# WORLDWIDE PDB PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 12:36 PM EDT

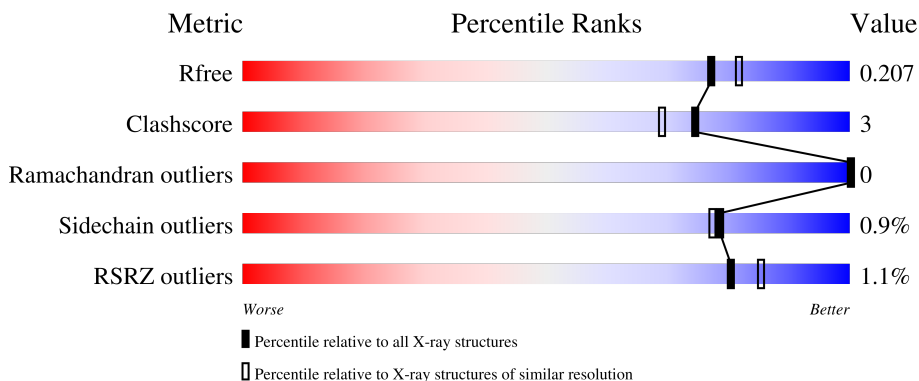| | | |
|---|---|---|
| PDB ID | : | 7TM9 |
| Title | : | Crystal structure of Bacterial alkaline phosphatase from Klebsiella pneumoniae |
| Authors | : | Seattle Structural Genomics Center for Infectious Disease (SSGCID) |
| Deposited on | : | 2022-01-19 |
| Resolution | : | 1.95 Å(reported) |

# 1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.95 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 | Percentile Ranks | Value |
|---|---|---|
| Rfree | | 0.207 |
| Clashscore | | 3 |
| Ramachandran outliers | | 0 |
| Sidechain outliers | | 0.9% |
| RSRZ outliers | | 1.1% |

*Worse*      *Better*

▊ Percentile relative to all X-ray structures

▉ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2580 (1.96-1.96) |
| Clashscore | 141614 | 2705 (1.96-1.96) |
| Ramachandran outliers | 138981 | 2678 (1.96-1.96) |
| Sidechain outliers | 138945 | 2678 (1.96-1.96) |
| RSRZ outliers | 127900 | 2539 (1.96-1.96) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 464 | 2%   89%   6%   5% |
| 1 | B | 464 | .%   88%   7%   5% |
| 1 | C | 464 | .%   90%   5%   5% |
| 1 | D | 464 | .%   87%   8%   5% |
| 1 | E | 464 | .%   88%   7%   5% |

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| Mol | Chain | Length | Quality of chain |
|:---:|:---:|:---:|:---|
| 1 | F | 464 | %<br>88%      7%   5% |
| 1 | G | 464 | %<br>87%      8%   5% |
| 1 | H | 464 | %<br>88%      7%   5% |

# 2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 29621 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 Bacterial alkaline phosphatase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 441 | Total<br>3228 | C<br>1992 | N<br>570 | O<br>654 | P<br>1 | S<br>11 | 0 | 0 | 0 |
| 1 | B | 441 | Total<br>3237 | C<br>1999 | N<br>569 | O<br>657 | P<br>1 | S<br>11 | 0 | 3 | 0 |
| 1 | C | 441 | Total<br>3238 | C<br>2000 | N<br>572 | O<br>654 | P<br>1 | S<br>11 | 0 | 2 | 0 |
| 1 | D | 441 | Total<br>3236 | C<br>1996 | N<br>570 | O<br>658 | P<br>1 | S<br>11 | 0 | 0 | 0 |
| 1 | E | 441 | Total<br>3229 | C<br>1993 | N<br>568 | O<br>656 | P<br>1 | S<br>11 | 0 | 1 | 0 |
| 1 | F | 441 | Total<br>3233 | C<br>1995 | N<br>572 | O<br>654 | P<br>1 | S<br>11 | 0 | 1 | 0 |
| 1 | G | 441 | Total<br>3241 | C<br>1998 | N<br>570 | O<br>661 | P<br>1 | S<br>11 | 0 | 2 | 0 |
| 1 | H | 441 | Total<br>3234 | C<br>1996 | N<br>570 | O<br>656 | P<br>1 | S<br>11 | 0 | 1 | 0 |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| A | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| A | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| A | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| A | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| A | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| A | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| A | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| B | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| B | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| B | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| B | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| B | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| B | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| B | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| B | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| C | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| C | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| C | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| C | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| C | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| C | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| C | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| C | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| D | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| D | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| D | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| D | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| D | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| D | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| D | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| D | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| E | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| E | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| E | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| E | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| E | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| E | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| E | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| E | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| F | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| F | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| F | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| F | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| F | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| F | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| F | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| F | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| G | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| G | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| G | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| G | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| G | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| G | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| G | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| G | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |
| H | 1 | MET | - | expression tag | UNP A0A0H3GK94 |
| H | 2 | ALA | - | expression tag | UNP A0A0H3GK94 |
| H | 3 | HIS | - | expression tag | UNP A0A0H3GK94 |
| H | 4 | HIS | - | expression tag | UNP A0A0H3GK94 |
| H | 5 | HIS | - | expression tag | UNP A0A0H3GK94 |
| H | 6 | HIS | - | expression tag | UNP A0A0H3GK94 |
| H | 7 | HIS | - | expression tag | UNP A0A0H3GK94 |
| H | 8 | HIS | - | expression tag | UNP A0A0H3GK94 |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 2 | A | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | B | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | C | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | D | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | E | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | F | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | G | 2 | Total 2 | Zn 2 | 0 | 0 |
| 2 | H | 2 | Total 2 | Zn 2 | 0 | 0 |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 3 | A | 1 | Total 1 | Mg 1 | 0 | 0 |
| 3 | B | 1 | Total 1 | Mg 1 | 0 | 0 |
| 3 | C | 1 | Total 1 | Mg 1 | 0 | 0 |
| 3 | D | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | E | 1 | Total 1 | Mg 1 | 0 | 0 |
| 3 | F | 1 | Total 1 | Mg 1 | 0 | 0 |
| 3 | G | 1 | Total 1 | Mg 1 | 0 | 0 |
| 3 | H | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | A | 424 | Total 424 | O 424 | 0 | 0 |
| 4 | B | 471 | Total 471 | O 471 | 0 | 0 |
| 4 | C | 454 | Total 454 | O 454 | 0 | 0 |
| 4 | D | 505 | Total 505 | O 505 | 0 | 0 |
| 4 | E | 469 | Total 469 | O 469 | 0 | 0 |
| 4 | F | 425 | Total 425 | O 425 | 0 | 0 |
| 4 | G | 524 | Total 524 | O 524 | 0 | 0 |
| 4 | H | 449 | Total 449 | O 449 | 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.
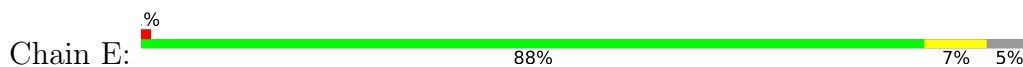
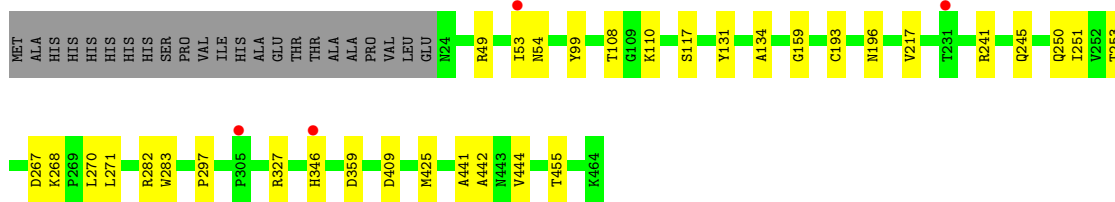- Molecule 1: Bacterial alkaline phosphatase
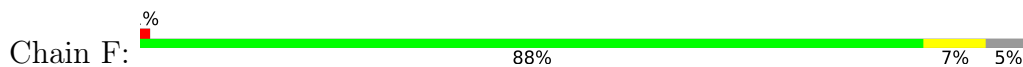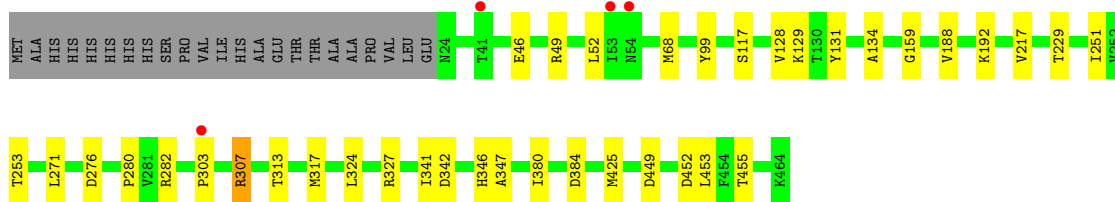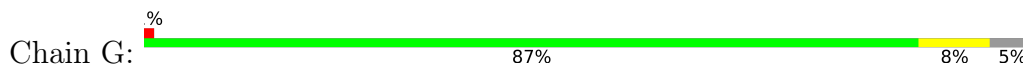


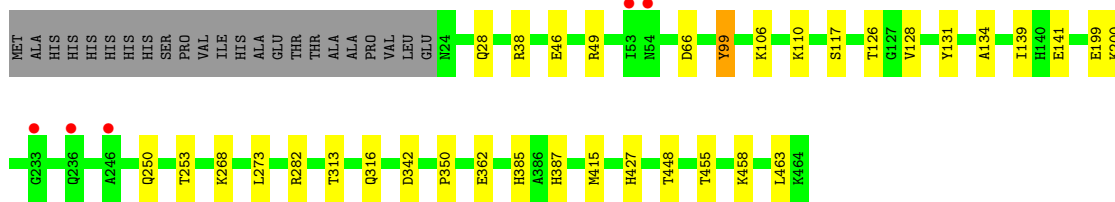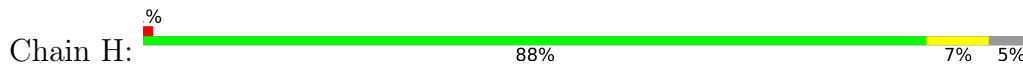- Molecule 1: Bacterial alkaline phosphatase



- Molecule 1: Bacterial alkaline phosphatase



- Molecule 1: Bacterial alkaline phosphatase

MET ALA HIS HIS HIS HIS HIS SER PRO VAL ILE HIS ALA GLU THR THR ALA ALA PRO VAL LEU GLU N24 R25 A50 S51 L52 I53 N54 K58 M68 F86 F87 K88 Y99 S117 A118 A134 K152 L156 P186 K203 R214 F226 A227 E228

L240 Q250 T253 E263 L270 R282 W283 K296 Q316 I341 D342 H346 N376 H387 A394 K397 V414 M425 T448 T455 K464

• Molecule 1: Bacterial alkaline phosphatase

Chain E:



