



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 02:50 am GMT

PDB ID : 7AQQ  
EMDB ID : EMD-11872  
Title : Cryo-EM structure of Arabidopsis thaliana Complex-I (membrane core)  
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.  
Deposited on : 2020-10-22  
Resolution : 3.06 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       | : <b>FAILED</b>  |
| Mogul                          | : 1.8.4, CSD as541be (2020)  |
| MolProbity                     | : 4.02b-467  |
| buster-report                  | : 1.1.7 (2018)   |
| Percentile statistics          | : 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ                           | : <b>FAILED</b>  |
| Ideal geometry (proteins)      | : Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : 2.39   |

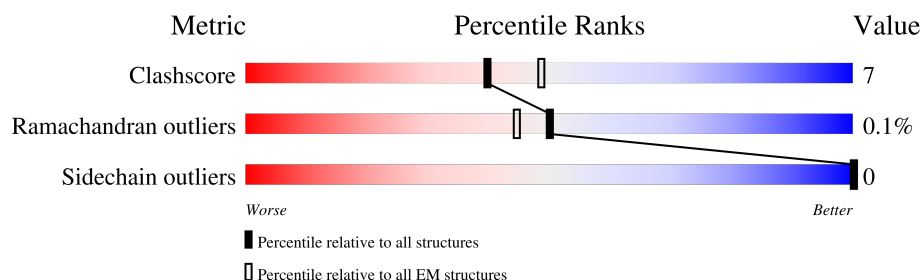
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.06 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.






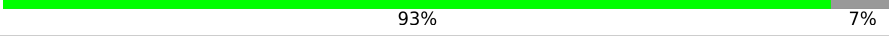

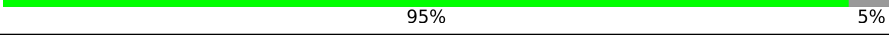

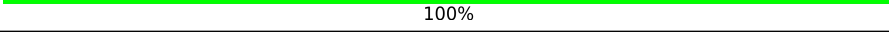


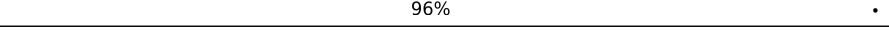

| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 119    | 54% 24% 23%      |
| 2   | H     | 325    | 79% 16% .        |
| 3   | J     | 205    | 57% 15% 28%      |
| 4   | K     | 100    | 78% 12% 10%      |
| 5   | L     | 669    | .. 96%           |
| 6   | M     | 495    | 43% 9% 47%       |
| 7   | N     | 499    | 81% 16% .        |
| 8   | O     | 159    | 69% 8% 23%       |
| 9   | X     | 106    | 80% 11% 8%       |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 10  | Z     | 143    |   |
| 11  | a     | 65     |   |
| 12  | b     | 65     |   |
| 13  | d     | 81     |   |
| 14  | e     | 83     |   |
| 15  | f     | 106    |   |
| 16  | i     | 98     |   |
| 17  | u     | 30     |   |
| 18  | v     | 113    |   |
| 19  | x     | 256    |   |
| 20  | y     | 278    |   |
| 21  | z     | 275    |  |

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 23281 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 NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 553 | 105 | 117 | 4 |         |       |

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | H     | 311      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2439  | 1659 | 372 | 393 | 15 |         |       |

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | J     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 784 | 179 | 191 | 8 |         |       |

- Molecule 4 is a protein called NADH dehydrogenase subunit 4L.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | K     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 476 | 109 | 115 | 7 |         |       |

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 5   | L     | 26       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 208   | 133 | 37 | 38 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 91      | PHE      | SER    | conflict | UNP B5TM94 |

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | M     | 262      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2126  | 1457 | 319 | 339 | 11 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| M     | 326     | LEU      | PRO    | conflict | UNP B5TM93 |
| M     | 378     | PHE      | SER    | conflict | UNP B5TM93 |

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | N     | 488      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3820  | 2573 | 577 | 642 | 28 |         |       |

- Molecule 8 is a protein called AT3G07480.1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | O     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 956   | 598 | 169 | 185 | 4 |         |       |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | X     | 97       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 767   | 480 | 132 | 143 | 12 |         |       |

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | Z     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 798   | 514 | 137 | 142 | 5 |         |       |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | a     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 469   | 302 | 84 | 78 | 5 |         |       |

- Molecule 12 is a protein called At2g46540/F11C10.23.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | b     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 295   | 195 | 48 | 49 | 3 |         |       |

