



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 01:58 PM JST

PDB ID : 9UTH / pdb_00009uth
Title : DPF3b in complex with H3K14cr peptide
Authors : Feng, F.; Huang, J.; Xiang, B.; Li, H.
Deposited on : 2025-05-03
Resolution : 2.69 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

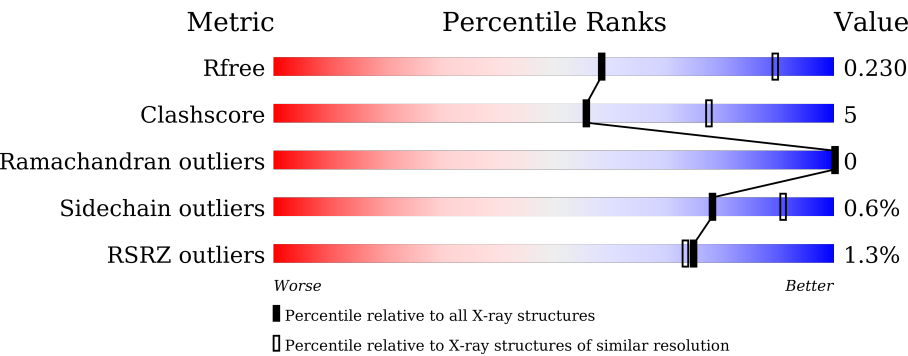
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	114	<div><div>0%</div><div><div>88%</div><div>11%</div><div>.</div></div></div>
1	C	114	<div><div>0%</div><div><div>88%</div><div>11%</div><div>..</div></div></div>
1	E	114	<div><div></div><div><div>85%</div><div>15%</div></div></div>
1	G	114	<div><div>2%</div><div><div>91%</div><div>8%</div><div>.</div></div></div>
2	B	26	<div><div></div><div><div>92%</div><div>8%</div></div></div>
2	D	26	<div><div>4%</div><div><div>69%</div><div>31%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	26	 4% 88% 12%
2	H	26	 4% 69% 31%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4431 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 Zinc finger protein DPF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			879	544	147	171	17			
1	C	113	Total	C	N	O	S	0	0	0
			875	541	146	171	17			
1	E	114	Total	C	N	O	S	0	0	0
			885	547	148	173	17			
1	G	113	Total	C	N	O	S	0	0	0
			875	541	146	171	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	SER	THR	conflict	UNP Q92784
C	255	SER	THR	conflict	UNP Q92784
E	255	SER	THR	conflict	UNP Q92784
G	255	SER	THR	conflict	UNP Q92784

- Molecule 2 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	26	Total	C	N	O	0	0	1
			189	114	42	33			
2	D	26	Total	C	N	O	0	0	1
			189	114	42	33			
2	F	26	Total	C	N	O	0	0	1
			189	114	42	33			
2	H	26	Total	C	N	O	0	0	1
			189	114	42	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ALA	ARG	conflict	UNP P84243
D	26	ALA	ARG	conflict	UNP P84243
F	26	ALA	ARG	conflict	UNP P84243
H	26	ALA	ARG	conflict	UNP P84243

- 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	4	Total Zn 4 4	0	0
3	C	4	Total Zn 4 4	0	0
3	E	4	Total Zn 4 4	0	0
3	G	4	Total Zn 4 4	0	0

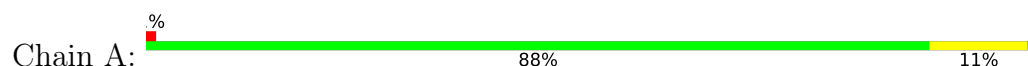
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	8	Total O 8 8	0	0
4	C	40	Total O 40 40	0	0
4	D	3	Total O 3 3	0	0
4	E	27	Total O 27 27	0	0
4	F	5	Total O 5 5	0	0
4	G	30	Total O 30 30	0	0
4	H	3	Total O 3 3	0	0

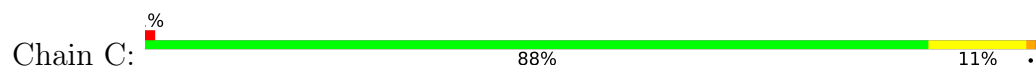
3 Residue-property plots

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

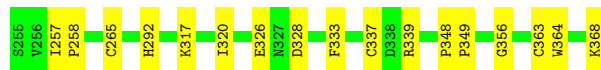
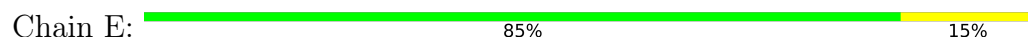
- Molecule 1: Zinc finger protein DPF3



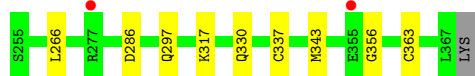
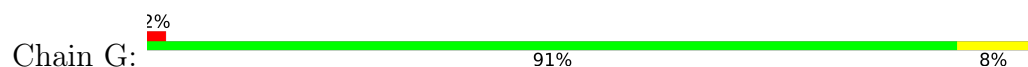
- Molecule 1: Zinc finger protein DPF3



- Molecule 1: Zinc finger protein DPF3



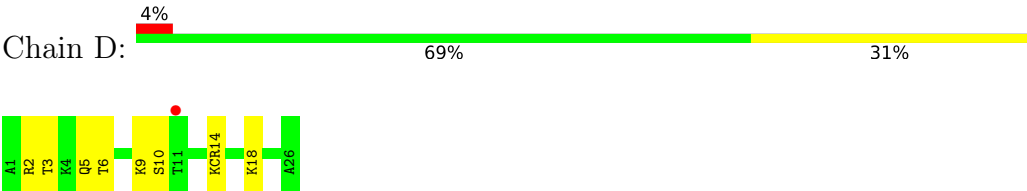
- Molecule 1: Zinc finger protein DPF3



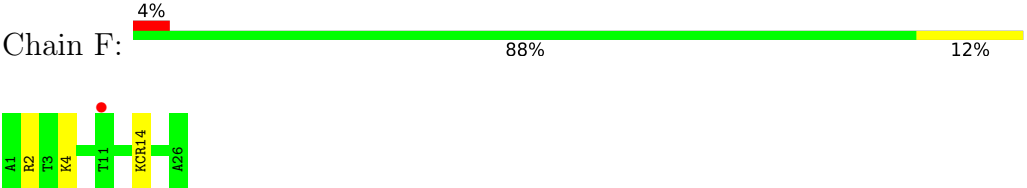
- Molecule 2: Histone H3.3



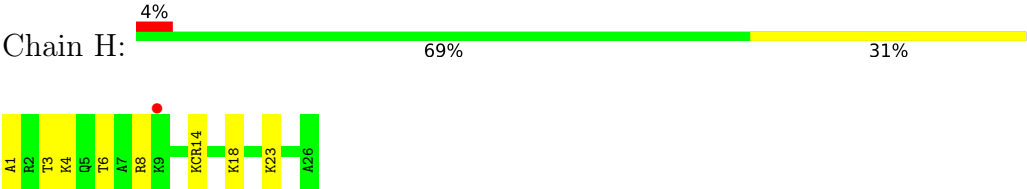
- Molecule 2: Histone H3.3



● Molecule 2: Histone H3.3



● Molecule 2: Histone H3.3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.09Å 84.25Å 111.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.11 – 2.69 36.11 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.11-2.69) 99.3 (36.11-2.69)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.181 , 0.230 0.180 , 0.230	Depositor DCC
R_{free} test set	1318 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4431	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 31.64 % 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 1.0715e-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, KCR

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	0.14	0/901	0.31	0/1220
1	C	0.14	0/897	0.34	0/1217
1	E	0.13	0/907	0.30	0/1228
1	G	0.13	0/897	0.29	0/1217
2	B	0.14	0/174	0.28	0/229
2	D	0.16	0/174	0.37	0/229
2	F	0.11	0/174	0.28	0/229
2	H	0.13	0/174	0.27	0/229
All	All	0.13	0/4298	0.31	0/5798

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	879	0	808	10	0
1	C	875	0	800	11	0
1	E	885	0	813	11	0
1	G	875	0	800	7	0
2	B	189	0	212	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	189	0	212	5	0
2	F	189	0	212	1	0
2	H	189	0	212	5	0
3	A	4	0	0	0	0
3	C	4	0	0	0	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
4	A	29	0	0	0	0
4	B	8	0	0	0	0
4	C	40	0	0	0	0
4	D	3	0	0	0	0
4	E	27	0	0	0	0
4	F	5	0	0	0	0
4	G	30	0	0	0	0
4	H	3	0	0	0	0
All	All	4431	0	4069	39	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 5.