MET ALA HIS HIS HIS HIS HIS SER PRO VAL ILE HIS ALA GLU THR THR ALA ALA PRO VAL LEU GLU N24 R38 T41 L48 R49 A50 S51 L52 I53 N54 K58 Y99 K110 S117 A121 W124 T125 T126 G127 V128 Y131 A134 L135 L148

G159 H177 V217 I251 L271 K296 T313 Q316 R327 N328 D342 H346 M425 T455 K464

• Molecule 1: Bacterial alkaline phosphatase

Chain F:



MET ALA HIS HIS HIS HIS HIS SER PRO VAL ILE HIS ALA GLU THR THR ALA ALA PRO VAL LEU GLU N24 R49 I53 N54 Y99 T108 G109 K110 S117 Y131 A134 G159 C193 N196 V217 T231 R241 Q245 Q250 I251 V252 T253

D267 K268 P269 L270 L271 R282 W283 P297 P305 R327 H346 D359 D409 M425 A441 A442 N443 V444 T455 K464

• Molecule 1: Bacterial alkaline phosphatase

Chain G:



MET ALA HIS HIS HIS HIS HIS SER PRO VAL ILE HIS ALA GLU THR THR ALA ALA PRO VAL LEU GLU N24 T41 E46 R49 L52 I53 N54 M68 Y99 S117 V128 K129 T130 Y131 A134 G159 V188 K192 V217 T229 I251 V252

T253 L271 D276 P280 V281 R282 P303 R307 T313 M317 L324 R327 I341 D342 H346 A347 I380 D384 M425 D449 D452 L453 F454 T455 K464

• Molecule 1: Bacterial alkaline phosphatase

Chain H:



MET ALA HIS HIS HIS HIS HIS SER PRO VAL ILE HIS ALA GLU THR THR ALA ALA PRO VAL LEU GLU N24 Q28 R38 E46 R49 I53 N54 D66 Y99 K106 K110 S117 T126 G127 V128 Y131 A134 I139 H140 E141 E199 K200

G233 Q236 A246 Q250 T253 K268 L273 R282 T313 Q316 D342 P350 E362 H385 A386 H387 M415 H427 T448 T455 K458 L463 K464

# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 71.95Å    240.60Å    101.48Å<br>90.00°    105.13°    90.00° | Depositor |
| Resolution (Å) | 46.09  –  1.95<br>49.66  –  1.95 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.9 (46.09-1.95)<br>97.7 (49.66-1.95) | Depositor<br>EDS |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.05 (at 1.95Å) | Xtriage |
| Refinement program | PHENIX 1.19.2_4158 | Depositor |
| R, $R_{free}$ | 0.172  ,  0.211<br>0.165  ,  0.207 | Depositor<br>DCC |
| $R_{free}$ test set | 11767 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 11.7 | Xtriage |
| Anisotropy | 0.454 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.35 , 52.7 | EDS |
| L-test for twinning[2] | $< |L| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o,F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 29621 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 15.0 | 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 56.01 % 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 2.9133e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

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

## 5   Model quality ⓘ

### 5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SEP, 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 | 0.50 | 0/3271 | 0.70 | 1/4446 (0.0%) |
| 1 | B | 0.52 | 0/3286 | 0.69 | 0/4469 |
| 1 | C | 0.53 | 0/3284 | 0.71 | 3/4464 (0.1%) |
| 1 | D | 0.52 | 0/3279 | 0.72 | 2/4456 (0.0%) |
| 1 | E | 0.52 | 0/3275 | 0.71 | 0/4454 |
| 1 | F | 0.51 | 0/3276 | 0.70 | 0/4453 |
| 1 | G | 0.54 | 0/3287 | 0.74 | 1/4470 (0.0%) |
| 1 | H | 0.52 | 0/3280 | 0.70 | 0/4458 |
| All | All | 0.52 | 0/26238 | 0.71 | 7/35670 (0.0%) |

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|-----|----------|-------|
| 1 | D | 342 | ASP | CB-CG-OD2 | -6.68 | 112.28 | 118.30 |
| 1 | C | 66 | ASP | CB-CG-OD2 | 6.10 | 123.79 | 118.30 |
| 1 | C | 99 | TYR | CA-CB-CG | 5.36 | 123.59 | 113.40 |
| 1 | D | 99 | TYR | CA-CB-CG | 5.33 | 123.53 | 113.40 |
| 1 | G | 384 | ASP | CB-CG-OD1 | 5.25 | 123.02 | 118.30 |

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 | 3228 | 0 | 3154 | 18 | 0 |
| 1 | B | 3237 | 0 | 3156 | 26 | 0 |
| 1 | C | 3238 | 0 | 3168 | 16 | 0 |
| 1 | D | 3236 | 0 | 3162 | 29 | 0 |
| 1 | E | 3229 | 0 | 3147 | 20 | 0 |
| 1 | F | 3233 | 0 | 3157 | 20 | 0 |
| 1 | G | 3241 | 0 | 3154 | 24 | 0 |
| 1 | H | 3234 | 0 | 3160 | 24 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 2 | C | 2 | 0 | 0 | 0 | 0 |
| 2 | D | 2 | 0 | 0 | 0 | 0 |
| 2 | E | 2 | 0 | 0 | 0 | 0 |
| 2 | F | 2 | 0 | 0 | 0 | 0 |
| 2 | G | 2 | 0 | 0 | 0 | 0 |
| 2 | H | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 424 | 0 | 0 | 3 | 0 |
| 4 | B | 471 | 0 | 0 | 9 | 0 |
| 4 | C | 454 | 0 | 0 | 5 | 0 |
| 4 | D | 505 | 0 | 0 | 5 | 0 |
| 4 | E | 469 | 0 | 0 | 5 | 0 |
| 4 | F | 425 | 0 | 0 | 2 | 0 |
| 4 | G | 524 | 0 | 0 | 7 | 0 |
| 4 | H | 449 | 0 | 0 | 4 | 0 |
| All | All | 29621 | 0 | 25258 | 163 | 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.

The worst 5 of 163 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:F:282:ARG:HG3 | 1:F:283:TRP:CD1 | 2.15 | 0.80 |
| 1:H:250:GLN:HG3 | 1:H:268:LYS:HE3 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:52:LEU:O | 1:F:49:ARG:NH2 | 2.30 | 0.65 |
| 1:H:110:LYS:HE2 | 4:H:673:HOH:O | 1.96 | 0.65 |
| 1:B:108:THR:HB | 4:B:1238:HOH:O | 1.95 | 0.65 |

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 | 438/464 (94%) | 431 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | B | 441/464 (95%) | 434 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | C | 440/464 (95%) | 434 (99%) | 6 (1%) | 0 | 100 | 100 |
| 1 | D | 438/464 (94%) | 433 (99%) | 5 (1%) | 0 | 100 | 100 |
| 1 | E | 439/464 (95%) | 434 (99%) | 5 (1%) | 0 | 100 | 100 |
| 1 | F | 439/464 (95%) | 433 (99%) | 6 (1%) | 0 | 100 | 100 |
| 1 | G | 440/464 (95%) | 436 (99%) | 4 (1%) | 0 | 100 | 100 |
| 1 | H | 439/464 (95%) | 435 (99%) | 4 (1%) | 0 | 100 | 100 |
| All | All | 3514/3712 (95%) | 3470 (99%) | 44 (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 | 328/352 (93%) | 325 (99%) | 3 (1%) | 78 | 77 |
| 1 | B | 329/352 (94%) | 327 (99%) | 2 (1%) | 86 | 85 |
| 1 | C | 329/352 (94%) | 326 (99%) | 3 (1%) | 78 | 77 |
| 1 | D | 330/352 (94%) | 327 (99%) | 3 (1%) | 78 | 77 |
| 1 | E | 328/352 (93%) | 324 (99%) | 4 (1%) | 71 | 68 |
| 1 | F | 328/352 (93%) | 325 (99%) | 3 (1%) | 78 | 77 |
| 1 | G | 330/352 (94%) | 326 (99%) | 4 (1%) | 71 | 68 |
| 1 | H | 329/352 (94%) | 327 (99%) | 2 (1%) | 86 | 85 |
| All | All | 2631/2816 (93%) | 2607 (99%) | 24 (1%) | 78 | 77 |

5 of 24 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 464 | LYS |
| 1 | F | 267 | ASP |
| 1 | F | 99 | TYR |
| 1 | G | 99 | TYR |
| 1 | C | 327 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 376 | ASN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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 | $\#\lvert Z\rvert > 2$ | Counts | RMSZ | $\#\lvert Z\rvert > 2$ |
| 1 | SEP | B | 117 | 1,2 | 8,9,10 | 1.64 | 2 (25%) | 8,12,14 | 1.57 | 1 (12%) |
| 1 | SEP | A | 117 | 1,2 | 8,9,10 | 1.63 | 2 (25%) | 8,12,14 | 1.58 | 2 (25%) |
| 1 | SEP | C | 117 | 1,2 | 8,9,10 | 1.56 | 1 (12%) | 8,12,14 | 1.47 | 3 (37%) |
| 1 | SEP | F | 117 | 1,2 | 8,9,10 | 1.75 | 1 (12%) | 8,12,14 | 1.13 | 0 |
| 1 | SEP | D | 117 | 1,2 | 8,9,10 | 1.78 | 1 (12%) | 8,12,14 | 1.09 | 1 (12%) |
| 1 | SEP | G | 117 | 1,2 | 8,9,10 | 1.73 | 1 (12%) | 8,12,14 | 1.67 | 2 (25%) |
| 1 | SEP | E | 117 | 1,2 | 8,9,10 | 1.59 | 1 (12%) | 8,12,14 | 1.63 | 2 (25%) |
| 1 | SEP | H | 117 | 1,2 | 8,9,10 | 1.60 | 1 (12%) | 8,12,14 | 1.61 | 2 (25%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | SEP | B | 117 | 1,2 | - | 1/5/8/10 | - |
| 1 | SEP | A | 117 | 1,2 | - | 1/5/8/10 | - |
| 1 | SEP | C | 117 | 1,2 | - | 0/5/8/10 | - |
| 1 | SEP | F | 117 | 1,2 | - | 0/5/8/10 | - |
| 1 | SEP | D | 117 | 1,2 | - | 1/5/8/10 | - |
| 1 | SEP | G | 117 | 1,2 | - | 1/5/8/10 | - |
| 1 | SEP | E | 117 | 1,2 | - | 1/5/8/10 | - |
| 1 | SEP | H | 117 | 1,2 | - | 1/5/8/10 | - |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | D | 117 | SEP | P-O1P | 3.94 | 1.63 | 1.50 |
| 1 | F | 117 | SEP | P-O1P | 3.73 | 1.62 | 1.50 |
| 1 | E | 117 | SEP | P-O1P | 3.51 | 1.61 | 1.50 |
| 1 | G | 117 | SEP | P-O1P | 3.39 | 1.61 | 1.50 |
| 1 | B | 117 | SEP | P-O1P | 3.07 | 1.60 | 1.50 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|----------|-------|----------------|-------------|
| 1 | B | 117 | SEP | OG-CB-CA | 3.70 | 111.74 | 108.14 |
| 1 | E | 117 | SEP | OG-CB-CA | 3.64 | 111.69 | 108.14 |
| 1 | A | 117 | SEP | OG-CB-CA | 3.39 | 111.45 | 108.14 |
| 1 | H | 117 | SEP | O2P-P-OG | -3.20 | 98.23 | 106.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | G | 117 | SEP | O2P-P-OG | -2.99 | 98.76 | 106.73 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 1 | A | 117 | SEP | CA-CB-OG-P |
| 1 | B | 117 | SEP | CA-CB-OG-P |
| 1 | D | 117 | SEP | CA-CB-OG-P |
| 1 | E | 117 | SEP | CA-CB-OG-P |
| 1 | G | 117 | SEP | CA-CB-OG-P |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