- Molecule 13 is a protein called Excitatory amino acid transporter.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 13  | d     | 75       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 592   | 382 | 106 | 99 | 5 |         |       |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | e     | 65       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 557   | 344 | 106 | 100 | 7 |         |       |

- Molecule 15 is a protein called At4g16450.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | f     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 763   | 490 | 126 | 142 | 5 |         |       |

- Molecule 16 is a protein called P1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | i     | 70       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 614   | 384 | 116 | 111 | 3 |         |       |

- Molecule 17 is a protein called unknown.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 17  | u     | 30       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 150   | 90 | 30 | 30 |         |       |

- Molecule 18 is a protein called Uncharacterized protein At2g27730, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 18  | v     | 30       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 226   | 147 | 39 | 40 |         |       |

- Molecule 19 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | x     | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1659  | 1063 | 285 | 306 | 5 |         |       |

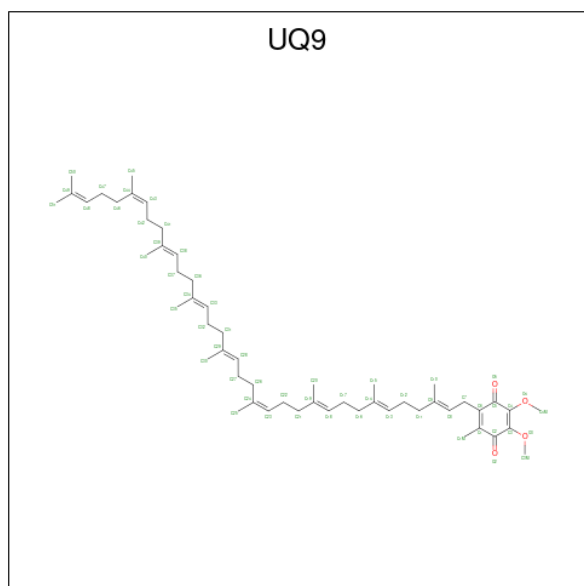
- Molecule 20 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | y     | 268      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2032  | 1271 | 363 | 391 | 7 |         |       |

- Molecule 21 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

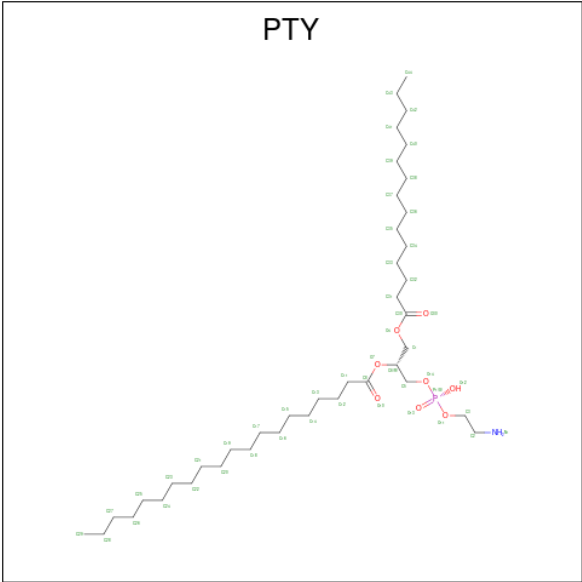
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | z     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1772  | 1111 | 325 | 330 | 6 |         |       |

- Molecule 22 is Ubiquinone-9 (three-letter code: UQ9) (formula:  $C_{54}H_{82}O_4$ ).



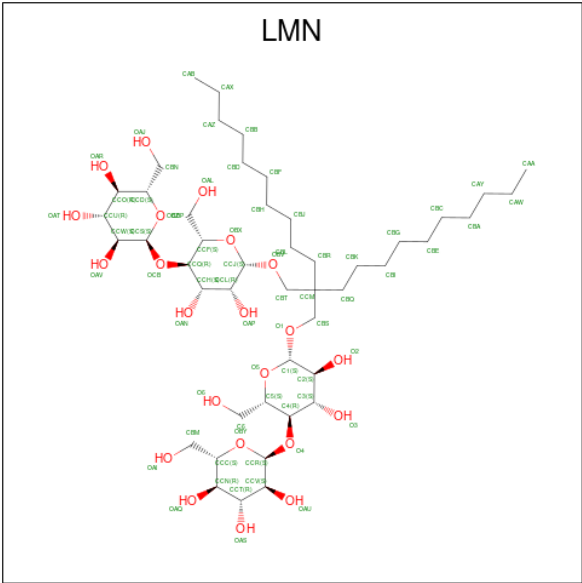
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 22  | H     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |

- Molecule 23 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 23  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 23  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |

- Molecule 24 is Lauryl Maltose Neopentyl Glycol (three-letter code: LMN) (formula: C<sub>47</sub>H<sub>88</sub>O<sub>22</sub>).



