



# wwPDB EM Validation Summary Report ⓘ

Aug 23, 2026 – 09:28 am BST

PDB ID : 30FF / pdb\_000030ff  
EMDB ID : EMD-57691  
Title : TFIID-containing RNA polymerase II pre-initiation complex in the presence of the +1 nucleosome  
Authors : Zhan, Y.; Abril-Garrido, J.; Grabbe, F.; Seweryn, P.; Neef, U.; Dienemann, C.; Cramer, P.  
Deposited on : 2026-04-22  
Resolution : 8.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

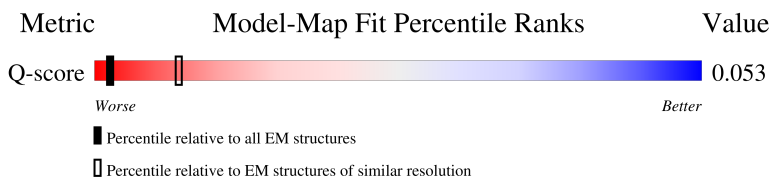
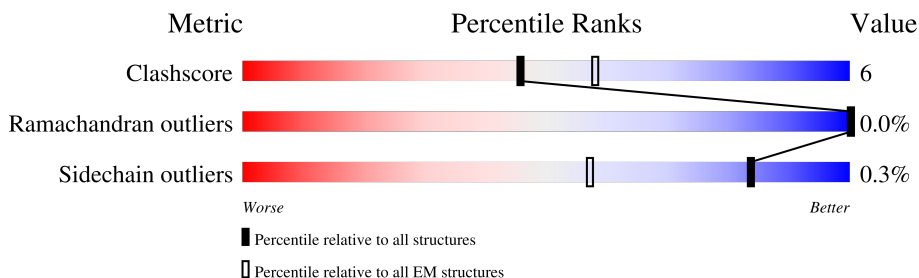
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 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.



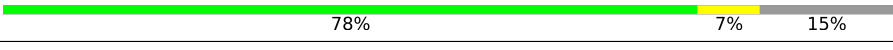
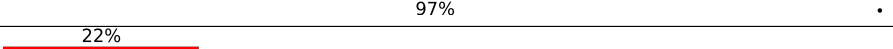
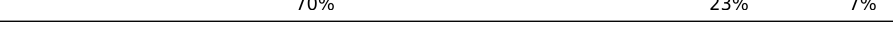
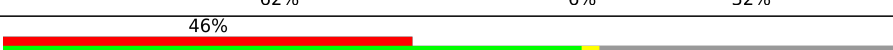
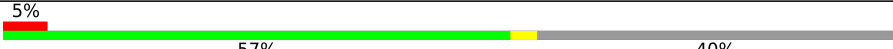
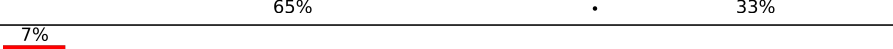
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 328 ( 8.00 - 9.00 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 782    | <br>70% 8% 23%   |
| 2   | 1     | 760    | <br>81% 13% 6%   |
| 3   | 2     | 548    | <br>45% 52%      |
| 4   | 3     | 462    | <br>85% 6% 9%    |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | 4     | 395    |    |
| 6   | 5     | 308    |    |
| 7   | 6     | 71     |    |
| 8   | 7     | 309    |    |
| 9   | 8     | 346    |    |
| 10  | 9     | 323    |    |
| 11  | A     | 1984   |    |
| 12  | B     | 1300   |    |
| 13  | C     | 275    |    |
| 14  | D     | 184    |   |
| 15  | DA    | 1893   |  |
| 16  | DB    | 1199   |  |
| 17  | DD    | 1085   |  |
| 17  | Dd    | 1085   |  |
| 18  | DE    | 800    |  |
| 18  | De    | 800    |  |
| 19  | DF    | 677    |  |
| 19  | Df    | 677    |  |
| 20  | DG    | 349    |  |
| 21  | DH    | 310    |  |
| 22  | DI    | 264    |  |
| 22  | Di    | 264    |  |
| 23  | DJ    | 218    |  |
| 23  | Dj    | 218    |  |
| 24  | DL    | 161    |  |

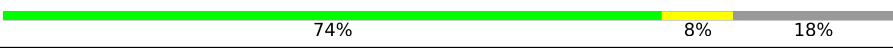
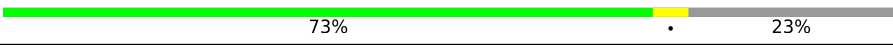
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 24  | Dl    | 161    |                  |
| 25  | Dc    | 929    |                  |
| 26  | Dk    | 211    |                  |
| 27  | Dm    | 124    |                  |
| 28  | E     | 210    |                  |
| 29  | F     | 127    |                  |
| 30  | G     | 172    |                  |
| 31  | H     | 150    |                  |
| 32  | I     | 125    |                  |
| 33  | J     | 67     |                  |
| 34  | K     | 117    |                  |
| 35  | L     | 58     |                  |
| 36  | M     | 316    |                  |
| 37  | N     | 227    |                  |
| 38  | O     | 339    |                  |
| 39  | Q     | 517    |                  |
| 40  | R     | 249    |                  |
| 41  | T     | 227    |                  |
| 42  | U     | 376    |                  |
| 43  | V     | 109    |                  |
| 44  | W     | 439    |                  |
| 45  | X     | 291    |                  |
| 46  | a     | 136    |                  |
| 46  | e     | 136    |                  |
| 47  | b     | 103    |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 47  | f     | 103    |  |
| 48  | c     | 130    |  |
| 48  | g     | 130    |  |
| 49  | d     | 126    |  |
| 49  | h     | 126    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 50  | 2A1  | 0     | 801 | -         | X        | -       | -                |
| 50  | 2A1  | 0     | 804 | -         | X        | -       | -                |
| 50  | 2A1  | 0     | 807 | -         | X        | -       | -                |
| 50  | 2A1  | 0     | 812 | -         | X        | -       | -                |
| 50  | 2A1  | 0     | 815 | -         | X        | -       | -                |
| 50  | 2A1  | 2     | 603 | -         | X        | -       | -                |
| 50  | 2A1  | 2     | 604 | -         | X        | -       | -                |
| 50  | 2A1  | N     | 301 | -         | X        | -       | -                |
| 50  | 2A1  | N     | 303 | -         | X        | -       | -                |
| 50  | 2A1  | N     | 304 | -         | X        | -       | -                |

## 2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 125749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 General transcription and DNA repair factor IIIH helicase subunit XPB.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 0     | 605      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4890  | 3127 | 848 | 885 | 30 |         |       |

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | 1     | 714      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5751  | 3683 | 999 | 1040 | 29 |         |       |

- Molecule 3 is a protein called General transcription factor IIIH subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 2     | 265      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2167  | 1382 | 378 | 395 | 12 |         |       |

- Molecule 4 is a protein called General transcription factor IIIH subunit 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 3     | 421      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3338  | 2154 | 584 | 587 | 13 |         |       |

- Molecule 5 is a protein called General transcription factor IIIH subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 4     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2732  | 1726 | 471 | 508 | 27 |         |       |

- Molecule 6 is a protein called General transcription factor IIIH subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 5     | 263      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2066  | 1323 | 344 | 380 | 19 |         |       |

- Molecule 7 is a protein called General transcription factor IIIH subunit 5.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 7   | 6     | 69       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 549   | 352 | 88 | 106 | 3 |         |       |

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | 7     | 212      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1724  | 1083 | 297 | 332 | 12 |         |       |

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | 8     | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2378  | 1535 | 406 | 426 | 11 |         |       |

- Molecule 10 is a protein called Cyclin-H.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | 9     | 287      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2334  | 1493 | 402 | 422 | 17 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 11  | A     | 1423     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11274 | 7092 | 2016 | 2094 | 72 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 12  | B     | 1136     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9076  | 5739 | 1597 | 1676 | 64 |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | C     | 257      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2059  | 1294 | 351 | 408 | 6 |         |       |

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | D     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1050  | 656 | 178 | 212 | 4 |         |       |

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | DA    | 558      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4563  | 2913 | 791 | 832 | 27 |         |       |

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 16  | DB    | 963      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7796  | 5011 | 1315 | 1412 | 58 |         |       |

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | DD    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1331  | 830 | 248 | 250 | 3 |         |       |
| 17  | Dd    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1308  | 814 | 238 | 253 | 3 |         |       |

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | DE    | 546      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4364  | 2766 | 757 | 820 | 21 |         |       |
| 18  | De    | 539      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4327  | 2746 | 748 | 814 | 19 |         |       |

There are 56 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DE    | 40      | THR      | PRO    | conflict | UNP Q8C092 |
| DE    | ?       | -        | GLY    | deletion | UNP Q8C092 |
| DE    | 53      | ALA      | VAL    | conflict | UNP Q8C092 |
| DE    | 54      | SER      | ALA    | conflict | UNP Q8C092 |
| DE    | 55      | SER      | ALA    | conflict | UNP Q8C092 |
| DE    | 56      | SER      | ALA    | conflict | UNP Q8C092 |
| DE    | 57      | THR      | ALA    | conflict | UNP Q8C092 |
| DE    | 67      | THR      | GLY    | conflict | UNP Q8C092 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DE    | 85      | ALA      | PRO    | conflict | UNP Q8C092 |
| DE    | 86      | PRO      | ALA    | conflict | UNP Q8C092 |
| DE    | 87      | ASP      | GLU    | conflict | UNP Q8C092 |
| DE    | 108     | LYS      | ASN    | conflict | UNP Q8C092 |
| DE    | 121     | GLY      | ARG    | conflict | UNP Q8C092 |
| DE    | 136     | VAL      | LEU    | conflict | UNP Q8C092 |
| DE    | 138     | SER      | GLY    | conflict | UNP Q8C092 |
| DE    | 143     | VAL      | ALA    | conflict | UNP Q8C092 |
| DE    | 144     | THR      | ALA    | conflict | UNP Q8C092 |
| DE    | 155     | ALA      | VAL    | conflict | UNP Q8C092 |
| DE    | 158     | PRO      | SER    | conflict | UNP Q8C092 |
| DE    | 162     | ASP      | GLU    | conflict | UNP Q8C092 |
| DE    | 170     | GLY      | VAL    | conflict | UNP Q8C092 |
| DE    | 171     | ALA      | THR    | conflict | UNP Q8C092 |
| DE    | 172     | THR      | SER    | conflict | UNP Q8C092 |
| DE    | 174     | VAL      | PHE    | conflict | UNP Q8C092 |
| DE    | 188     | GLY      | ALA    | conflict | UNP Q8C092 |
| DE    | 310     | SER      | TYR    | conflict | UNP Q8C092 |
| DE    | 635     | PHE      | TYR    | conflict | UNP Q8C092 |
| DE    | 741     | ILE      | VAL    | conflict | UNP Q8C092 |
| De    | 40      | THR      | PRO    | conflict | UNP Q8C092 |
| De    | ?       | -        | GLY    | deletion | UNP Q8C092 |
| De    | 53      | ALA      | VAL    | conflict | UNP Q8C092 |
| De    | 54      | SER      | ALA    | conflict | UNP Q8C092 |
| De    | 55      | SER      | ALA    | conflict | UNP Q8C092 |
| De    | 56      | SER      | ALA    | conflict | UNP Q8C092 |
| De    | 57      | THR      | ALA    | conflict | UNP Q8C092 |
| De    | 67      | THR      | GLY    | conflict | UNP Q8C092 |
| De    | 85      | ALA      | PRO    | conflict | UNP Q8C092 |
| De    | 86      | PRO      | ALA    | conflict | UNP Q8C092 |
| De    | 87      | ASP      | GLU    | conflict | UNP Q8C092 |
| De    | 108     | LYS      | ASN    | conflict | UNP Q8C092 |
| De    | 121     | GLY      | ARG    | conflict | UNP Q8C092 |
| De    | 136     | VAL      | LEU    | conflict | UNP Q8C092 |
| De    | 138     | SER      | GLY    | conflict | UNP Q8C092 |
| De    | 143     | VAL      | ALA    | conflict | UNP Q8C092 |
| De    | 144     | THR      | ALA    | conflict | UNP Q8C092 |
| De    | 155     | ALA      | VAL    | conflict | UNP Q8C092 |
| De    | 158     | PRO      | SER    | conflict | UNP Q8C092 |
| De    | 162     | ASP      | GLU    | conflict | UNP Q8C092 |
| De    | 170     | GLY      | VAL    | conflict | UNP Q8C092 |
| De    | 171     | ALA      | THR    | conflict | UNP Q8C092 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| De    | 172     | THR      | SER    | conflict | UNP Q8C092 |
| De    | 174     | VAL      | PHE    | conflict | UNP Q8C092 |
| De    | 188     | GLY      | ALA    | conflict | UNP Q8C092 |
| De    | 310     | SER      | TYR    | conflict | UNP Q8C092 |
| De    | 635     | PHE      | TYR    | conflict | UNP Q8C092 |
| De    | 741     | ILE      | VAL    | conflict | UNP Q8C092 |

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | DF    | 408      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3109  | 1970 | 542 | 579 | 18 |         |       |
| 19  | Df    | 403      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3081  | 1954 | 533 | 576 | 18 |         |       |

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | DG    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1180  | 748 | 217 | 211 | 4 |         |       |

- Molecule 21 is a protein called Transcription initiation factor TFIID subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | DH    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 1034 | 283 | 311 | 5 |         |       |

- Molecule 22 is a protein called Transcription initiation factor TFIID subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | DI    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 959   | 610 | 166 | 177 | 6 |         |       |
| 22  | Di    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 615 | 167 | 178 | 7 |         |       |

There are 18 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DI    | 6       | THR      | MET    | conflict | UNP Q17QQ4 |
| DI    | 138     | THR      | ALA    | conflict | UNP Q17QQ4 |
| DI    | 168     | GLN      | PRO    | conflict | UNP Q17QQ4 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DI    | 169     | THR      | ALA    | conflict | UNP Q17QQ4 |
| DI    | 180     | MET      | VAL    | conflict | UNP Q17QQ4 |
| DI    | 231     | MET      | VAL    | conflict | UNP Q17QQ4 |
| DI    | 240     | SER      | ALA    | conflict | UNP Q17QQ4 |
| DI    | 248     | ARG      | HIS    | conflict | UNP Q17QQ4 |
| DI    | 249     | GLU      | ASP    | conflict | UNP Q17QQ4 |
| Di    | 6       | THR      | MET    | conflict | UNP Q17QQ4 |
| Di    | 138     | THR      | ALA    | conflict | UNP Q17QQ4 |
| Di    | 168     | GLN      | PRO    | conflict | UNP Q17QQ4 |
| Di    | 169     | THR      | ALA    | conflict | UNP Q17QQ4 |
| Di    | 180     | MET      | VAL    | conflict | UNP Q17QQ4 |
| Di    | 231     | MET      | VAL    | conflict | UNP Q17QQ4 |
| Di    | 240     | SER      | ALA    | conflict | UNP Q17QQ4 |
| Di    | 248     | ARG      | HIS    | conflict | UNP Q17QQ4 |
| Di    | 249     | GLU      | ASP    | conflict | UNP Q17QQ4 |

- Molecule 23 is a protein called Transcription initiation factor TFIID subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | DJ    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 720   | 466 | 115 | 135 | 4 |         |       |
| 23  | Dj    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 760   | 488 | 124 | 144 | 4 |         |       |

- Molecule 24 is a protein called Transcription initiation factor TFIID subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | DL    | 74       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 605   | 379 | 105 | 118 | 3 |         |       |
| 24  | DI    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 547 | 158 | 167 | 5 |         |       |

- Molecule 25 is a protein called Transcription initiation factor TFIID subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Dc    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 638 | 174 | 193 | 6 |         |       |

- Molecule 26 is a protein called Transcription initiation factor TFIID subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Dk    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 499 | 142 | 140 | 5 |         |       |

- Molecule 27 is a protein called Transcription initiation factor TFIID subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Dm    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 724   | 456 | 131 | 131 | 6 |         |       |

- Molecule 28 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | E     | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1721  | 1089 | 300 | 324 | 8 |         |       |

- Molecule 29 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | F     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 406 | 108 | 117 | 5 |         |       |

- Molecule 30 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | G     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1351  | 875 | 219 | 249 | 8 |         |       |

- Molecule 31 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | H     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1186  | 750 | 194 | 237 | 5 |         |       |

- Molecule 32 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 32  | I     | 114      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 928   | 571 | 166 | 180 | 11 |         |       |

- Molecule 33 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | J     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 507   | 328 | 86 | 87 | 6 |         |       |

- Molecule 34 is a protein called RNA polymerase II subunit J.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | K     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 920   | 593 | 152 | 173 | 2 |         |       |

- Molecule 35 is a protein called RNA polymerase II subunit K.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | L     | 44       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 373   | 231 | 72 | 64 | 6 |         |       |

- Molecule 36 is a protein called Transcription initiation factor IIB.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | M     | 252      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1954  | 1224 | 346 | 367 | 17 |         |       |

- Molecule 37 is a DNA chain called Non-template DNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 37  | N     | 227      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 4645  | 2201 | 862 | 1356 | 226 |         |       |

- Molecule 38 is a protein called TATA-box-binding protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | O     | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1422  | 923 | 251 | 241 | 7 |         |       |

- Molecule 39 is a protein called General transcription factor IIF subunit 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | Q     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1138  | 719 | 208 | 208 | 3 |         |       |

- Molecule 40 is a protein called General transcription factor IIF subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | R     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1788  | 1127 | 320 | 338 | 3 |         |       |

- Molecule 41 is a DNA chain called Template DNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 41  | T     | 227      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 4656  | 2206 | 860 | 1364 | 226 |         |       |

- Molecule 42 is a protein called Transcription initiation factor IIA subunit 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | U     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 931   | 585 | 152 | 190 | 4 |         |       |

- Molecule 43 is a protein called Transcription initiation factor IIA subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | V     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 806   | 510 | 142 | 151 | 3 |         |       |

- Molecule 44 is a protein called General transcription factor IIE subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | W     | 202      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1659  | 1042 | 299 | 307 | 11 |         |       |

- Molecule 45 is a protein called Transcription initiation factor IIE subunit beta.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | X     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1403  | 895 | 243 | 261 | 4 |         |       |

- Molecule 46 is a protein called Histone H3.2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | a     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 801   | 505 | 155 | 138 | 3 |         |       |
| 46  | e     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 511 | 157 | 139 | 3 |         |       |

- Molecule 47 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | b     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 653   | 412 | 127 | 113 | 1 |         |       |
| 47  | f     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 401 | 125 | 111 | 1 |         |       |

- Molecule 48 is a protein called Histone H2A type 1.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 48  | c     | 109      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 843   | 531 | 167 | 145 |  |         |       |
| 48  | g     | 106      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 818   | 516 | 160 | 142 |  |         |       |

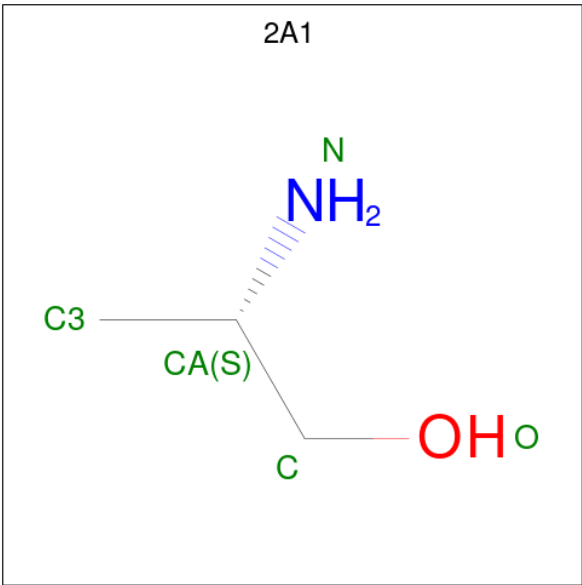
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| c     | 100     | ARG      | GLY    | engineered mutation | UNP P06897 |
| g     | 100     | ARG      | GLY    | engineered mutation | UNP P06897 |

- Molecule 49 is a protein called Histone H2B 1.1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | d     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 766   | 480 | 142 | 142 | 2 |         |       |
| 49  | h     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 744   | 468 | 134 | 140 | 2 |         |       |

- Molecule 50 is (2S)-2-aminopropan-1-ol (CCD ID: 2A1) (formula: C<sub>3</sub>H<sub>9</sub>NO) (labeled as "Ligand of Interest" by depositor).



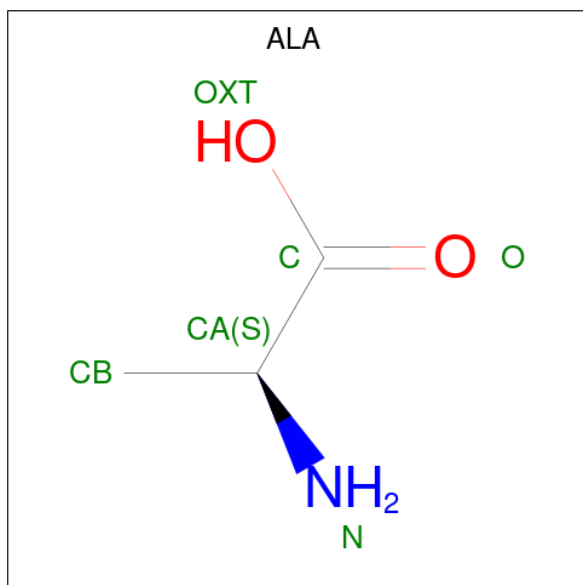
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |

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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 50  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 50  | N     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |

- Molecule 51 is ALANINE (CCD ID: ALA) (formula:  $C_3H_7NO_2$ ).



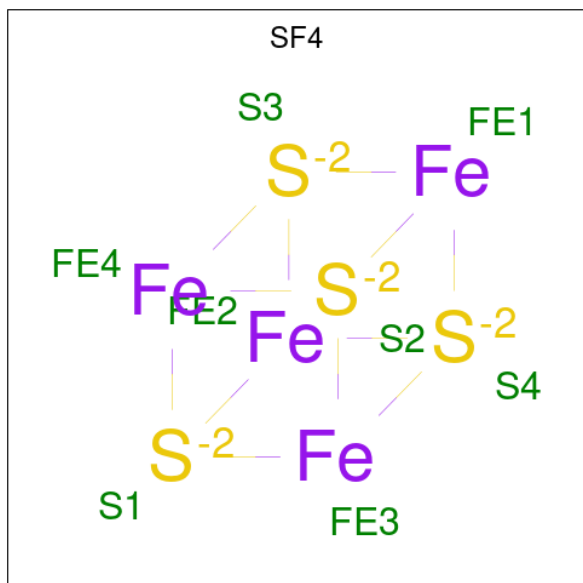
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 51  | 0     | 1        | Total | C | N | O | 0       |
|     |       |          | 6     | 3 | 1 | 2 |         |

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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 51  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |
| 51  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 6     | 3 | 1 | 2 |         |

- Molecule 52 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 52  | 1     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 53  | 4     | 3        | Total | Zn | 0       |
|     |       |          | 3     | 3  |         |
| 53  | 5     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 53  | 7     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 53  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 53  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 53  | C     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 53  | I     | 2        | Total<br>2 | Zn<br>2 | 0       |
| 53  | J     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 53  | L     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 53  | M     | 1        | Total<br>1 | Zn<br>1 | 0       |
| 53  | W     | 1        | Total<br>1 | Zn<br>1 | 0       |

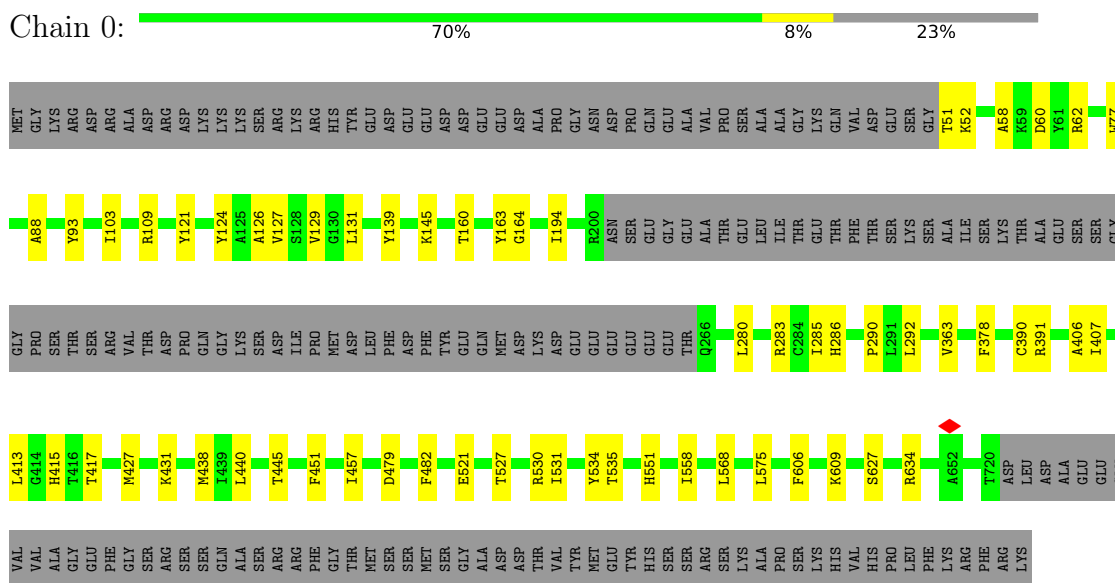
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 54  | A     | 1        | Total<br>1 | Mg<br>1 | 0       |

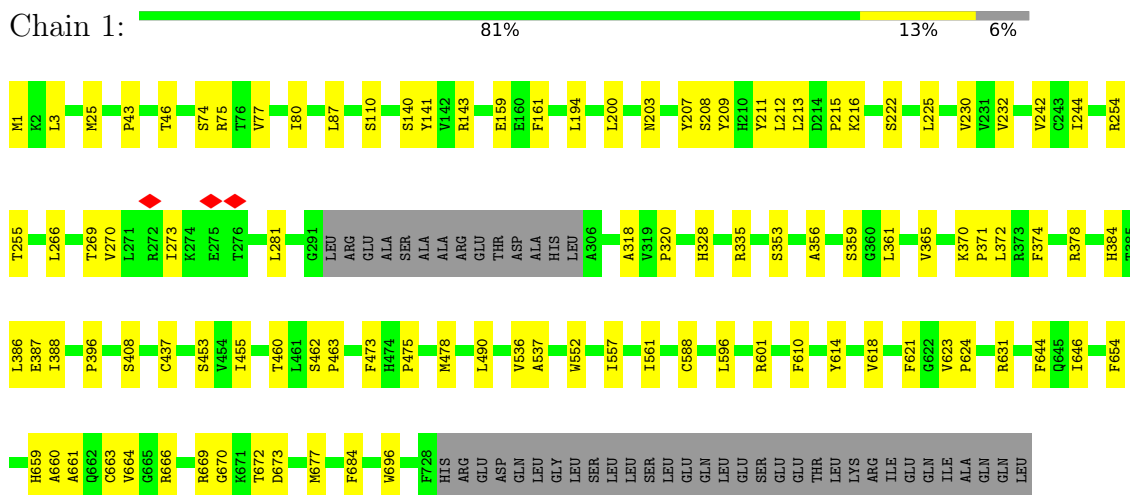
### 3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: General transcription and DNA repair factor IIH helicase subunit XPB



- Molecule 2: TFIIH basal transcription factor complex helicase XPD subunit



- Molecule 3: General transcription factor IIH subunit 1

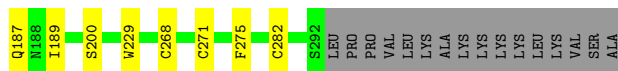
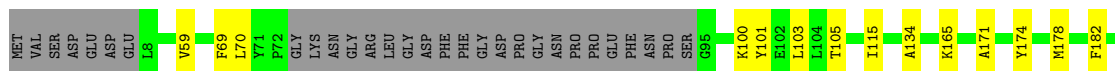
- Molecule 4: General transcription factor IIH subunit 4

- Molecule 5: General transcription factor IIH subunit 2

- Molecule 6: General transcription factor IIH subunit 3

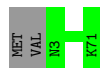


WORLD WIDE  
PDB  
PROTEIN DATA BANK



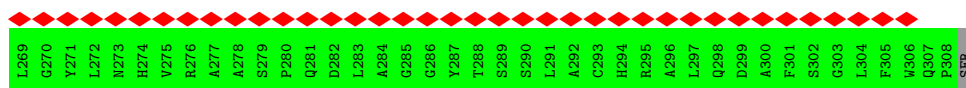
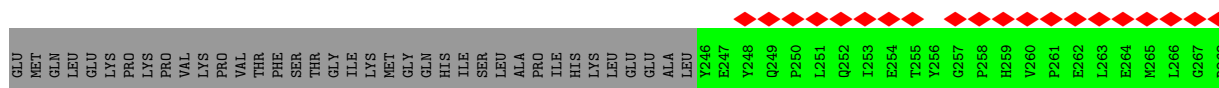
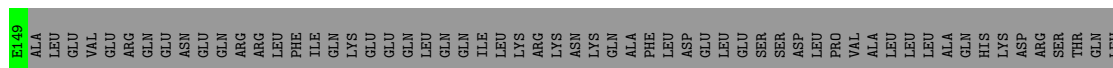
- Molecule 7: General transcription factor IIH subunit 5

Chain 6: 97%



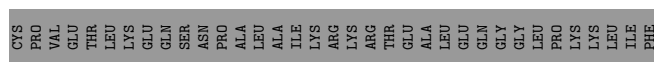
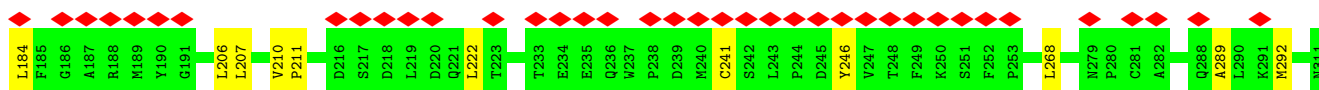
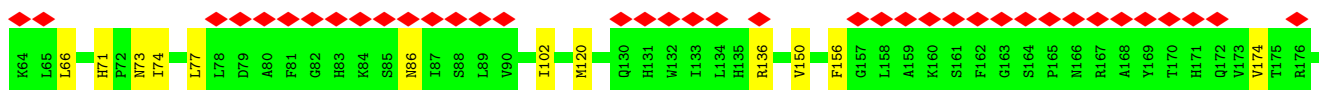
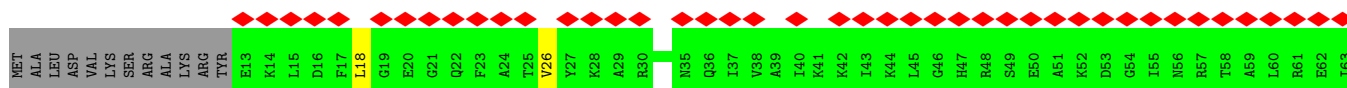
- Molecule 8: CDK-activating kinase assembly factor MAT1