All (39) 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:G:266:LEU:HD22	2:H:23:LYS:HG3	1.66	0.78
1:C:286:ASP:HB3	2:H:18:LYS:HD3	1.77	0.66
1:G:330:GLN:HA	1:G:343:MET:HE2	1.86	0.57
1:C:297:GLN:NE2	2:D:10:SER:O	2.29	0.55
2:D:3:THR:H	2:D:6:THR:HB	1.72	0.55
1:C:333:PHE:HB2	2:D:2:ARG:HB3	1.89	0.55
1:E:356:GLY:HA2	1:G:297:GLN:HG2	1.89	0.54
1:C:303:THR:HG22	1:C:307:LYS:HE2	1.90	0.54
2:D:18:LYS:HG3	1:G:286:ASP:HB3	1.92	0.52
1:E:257:ILE:HG13	1:E:258:PRO:HD2	1.93	0.51
1:A:355:GLU:OE1	1:A:355:GLU:N	2.41	0.50
1:A:317:LYS:HD2	1:A:333:PHE:CE1	2.46	0.50
1:E:337:CYS:HB3	1:E:363:CYS:SG	2.51	0.49
2:H:3:THR:HB	2:H:6:THR:HG23	1.94	0.48
1:A:297:GLN:HG2	1:C:356:GLY:HA2	1.96	0.48
1:A:299:THR:HG22	1:C:335:ASP:HB3	1.96	0.48
1:C:317:LYS:HE3	1:C:338:ASP:O	2.12	0.48
1:A:330:GLN:HA	1:A:343:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:337:CYS:HB3	1:G:363:CYS:SG	2.55	0.47
1:G:317:LYS:HE3	1:G:317:LYS:HB2	1.75	0.47
1:G:356:GLY:O	2:H:1:ALA:N	2.42	0.47
2:D:5:GLN:O	2:D:9:LYS:HG2	2.15	0.47
1:E:364:TRP:O	1:E:368:LYS:HB3	2.14	0.46
1:A:331:LEU:HD23	2:B:4:LYS:HE3	1.98	0.46
1:E:320:ILE:HG13	1:E:339:ARG:HD3	1.98	0.45
1:A:342:HIS:HB2	1:A:345:CYS:HB2	1.99	0.45
1:E:317:LYS:HD2	1:E:333:PHE:CE1	2.52	0.44
1:E:368:LYS:HB3	1:E:368:LYS:HE2	1.77	0.44
2:H:4:LYS:O	2:H:8:ARG:HB2	2.18	0.43
1:E:348:PRO:HA	1:E:349:PRO:HD3	1.93	0.43
1:E:328:ASP:HB3	2:F:4:LYS:HD2	2.00	0.43
1:A:324:THR:OG1	1:A:326:GLU:OE1	2.29	0.42
1:E:317:LYS:HD2	1:E:333:PHE:CZ	2.55	0.42
1:A:330:GLN:HG2	1:A:343:MET:HE3	2.02	0.41
1:A:368:LYS:HD3	1:C:303:THR:HG21	2.03	0.41
1:C:328:ASP:OD1	1:C:328:ASP:N	2.53	0.41
1:E:265:CYS:SG	1:E:292:HIS:CE1	3.14	0.41
1:C:332:LEU:HD23	1:C:332:LEU:HA	1.89	0.41
1:C:272:ASN:HA	1:C:292:HIS:CE1	2.57	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	111/114 (97%)	109 (98%)	2 (2%)	0	100	100
1	C	111/114 (97%)	110 (99%)	1 (1%)	0	100	100
1	E	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	G	111/114 (97%)	107 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	23/26 (88%)	23 (100%)	0	0	100	100
2	D	23/26 (88%)	23 (100%)	0	0	100	100
2	F	23/26 (88%)	23 (100%)	0	0	100	100
2	H	23/26 (88%)	23 (100%)	0	0	100	100
All	All	537/560 (96%)	527 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	102/103 (99%)	102 (100%)	0	100	100
1	C	102/103 (99%)	101 (99%)	1 (1%)	68	86
1	E	103/103 (100%)	102 (99%)	1 (1%)	68	86
1	G	102/103 (99%)	102 (100%)	0	100	100
2	B	16/16 (100%)	16 (100%)	0	100	100
2	D	16/16 (100%)	16 (100%)	0	100	100
2	F	16/16 (100%)	15 (94%)	1 (6%)	16	39
2	H	16/16 (100%)	16 (100%)	0	100	100
All	All	473/476 (99%)	470 (99%)	3 (1%)	78	91

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

Mol	Chain	Res	Type
1	C	332	LEU
1	E	326	GLU
2	F	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	327	ASN
1	A	330	GLN
1	G	327	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	KCR	F	14	2	12,13,14	1.60	1 (8%)	9,14,16	1.49	2 (22%)
2	KCR	H	14	2	12,13,14	1.64	1 (8%)	9,14,16	2.28	4 (44%)
2	KCR	B	14	2	12,13,14	1.51	1 (8%)	9,14,16	1.58	2 (22%)
2	KCR	D	14	2	12,13,14	1.57	1 (8%)	9,14,16	1.62	2 (22%)

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	KCR	F	14	2	-	2/12/13/15	-
2	KCR	H	14	2	-	2/12/13/15	-
2	KCR	B	14	2	-	3/12/13/15	-
2	KCR	D	14	2	-	1/12/13/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	14	KCR	CH-NZ	3.86	1.42	1.34
2	F	14	KCR	CH-NZ	3.78	1.42	1.34
2	D	14	KCR	CH-NZ	3.66	1.42	1.34
2	B	14	KCR	CH-NZ	3.64	1.42	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	14	KCR	CX-CH-NZ	4.47	123.40	114.97
2	H	14	KCR	CY-CX-CH	-3.66	116.48	120.88
2	D	14	KCR	CH3-CY-CX	-3.12	119.19	125.34
2	F	14	KCR	CH3-CY-CX	-2.62	120.17	125.34
2	D	14	KCR	CX-CH-NZ	2.60	119.87	114.97
2	B	14	KCR	CH3-CY-CX	-2.59	120.22	125.34
2	B	14	KCR	CX-CH-NZ	2.48	119.64	114.97
2	F	14	KCR	CX-CH-NZ	2.45	119.59	114.97
2	H	14	KCR	OH-CH-NZ	-2.24	118.52	122.23
2	H	14	KCR	OH-CH-CX	-2.17	118.08	123.03

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	14	KCR	OH-CH-NZ-CE
2	H	14	KCR	CX-CH-NZ-CE
2	F	14	KCR	NZ-CH-CX-CY
2	B	14	KCR	OH-CH-CX-CY
2	F	14	KCR	OH-CH-CX-CY
2	B	14	KCR	NZ-CH-CX-CY
2	D	14	KCR	C-CA-CB-CG
2	B	14	KCR	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	113/114 (99%)	-0.30	1 (0%) 81 80	19, 27, 47, 64	0
1	C	113/114 (99%)	-0.30	1 (0%) 81 80	14, 27, 49, 63	0
1	E	114/114 (100%)	-0.06	0 100 100	18, 37, 63, 71	0
1	G	113/114 (99%)	-0.13	2 (1%) 67 65	18, 29, 58, 80	0
2	B	25/26 (96%)	-0.16	0 100 100	22, 32, 54, 64	0
2	D	25/26 (96%)	0.50	1 (4%) 42 38	24, 41, 59, 67	0
2	F	25/26 (96%)	0.42	1 (4%) 42 38	30, 39, 70, 82	0
2	H	25/26 (96%)	0.48	1 (4%) 42 38	32, 44, 66, 77	0
All	All	553/560 (98%)	-0.11	7 (1%) 75 73	14, 32, 63, 82	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	355	GLU	2.6
1	C	364	TRP	2.6
2	F	11	THR	2.3
1	A	256	VAL	2.3
2	D	11	THR	2.2
1	G	277	ARG	2.2
2	H	9	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
2	KCR	H	14	14/15	0.89	0.10	25,32,38,40	0
2	KCR	F	14	14/15	0.91	0.10	28,39,43,44	0
2	KCR	D	14	14/15	0.94	0.08	21,26,31,32	0
2	KCR	B	14	14/15	0.95	0.08	18,23,26,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