# 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, $95^{th}$ 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(Å²) | Q<0.9 |
|-----|-------|----------|--------|---------|-----|-----|----------|-------|
| 1 | A | 440/464 (94%) | 0.11 | 8 (1%) | 68 | 76 | 6, 13, 27, 40 | 0 |
| 1 | B | 440/464 (94%) | -0.02 | 3 (0%) | 87 | 92 | 5, 11, 25, 47 | 0 |
| 1 | C | 440/464 (94%) | 0.03 | 6 (1%) | 75 | 82 | 5, 12, 24, 37 | 0 |
| 1 | D | 440/464 (94%) | -0.04 | 4 (0%) | 84 | 89 | 5, 11, 25, 41 | 0 |
| 1 | E | 440/464 (94%) | -0.02 | 5 (1%) | 80 | 85 | 5, 13, 26, 46 | 0 |
| 1 | F | 440/464 (94%) | 0.04 | 4 (0%) | 84 | 89 | 6, 13, 27, 41 | 0 |
| 1 | G | 440/464 (94%) | -0.08 | 4 (0%) | 84 | 89 | 4, 11, 24, 39 | 0 |
| 1 | H | 440/464 (94%) | 0.03 | 5 (1%) | 80 | 85 | 5, 13, 28, 37 | 0 |
| All | All | 3520/3712 (94%) | 0.01 | 39 (1%) | 80 | 85 | 4, 12, 27, 47 | 0 |

The worst 5 of 39 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 53 | ILE | 4.7 |
| 1 | B | 53 | ILE | 4.5 |
| 1 | G | 54 | ASN | 3.8 |
| 1 | F | 305 | PRO | 3.7 |
| 1 | A | 53 | ILE | 3.4 |

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

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, $95^{th}$ 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(Å²) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|---------------|-------|
| 1 | SEP | F | 117 | 10/11 | 0.83 | 0.19 | 4,13,27,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å²) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|---------------|-------|
| 1 | SEP | H | 117 | 10/11 | 0.85 | 0.19 | 9,15,25,27 | 0 |
| 1 | SEP | D | 117 | 10/11 | 0.86 | 0.15 | 6,10,28,31 | 0 |
| 1 | SEP | A | 117 | 10/11 | 0.87 | 0.17 | 6,14,25,27 | 0 |
| 1 | SEP | B | 117 | 10/11 | 0.87 | 0.16 | 5,11,26,27 | 0 |
| 1 | SEP | C | 117 | 10/11 | 0.87 | 0.17 | 5,14,29,30 | 0 |
| 1 | SEP | G | 117 | 10/11 | 0.88 | 0.15 | 5,12,22,30 | 0 |
| 1 | SEP | E | 117 | 10/11 | 0.88 | 0.15 | 5,10,25,25 | 0 |

## 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, $95^{th}$ 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(Å²) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|---------------|-------|
| 3 | MG | F | 503 | 1/1 | 0.93 | 0.08 | 13,13,13,13 | 0 |
| 3 | MG | A | 503 | 1/1 | 0.94 | 0.05 | 14,14,14,14 | 0 |
| 3 | MG | H | 503 | 1/1 | 0.95 | 0.06 | 12,12,12,12 | 0 |
| 3 | MG | D | 503 | 1/1 | 0.96 | 0.09 | 8,8,8,8 | 0 |
| 2 | ZN | B | 501 | 1/1 | 0.97 | 0.11 | 37,37,37,37 | 0 |
| 2 | ZN | C | 502 | 1/1 | 0.97 | 0.11 | 39,39,39,39 | 0 |
| 2 | ZN | F | 501 | 1/1 | 0.97 | 0.17 | 41,41,41,41 | 0 |
| 2 | ZN | F | 502 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 2 | ZN | B | 502 | 1/1 | 0.98 | 0.08 | 32,32,32,32 | 0 |
| 2 | ZN | H | 501 | 1/1 | 0.98 | 0.14 | 38,38,38,38 | 0 |
| 2 | ZN | C | 501 | 1/1 | 0.98 | 0.18 | 42,42,42,42 | 0 |
| 3 | MG | C | 503 | 1/1 | 0.98 | 0.04 | 8,8,8,8 | 0 |
| 2 | ZN | A | 502 | 1/1 | 0.98 | 0.10 | 34,34,34,34 | 0 |
| 3 | MG | E | 503 | 1/1 | 0.98 | 0.04 | 7,7,7,7 | 0 |
| 2 | ZN | D | 502 | 1/1 | 0.98 | 0.10 | 33,33,33,33 | 0 |
| 2 | ZN | A | 501 | 1/1 | 0.98 | 0.17 | 39,39,39,39 | 0 |
| 2 | ZN | D | 501 | 1/1 | 0.99 | 0.12 | 42,42,42,42 | 0 |
| 3 | MG | B | 503 | 1/1 | 0.99 | 0.07 | 10,10,10,10 | 0 |
| 2 | ZN | E | 501 | 1/1 | 0.99 | 0.13 | 36,36,36,36 | 0 |
| 2 | ZN | G | 501 | 1/1 | 0.99 | 0.13 | 34,34,34,34 | 0 |
| 2 | ZN | G | 502 | 1/1 | 0.99 | 0.10 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors($Å^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------------------|-------|
| 2 | ZN | E | 502 | 1/1 | 0.99 | 0.08 | 31,31,31,31 | 0 |
| 3 | MG | G | 503 | 1/1 | 0.99 | 0.04 | 8,8,8,8 | 0 |
| 2 | ZN | H | 502 | 1/1 | 0.99 | 0.13 | 37,37,37,37 | 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.
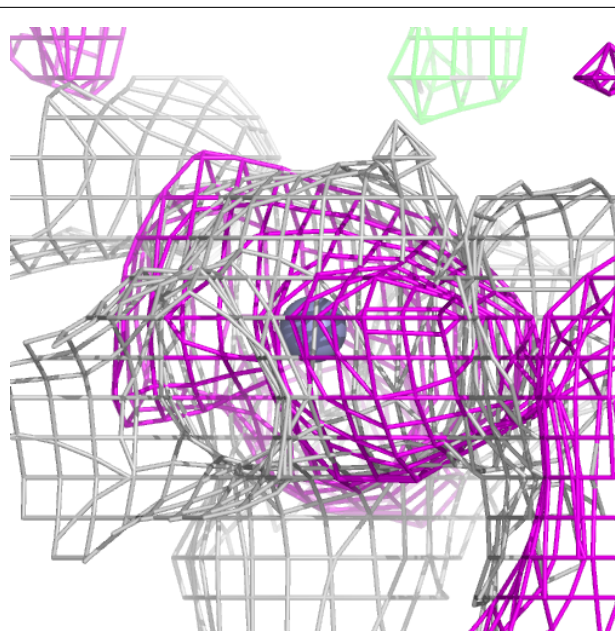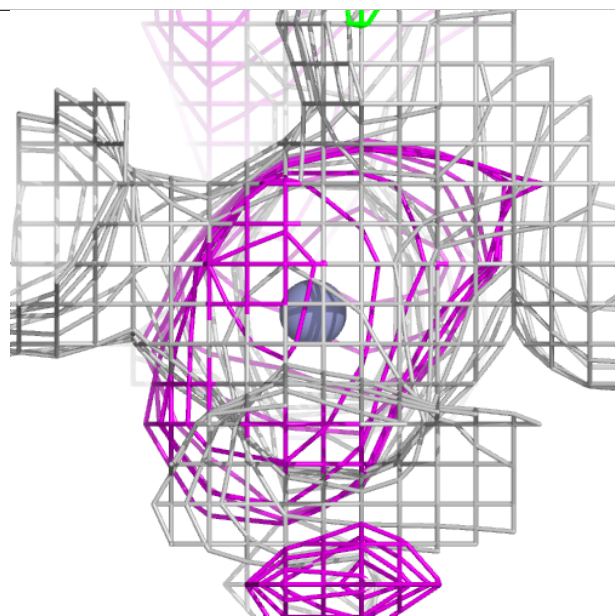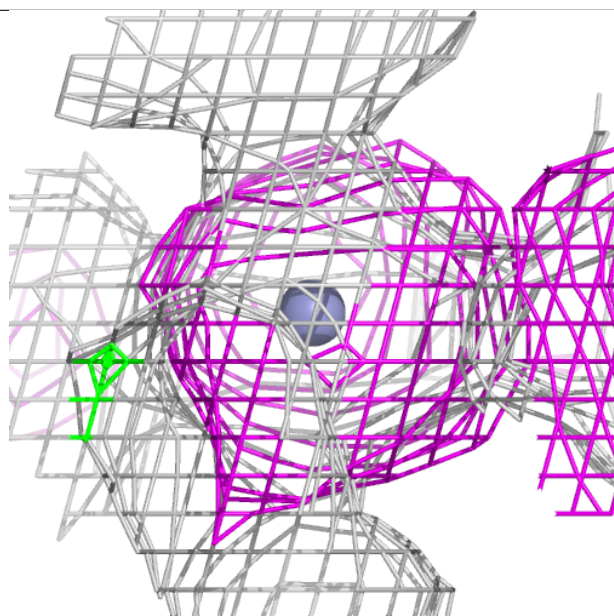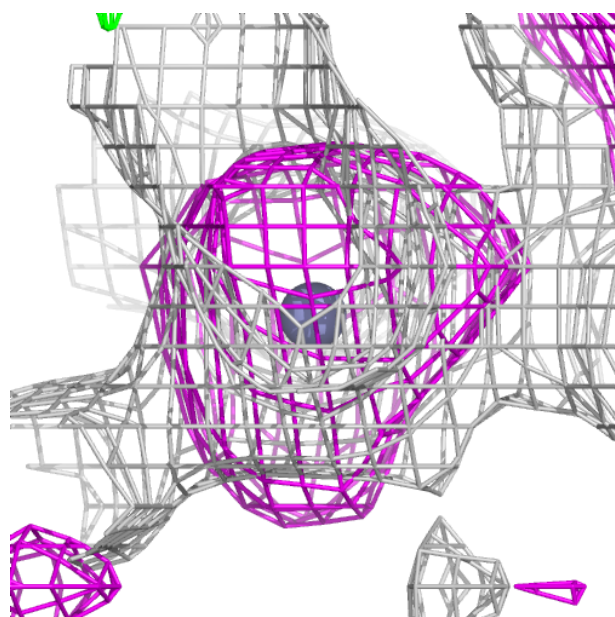