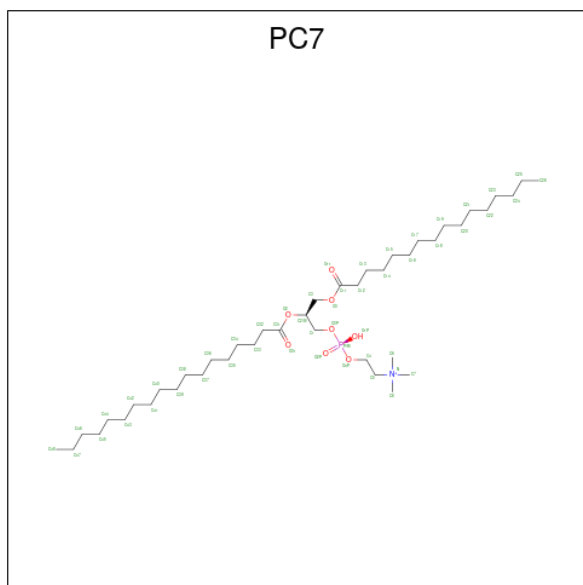
| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 24  | M     | 1        | Total | C  | O  | 0       |
|     |       |          | 69    | 47 | 22 |         |

- Molecule 25 is FE (III) ION (three-letter code: FE) (formula: Fe).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 25  | O     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 26 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P).

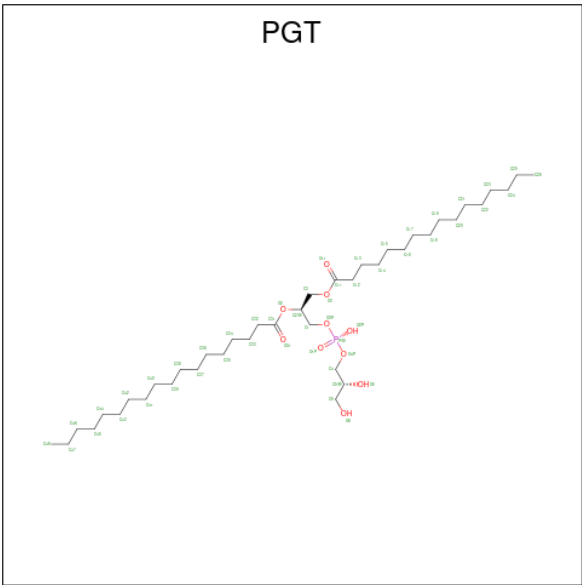


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 26  | v     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

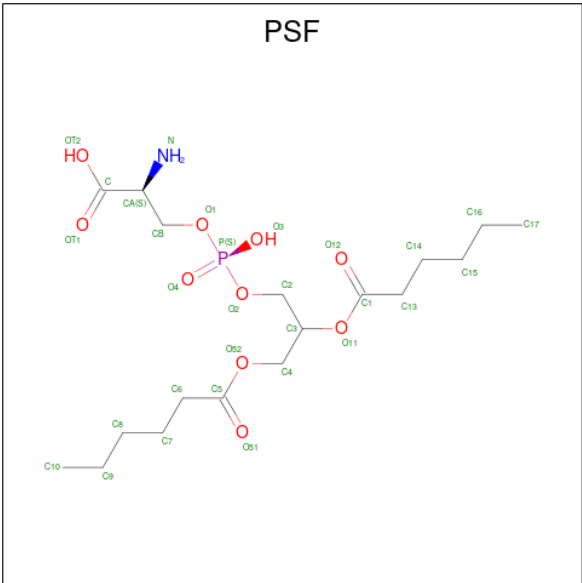
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 27  | y     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 28 is (1S)-2-{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