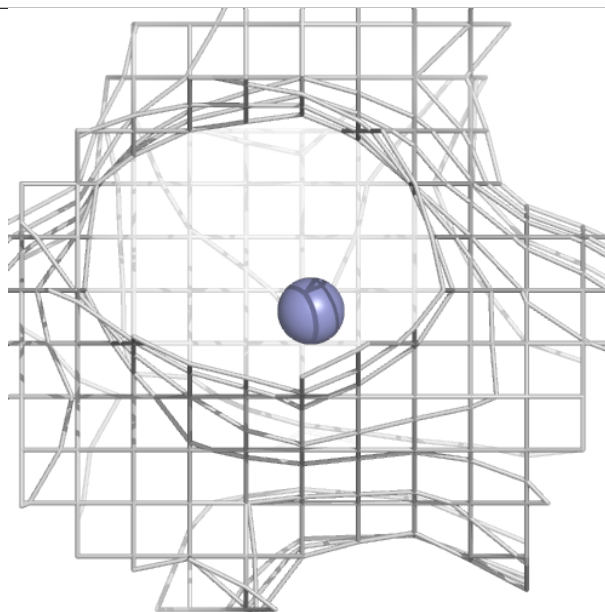
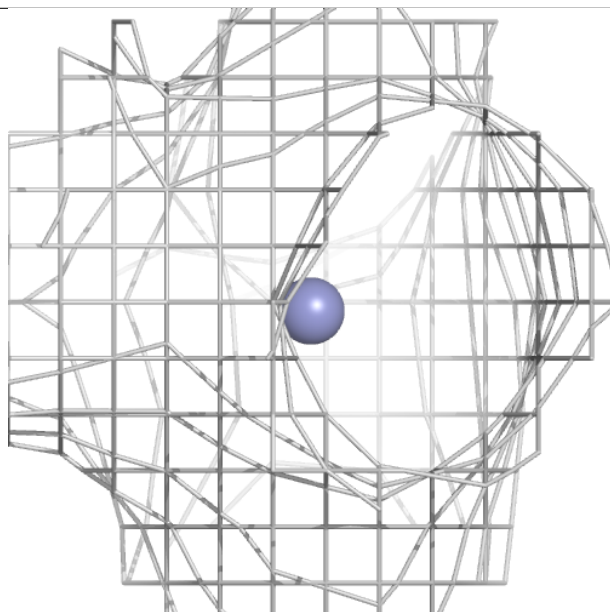
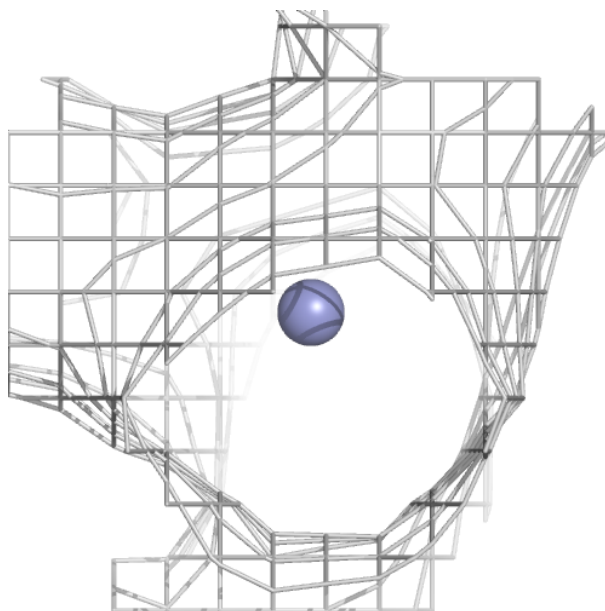
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	401	1/1	0.98	0.03	27,27,27,27	0
3	ZN	A	403	1/1	0.98	0.04	30,30,30,30	0
3	ZN	E	402	1/1	0.98	0.03	36,36,36,36	0
3	ZN	A	404	1/1	0.99	0.02	17,17,17,17	0
3	ZN	C	401	1/1	0.99	0.02	27,27,27,27	0
3	ZN	C	402	1/1	0.99	0.03	20,20,20,20	0
3	ZN	E	401	1/1	0.99	0.02	33,33,33,33	0
3	ZN	A	402	1/1	0.99	0.03	24,24,24,24	0
3	ZN	E	403	1/1	0.99	0.02	19,19,19,19	0
3	ZN	E	404	1/1	0.99	0.03	38,38,38,38	0
3	ZN	G	401	1/1	0.99	0.03	31,31,31,31	0
3	ZN	G	402	1/1	0.99	0.03	21,21,21,21	0
3	ZN	G	403	1/1	0.99	0.02	26,26,26,26	0
3	ZN	C	404	1/1	1.00	0.01	19,19,19,19	0
3	ZN	C	403	1/1	1.00	0.01	21,21,21,21	0
3	ZN	G	404	1/1	1.00	0.01	19,19,19,19	0

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

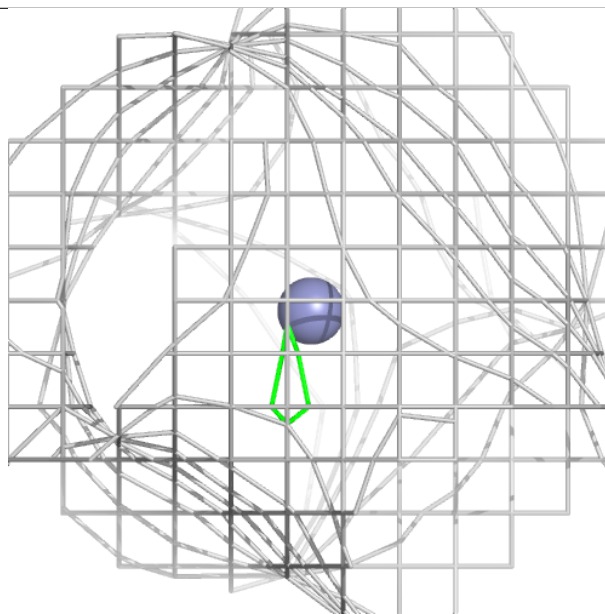
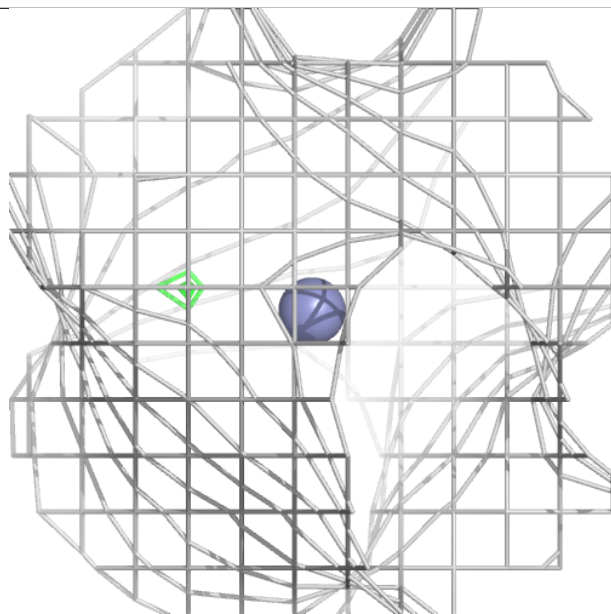
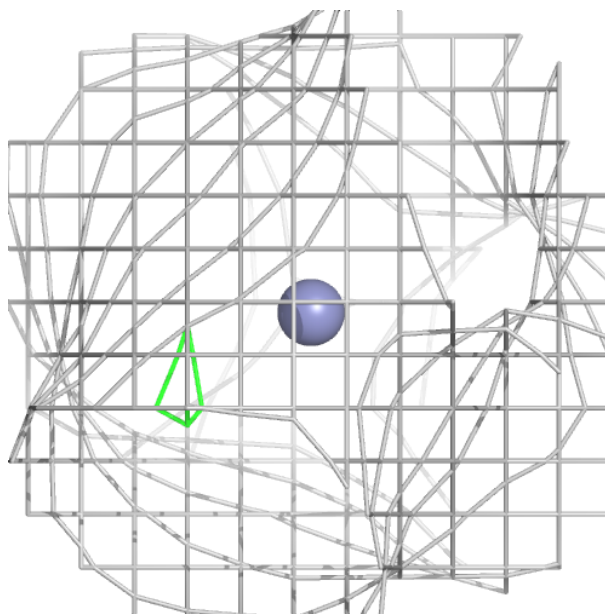
Electron density around ZN A 401:

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



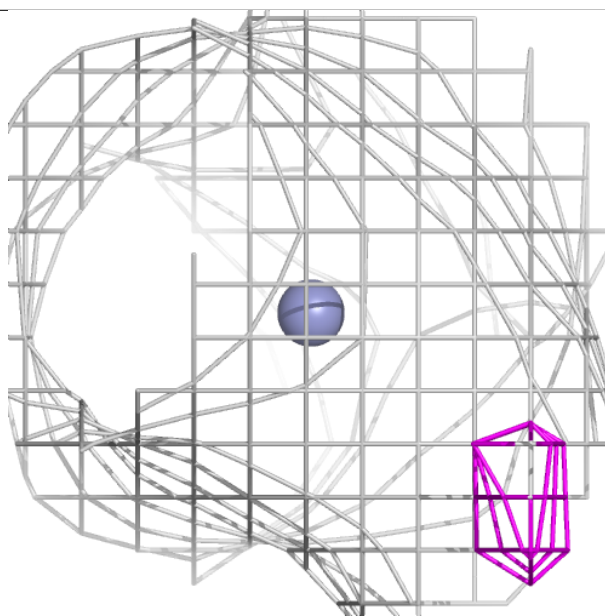
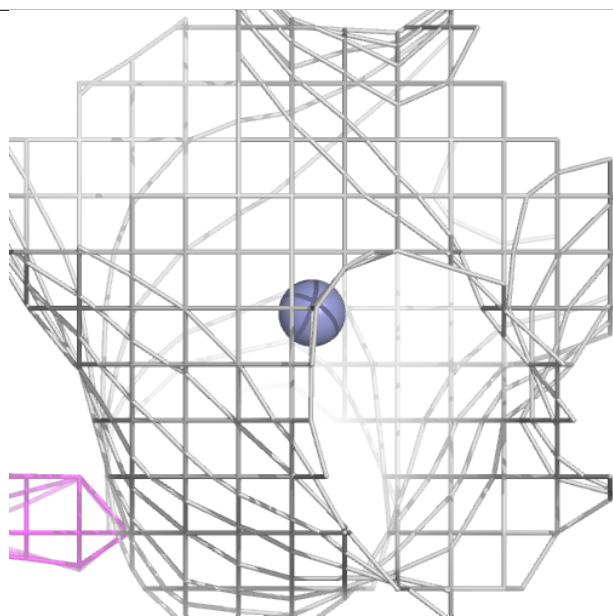
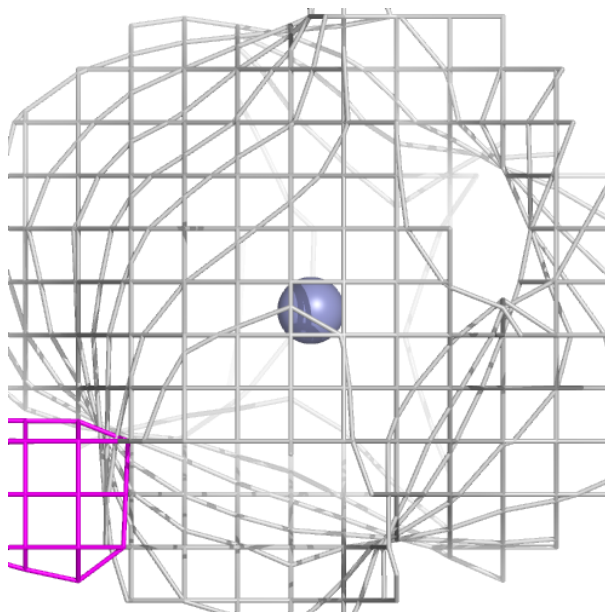
Electron density around ZN A 403:

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and green (positive)



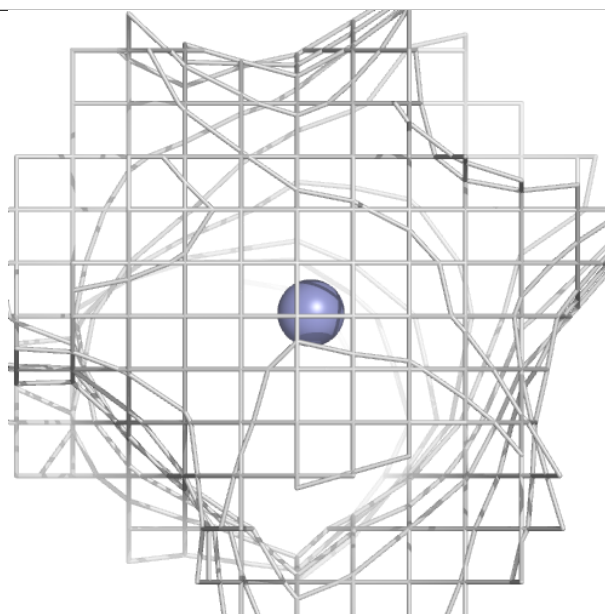
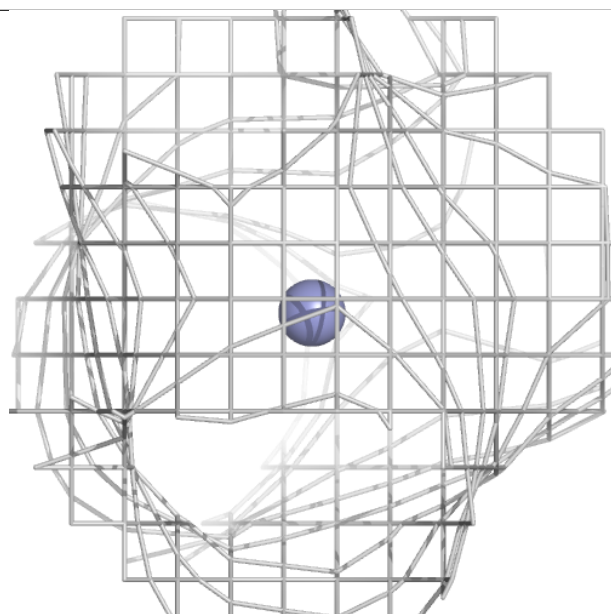
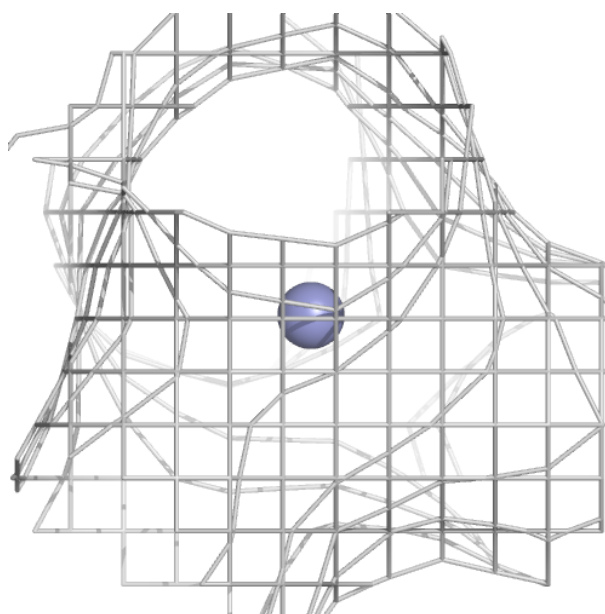
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and green (positive)



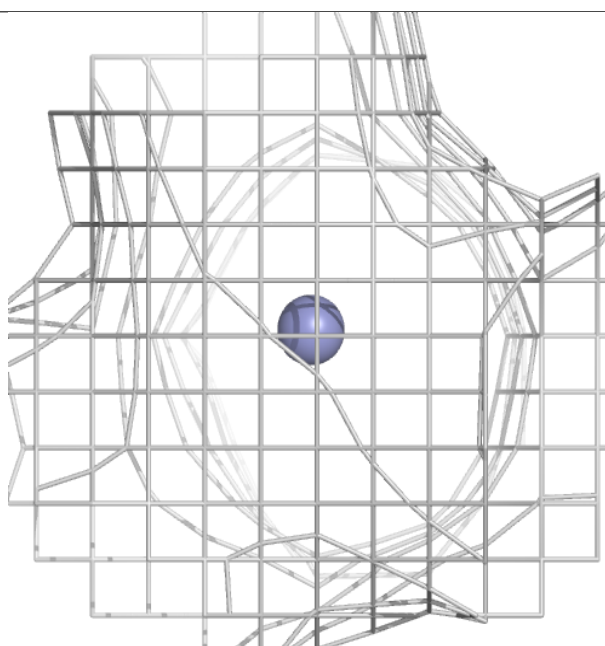
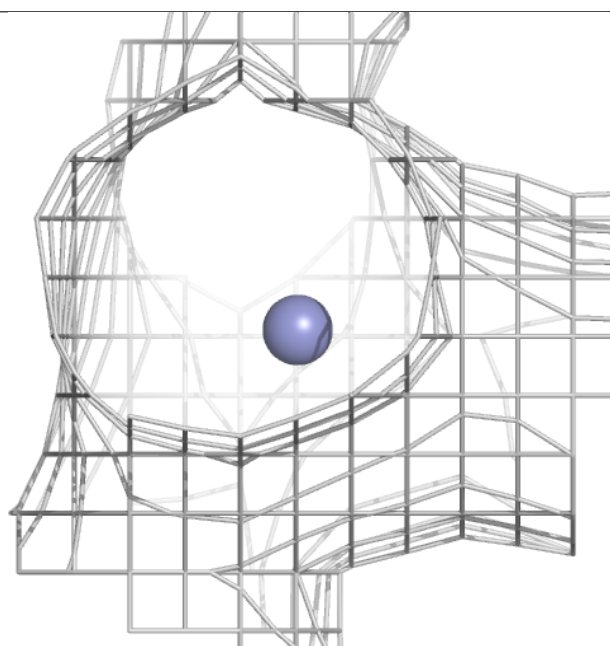
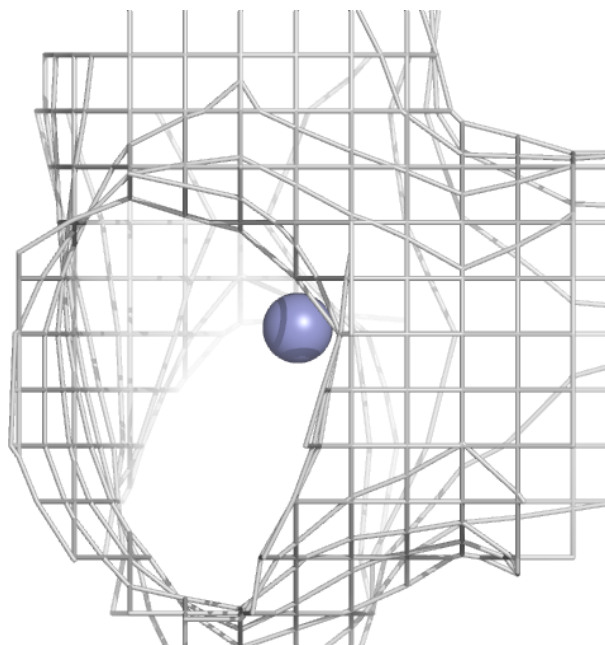
Electron density around ZN A 404:

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and green (positive)



