



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2021 – 02:38 PM EST

PDB ID : 5BKN
Title : Crystallographic structure of a cubic crystal form of STMV (84.5 degree rotation) grown from chloride
Authors : McPherson, A.
Deposited on : 2021-03-20
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.24 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.24 |

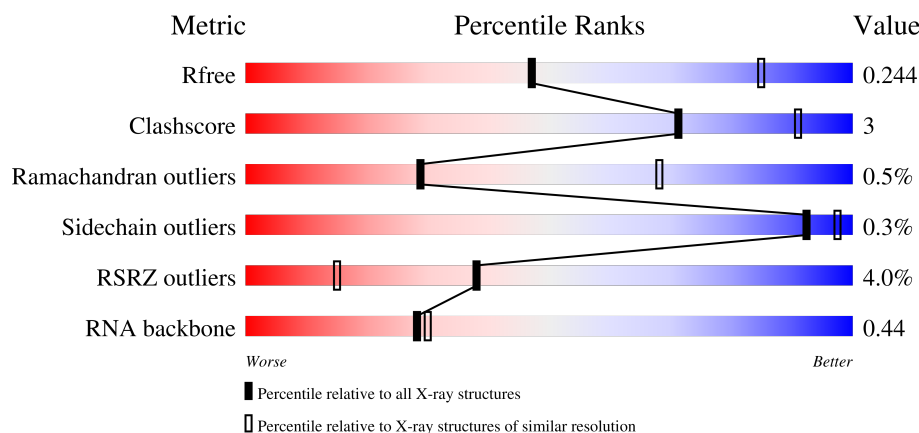
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




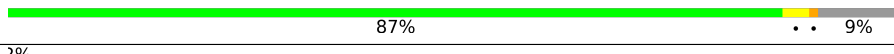

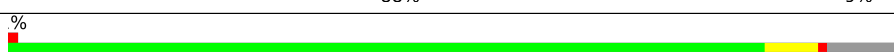



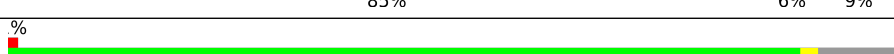
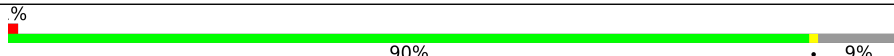
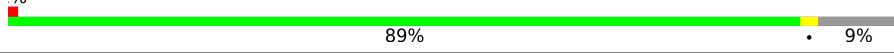
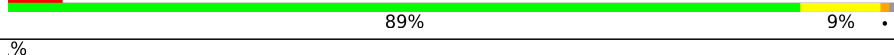
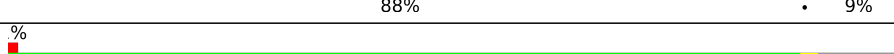
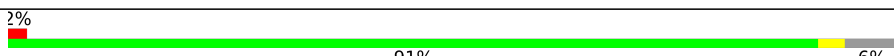




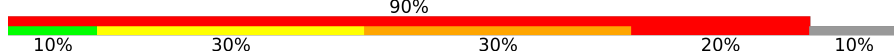

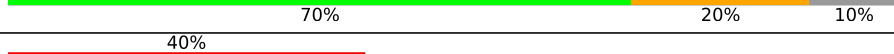
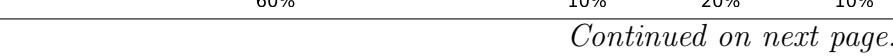


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |
| RNA backbone | 3102 | 1173 (3.30-2.70) |

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 | 159 | 89% 9% |
| 1 | B | 159 | 80% 10% 9% |
| 1 | C | 159 | 87% 10% |
| 1 | D | 159 | 89% 9% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | E | 159 |  |
| 1 | F | 159 |  |
| 1 | G | 159 |  |
| 1 | GG | 159 |  |
| 1 | H | 159 |  |
| 1 | HH | 159 |  |
| 1 | I | 159 |  |
| 1 | II | 159 |  |
| 1 | J | 159 |  |
| 1 | JJ | 159 |  |
| 1 | K | 159 |  |
| 1 | KK | 159 |  |
| 1 | L | 159 |  |
| 1 | M | 159 |  |
| 1 | N | 159 |  |
| 1 | O | 159 |  |
| 2 | P | 8 |  |
| 2 | S | 8 |  |
| 2 | a | 8 |  |
| 3 | T | 6 |  |
| 4 | V | 9 |  |
| 5 | TT | 10 |  |
| 5 | UU | 10 |  |
| 5 | UU | 10 | |
| 5 | UU | 10 | |
| 5 | X | 10 | |
| 5 | Y | 10 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6 | e | 12 | |
| 6 | qq | 12 | |
| 7 | h | 7 | |
| 8 | i | 6 | |
| 8 | ll | 6 | |
| 9 | WW | 9 | |
| 9 | kk | 9 | |
| 9 | m | 9 | |
| 10 | n | 8 | |
| 11 | bb | 12 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 12 | CL | A | 201 | - | - | - | X |
| 12 | CL | E | 202 | - | - | - | X |
| 12 | CL | I | 502 | - | - | X | - |

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 50179 atoms, of which 23685 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 Coat protein.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|-----------|----------|----------|--------|---------|---------|-------|
| 1 | A | 144 | Total 2278 | C 716 | H 1145 | N 200 | O 210 | S 7 | 0 | 13 | 0 |
| 1 | B | 144 | Total 2218 | C 707 | H 1095 | N 199 | O 210 | S 7 | 0 | 11 | 0 |
| 1 | C | 143 | Total 2239 | C 708 | H 1115 | N 199 | O 210 | S 7 | 0 | 20 | 0 |
| 1 | D | 144 | Total 2258 | C 712 | H 1128 | N 200 | O 211 | S 7 | 0 | 18 | 0 |
| 1 | E | 144 | Total 2242 | C 712 | H 1112 | N 200 | O 211 | S 7 | 0 | 19 | 0 |
| 1 | F | 144 | Total 2298 | C 723 | H 1152 | N 202 | O 214 | S 7 | 0 | 17 | 0 |
| 1 | G | 146 | Total 2264 | C 720 | H 1120 | N 202 | O 215 | S 7 | 0 | 13 | 0 |
| 1 | H | 145 | Total 2311 | C 729 | H 1157 | N 203 | O 215 | S 7 | 0 | 19 | 0 |
| 1 | I | 144 | Total 2259 | C 711 | H 1130 | N 200 | O 211 | S 7 | 0 | 13 | 0 |
| 1 | J | 144 | Total 2265 | C 717 | H 1127 | N 201 | O 213 | S 7 | 0 | 13 | 0 |
| 1 | K | 145 | Total 2320 | C 729 | H 1160 | N 207 | O 218 | S 6 | 1 | 12 | 0 |
| 1 | L | 156 | Total 2429 | C 786 | H 1181 | N 223 | O 232 | S 7 | 2 | 13 | 0 |
| 1 | M | 144 | Total 2339 | C 733 | H 1178 | N 204 | O 217 | S 7 | 1 | 11 | 0 |
| 1 | N | 144 | Total 2276 | C 717 | H 1138 | N 200 | O 214 | S 7 | 0 | 6 | 0 |
| 1 | O | 149 | Total 2297 | C 733 | H 1129 | N 206 | O 222 | S 7 | 0 | 24 | 0 |
| 1 | GG | 145 | Total 2254 | C 711 | H 1123 | N 200 | O 213 | S 7 | 0 | 19 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | HH | 144 | Total | C | H | N | O | S | 0 | 14 | 0 |
| | | | 2262 | 713 | 1132 | 199 | 211 | 7 | | | |
| 1 | II | 144 | Total | C | H | N | O | S | 0 | 12 | 0 |
| | | | 2200 | 707 | 1077 | 199 | 210 | 7 | | | |
| 1 | JJ | 144 | Total | C | H | N | O | S | 0 | 16 | 0 |
| | | | 2230 | 703 | 1112 | 199 | 210 | 6 | | | |
| 1 | KK | 144 | Total | C | H | N | O | S | 0 | 14 | 0 |
| | | | 2247 | 707 | 1124 | 199 | 210 | 7 | | | |

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|--------|---------|---------|-------|
| 2 | P | 7 | Total 220 | C 70 | H 66 | N 35 | O 42 | P 7 | 0 | 7 | 0 |
| 2 | S | 6 | Total 187 | C 60 | H 55 | N 30 | O 36 | P 6 | 0 | 6 | 0 |
| 2 | a | 4 | Total 132 | C 40 | H 44 | N 20 | O 24 | P 4 | 0 | 4 | 0 |

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 3 | T | 5 | Total | C | H | N | O | P | 0 | 5 | 0 |
| | | | 156 | 50 | 46 | 25 | 30 | 5 | | | |

- Molecule 4 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 4 | V | 8 | Total | C | H | N | O | P | 0 | 6 | 0 |
| | | | 233 | 80 | 57 | 40 | 48 | 8 | | | |

- Molecule 5 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 5 | X | 9 | Total | C | H | N | O | P | 0 | 8 | 0 |
| | | | 286 | 90 | 88 | 45 | 54 | 9 | | | |
| 5 | Y | 9 | Total | C | H | N | O | P | 0 | 6 | 0 |
| | | | 258 | 90 | 60 | 45 | 54 | 9 | | | |
| 5 | TT | 9 | Total | C | H | N | O | P | 0 | 6 | 0 |
| | | | 258 | 90 | 60 | 45 | 54 | 9 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 5 | UU | 9 | Total | C | H | N | O | P | 0 | 7 | 0 |
| | | | 261 | 90 | 63 | 45 | 54 | 9 | | | |

- Molecule 6 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|---------|---------|---------|-------|
| 6 | e | 11 | Total 300 | C 99 | H 80 | N 22 | O 88 | P 11 | 0 | 10 | 0 |
| 6 | qq | 6 | Total 152 | C 54 | H 32 | N 12 | O 48 | P 6 | 0 | 4 | 0 |

- Molecule 7 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 7 | h | 6 | Total | C | H | N | O | P | 0 | 6 | 0 |
| | | | 169 | 54 | 49 | 12 | 48 | 6 | | | |

- Molecule 8 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|--------|---------|---------|-------|
| 8 | i | 5 | Total 140 | C 45 | H 40 | N 10 | O 40 | P 5 | 0 | 5 | 0 |
| 8 | ll | 5 | Total 140 | C 45 | H 40 | N 10 | O 40 | P 5 | 0 | 5 | 0 |

- Molecule 9 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 9 | m | 8 | Total | C | H | N | O | P | 0 | 8 | 0 |
| | | | 240 | 72 | 80 | 16 | 64 | 8 | | | |
| 9 | WW | 8 | Total | C | H | N | O | P | 0 | 2 | 0 |
| | | | 171 | 72 | 11 | 16 | 64 | 8 | | | |
| 9 | kk | 8 | Total | C | H | N | O | P | 0 | 6 | 0 |
| | | | 209 | 72 | 49 | 16 | 64 | 8 | | | |

- Molecule 10 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*U)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---|---------|---------|-------|
| 10 | n | 7 | Total | C | H | N | O | P | 0 | 7 | 0 |
| | | | 198 | 63 | 58 | 14 | 56 | 7 | | | |

- Molecule 11 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*A P*AP*A)-3').

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|----|---------|---------|-------|
| 11 | bb | 11 | Total | C | H | N | O | P | 0 | 8 | 0 |
| | | | 314 | 110 | 72 | 55 | 66 | 11 | | | |

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 12 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 12 | B | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 12 | E | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 12 | F | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 12 | H | 3 | Total | Cl | 0 | 0 |
| | | | 3 | 3 | | |
| 12 | I | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 12 | J | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 12 | K | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 12 | M | 5 | Total | Cl | 0 | 0 |
| | | | 5 | 5 | | |
| 12 | O | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 12 | S | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 12 | n | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 12 | GG | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 12 | KK | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 13 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 13 | B | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | F | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | G | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | H | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | J | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | K | 3 | Total 3 | Mg 3 | 0 | 0 |
| 13 | L | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | M | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | O | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | II | 1 | Total 1 | Mg 1 | 0 | 0 |
| 13 | JJ | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 14 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14 | A | 51 | Total 51 | O 51 | 0 | 0 |
| 14 | B | 33 | Total 33 | O 33 | 0 | 0 |
| 14 | C | 17 | Total 17 | O 17 | 0 | 0 |
| 14 | D | 30 | Total 30 | O 30 | 0 | 0 |
| 14 | E | 30 | Total 30 | O 30 | 0 | 0 |
| 14 | F | 25 | Total 25 | O 25 | 0 | 0 |
| 14 | G | 24 | Total 24 | O 24 | 0 | 0 |
| 14 | H | 24 | Total 24 | O 24 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14 | I | 14 | Total 14 | O 14 | 0 | 0 |
| 14 | J | 36 | Total 36 | O 36 | 0 | 0 |
| 14 | K | 32 | Total 32 | O 32 | 0 | 0 |
| 14 | L | 35 | Total 35 | O 35 | 0 | 0 |
| 14 | M | 28 | Total 28 | O 28 | 0 | 0 |
| 14 | N | 22 | Total 22 | O 22 | 0 | 0 |
| 14 | O | 56 | Total 56 | O 56 | 0 | 0 |
| 14 | P | 6 | Total 6 | O 6 | 0 | 0 |
| 14 | S | 2 | Total 2 | O 2 | 0 | 0 |
| 14 | T | 3 | Total 3 | O 3 | 0 | 0 |
| 14 | V | 1 | Total 1 | O 1 | 0 | 0 |
| 14 | X | 2 | Total 2 | O 2 | 0 | 0 |
| 14 | Y | 4 | Total 4 | O 4 | 0 | 0 |
| 14 | a | 5 | Total 5 | O 5 | 0 | 0 |
| 14 | e | 3 | Total 3 | O 3 | 0 | 0 |
| 14 | h | 1 | Total 1 | O 1 | 0 | 0 |
| 14 | i | 1 | Total 1 | O 1 | 0 | 0 |
| 14 | m | 5 | Total 5 | O 5 | 0 | 0 |
| 14 | n | 3 | Total 3 | O 3 | 0 | 0 |
| 14 | GG | 22 | Total 22 | O 22 | 0 | 0 |
| 14 | HH | 29 | Total 29 | O 29 | 0 | 0 |

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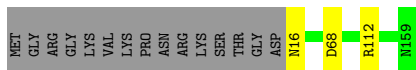
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14 | II | 20 | Total 20 | O 20 | 0 | 0 |
| 14 | JJ | 11 | Total 11 | O 11 | 0 | 0 |
| 14 | KK | 2 | Total 2 | O 2 | 0 | 0 |
| 14 | TT | 2 | Total 2 | O 2 | 0 | 0 |
| 14 | UU | 18 | Total 18 | O 18 | 0 | 0 |
| 14 | WW | 4 | Total 4 | O 4 | 0 | 0 |
| 14 | bb | 27 | Total 27 | O 27 | 0 | 0 |
| 14 | kk | 1 | Total 1 | O 1 | 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: Coat protein

Chain A: 




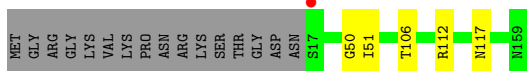
- Molecule 1: Coat protein

Chain B: 

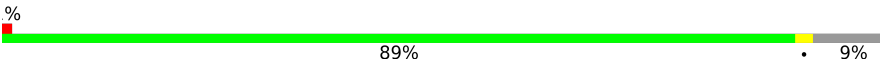


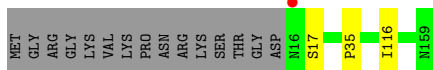
- Molecule 1: Coat protein

Chain C: 




- Molecule 1: Coat protein

Chain D: 




- Molecule 1: Coat protein

Chain E: 




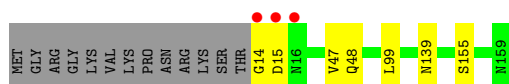
- Molecule 1: Coat protein

Chain F:  87% 9%




• Molecule 1: Coat protein

Chain G:  87% 8%




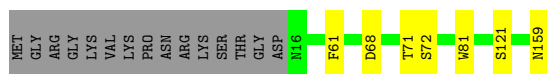
• Molecule 1: Coat protein

Chain H:  85% 6% 9%




• Molecule 1: Coat protein

Chain I:  86% 9%

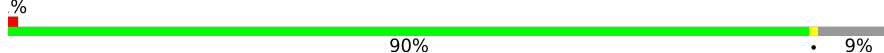


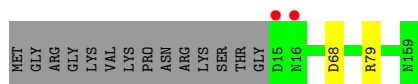
• Molecule 1: Coat protein

Chain J:  85% 6% 9%




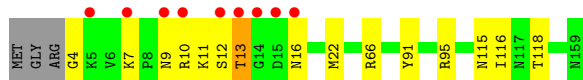
• Molecule 1: Coat protein

Chain K:  90% 9%

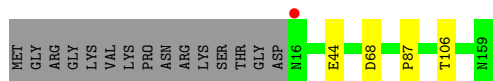
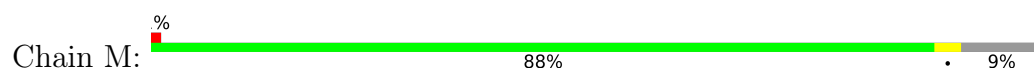