Chain 7: 22% 60% 8% 31%

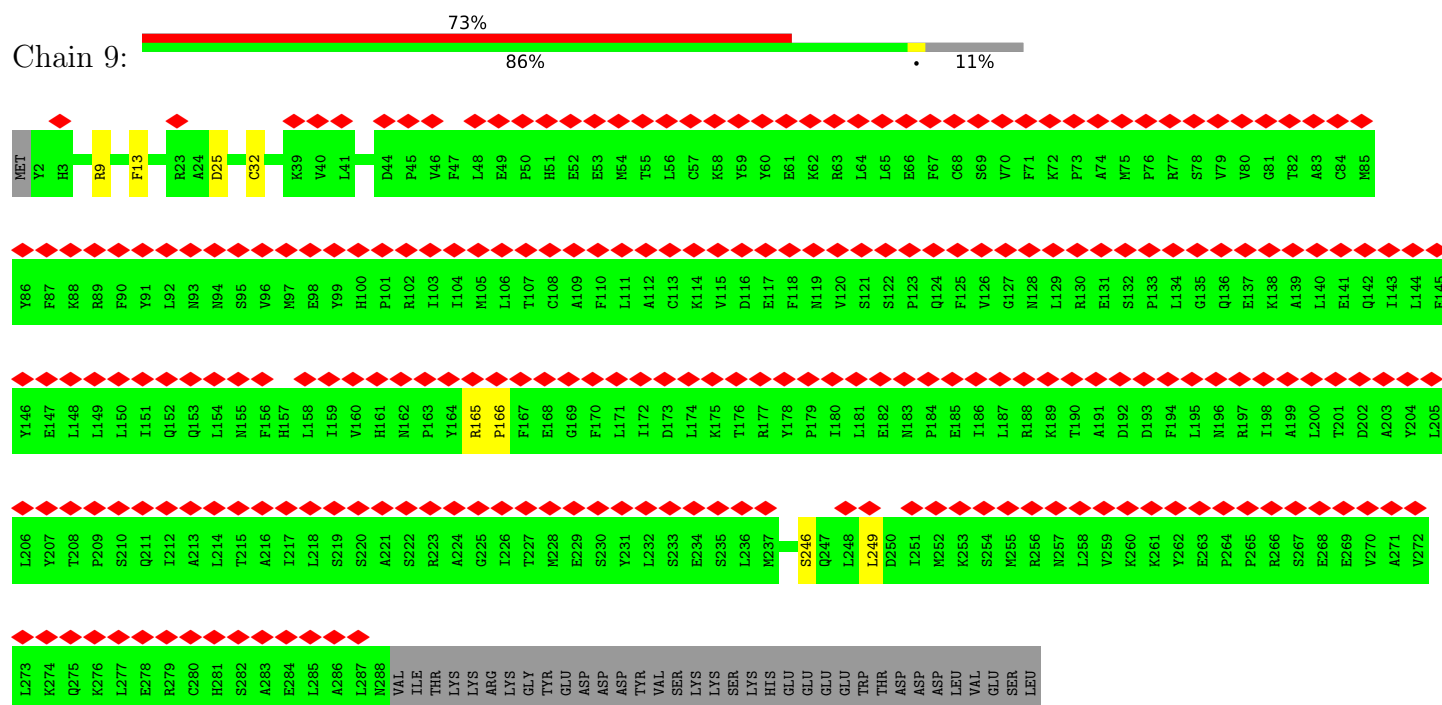


- Molecule 9: Cyclin-dependent kinase 7

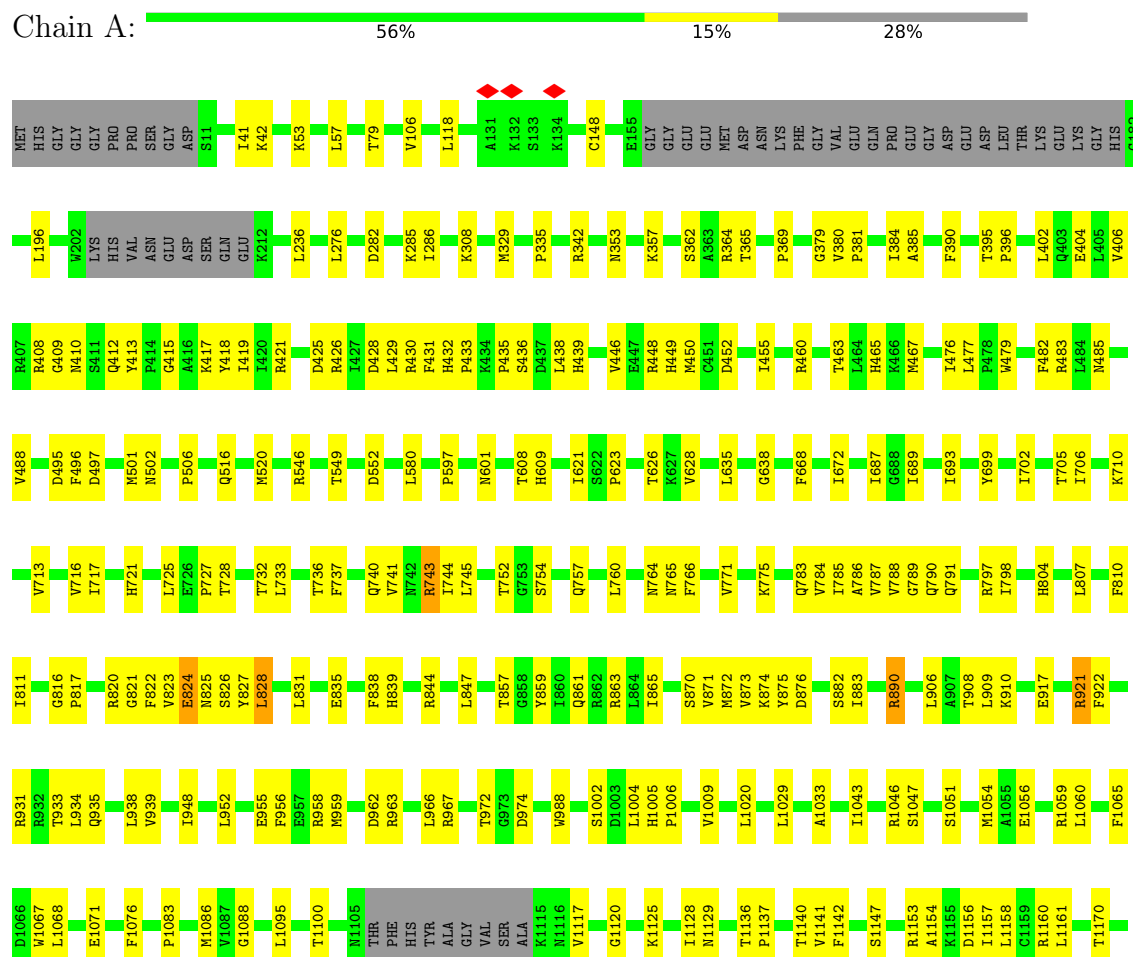
Chain 8: 34% 79% 7% 14%



- Molecule 10: Cyclin-H



- Molecule 11: DNA-directed RNA polymerase subunit







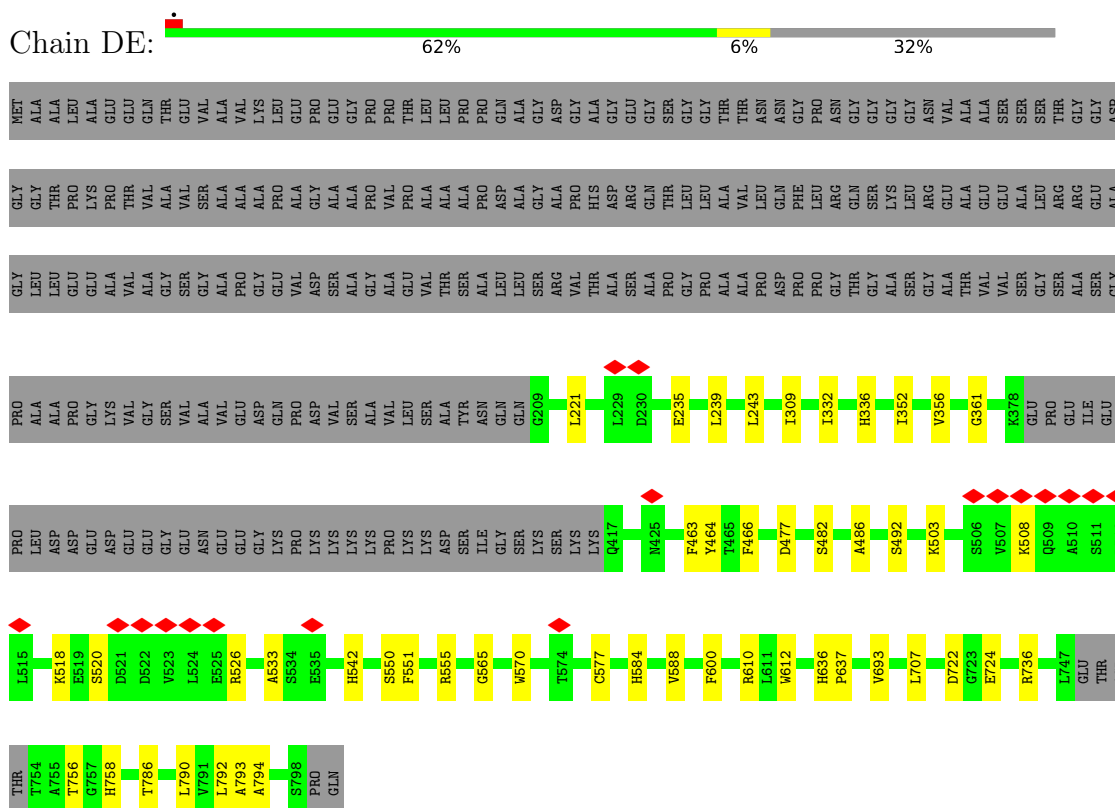








- Molecule 18: Transcription initiation factor TFIID subunit 5

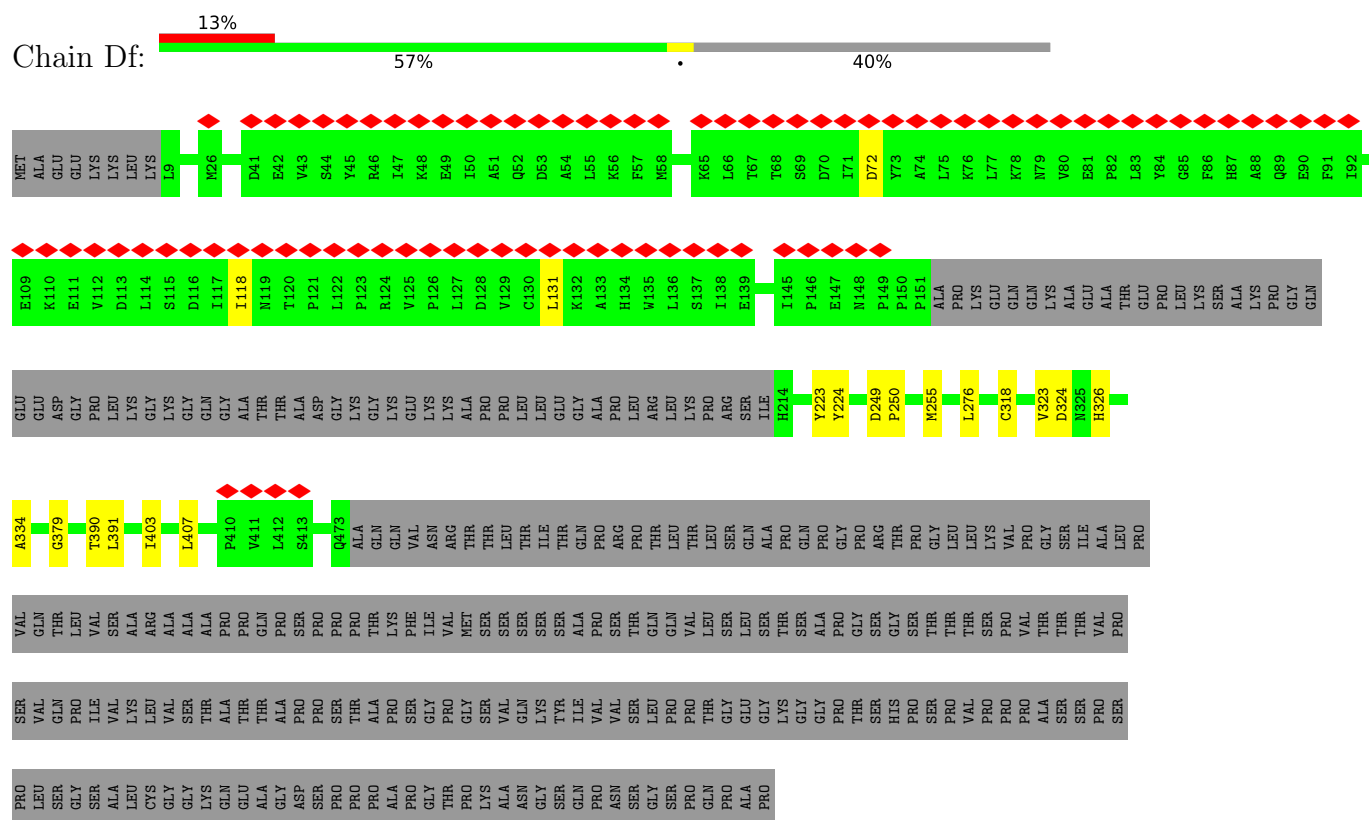


- Molecule 18: Transcription initiation factor TFIID subunit 5

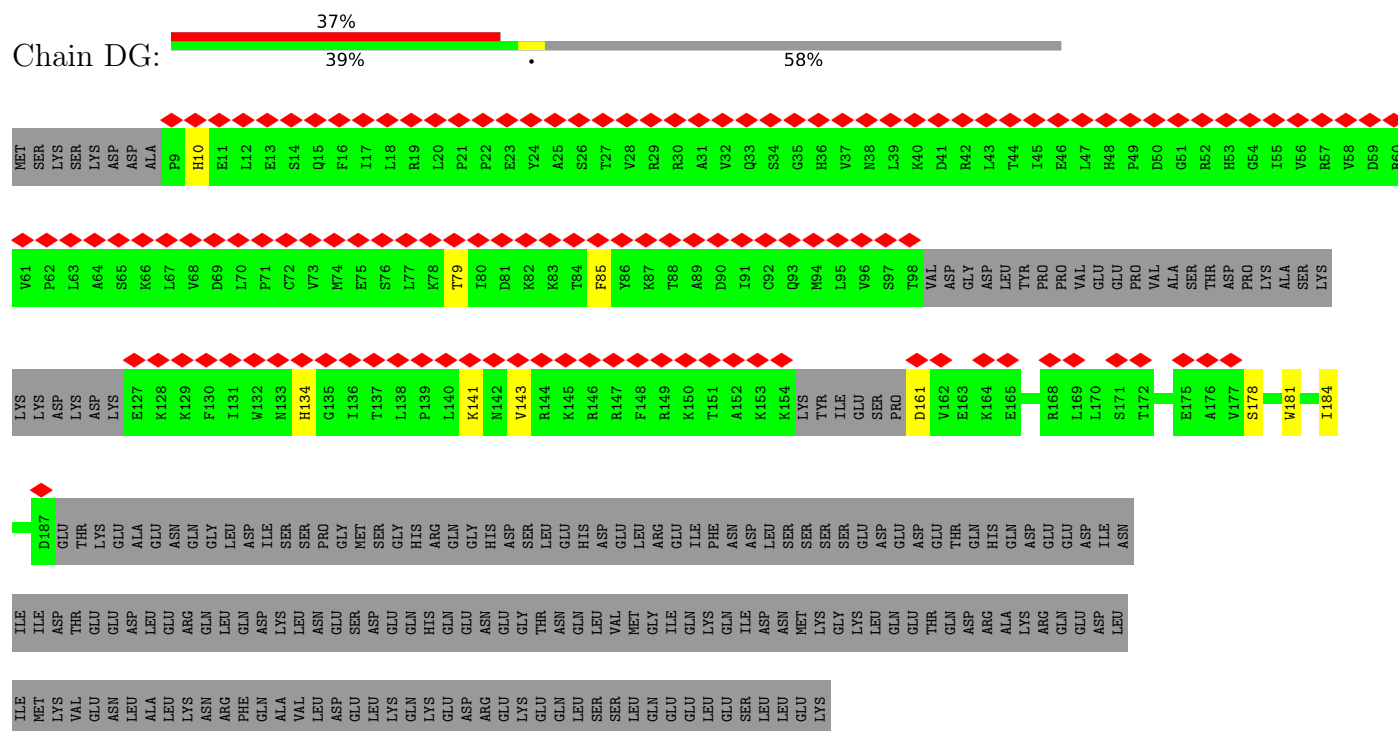




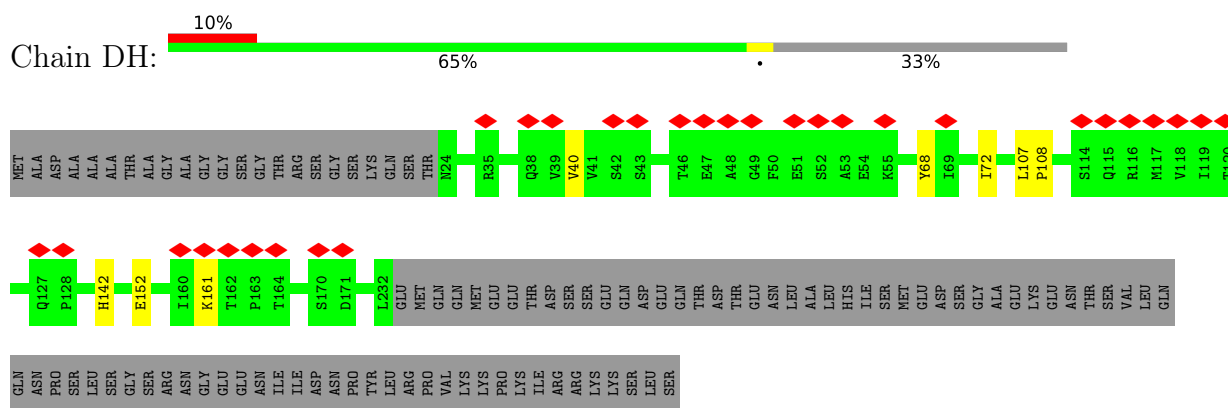
• Molecule 19: Transcription initiation factor TFIID subunit 6



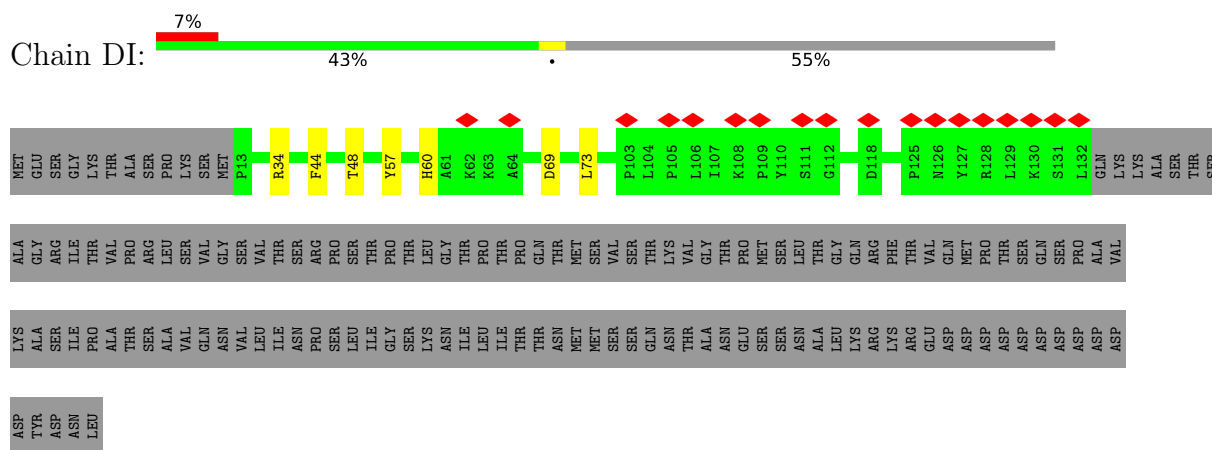
• Molecule 20: Transcription initiation factor TFIID subunit 7



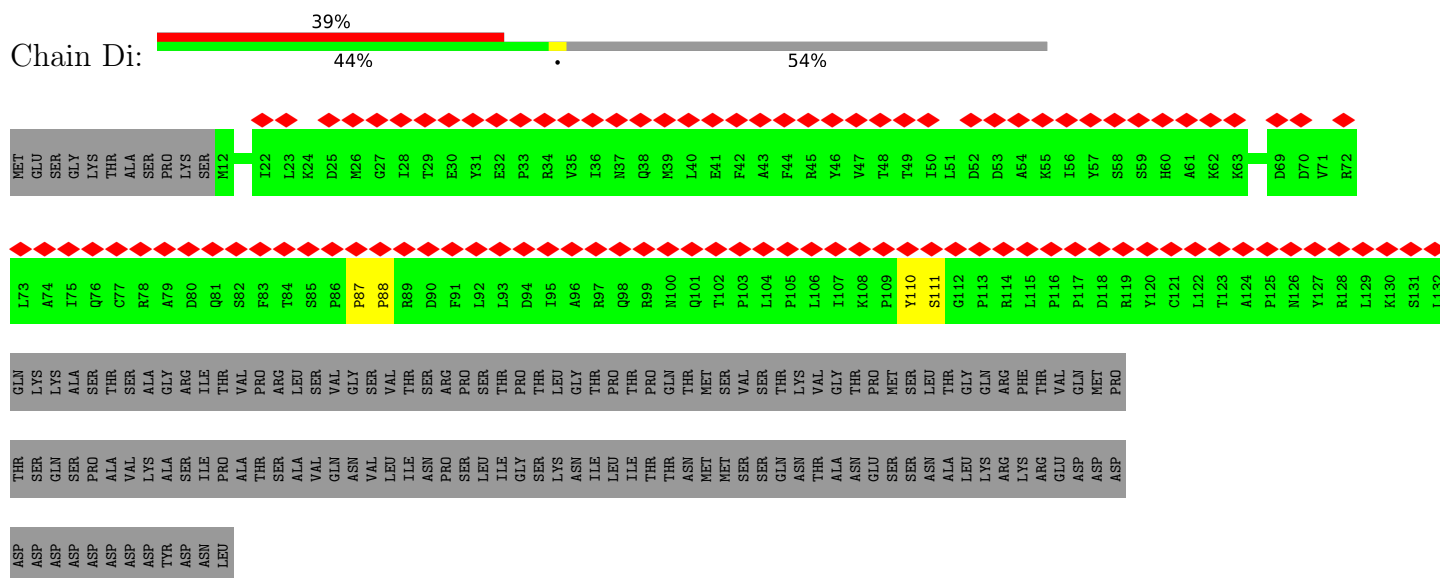
• Molecule 21: Transcription initiation factor TFIID subunit 8



• Molecule 22: Transcription initiation factor TFIID subunit 9

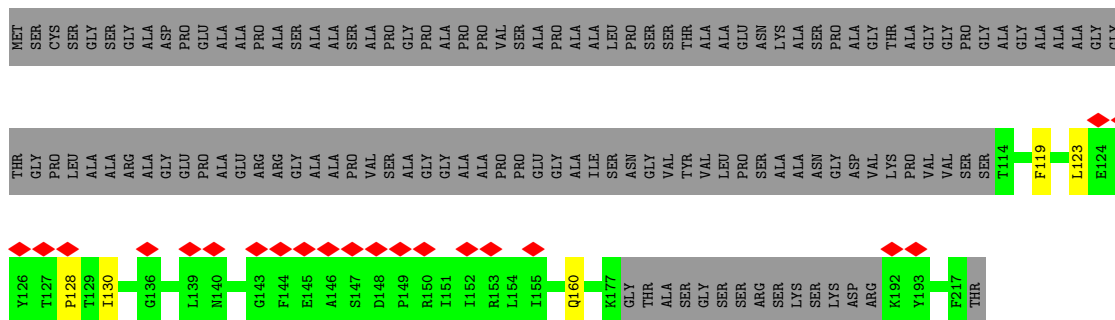


• Molecule 22: Transcription initiation factor TFIID subunit 9

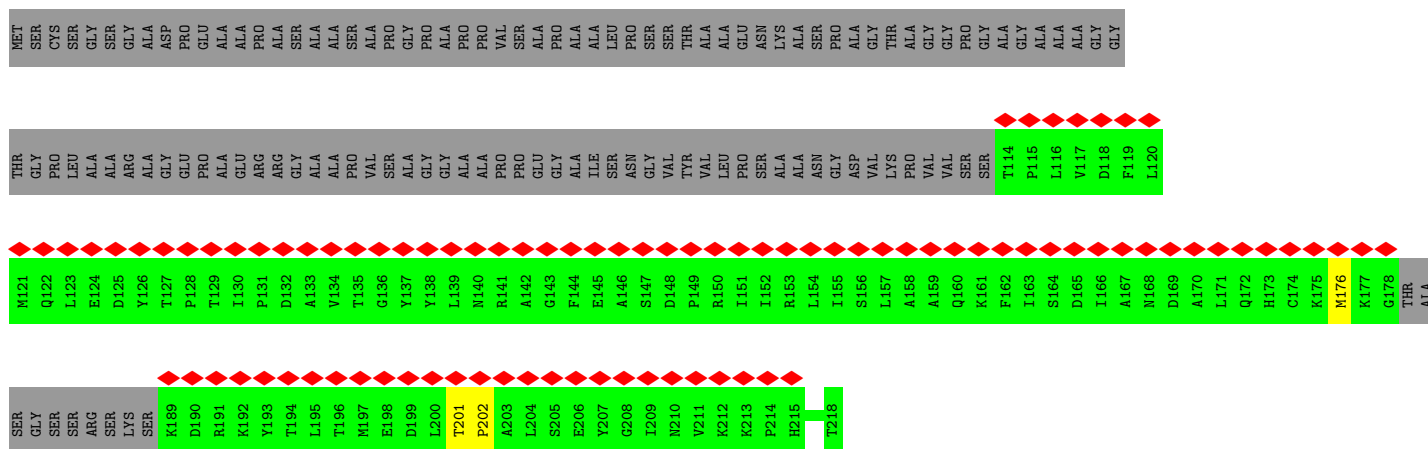
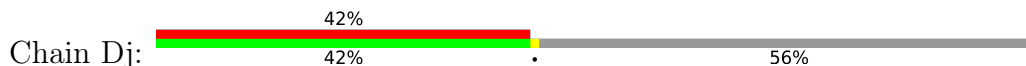


• Molecule 23: Transcription initiation factor TFIID subunit 10

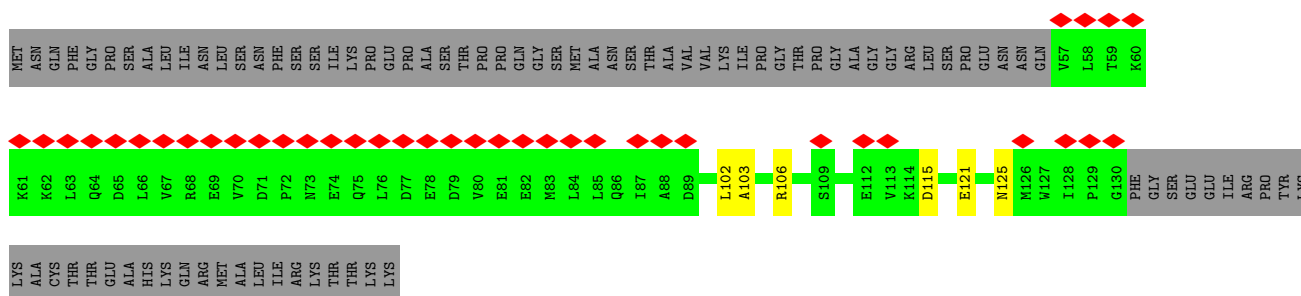
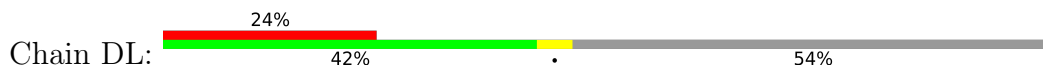




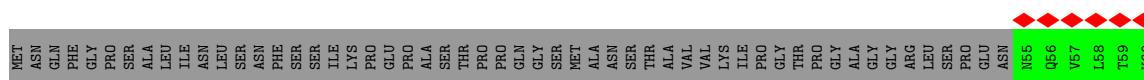
- Molecule 23: Transcription initiation factor TFIID subunit 10