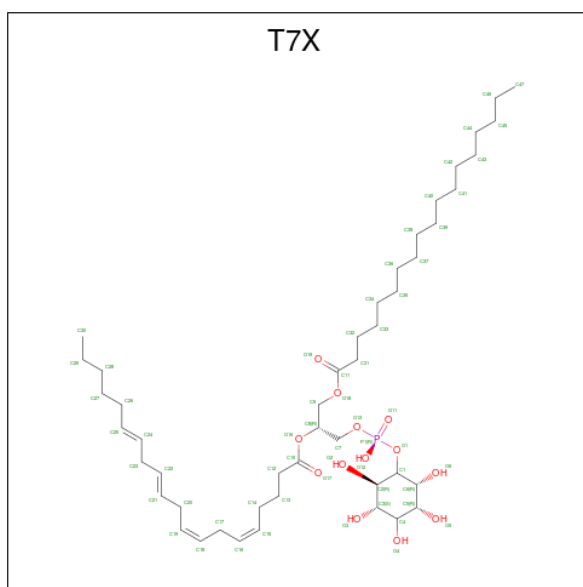
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 28  | y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 41    | 30 | 10 | 1 |         |

- Molecule 29 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (three-letter code: PSF) (formula: C<sub>18</sub>H<sub>34</sub>NO<sub>10</sub>P).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 29  | z     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 30    | 18 | 1 | 10 | 1 |         |

- Molecule 30 is Phosphatidylinositol (three-letter code: T7X) (formula: C<sub>47</sub>H<sub>83</sub>O<sub>13</sub>P).

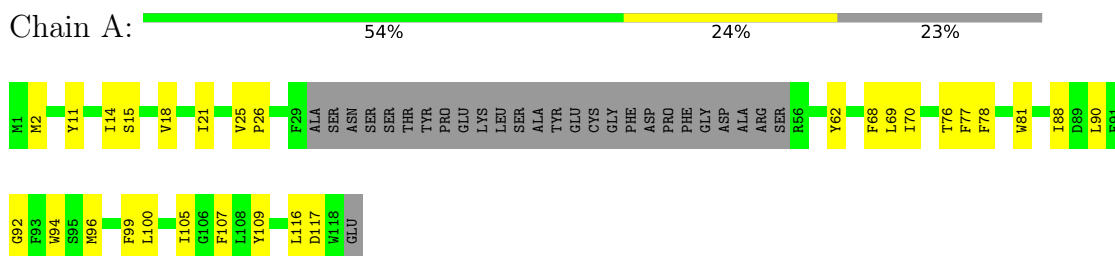


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 30  | z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 61    | 47 | 13 | 1 |         |

### 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. 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. 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.

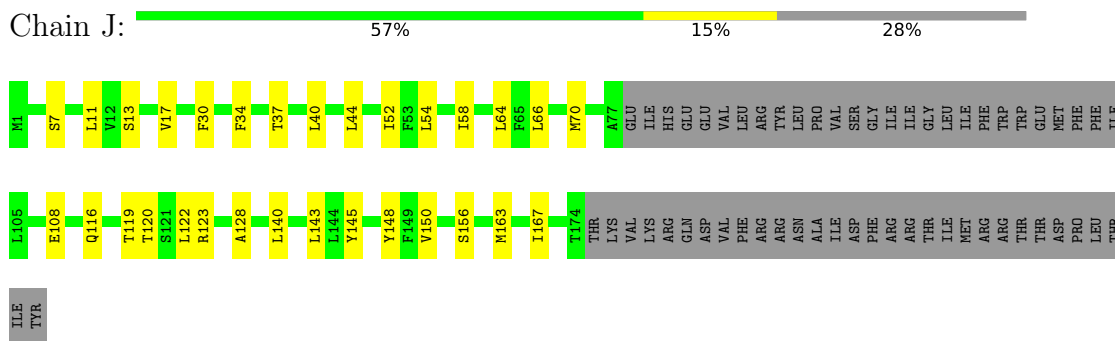
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



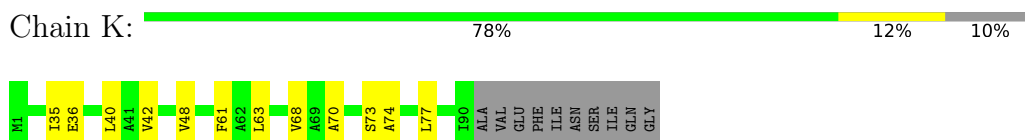
- Molecule 2: NADH-ubiquinone oxidoreductase chain 1



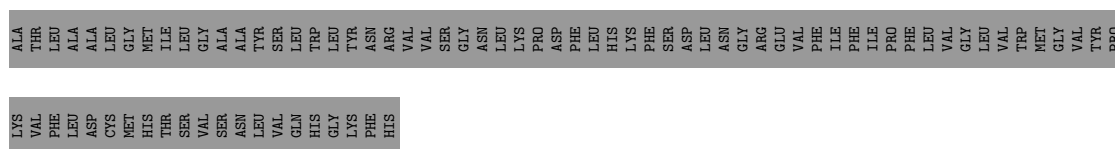
- Molecule 3: NADH-ubiquinone oxidoreductase chain 6



