
2	P	64/70 (91%)	64 (100%)	0	0	100	100
All	All	1280/1400 (91%)	1268 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/93 (91%)	85 (100%)	0	100	100
1	C	85/93 (91%)	84 (99%)	1 (1%)	63	78
1	E	84/93 (90%)	84 (100%)	0	100	100
1	G	85/93 (91%)	84 (99%)	1 (1%)	63	78
1	I	83/93 (89%)	82 (99%)	1 (1%)	63	78
1	K	84/93 (90%)	84 (100%)	0	100	100
1	M	85/93 (91%)	85 (100%)	0	100	100
1	O	85/93 (91%)	85 (100%)	0	100	100
2	B	58/61 (95%)	58 (100%)	0	100	100
2	D	57/61 (93%)	57 (100%)	0	100	100
2	F	57/61 (93%)	57 (100%)	0	100	100
2	H	59/61 (97%)	59 (100%)	0	100	100
2	J	55/61 (90%)	55 (100%)	0	100	100
2	L	60/61 (98%)	60 (100%)	0	100	100
2	N	56/61 (92%)	56 (100%)	0	100	100
2	P	55/61 (90%)	55 (100%)	0	100	100
All	All	1133/1232 (92%)	1130 (100%)	3 (0%)	86	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	57	LYS
1	G	86	LYS
1	I	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	131	GLN
2	B	105	GLN
2	D	77	GLN
2	D	105	GLN
1	E	131	GLN
2	F	105	GLN
1	G	118	GLN
1	G	131	GLN
2	J	105	GLN
2	L	105	GLN
1	O	48	ASN
1	O	89	ASN
2	P	77	GLN

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 20 ligands modelled in this entry, 20 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	97/105 (92%)	0.76	9 (9%) 14 12	46, 68, 100, 107	0
1	C	96/105 (91%)	0.54	5 (5%) 33 29	52, 71, 102, 119	0
1	E	97/105 (92%)	0.74	9 (9%) 14 12	48, 68, 98, 105	0
1	G	97/105 (92%)	0.35	4 (4%) 41 38	44, 58, 82, 94	0
1	I	97/105 (92%)	0.97	11 (11%) 10 8	44, 74, 104, 127	0
1	K	97/105 (92%)	0.80	8 (8%) 17 15	45, 68, 100, 108	0
1	M	97/105 (92%)	0.39	1 (1%) 79 77	38, 66, 94, 113	0
1	O	97/105 (92%)	0.58	5 (5%) 33 29	41, 66, 93, 126	0
2	B	67/70 (95%)	0.37	4 (5%) 27 24	41, 55, 83, 123	0
2	D	67/70 (95%)	0.79	8 (11%) 9 7	48, 65, 102, 125	0
2	F	67/70 (95%)	0.32	3 (4%) 38 35	40, 54, 76, 85	0
2	H	68/70 (97%)	0.34	2 (2%) 53 50	46, 58, 81, 108	0
2	J	66/70 (94%)	0.87	10 (15%) 5 4	43, 66, 104, 112	0
2	L	70/70 (100%)	0.21	2 (2%) 53 50	46, 57, 77, 103	0
2	N	66/70 (94%)	0.66	5 (7%) 20 17	43, 66, 91, 113	0
2	P	66/70 (94%)	0.93	12 (18%) 3 2	43, 65, 92, 99	0
All	All	1312/1400 (93%)	0.61	98 (7%) 20 17	38, 65, 97, 127	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	TYR	7.6
1	K	132	TYR	7.1
2	N	62	LEU	6.6
1	G	132	TYR	6.1
1	C	132	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
1	O	132	TYR	5.8
1	E	132	TYR	5.8
2	D	62	LEU	5.6
1	M	132	TYR	5.1
1	I	132	TYR	4.7
2	D	127	LEU	4.4
1	E	41	ASP	4.2
2	P	62	LEU	4.1
2	J	62	LEU	4.1
2	F	61	ARG	3.9
2	J	61	ARG	3.8
2	P	126	ARG	3.5
1	I	109	ASP	3.4
1	K	92	LEU	3.4
1	A	41	ASP	3.3
2	J	126	ARG	3.2
1	O	36	GLU	3.2
2	L	127	LEU	3.2
2	D	120	LYS	3.1
1	K	65	PHE	3.1
2	H	60	SER	3.1
2	B	127	LEU	3.1
1	I	119	ILE	3.1
2	N	119	ALA	3.1
2	J	114	PRO	3.0
1	I	92	LEU	3.0
1	I	36	GLU	3.0
2	N	67	ARG	2.9
1	I	89	ASN	2.9
2	P	61	ARG	2.8
2	L	59	PRO	2.8
2	B	62	LEU	2.8
1	K	99	PHE	2.8
2	J	119	ALA	2.8
1	A	40	GLY	2.7
2	D	126	ARG	2.7
2	J	118	GLU	2.7
2	P	98	GLY	2.7
2	N	126	ARG	2.7
1	E	44	ILE	2.6
1	I	44	ILE	2.6
1	C	120	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	P	114	PRO	2.6
1	E	38	PHE	2.6
1	I	54	ILE	2.6
1	O	44	ILE	2.5
1	C	57	LYS	2.5
1	E	63	LYS	2.5
1	E	65	PHE	2.4
1	A	63	LYS	2.4
2	D	69	THR	2.4
1	G	65	PHE	2.4
1	O	52	ILE	2.4
1	A	114	GLU	2.4
1	A	123	ALA	2.4
2	P	70	VAL	2.4
1	K	40	GLY	2.4
1	C	92	LEU	2.4
2	P	119	ALA	2.3
2	B	61	ARG	2.3
1	G	52	ILE	2.3
2	J	117	ASP	2.3
1	E	36	GLU	2.3
1	K	52	ILE	2.3
1	I	88	LYS	2.3
2	F	118	GLU	2.3
2	F	125	ARG	2.2
2	H	118	GLU	2.2
2	P	120	LYS	2.2
2	P	99	VAL	2.2
1	A	124	LYS	2.2
1	A	54	ILE	2.2
1	A	92	LEU	2.2
2	N	127	LEU	2.2
1	I	39	VAL	2.2
2	D	61	ARG	2.2
2	P	67	ARG	2.2
2	J	98	GLY	2.2
2	B	119	ALA	2.2
1	C	113	LEU	2.1
1	O	54	ILE	2.1
2	P	96	VAL	2.1
2	P	100	ARG	2.1
1	E	52	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	117	ASP	2.1
1	I	110	LYS	2.1
1	K	91	PRO	2.1
1	E	45	VAL	2.1
1	K	39	VAL	2.0
2	J	120	LYS	2.0
1	G	92	LEU	2.0
2	D	67	ARG	2.0
2	J	81	ARG	2.0

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](#)

There are no oligosaccharides 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
3	ZN	H	201	1/1	0.92	0.16	121,121,121,121	0
3	ZN	E	201	1/1	0.98	0.09	83,83,83,83	0
3	ZN	J	201	1/1	0.98	0.04	47,47,47,47	0
3	ZN	L	201	1/1	0.98	0.09	76,76,76,76	0
3	ZN	P	201	1/1	0.98	0.03	51,51,51,51	0
3	ZN	D	201	1/1	0.99	0.02	56,56,56,56	0
3	ZN	J	202	1/1	0.99	0.03	66,66,66,66	0
3	ZN	A	201	1/1	0.99	0.03	66,66,66,66	0
3	ZN	N	201	1/1	0.99	0.03	53,53,53,53	0
3	ZN	B	202	1/1	0.99	0.03	63,63,63,63	0
3	ZN	H	203	1/1	1.00	0.01	53,53,53,53	0
3	ZN	B	201	1/1	1.00	0.02	47,47,47,47	0
3	ZN	F	201	1/1	1.00	0.02	48,48,48,48	0
3	ZN	F	202	1/1	1.00	0.01	54,54,54,54	0

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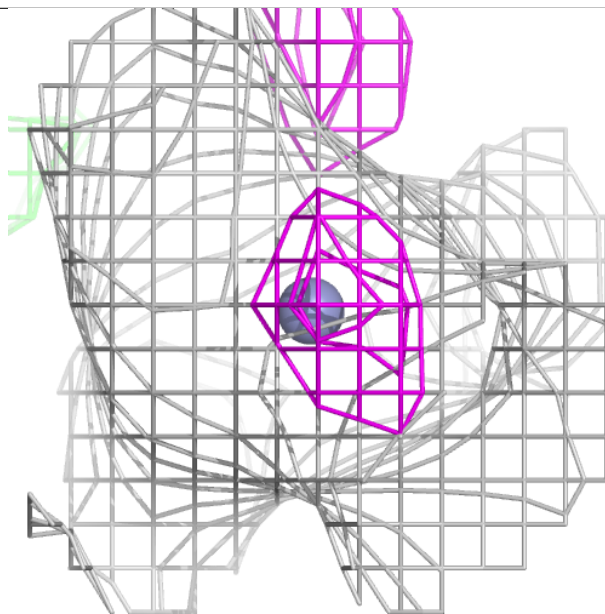
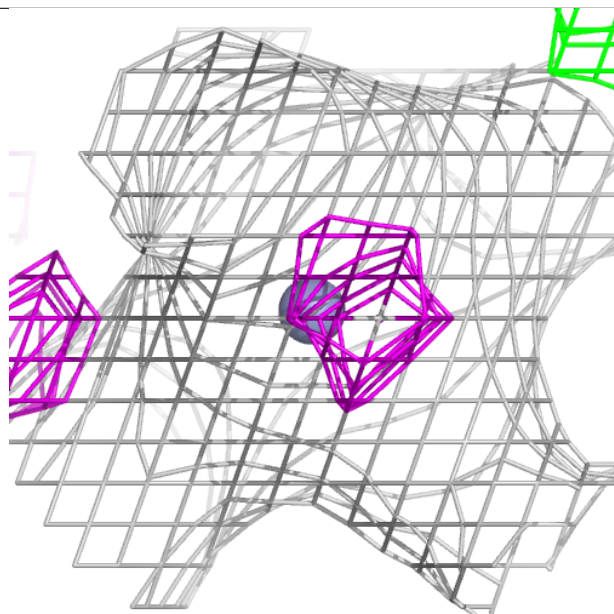
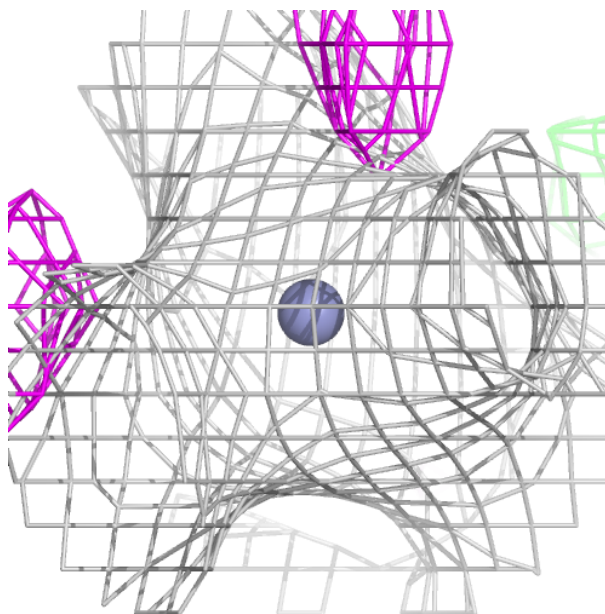
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	L	202	1/1	1.00	0.02	50,50,50,50	0
3	ZN	L	203	1/1	1.00	0.02	54,54,54,54	0
3	ZN	D	202	1/1	1.00	0.02	60,60,60,60	0
3	ZN	N	202	1/1	1.00	0.02	62,62,62,62	0
3	ZN	H	202	1/1	1.00	0.02	48,48,48,48	0
3	ZN	P	202	1/1	1.00	0.02	61,61,61,61	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.