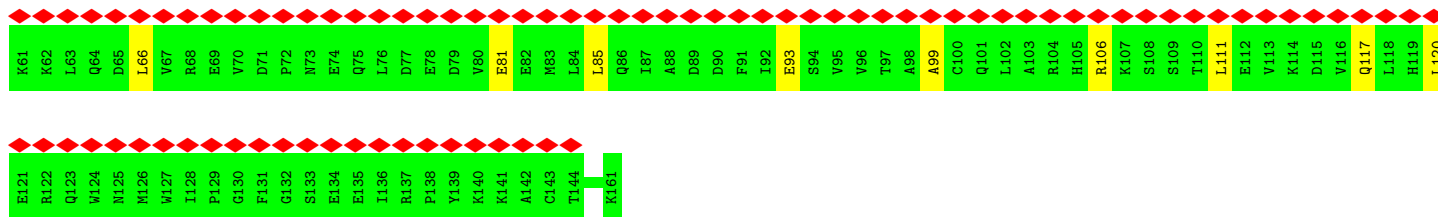


- Molecule 24: Transcription initiation factor TFIID subunit 12

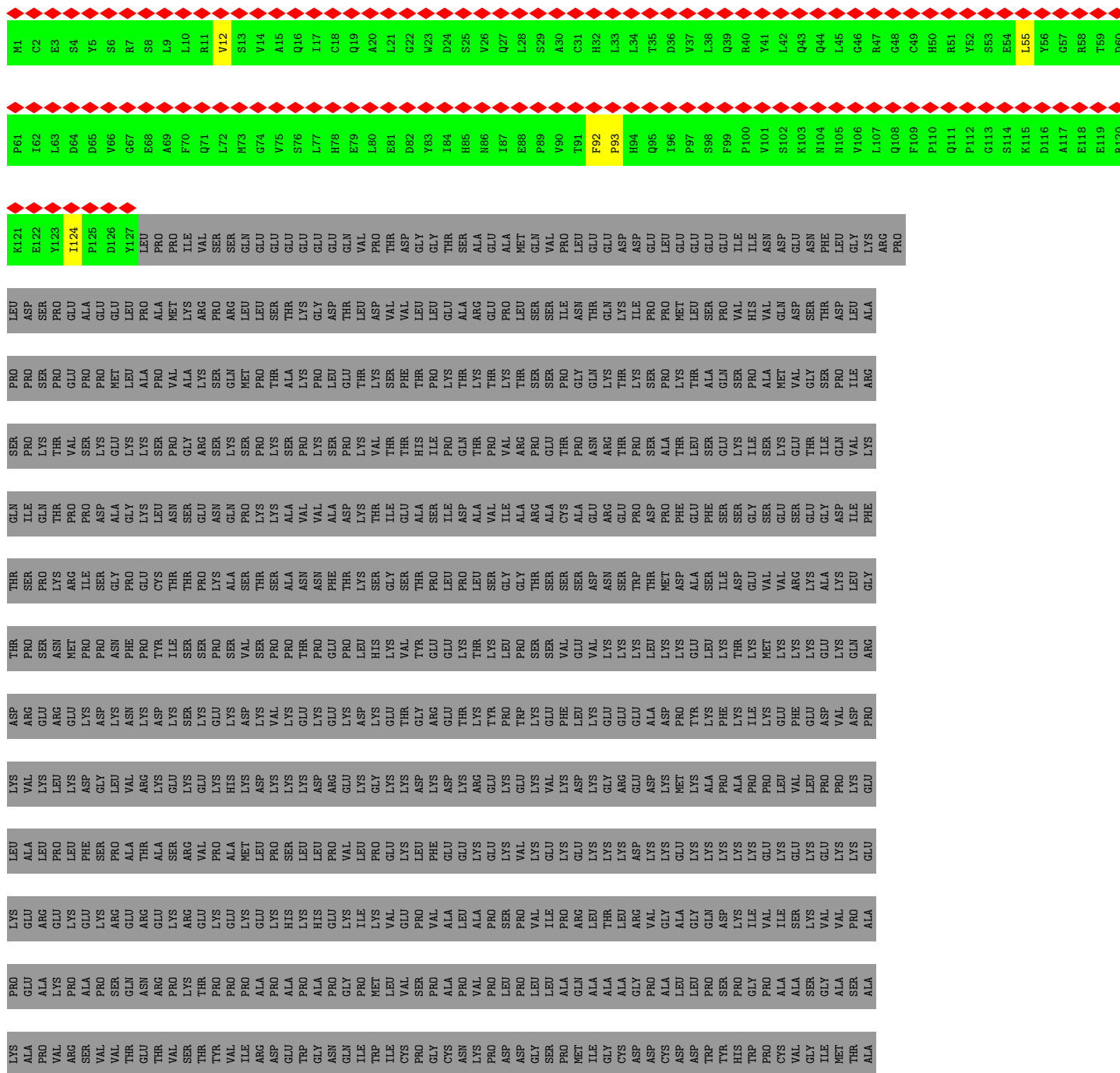


- Molecule 24: Transcription initiation factor TFIID subunit 12





• Molecule 25: Transcription initiation factor TFIID subunit 3

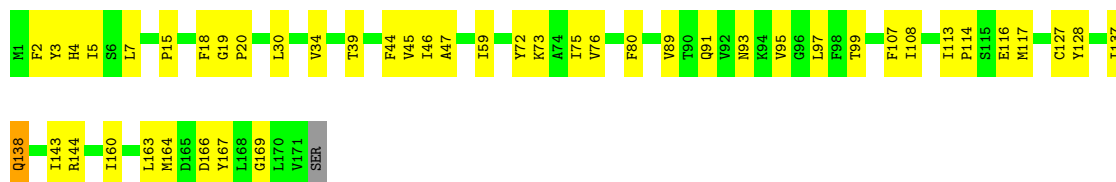






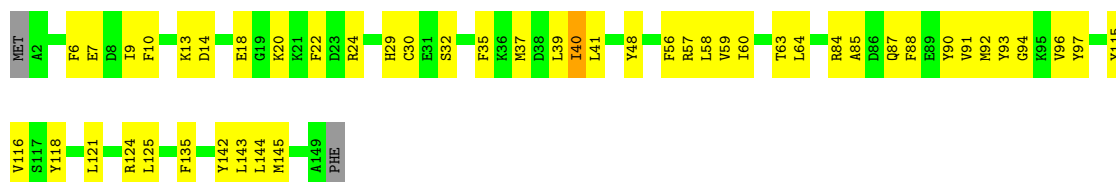
- Molecule 30: DNA-directed RNA polymerase II subunit RPB7

Chain G: 73% 26% ..



- Molecule 31: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 67% 31% ..



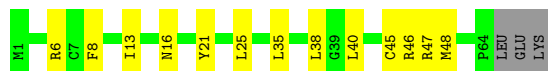
- Molecule 32: DNA-directed RNA polymerase II subunit RPB9

Chain I: 70% 21% 9%



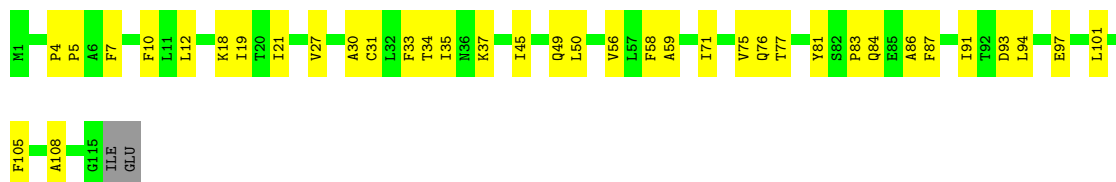
- Molecule 33: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 76% 19%



- Molecule 34: RNA polymerase II subunit J

Chain K: 67% 32%



- Molecule 35: RNA polymerase II subunit K

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ASP | THR | GLN | LYS | ASP | VAL | GLN | PRO | PRO | LYS | GLN | GLN | PRO | M15 | M16 | Y17 | I28 | K29 | S30 | R31 | D32 | R42 | I43 | M44 | Y45 | A57 | R58 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

Chain M:  65% 15% 20%

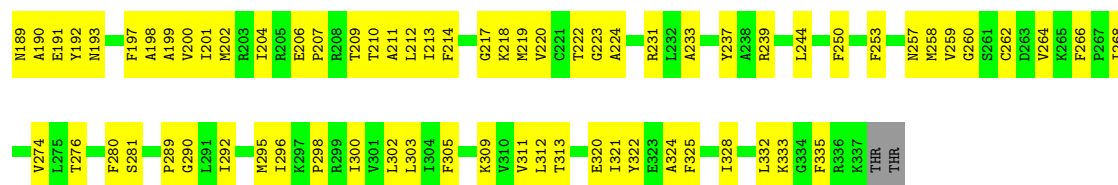
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|
| A261 | A262 | A263 | A264 | S265 | K268 | Y289 | L292 | Y293 | L299 | F300 | P301 | F304 | K305 | F306 | D307 | T308 | P309 | V310 | D311 | K312 | L313 | P314 | Q315 | L316 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |
| ALA  | SER  | PHE  | GLU  | PHE  | GLY  | ASN  | SER  | LYS  | TYR  | GLN  | ASN  | ARG  | ARG  | T106 | A125 | D126 | R127 | L130 | P131 | I134 | V183 | F195 | L199 | F214 | F218 | C219 | P225 | V228 | Q229 | P230 | A231 | A232 | I235 | L242 | D243 | L244 | V245 | P246 | G247 | R248 | A256 | A257 | I258 | Y259 |     |     |     |     |
| MET  | ALA  | SER  | THR  | SER  | ARG  | LEU  | ASP  | ALA  | LEU  | PRO  | ARG  | VAL  | T114 | G114 | D26  | I23  | C37  | G38  | L39  | T34  | PHE  | SER  | ASN  | ASP  | LYS  | ALA  | THR  | LYS  | ASP  | PRO  | SER  | ARG  | VAL  | GLY  | ASP  | SER  | GLN  | ASP  | LEU  | SER  | THR  | MET  | ILE  | GLY  | LYS | GLY | THR | GLY |

Chain N:  22% 34% 63%

[illegible]

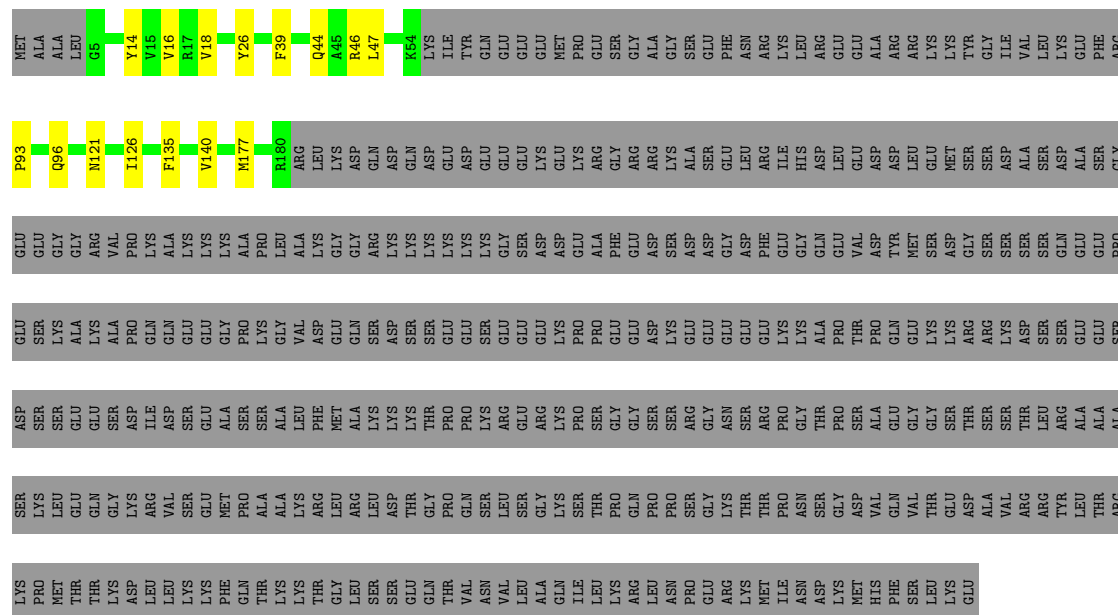
Chain 0:  29% 24% 47%

[illegible]



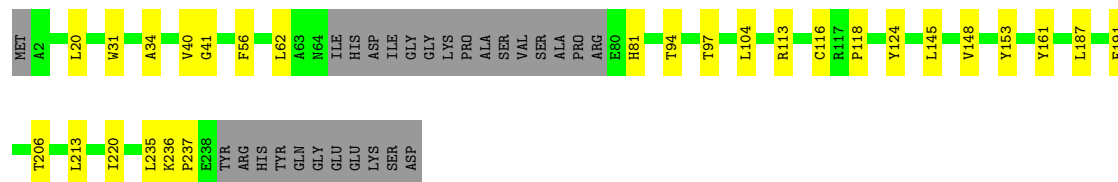
• Molecule 39: General transcription factor IIF subunit 1

Chain Q: 24% 73%



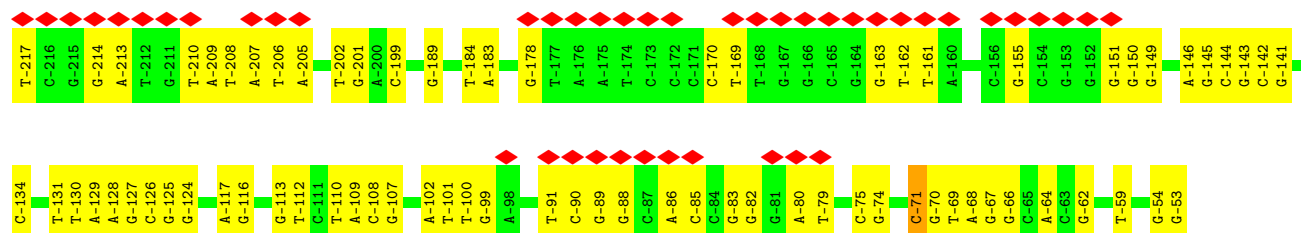
• Molecule 40: General transcription factor IIF subunit 2

Chain R: 78% 11% 11%



• Molecule 41: Template DNA

Chain T: 20% 55% 44%





SER TYR  
GLU SER  
VAL SER  
GLN SER  
ARG ARG  
PRO PRO  
LEU LEU  
VAL VAL  
ALA VAL  
GLN VAL  
MET MET  
THR THR  
PRO PRO  
GLU GLU  
GLY LYS

- Molecule 45: Transcription initiation factor IIE subunit beta

Chain X: 42% 17% 41%

MET ASP  
PRO PRO  
SER SER  
LEU LEU  
VAL VAL  
ARG ARG  
GLU GLU  
SER SER  
LEU LEU  
PHE PHE  
LYS LYS  
LYS LYS  
ARG ARG  
ALA ALA  
LEU LEU  
SER SER  
THR THR  
PRO PRO  
VAL VAL  
VAL VAL  
GLU GLU  
TYR TYR  
ILE ILE  
ALA ALA  
MET MET  
GLY GLY  
GLN GLN  
ARG ARG  
MET MET  
PHE PHE  
GLU GLU  
ASP ASP  
PHE PHE  
GLU GLU

SER PHE  
ASN ASN  
LEU LEU  
LYS LYS  
ALA ALA  
LEU LEU  
SER SER  
GLY GLY  
SER SER  
G72 G72  
F75 F75  
G76 G76  
V77 V77  
L78 L78  
I81 I81  
R85 R85  
R88 R88  
H89 H89  
T94 T94  
L97 L97  
T98 T98  
L99 L99  
L103 L103  
L109 L109  
D110 D110  
I111 I111  
Q115 Q115  
K116 K116  
L119 L119  
M120 M120  
L124 L124  
K129 K129  
I133 I133  
Y137 Y137  
A138 A138  
F139 F139  
M144 M144  
V145 V145  
R146 R146  
D147 D147  
K148 K148  
L151 L151

L155 L155  
H158 H158  
G165 G165  
I166 I166  
L167 L167  
I171 I171  
E172 E172  
E173 E173  
A174 A174  
L175 L175  
S178 S178  
L185 L185  
V192 V192  
N193 N193  
R194 R194  
T200 T200  
L201 L201  
F202 F202  
V212 V212  
F216 F216  
L219 L219  
W220 W220  
V223 V223  
T242 T242  
SER SER  
MET MET  
GLN GLN  
SER SER  
GLY GLY  
PRO PRO  
LYS LYS  
LYS LYS  
VAL VAL  
ALA ALA  
PRO PRO  
ILE ILE  
GLN GLN  
ARG ARG  
LYS LYS  
LYS LYS  
PRO PRO  
ALA ALA  
SER SER

GLN LYS  
LYS LYS  
ARG ARG  
PHE PHE  
LYS LYS  
THR THR  
HIS HIS  
ASN ASN  
SER SER  
HIS HIS  
E172 E172  
E173 E173  
ALA ALA  
VAL VAL  
LEU LEU  
LYS LYS  
ASP ASP  
TYR TYR  
SER SER  
ASP ASP  
ILE ILE  
THR THR  
SER SER  
SER SER  
LYS LYS

- Molecule 46: Histone H3.2

Chain a: 67% 29%

MET ALA  
ALA ARG  
THR THR  
LYS LYS  
GLN GLN  
THR THR  
ALA ALA  
ARG ARG  
LYS LYS  
SER SER  
THR THR  
GLY GLY  
LYS LYS  
PRO PRO  
ARG ARG  
LYS LYS  
GLN GLN  
LEU LEU  
ALA ALA  
ALA ALA  
ARG ARG  
LYS LYS  
ALA ALA  
ALA ALA  
ARG ARG  
LYS LYS  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
GLY GLY  
GLY GLY  
VAL VAL  
LYS LYS  
P39 P39  
H40 H40  
R43 R43  
L66 L66  
P67 P67  
A76 A76  
L83 L83  
R135 R135  
ALA ALA

- Molecule 46: Histone H3.2

Chain e: 68% 28%

MET ALA  
ALA ARG  
THR THR  
LYS LYS  
GLN GLN  
THR THR  
ALA ALA  
ARG ARG  
LYS LYS  
SER SER  
THR THR  
GLY GLY  
LYS LYS  
PRO PRO  
ARG ARG  
LYS LYS  
GLN GLN  
LEU LEU  
ALA ALA  
ALA ALA  
ARG ARG  
LYS LYS  
SER SER  
PRO PRO  
ALA ALA  
THR THR  
GLY GLY  
GLY GLY  
VAL VAL  
LYS LYS  
K38 K38  
P39 P39  
V47 V47  
R84 R84  
F85 F85  
V102 V102  
I113 I113  
R135 R135  
ALA ALA

- Molecule 47: Histone H4

Chain b: 75% 20%

MET SER  
SER GLY  
GLY ARG  
GLY GLY  
LYS LYS  
GLY GLY  
GLY GLY  
GLY GLY  
GLY GLY  
LEU LEU  
LYS LYS  
LYS LYS  
GLY GLY  
GLY GLY  
ALA ALA  
LYS LYS  
ARG ARG  
HIS HIS  
ARG ARG  
LYS LYS  
VAL VAL  
LEU LEU  
R24 R24  
V22 V22  
L23 L23  
R24 R24  
T31 T31  
K32 K32  
I35 I35  
Y52 Y52  
G103 G103

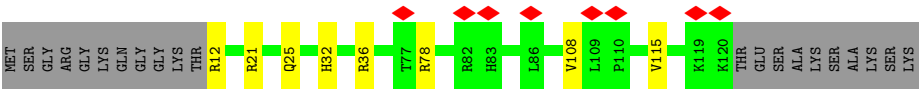
- Molecule 47: Histone H4

Chain f: 76% 22%

MET SER  
SER GLY  
GLY ARG  
GLY GLY  
LYS LYS  
GLY GLY  
GLY GLY  
GLY GLY  
LEU LEU  
LYS LYS  
LYS LYS  
GLY GLY  
GLY GLY  
ALA ALA  
LYS LYS  
ARG ARG  
HIS HIS  
ARG ARG  
LYS LYS  
VAL VAL  
LEU LEU  
R24 R24  
K30 K30  
T81 T81  
R82 R82  
L91 L91  
R96 R96  
G103 G103

- Molecule 48: Histone H2A type 1

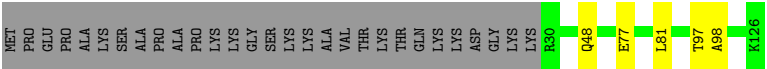
Chain c: 6% 78% 6% 16%



● Molecule 48: Histone H2A type 1



● Molecule 49: Histone H2B 1.1



● Molecule 49: Histone H2B 1.1



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 30253                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40.00                                   | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1500                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.014                                   | Depositor |
| Minimum map value                    | -0.003                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.0012                                  | Depositor |
| Map size (Å)                         | 537.6, 537.6, 537.6                     | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.05, 1.05, 1.05                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, MG, 2A1

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   | 0     | 0.24         | 0/4994      | 0.69        | 0/6745         |
| 2   | 1     | 0.25         | 0/5875      | 0.76        | 1/7955 (0.0%)  |
| 3   | 2     | 0.27         | 0/2210      | 0.73        | 0/2975         |
| 4   | 3     | 0.24         | 0/3412      | 0.68        | 0/4622         |
| 5   | 4     | 0.25         | 0/2793      | 0.68        | 0/3780         |
| 6   | 5     | 0.24         | 0/2103      | 0.66        | 0/2846         |
| 7   | 6     | 0.24         | 0/555       | 0.71        | 0/747          |
| 8   | 7     | 0.31         | 0/1756      | 0.83        | 4/2367 (0.2%)  |
| 9   | 8     | 0.25         | 0/2437      | 0.70        | 0/3306         |
| 10  | 9     | 0.31         | 0/2384      | 0.80        | 0/3220         |
| 11  | A     | 0.39         | 0/11479     | 0.82        | 5/15496 (0.0%) |
| 12  | B     | 0.41         | 0/9257      | 0.83        | 5/12493 (0.0%) |
| 13  | C     | 0.41         | 0/2102      | 0.76        | 0/2857         |
| 14  | D     | 0.27         | 0/1064      | 0.70        | 0/1428         |
| 15  | DA    | 0.27         | 0/4679      | 0.72        | 2/6320 (0.0%)  |
| 16  | DB    | 0.25         | 0/7993      | 0.66        | 2/10836 (0.0%) |
| 17  | DD    | 0.27         | 0/1344      | 0.76        | 0/1795         |
| 17  | Dd    | 0.22         | 0/1322      | 0.66        | 0/1772         |
| 18  | DE    | 0.24         | 0/4469      | 0.70        | 1/6050 (0.0%)  |
| 18  | De    | 0.25         | 0/4433      | 0.71        | 0/6004         |
| 19  | DF    | 0.27         | 0/3167      | 0.77        | 4/4303 (0.1%)  |
| 19  | Df    | 0.25         | 0/3140      | 0.68        | 0/4268         |
| 20  | DG    | 0.30         | 0/1199      | 0.74        | 0/1612         |
| 21  | DH    | 0.31         | 0/1673      | 0.81        | 0/2285         |
| 22  | DI    | 0.31         | 0/981       | 0.76        | 0/1332         |
| 22  | Di    | 0.30         | 0/989       | 0.72        | 0/1343         |
| 23  | DJ    | 0.23         | 0/736       | 0.64        | 0/998          |
| 23  | Dj    | 0.28         | 0/776       | 0.68        | 0/1049         |
| 24  | DL    | 0.22         | 0/613       | 0.67        | 0/829          |
| 24  | Di    | 0.19         | 0/889       | 0.61        | 0/1194         |
| 25  | Dc    | 0.26         | 0/1035      | 0.69        | 0/1406         |
| 26  | Dk    | 0.19         | 0/800       | 0.60        | 0/1070         |

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 27  | Dm    | 0.18         | 0/733       | 0.57        | 0/977            |
| 28  | E     | 0.42         | 0/1752      | 0.73        | 0/2366           |
| 29  | F     | 0.48         | 0/646       | 0.73        | 0/871            |
| 30  | G     | 0.37         | 0/1382      | 0.73        | 0/1874           |
| 31  | H     | 0.55         | 0/1207      | 0.76        | 1/1628 (0.1%)    |
| 32  | I     | 0.39         | 0/949       | 0.73        | 0/1284           |
| 33  | J     | 0.32         | 0/516       | 0.70        | 0/696            |
| 34  | K     | 0.49         | 0/939       | 0.78        | 0/1271           |
| 35  | L     | 0.30         | 0/378       | 0.72        | 0/500            |
| 36  | M     | 0.35         | 0/1984      | 0.70        | 1/2679 (0.0%)    |
| 37  | N     | 0.45         | 0/5211      | 0.94        | 9/8039 (0.1%)    |
| 38  | O     | 0.48         | 0/1448      | 0.73        | 0/1948           |
| 39  | Q     | 0.30         | 0/1167      | 0.74        | 0/1576           |
| 40  | R     | 0.27         | 0/1817      | 0.69        | 0/2445           |
| 41  | T     | 0.43         | 0/5223      | 0.85        | 2/8062 (0.0%)    |
| 42  | U     | 0.27         | 0/946       | 0.76        | 1/1274 (0.1%)    |
| 43  | V     | 0.31         | 0/816       | 0.71        | 1/1105 (0.1%)    |
| 44  | W     | 0.32         | 0/1686      | 0.71        | 0/2266           |
| 45  | X     | 0.31         | 0/1427      | 0.78        | 0/1916           |
| 46  | a     | 0.29         | 0/813       | 0.78        | 0/1090           |
| 46  | e     | 0.32         | 0/822       | 0.75        | 0/1102           |
| 47  | b     | 0.26         | 0/660       | 0.79        | 0/883            |
| 47  | f     | 0.26         | 0/645       | 0.77        | 0/862            |
| 48  | c     | 0.28         | 0/853       | 0.84        | 0/1149           |
| 48  | g     | 0.27         | 0/828       | 0.79        | 0/1117           |
| 49  | d     | 0.29         | 0/777       | 0.78        | 0/1041           |
| 49  | h     | 0.26         | 0/755       | 0.65        | 0/1013           |
| All | All   | 0.33         | 0/129039    | 0.76        | 39/176337 (0.0%) |

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   | 0     | 0                   | 2                   |
| 2   | 1     | 0                   | 5                   |
| 4   | 3     | 0                   | 1                   |
| 5   | 4     | 0                   | 1                   |
| 10  | 9     | 0                   | 1                   |
| 11  | A     | 0                   | 3                   |
| 13  | C     | 0                   | 1                   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 18  | DE    | 0                   | 2                   |
| 19  | DF    | 0                   | 1                   |
| 22  | DI    | 0                   | 1                   |
| 28  | E     | 0                   | 1                   |
| 36  | M     | 0                   | 1                   |
| 46  | a     | 0                   | 1                   |
| 47  | b     | 0                   | 1                   |
| 48  | c     | 0                   | 1                   |
| 48  | g     | 0                   | 1                   |
| All | All   | 0                   | 24                  |

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | N     | 71  | DG   | O4'-C1'-N9  | 11.01 | 124.92      | 108.40   |
| 11  | A     | 824 | GLU  | N-CA-CB     | -9.08 | 96.31       | 110.30   |
| 37  | N     | 71  | DG   | C1'-O4'-C4' | -8.42 | 97.06       | 109.70   |
| 16  | DB    | 965 | TRP  | CA-CB-CG    | 7.32  | 127.51      | 113.60   |
| 42  | U     | 32  | ASP  | N-CA-C      | 6.65  | 124.96      | 110.80   |

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 0     | 109 | ARG  | Sidechain |
| 1   | 0     | 391 | ARG  | Sidechain |
| 2   | 1     | 254 | ARG  | Sidechain |
| 2   | 1     | 378 | ARG  | Sidechain |
| 2   | 1     | 631 | ARG  | Sidechain |

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 4890  | 0        | 4949     | 38      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | 1     | 5751  | 0        | 5794     | 61      | 0            |
| 3   | 2     | 2167  | 0        | 2175     | 13      | 0            |
| 4   | 3     | 3338  | 0        | 3343     | 16      | 0            |
| 5   | 4     | 2732  | 0        | 2703     | 20      | 0            |
| 6   | 5     | 2066  | 0        | 2100     | 16      | 0            |
| 7   | 6     | 549   | 0        | 558      | 0       | 0            |
| 8   | 7     | 1724  | 0        | 1697     | 22      | 0            |
| 9   | 8     | 2378  | 0        | 2397     | 13      | 0            |
| 10  | 9     | 2334  | 0        | 2357     | 6       | 0            |
| 11  | A     | 11274 | 0        | 11408    | 259     | 0            |
| 12  | B     | 9076  | 0        | 9116     | 178     | 0            |
| 13  | C     | 2059  | 0        | 2008     | 55      | 0            |
| 14  | D     | 1050  | 0        | 1033     | 23      | 0            |
| 15  | DA    | 4563  | 0        | 4485     | 24      | 0            |
| 16  | DB    | 7796  | 0        | 7751     | 13      | 0            |
| 17  | DD    | 1331  | 0        | 1351     | 5       | 0            |
| 17  | Dd    | 1308  | 0        | 1318     | 13      | 0            |
| 18  | DE    | 4364  | 0        | 4244     | 24      | 0            |
| 18  | De    | 4327  | 0        | 4197     | 9       | 0            |
| 19  | DF    | 3109  | 0        | 3045     | 7       | 0            |
| 19  | Df    | 3081  | 0        | 3012     | 10      | 0            |
| 20  | DG    | 1180  | 0        | 1235     | 6       | 0            |
| 21  | DH    | 1633  | 0        | 1621     | 4       | 0            |
| 22  | DI    | 959   | 0        | 969      | 8       | 0            |
| 22  | Di    | 967   | 0        | 977      | 2       | 0            |
| 23  | DJ    | 720   | 0        | 719      | 3       | 0            |
| 23  | Dj    | 760   | 0        | 759      | 2       | 0            |
| 24  | DL    | 605   | 0        | 606      | 7       | 0            |
| 24  | DI    | 877   | 0        | 893      | 7       | 0            |
| 25  | Dc    | 1011  | 0        | 975      | 5       | 0            |
| 26  | Dk    | 786   | 0        | 818      | 3       | 0            |
| 27  | Dm    | 724   | 0        | 744      | 2       | 0            |
| 28  | E     | 1721  | 0        | 1737     | 52      | 0            |
| 29  | F     | 636   | 0        | 665      | 39      | 0            |
| 30  | G     | 1351  | 0        | 1358     | 41      | 0            |
| 31  | H     | 1186  | 0        | 1147     | 49      | 0            |
| 32  | I     | 928   | 0        | 859      | 22      | 0            |
| 33  | J     | 507   | 0        | 523      | 13      | 0            |
| 34  | K     | 920   | 0        | 942      | 37      | 0            |
| 35  | L     | 373   | 0        | 381      | 9       | 0            |
| 36  | M     | 1954  | 0        | 1990     | 38      | 0            |
| 37  | N     | 4645  | 0        | 2544     | 159     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 38  | O     | 1422   | 0        | 1514     | 83      | 0            |
| 39  | Q     | 1138   | 0        | 1103     | 11      | 0            |
| 40  | R     | 1788   | 0        | 1819     | 26      | 0            |
| 41  | T     | 4656   | 0        | 2548     | 102     | 0            |
| 42  | U     | 931    | 0        | 888      | 22      | 0            |
| 43  | V     | 806    | 0        | 818      | 25      | 0            |
| 44  | W     | 1659   | 0        | 1665     | 51      | 0            |
| 45  | X     | 1403   | 0        | 1428     | 45      | 0            |
| 46  | a     | 801    | 0        | 839      | 3       | 0            |
| 46  | e     | 810    | 0        | 851      | 4       | 0            |
| 47  | b     | 653    | 0        | 696      | 4       | 0            |
| 47  | f     | 638    | 0        | 676      | 1       | 0            |
| 48  | c     | 843    | 0        | 908      | 6       | 0            |
| 48  | g     | 818    | 0        | 877      | 7       | 0            |
| 49  | d     | 766    | 0        | 797      | 3       | 0            |
| 49  | h     | 744    | 0        | 771      | 3       | 0            |
| 50  | 0     | 70     | 0        | 0        | 3       | 0            |
| 50  | 2     | 20     | 0        | 0        | 0       | 0            |
| 50  | N     | 30     | 0        | 0        | 0       | 0            |
| 51  | 0     | 6      | 0        | 5        | 1       | 0            |
| 51  | 2     | 11     | 0        | 10       | 0       | 0            |
| 52  | 1     | 8      | 0        | 0        | 0       | 0            |
| 53  | 4     | 3      | 0        | 0        | 0       | 0            |
| 53  | 5     | 2      | 0        | 0        | 0       | 0            |
| 53  | 7     | 2      | 0        | 0        | 0       | 0            |
| 53  | A     | 2      | 0        | 0        | 0       | 0            |
| 53  | B     | 1      | 0        | 0        | 0       | 0            |
| 53  | C     | 1      | 0        | 0        | 0       | 0            |
| 53  | I     | 2      | 0        | 0        | 0       | 0            |
| 53  | J     | 1      | 0        | 0        | 0       | 0            |
| 53  | L     | 1      | 0        | 0        | 0       | 0            |
| 53  | M     | 1      | 0        | 0        | 0       | 0            |
| 53  | W     | 1      | 0        | 0        | 0       | 0            |
| 54  | A     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 125749 | 0        | 121716   | 1502    | 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 6.