- Molecule 4: NADH dehydrogenase subunit 4L

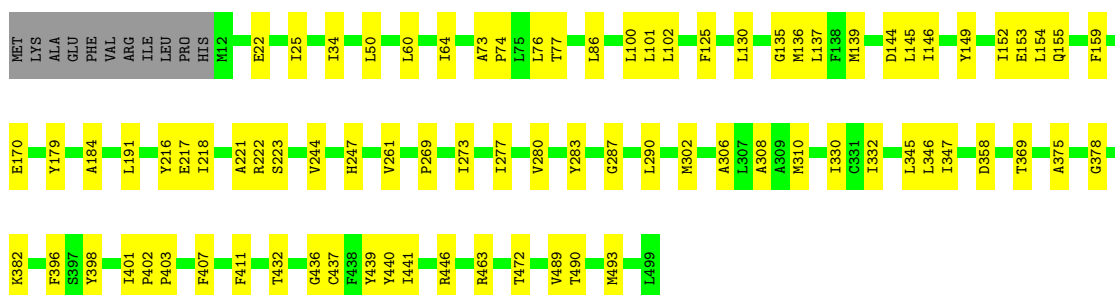






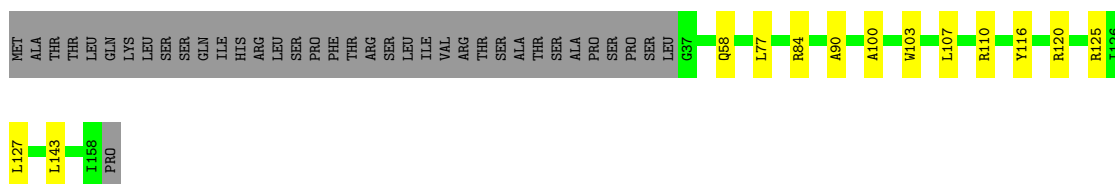
• Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N: 81% 16%



• Molecule 8: AT3G07480.1

Chain O: 69% 8% 23%



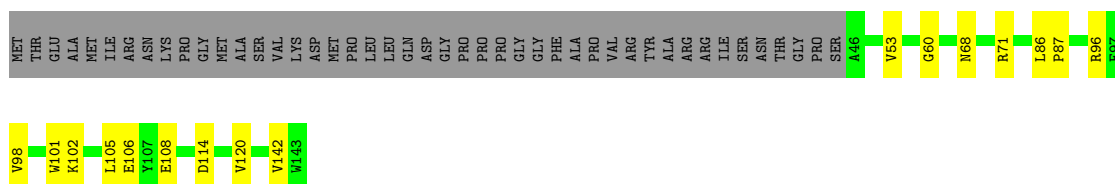
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B

Chain X: 80% 11% 8%



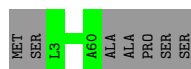
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A

Chain Z: 57% 11% 31%



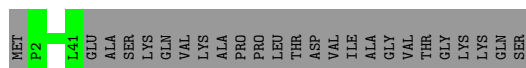
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a: 89% 11%



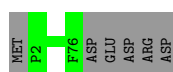
- Molecule 12: At2g46540/F11C10.23

Chain b: 62% 38%



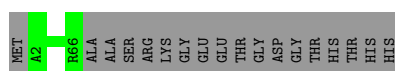
- Molecule 13: Excitatory amino acid transporter

Chain d: 93% 7%



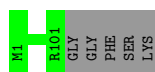
- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B

Chain e: 78% 22%



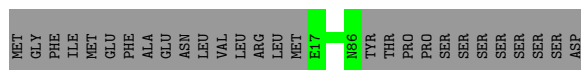
- Molecule 15: At4g16450

Chain f: 95% 5%



- Molecule 16: P1

Chain i: 71% 29%



- Molecule 17: unknown

Chain u: 100%

There are no outlier residues recorded for this chain.