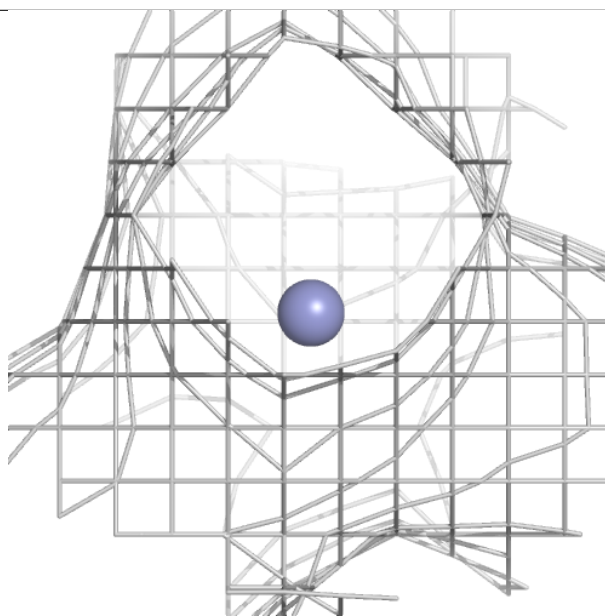
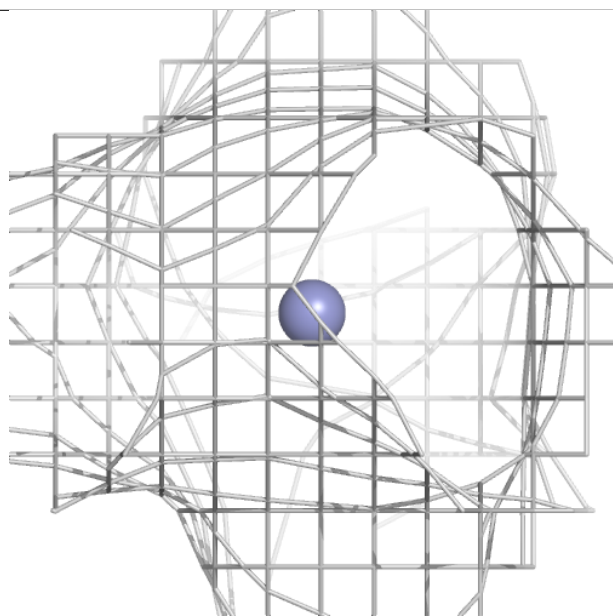
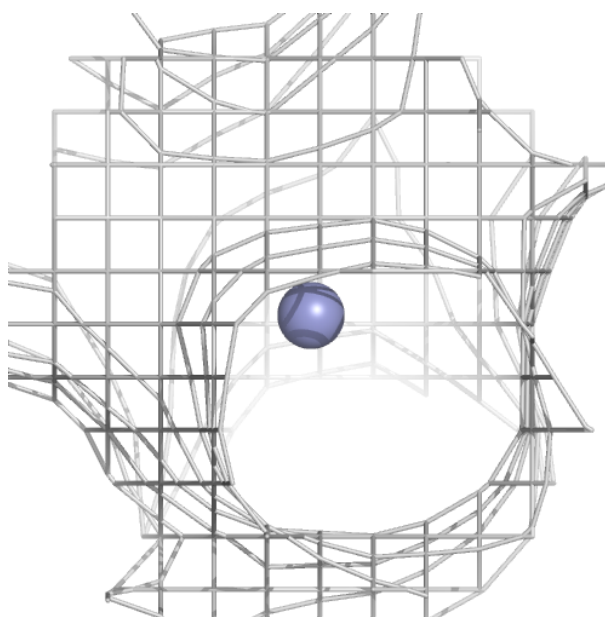
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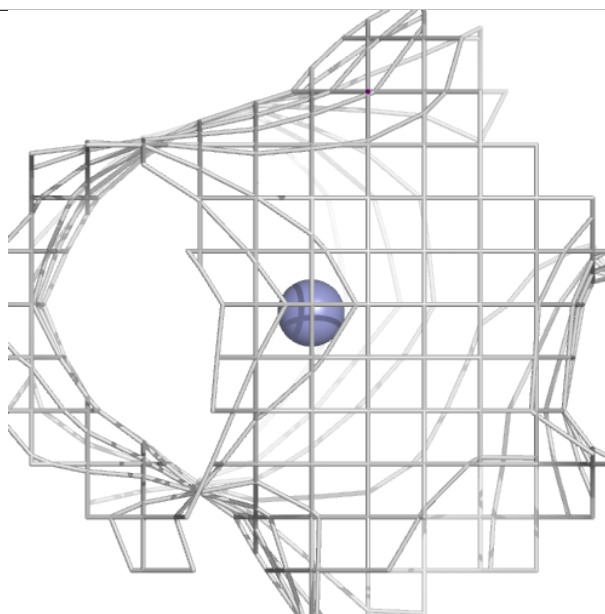
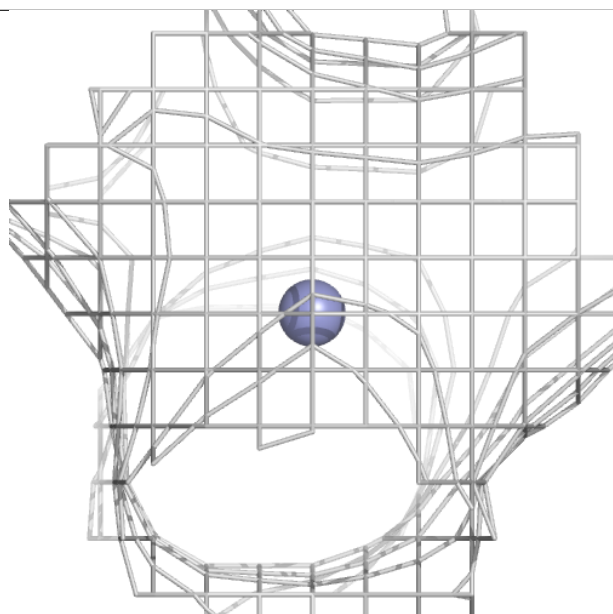
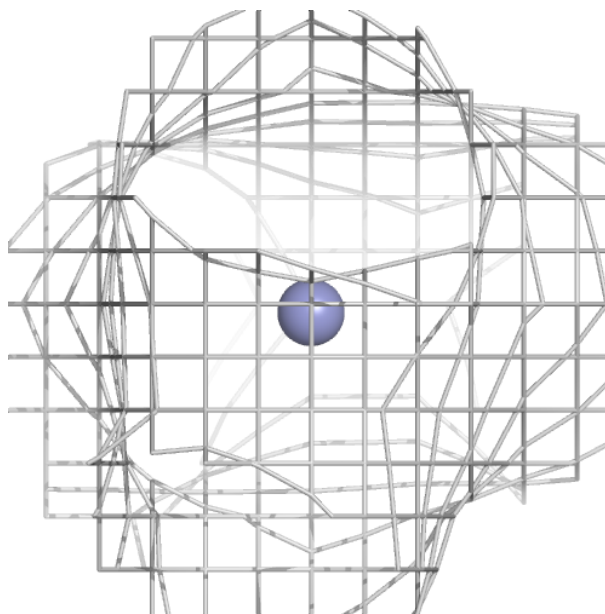
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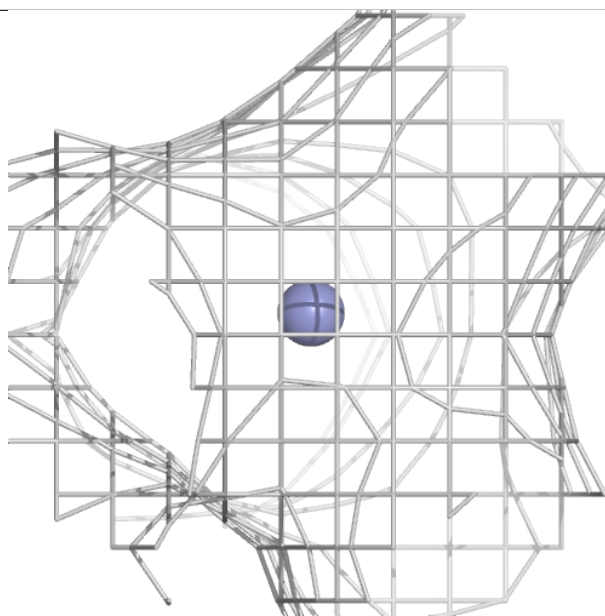
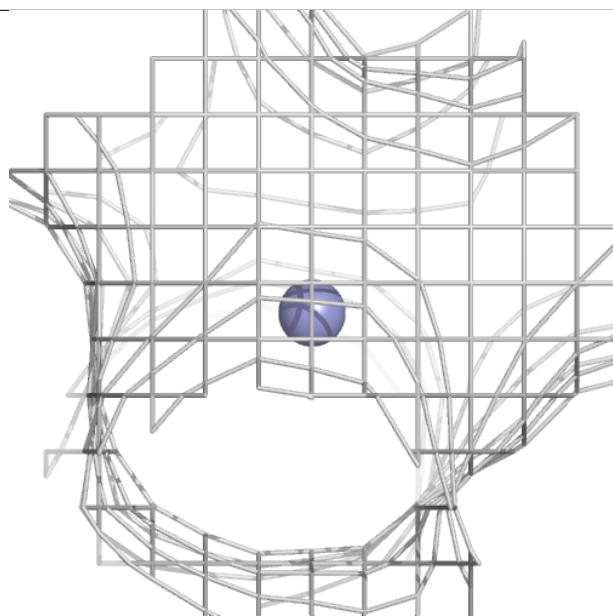
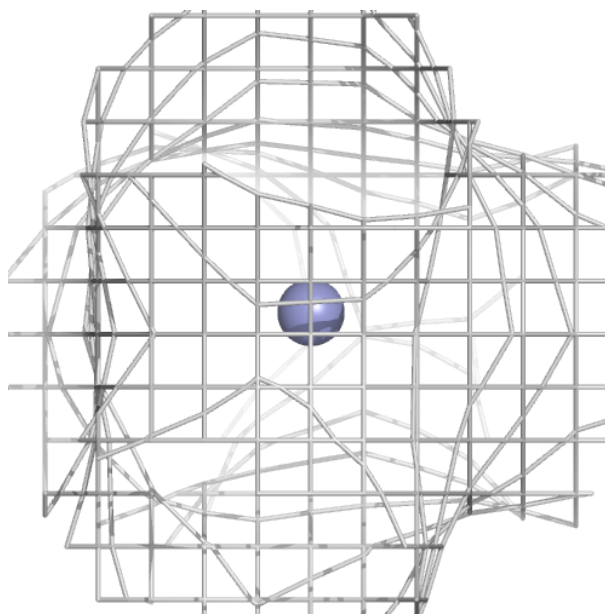
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and green (positive)