The worst 5 of 1502 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:N:178:DC:O2    | 41:T:-178:DG:N2   | 1.89                     | 1.03              |
| 11:A:608:THR:HG21 | 11:A:771:VAL:HG13 | 1.55                     | 0.88              |
| 41:T:-207:DA:H2'  | 41:T:-206:DT:H71  | 1.62                     | 0.82              |
| 11:A:706:ILE:HG22 | 11:A:710:LYS:HE3  | 1.62                     | 0.81              |
| 12:B:849:ASP:HB3  | 35:L:15:MET:HE1   | 1.63                     | 0.79              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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   | 0     | 601/782 (77%)   | 583 (97%)  | 18 (3%) | 0        | 100         | 100 |
| 2   | 1     | 710/760 (93%)   | 679 (96%)  | 31 (4%) | 0        | 100         | 100 |
| 3   | 2     | 253/548 (46%)   | 245 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 4   | 3     | 413/462 (89%)   | 400 (97%)  | 13 (3%) | 0        | 100         | 100 |
| 5   | 4     | 341/395 (86%)   | 334 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 6   | 5     | 259/308 (84%)   | 246 (95%)  | 13 (5%) | 0        | 100         | 100 |
| 7   | 6     | 67/71 (94%)     | 65 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 8   | 7     | 208/309 (67%)   | 196 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 9   | 8     | 297/346 (86%)   | 287 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 10  | 9     | 285/323 (88%)   | 279 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 11  | A     | 1413/1984 (71%) | 1379 (98%) | 34 (2%) | 0        | 100         | 100 |
| 12  | B     | 1130/1300 (87%) | 1096 (97%) | 34 (3%) | 0        | 100         | 100 |
| 13  | C     | 253/275 (92%)   | 247 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 14  | D     | 126/184 (68%)   | 122 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 15  | DA    | 542/1893 (29%)  | 526 (97%)  | 16 (3%) | 0        | 100         | 100 |
| 16  | DB    | 959/1199 (80%)  | 928 (97%)  | 31 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 17  | DD    | 153/1085 (14%) | 152 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 17  | Dd    | 154/1085 (14%) | 151 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 18  | DE    | 540/800 (68%)  | 526 (97%) | 14 (3%) | 0        | 100         | 100 |
| 18  | De    | 531/800 (66%)  | 507 (96%) | 24 (4%) | 0        | 100         | 100 |
| 19  | DF    | 404/677 (60%)  | 393 (97%) | 11 (3%) | 0        | 100         | 100 |
| 19  | Df    | 399/677 (59%)  | 388 (97%) | 11 (3%) | 0        | 100         | 100 |
| 20  | DG    | 139/349 (40%)  | 132 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 21  | DH    | 207/310 (67%)  | 196 (95%) | 11 (5%) | 0        | 100         | 100 |
| 22  | DI    | 118/264 (45%)  | 114 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 22  | Di    | 119/264 (45%)  | 114 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 23  | DJ    | 86/218 (39%)   | 80 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 23  | Dj    | 91/218 (42%)   | 84 (92%)  | 7 (8%)  | 0        | 100         | 100 |
| 24  | DL    | 72/161 (45%)   | 70 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 24  | DI    | 105/161 (65%)  | 101 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 25  | Dc    | 125/929 (14%)  | 124 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 26  | Dk    | 96/211 (46%)   | 94 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 27  | Dm    | 85/124 (68%)   | 80 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 28  | E     | 207/210 (99%)  | 204 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 29  | F     | 77/127 (61%)   | 76 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 30  | G     | 169/172 (98%)  | 160 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 31  | H     | 146/150 (97%)  | 143 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 32  | I     | 112/125 (90%)  | 104 (93%) | 8 (7%)  | 0        | 100         | 100 |
| 33  | J     | 62/67 (92%)    | 61 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 34  | K     | 113/117 (97%)  | 109 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 35  | L     | 42/58 (72%)    | 41 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 36  | M     | 248/316 (78%)  | 241 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 38  | O     | 177/339 (52%)  | 175 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 39  | Q     | 134/517 (26%)  | 129 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 40  | R     | 218/249 (88%)  | 215 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 42  | U     | 109/376 (29%)  | 104 (95%) | 5 (5%)  | 0        | 100         | 100 |
| 43  | V     | 97/109 (89%)   | 93 (96%)  | 4 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 44  | W     | 198/439 (45%)     | 197 (100%)  | 1 (0%)   | 0        | 100         | 100 |
| 45  | X     | 169/291 (58%)     | 163 (96%)   | 6 (4%)   | 0        | 100         | 100 |
| 46  | a     | 95/136 (70%)      | 95 (100%)   | 0        | 0        | 100         | 100 |
| 46  | e     | 96/136 (71%)      | 95 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 47  | b     | 80/103 (78%)      | 78 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 47  | f     | 78/103 (76%)      | 77 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 48  | c     | 107/130 (82%)     | 106 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 48  | g     | 104/130 (80%)     | 101 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 49  | d     | 95/126 (75%)      | 94 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 49  | h     | 93/126 (74%)      | 93 (100%)   | 0        | 0        | 100         | 100 |
| All | All   | 14307/24124 (59%) | 13872 (97%) | 435 (3%) | 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 PDB entries followed by that with respect to all EM entries.

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   | 0     | 536/688 (78%)   | 535 (100%)  | 1 (0%)   | 87          | 87  |
| 2   | 1     | 624/664 (94%)   | 621 (100%)  | 3 (0%)   | 81          | 83  |
| 3   | 2     | 241/484 (50%)   | 241 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 351/399 (88%)   | 351 (100%)  | 0        | 100         | 100 |
| 5   | 4     | 311/352 (88%)   | 309 (99%)   | 2 (1%)   | 78          | 83  |
| 6   | 5     | 234/272 (86%)   | 234 (100%)  | 0        | 100         | 100 |
| 7   | 6     | 62/64 (97%)     | 62 (100%)   | 0        | 100         | 100 |
| 8   | 7     | 194/283 (69%)   | 194 (100%)  | 0        | 100         | 100 |
| 9   | 8     | 259/299 (87%)   | 258 (100%)  | 1 (0%)   | 84          | 84  |
| 10  | 9     | 259/296 (88%)   | 259 (100%)  | 0        | 100         | 100 |
| 11  | A     | 1254/1763 (71%) | 1252 (100%) | 2 (0%)   | 87          | 87  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 12  | B     | 994/1127 (88%) | 994 (100%) | 0        | 100         | 100 |
| 13  | C     | 234/252 (93%)  | 234 (100%) | 0        | 100         | 100 |
| 14  | D     | 118/160 (74%)  | 117 (99%)  | 1 (1%)   | 73          | 80  |
| 15  | DA    | 495/1682 (29%) | 492 (99%)  | 3 (1%)   | 78          | 83  |
| 16  | DB    | 876/1083 (81%) | 875 (100%) | 1 (0%)   | 88          | 89  |
| 17  | DD    | 144/815 (18%)  | 143 (99%)  | 1 (1%)   | 76          | 81  |
| 17  | Dd    | 146/815 (18%)  | 145 (99%)  | 1 (1%)   | 76          | 81  |
| 18  | DE    | 478/657 (73%)  | 478 (100%) | 0        | 100         | 100 |
| 18  | De    | 475/657 (72%)  | 473 (100%) | 2 (0%)   | 84          | 84  |
| 19  | DF    | 324/574 (56%)  | 321 (99%)  | 3 (1%)   | 70          | 79  |
| 19  | Df    | 322/574 (56%)  | 320 (99%)  | 2 (1%)   | 78          | 83  |
| 20  | DG    | 133/322 (41%)  | 130 (98%)  | 3 (2%)   | 44          | 64  |
| 21  | DH    | 181/270 (67%)  | 180 (99%)  | 1 (1%)   | 78          | 83  |
| 22  | DI    | 106/235 (45%)  | 105 (99%)  | 1 (1%)   | 70          | 79  |
| 22  | Di    | 107/235 (46%)  | 107 (100%) | 0        | 100         | 100 |
| 23  | DJ    | 79/154 (51%)   | 79 (100%)  | 0        | 100         | 100 |
| 23  | Dj    | 83/154 (54%)   | 83 (100%)  | 0        | 100         | 100 |
| 24  | DL    | 69/141 (49%)   | 69 (100%)  | 0        | 100         | 100 |
| 24  | Dl    | 98/141 (70%)   | 97 (99%)   | 1 (1%)   | 68          | 78  |
| 25  | Dc    | 113/833 (14%)  | 113 (100%) | 0        | 100         | 100 |
| 26  | Dk    | 87/182 (48%)   | 87 (100%)  | 0        | 100         | 100 |
| 27  | Dm    | 80/106 (76%)   | 79 (99%)   | 1 (1%)   | 61          | 74  |
| 28  | E     | 191/192 (100%) | 191 (100%) | 0        | 100         | 100 |
| 29  | F     | 69/111 (62%)   | 69 (100%)  | 0        | 100         | 100 |
| 30  | G     | 152/153 (99%)  | 149 (98%)  | 3 (2%)   | 48          | 66  |
| 31  | H     | 129/131 (98%)  | 129 (100%) | 0        | 100         | 100 |
| 32  | I     | 103/112 (92%)  | 103 (100%) | 0        | 100         | 100 |
| 33  | J     | 53/56 (95%)    | 53 (100%)  | 0        | 100         | 100 |
| 34  | K     | 104/106 (98%)  | 104 (100%) | 0        | 100         | 100 |
| 35  | L     | 41/55 (74%)    | 41 (100%)  | 0        | 100         | 100 |
| 36  | M     | 215/268 (80%)  | 215 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 38  | O     | 154/293 (53%)     | 154 (100%)   | 0        | 100         | 100 |
| 39  | Q     | 121/448 (27%)     | 121 (100%)   | 0        | 100         | 100 |
| 40  | R     | 196/218 (90%)     | 196 (100%)   | 0        | 100         | 100 |
| 42  | U     | 105/324 (32%)     | 105 (100%)   | 0        | 100         | 100 |
| 43  | V     | 90/98 (92%)       | 90 (100%)    | 0        | 100         | 100 |
| 44  | W     | 182/373 (49%)     | 182 (100%)   | 0        | 100         | 100 |
| 45  | X     | 154/261 (59%)     | 154 (100%)   | 0        | 100         | 100 |
| 46  | a     | 85/111 (77%)      | 85 (100%)    | 0        | 100         | 100 |
| 46  | e     | 86/111 (78%)      | 86 (100%)    | 0        | 100         | 100 |
| 47  | b     | 67/79 (85%)       | 67 (100%)    | 0        | 100         | 100 |
| 47  | f     | 65/79 (82%)       | 65 (100%)    | 0        | 100         | 100 |
| 48  | c     | 86/101 (85%)      | 86 (100%)    | 0        | 100         | 100 |
| 48  | g     | 84/101 (83%)      | 84 (100%)    | 0        | 100         | 100 |
| 49  | d     | 83/106 (78%)      | 83 (100%)    | 0        | 100         | 100 |
| 49  | h     | 81/106 (76%)      | 81 (100%)    | 0        | 100         | 100 |
| All | All   | 12763/20726 (62%) | 12730 (100%) | 33 (0%)  | 84          | 86  |

5 of 33 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 24  | Dl    | 106  | ARG  |
| 27  | Dm    | 31   | LEU  |
| 30  | G     | 166  | ASP  |
| 15  | DA    | 1165 | LEU  |
| 15  | DA    | 475  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | Q     | 10  | ASN  |
| 43  | V     | 35  | GLN  |
| 16  | DB    | 348 | GLN  |
| 16  | DB    | 285 | HIS  |
| 43  | V     | 70  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 46 ligands modelled in this entry, 18 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |       |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|-------|-------------|
|     |      |       |     |       | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ  | # $ Z  > 2$ |
| 50  | 2A1  | 0     | 812 | 50    | 4,4,4        | 2.82 | 2 (50%)     | 3,4,4       | 1.76  | 1 (33%)     |
| 50  | 2A1  | 0     | 803 | 50    | 4,4,4        | 2.20 | 1 (25%)     | 3,4,4       | 3.86  | 2 (66%)     |
| 50  | 2A1  | 0     | 806 | 50    | 4,4,4        | 2.23 | 1 (25%)     | 3,4,4       | 4.00  | 1 (33%)     |
| 51  | ALA  | 2     | 602 | 50    | 3,4,5        | 0.41 | 0           | 2,4,6       | 17.08 | 1 (50%)     |
| 50  | 2A1  | 0     | 807 | 51,50 | 4,4,4        | 3.67 | 2 (50%)     | 3,4,4       | 0.88  | 0           |
| 50  | 2A1  | 2     | 604 | 50    | 4,4,4        | 3.04 | 3 (75%)     | 3,4,4       | 4.06  | 2 (66%)     |
| 50  | 2A1  | N     | 305 | 50    | 4,4,4        | 3.05 | 2 (50%)     | 3,4,4       | 3.49  | 1 (33%)     |
| 50  | 2A1  | 2     | 605 | 51,50 | 4,4,4        | 2.42 | 1 (25%)     | 3,4,4       | 2.59  | 1 (33%)     |
| 50  | 2A1  | 0     | 813 | 50    | 4,4,4        | 3.19 | 2 (50%)     | 3,4,4       | 3.19  | 1 (33%)     |
| 50  | 2A1  | 0     | 814 | 50    | 4,4,4        | 2.53 | 2 (50%)     | 3,4,4       | 4.84  | 1 (33%)     |
| 50  | 2A1  | 0     | 805 | 50    | 4,4,4        | 2.42 | 1 (25%)     | 3,4,4       | 3.74  | 2 (66%)     |
| 50  | 2A1  | N     | 306 | -     | 4,4,4        | 2.31 | 1 (25%)     | 3,4,4       | 2.76  | 1 (33%)     |
| 51  | ALA  | 0     | 808 | 50    | 5,5,5        | 1.61 | 2 (40%)     | 6,6,6       | 2.72  | 2 (33%)     |
| 50  | 2A1  | 2     | 601 | 51    | 4,4,4        | 2.29 | 1 (25%)     | 3,4,4       | 3.38  | 1 (33%)     |

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 50  | 2A1  | N     | 302  | 50    | 4,4,4        | 1.73 | 1 (25%)  | 3,4,4       | 3.88 | 2 (66%)  |
| 51  | ALA  | 2     | 606  | 50    | 5,5,5        | 1.47 | 0        | 6,6,6       | 1.15 | 0        |
| 52  | SF4  | 1     | 1000 | 2     | 0,12,12      | -    | -        | -           | -    | -        |
| 50  | 2A1  | 2     | 603  | 51,50 | 4,4,4        | 2.58 | 2 (50%)  | 3,4,4       | 1.98 | 1 (33%)  |
| 50  | 2A1  | 0     | 810  | 50    | 4,4,4        | 1.90 | 1 (25%)  | 3,4,4       | 0.90 | 0        |
| 50  | 2A1  | 0     | 804  | 50    | 4,4,4        | 2.00 | 1 (25%)  | 3,4,4       | 3.66 | 2 (66%)  |
| 50  | 2A1  | 0     | 811  | 50    | 4,4,4        | 2.34 | 1 (25%)  | 3,4,4       | 3.32 | 1 (33%)  |
| 50  | 2A1  | 0     | 809  | -     | 4,4,4        | 2.30 | 1 (25%)  | 3,4,4       | 2.71 | 1 (33%)  |
| 50  | 2A1  | N     | 304  | 50    | 4,4,4        | 3.11 | 2 (50%)  | 3,4,4       | 5.59 | 2 (66%)  |
| 50  | 2A1  | 0     | 802  | 50    | 4,4,4        | 2.75 | 1 (25%)  | 3,4,4       | 0.83 | 0        |
| 50  | 2A1  | N     | 301  | 50    | 4,4,4        | 2.46 | 1 (25%)  | 3,4,4       | 2.50 | 1 (33%)  |
| 50  | 2A1  | 0     | 801  | 50    | 4,4,4        | 2.12 | 3 (75%)  | 3,4,4       | 0.38 | 0        |
| 50  | 2A1  | 0     | 815  | 50    | 4,4,4        | 2.12 | 1 (25%)  | 3,4,4       | 4.72 | 2 (66%)  |
| 50  | 2A1  | N     | 303  | 50    | 4,4,4        | 2.00 | 1 (25%)  | 3,4,4       | 3.83 | 1 (33%)  |

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   |
|-----|------|-------|------|-------|---------|----------|---------|
| 50  | 2A1  | 0     | 812  | 50    | -       | 2/2/2/2  | -       |
| 50  | 2A1  | 0     | 803  | 50    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | 0     | 806  | 50    | -       | 1/2/2/2  | -       |
| 51  | ALA  | 2     | 602  | 50    | -       | 0/0/2/4  | -       |
| 50  | 2A1  | 0     | 807  | 51,50 | -       | 2/2/2/2  | -       |
| 50  | 2A1  | 2     | 604  | 50    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | N     | 305  | 50    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | 2     | 605  | 51,50 | -       | 1/2/2/2  | -       |
| 50  | 2A1  | 0     | 813  | 50    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | 0     | 814  | 50    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | 0     | 805  | 50    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | N     | 306  | -     | -       | 1/2/2/2  | -       |
| 51  | ALA  | 0     | 808  | 50    | -       | 0/4/4/4  | -       |
| 50  | 2A1  | 2     | 601  | 51    | -       | 0/2/2/2  | -       |
| 50  | 2A1  | N     | 302  | 50    | -       | 0/2/2/2  | -       |
| 51  | ALA  | 2     | 606  | 50    | -       | 0/4/4/4  | -       |
| 52  | SF4  | 1     | 1000 | 2     | -       | -        | 0/6/5/5 |
| 50  | 2A1  | 2     | 603  | 51,50 | -       | 1/2/2/2  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 50  | 2A1  | 0     | 810 | 50   | -       | 0/2/2/2  | -     |
| 50  | 2A1  | 0     | 804 | 50   | -       | 2/2/2/2  | -     |
| 50  | 2A1  | 0     | 811 | 50   | -       | 0/2/2/2  | -     |
| 50  | 2A1  | 0     | 809 | -    | -       | 0/2/2/2  | -     |
| 50  | 2A1  | N     | 304 | 50   | -       | 2/2/2/2  | -     |
| 50  | 2A1  | 0     | 802 | 50   | -       | 2/2/2/2  | -     |
| 50  | 2A1  | N     | 301 | 50   | -       | 2/2/2/2  | -     |
| 50  | 2A1  | 0     | 801 | 50   | -       | 2/2/2/2  | -     |
| 50  | 2A1  | 0     | 815 | 50   | -       | 2/2/2/2  | -     |
| 50  | 2A1  | N     | 303 | 50   | -       | 2/2/2/2  | -     |

The worst 5 of 37 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 50  | 0     | 807 | 2A1  | O-C   | -5.70 | 1.18        | 1.42     |
| 50  | N     | 304 | 2A1  | O-C   | -5.51 | 1.19        | 1.42     |
| 50  | 0     | 802 | 2A1  | O-C   | -4.89 | 1.21        | 1.42     |
| 50  | 0     | 813 | 2A1  | O-C   | -4.67 | 1.22        | 1.42     |
| 50  | N     | 301 | 2A1  | O-C   | -4.65 | 1.22        | 1.42     |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 51  | 2     | 602 | ALA  | O-C-CA | -24.15 | 47.80       | 124.28   |
| 50  | N     | 304 | 2A1  | O-C-CA | 9.19   | 129.31      | 112.42   |
| 50  | 0     | 814 | 2A1  | O-C-CA | 8.12   | 127.34      | 112.42   |
| 50  | 0     | 815 | 2A1  | O-C-CA | 7.33   | 125.90      | 112.42   |
| 50  | 0     | 806 | 2A1  | O-C-CA | 6.69   | 124.72      | 112.42   |

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

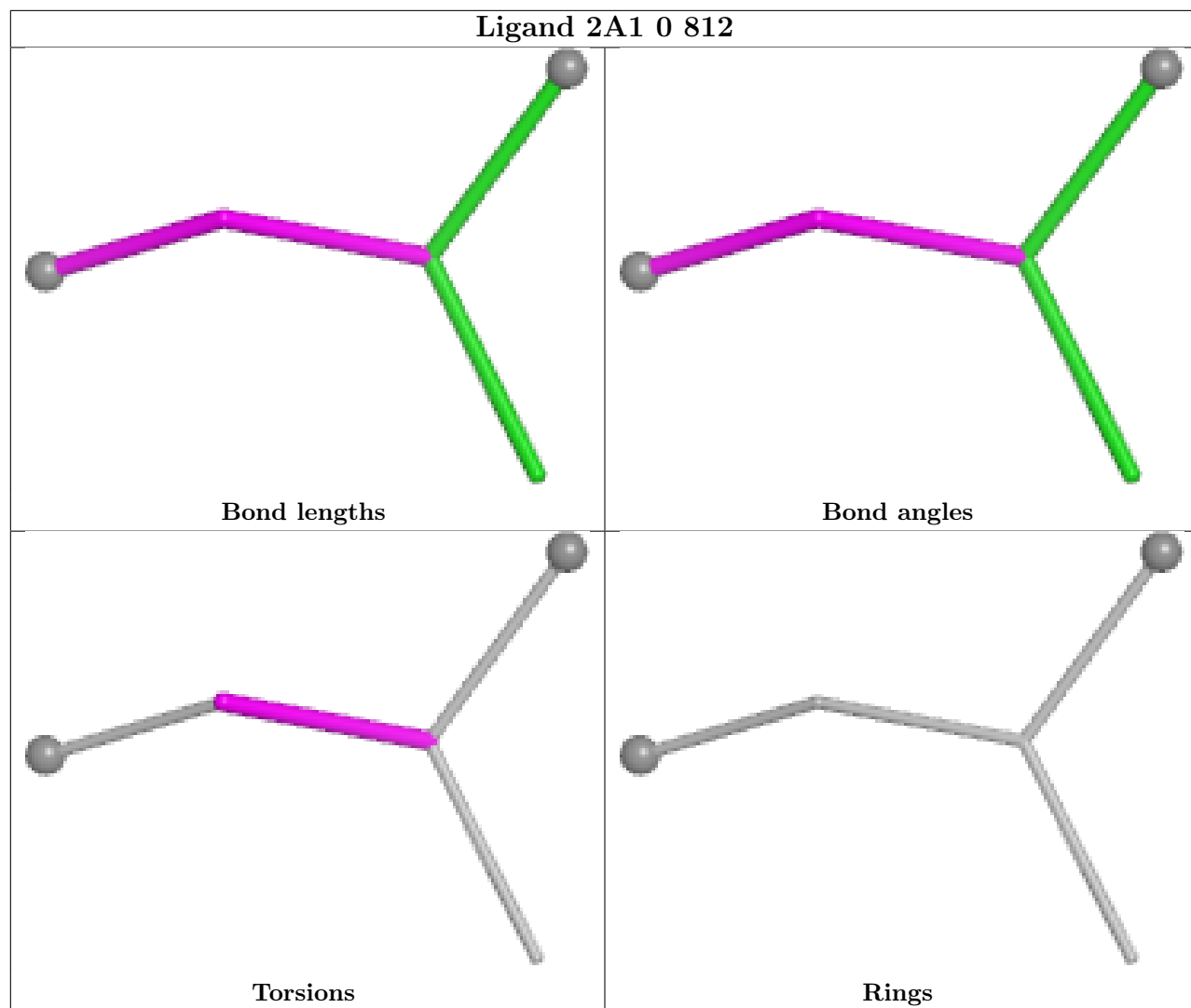
| Mol | Chain | Res | Type | Atoms     |
|-----|-------|-----|------|-----------|
| 50  | 0     | 801 | 2A1  | O-C-CA-N  |
| 50  | 0     | 801 | 2A1  | O-C-CA-C3 |
| 50  | 0     | 802 | 2A1  | O-C-CA-N  |
| 50  | 0     | 802 | 2A1  | O-C-CA-C3 |
| 50  | 0     | 804 | 2A1  | O-C-CA-N  |

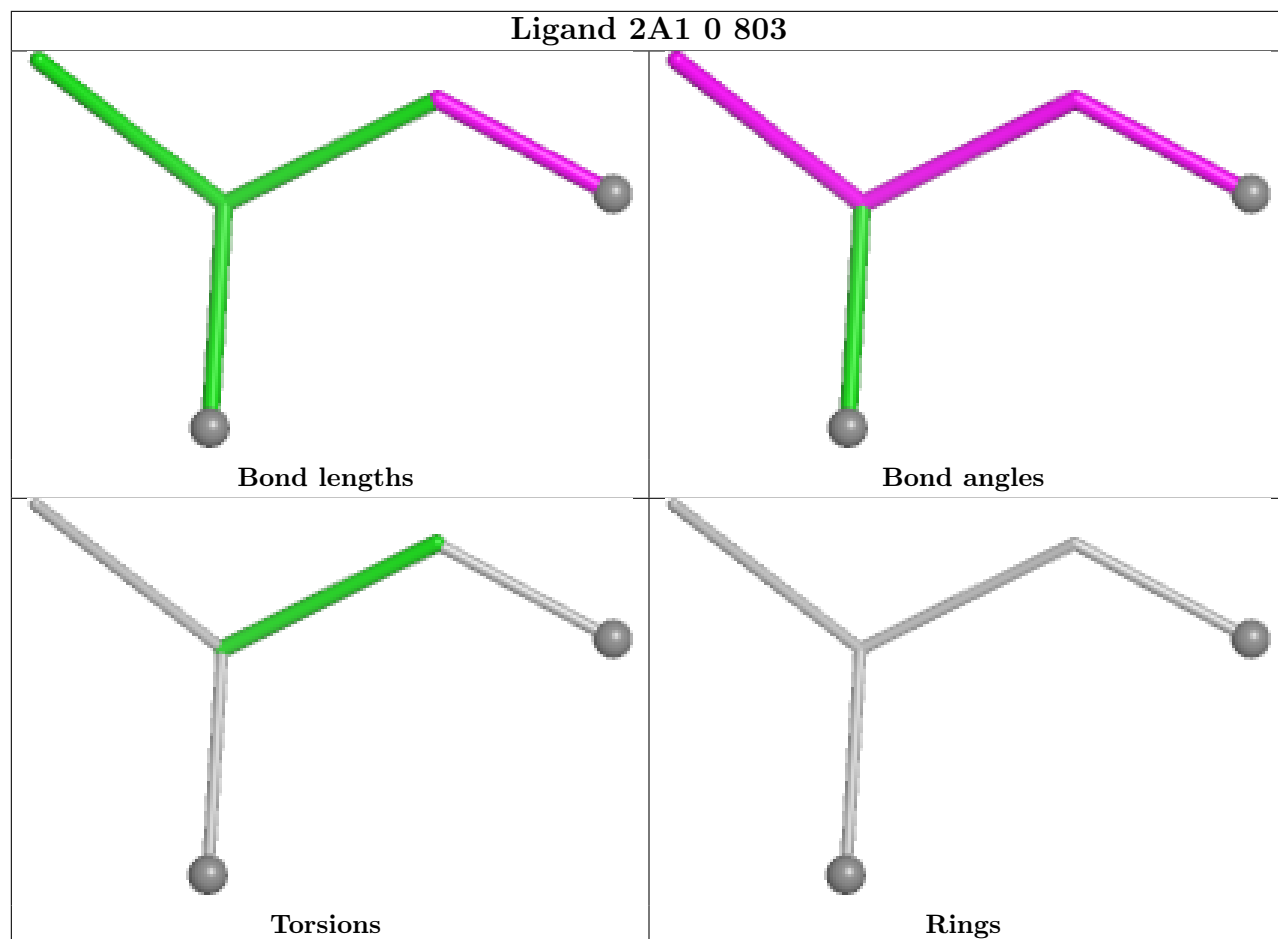
There are no ring outliers.