• Molecule 1: Coat protein

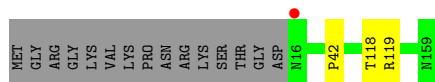
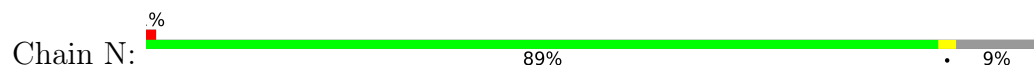
Chain L:  89% 9% 6%



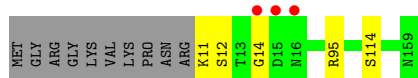
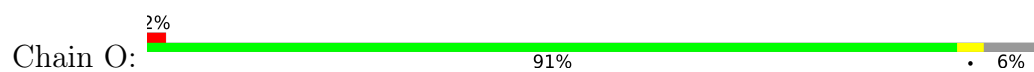
• Molecule 1: Coat protein



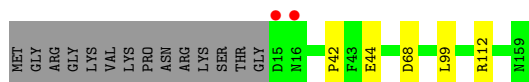
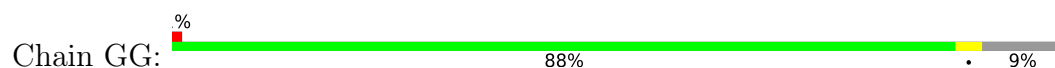
• Molecule 1: Coat protein



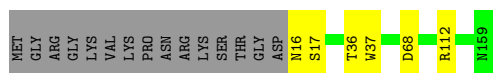
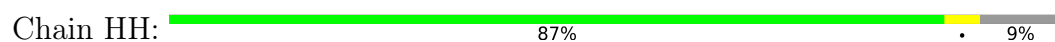
• Molecule 1: Coat protein



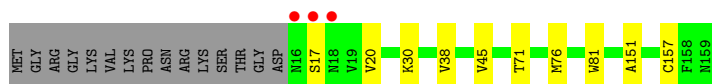
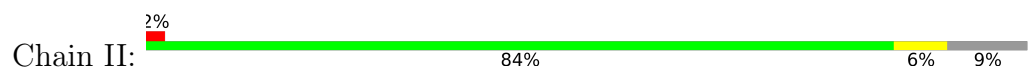
• Molecule 1: Coat protein



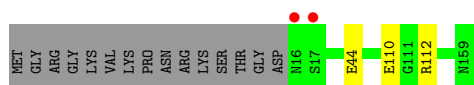
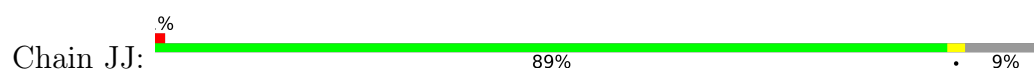
• Molecule 1: Coat protein



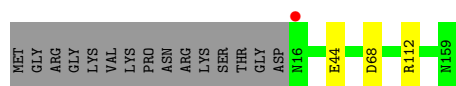
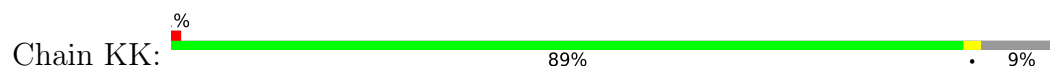
• Molecule 1: Coat protein



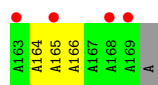
• Molecule 1: Coat protein



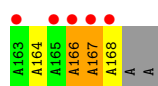
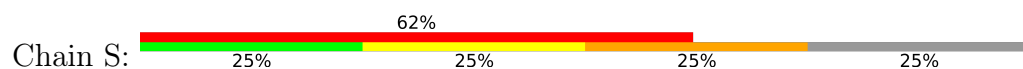
- Molecule 1: Coat protein



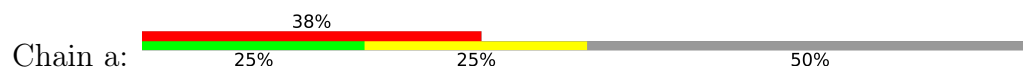
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*A)-3')



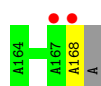
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*A)-3')



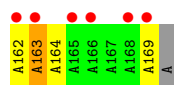
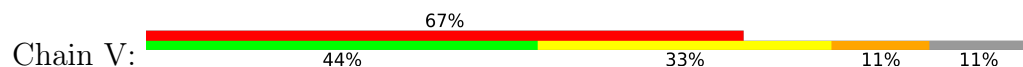
- Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*A)-3')



- Molecule 3: RNA (5'-R(P*AP*AP*AP*AP*AP*A)-3')

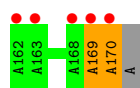


- Molecule 4: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*A)-3')

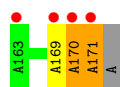
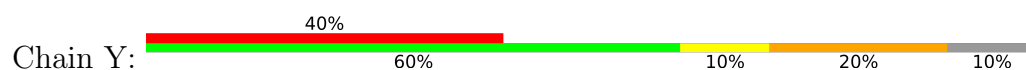


- Molecule 5: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

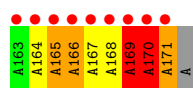
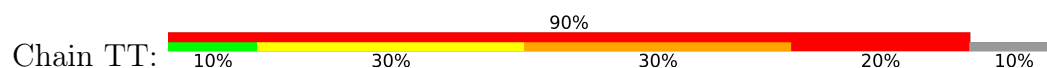




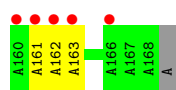
- Molecule 5: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



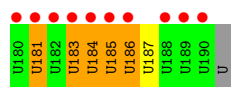
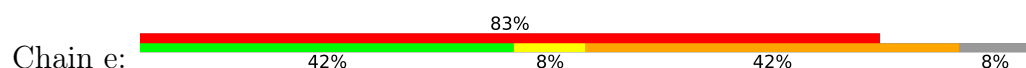
- Molecule 5: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



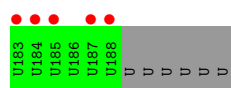
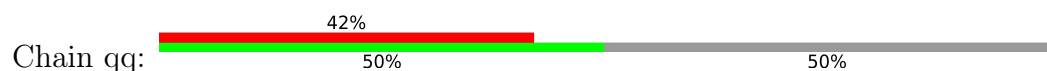
- Molecule 5: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



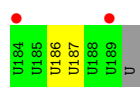
- Molecule 6: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



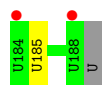
- Molecule 6: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 7: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*U)-3')



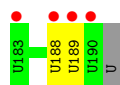
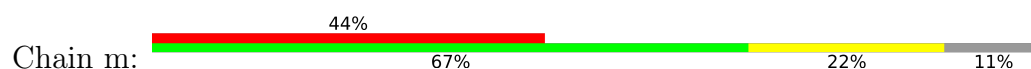
- Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3')



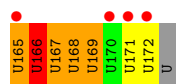
- Molecule 8: RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3')



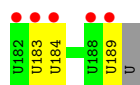
- Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



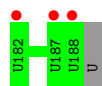
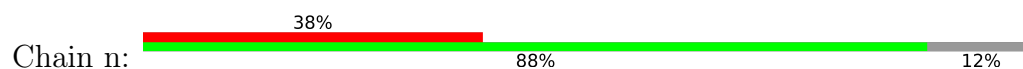
- Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



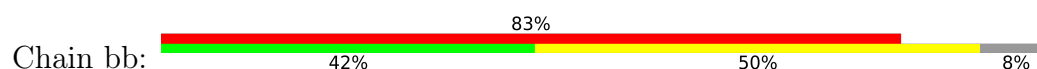
- Molecule 9: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 10: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 11: RNA (5'-R(P*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 2 3 | Depositor |
| Cell constants a, b, c, α , β , γ | 234.65Å 234.65Å 234.65Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 65.08 – 3.00 104.94 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 99.5 (65.08-3.00) 92.0 (104.94-3.00) | Depositor EDS |
| R_{merge} | 0.13 | Depositor |
| R_{sym} | 0.13 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.42 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX 1.19_4092 | Depositor |
| R, R_{free} | 0.208 , 0.255 0.199 , 0.244 | Depositor DCC |
| R_{free} test set | 4529 reflections (5.27%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 39.1 | Xtriage |
| Anisotropy | 0.000 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 36.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | 0.024 for l,-k,h | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 50179 | wwPDB-VP |
| Average B, all atoms (Å ²) | 48.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.34 | 0/1181 | 0.55 | 0/1608 |
| 1 | B | 0.35 | 0/1150 | 0.56 | 0/1566 |
| 1 | C | 0.32 | 0/1151 | 0.54 | 0/1567 |
| 1 | D | 0.33 | 0/1166 | 0.53 | 0/1588 |
| 1 | E | 0.33 | 0/1184 | 0.54 | 0/1612 |
| 1 | F | 0.33 | 0/1222 | 0.54 | 0/1665 |
| 1 | G | 0.32 | 0/1189 | 0.54 | 0/1619 |
| 1 | GG | 0.31 | 0/1174 | 0.54 | 0/1599 |
| 1 | H | 0.35 | 0/1218 | 0.56 | 0/1660 |
| 1 | HH | 0.32 | 0/1187 | 0.53 | 0/1617 |
| 1 | I | 0.34 | 0/1167 | 0.55 | 0/1589 |
| 1 | II | 0.32 | 0/1171 | 0.53 | 0/1595 |
| 1 | J | 0.36 | 0/1189 | 0.54 | 0/1617 |
| 1 | JJ | 0.31 | 0/1142 | 0.55 | 0/1556 |
| 1 | K | 0.32 | 0/1230 | 0.53 | 0/1675 |
| 1 | KK | 0.30 | 0/1177 | 0.52 | 0/1602 |
| 1 | L | 0.35 | 0/1332 | 0.56 | 0/1809 |
| 1 | M | 0.34 | 0/1231 | 0.54 | 0/1675 |
| 1 | N | 0.34 | 0/1186 | 0.55 | 0/1614 |
| 1 | O | 0.35 | 0/1201 | 0.55 | 0/1634 |
| 2 | P | 0.32 | 0/174 | 0.74 | 0/269 |
| 2 | S | 0.43 | 0/149 | 0.87 | 0/230 |
| 2 | a | 0.43 | 0/99 | 0.95 | 0/152 |
| 3 | T | 0.43 | 0/124 | 0.71 | 0/191 |
| 4 | V | 0.34 | 0/199 | 0.75 | 0/308 |
| 5 | TT | 1.02 | 2/224 (0.9%) | 2.85 | 11/347 (3.2%) |
| 5 | UU | 0.29 | 0/224 | 0.75 | 0/347 |
| 5 | X | 0.35 | 0/224 | 0.72 | 0/347 |
| 5 | Y | 0.34 | 0/224 | 0.71 | 0/347 |
| 6 | e | 0.91 | 0/241 | 3.56 | 25/370 (6.8%) |
| 6 | qq | 0.31 | 0/131 | 1.06 | 0/200 |
| 7 | h | 0.27 | 0/131 | 0.78 | 0/200 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 8 | i | 0.37 | 0/109 | 1.02 | 0/166 |
| 8 | ll | 0.34 | 0/109 | 0.76 | 0/166 |
| 9 | WW | 0.29 | 0/175 | 1.02 | 2/268 (0.7%) |
| 9 | kk | 0.27 | 0/175 | 0.74 | 0/268 |
| 9 | m | 0.24 | 0/175 | 0.79 | 0/268 |
| 10 | n | 0.26 | 0/153 | 0.73 | 0/234 |
| 11 | bb | 0.25 | 0/274 | 0.67 | 0/425 |
| All | All | 0.35 | 2/27162 (0.0%) | 0.73 | 38/37570 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | B | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 5 | TT | 166[A] | A | C5'-C4' | 8.04 | 1.61 | 1.51 |
| 5 | TT | 166[A] | A | N9-C4 | 6.26 | 1.41 | 1.37 |

The worst 5 of 38 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|--------|-------------|----------|
| 5 | TT | 166[A] | A | O5'-P-OP2 | -38.53 | 64.46 | 110.70 |
| 6 | e | 184[A] | U | O5'-P-OP1 | -31.59 | 72.79 | 110.70 |
| 6 | e | 184[A] | U | O5'-P-OP2 | -23.84 | 82.09 | 110.70 |
| 6 | e | 185[A] | U | O4'-C1'-N1 | 20.01 | 124.21 | 108.20 |
| 6 | e | 185[A] | U | C2-N1-C1' | 17.27 | 138.43 | 117.70 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 24 | ARG | Sidechain |