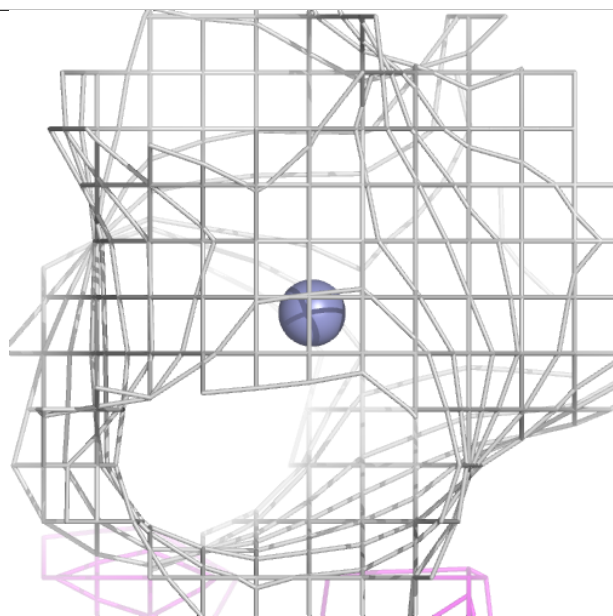
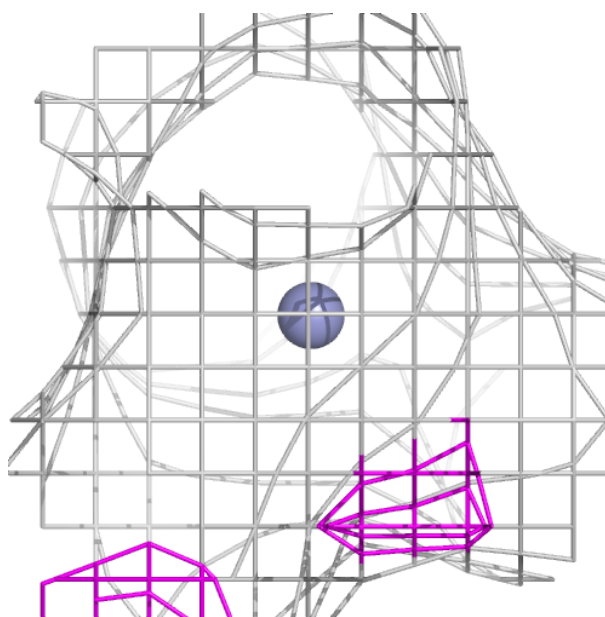
Electron density around ZN A 402:

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and green (positive)



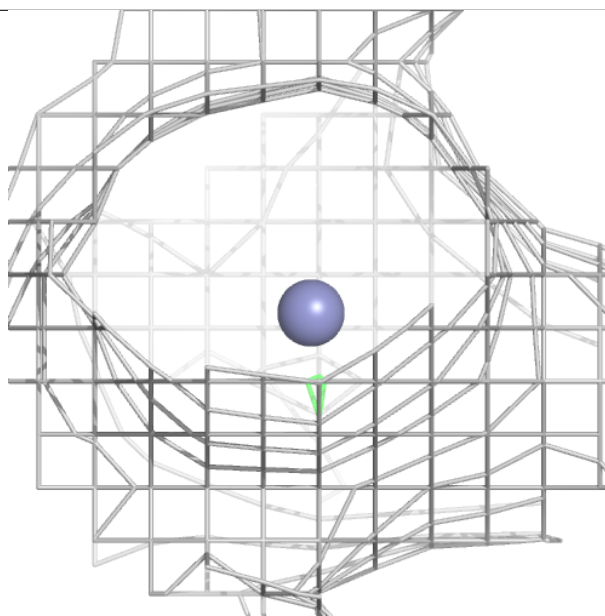
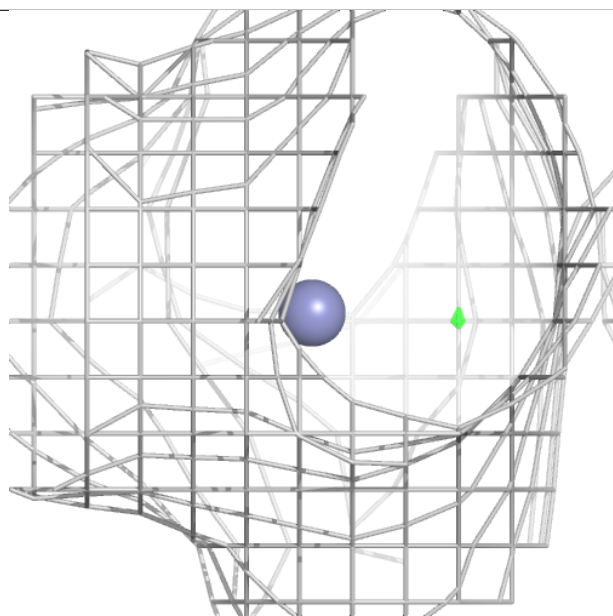
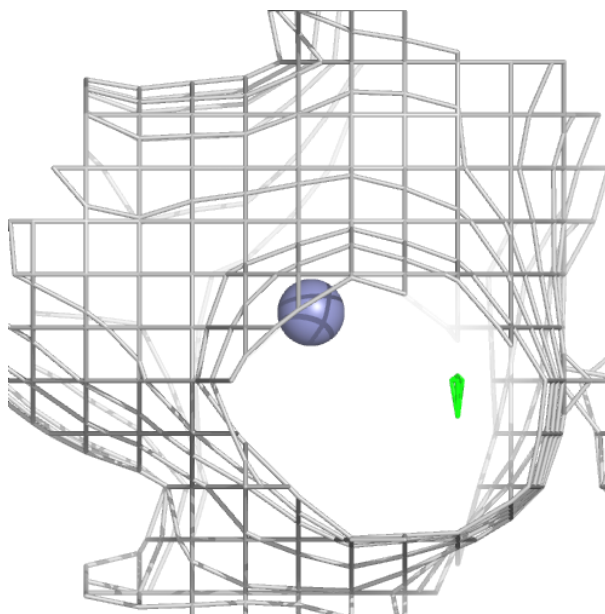
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and green (positive)



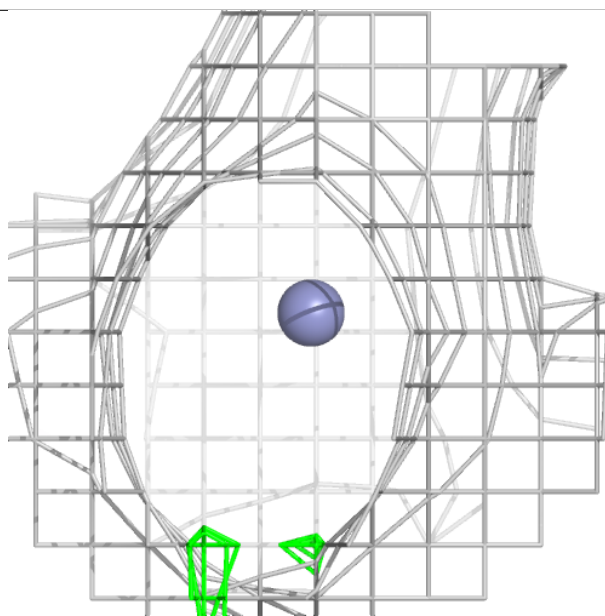
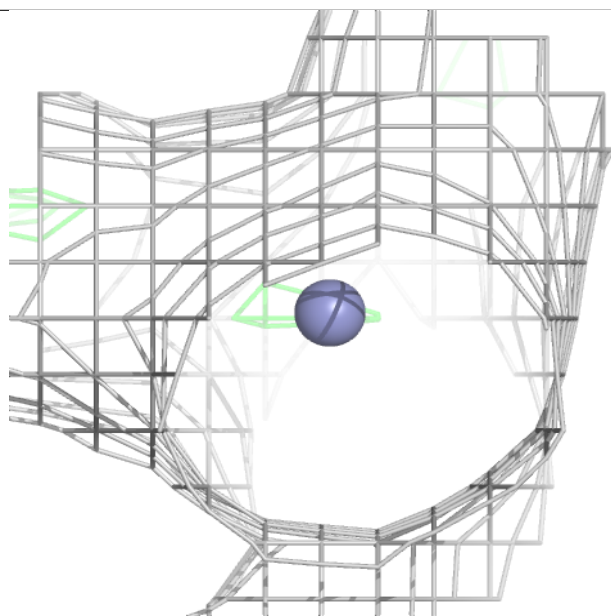
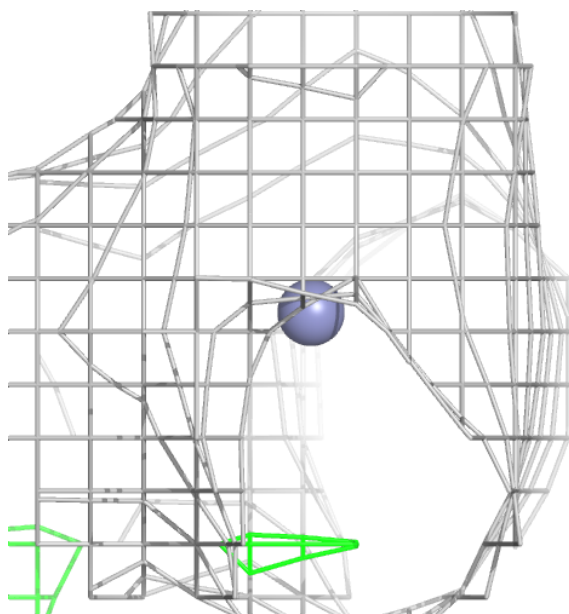
Electron density around ZN E 404:

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and green (positive)



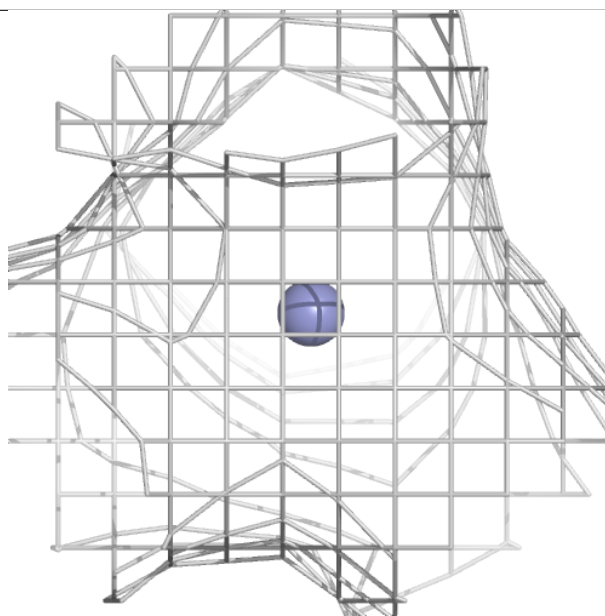
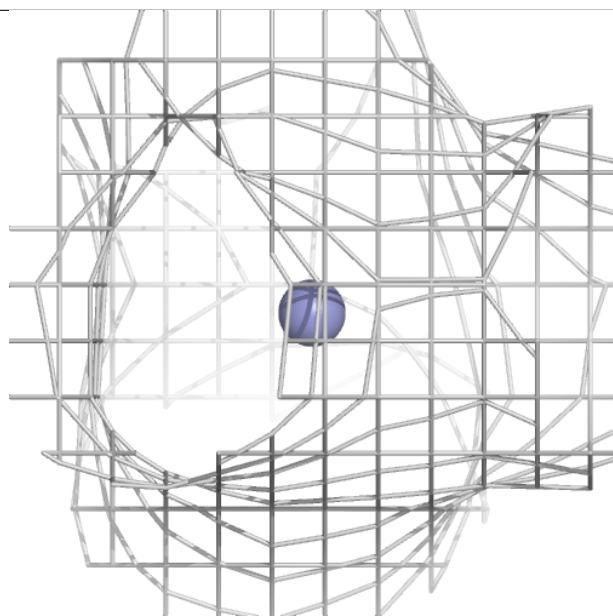
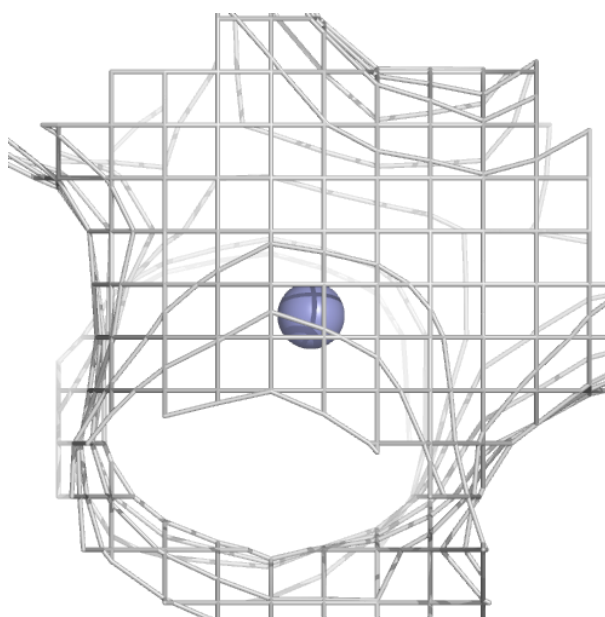
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and green (positive)



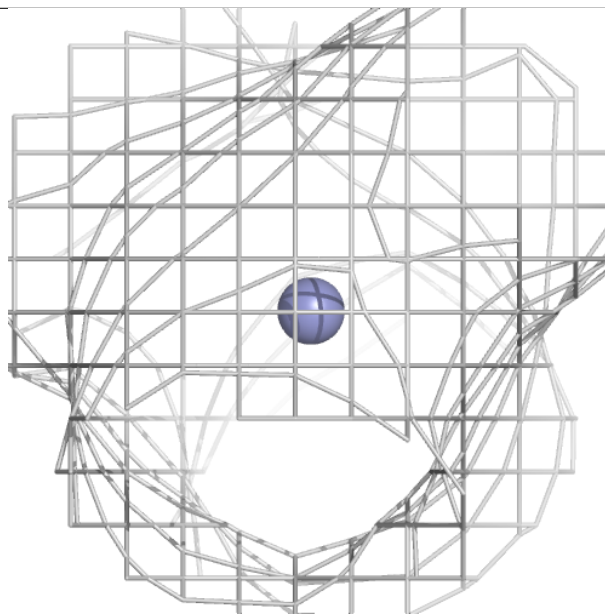
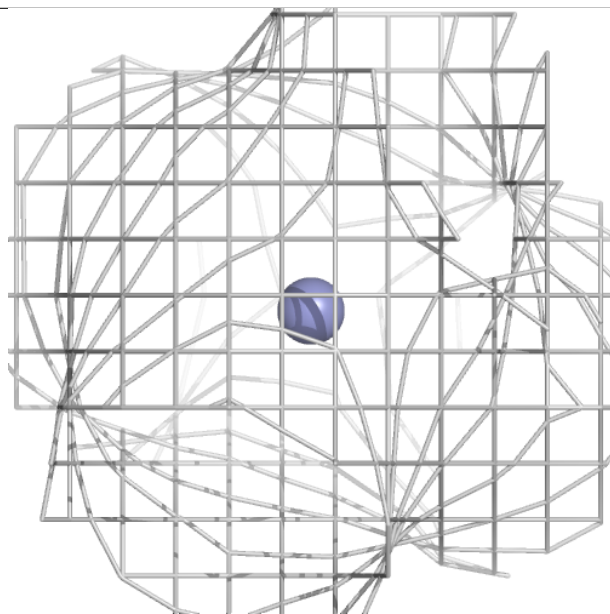
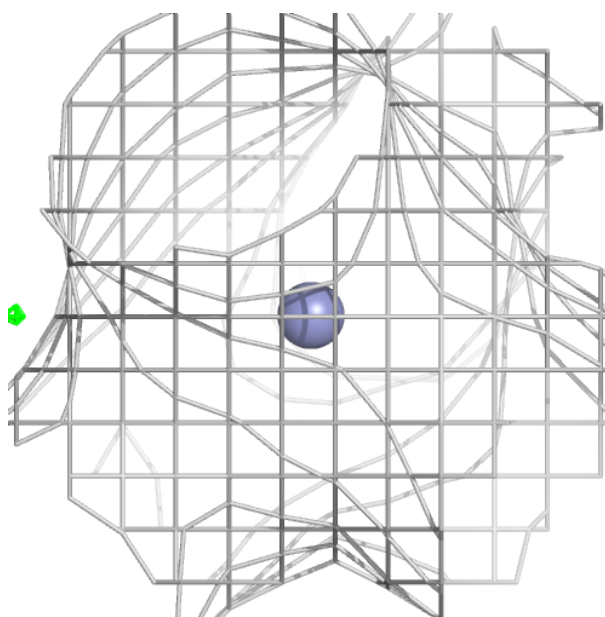
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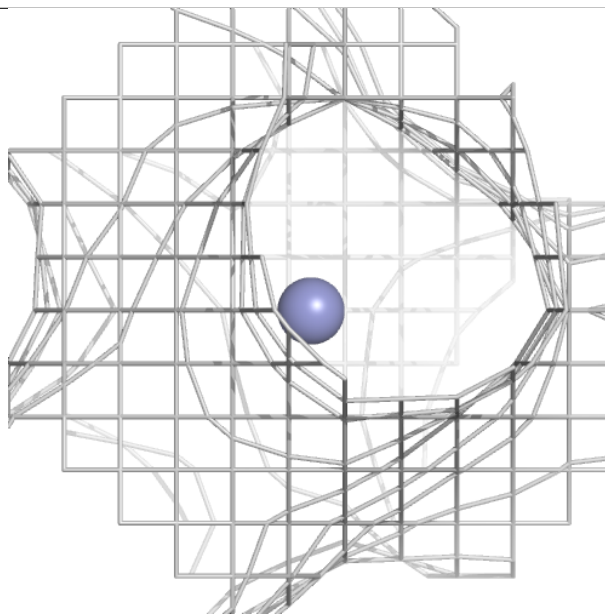
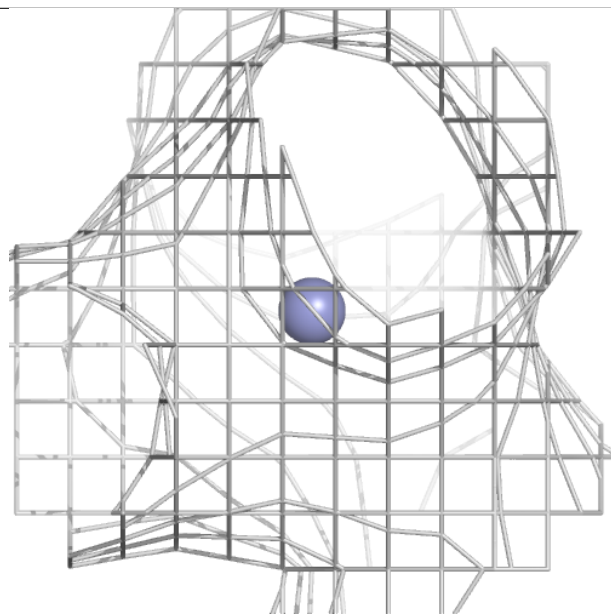
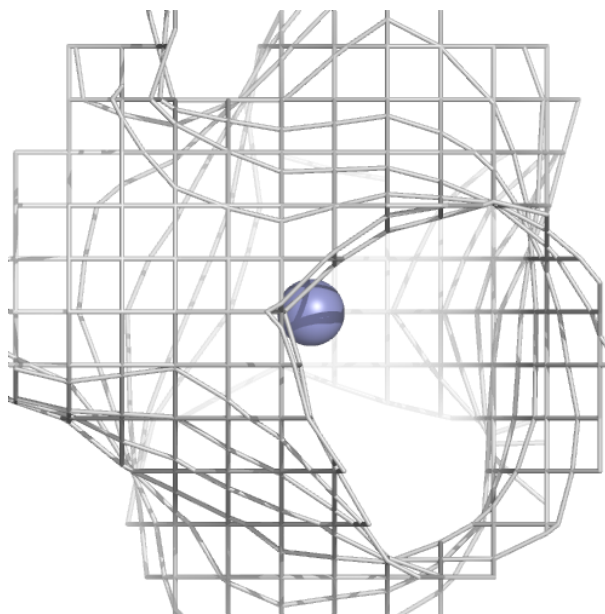
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and green (positive)