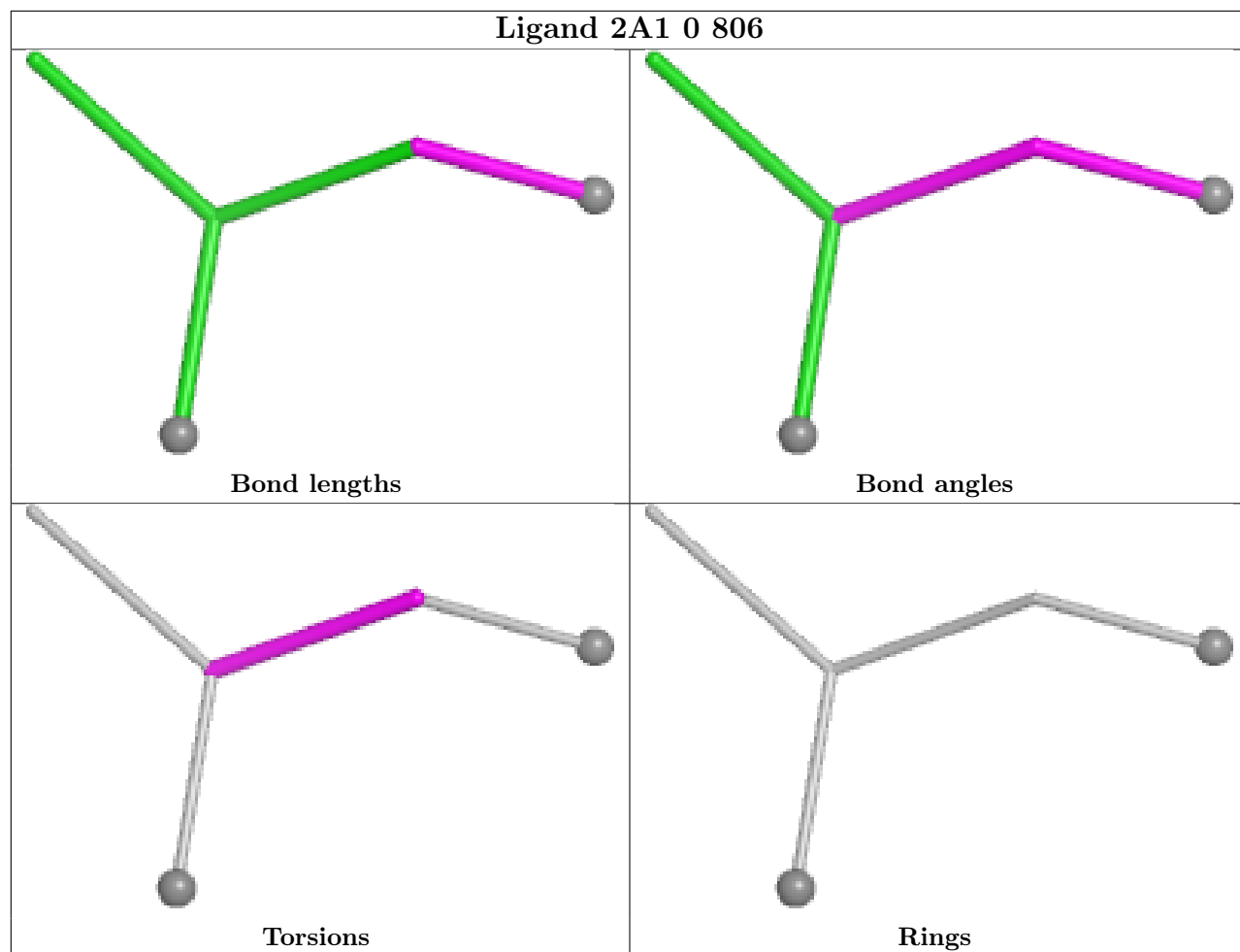
6 monomers are involved in 3 short contacts:

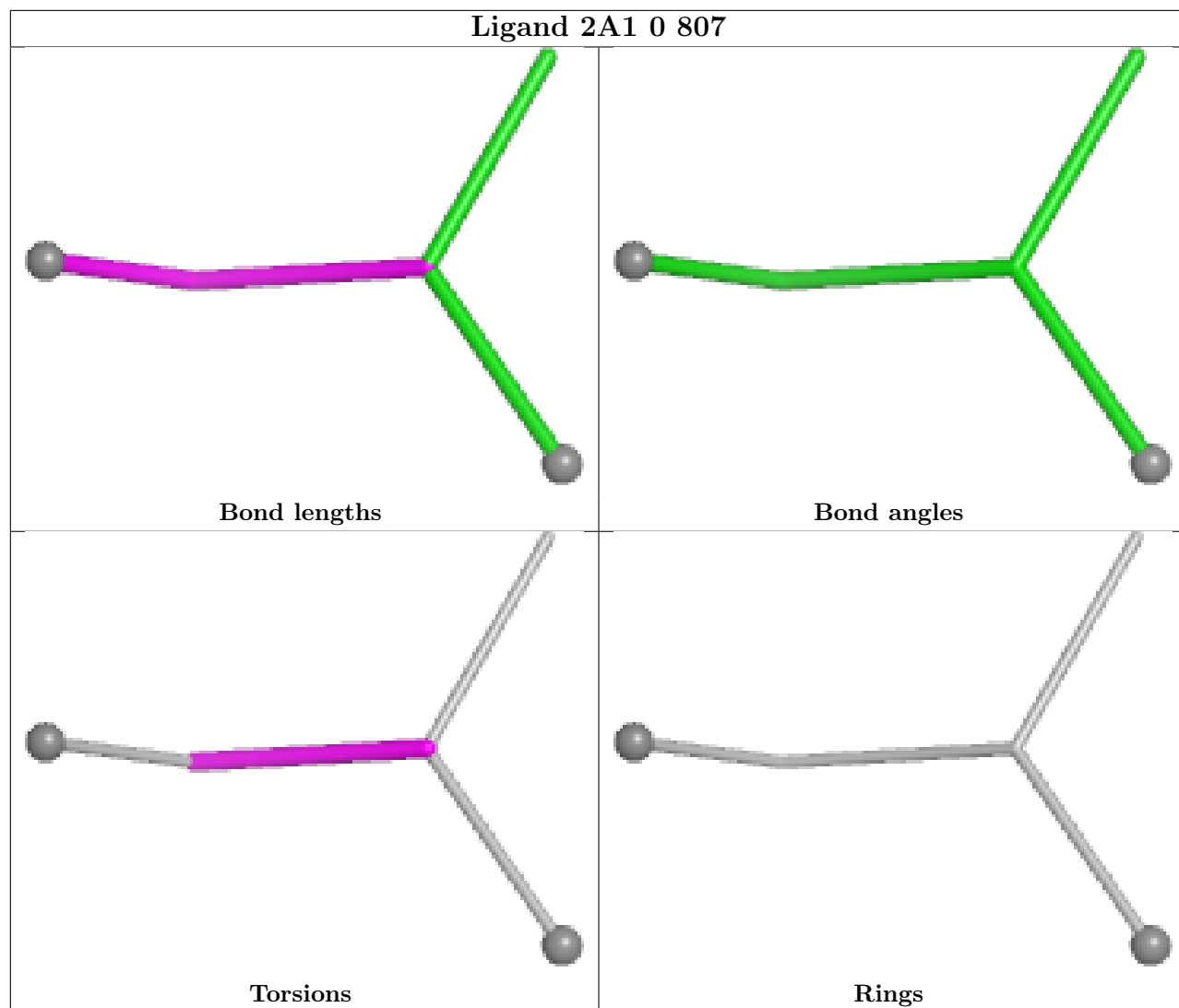
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 50  | 0     | 812 | 2A1  | 1       | 0            |
| 50  | 0     | 807 | 2A1  | 1       | 0            |
| 50  | 0     | 813 | 2A1  | 1       | 0            |
| 51  | 0     | 808 | ALA  | 1       | 0            |
| 50  | 0     | 802 | 2A1  | 1       | 0            |
| 50  | 0     | 801 | 2A1  | 1       | 0            |

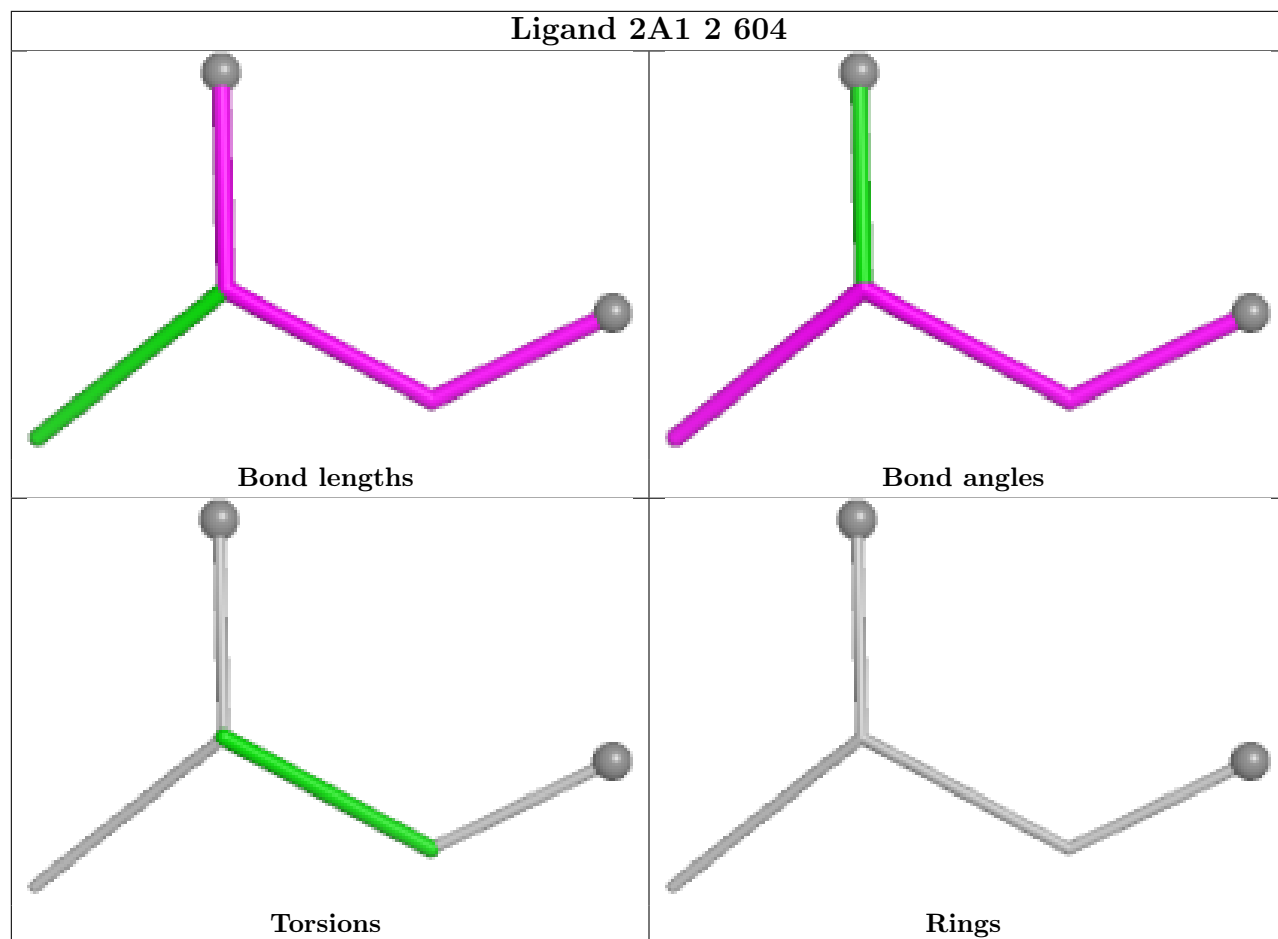
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