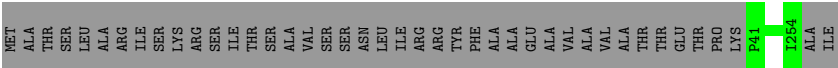
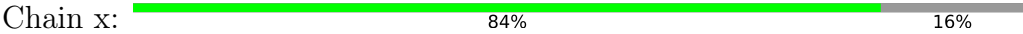
- Molecule 18: Uncharacterized protein At2g27730, mitochondrial

Chain v: 27% 73%

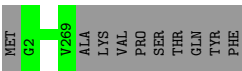




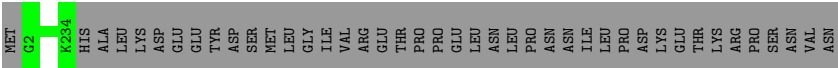
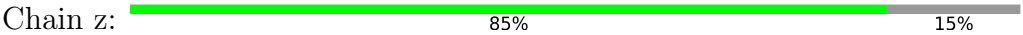
- Molecule 19: Gamma carbonic anhydrase-like 2, mitochondrial



- Molecule 20: Gamma carbonic anhydrase 2, mitochondrial



- Molecule 21: Gamma carbonic anhydrase 1, mitochondrial





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 459177                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 43                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T7X, UQ9, PTY, ZN, LMN, FE, PSF, PC7, PGT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.28         | 0/807       | 0.44        | 0/1096      |
| 2   | H     | 0.29         | 0/2510      | 0.49        | 0/3416      |
| 3   | J     | 0.28         | 0/1187      | 0.47        | 0/1617      |
| 4   | K     | 0.28         | 0/717       | 0.47        | 0/969       |
| 5   | L     | 0.23         | 0/211       | 0.54        | 0/282       |
| 6   | M     | 0.27         | 0/2188      | 0.44        | 0/2976      |
| 7   | N     | 0.28         | 0/3924      | 0.46        | 0/5327      |
| 8   | O     | 0.24         | 0/971       | 0.49        | 0/1314      |
| 9   | X     | 0.26         | 0/781       | 0.45        | 0/1049      |
| 10  | Z     | 0.28         | 0/820       | 0.51        | 0/1108      |
| 11  | a     | 0.25         | 0/481       | 0.50        | 0/646       |
| 12  | b     | 0.25         | 0/300       | 0.46        | 0/407       |
| 13  | d     | 0.26         | 0/605       | 0.49        | 0/815       |
| 14  | e     | 0.27         | 0/570       | 0.49        | 0/759       |
| 15  | f     | 0.28         | 0/779       | 0.46        | 0/1052      |
| 16  | i     | 0.26         | 0/632       | 0.50        | 0/852       |
| 18  | v     | 0.24         | 0/230       | 0.39        | 0/311       |
| 19  | x     | 0.28         | 0/1700      | 0.50        | 0/2320      |
| 20  | y     | 0.27         | 0/2066      | 0.48        | 0/2800      |
| 21  | z     | 0.27         | 0/1804      | 0.50        | 0/2441      |
| All | All   | 0.27         | 0/23283     | 0.48        | 0/31557     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 779   | 0        | 796      | 22      | 0            |
| 2   | H     | 2439  | 0        | 2554     | 39      | 0            |
| 3   | J     | 1162  | 0        | 1238     | 26      | 0            |
| 4   | K     | 707   | 0        | 771      | 15      | 0            |
| 5   | L     | 208   | 0        | 211      | 8       | 0            |
| 6   | M     | 2126  | 0        | 2227     | 33      | 0            |
| 7   | N     | 3820  | 0        | 3926     | 66      | 0            |
| 8   | O     | 956   | 0        | 968      | 8       | 0            |
| 9   | X     | 767   | 0        | 766      | 8       | 0            |
| 10  | Z     | 798   | 0        | 780      | 12      | 0            |
| 11  | a     | 469   | 0        | 472      | 0       | 0            |
| 12  | b     | 295   | 0        | 322      | 0       | 0            |
| 13  | d     | 592   | 0        | 610      | 0       | 0            |
| 14  | e     | 557   | 0        | 525      | 0       | 0            |
| 15  | f     | 763   | 0        | 767      | 0       | 0            |
| 16  | i     | 614   | 0        | 577      | 0       | 0            |
| 17  | u     | 150   | 0        | 34       | 0       | 0            |
| 18  | v     | 226   | 0        | 235      | 0       | 0            |
| 19  | x     | 1659  | 0        | 1673     | 0       | 0            |
| 20  | y     | 2032  | 0        | 2044     | 0       | 0            |
| 21  | z     | 1772  | 0        | 1771     | 0       | 0            |
| 22  | H     | 35    | 0        | 43       | 2       | 0            |
| 23  | H     | 50    | 0        | 79       | 4       | 0            |
| 23  | N     | 50    | 0        | 79       | 5       | 0            |
| 24  | M     | 69    | 0        | 88       | 1       | 0            |
| 25  | O     | 1     | 0        | 0        | 0       | 0            |
| 26  | v     | 52    | 0        | 84       | 0       | 0            |
| 27  | y     | 1     | 0        | 0        | 0       | 0            |
| 28  | y     | 41    | 0        | 52       | 0       | 0            |
| 29  | z     | 30    | 0        | 32       | 0       | 0            |
| 30  | z     | 61    | 0        | 0        | 0       | 0            |
| All | All   | 23281 | 0        | 23724    | 198     | 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 7.