**Electron density around ZN B 501:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
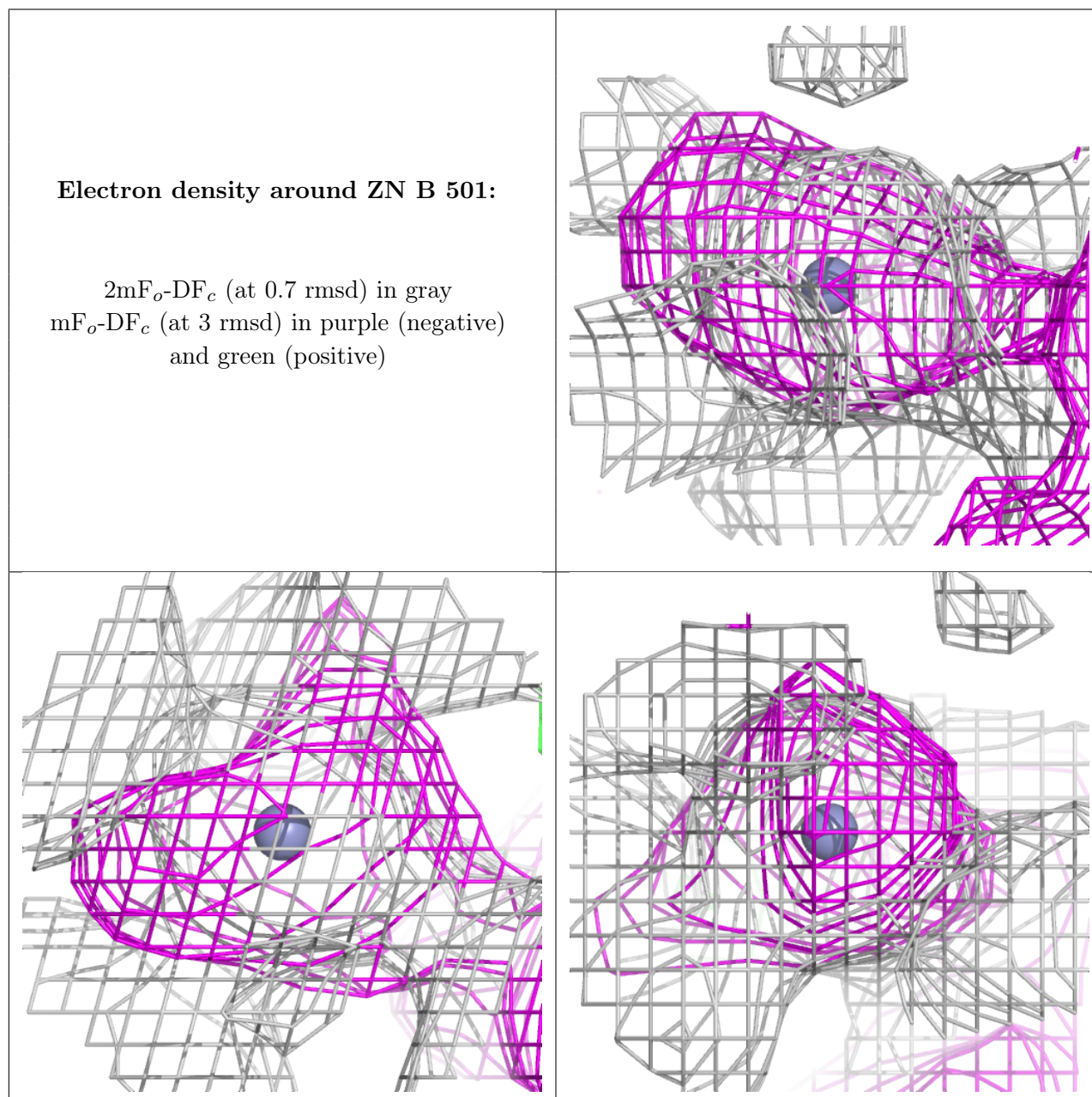
**Electron density around ZN C 502:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
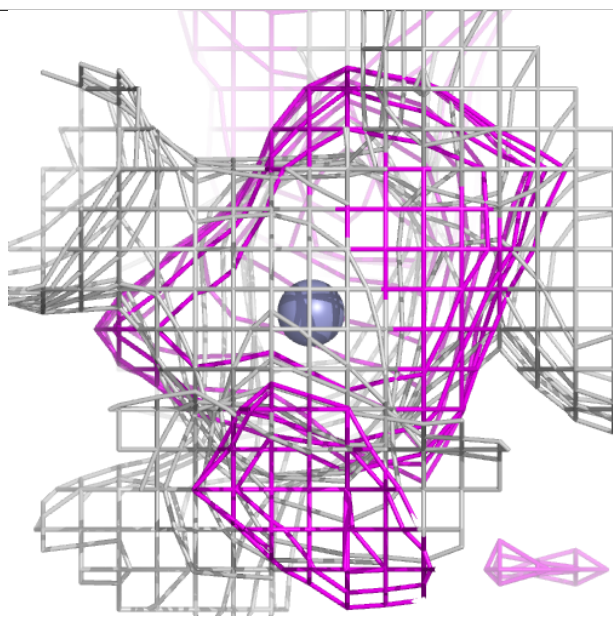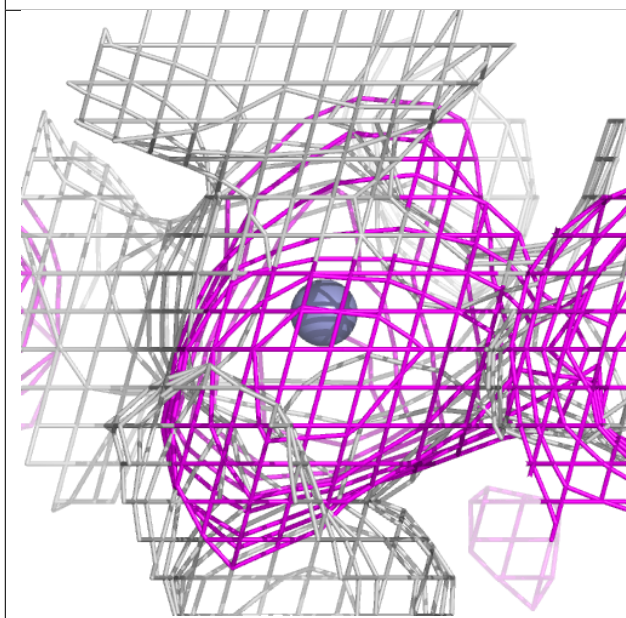and green (positive)
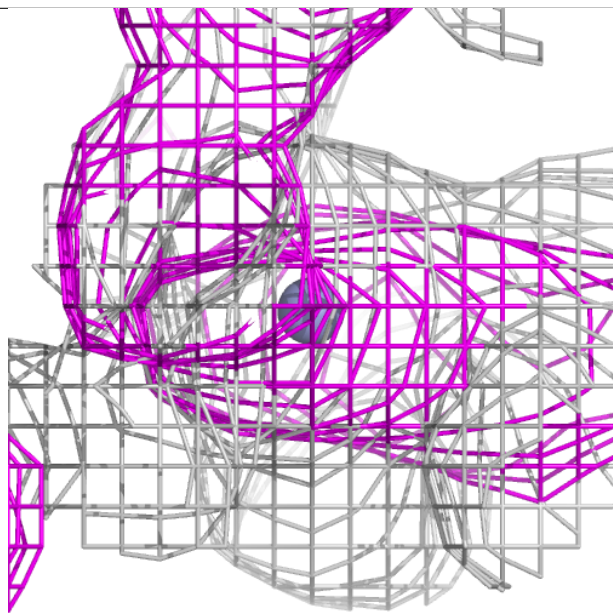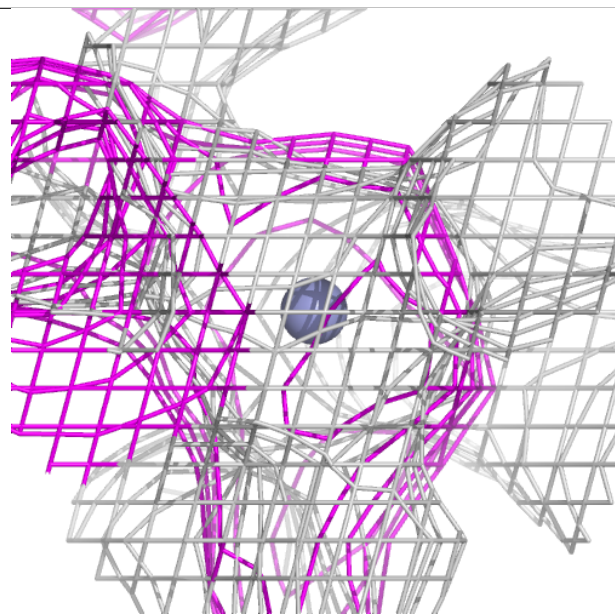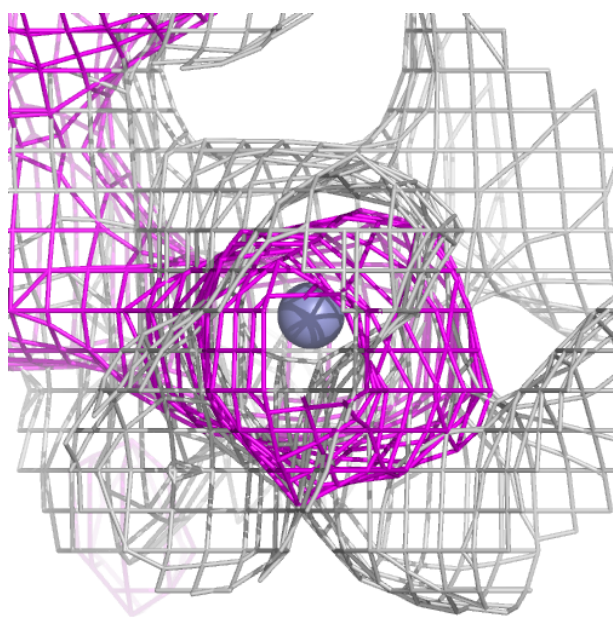
**Electron density around ZN F 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
$mF_o-DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
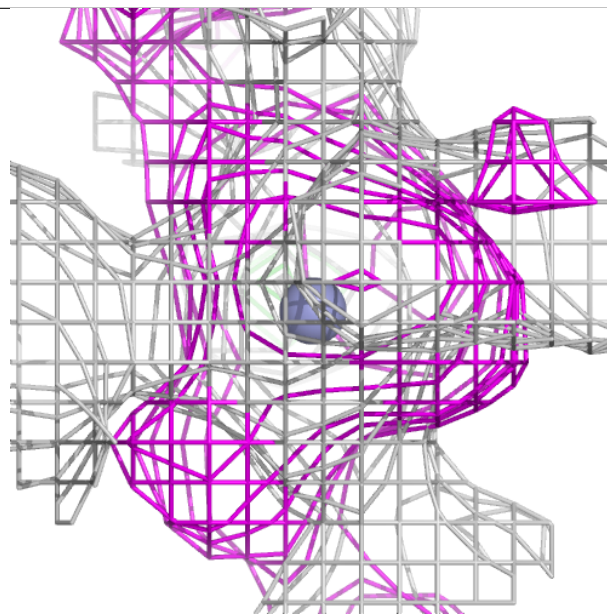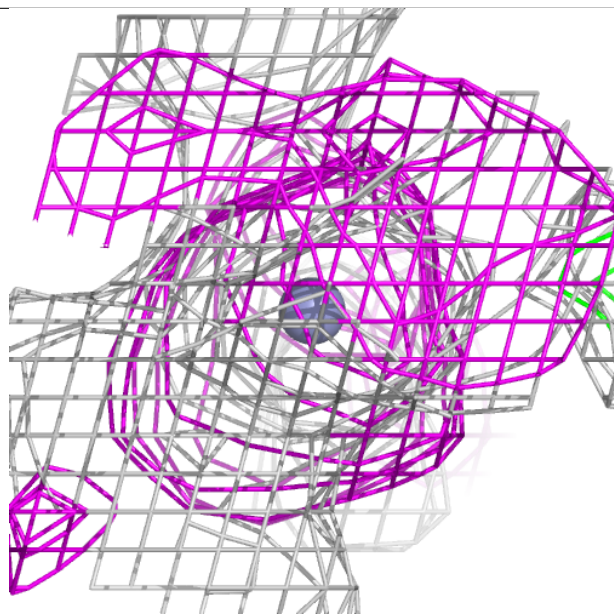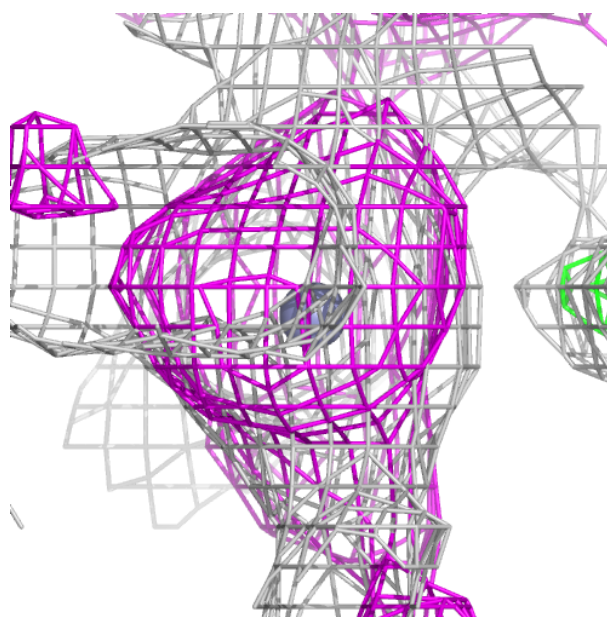