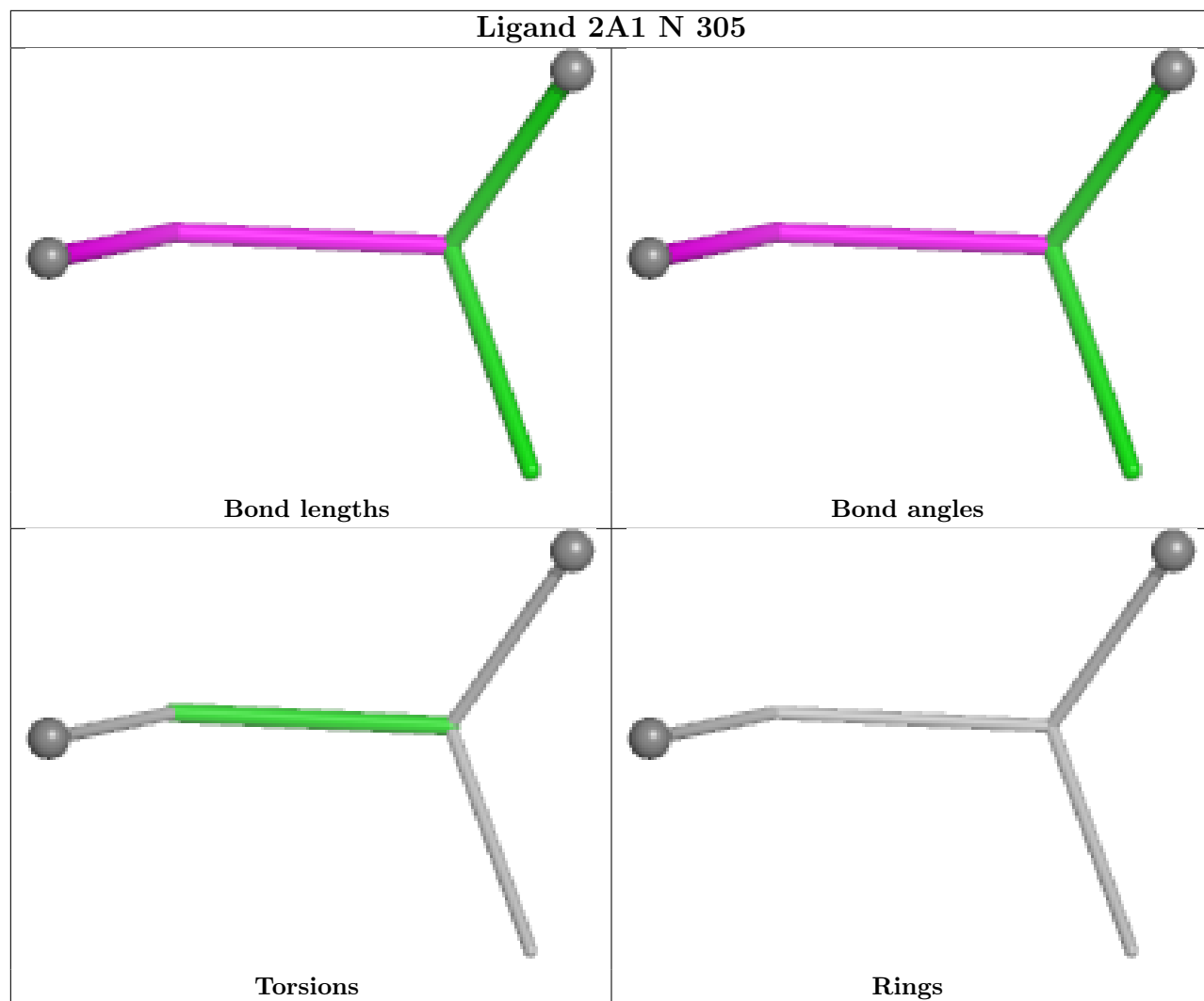


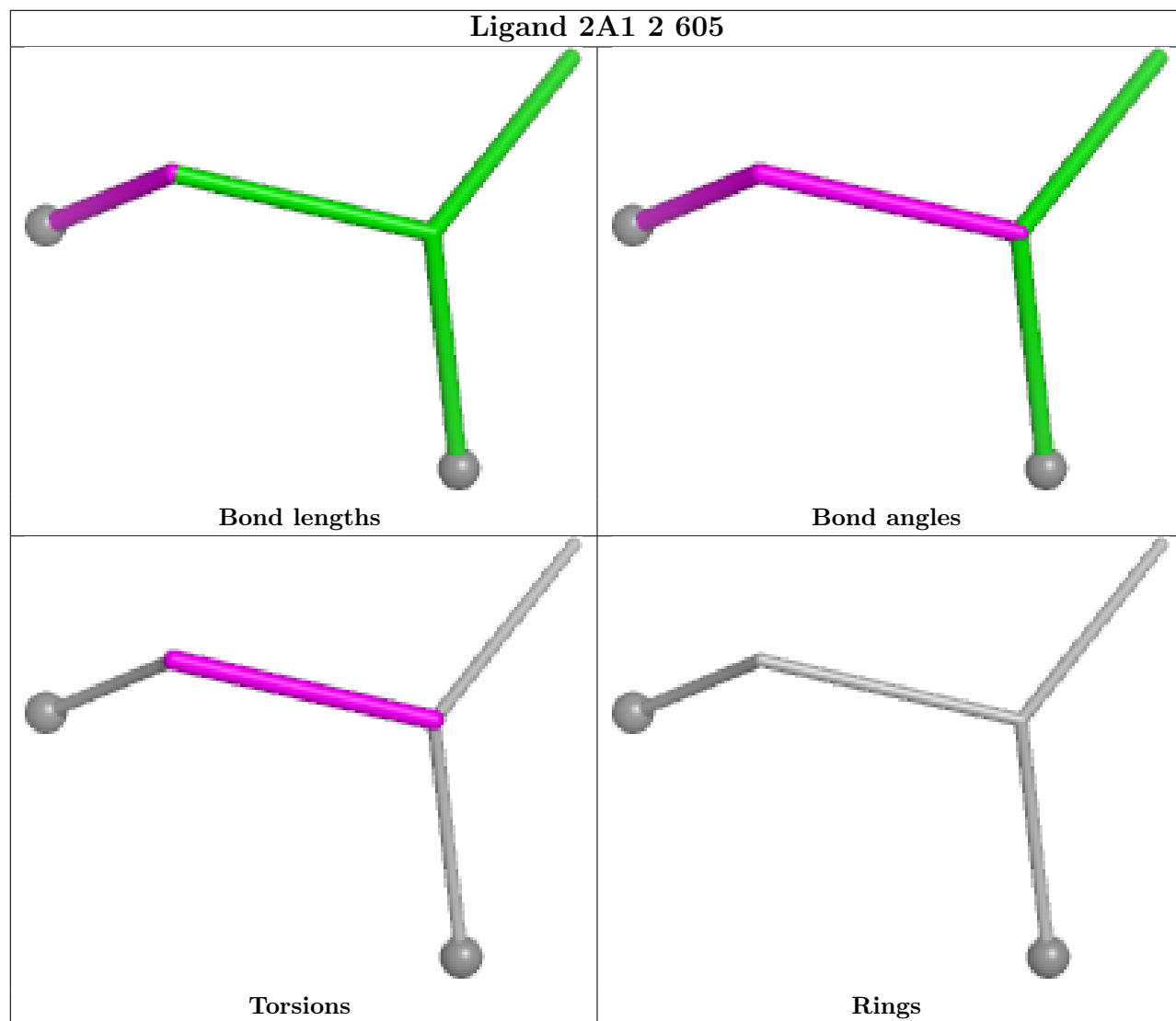


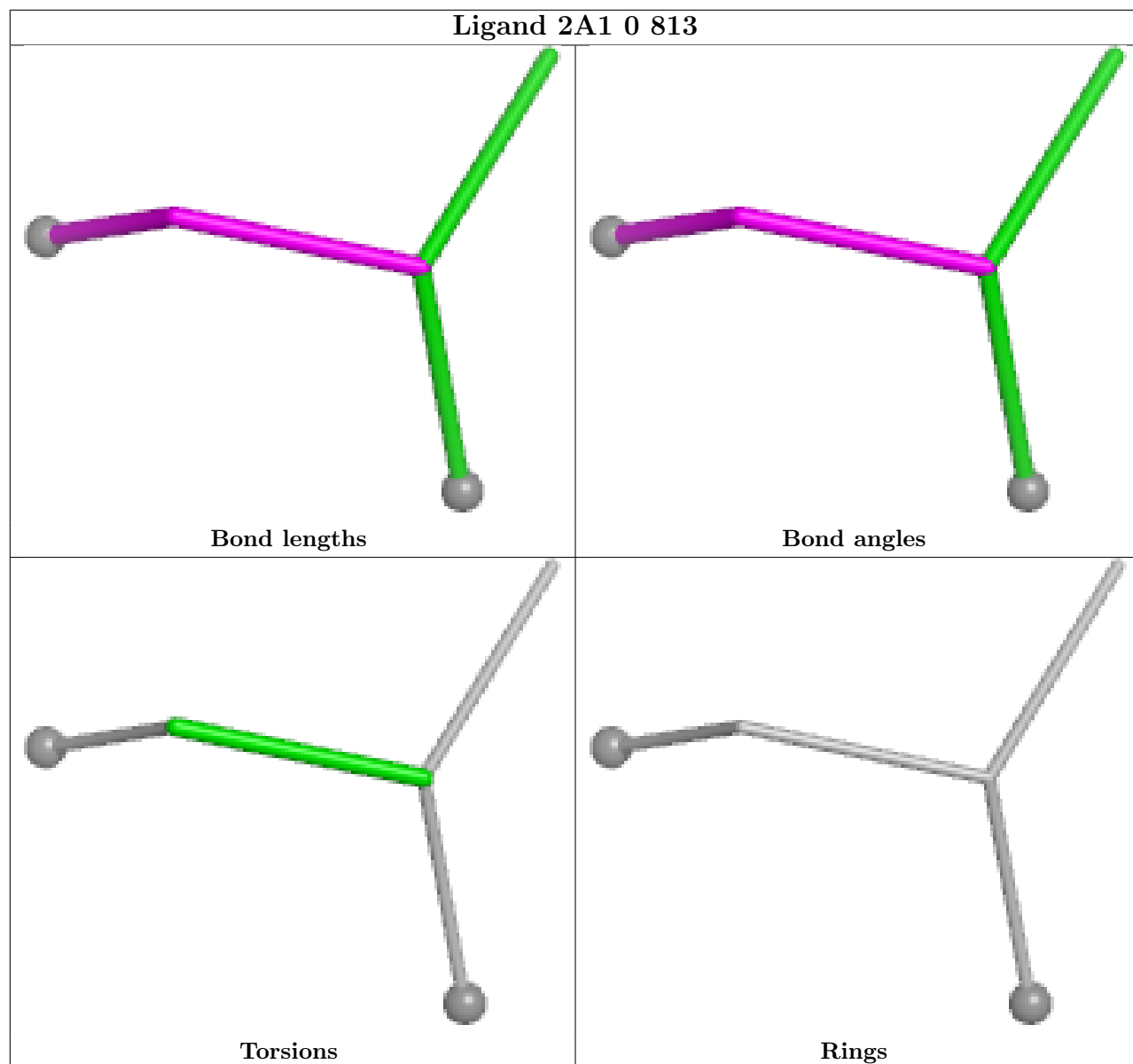


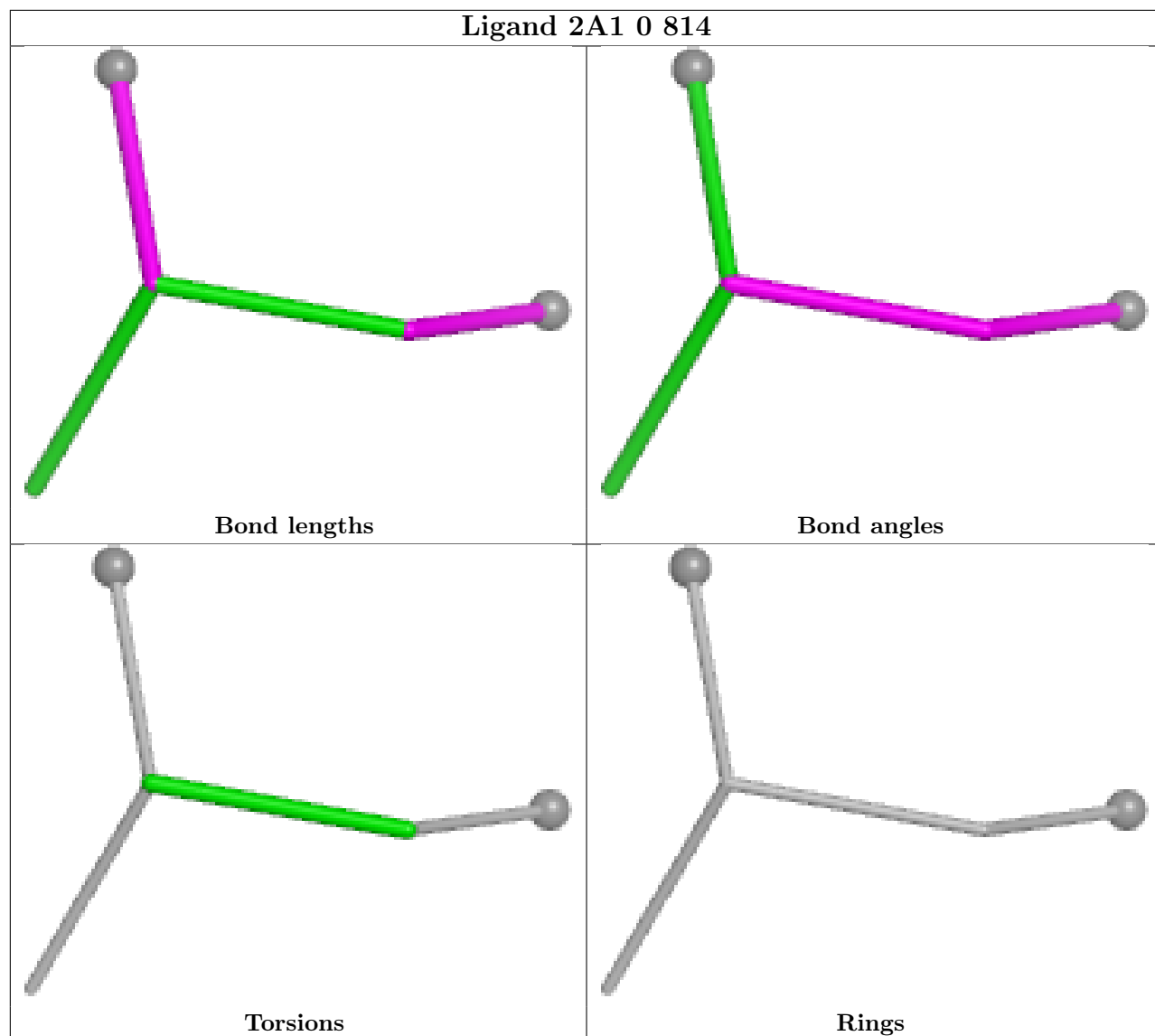


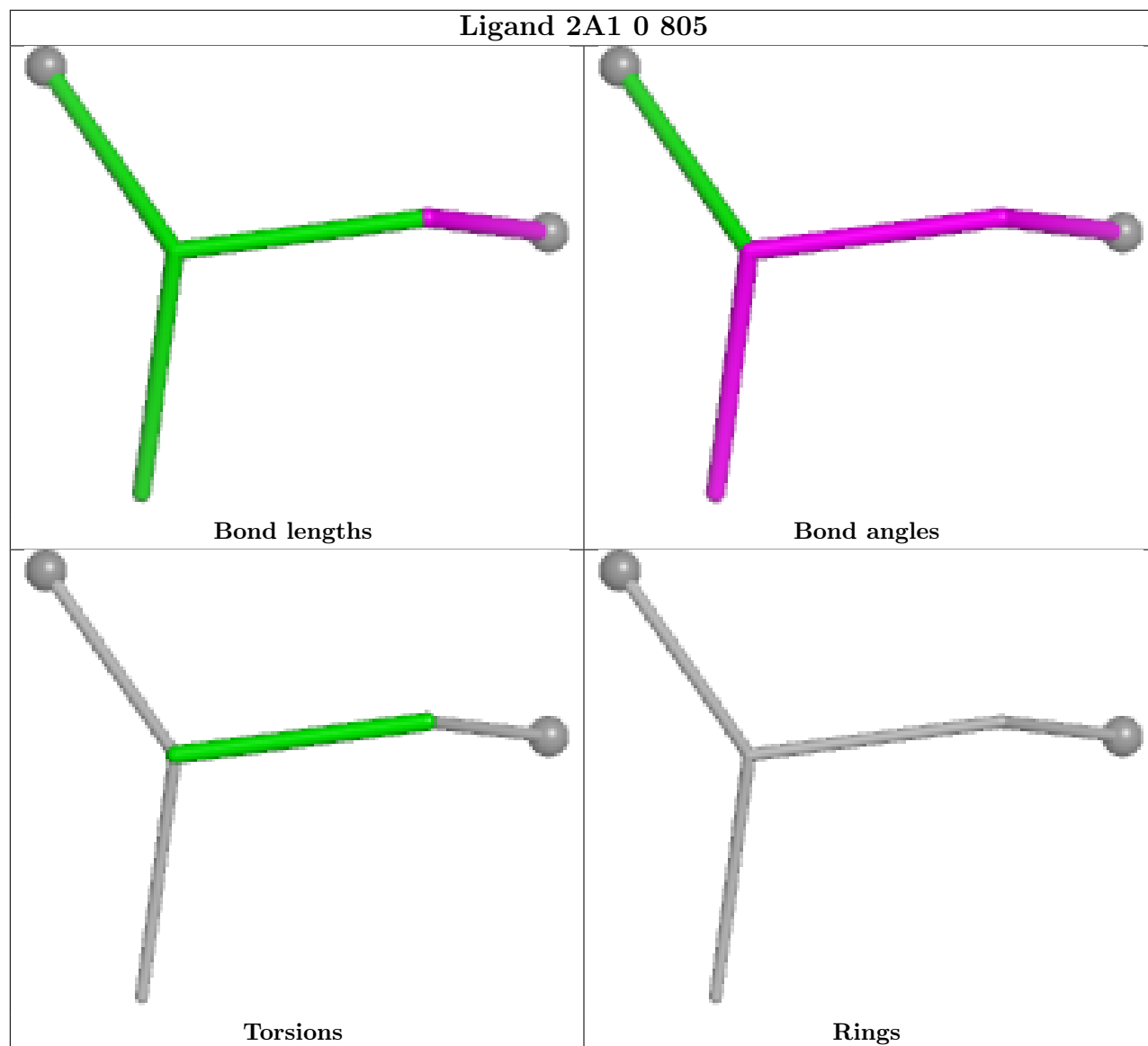


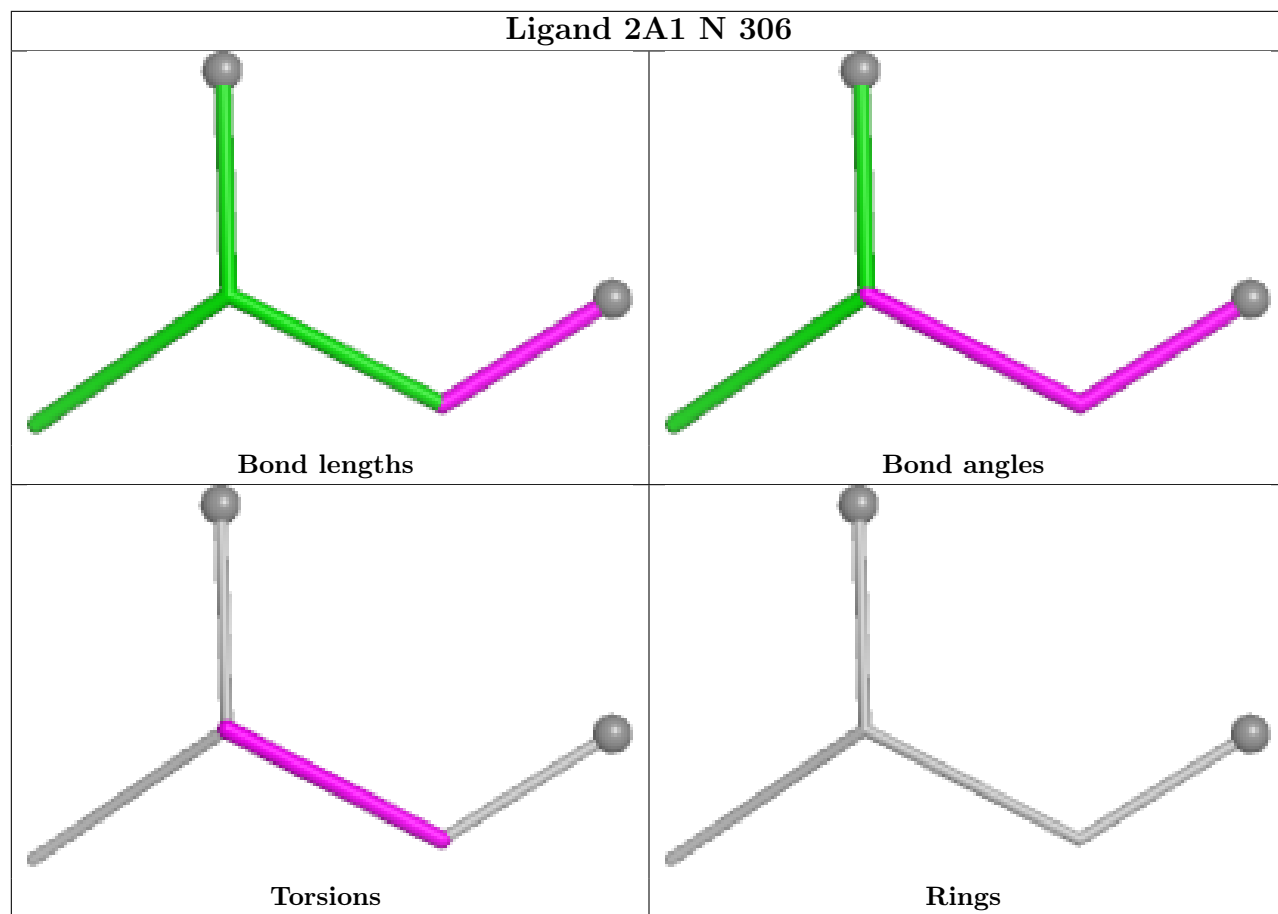


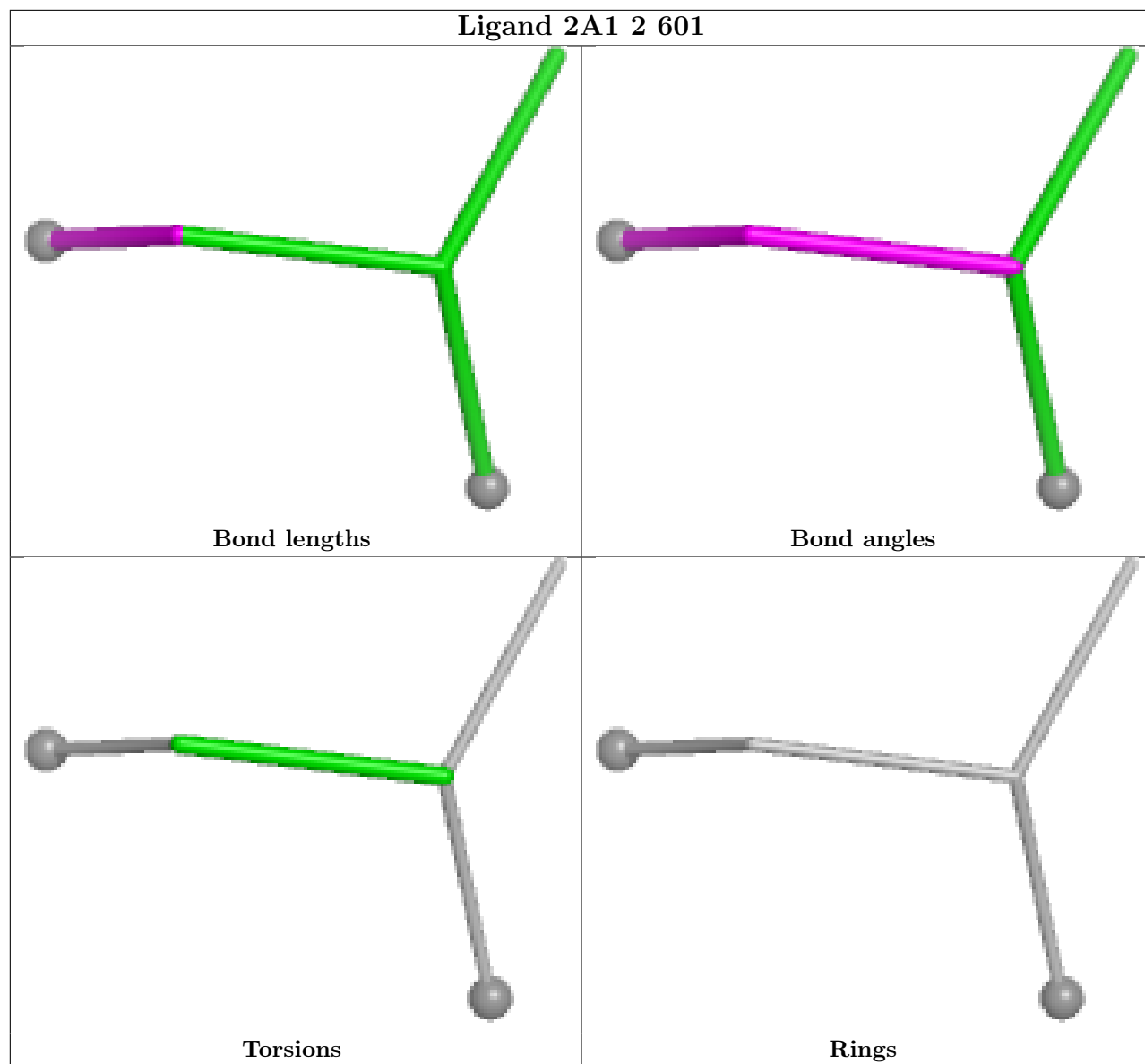


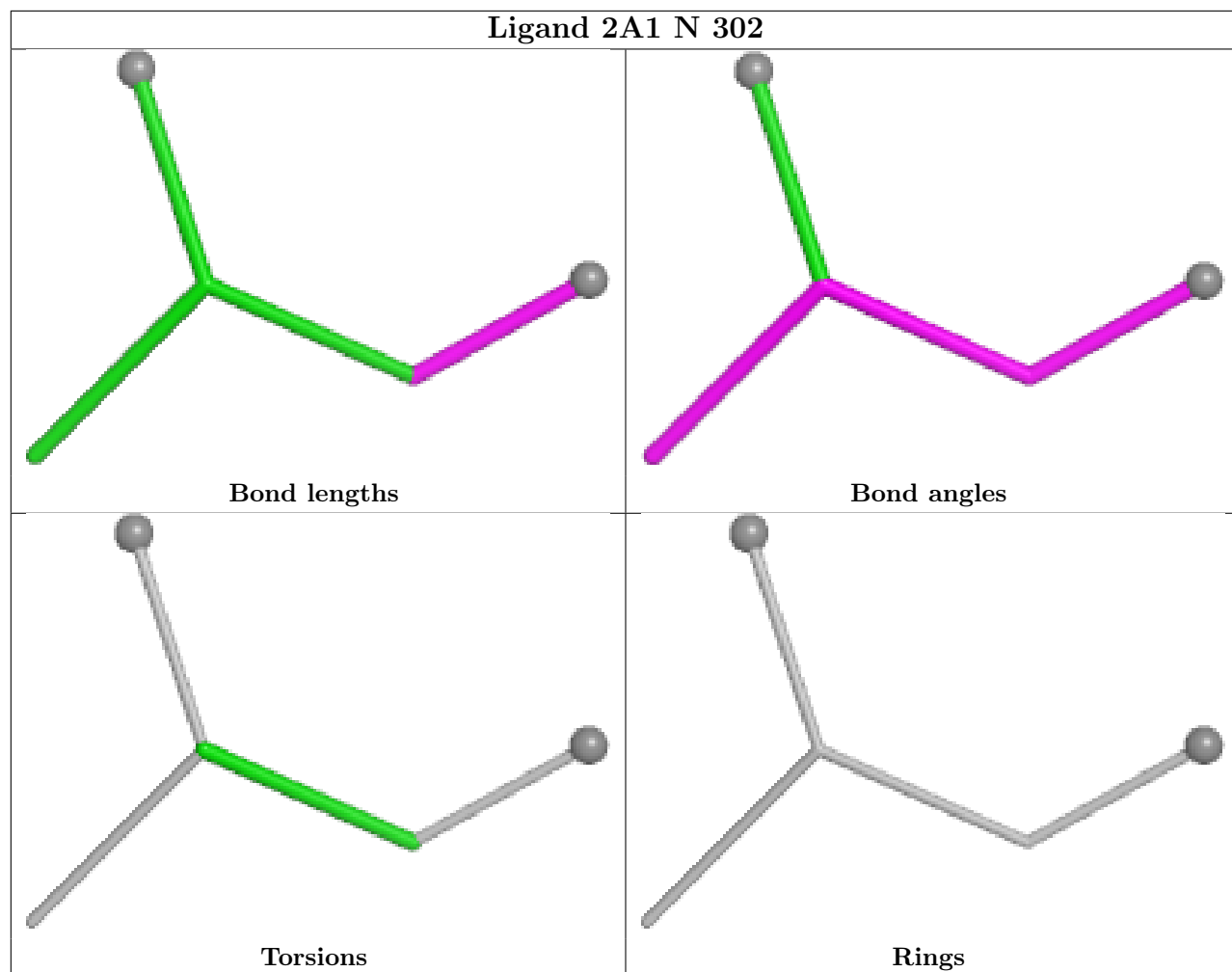


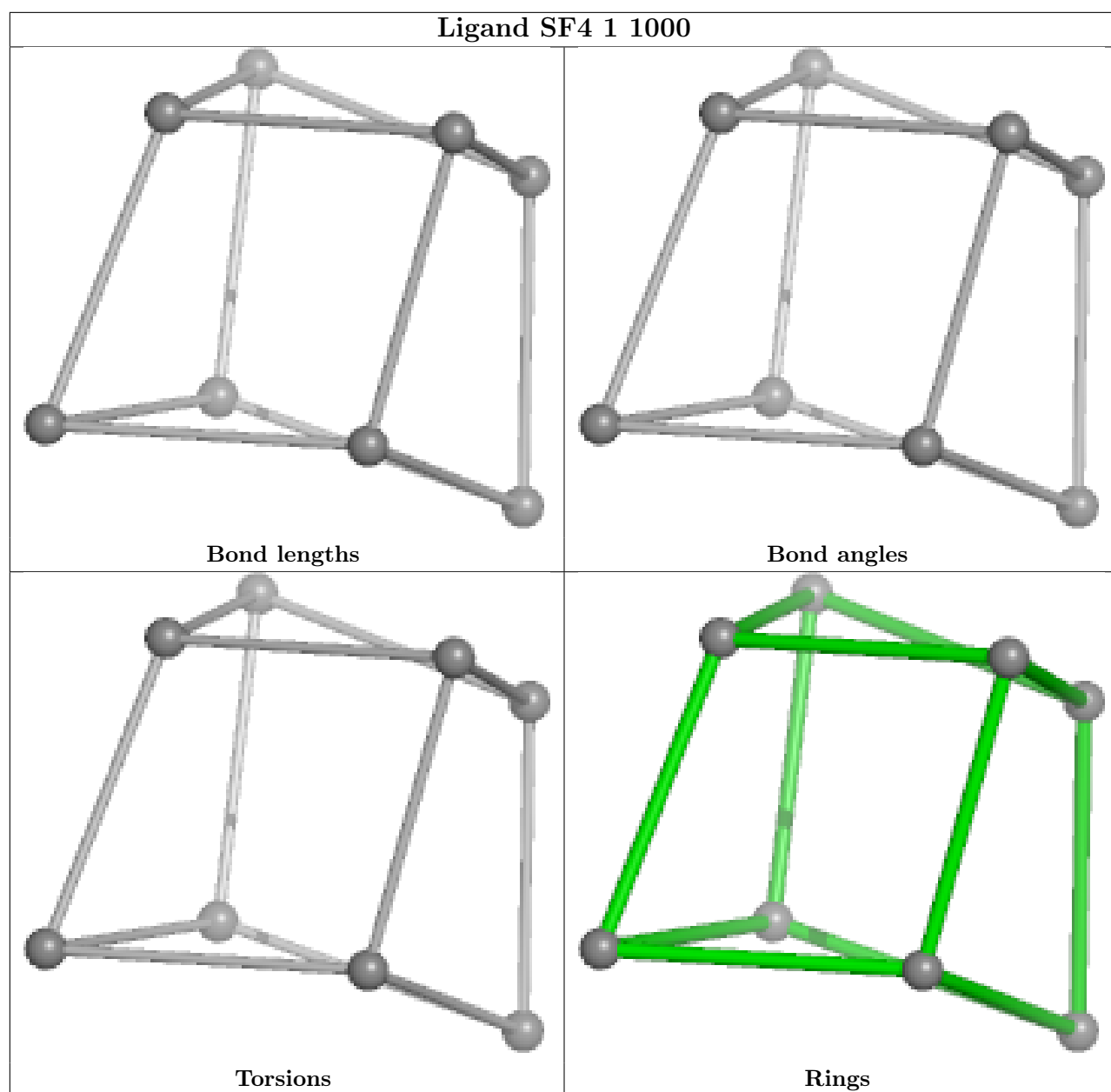


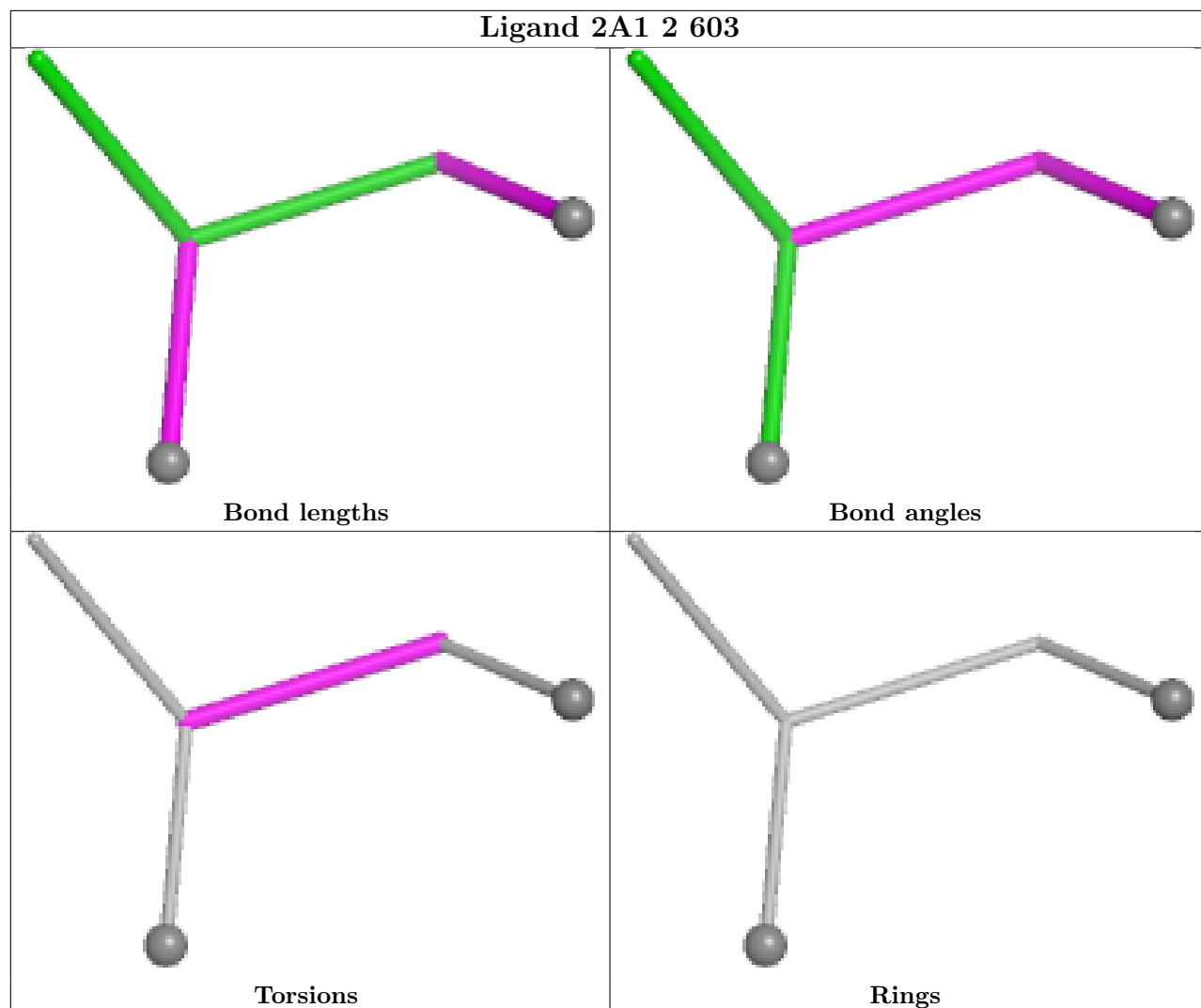


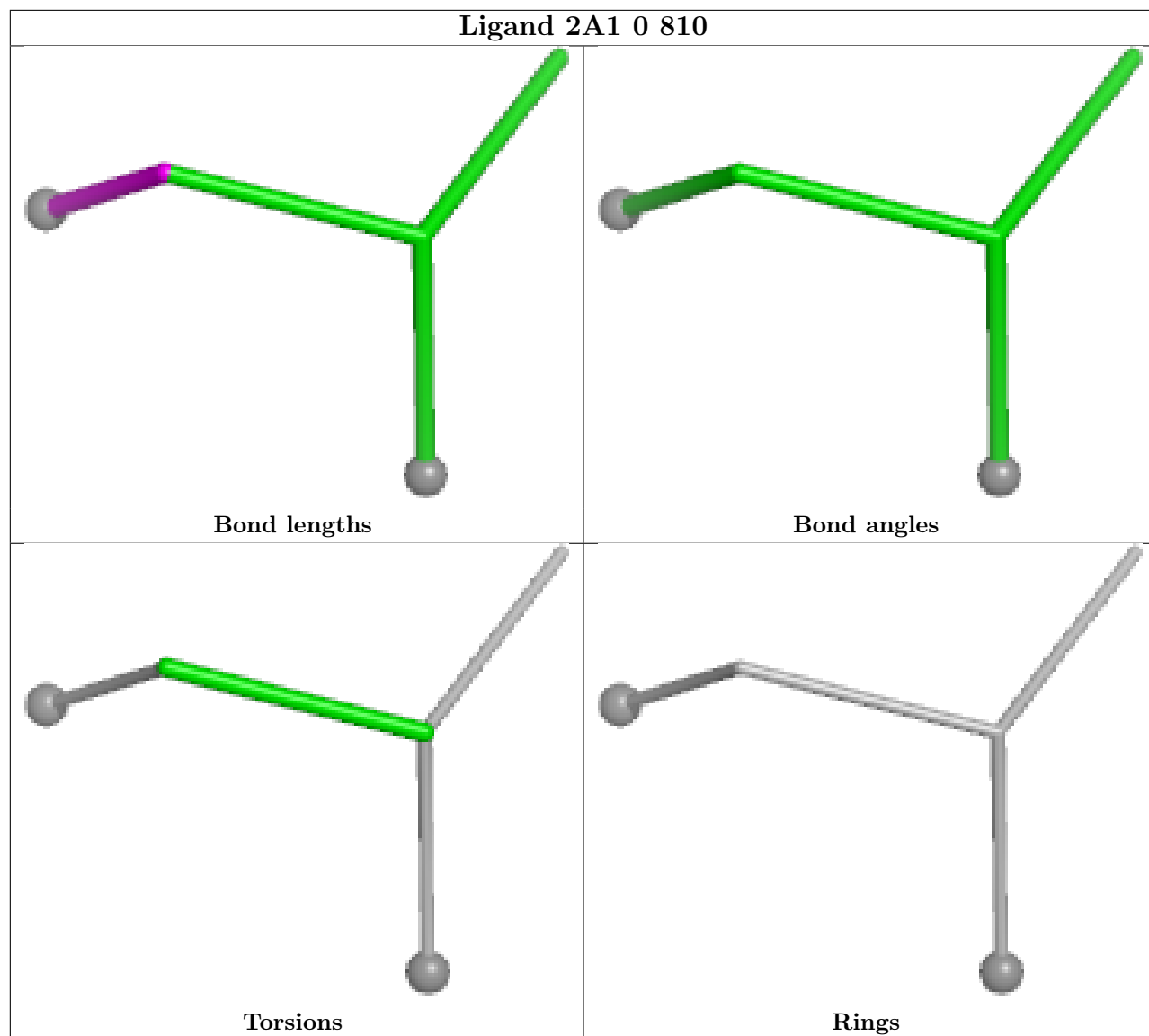




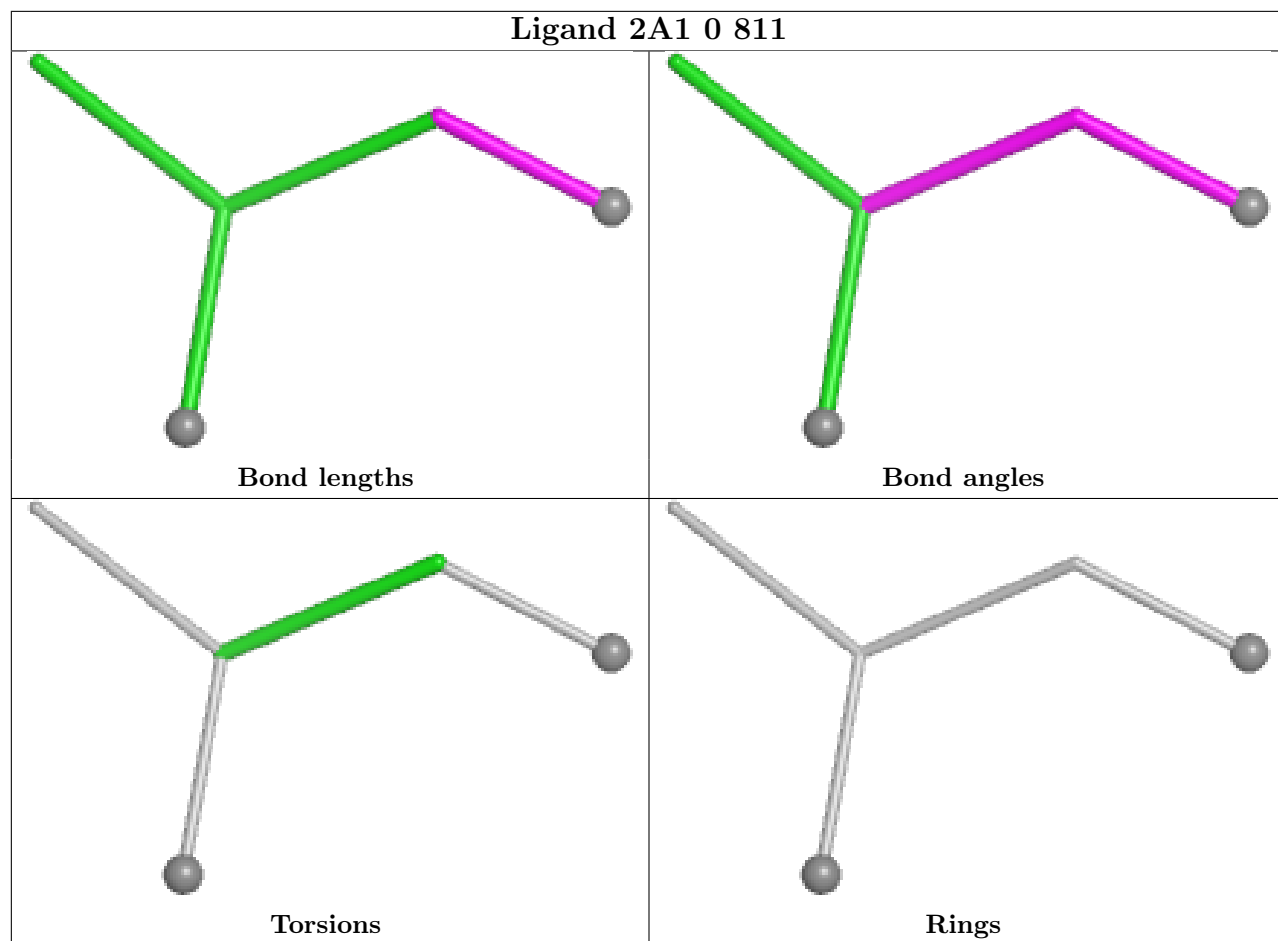


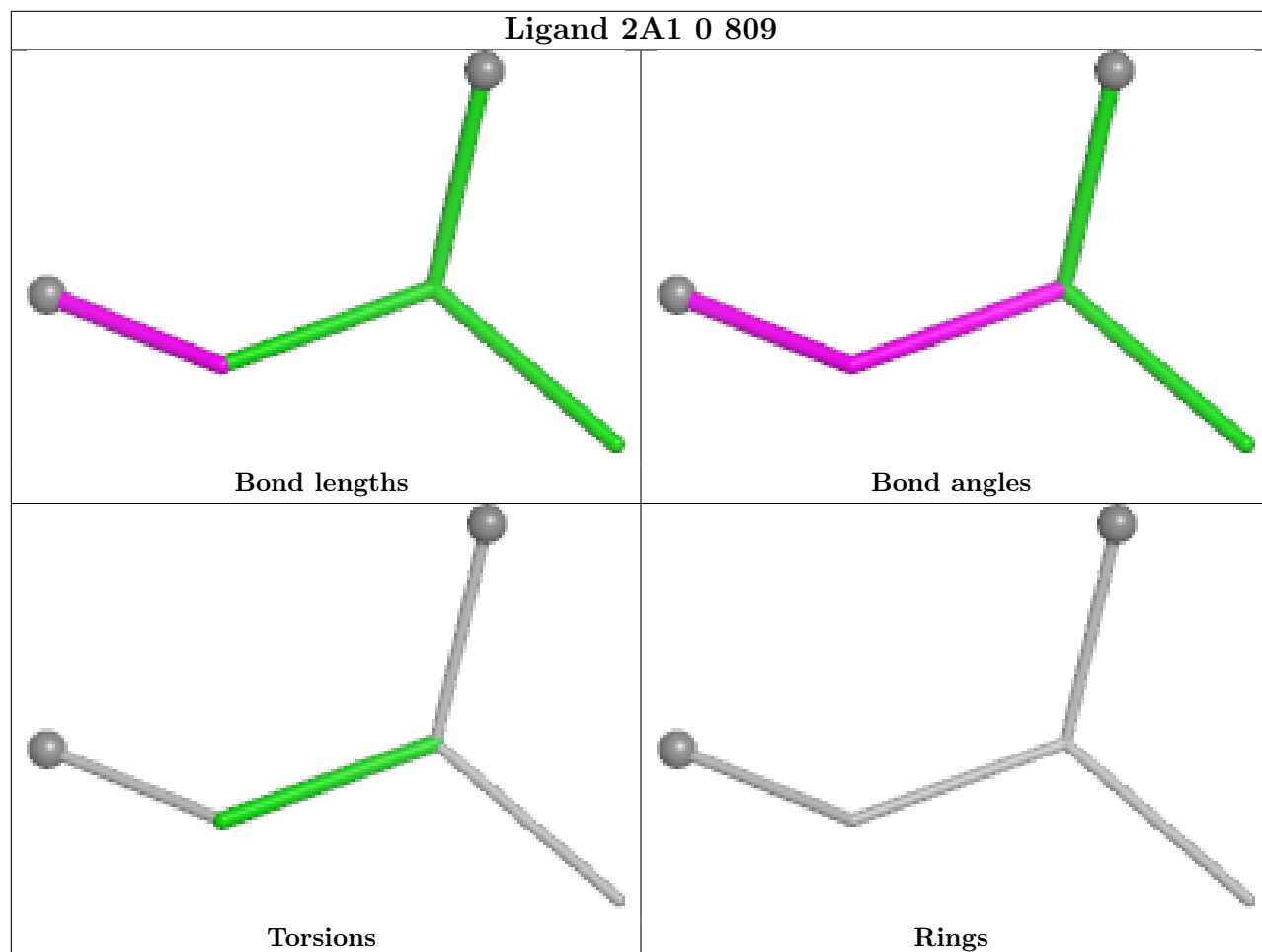


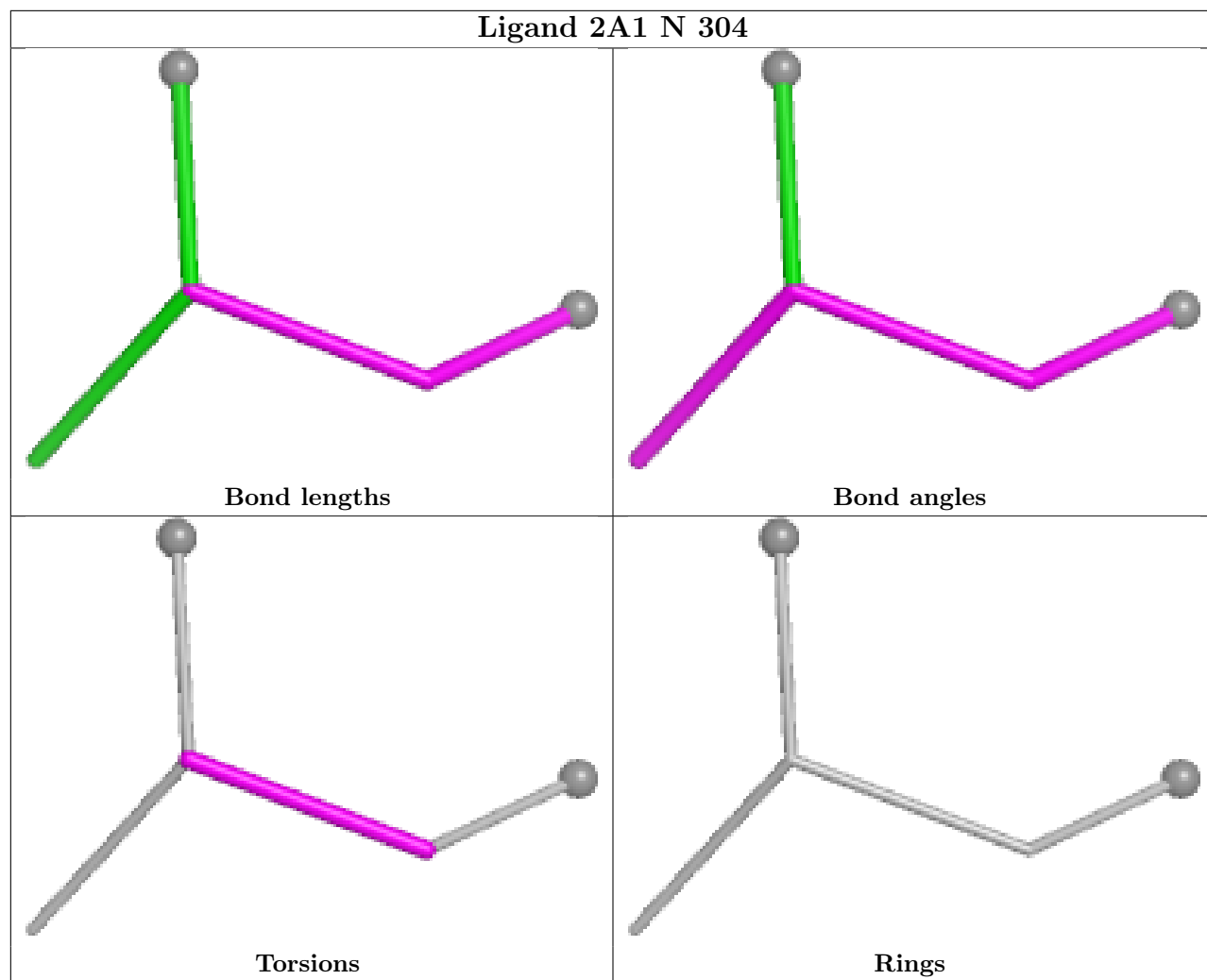


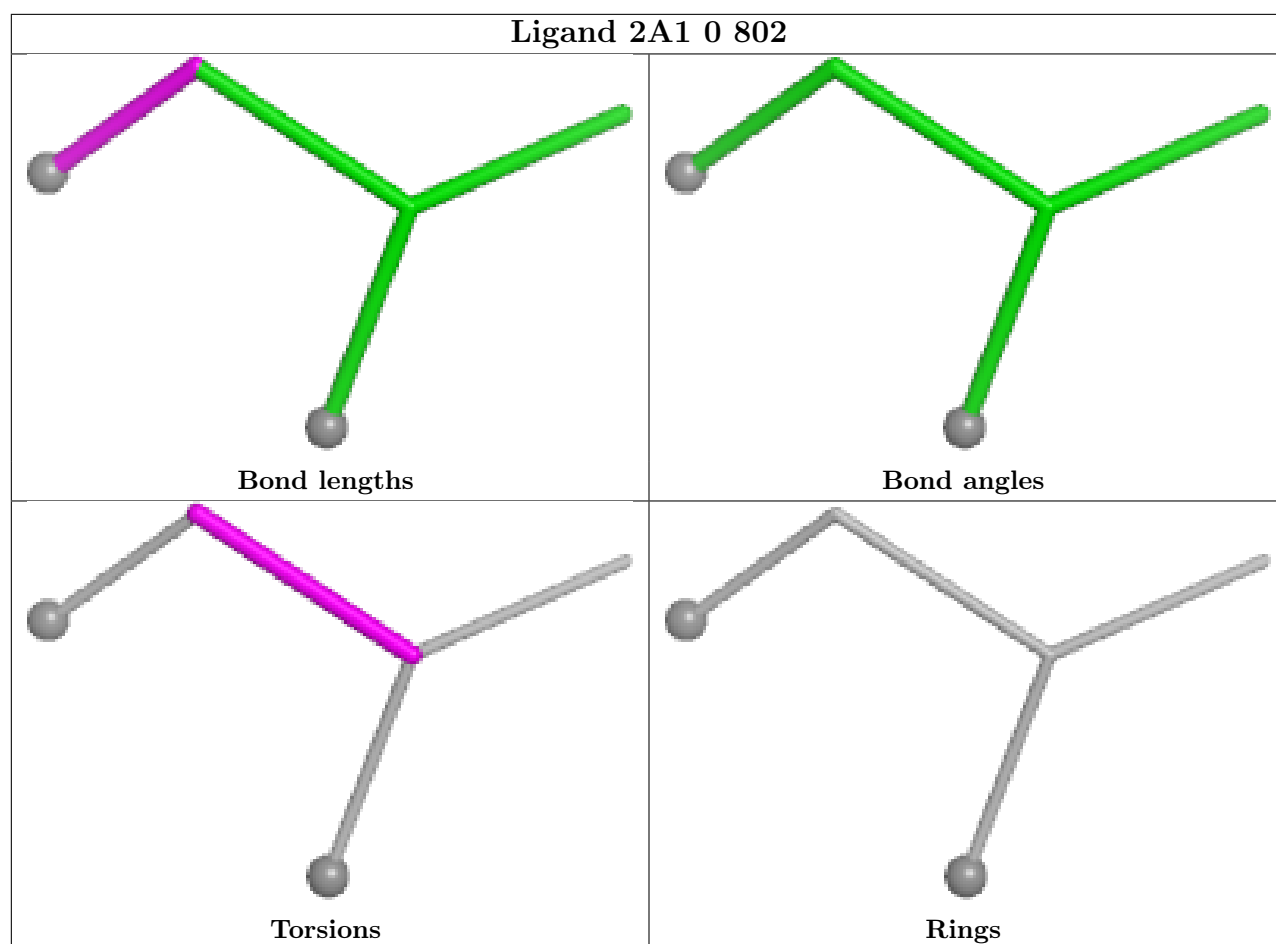


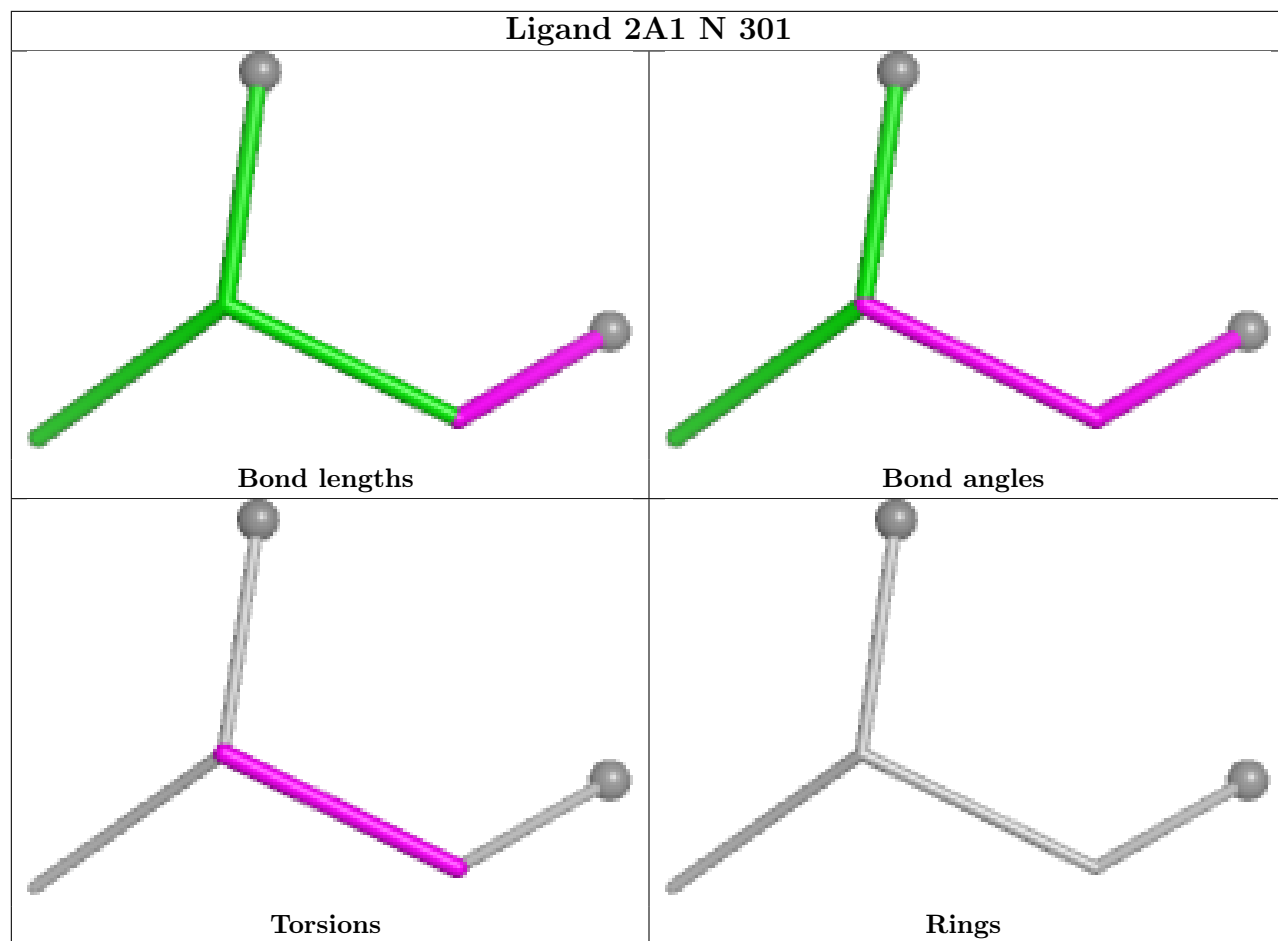




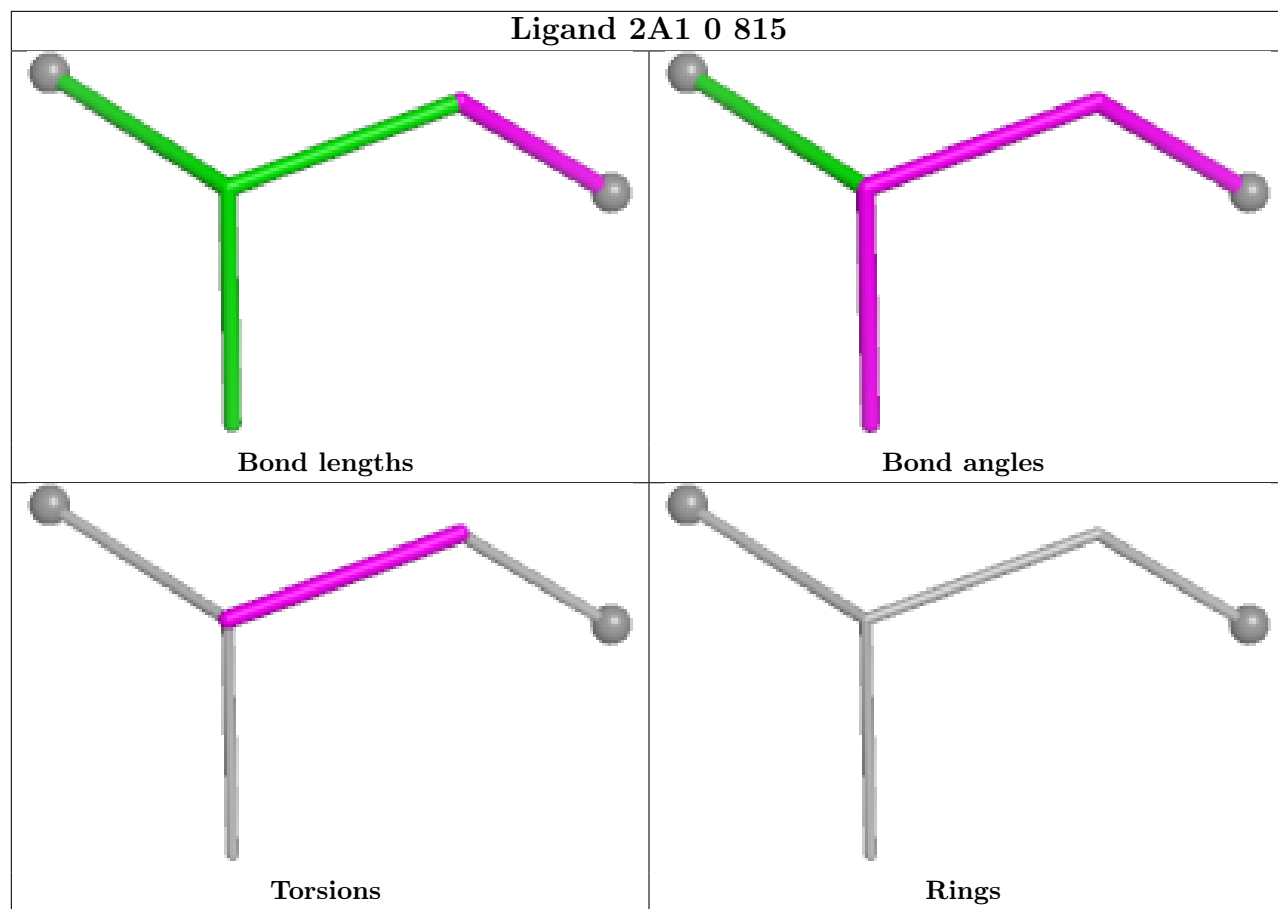


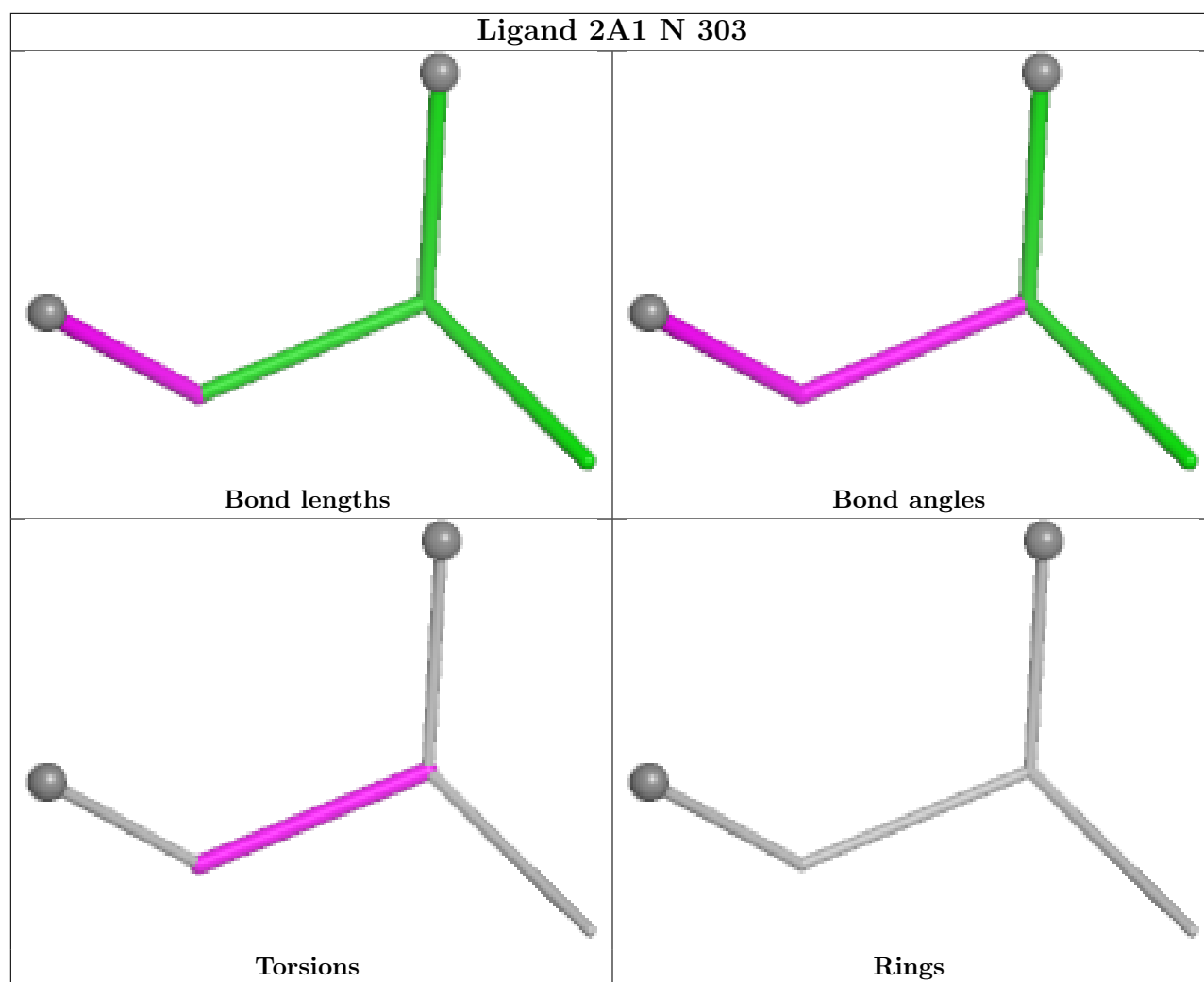












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

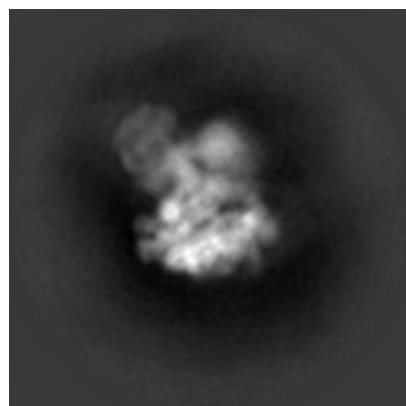
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57691. These allow visual inspection of the internal detail of the map and identification of artifacts.

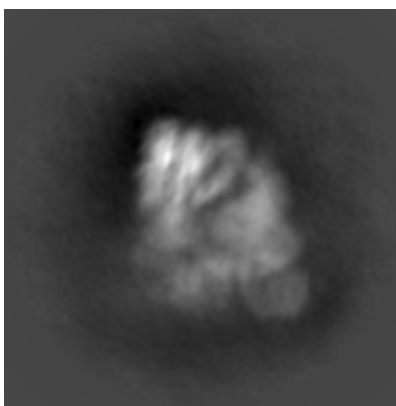
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

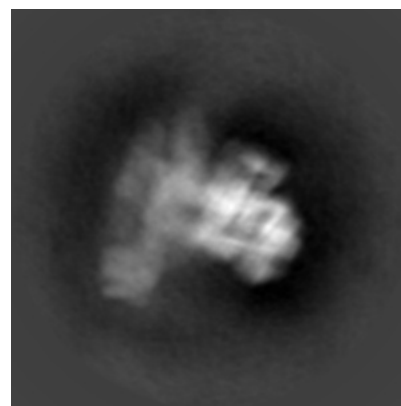
#### 6.1.1 Primary map



X

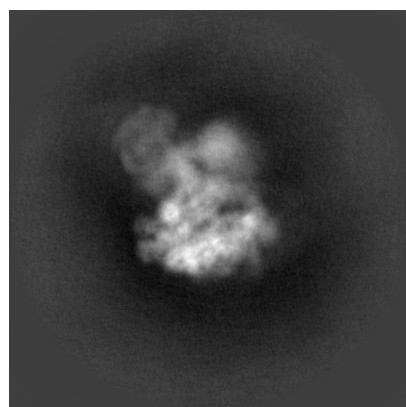


Y

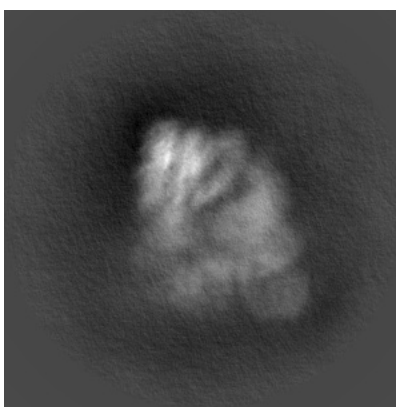


Z