The worst 5 of 198 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 6:M:142:PHE:O   | 6:M:146:PHE:HB2 | 1.78                     | 0.83              |
| 4:K:36:GLU:OE1  | 4:K:73:SER:OG   | 1.99                     | 0.79              |
| 4:K:42:VAL:HG11 | 7:N:191:LEU:HG  | 1.66                     | 0.76              |
| 3:J:37:THR:HG21 | 4:K:40:LEU:HD11 | 1.65                     | 0.76              |
| 1:A:88:ILE:HD12 | 1:A:92:GLY:HA3  | 1.69                     | 0.73              |

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   | A     | 88/119 (74%)  | 86 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 2   | H     | 307/325 (94%) | 287 (94%) | 19 (6%) | 1 (0%)   | 37          | 64  |
| 3   | J     | 143/205 (70%) | 136 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 4   | K     | 88/100 (88%)  | 86 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 5   | L     | 24/669 (4%)   | 21 (88%)  | 3 (12%) | 0        | 100         | 100 |
| 6   | M     | 260/495 (52%) | 256 (98%) | 3 (1%)  | 1 (0%)   | 30          | 58  |
| 7   | N     | 486/499 (97%) | 475 (98%) | 11 (2%) | 0        | 100         | 100 |
| 8   | O     | 120/159 (76%) | 114 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 9   | X     | 95/106 (90%)  | 94 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 10  | Z     | 96/143 (67%)  | 91 (95%)  | 4 (4%)  | 1 (1%)   | 13          | 38  |
| 11  | a     | 56/65 (86%)   | 56 (100%) | 0       | 0        | 100         | 100 |
| 12  | b     | 38/65 (58%)   | 38 (100%) | 0       | 0        | 100         | 100 |
| 13  | d     | 73/81 (90%)   | 71 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 14  | e     | 63/83 (76%)   | 63 (100%) | 0       | 0        | 100         | 100 |
| 15  | f     | 99/106 (93%)  | 96 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 16  | i     | 68/98 (69%)   | 66 (97%)  | 2 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 18  | v     | 28/113 (25%)    | 27 (96%)   | 1 (4%)  | 0        | 100         | 100 |
| 19  | x     | 212/256 (83%)   | 207 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 20  | y     | 266/278 (96%)   | 252 (95%)  | 14 (5%) | 0        | 100         | 100 |
| 21  | z     | 231/275 (84%)   | 227 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| All | All   | 2841/4240 (67%) | 2749 (97%) | 89 (3%) | 3 (0%)   | 50          | 77  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 201 | ALA  |
| 6   | M     | 231 | VAL  |
| 10  | Z     | 120 | VAL  |