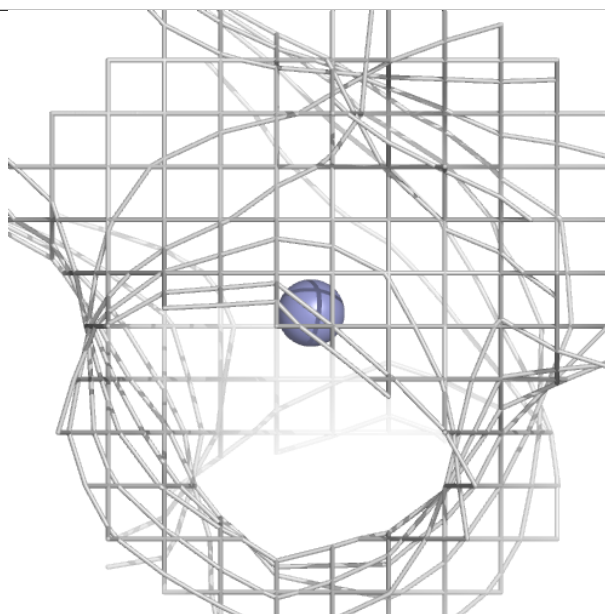
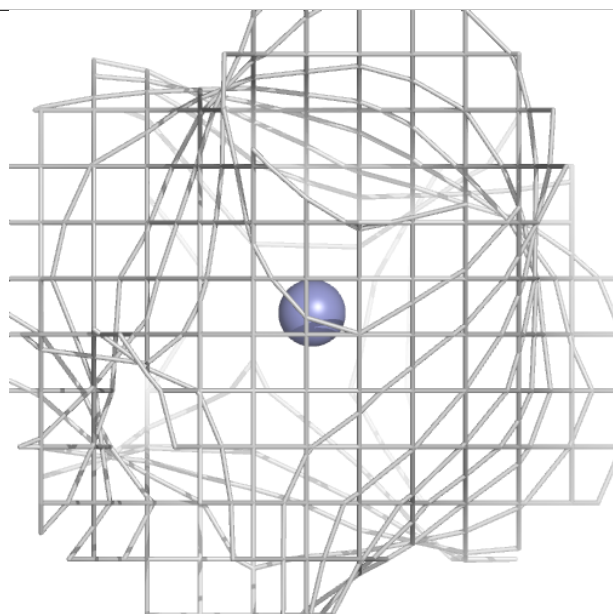
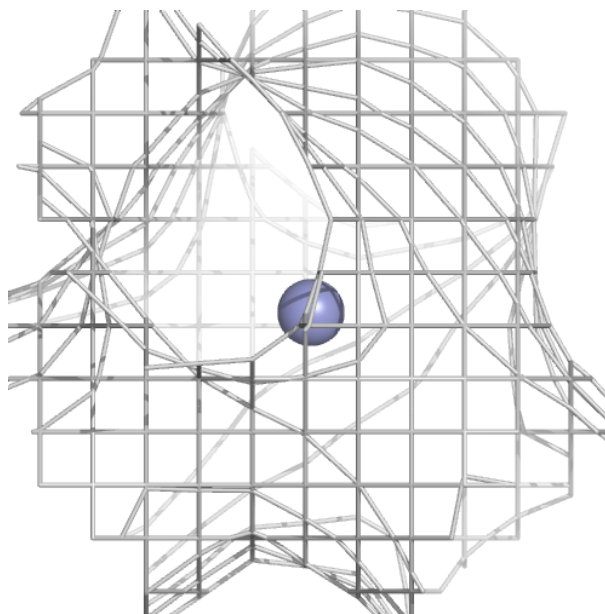
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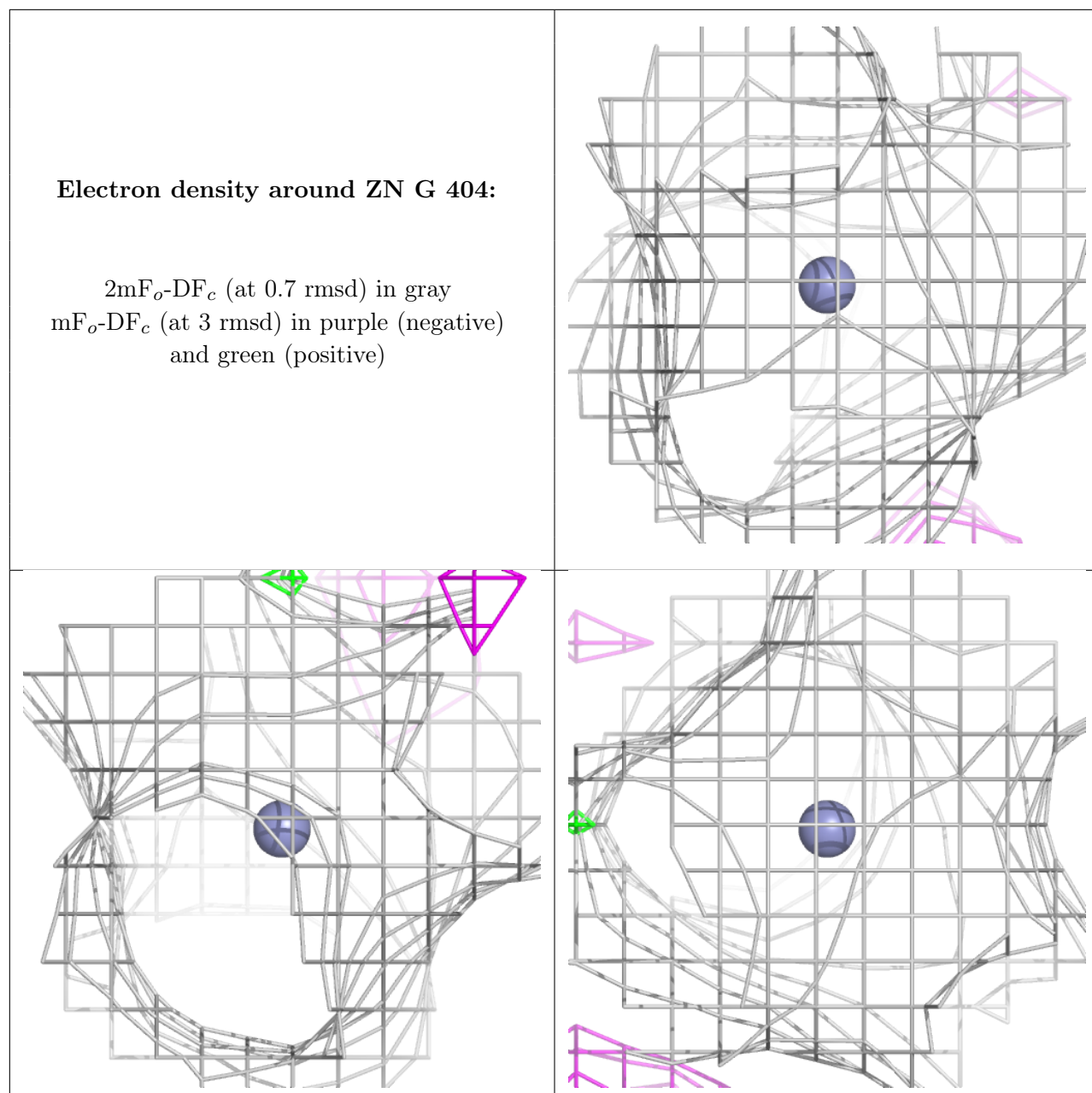
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and green (positive)



Electron density around ZN C 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.