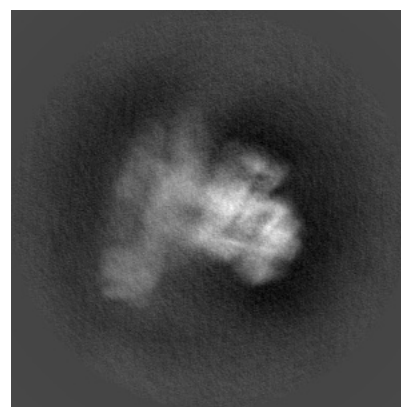
#### 6.1.2 Raw map



X



Y

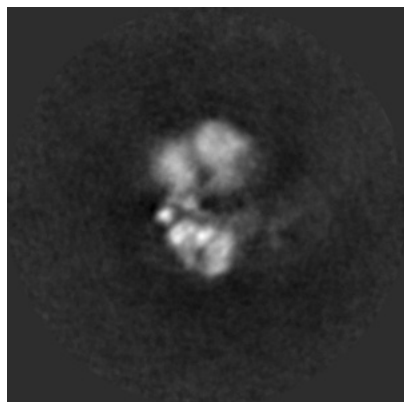


Z

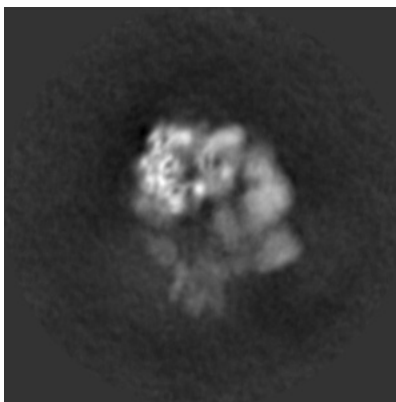
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

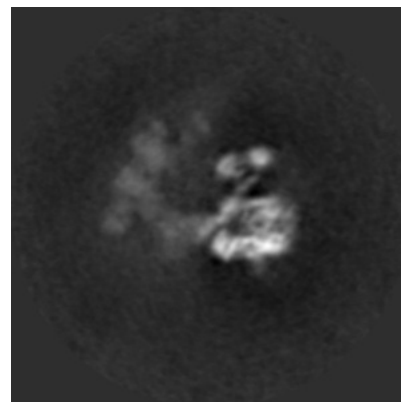
### 6.2.1 Primary map



X Index: 256

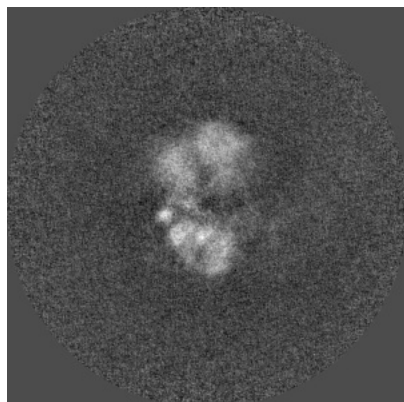


Y Index: 256

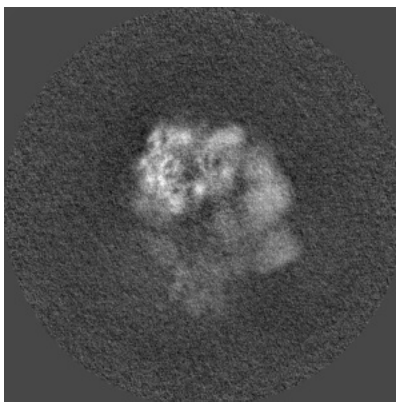


Z Index: 256

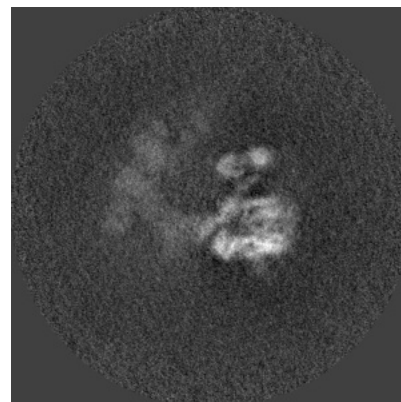
### 6.2.2 Raw map



X Index: 256



Y Index: 256

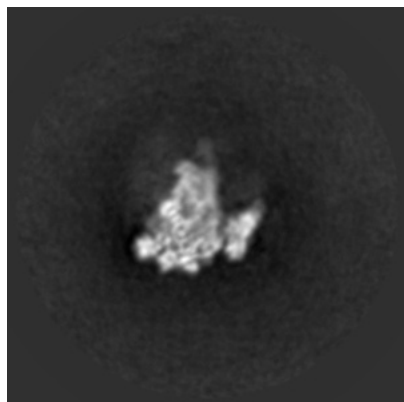


Z Index: 256

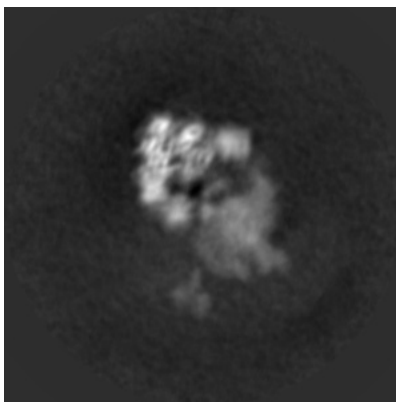
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

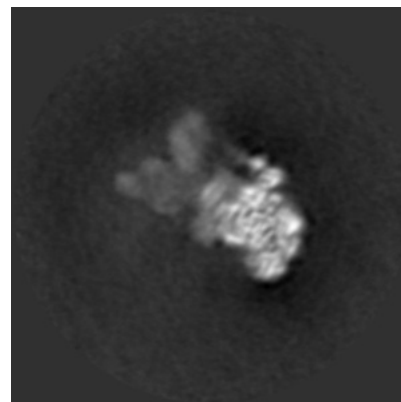
### 6.3.1 Primary map



X Index: 334

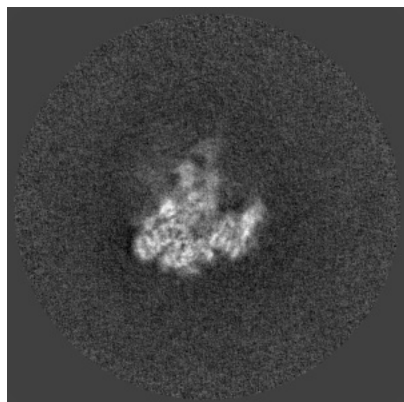


Y Index: 228

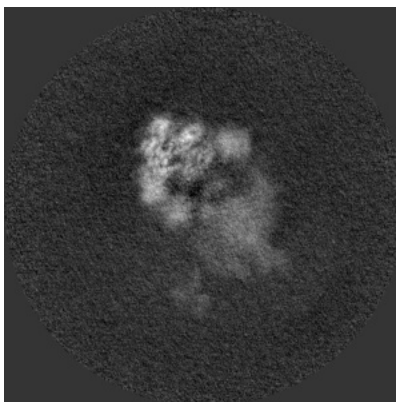


Z Index: 204

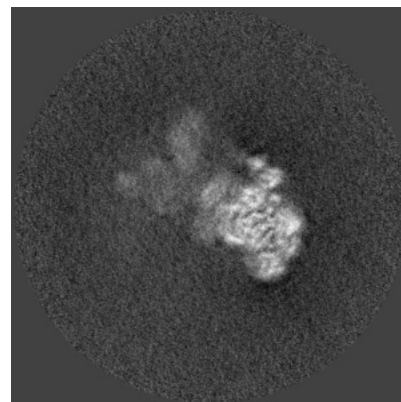
### 6.3.2 Raw map



X Index: 327



Y Index: 228



Z Index: 203

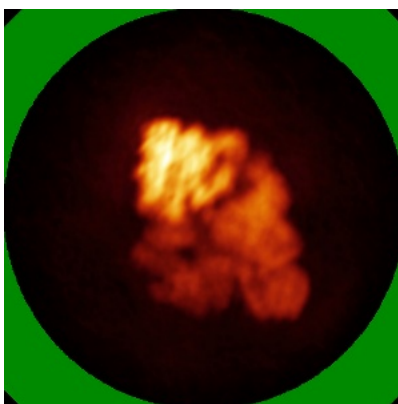
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

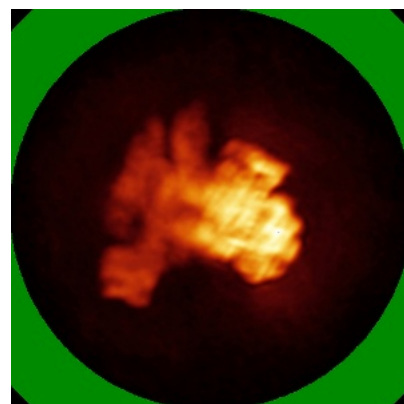
### 6.4.1 Primary map



X

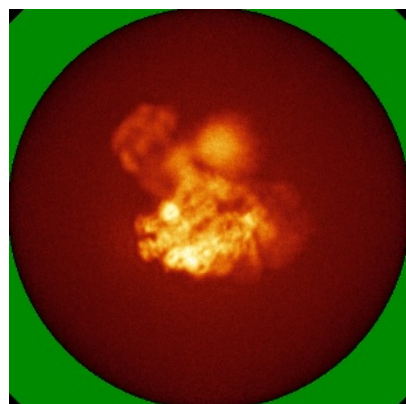


Y

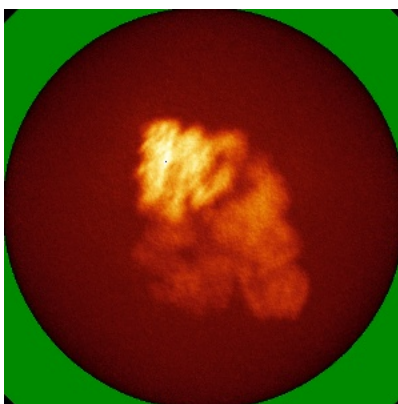


Z

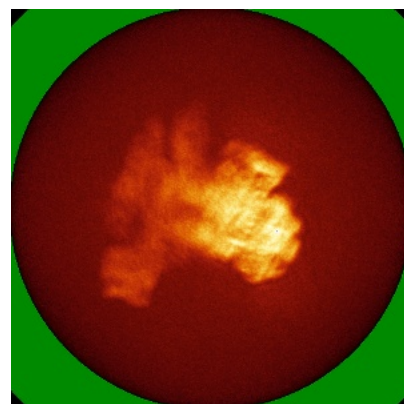
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