**Electron density around ZN F 502:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
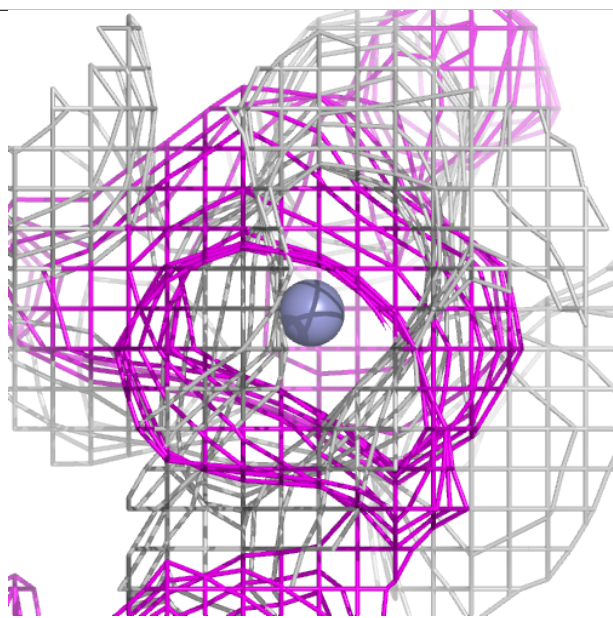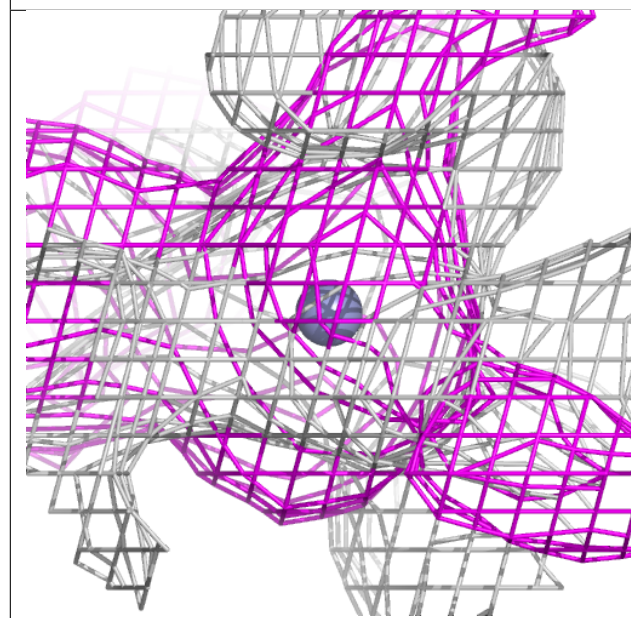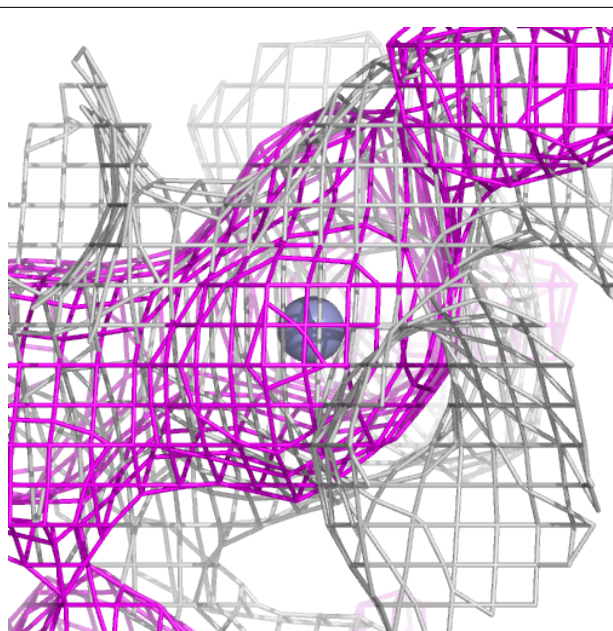
**Electron density around ZN B 502:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
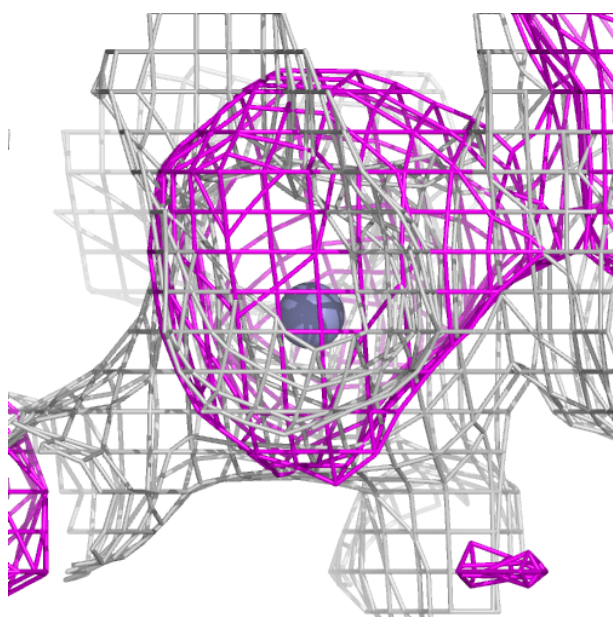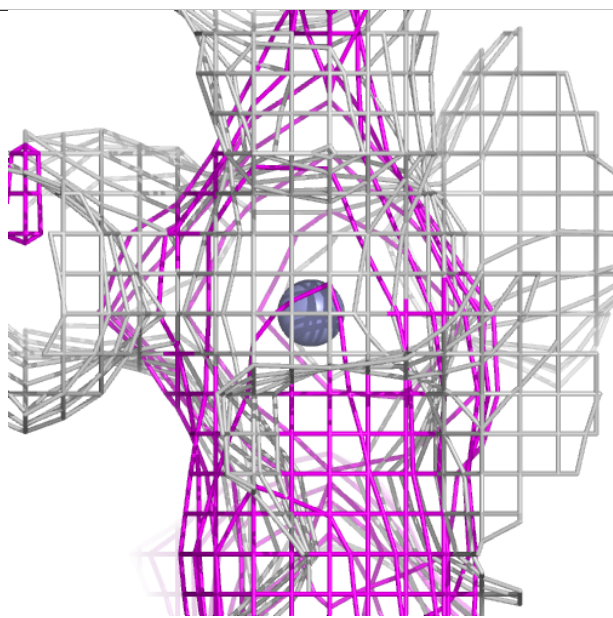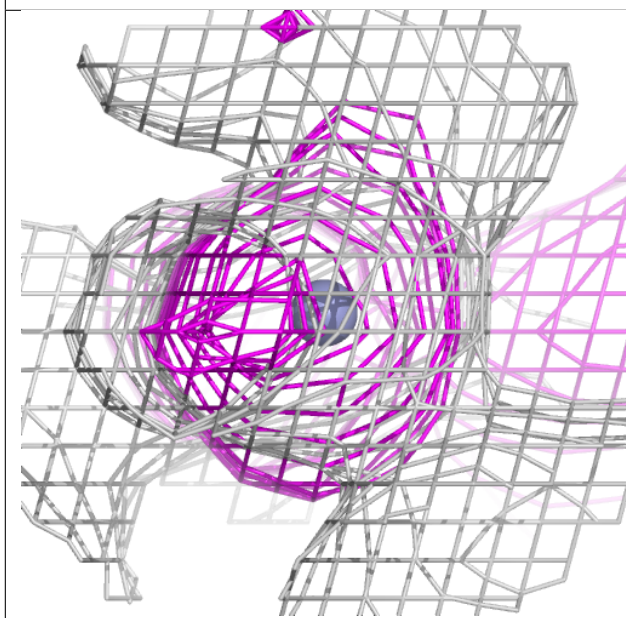and green (positive)
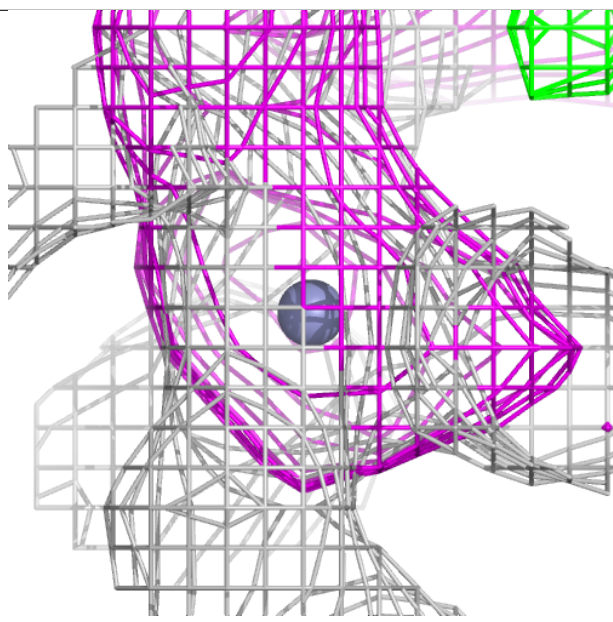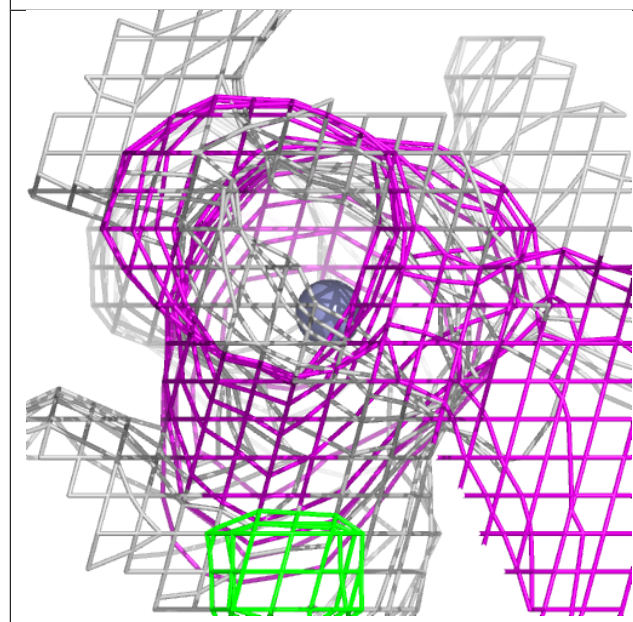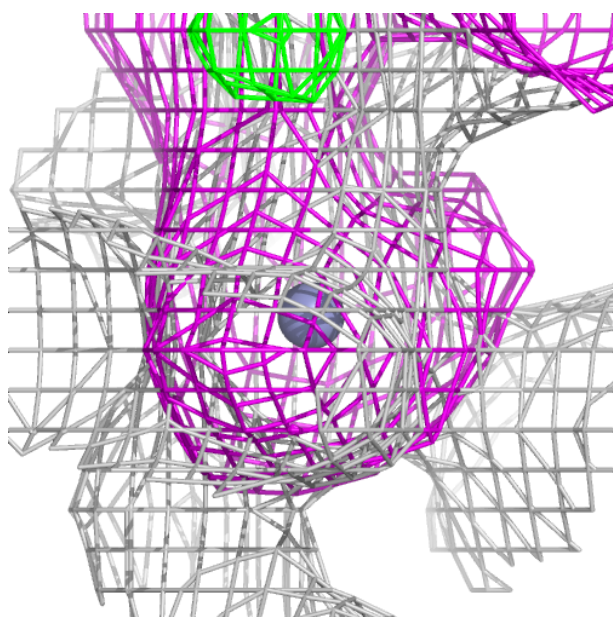