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 | 1133 | 1145 | 1105 | 2 | 0 |
| 1 | B | 1123 | 1095 | 1108 | 9 | 0 |
| 1 | C | 1124 | 1115 | 1079 | 5 | 0 |
| 1 | D | 1130 | 1128 | 1091 | 3 | 0 |
| 1 | E | 1130 | 1112 | 1075 | 5 | 0 |
| 1 | F | 1146 | 1152 | 1086 | 5 | 0 |
| 1 | G | 1144 | 1120 | 1112 | 7 | 0 |
| 1 | GG | 1131 | 1123 | 1057 | 4 | 0 |
| 1 | H | 1154 | 1157 | 1106 | 6 | 0 |
| 1 | HH | 1130 | 1132 | 1096 | 5 | 0 |
| 1 | I | 1129 | 1130 | 1096 | 6 | 0 |
| 1 | II | 1123 | 1077 | 1095 | 6 | 0 |
| 1 | J | 1138 | 1127 | 1118 | 9 | 0 |
| 1 | JJ | 1118 | 1112 | 1079 | 2 | 0 |
| 1 | K | 1160 | 1160 | 1120 | 2 | 0 |
| 1 | KK | 1123 | 1124 | 1075 | 3 | 0 |
| 1 | L | 1248 | 1181 | 1236 | 13 | 0 |
| 1 | M | 1161 | 1178 | 1159 | 4 | 0 |
| 1 | N | 1138 | 1138 | 1136 | 2 | 0 |
| 1 | O | 1168 | 1129 | 1113 | 5 | 0 |
| 2 | P | 154 | 66 | 78 | 5 | 0 |
| 2 | S | 132 | 55 | 67 | 4 | 0 |
| 2 | a | 88 | 44 | 45 | 0 | 0 |
| 3 | T | 110 | 46 | 56 | 0 | 0 |
| 4 | V | 176 | 57 | 89 | 4 | 0 |
| 5 | TT | 198 | 60 | 100 | 5 | 0 |
| 5 | UU | 198 | 63 | 100 | 2 | 0 |
| 5 | X | 198 | 88 | 100 | 1 | 0 |
| 5 | Y | 198 | 60 | 100 | 4 | 0 |
| 6 | e | 220 | 80 | 111 | 0 | 0 |
| 6 | qq | 120 | 32 | 61 | 0 | 0 |
| 7 | h | 120 | 49 | 61 | 0 | 0 |
| 8 | i | 100 | 40 | 51 | 0 | 0 |
| 8 | ll | 100 | 40 | 51 | 0 | 0 |
| 9 | WW | 160 | 11 | 75 | 7 | 0 |
| 9 | kk | 160 | 49 | 81 | 0 | 2 |
| 9 | m | 160 | 80 | 81 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10 | n | 140 | 58 | 71 | 0 | 0 |
| 11 | bb | 242 | 72 | 122 | 0 | 0 |
| 12 | A | 2 | 0 | 0 | 1 | 0 |
| 12 | B | 2 | 0 | 0 | 0 | 0 |
| 12 | E | 2 | 0 | 0 | 0 | 0 |
| 12 | F | 2 | 0 | 0 | 0 | 0 |
| 12 | GG | 2 | 0 | 0 | 0 | 0 |
| 12 | H | 3 | 0 | 0 | 1 | 0 |
| 12 | I | 2 | 0 | 0 | 3 | 0 |
| 12 | J | 1 | 0 | 0 | 0 | 0 |
| 12 | K | 1 | 0 | 0 | 0 | 0 |
| 12 | KK | 1 | 0 | 0 | 0 | 0 |
| 12 | M | 5 | 0 | 0 | 1 | 0 |
| 12 | O | 1 | 0 | 0 | 1 | 0 |
| 12 | S | 1 | 0 | 0 | 1 | 0 |
| 12 | n | 1 | 0 | 0 | 0 | 0 |
| 13 | A | 1 | 0 | 0 | 0 | 0 |
| 13 | B | 1 | 0 | 0 | 0 | 0 |
| 13 | F | 1 | 0 | 0 | 0 | 0 |
| 13 | G | 1 | 0 | 0 | 0 | 0 |
| 13 | H | 1 | 0 | 0 | 0 | 0 |
| 13 | II | 1 | 0 | 0 | 0 | 0 |
| 13 | J | 1 | 0 | 0 | 0 | 0 |
| 13 | JJ | 1 | 0 | 0 | 0 | 0 |
| 13 | K | 3 | 0 | 0 | 0 | 0 |
| 13 | L | 1 | 0 | 0 | 0 | 0 |
| 13 | M | 1 | 0 | 0 | 0 | 0 |
| 13 | O | 1 | 0 | 0 | 0 | 0 |
| 14 | A | 51 | 0 | 0 | 1 | 1 |
| 14 | B | 33 | 0 | 0 | 1 | 2 |
| 14 | C | 17 | 0 | 0 | 0 | 0 |
| 14 | D | 30 | 0 | 0 | 0 | 0 |
| 14 | E | 30 | 0 | 0 | 2 | 0 |
| 14 | F | 25 | 0 | 0 | 0 | 0 |
| 14 | G | 24 | 0 | 0 | 2 | 0 |
| 14 | GG | 22 | 0 | 0 | 2 | 0 |
| 14 | H | 24 | 0 | 0 | 2 | 0 |
| 14 | HH | 29 | 0 | 0 | 1 | 1 |
| 14 | I | 14 | 0 | 0 | 2 | 0 |
| 14 | II | 20 | 0 | 0 | 1 | 0 |
| 14 | J | 36 | 0 | 0 | 1 | 0 |
| 14 | JJ | 11 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14 | K | 32 | 0 | 0 | 1 | 0 |
| 14 | KK | 2 | 0 | 0 | 0 | 0 |
| 14 | L | 35 | 0 | 0 | 4 | 1 |
| 14 | M | 28 | 0 | 0 | 1 | 1 |
| 14 | N | 22 | 0 | 0 | 0 | 0 |
| 14 | O | 56 | 0 | 0 | 1 | 0 |
| 14 | P | 6 | 0 | 0 | 2 | 0 |
| 14 | S | 2 | 0 | 0 | 1 | 0 |
| 14 | T | 3 | 0 | 0 | 0 | 0 |
| 14 | TT | 2 | 0 | 0 | 0 | 0 |
| 14 | UU | 18 | 0 | 0 | 0 | 0 |
| 14 | V | 1 | 0 | 0 | 0 | 0 |
| 14 | WW | 4 | 0 | 0 | 1 | 0 |
| 14 | X | 2 | 0 | 0 | 0 | 0 |
| 14 | Y | 4 | 0 | 0 | 2 | 0 |
| 14 | a | 5 | 0 | 0 | 0 | 0 |
| 14 | bb | 27 | 0 | 0 | 0 | 0 |
| 14 | e | 3 | 0 | 0 | 0 | 0 |
| 14 | h | 1 | 0 | 0 | 0 | 0 |
| 14 | i | 1 | 0 | 0 | 0 | 0 |
| 14 | kk | 1 | 0 | 0 | 0 | 0 |
| 14 | m | 5 | 0 | 0 | 0 | 0 |
| 14 | n | 3 | 0 | 0 | 0 | 0 |
| All | All | 26494 | 23685 | 23642 | 117 | 4 |

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 117 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:L:4:GLY:N | 14:L:301:HOH:O | 1.95 | 0.96 |
| 2:S:164[A]:A:O2' | 12:S:201:CL:CL | 2.21 | 0.95 |
| 9:WW:167[A]:U:H2' | 9:WW:168:U:H5'' | 1.47 | 0.95 |
| 1:M:68[B]:ASP:OD1 | 14:M:601:HOH:O | 1.88 | 0.90 |
| 1:J:148:ARG:NH1 | 14:J:1401:HOH:O | 2.05 | 0.88 |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 14:L:335:HOH:O | 14:M:622:HOH:O[8_656] | 1.98 | 0.22 |
| 9:kk:189:U:O3' | 14:B:325:HOH:O[6_566] | 2.06 | 0.14 |
| 9:kk:189:U:O2' | 14:B:325:HOH:O[6_566] | 2.07 | 0.13 |
| 14:A:342:HOH:O | 14:HH:228:HOH:O[9_565] | 2.15 | 0.05 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | A | 147/159 (92%) | 140 (95%) | 7 (5%) | 0 | 100 | 100 |
| 1 | B | 143/159 (90%) | 131 (92%) | 9 (6%) | 3 (2%) | 7 | 33 |
| 1 | C | 143/159 (90%) | 134 (94%) | 9 (6%) | 0 | 100 | 100 |
| 1 | D | 145/159 (91%) | 135 (93%) | 10 (7%) | 0 | 100 | 100 |
| 1 | E | 147/159 (92%) | 140 (95%) | 7 (5%) | 0 | 100 | 100 |
| 1 | F | 152/159 (96%) | 140 (92%) | 12 (8%) | 0 | 100 | 100 |
| 1 | G | 148/159 (93%) | 139 (94%) | 9 (6%) | 0 | 100 | 100 |
| 1 | GG | 146/159 (92%) | 135 (92%) | 10 (7%) | 1 (1%) | 22 | 60 |
| 1 | H | 152/159 (96%) | 143 (94%) | 7 (5%) | 2 (1%) | 12 | 45 |
| 1 | HH | 148/159 (93%) | 138 (93%) | 10 (7%) | 0 | 100 | 100 |
| 1 | I | 145/159 (91%) | 139 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | II | 146/159 (92%) | 134 (92%) | 11 (8%) | 1 (1%) | 22 | 60 |
| 1 | J | 147/159 (92%) | 139 (95%) | 7 (5%) | 1 (1%) | 22 | 60 |
| 1 | JJ | 142/159 (89%) | 135 (95%) | 7 (5%) | 0 | 100 | 100 |
| 1 | K | 152/159 (96%) | 146 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | KK | 146/159 (92%) | 136 (93%) | 10 (7%) | 0 | 100 | 100 |
| 1 | L | 167/159 (105%) | 152 (91%) | 13 (8%) | 2 (1%) | 13 | 48 |
| 1 | M | 153/159 (96%) | 145 (95%) | 7 (5%) | 1 (1%) | 22 | 60 |
| 1 | N | 148/159 (93%) | 139 (94%) | 8 (5%) | 1 (1%) | 22 | 60 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|----------|-------------|
| 1 | O | 150/159 (94%) | 139 (93%) | 10 (7%) | 1 (1%) | 22 60 |
| All | All | 2967/3180 (93%) | 2779 (94%) | 175 (6%) | 13 (0%) | 29 72 |

5 of 13 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 122 | VAL |
| 1 | L | 16 | ASN |
| 1 | B | 37 | TRP |
| 1 | L | 13 | THR |
| 1 | N | 42 | PRO |

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 | 133/140 (95%) | 132 (99%) | 1 (1%) | 81 93 |
| 1 | B | 129/140 (92%) | 128 (99%) | 1 (1%) | 81 93 |
| 1 | C | 129/140 (92%) | 129 (100%) | 0 | 100 100 |
| 1 | D | 131/140 (94%) | 131 (100%) | 0 | 100 100 |
| 1 | E | 133/140 (95%) | 133 (100%) | 0 | 100 100 |
| 1 | F | 138/140 (99%) | 137 (99%) | 1 (1%) | 84 94 |
| 1 | G | 133/140 (95%) | 133 (100%) | 0 | 100 100 |
| 1 | GG | 132/140 (94%) | 132 (100%) | 0 | 100 100 |
| 1 | H | 138/140 (99%) | 137 (99%) | 1 (1%) | 84 94 |
| 1 | HH | 134/140 (96%) | 134 (100%) | 0 | 100 100 |
| 1 | I | 131/140 (94%) | 131 (100%) | 0 | 100 100 |
| 1 | II | 132/140 (94%) | 131 (99%) | 1 (1%) | 81 93 |
| 1 | J | 133/140 (95%) | 133 (100%) | 0 | 100 100 |
| 1 | JJ | 128/140 (91%) | 128 (100%) | 0 | 100 100 |
| 1 | K | 138/140 (99%) | 138 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1 | KK | 132/140 (94%) | 132 (100%) | 0 | 100 | 100 |
| 1 | L | 150/140 (107%) | 147 (98%) | 3 (2%) | 55 | 83 |
| 1 | M | 139/140 (99%) | 139 (100%) | 0 | 100 | 100 |
| 1 | N | 134/140 (96%) | 134 (100%) | 0 | 100 | 100 |
| 1 | O | 135/140 (96%) | 135 (100%) | 0 | 100 | 100 |
| All | All | 2682/2800 (96%) | 2674 (100%) | 8 (0%) | 92 | 97 |

5 of 8 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | II | 45 | VAL |
| 1 | L | 13 | THR |
| 1 | L | 9 | ASN |
| 1 | H | 122 | VAL |
| 1 | L | 11 | LYS |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | JJ | 117 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 10 | n | 6/8 (75%) | 0 | 0 |
| 11 | bb | 10/12 (83%) | 6 (60%) | 0 |
| 2 | P | 6/8 (75%) | 0 | 0 |
| 2 | S | 5/8 (62%) | 3 (60%) | 0 |
| 2 | a | 3/8 (37%) | 2 (66%) | 0 |
| 3 | T | 4/6 (66%) | 1 (25%) | 0 |
| 4 | V | 7/9 (77%) | 2 (28%) | 0 |
| 5 | TT | 8/10 (80%) | 7 (87%) | 0 |
| 5 | UU | 8/10 (80%) | 1 (12%) | 0 |
| 5 | X | 8/10 (80%) | 1 (12%) | 1 (12%) |
| 5 | Y | 8/10 (80%) | 2 (25%) | 0 |
| 6 | e | 10/12 (83%) | 6 (60%) | 0 |
| 6 | qq | 5/12 (41%) | 0 | 0 |
| 7 | h | 5/7 (71%) | 2 (40%) | 0 |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 8 | i | 4/6 (66%) | 1 (25%) | 0 |
| 8 | ll | 4/6 (66%) | 1 (25%) | 0 |
| 9 | WW | 8/9 (88%) | 6 (75%) | 1 (12%) |
| 9 | kk | 7/9 (77%) | 2 (28%) | 0 |
| 9 | m | 7/9 (77%) | 2 (28%) | 0 |
| All | All | 123/169 (72%) | 45 (36%) | 2 (1%) |

5 of 45 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | S | 166[A] | A |
| 2 | S | 167[A] | A |
| 2 | S | 168[A] | A |
| 3 | T | 168[A] | A |
| 4 | V | 163 | A |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 5 | X | 169[A] | A |
| 9 | WW | 165 | U |

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 40 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 | 144/159 (90%) | -0.21 | 0 100 100 | 24, 34, 46, 71 | 1 (0%) |
| 1 | B | 144/159 (90%) | -0.14 | 0 100 100 | 26, 36, 49, 80 | 2 (1%) |
| 1 | C | 143/159 (89%) | -0.10 | 1 (0%) 87 69 | 32, 43, 55, 84 | 0 |
| 1 | D | 144/159 (90%) | -0.00 | 1 (0%) 87 69 | 35, 47, 58, 81 | 0 |
| 1 | E | 144/159 (90%) | -0.20 | 1 (0%) 87 69 | 29, 39, 49, 74 | 0 |
| 1 | F | 144/159 (90%) | -0.20 | 0 100 100 | 25, 33, 42, 83 | 0 |
| 1 | G | 146/159 (91%) | 0.02 | 3 (2%) 63 34 | 29, 42, 61, 104 | 2 (1%) |
| 1 | GG | 145/159 (91%) | 0.13 | 2 (1%) 75 49 | 33, 55, 76, 110 | 0 |
| 1 | H | 145/159 (91%) | -0.09 | 2 (1%) 75 49 | 29, 39, 50, 109 | 2 (1%) |
| 1 | HH | 144/159 (90%) | 0.28 | 0 100 100 | 30, 50, 66, 82 | 2 (1%) |
| 1 | I | 144/159 (90%) | -0.25 | 0 100 100 | 17, 32, 48, 73 | 0 |
| 1 | II | 144/159 (90%) | 0.24 | 3 (2%) 63 34 | 36, 49, 65, 87 | 0 |
| 1 | J | 144/159 (90%) | -0.23 | 0 100 100 | 20, 29, 42, 72 | 1 (0%) |
| 1 | JJ | 144/159 (90%) | 0.12 | 2 (1%) 75 49 | 45, 56, 69, 96 | 1 (0%) |
| 1 | K | 145/159 (91%) | -0.08 | 2 (1%) 75 49 | 23, 30, 43, 97 | 0 |
| 1 | KK | 144/159 (90%) | 0.19 | 1 (0%) 87 69 | 47, 61, 75, 95 | 0 |
| 1 | L | 156/159 (98%) | -0.03 | 9 (5%) 23 7 | 20, 28, 68, 102 | 1 (0%) |
| 1 | M | 144/159 (90%) | -0.27 | 1 (0%) 87 69 | 19, 26, 36, 84 | 0 |
| 1 | N | 144/159 (90%) | -0.28 | 1 (0%) 87 69 | 20, 27, 41, 76 | 0 |
| 1 | O | 149/159 (93%) | -0.08 | 3 (2%) 65 36 | 22, 30, 52, 99 | 2 (1%) |
| 2 | P | 7/8 (87%) | 2.88 | 4 (57%) 0 0 | 61, 66, 95, 108 | 7 (100%) |
| 2 | S | 6/8 (75%) | 3.41 | 5 (83%) 0 0 | 63, 74, 91, 98 | 6 (100%) |
| 2 | a | 4/8 (50%) | 3.19 | 3 (75%) 0 0 | 41, 43, 77, 97 | 4 (100%) |
| 3 | T | 5/6 (83%) | 2.15 | 2 (40%) 0 0 | 56, 58, 61, 70 | 5 (100%) |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-----------|
| 4 | V | 8/9 (88%) | 3.34 | 6 (75%) 0 0 | 69, 97, 149, 152 | 6 (75%) |
| 5 | TT | 9/10 (90%) | 5.35 | 9 (100%) 0 0 | 78, 101, 133, 150 | 5 (55%) |
| 5 | UU | 9/10 (90%) | 3.12 | 5 (55%) 0 0 | 65, 76, 101, 119 | 9 (100%) |
| 5 | X | 9/10 (90%) | 2.66 | 5 (55%) 0 0 | 50, 61, 94, 117 | 9 (100%) |
| 5 | Y | 9/10 (90%) | 3.03 | 4 (44%) 0 0 | 45, 53, 95, 104 | 9 (100%) |
| 6 | e | 11/12 (91%) | 5.85 | 10 (90%) 0 0 | 80, 95, 112, 114 | 11 (100%) |
| 6 | qq | 6/12 (50%) | 4.03 | 5 (83%) 0 0 | 83, 92, 121, 141 | 4 (66%) |
| 7 | h | 6/7 (85%) | 2.32 | 2 (33%) 0 0 | 62, 66, 82, 93 | 6 (100%) |
| 8 | i | 5/6 (83%) | 2.80 | 2 (40%) 0 0 | 50, 60, 82, 98 | 5 (100%) |
| 8 | ll | 5/6 (83%) | 1.62 | 1 (20%) 1 0 | 72, 72, 81, 90 | 5 (100%) |
| 9 | WW | 8/9 (88%) | 3.12 | 4 (50%) 0 0 | 77, 106, 116, 143 | 4 (50%) |
| 9 | kk | 8/9 (88%) | 3.02 | 5 (62%) 0 0 | 63, 77, 109, 118 | 8 (100%) |
| 9 | m | 8/9 (88%) | 3.06 | 4 (50%) 0 0 | 50, 65, 98, 102 | 8 (100%) |
| 10 | n | 7/8 (87%) | 1.60 | 3 (42%) 0 0 | 46, 55, 91, 91 | 7 (100%) |
| 11 | bb | 11/12 (91%) | 5.31 | 10 (90%) 0 0 | 76, 89, 103, 105 | 11 (100%) |
| All | All | 3042/3349 (90%) | 0.10 | 121 (3%) 38 15 | 17, 39, 75, 152 | 143 (4%) |