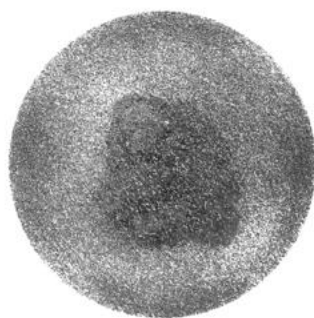
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

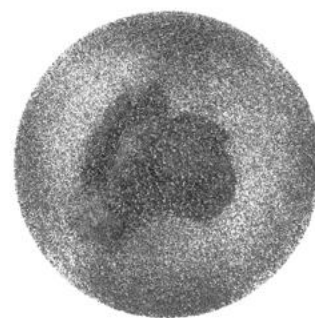
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

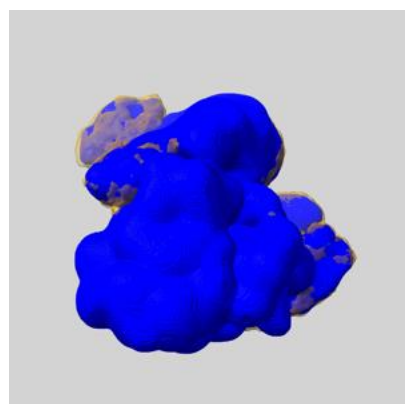
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

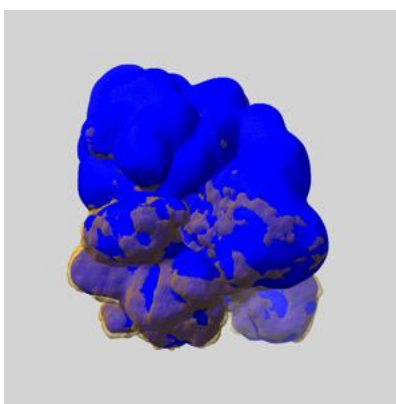
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

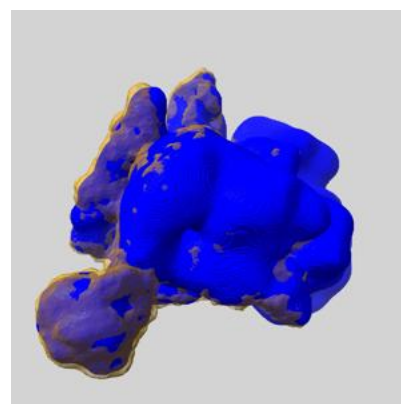
### 6.6.1 emd\_57691\_msk\_1.map [i](#)



X



Y

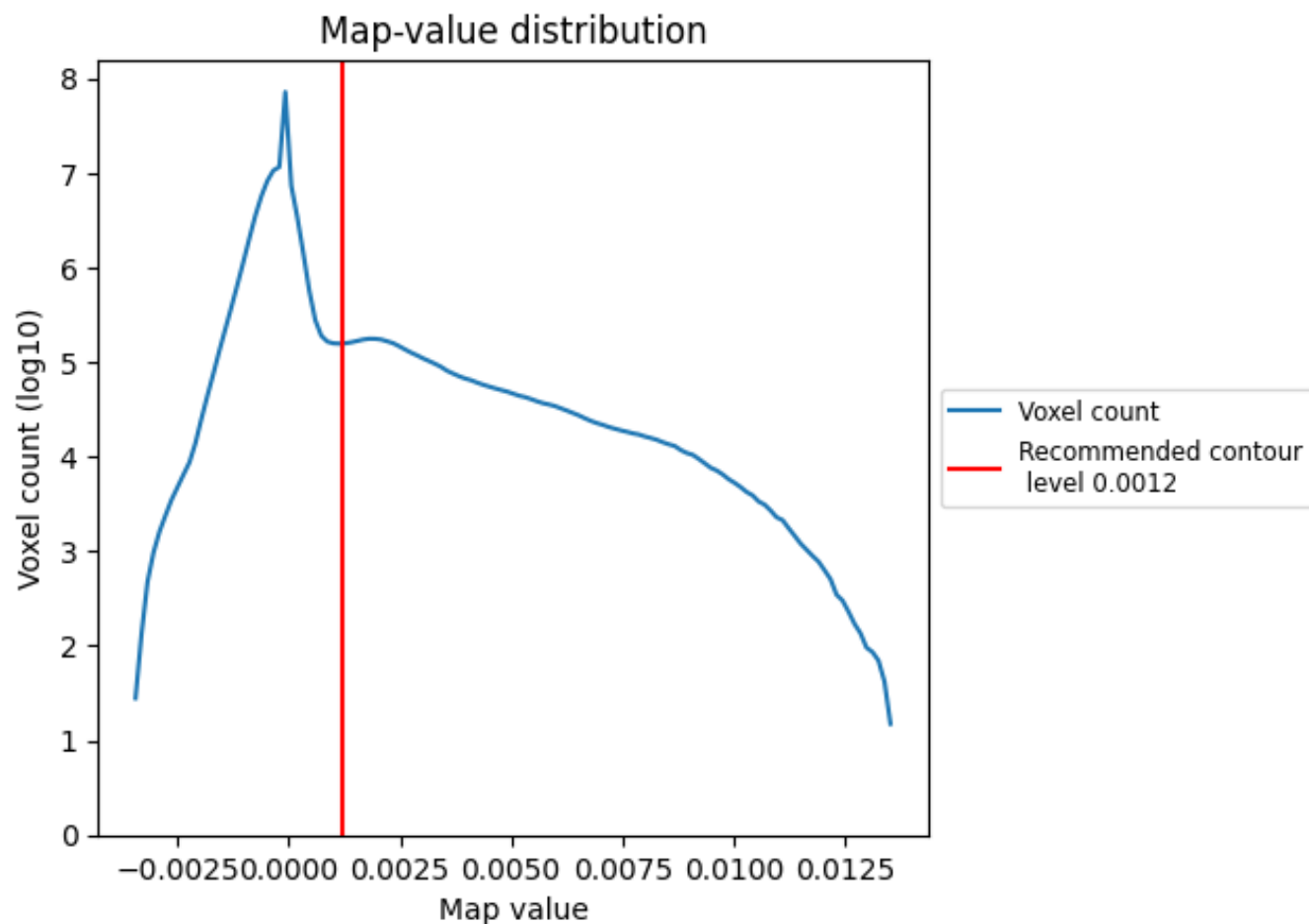


Z

## 7 Map analysis [i](#)

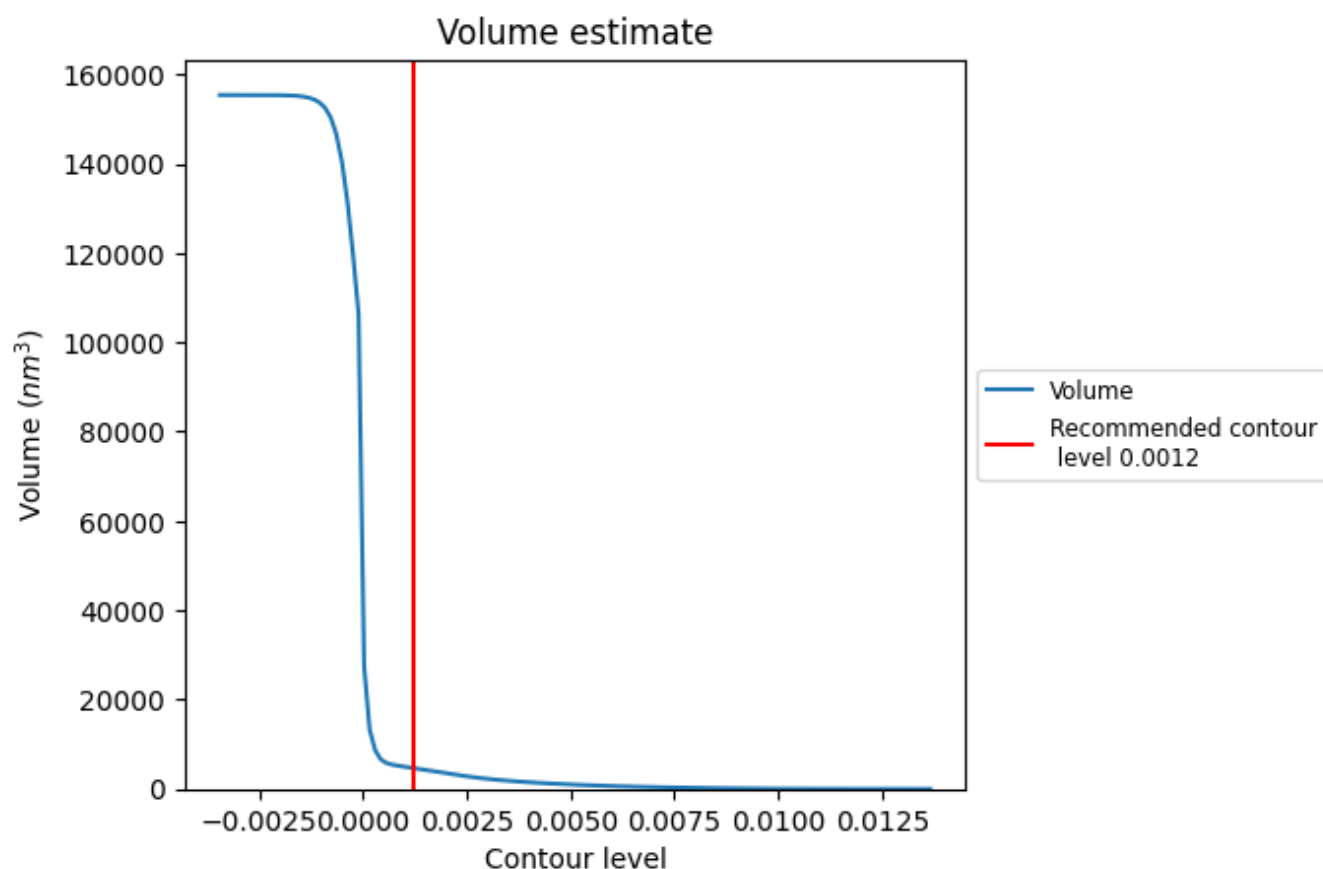
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

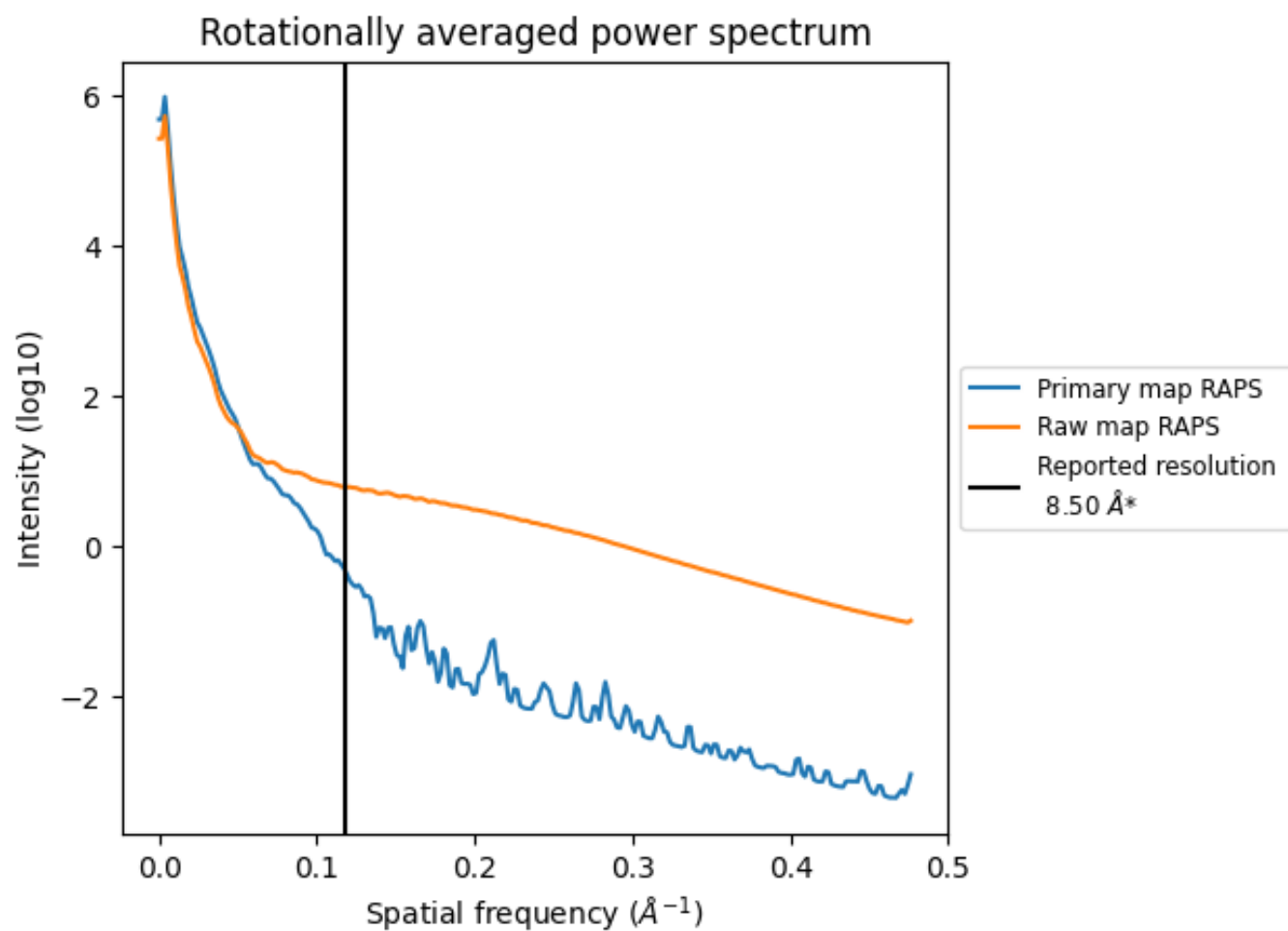
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4699  $\text{nm}^3$ ; this corresponds to an approximate mass of 4245 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

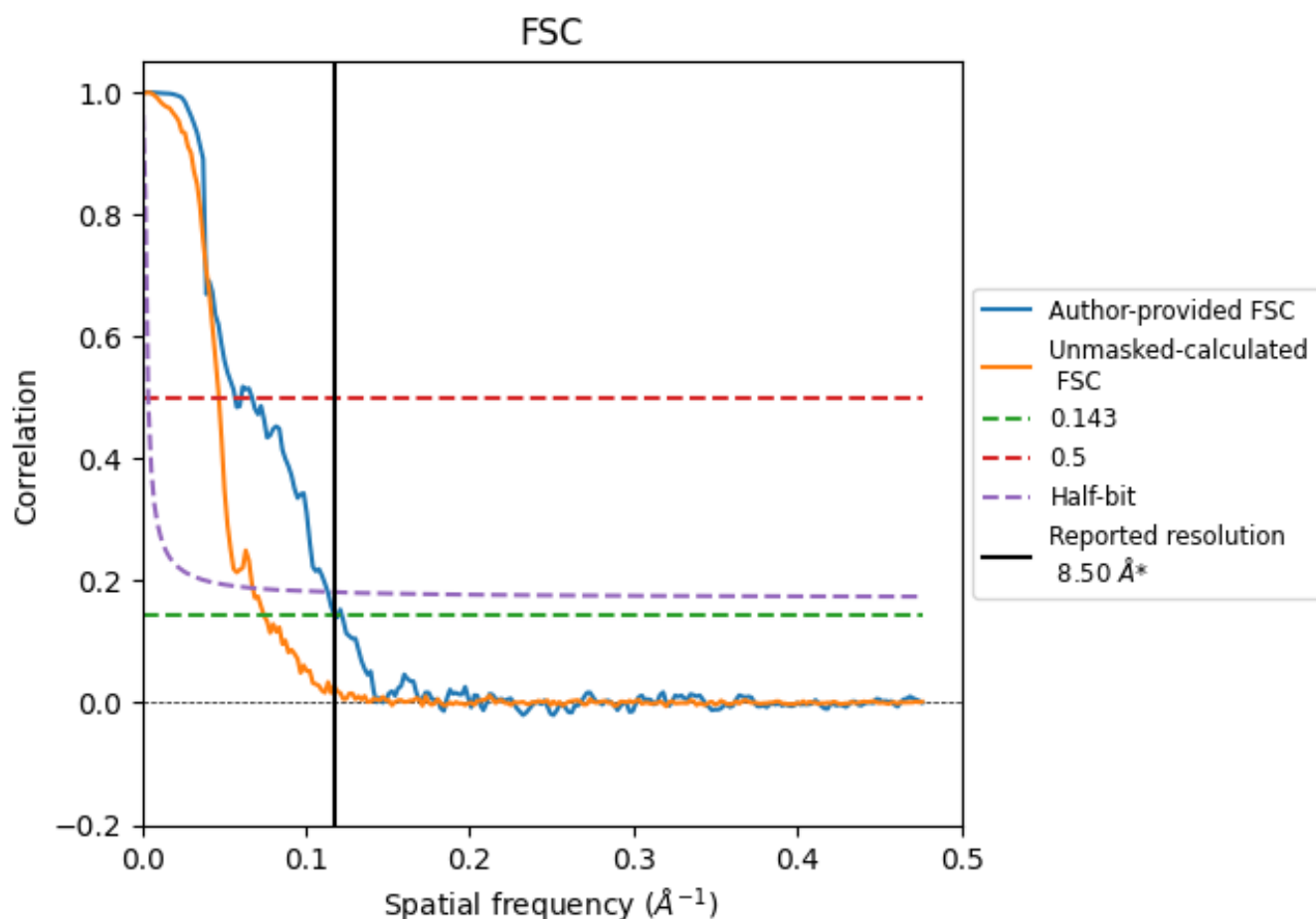


\*Reported resolution corresponds to spatial frequency of 0.118 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.118 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

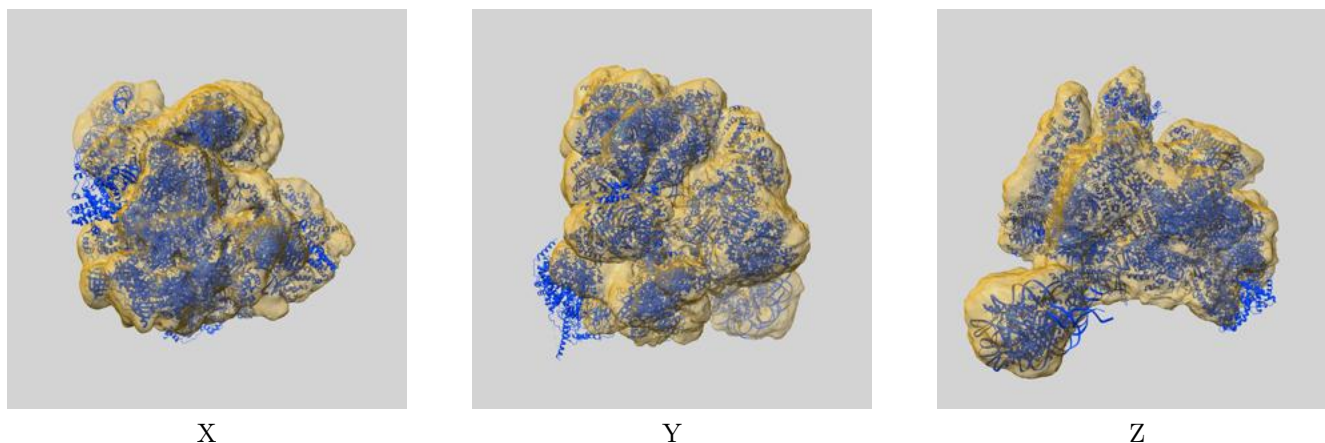
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 8.50                               | -     | -        |
| Author-provided FSC curve | 8.47                               | 17.67 | 8.83     |
| Unmasked-calculated*      | 13.44                              | 21.37 | 14.81    |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 13.44 differs from the reported value 8.5 by more than 10 %

## 9 Map-model fit [i](#)

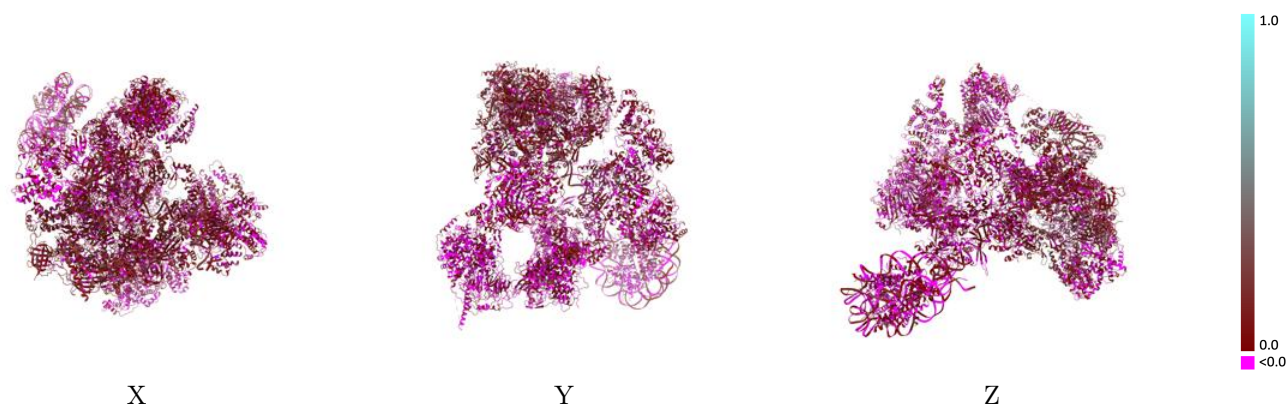
This section contains information regarding the fit between EMDB map EMD-57691 and PDB model 30FF. Per-residue inclusion information can be found in section [3](#) on page [20](#).

### 9.1 Map-model overlay [i](#)



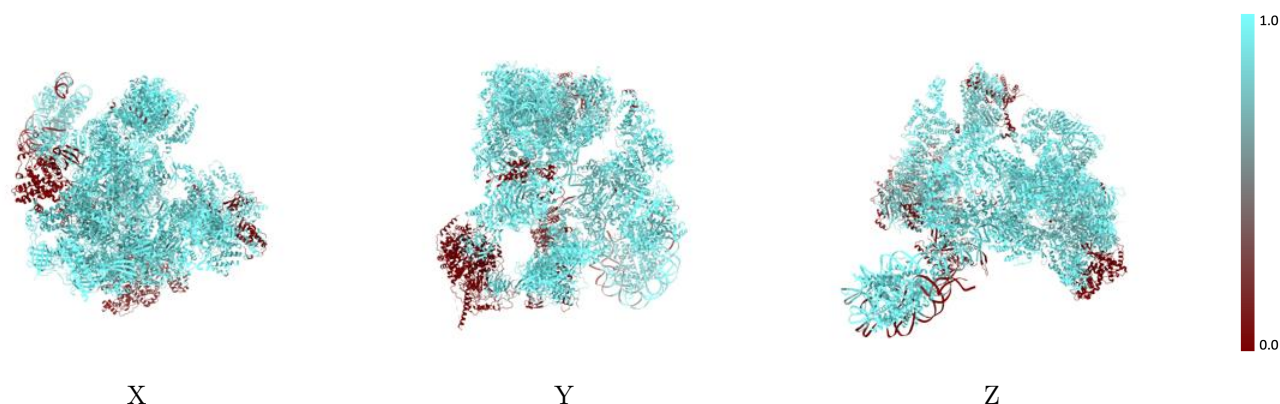
The images above show the 3D surface view of the map at the recommended contour level 0.0012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



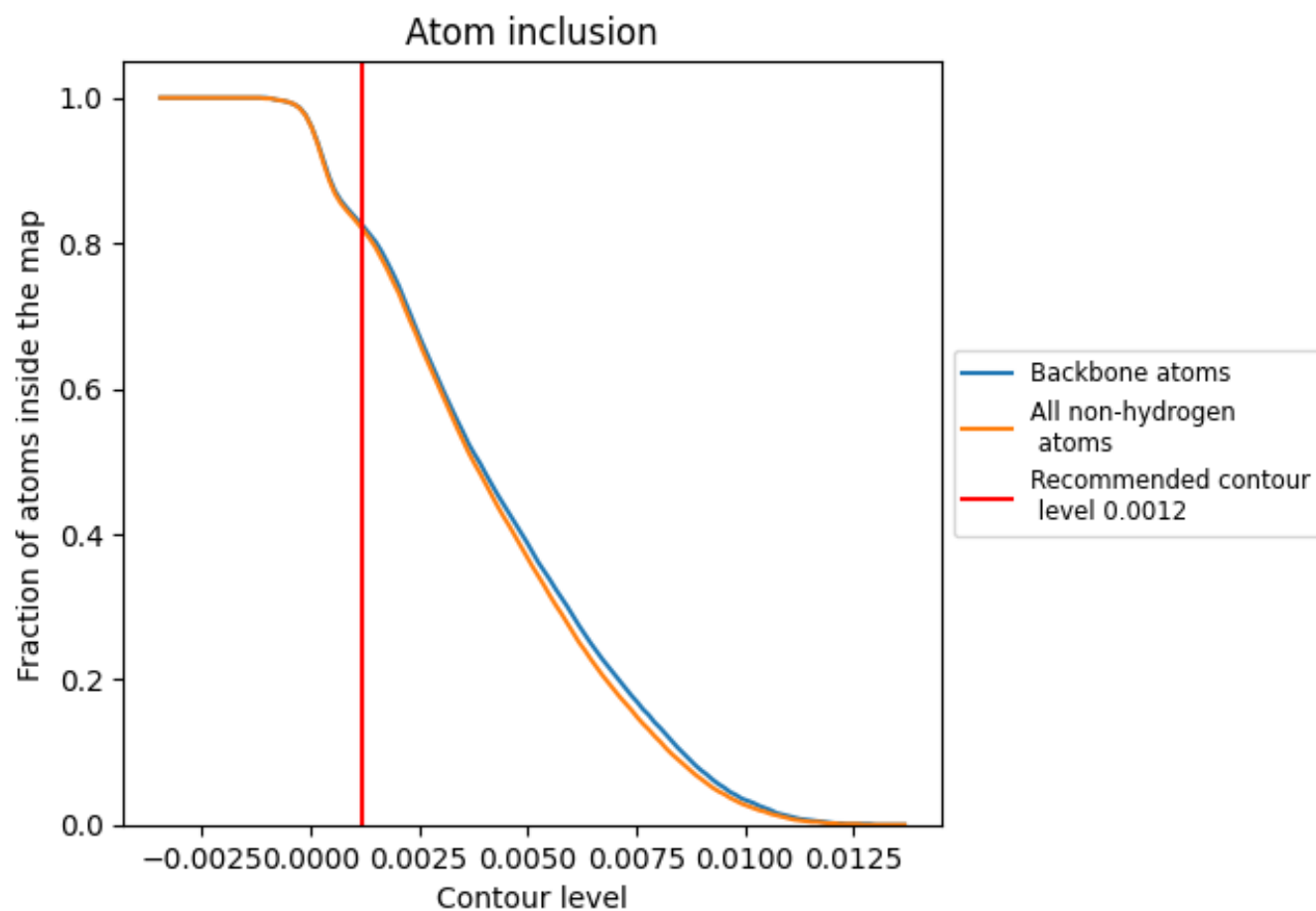
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0012) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| All   |  0.8190   |  0.0530    |
| 0     |  0.9960   |  0.0420    |
| 1     |  0.9920   |  0.0500    |
| 2     |  1.0000   |  0.0480    |
| 3     |  0.9860   |  0.0470    |
| 4     |  0.9780   |  0.0490    |
| 5     |  1.0000   |  0.0320    |
| 6     |  1.0000   |  0.0330    |
| 7     |  0.6810   |  0.0350    |
| 8     |  0.5810   |  0.0290    |
| 9     |  0.1680   |  -0.0070   |
| A     |  0.9970   |  0.1070    |
| B     |  1.0000   |  0.1120    |
| C     |  0.9990   |  0.1280    |
| D     |  0.9990  |  0.0920   |
| DA    |  0.5590 |  0.0160  |
| DB    |  0.8010 |  0.0130  |
| DD    |  0.5470 |  0.0170  |
| DE    |  0.9520 |  0.0380  |
| DF    |  0.9020 |  0.0280  |
| DG    |  0.1030 |  -0.0060 |
| DH    |  0.8400 |  0.0440  |
| DI    |  0.8400 |  0.0250  |
| DJ    |  0.7150 |  0.0360  |
| DL    |  0.4590 |  0.0110  |
| Dc    |  0.0000 |  0.0020  |
| Dd    |  0.0000 |  0.0020  |
| De    |  0.3160 |  0.0020  |
| Df    |  0.7590 |  0.0260  |
| Di    |  0.1280 |  -0.0260 |
| Dj    |  0.0430 |  0.0220  |
| Dk    |  0.0000 |  -0.0200 |
| Dl    |  0.1430 |  0.0070  |
| Dm    |  0.0000 |  -0.0230 |
| E     |  0.9980 |  0.1150  |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| F     |  1.0000   |  0.1280    |
| G     |  0.9990   |  0.0930    |
| H     |  0.9990   |  0.1120    |
| I     |  1.0000   |  0.0770    |
| J     |  1.0000   |  0.1090    |
| K     |  1.0000   |  0.1170    |
| L     |  1.0000   |  0.1050    |
| M     |  0.9980   |  0.1110    |
| N     |  0.7700   |  0.0550    |
| O     |  1.0000   |  0.0970    |
| Q     |  1.0000   |  0.0650    |
| R     |  0.9990   |  0.0990    |
| T     |  0.7490   |  0.0470    |
| U     |  0.9850   |  0.0880    |
| V     |  0.9820   |  0.0840    |
| W     |  0.9850   |  0.0930    |
| X     |  1.0000   |  0.1010    |
| a     |  0.9640   |  0.0110    |
| b     |  0.9790   |  -0.0030   |
| c     |  0.9240  |  -0.0050  |
| d     |  0.9990 |  0.0130  |
| e     |  0.9340 |  0.0360  |
| f     |  0.9440 |  -0.0080 |
| g     |  0.9960 |  0.0280  |
| h     |  0.9960 |  0.0210  |