**Electron density around ZN H 501:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
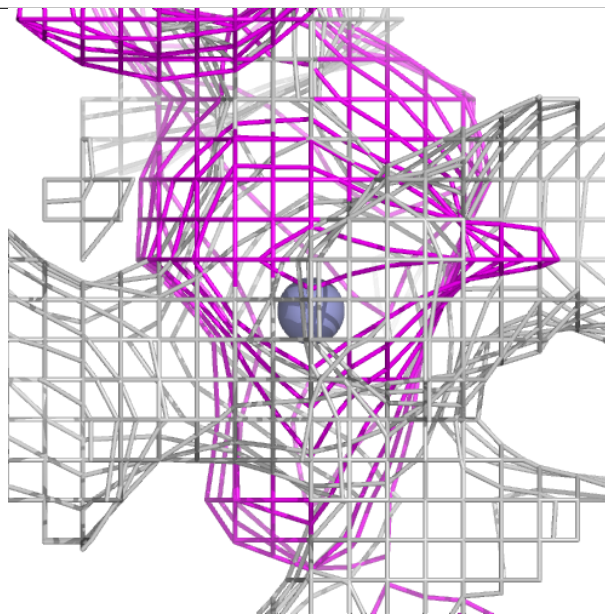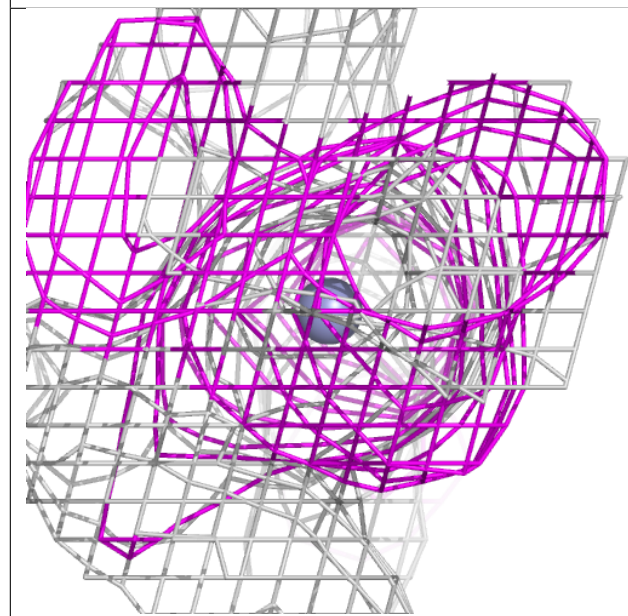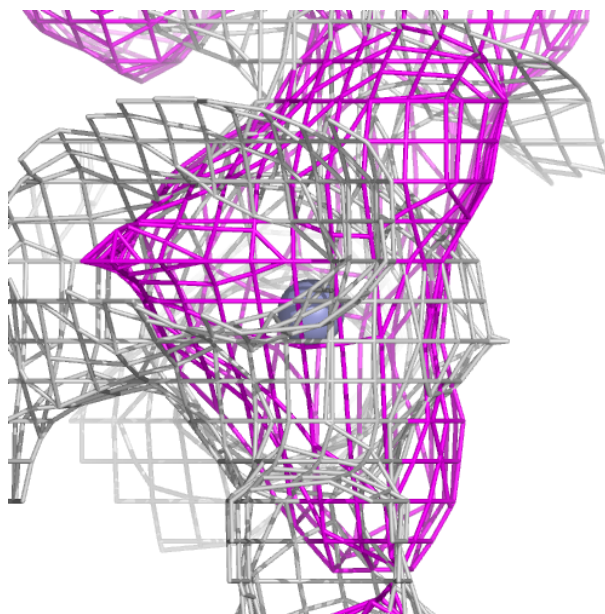
**Electron density around ZN C 501:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
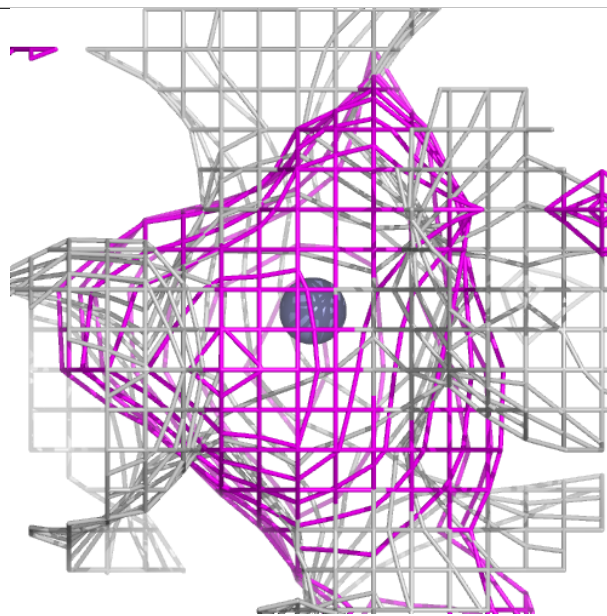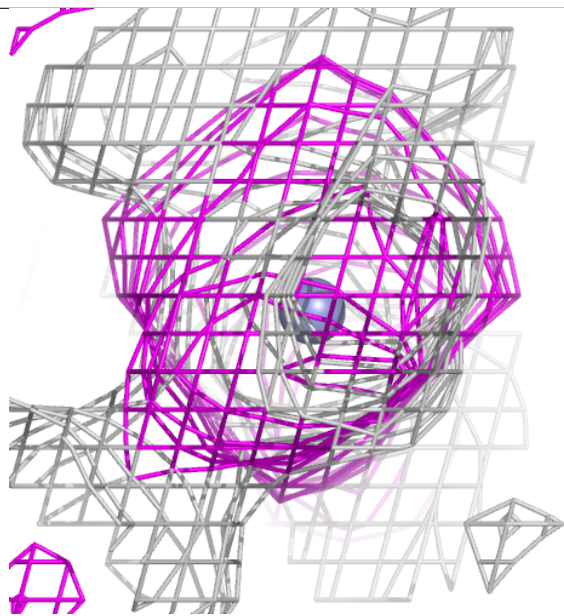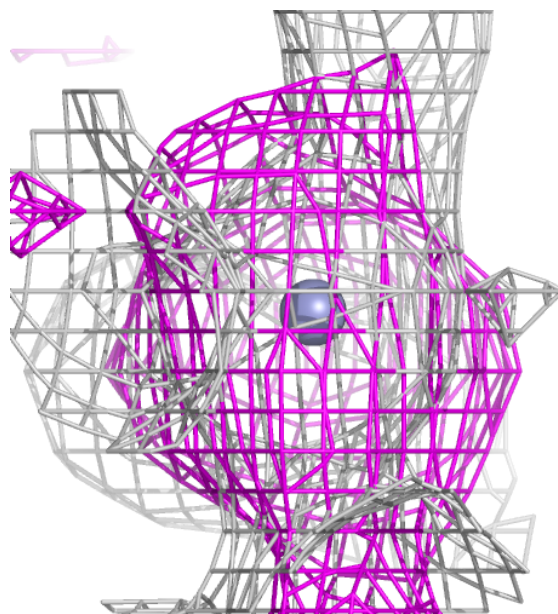
**Electron density around ZN A 502:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
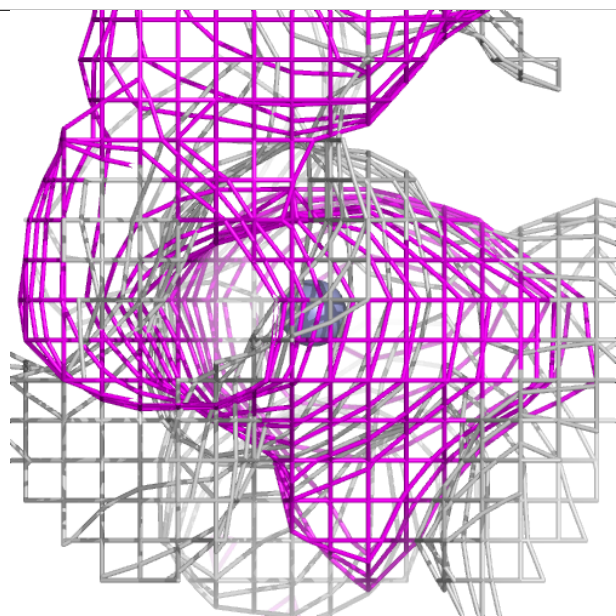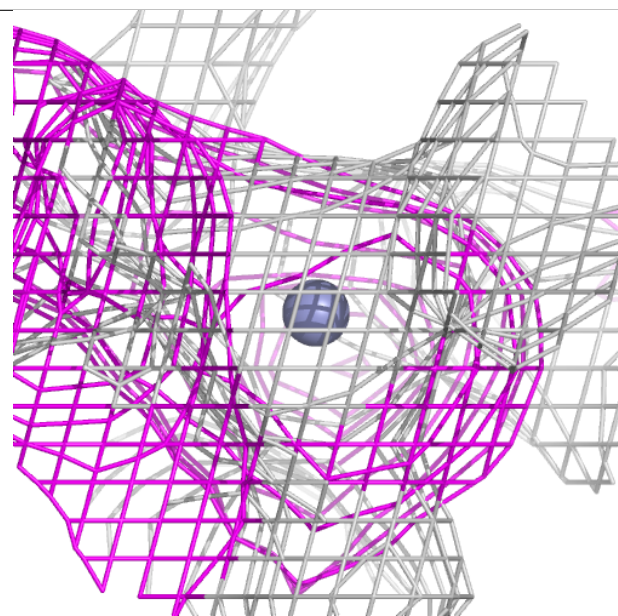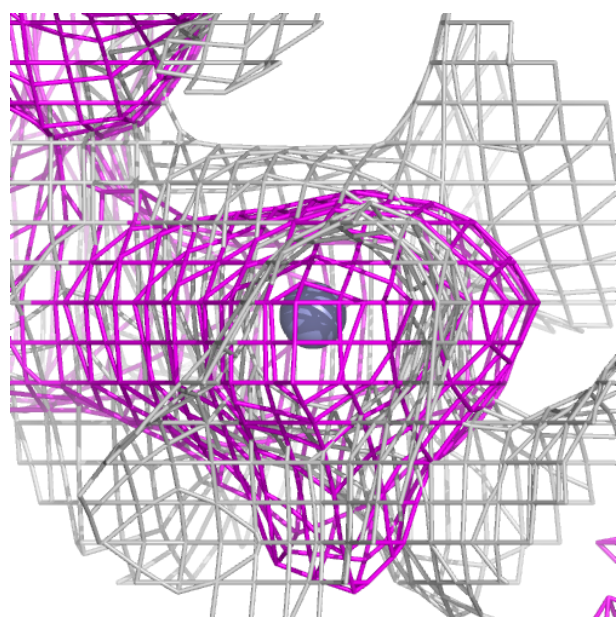
**Electron density around ZN D 502:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
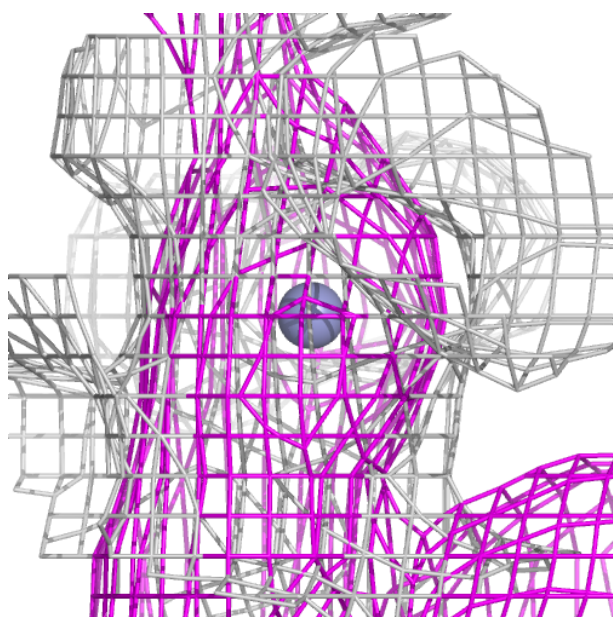$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