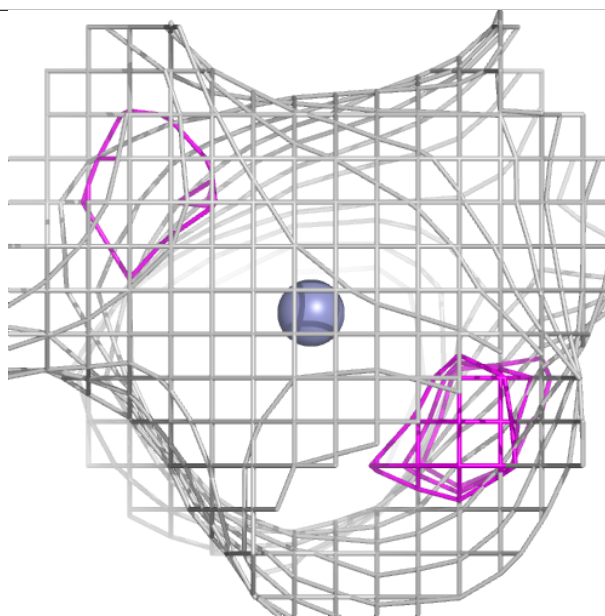
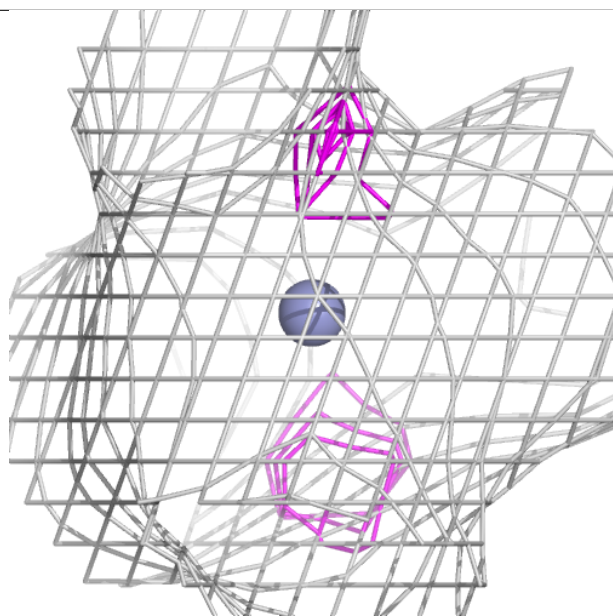
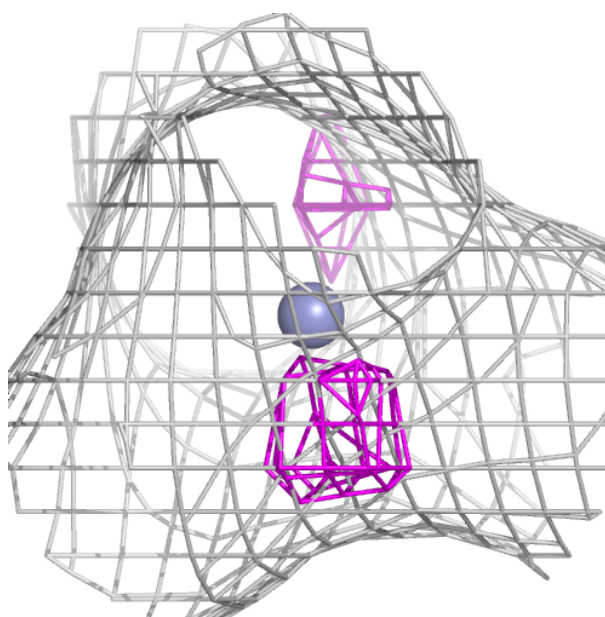
Electron density around ZN H 201:

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



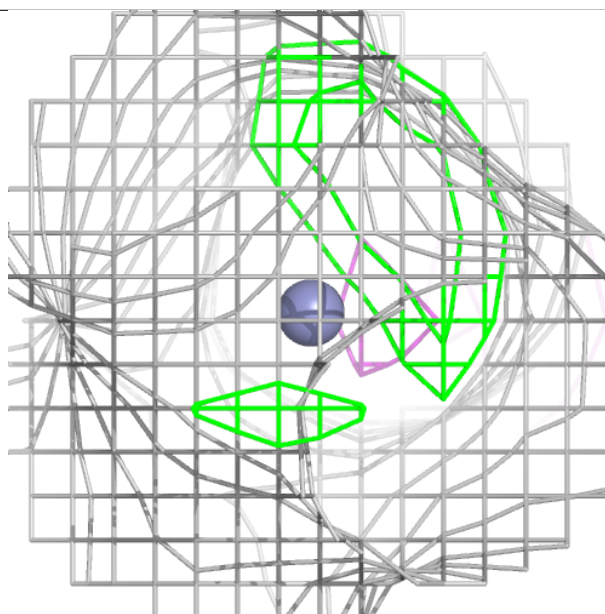
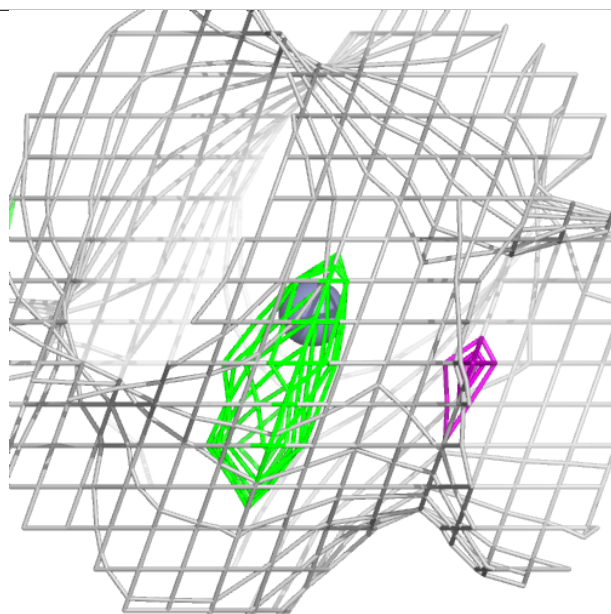
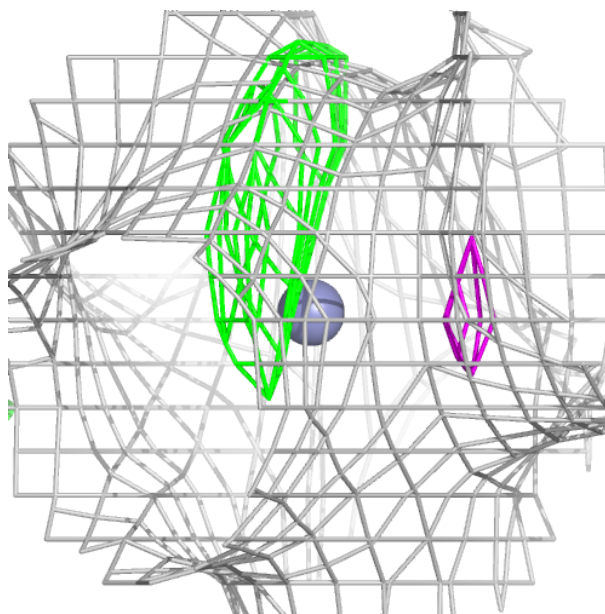
Electron density around ZN E 201:

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



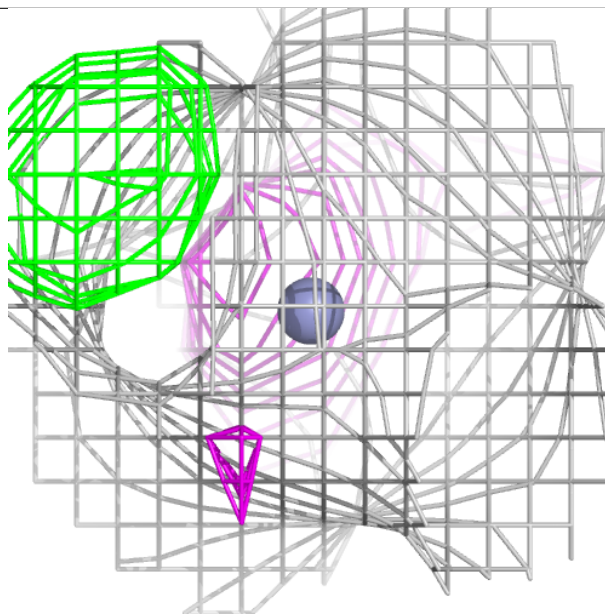
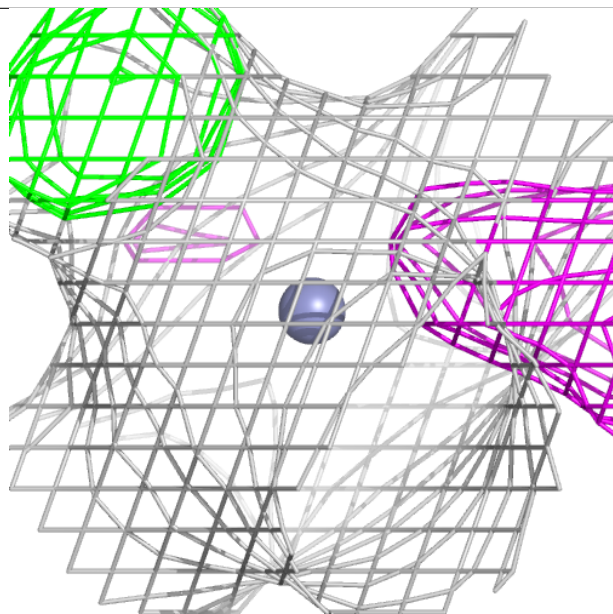
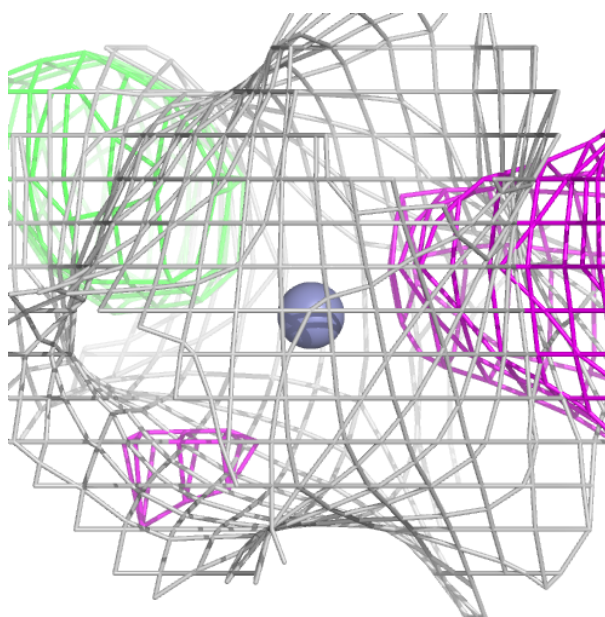
Electron density around ZN J 201:

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



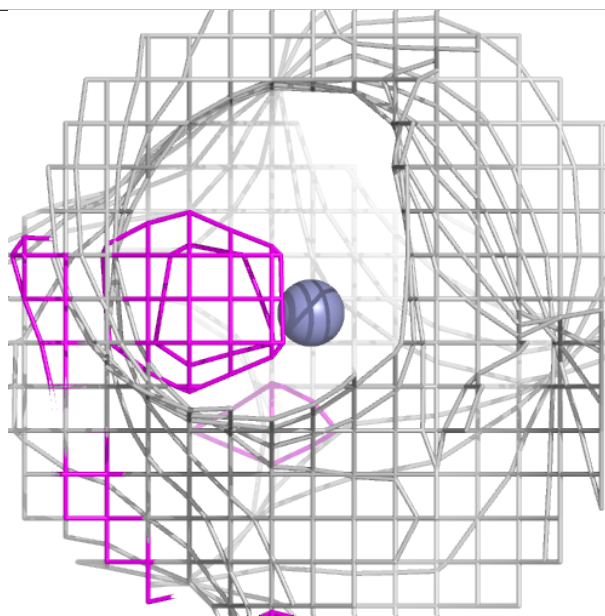
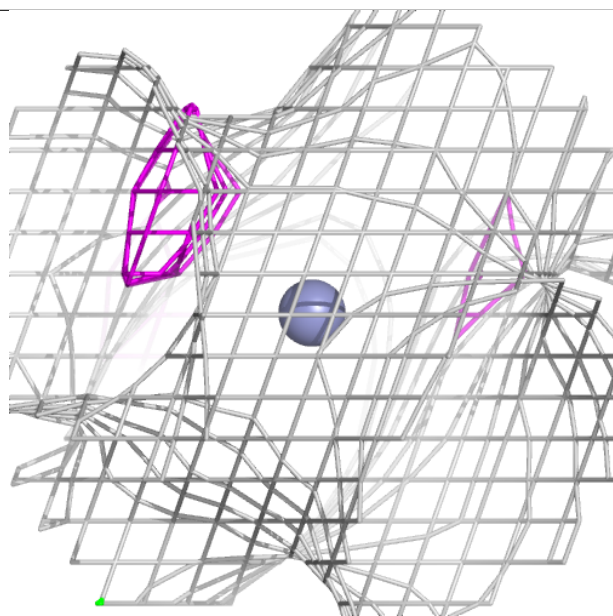
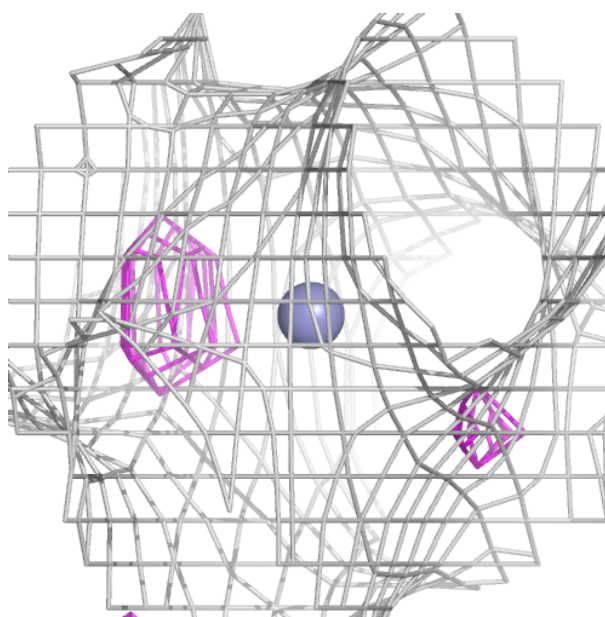
Electron density around ZN L 201:

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



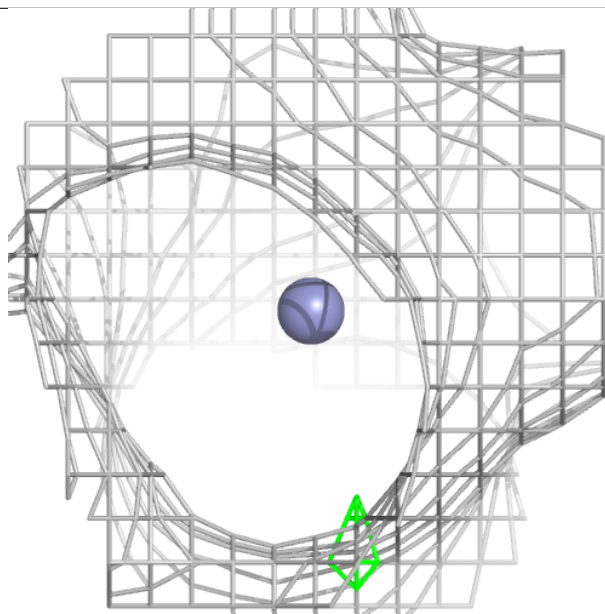
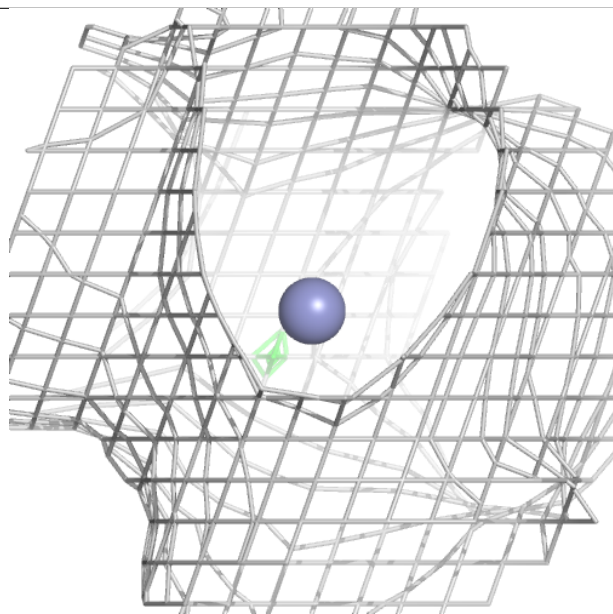
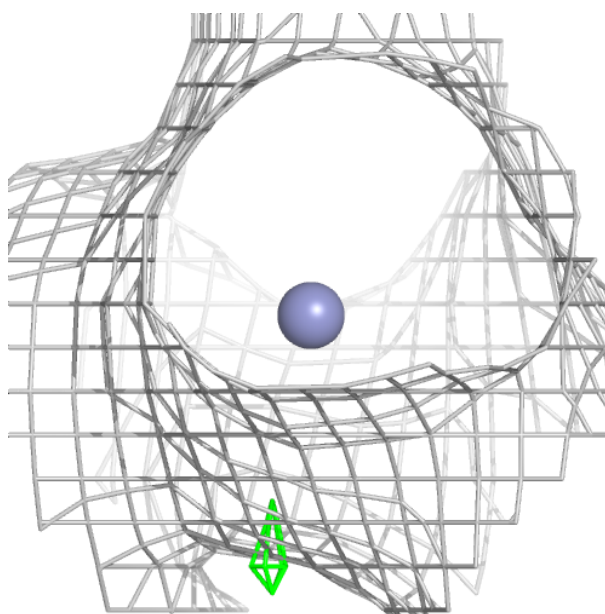
Electron density around ZN P 201:

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



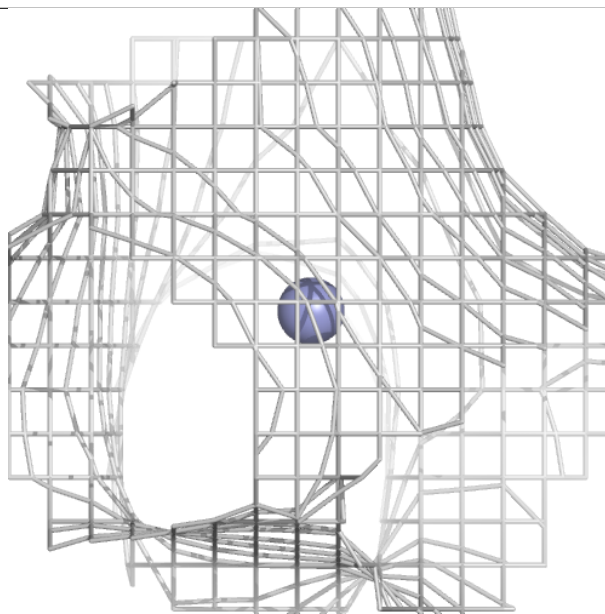
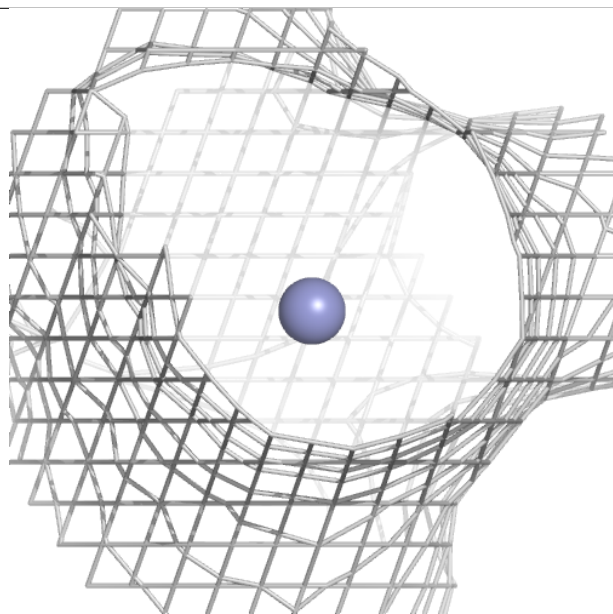
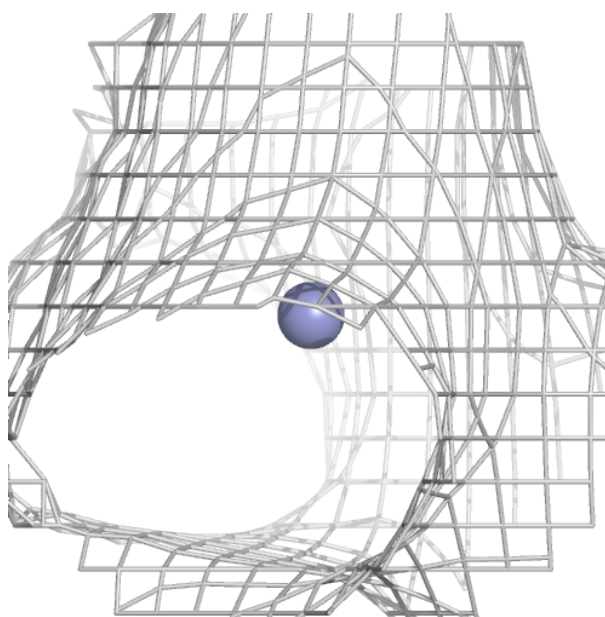
Electron density around ZN D 201:

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



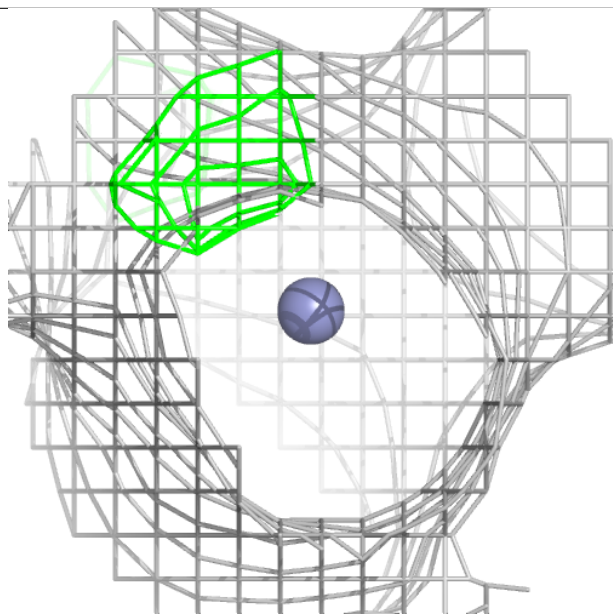
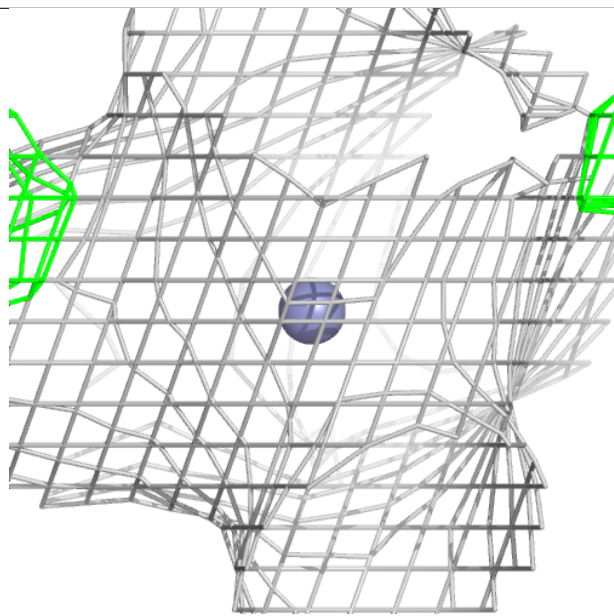
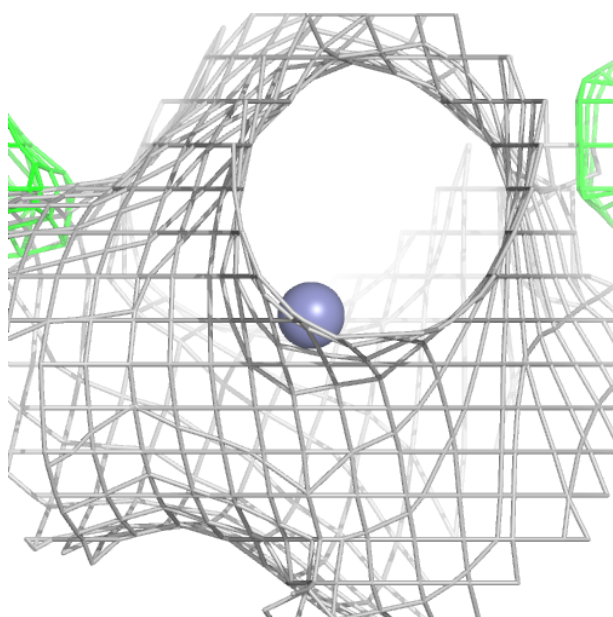
Electron density around ZN J 202:

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



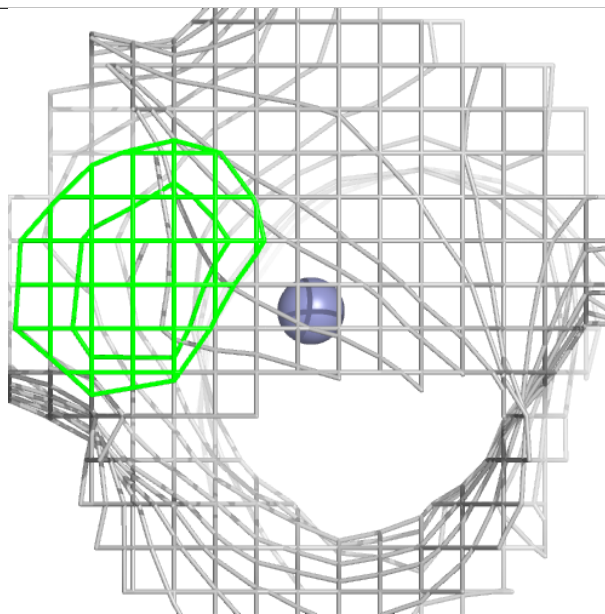
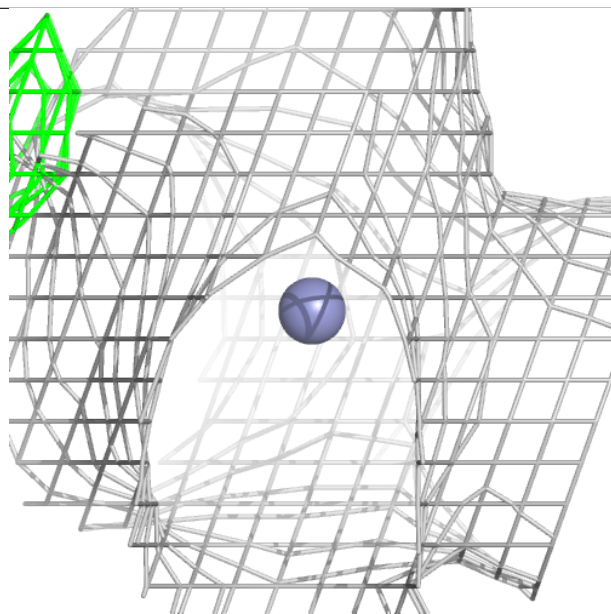
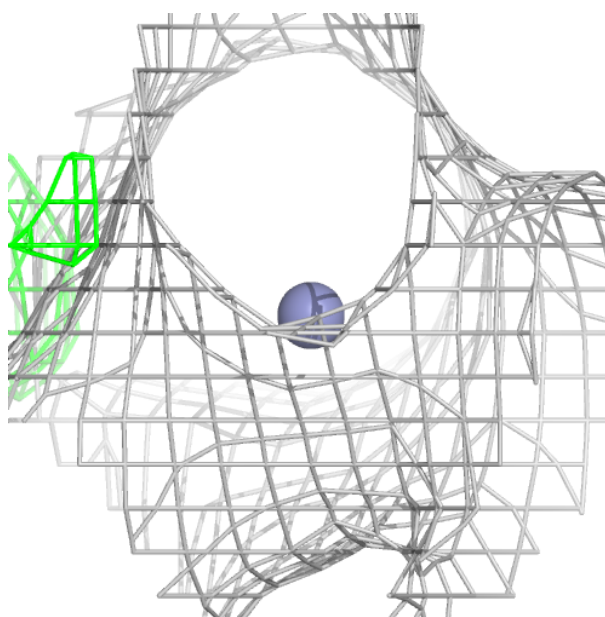
Electron density around ZN A 201:

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



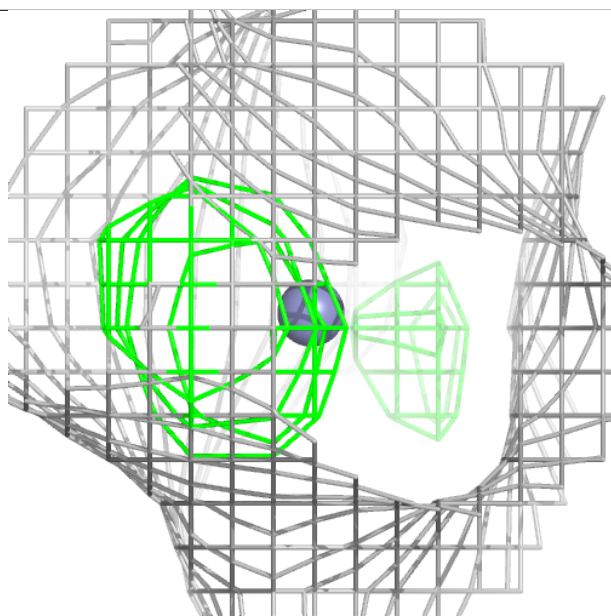
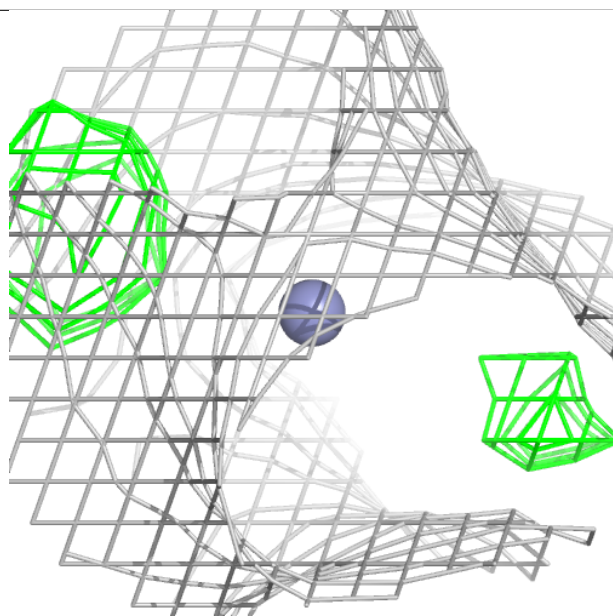
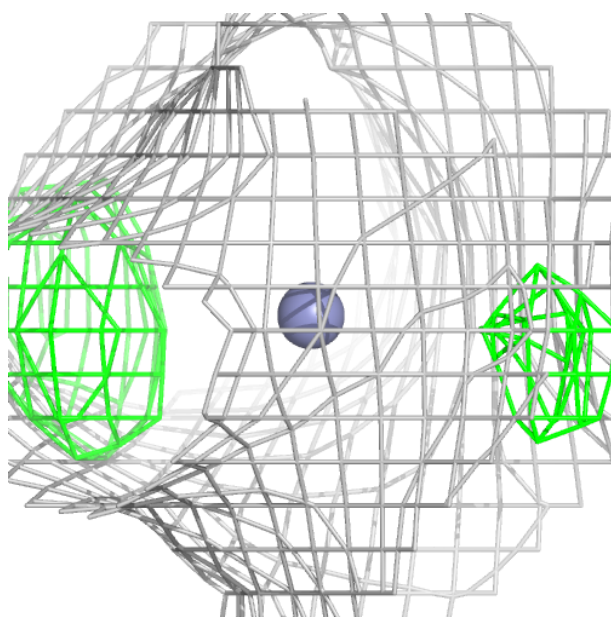
Electron density around ZN N 201:

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



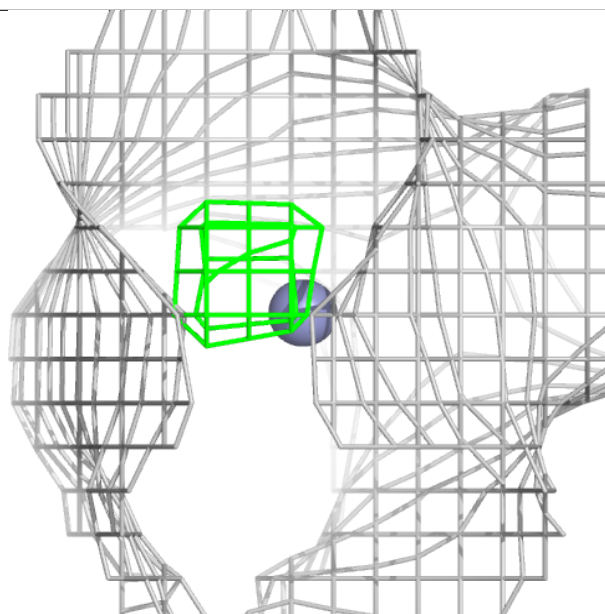
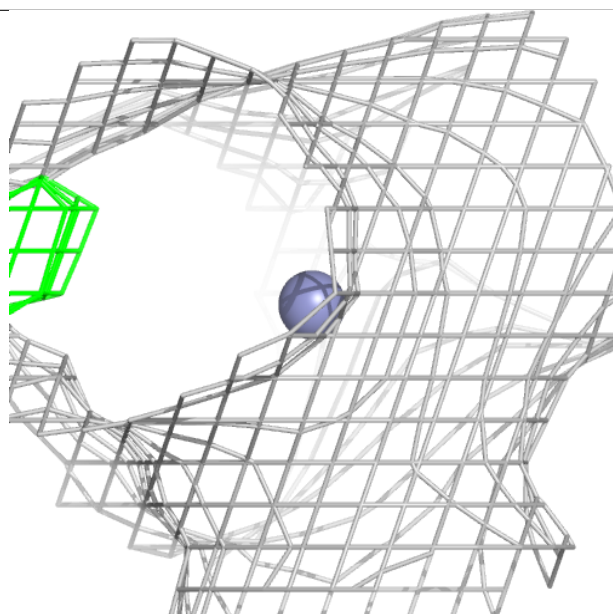
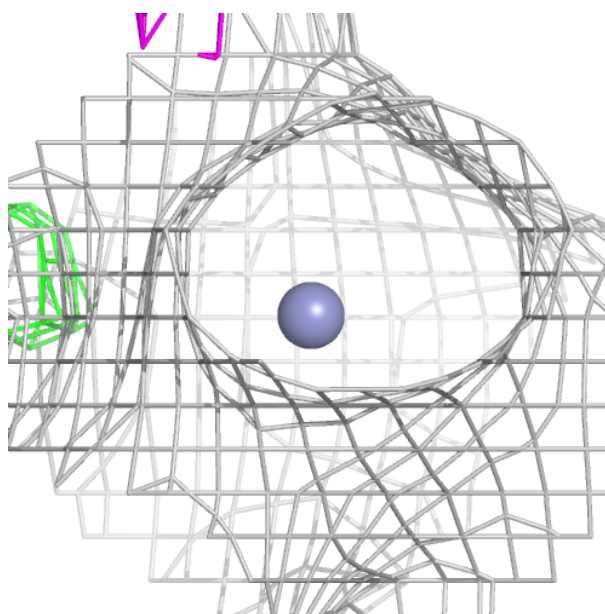
Electron density around ZN B 202:

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



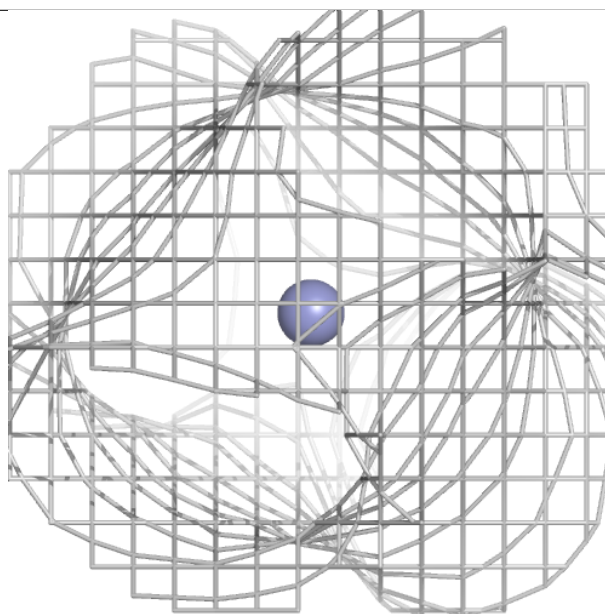
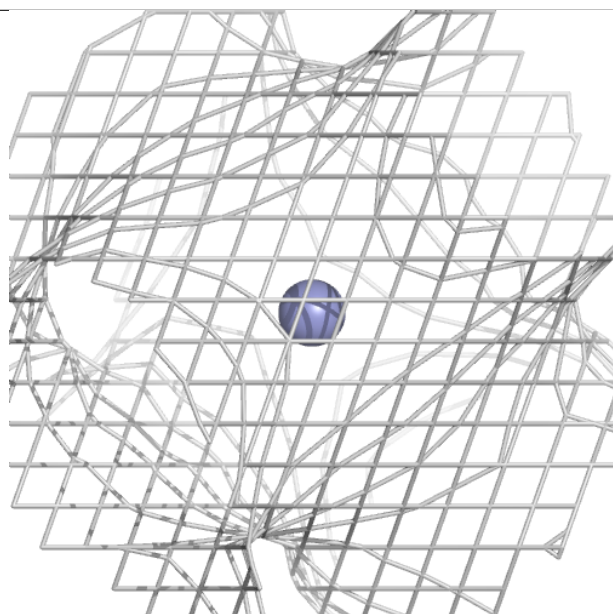
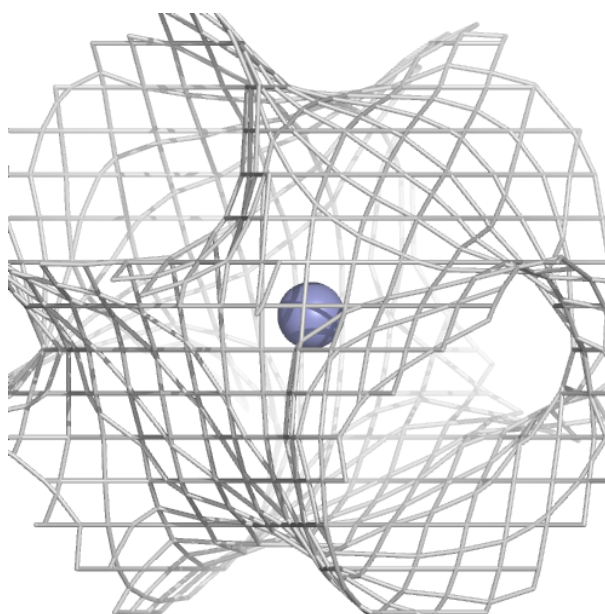
Electron density around ZN H 203:

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



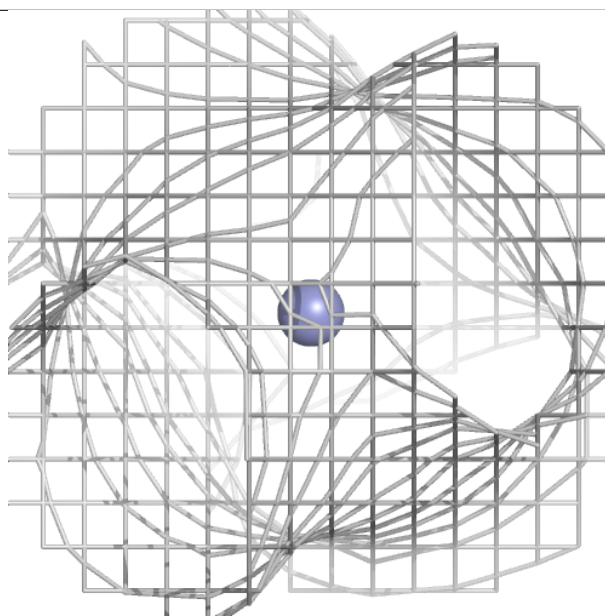
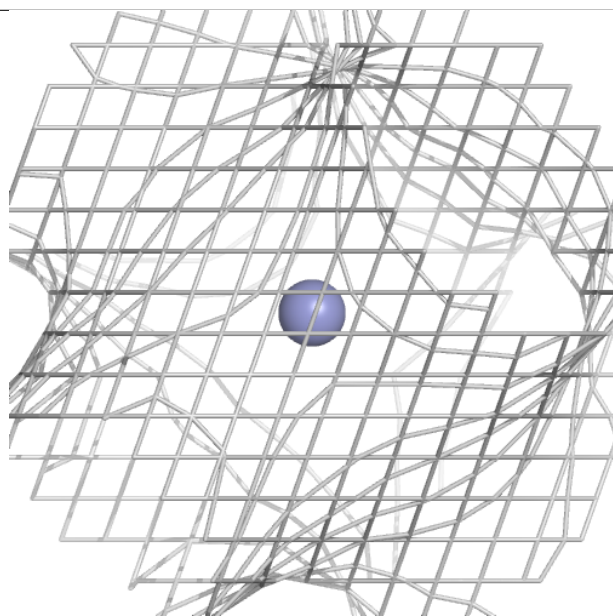
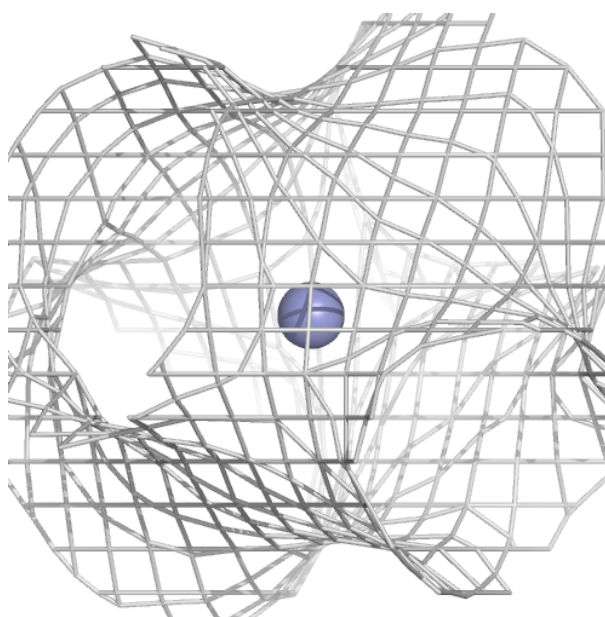
Electron density around ZN B 201:

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



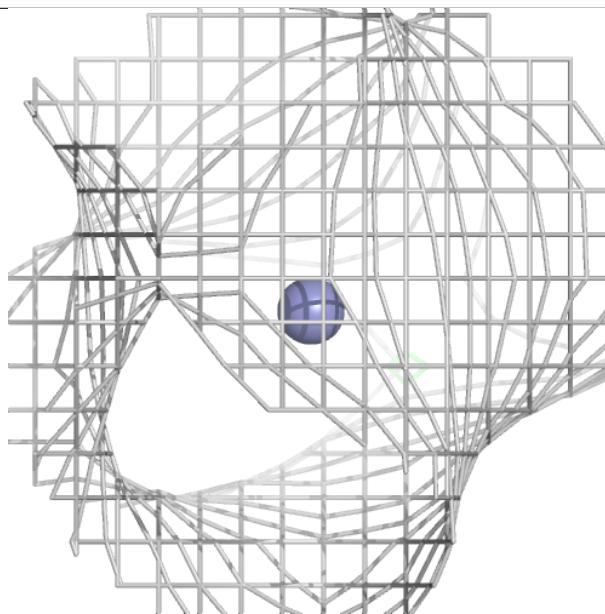
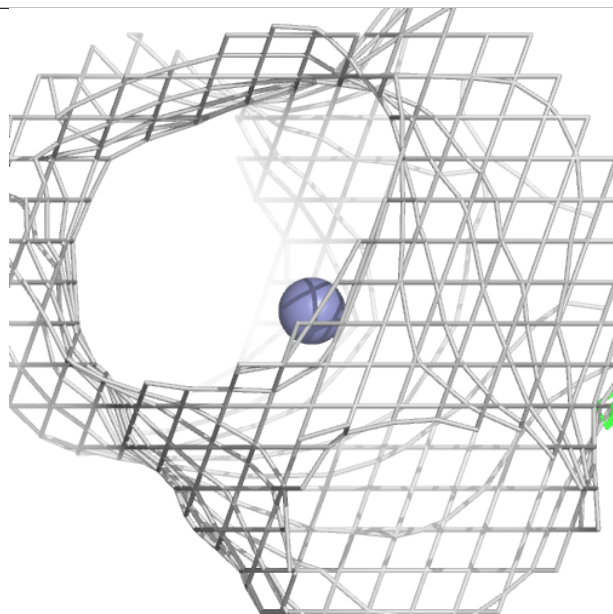
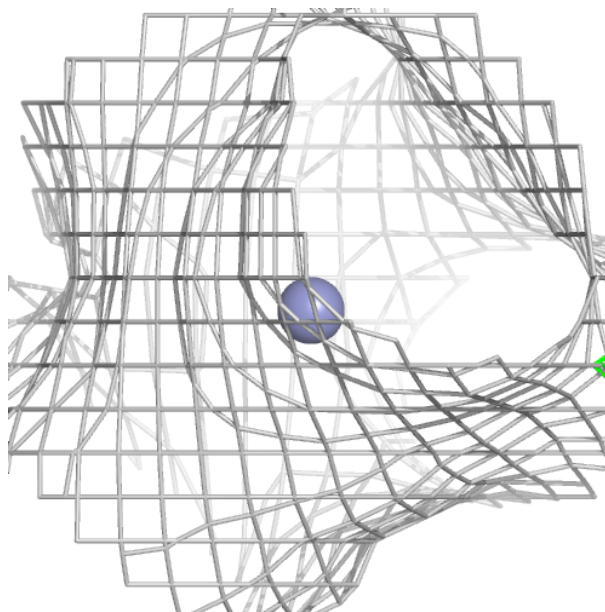
Electron density around ZN F 201:

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



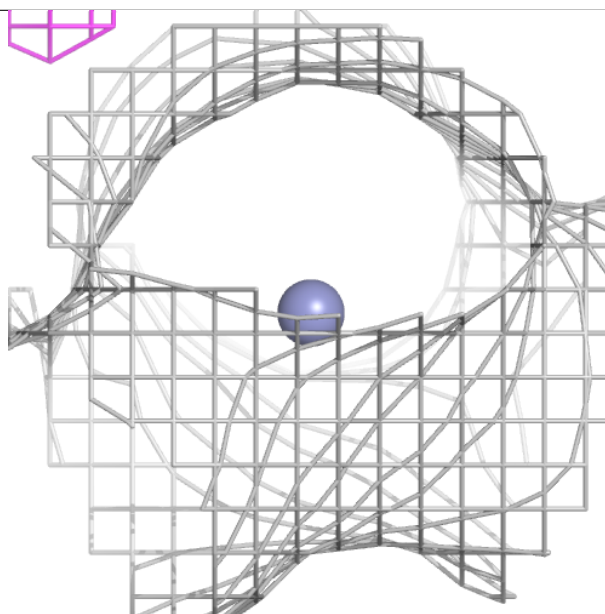
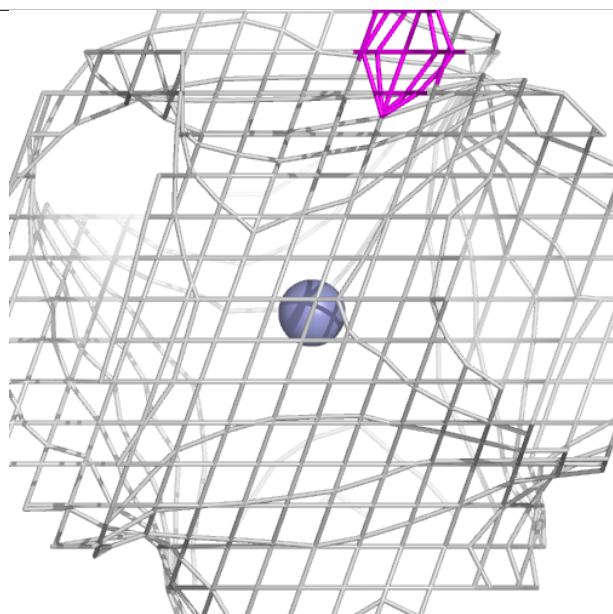
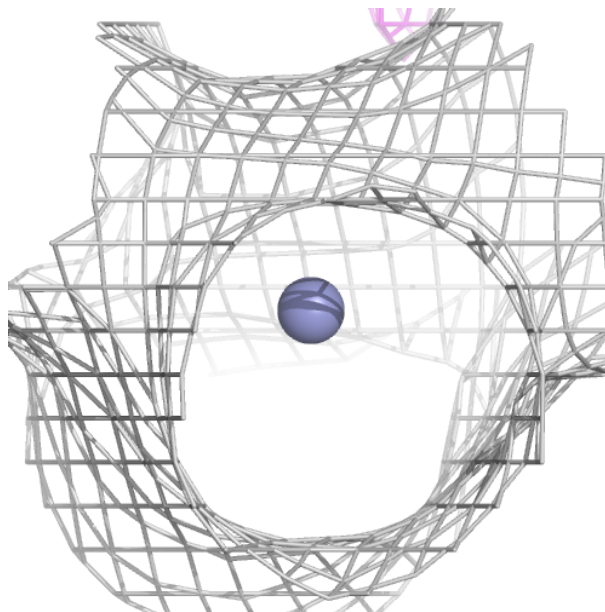
Electron density around ZN F 202:

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



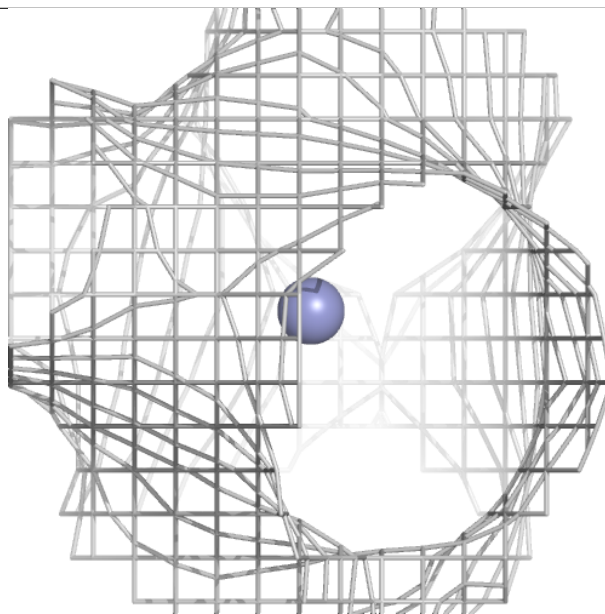
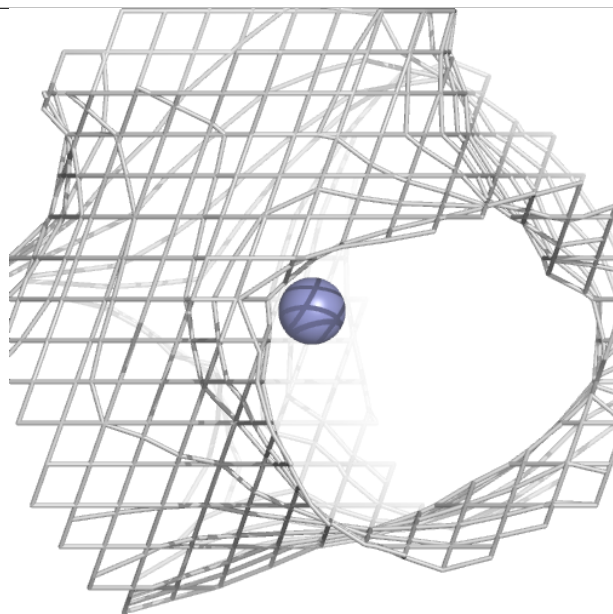
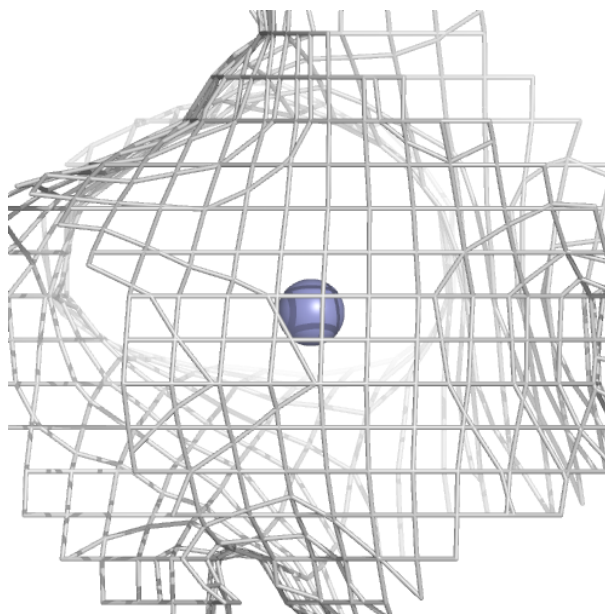
Electron density around ZN L 202:

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



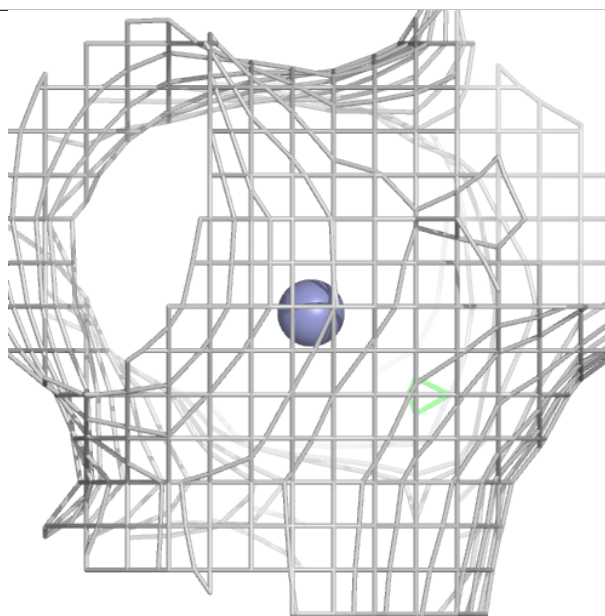
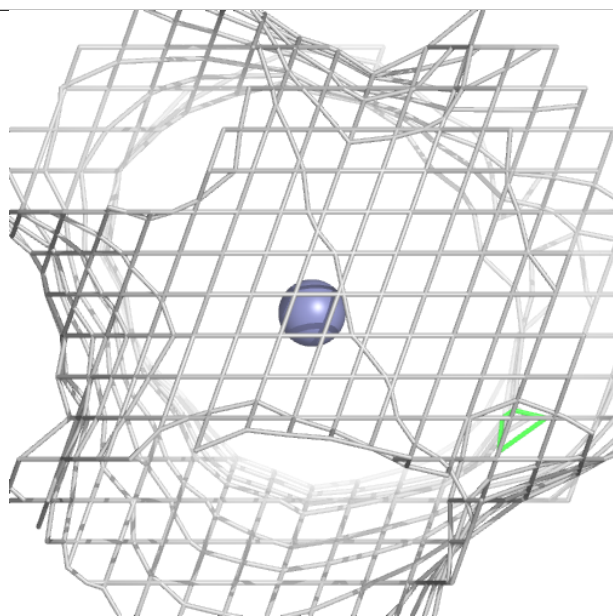
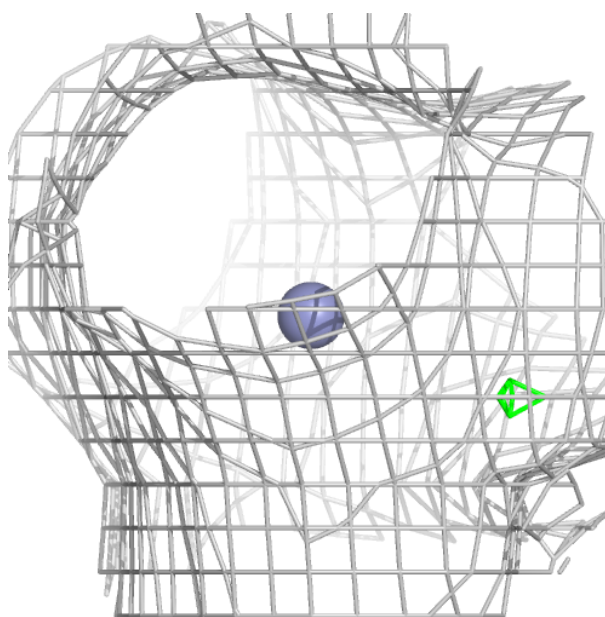
Electron density around ZN L 203:

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



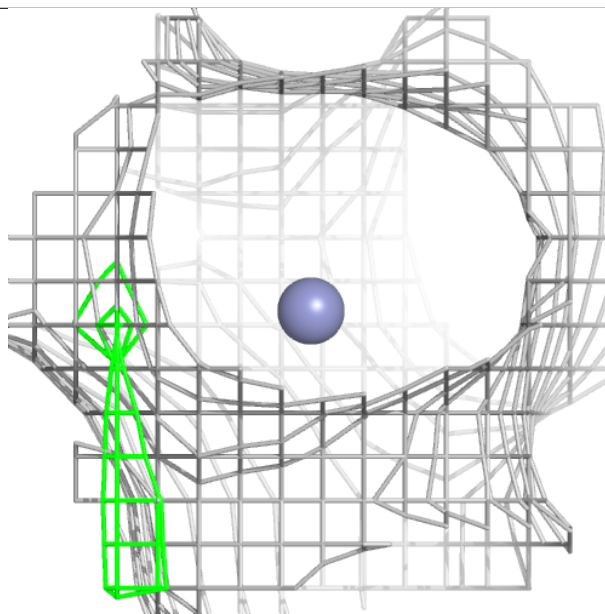
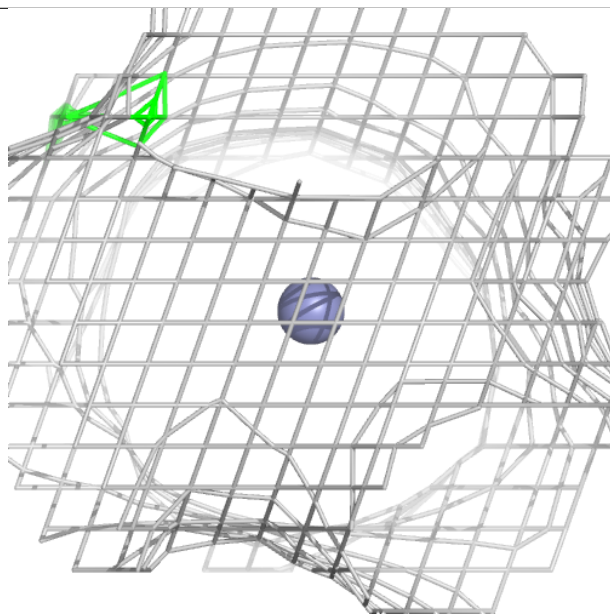
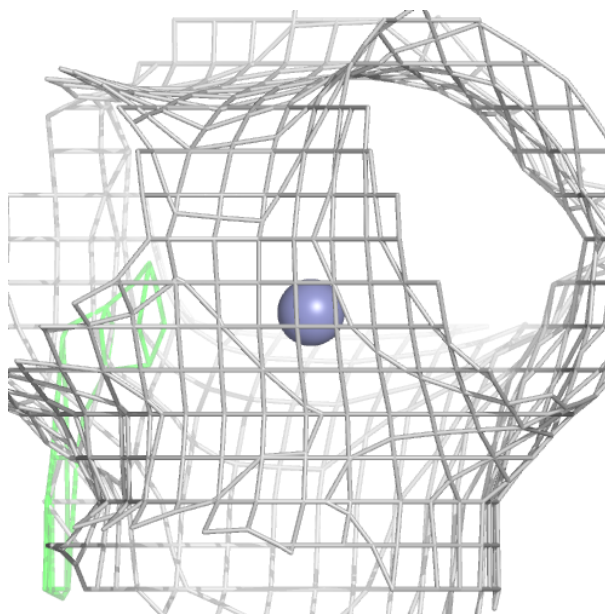
Electron density around ZN D 202:

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



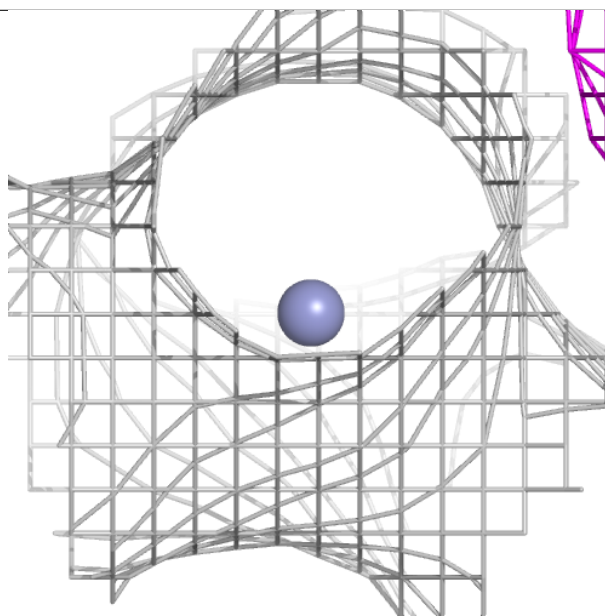
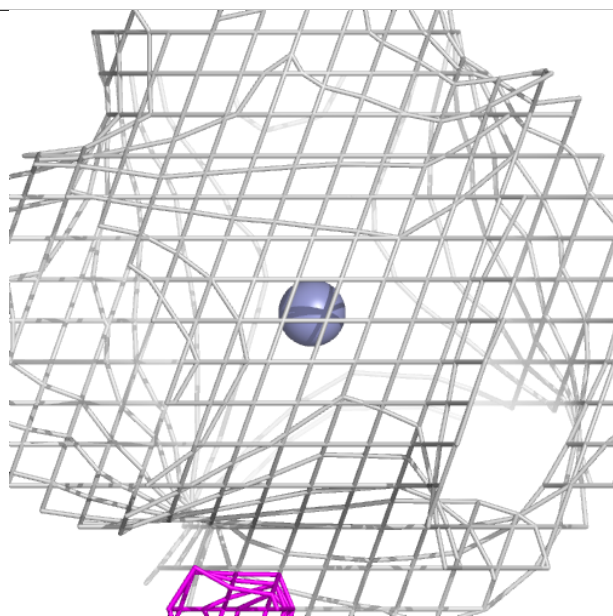
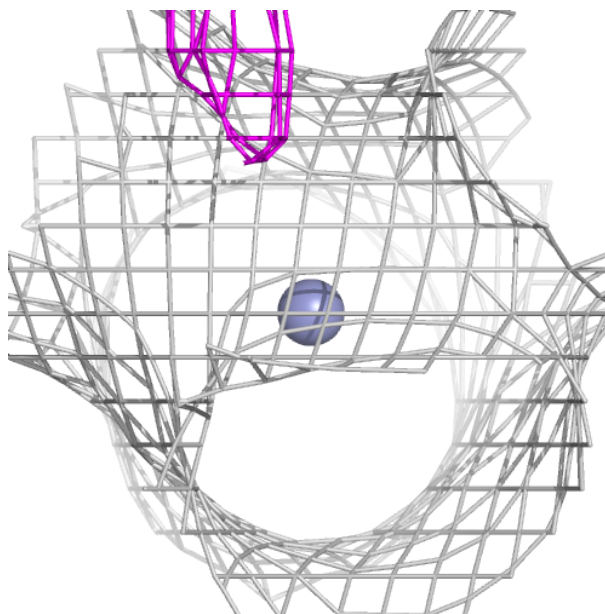
Electron density around ZN N 202:

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



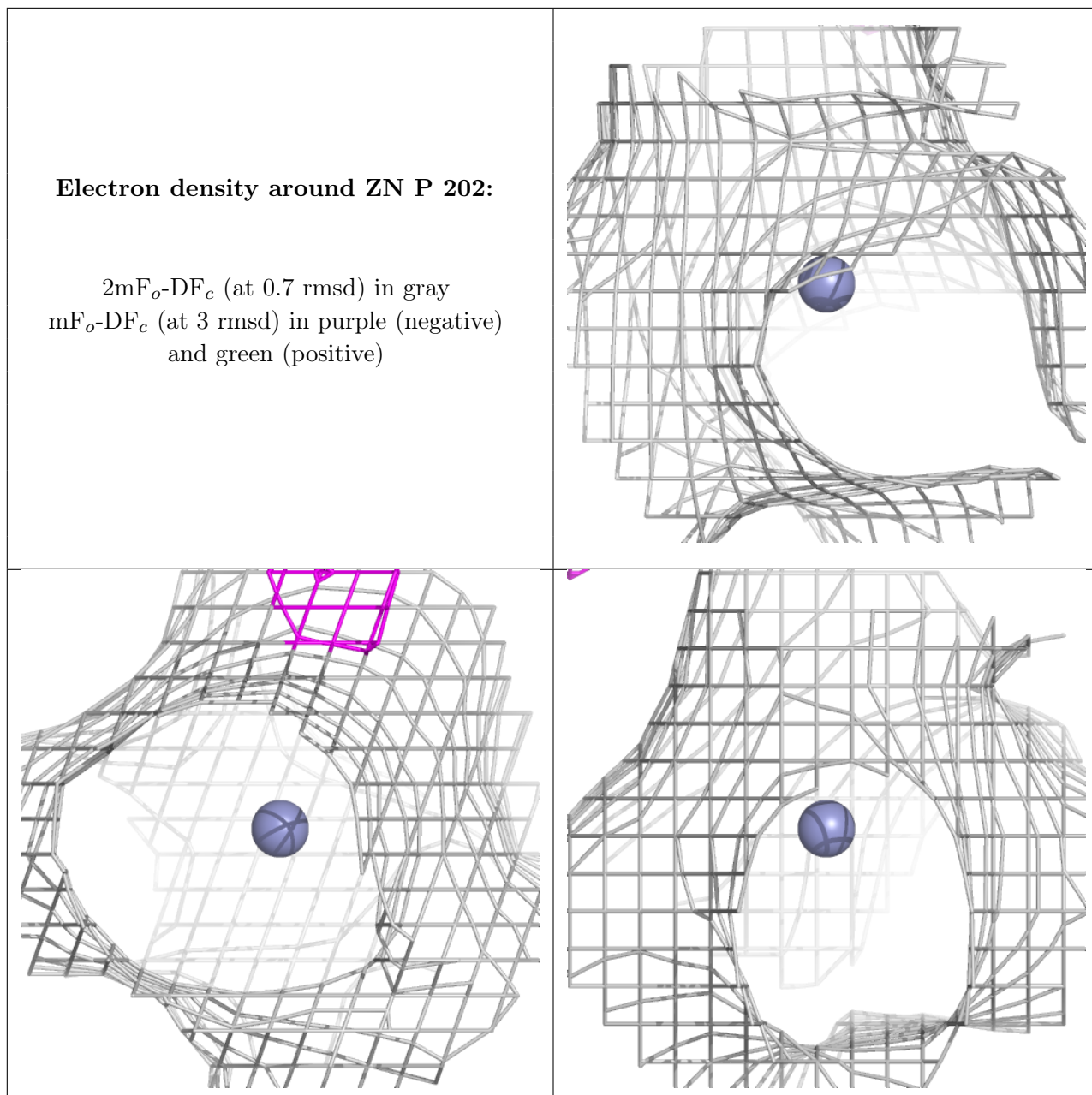
Electron density around ZN H 202:

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



Electron density around ZN P 202:

$2mF_o-DF_c$ (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.