The worst 5 of 121 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 6 | e | 180 | U | 10.3 |
| 11 | bb | 161[A] | A | 9.6 |
| 6 | e | 182[A] | U | 9.5 |
| 11 | bb | 162[A] | A | 8.7 |
| 6 | e | 181[A] | U | 8.7 |

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

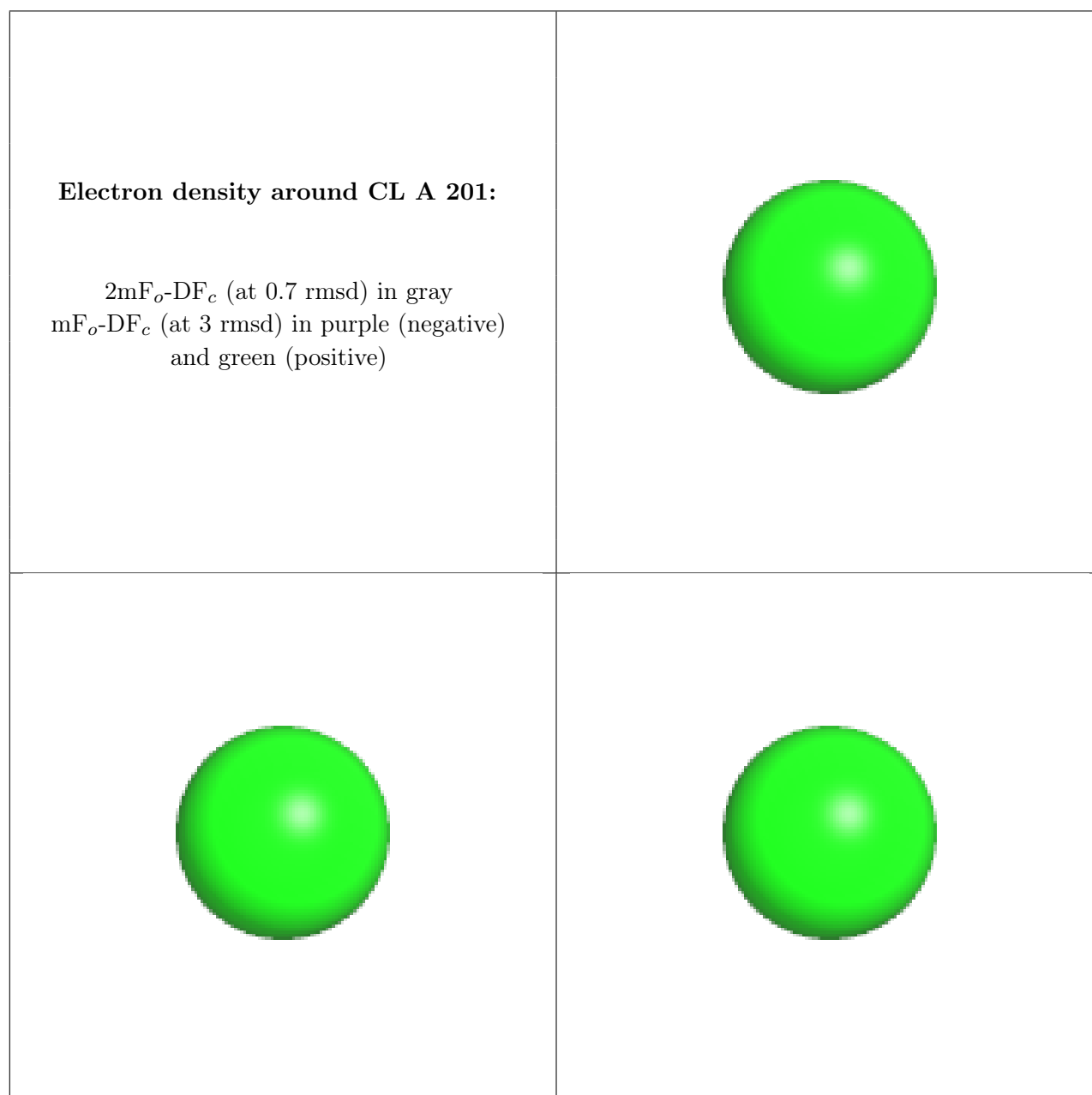
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 12 | CL | A | 201 | 1/1 | 0.62 | 1.08 | 84,84,84,84 | 0 |
| 12 | CL | H | 203 | 1/1 | 0.75 | 0.34 | 72,72,72,72 | 0 |
| 12 | CL | E | 202 | 1/1 | 0.79 | 0.93 | 64,64,64,64 | 0 |
| 12 | CL | M | 501 | 1/1 | 0.82 | 0.57 | 51,51,51,51 | 0 |
| 12 | CL | O | 201 | 1/1 | 0.83 | 0.61 | 67,67,67,67 | 0 |
| 12 | CL | S | 201 | 1/1 | 0.84 | 0.43 | 68,68,68,68 | 0 |
| 12 | CL | I | 502 | 1/1 | 0.85 | 0.54 | 58,58,58,58 | 0 |
| 12 | CL | E | 201 | 1/1 | 0.85 | 0.30 | 59,59,59,59 | 0 |
| 12 | CL | H | 202 | 1/1 | 0.88 | 0.27 | 74,74,74,74 | 0 |
| 12 | CL | GG | 201 | 1/1 | 0.91 | 0.13 | 59,59,59,59 | 0 |
| 13 | MG | JJ | 201 | 1/1 | 0.92 | 0.22 | 60,60,60,60 | 0 |
| 13 | MG | A | 203 | 1/1 | 0.93 | 0.30 | 42,42,42,42 | 0 |
| 12 | CL | F | 302 | 1/1 | 0.94 | 0.49 | 67,67,67,67 | 0 |
| 12 | CL | H | 201 | 1/1 | 0.94 | 0.37 | 62,62,62,62 | 0 |
| 12 | CL | J | 1301 | 1/1 | 0.94 | 0.14 | 52,52,52,52 | 0 |
| 12 | CL | B | 202 | 1/1 | 0.94 | 0.14 | 42,42,42,42 | 0 |
| 12 | CL | M | 504 | 1/1 | 0.94 | 0.28 | 59,59,59,59 | 0 |
| 12 | CL | GG | 202 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 12 | CL | B | 201 | 1/1 | 0.95 | 0.15 | 34,34,34,34 | 0 |
| 13 | MG | J | 1302 | 1/1 | 0.95 | 0.48 | 37,37,37,37 | 0 |
| 13 | MG | K | 303 | 1/1 | 0.95 | 0.53 | 35,35,35,35 | 0 |
| 12 | CL | M | 503 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 12 | CL | I | 501 | 1/1 | 0.96 | 0.33 | 67,67,67,67 | 0 |
| 13 | MG | B | 203 | 1/1 | 0.96 | 0.33 | 43,43,43,43 | 0 |
| 13 | MG | H | 204 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 12 | CL | A | 202 | 1/1 | 0.96 | 0.11 | 46,46,46,46 | 0 |
| 12 | CL | M | 502 | 1/1 | 0.96 | 0.67 | 58,58,58,58 | 0 |
| 13 | MG | K | 304 | 1/1 | 0.96 | 0.45 | 37,37,37,37 | 0 |
| 13 | MG | O | 202 | 1/1 | 0.96 | 0.60 | 31,31,31,31 | 0 |
| 13 | MG | II | 201 | 1/1 | 0.96 | 0.43 | 52,52,52,52 | 0 |
| 12 | CL | KK | 201 | 1/1 | 0.96 | 0.18 | 62,62,62,62 | 1 |
| 12 | CL | n | 401 | 1/1 | 0.97 | 0.17 | 45,45,45,45 | 0 |
| 12 | CL | F | 301 | 1/1 | 0.97 | 0.18 | 34,34,34,34 | 0 |
| 13 | MG | K | 302 | 1/1 | 0.97 | 0.33 | 25,25,25,25 | 0 |
| 13 | MG | G | 201 | 1/1 | 0.97 | 0.17 | 39,39,39,39 | 0 |
| 12 | CL | M | 505 | 1/1 | 0.98 | 0.31 | 45,45,45,45 | 0 |
| 13 | MG | L | 201 | 1/1 | 0.98 | 0.45 | 36,36,36,36 | 0 |

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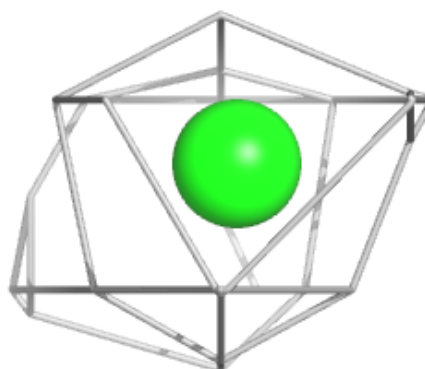
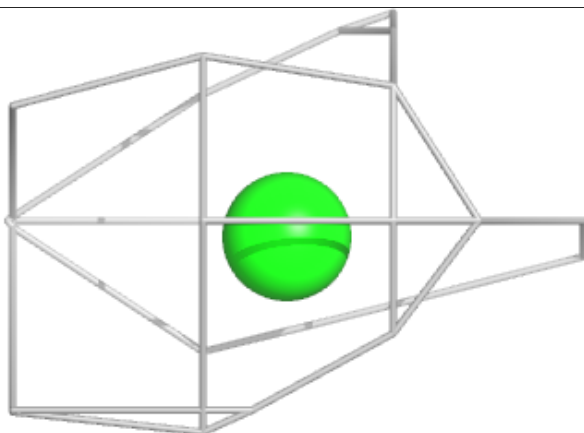
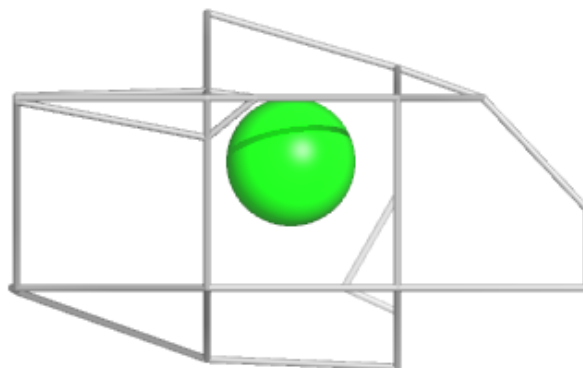
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 13 | MG | M | 506 | 1/1 | 0.98 | 0.26 | 32,32,32,32 | 0 |
| 13 | MG | F | 303 | 1/1 | 0.99 | 0.28 | 36,36,36,36 | 0 |
| 12 | CL | K | 301 | 1/1 | 0.99 | 0.15 | 25,25,25,25 | 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.



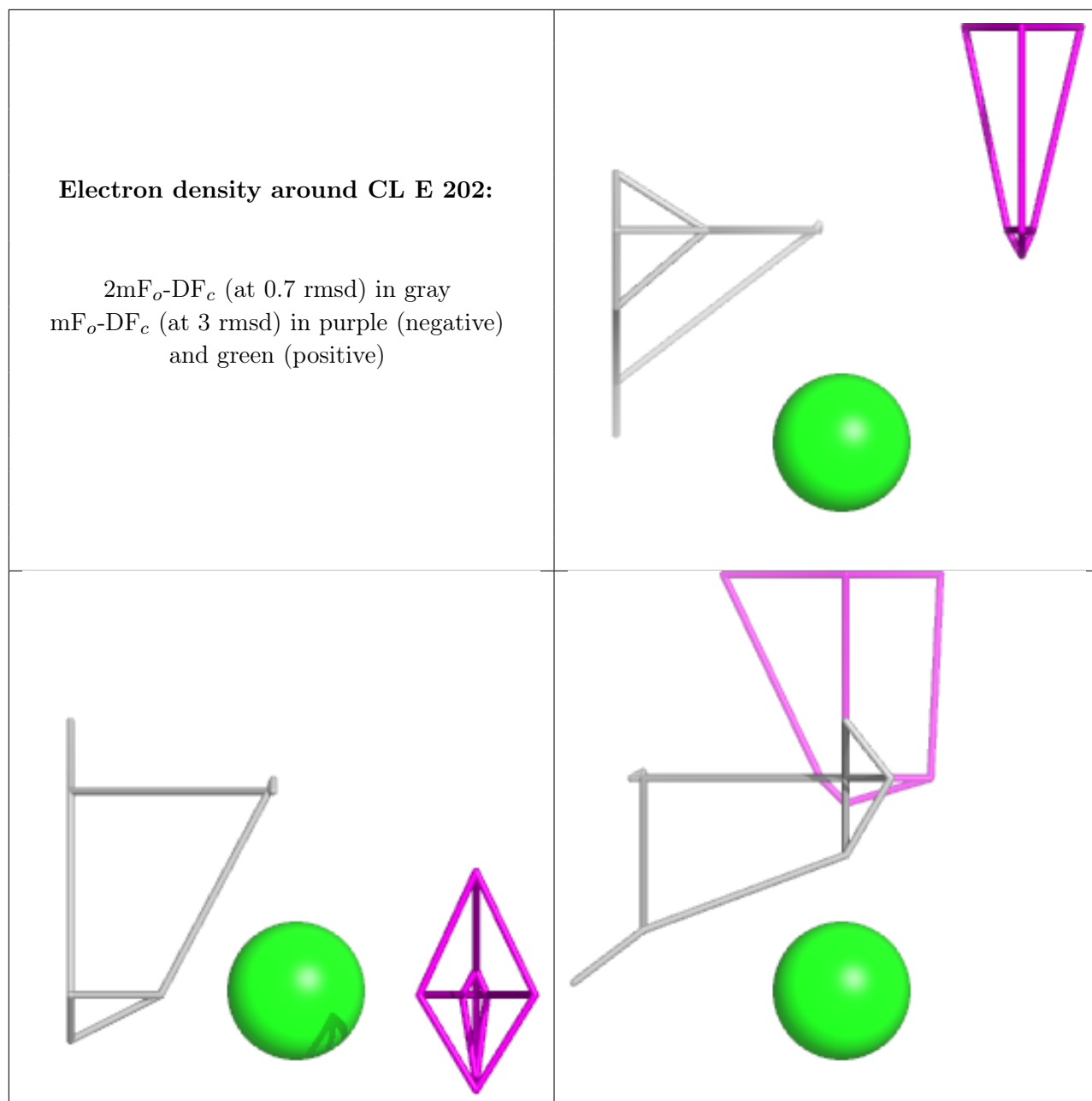
Electron density around CL H 203:

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



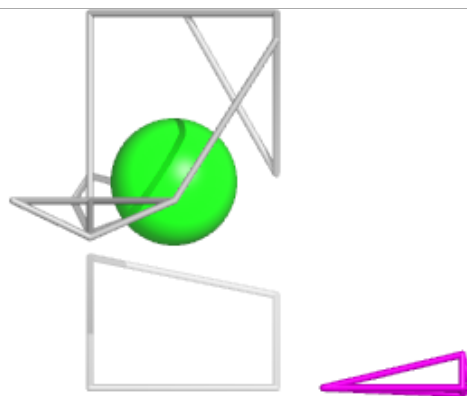
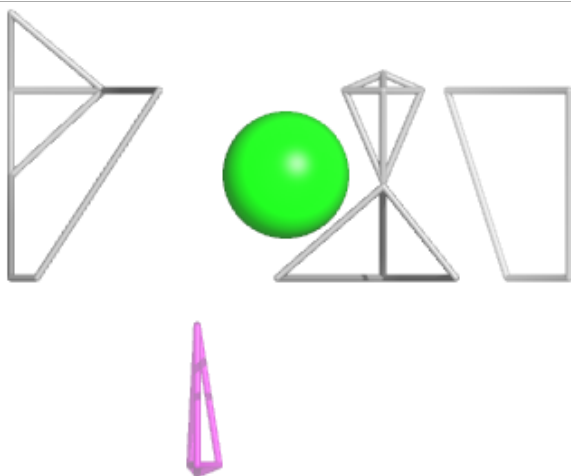
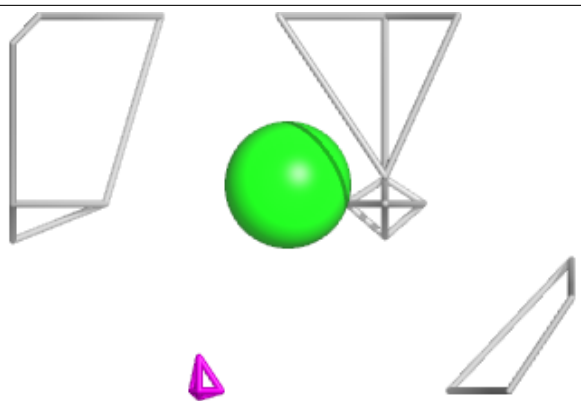
Electron density around CL E 202:

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



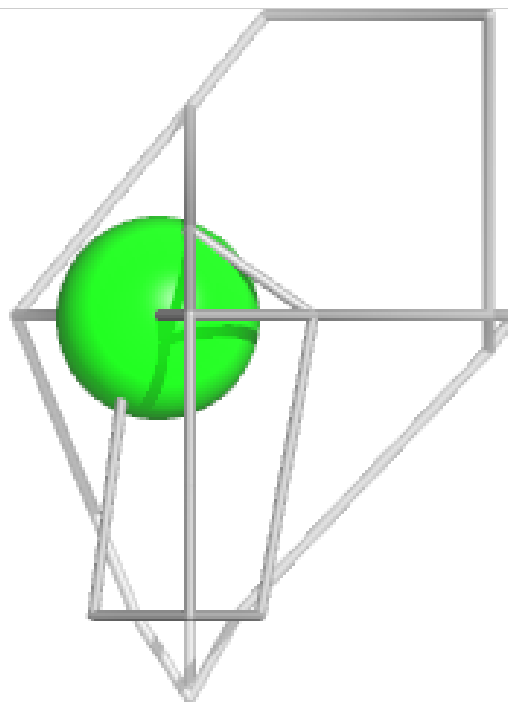
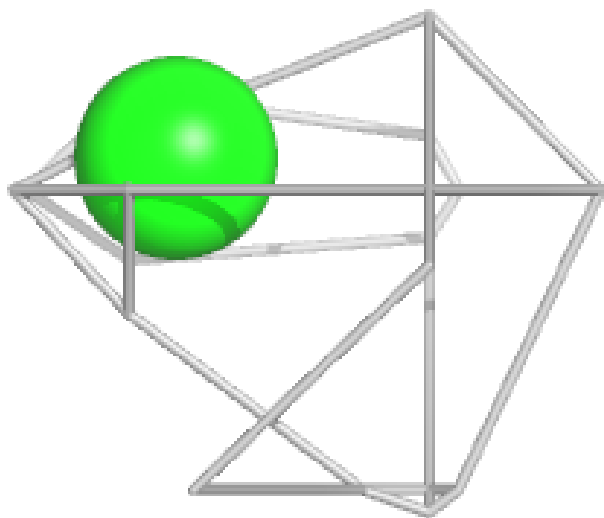
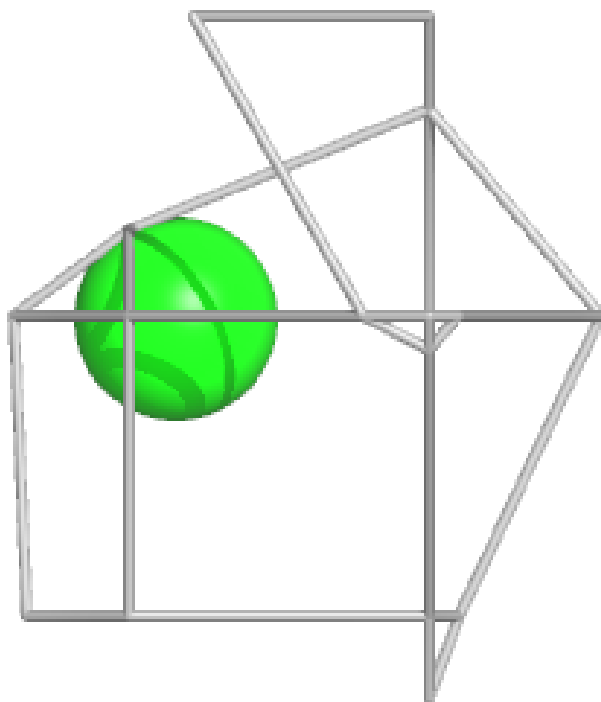
Electron density around CL M 501:

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



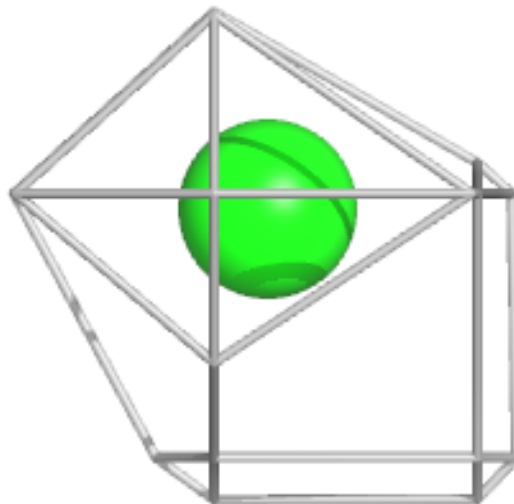
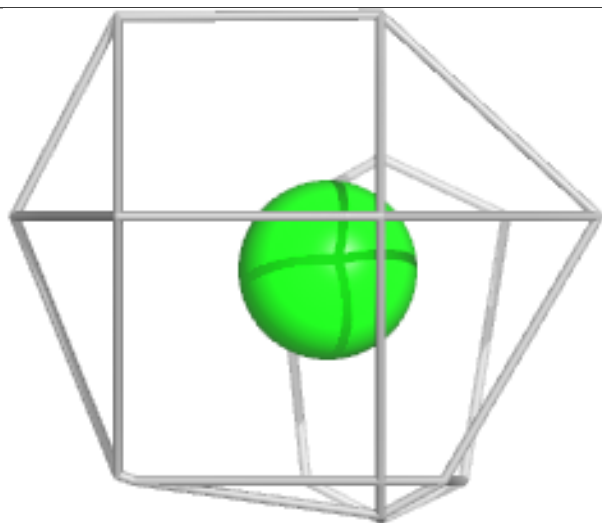
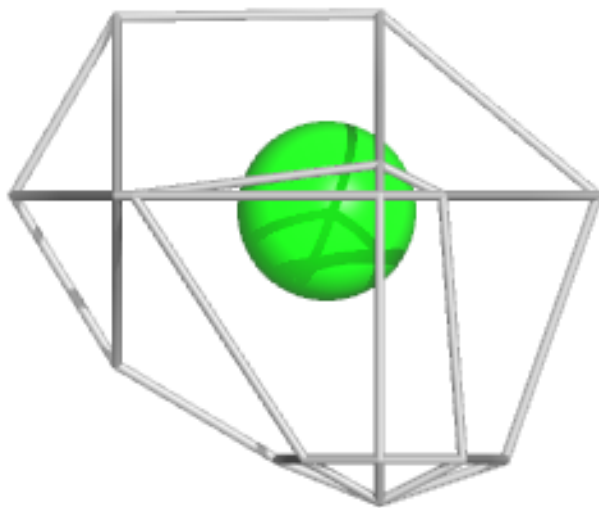
Electron density around CL O 201:

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



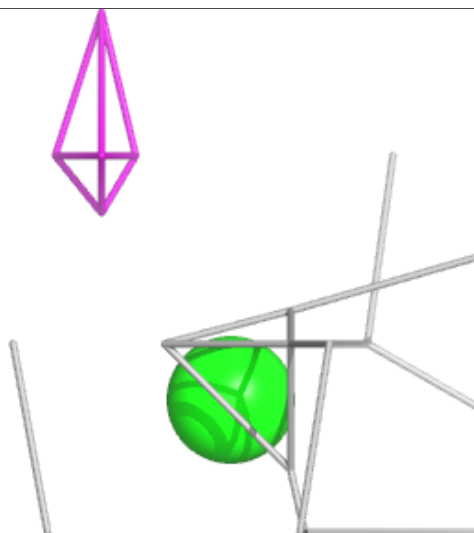
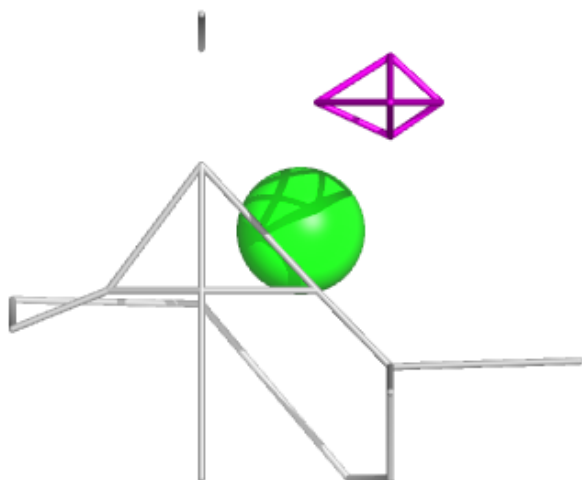
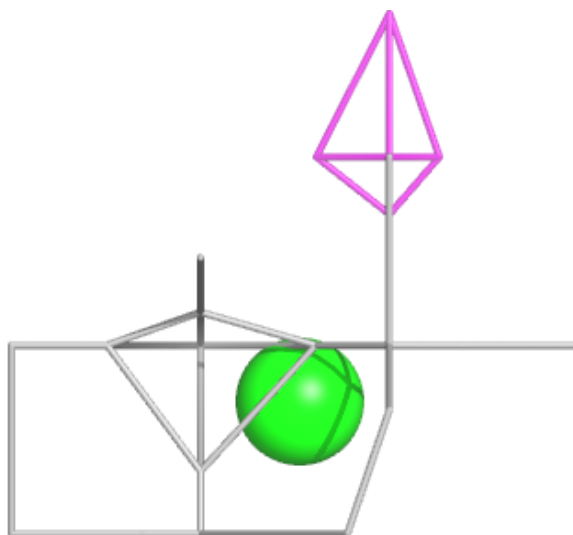
Electron density around CL S 201:

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



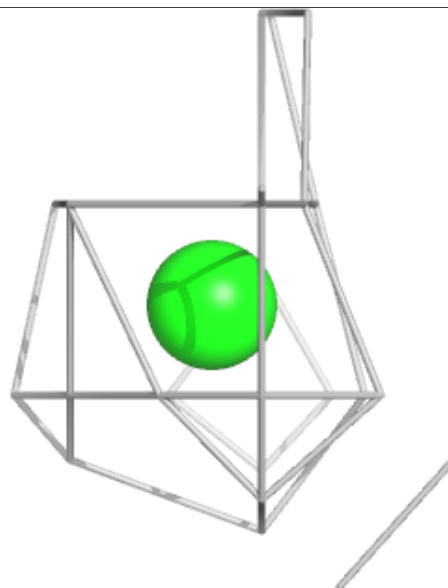
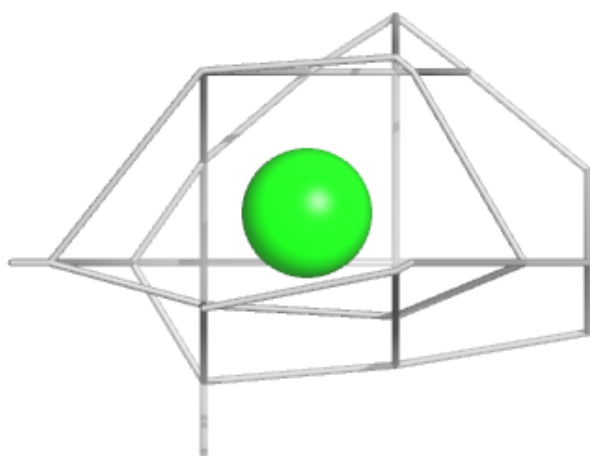
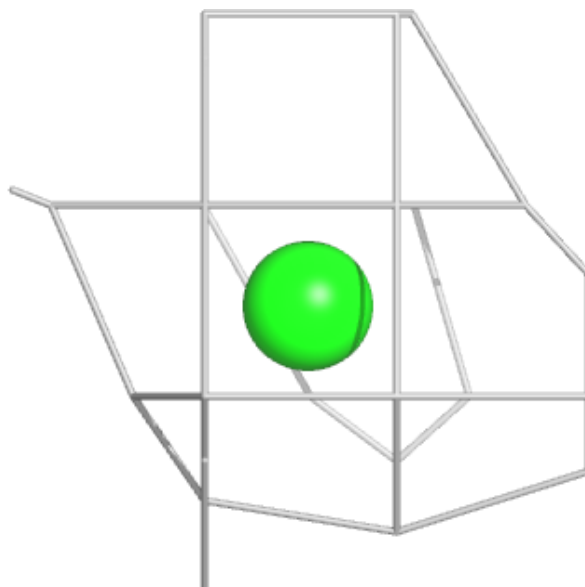
Electron density around CL I 502:

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



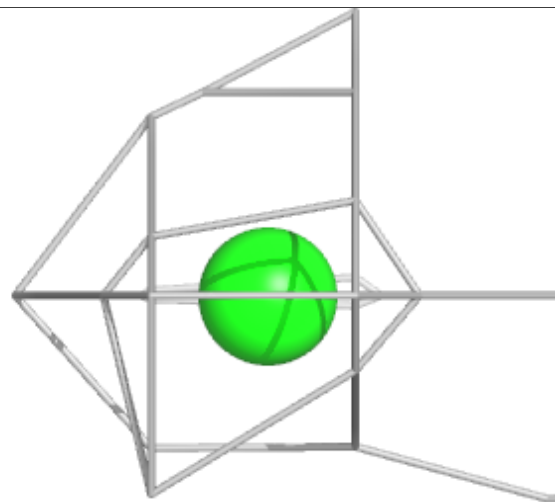
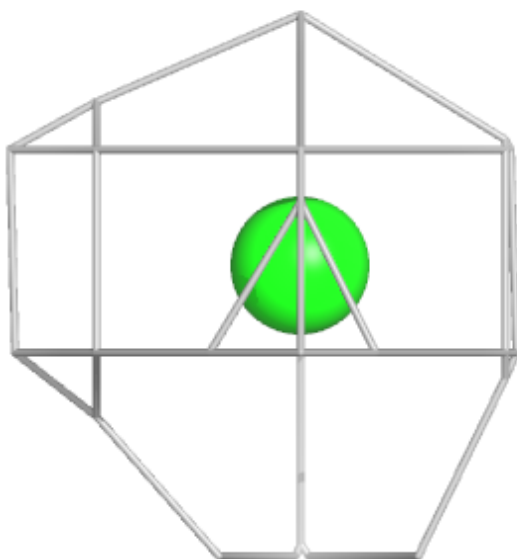
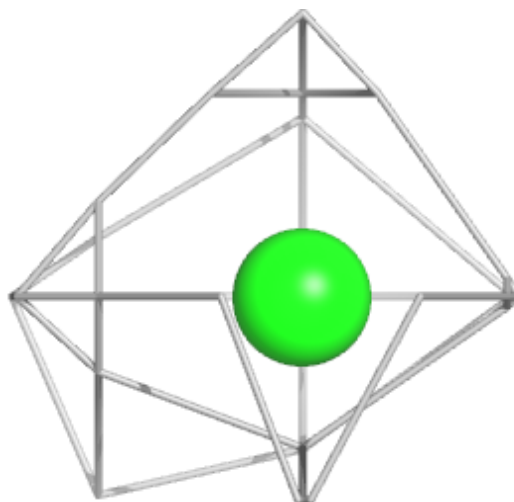
Electron density around CL E 201:

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



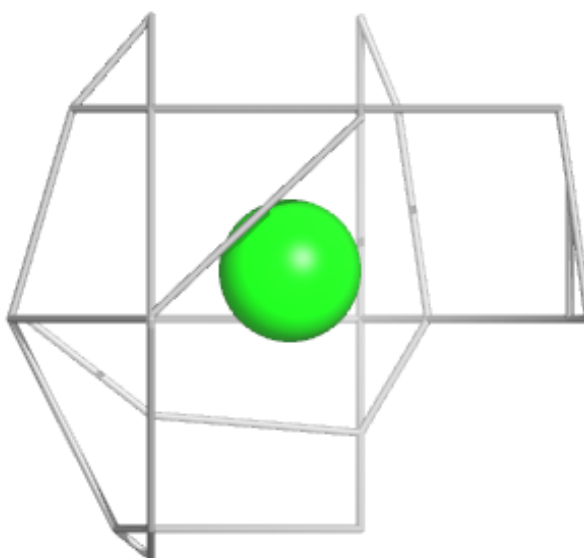
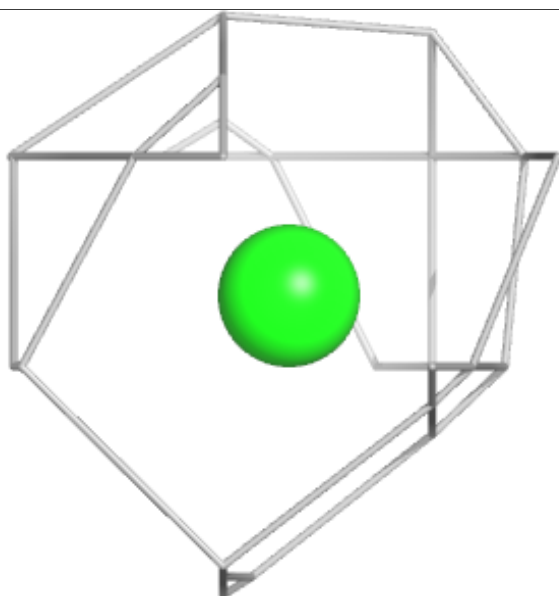
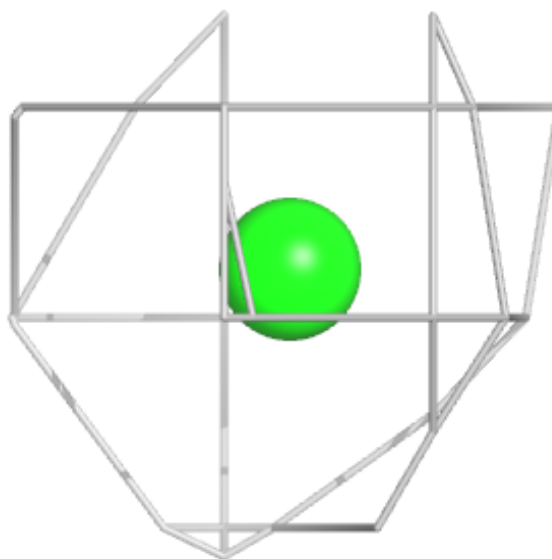
Electron density around CL H 202:

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



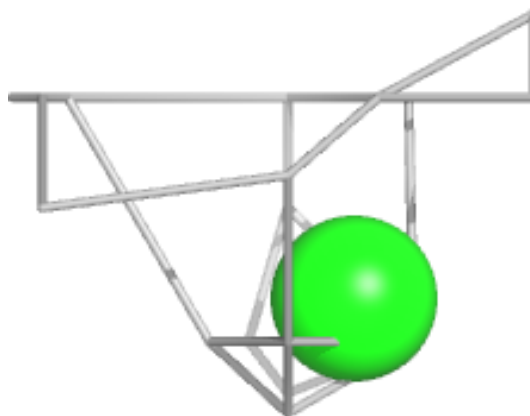
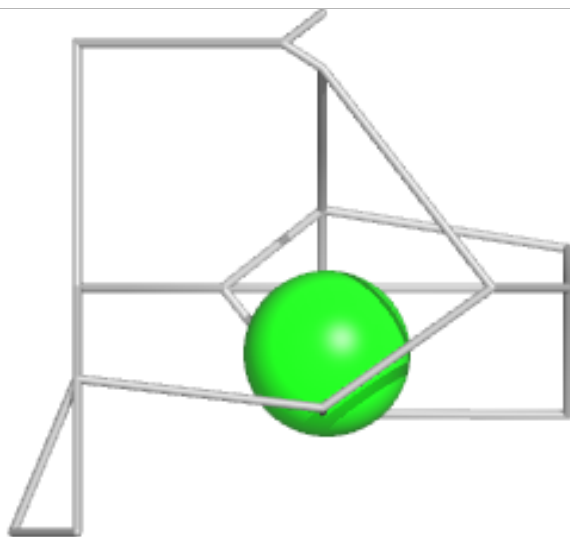
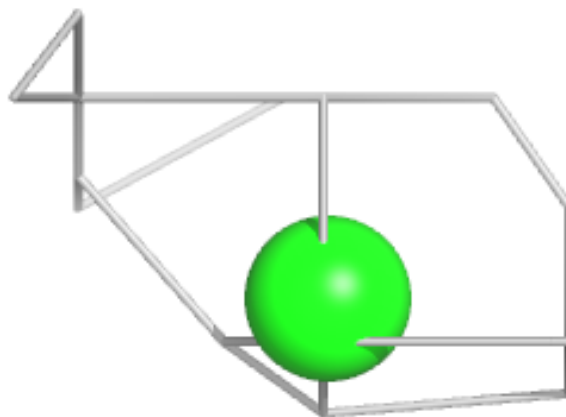
Electron density around CL GG 201:

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



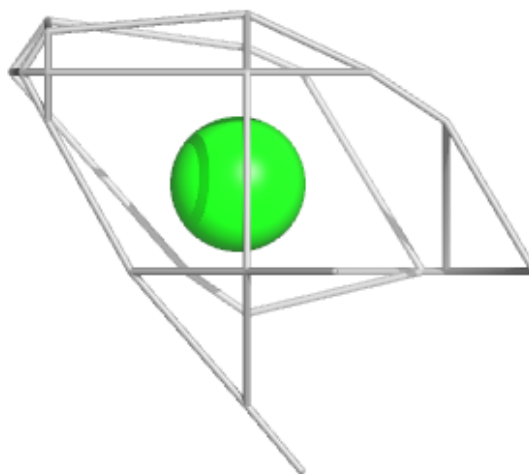
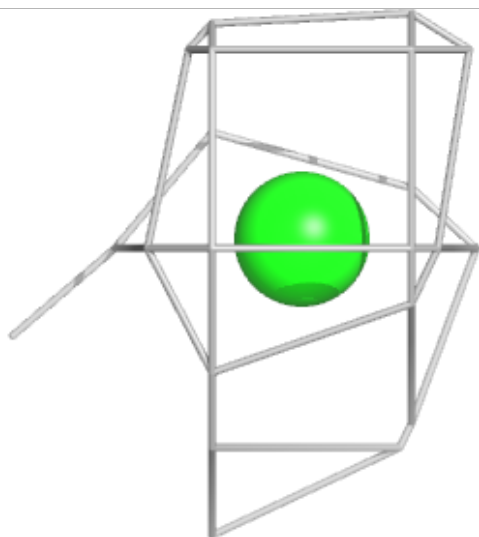
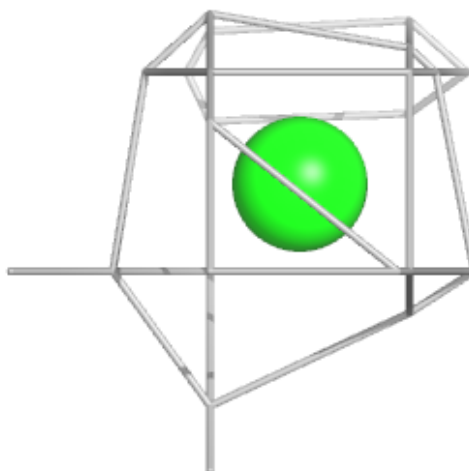
Electron density around CL F 302:

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



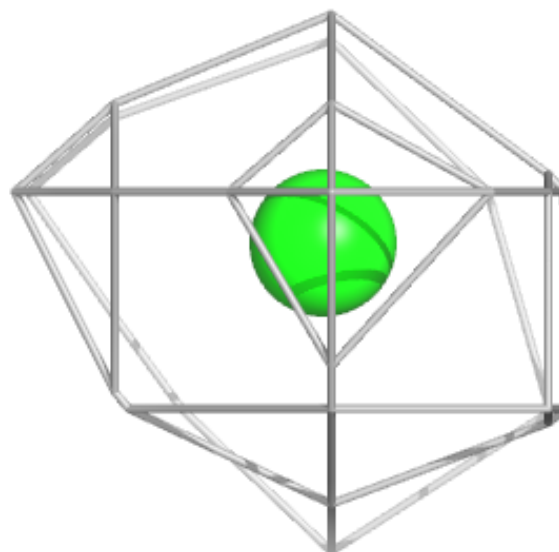
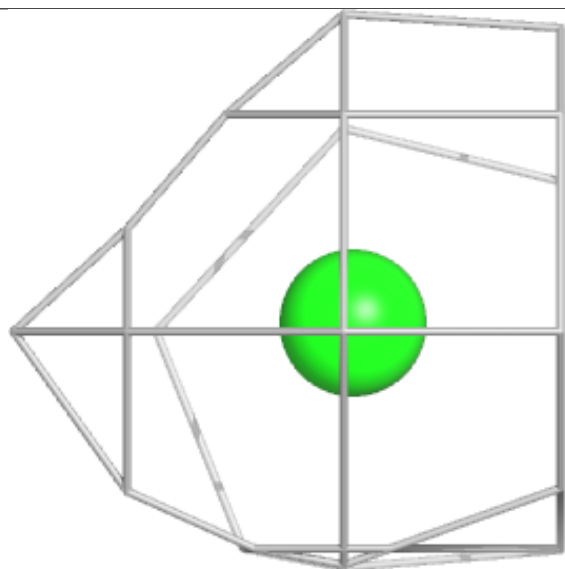
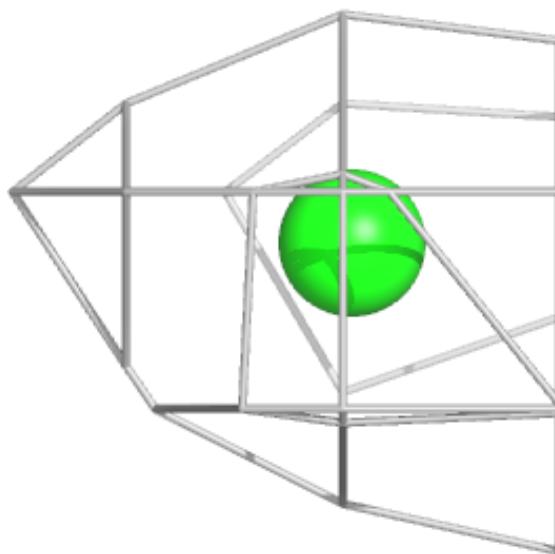
Electron density around CL H 201:

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



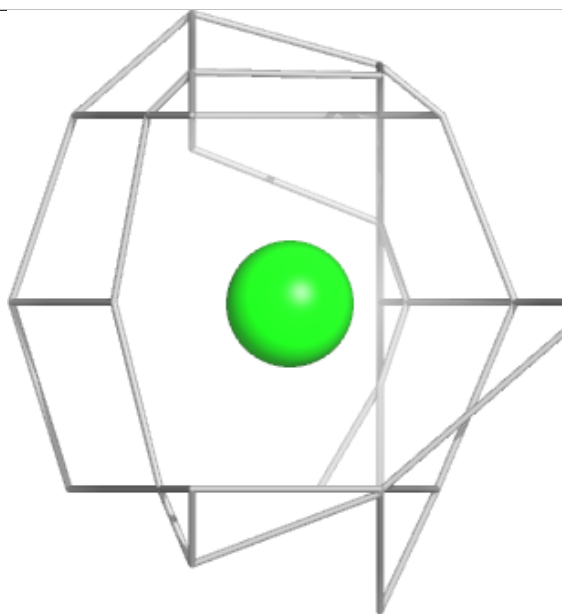
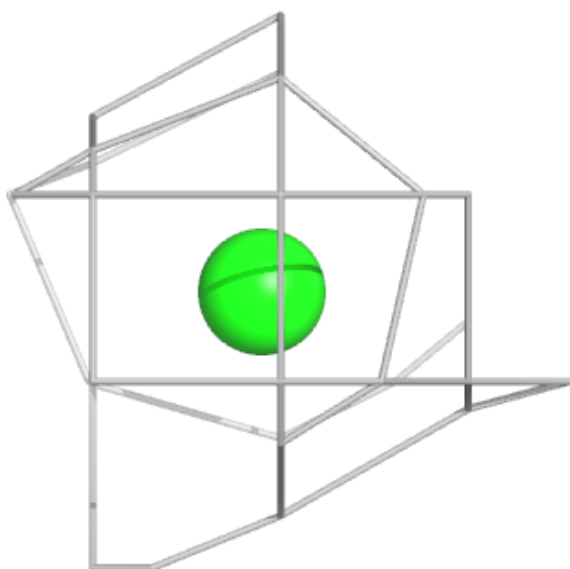
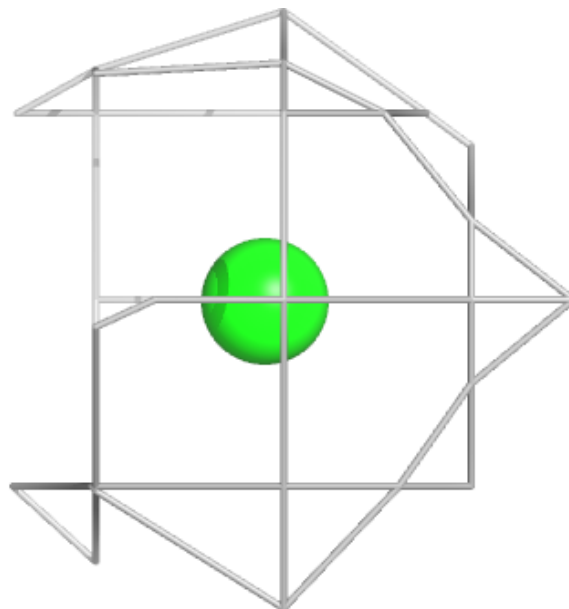
Electron density around CL J 1301:

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



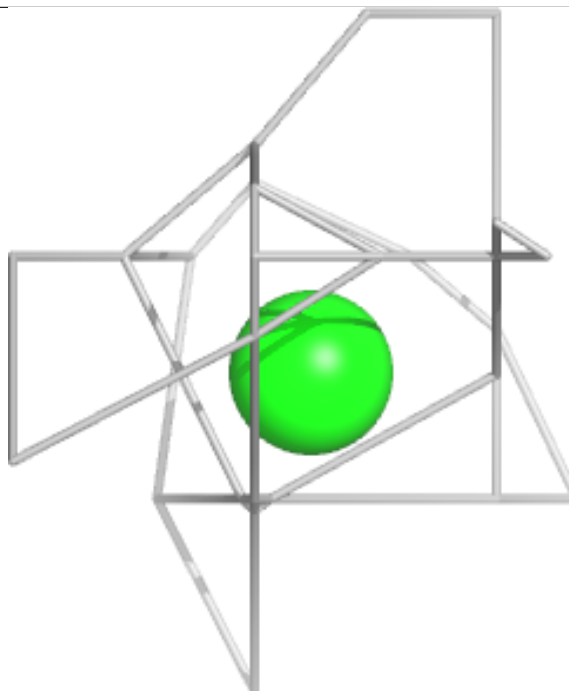
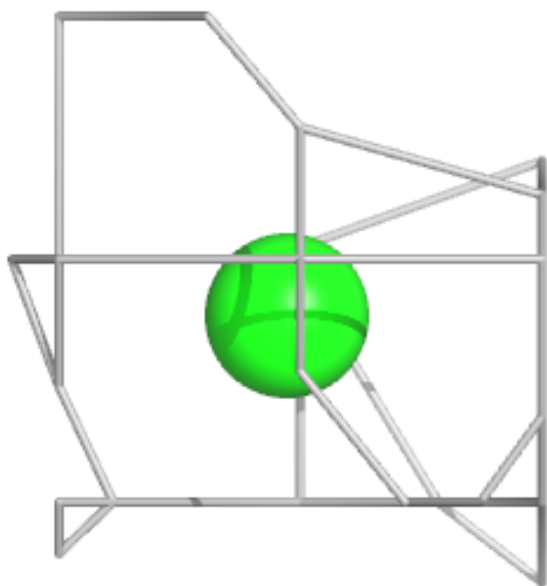
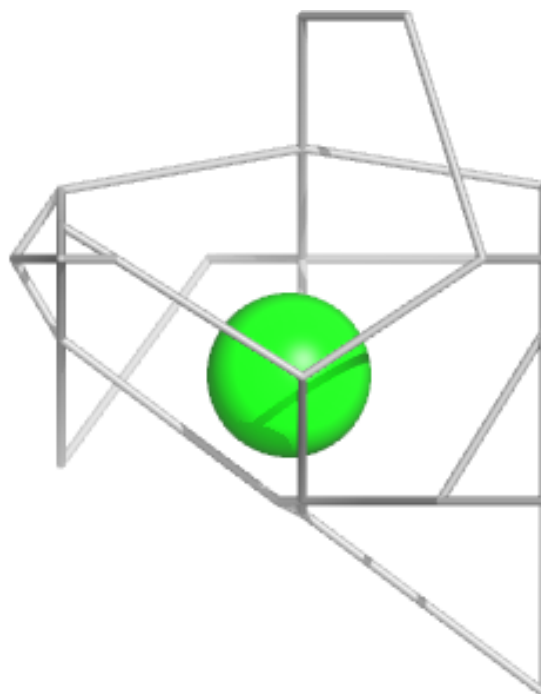
Electron density around CL B 202:

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



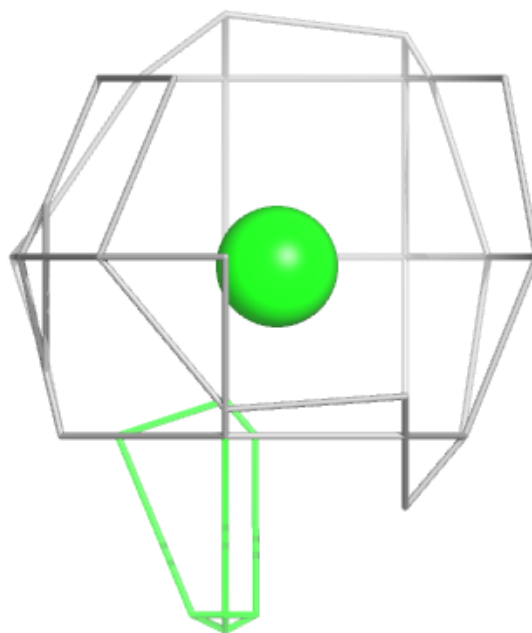
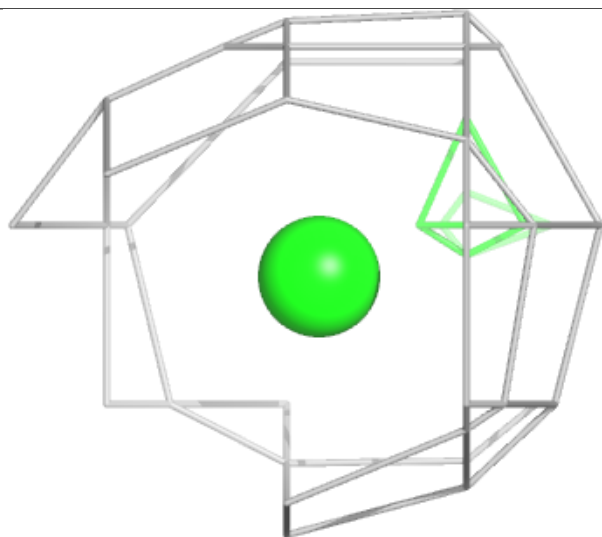
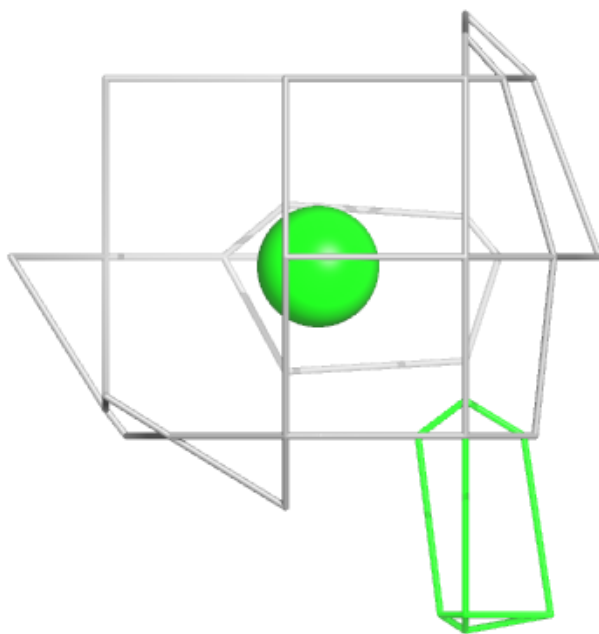
Electron density around CL M 504:

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



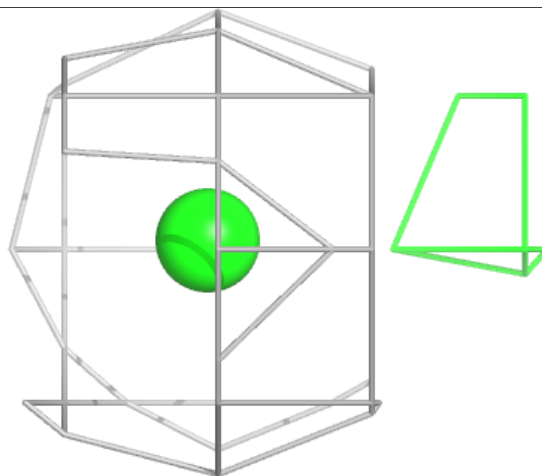
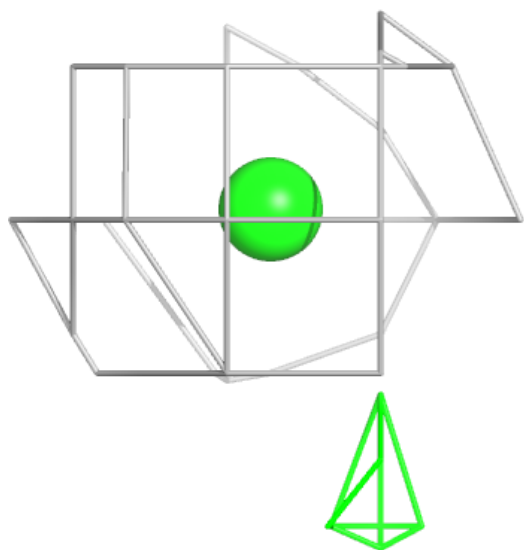
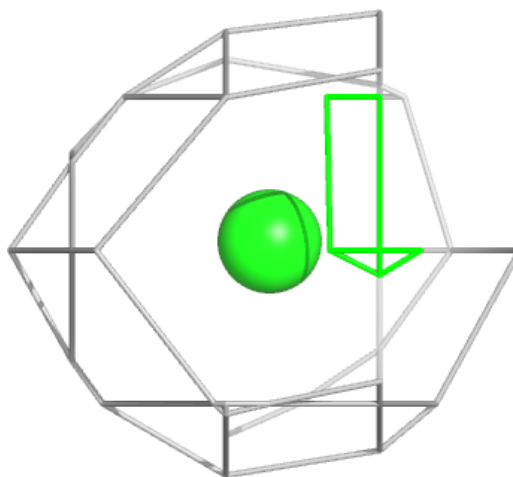
Electron density around CL GG 202:

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



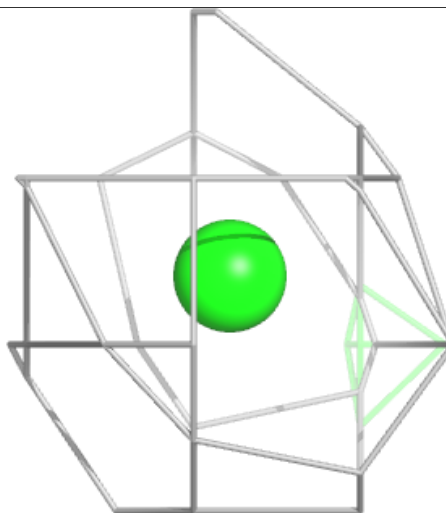
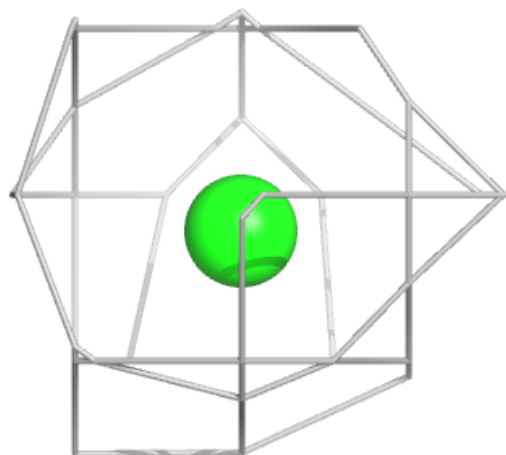
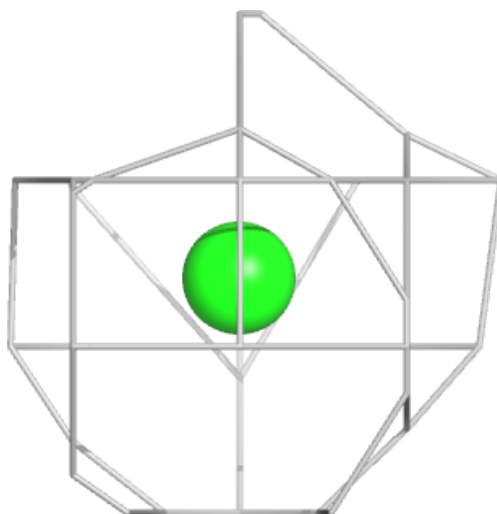
Electron density around CL B 201:

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



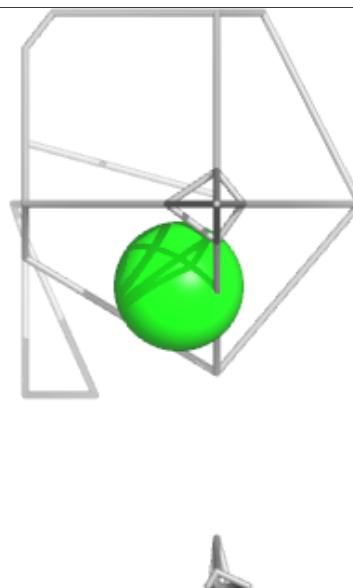
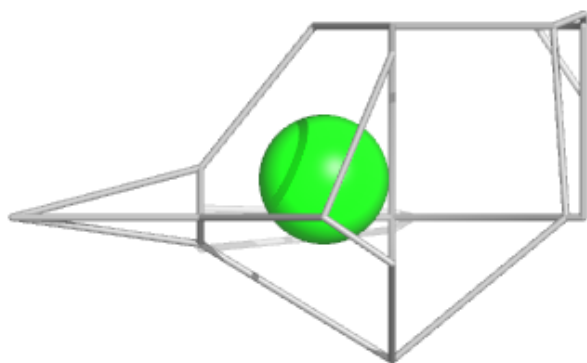
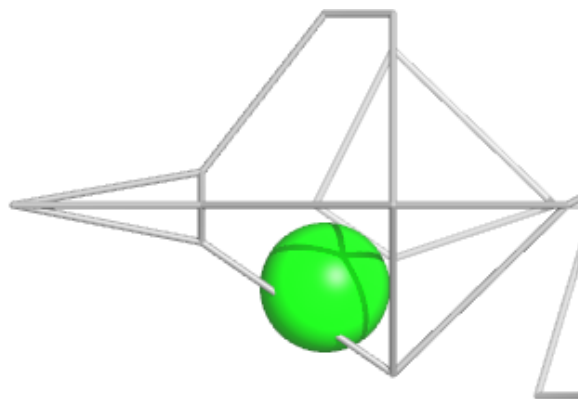
Electron density around CL M 503:

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



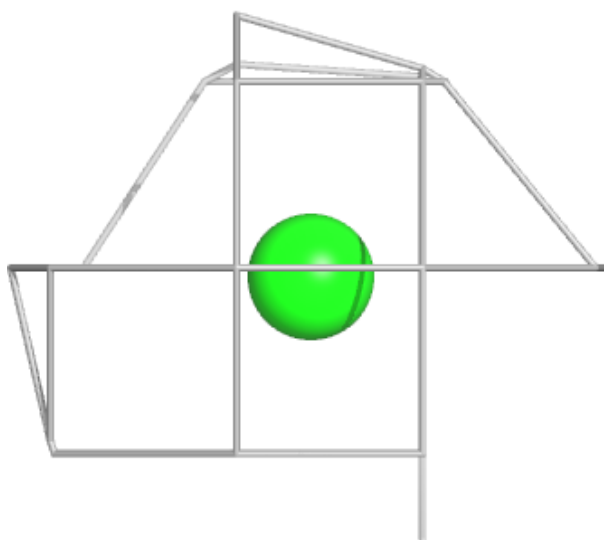
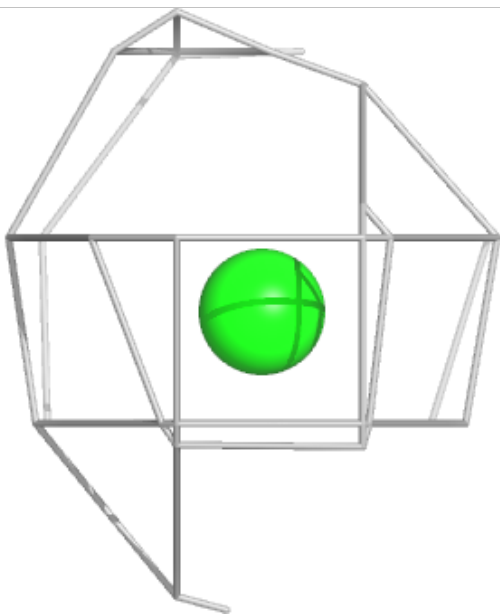
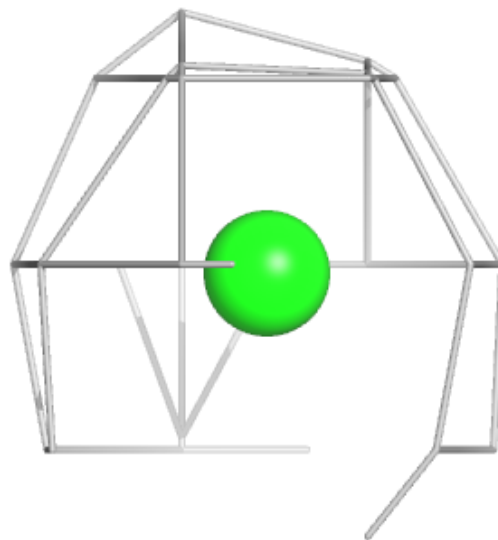
Electron density around CL I 501:

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



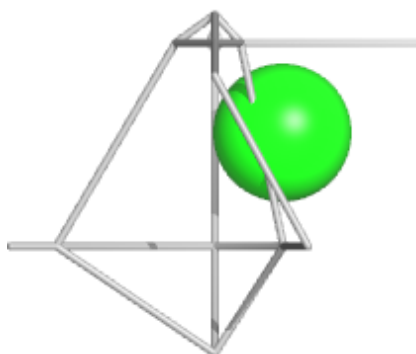
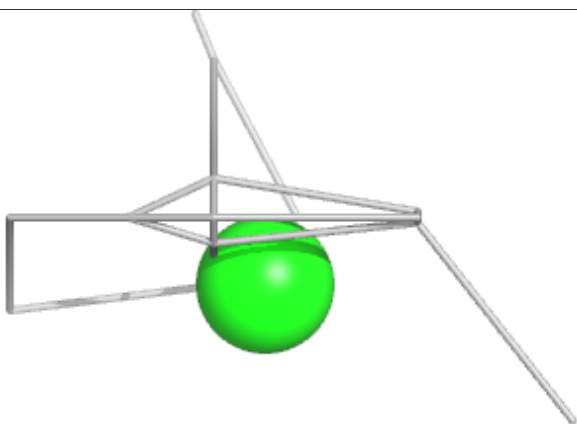
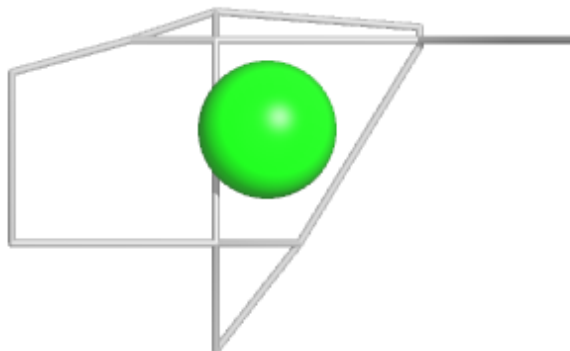
Electron density around CL A 202:

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



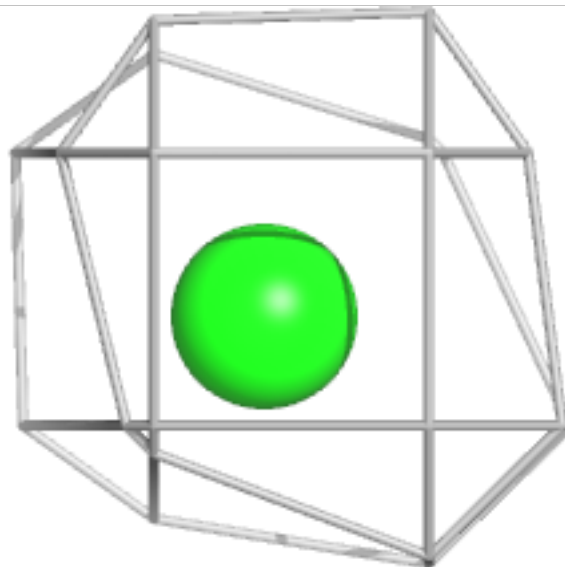
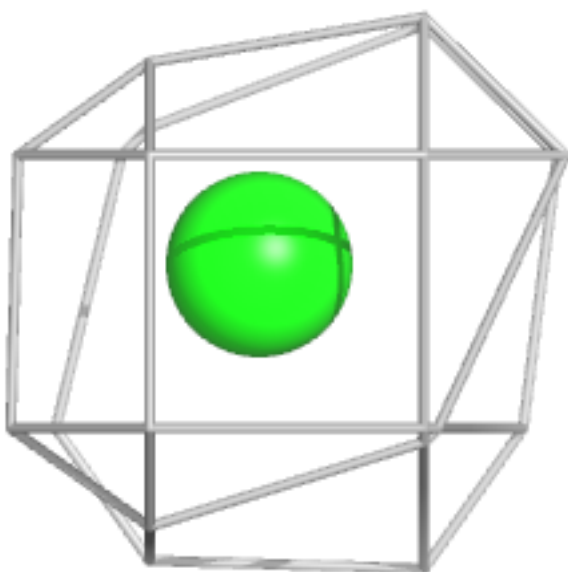
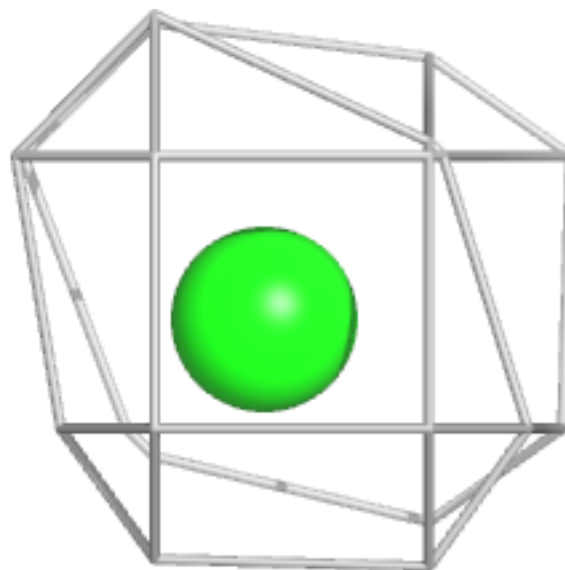
Electron density around CL M 502:

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



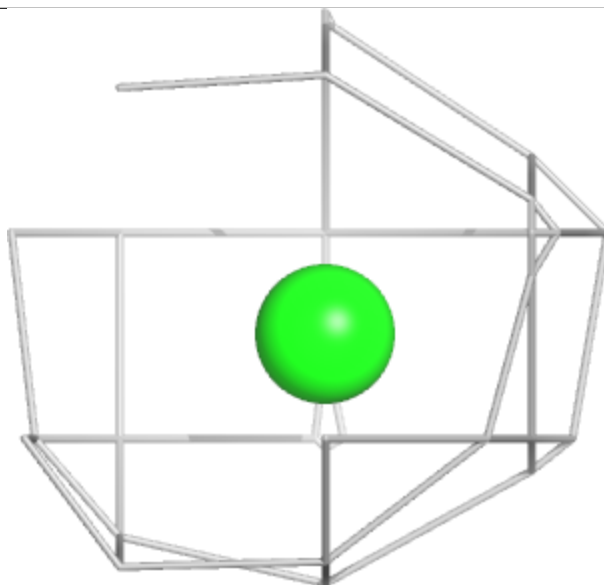
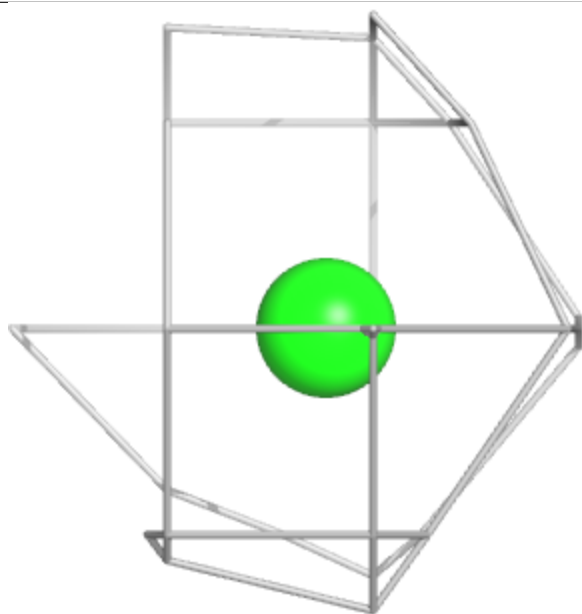
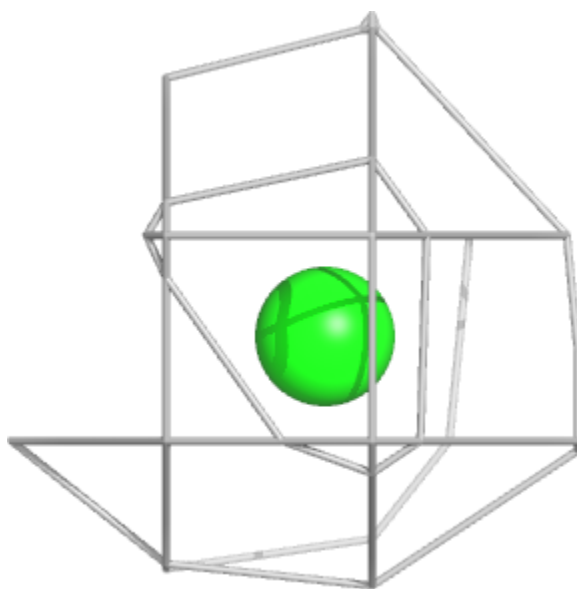
Electron density around CL KK 201:

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



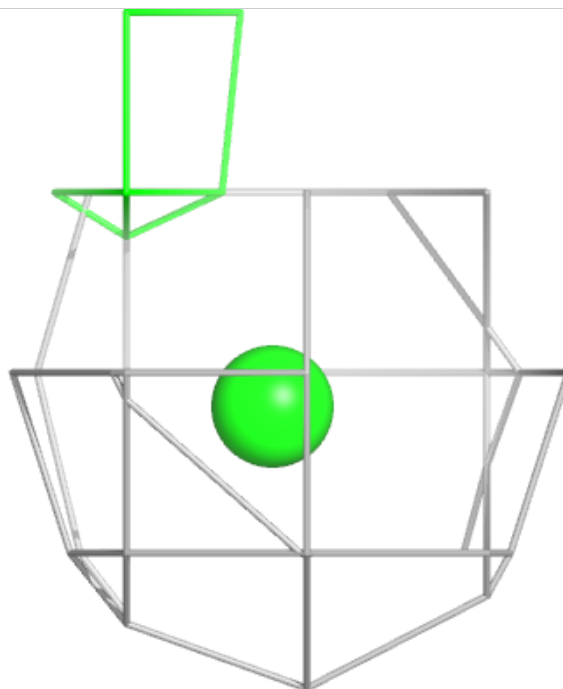
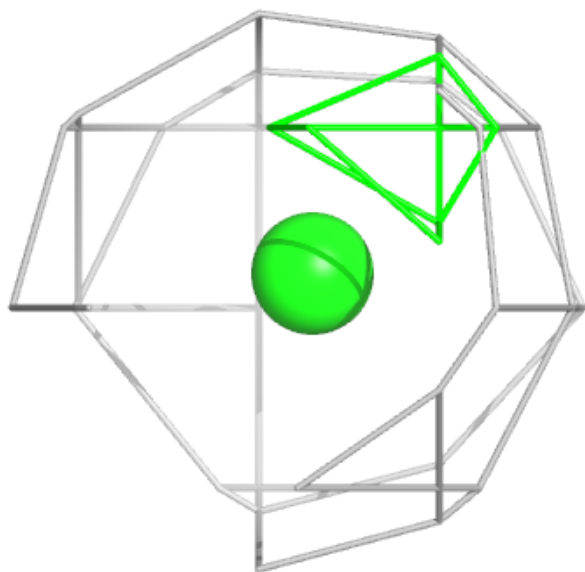
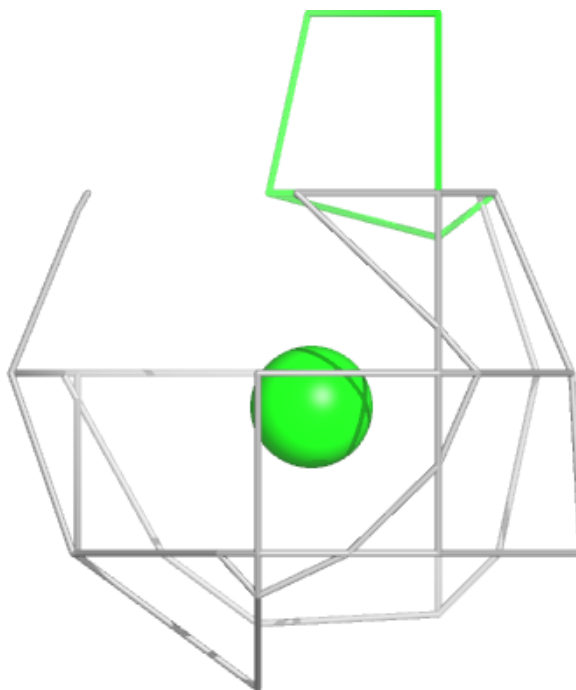
Electron density around CL n 401:

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



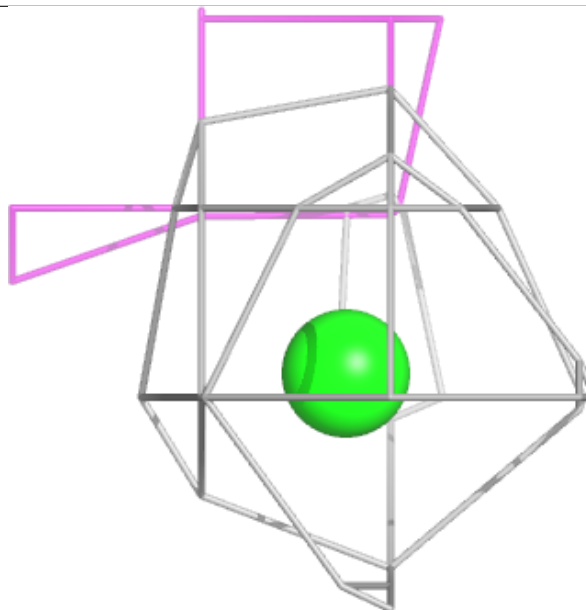
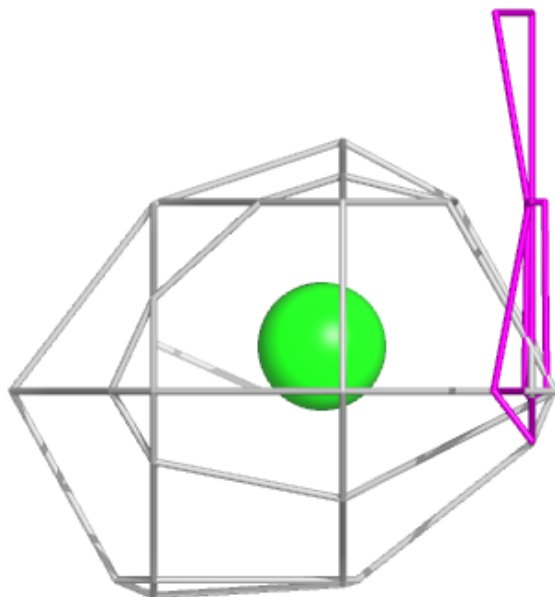
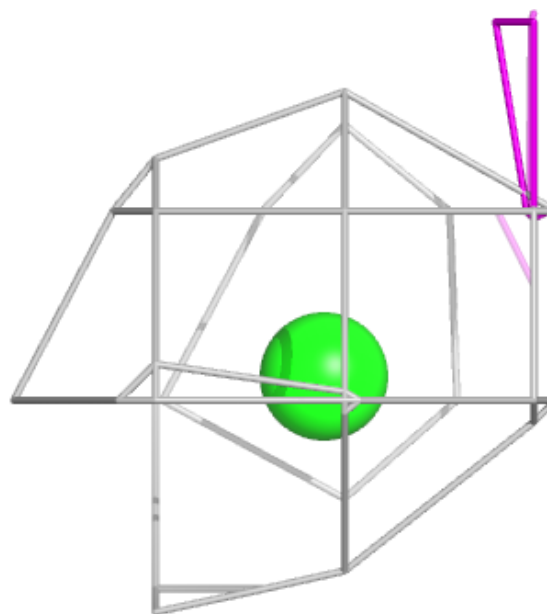
Electron density around CL F 301:

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



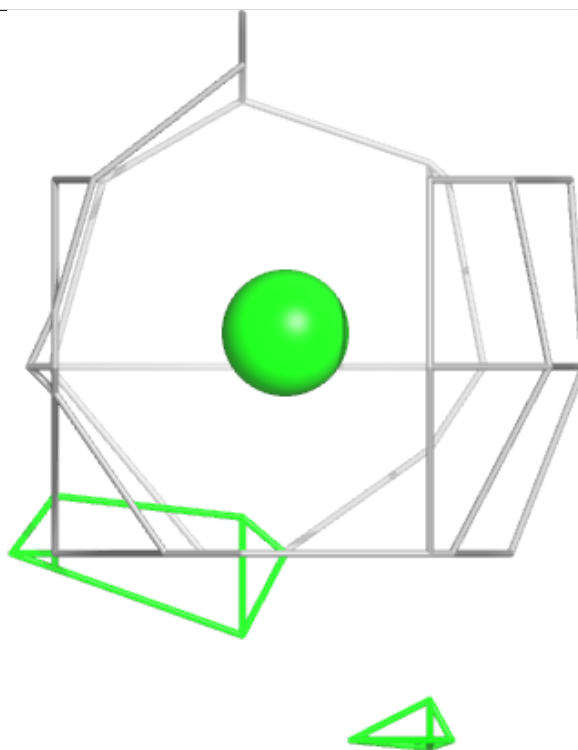
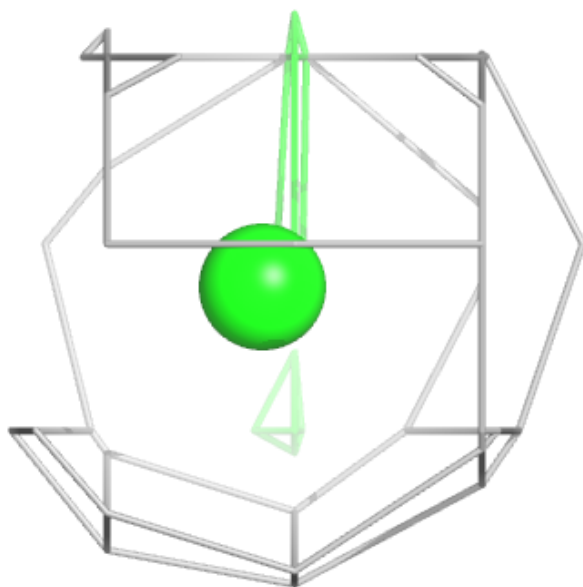
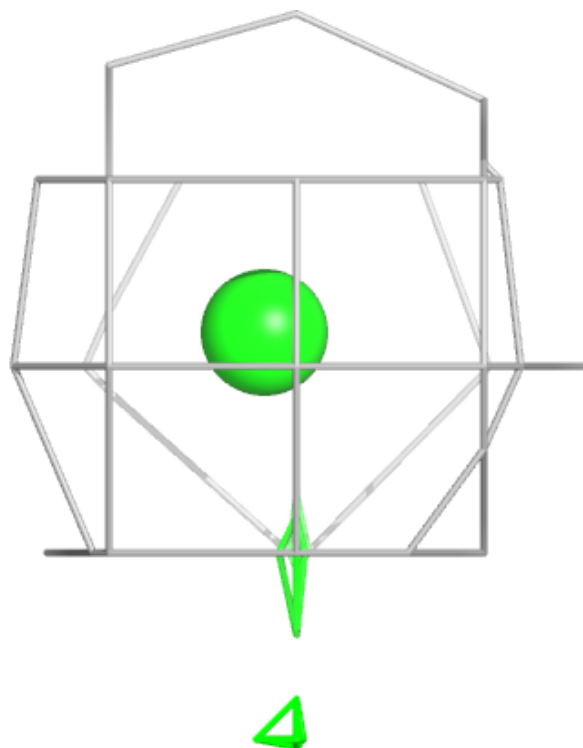
Electron density around CL M 505:

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



Electron density around CL K 301:

$2mF_o - DF_c$ (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.