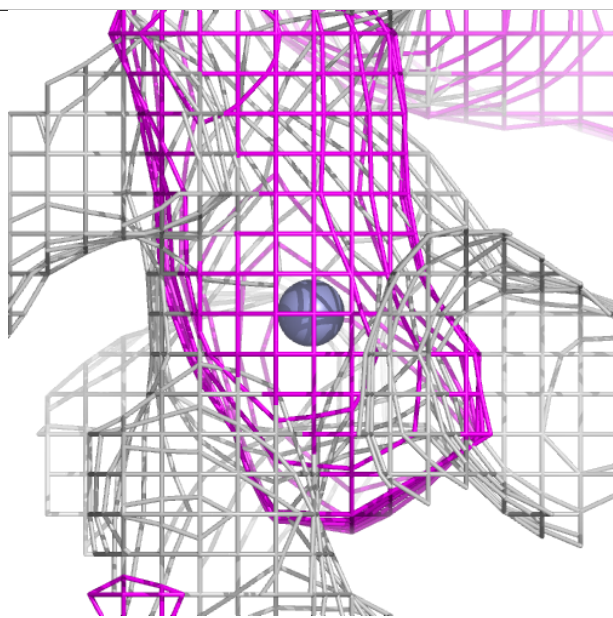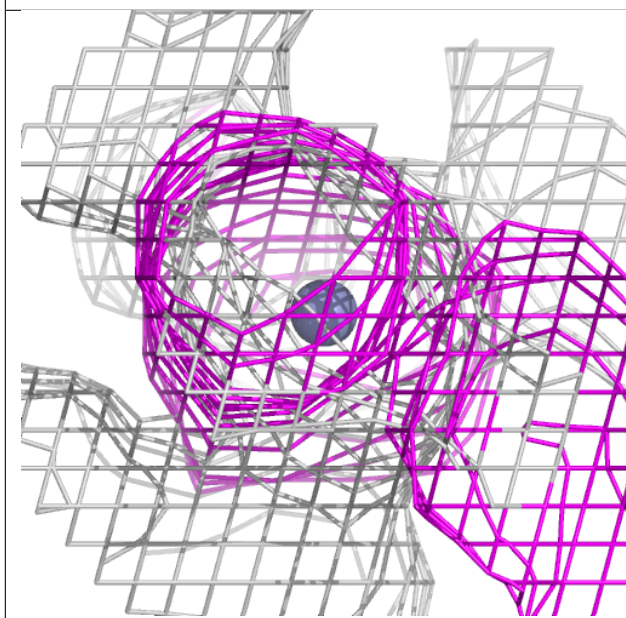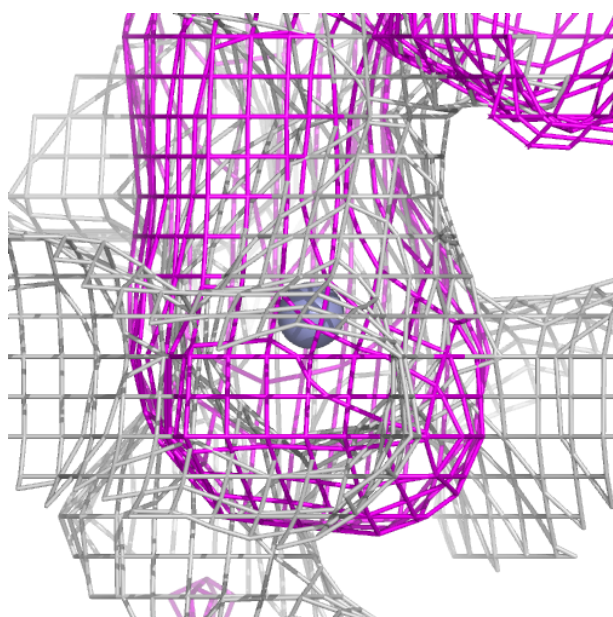
**Electron density around ZN A 501:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
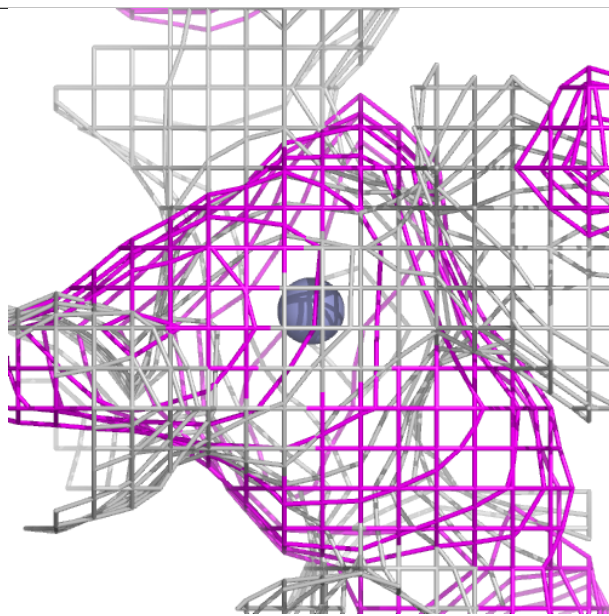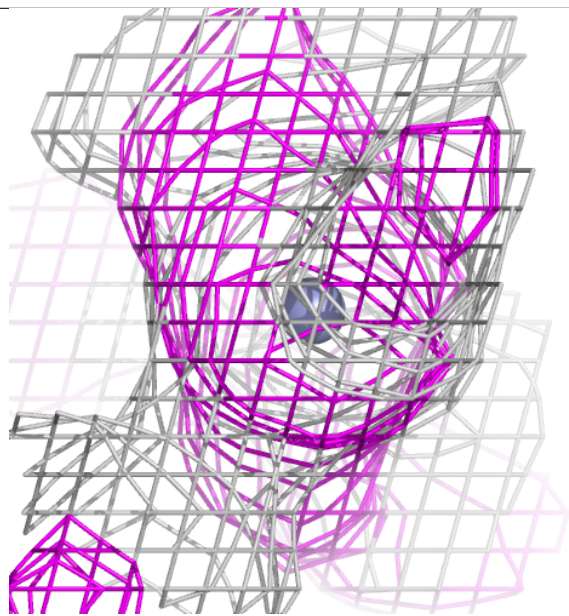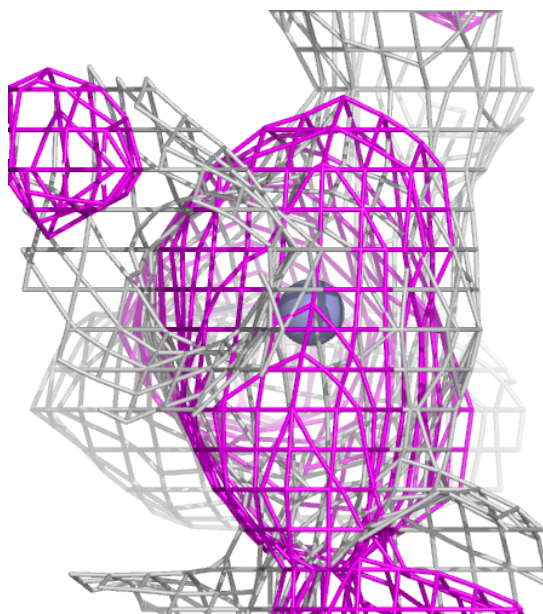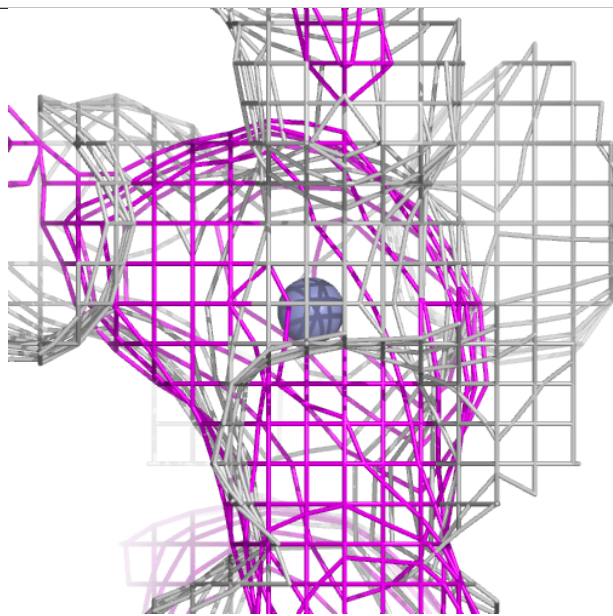
**Electron density around ZN D 501:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
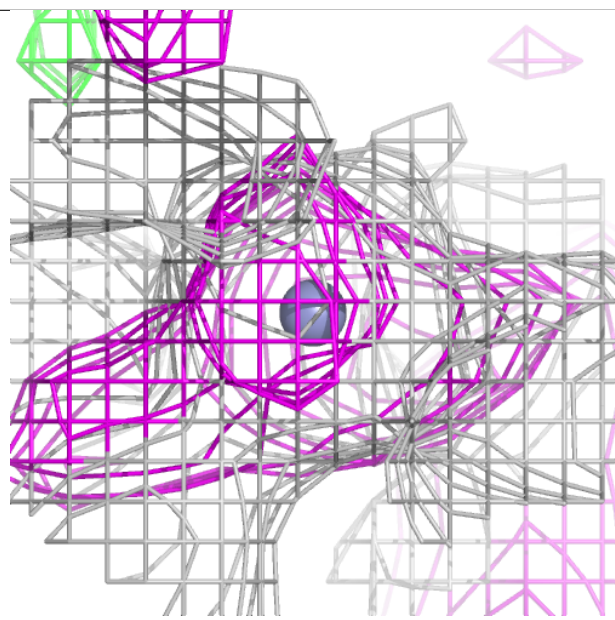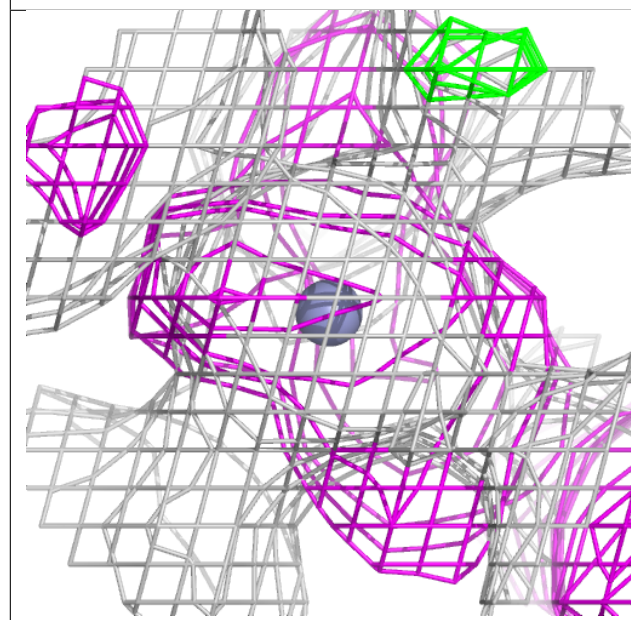
**Electron density around ZN E 501:**

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

**Electron density around ZN G 501:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
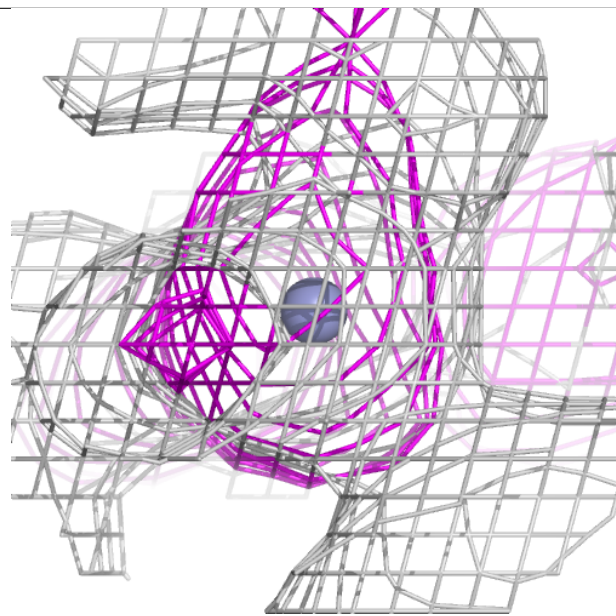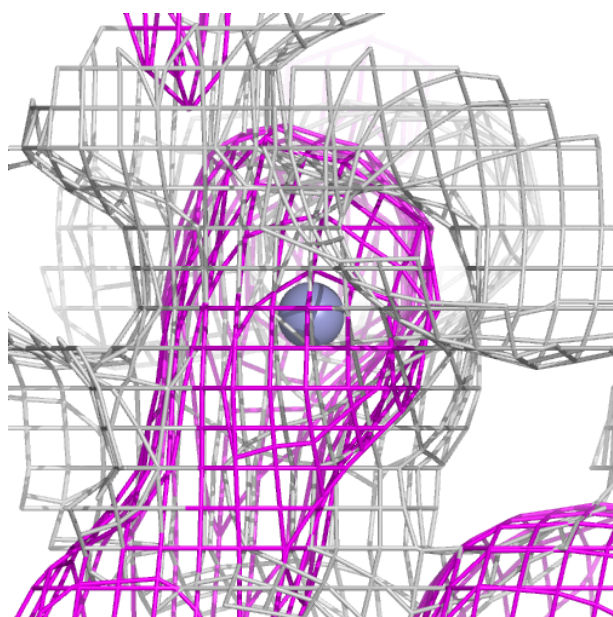
**Electron density around ZN G 502:**

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

**Electron density around ZN E 502:**

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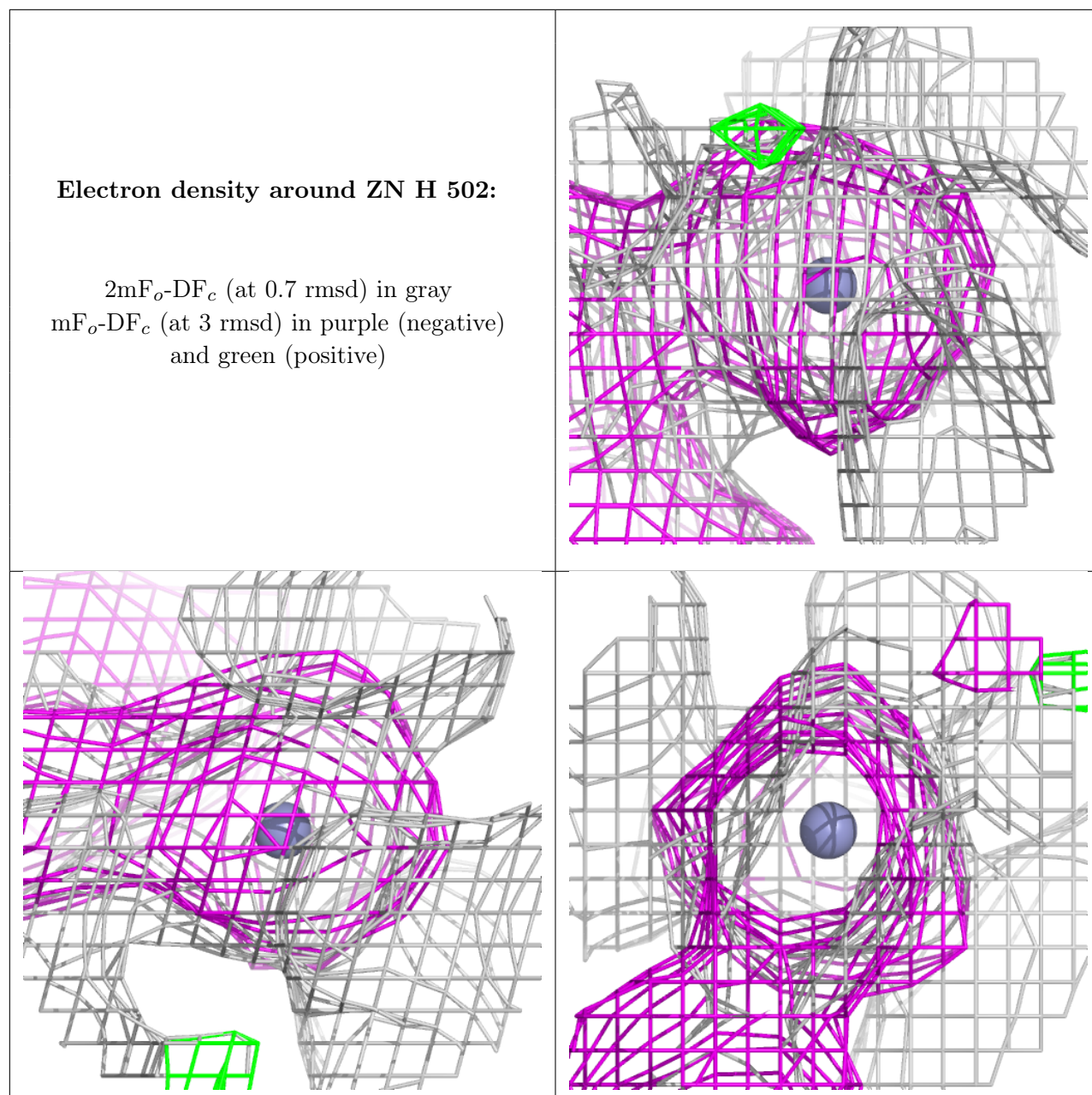and green (positive)

**Electron density around ZN H 502:**

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

## 6.5 Other polymers ⓘ

There are no such residues in this entry.