### 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   | A     | 83/106 (78%)  | 83 (100%)  | 0        | 100         | 100 |
| 2   | H     | 262/272 (96%) | 262 (100%) | 0        | 100         | 100 |
| 3   | J     | 131/186 (70%) | 131 (100%) | 0        | 100         | 100 |
| 4   | K     | 78/86 (91%)   | 78 (100%)  | 0        | 100         | 100 |
| 5   | L     | 21/568 (4%)   | 21 (100%)  | 0        | 100         | 100 |
| 6   | M     | 232/434 (54%) | 232 (100%) | 0        | 100         | 100 |
| 7   | N     | 406/416 (98%) | 406 (100%) | 0        | 100         | 100 |
| 8   | O     | 107/141 (76%) | 107 (100%) | 0        | 100         | 100 |
| 9   | X     | 87/94 (93%)   | 87 (100%)  | 0        | 100         | 100 |
| 10  | Z     | 79/115 (69%)  | 79 (100%)  | 0        | 100         | 100 |
| 11  | a     | 48/53 (91%)   | 48 (100%)  | 0        | 100         | 100 |
| 12  | b     | 33/53 (62%)   | 33 (100%)  | 0        | 100         | 100 |
| 13  | d     | 60/66 (91%)   | 60 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 14  | e     | 60/73 (82%)     | 60 (100%)   | 0        | 100         | 100 |
| 15  | f     | 81/84 (96%)     | 81 (100%)   | 0        | 100         | 100 |
| 16  | i     | 64/90 (71%)     | 64 (100%)   | 0        | 100         | 100 |
| 18  | v     | 23/84 (27%)     | 23 (100%)   | 0        | 100         | 100 |
| 19  | x     | 183/216 (85%)   | 183 (100%)  | 0        | 100         | 100 |
| 20  | y     | 223/232 (96%)   | 223 (100%)  | 0        | 100         | 100 |
| 21  | z     | 188/228 (82%)   | 188 (100%)  | 0        | 100         | 100 |
| All | All   | 2449/3597 (68%) | 2449 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | M     | 31  | ASN  |
| 7   | N     | 53  | ASN  |
| 9   | X     | 45  | ASN  |
| 19  | x     | 116 | ASN  |
| 21  | z     | 101 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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 | $\# Z  > 2$ |
| 28  | PGT  | y     | 302 | -    | 40,40,50     | 1.16 | 3 (7%)      | 43,46,56    | 1.10 | 2 (4%)      |
| 26  | PC7  | v     | 201 | -    | 51,51,51     | 0.95 | 4 (7%)      | 57,59,59    | 1.04 | 2 (3%)      |
| 30  | T7X  | z     | 302 | -    | 61,61,61     | 0.84 | 4 (6%)      | 71,73,73    | 1.07 | 3 (4%)      |
| 23  | PTY  | N     | 501 | -    | 49,49,49     | 0.86 | 4 (8%)      | 52,54,54    | 1.12 | 2 (3%)      |
| 23  | PTY  | H     | 402 | -    | 49,49,49     | 0.87 | 4 (8%)      | 52,54,54    | 1.12 | 2 (3%)      |
| 24  | LMN  | M     | 501 | -    | 72,72,72     | 1.65 | 14 (19%)    | 96,98,98    | 1.02 | 3 (3%)      |
| 29  | PSF  | z     | 301 | -    | 28,29,29     | 1.18 | 4 (14%)     | 32,36,36    | 1.22 | 2 (6%)      |
| 22  | UQ9  | H     | 401 | -    | 35,35,58     | 2.51 | 12 (34%)    | 42,45,73    | 1.86 | 12 (28%)    |

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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 28  | PGT  | y     | 302 | -    | -       | 22/45/45/55   | -       |
| 26  | PC7  | v     | 201 | -    | -       | 23/55/55/55   | -       |
| 30  | T7X  | z     | 302 | -    | -       | 29/56/80/80   | 0/1/1/1 |
| 23  | PTY  | N     | 501 | -    | -       | 26/53/53/53   | -       |
| 23  | PTY  | H     | 402 | -    | -       | 19/53/53/53   | -       |
| 24  | LMN  | M     | 501 | -    | -       | 34/50/130/130 | 0/4/4/4 |
| 29  | PSF  | z     | 301 | -    | -       | 12/35/35/35   | -       |
| 22  | UQ9  | H     | 401 | -    | -       | 8/30/54/81    | 0/1/1/1 |

The worst 5 of 49 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 22  | H     | 401 | UQ9  | C6-C1   | 9.90 | 1.53        | 1.35     |
| 24  | M     | 501 | LMN  | O5-C1   | 4.69 | 1.53        | 1.41     |
| 22  | H     | 401 | UQ9  | C4-C3   | 4.32 | 1.53        | 1.36     |
| 24  | M     | 501 | LMN  | CBS-CCM | 4.16 | 1.63        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 24  | M     | 501 | LMN  | CBT-CCM | 4.07 | 1.62        | 1.53     |

The worst 5 of 28 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 22  | H     | 401 | UQ9  | C7-C6-C5    | 4.75 | 124.20      | 118.48   |
| 30  | z     | 302 | T7X  | O16-C10-C12 | 4.26 | 120.69      | 111.50   |
| 23  | N     | 501 | PTY  | O7-C8-C11   | 4.17 | 120.49      | 111.50   |
| 28  | y     | 302 | PGT  | O2-C31-C32  | 4.08 | 120.29      | 111.50   |
| 23  | H     | 402 | PTY  | O7-C8-C11   | 4.07 | 120.27      | 111.50   |

There are no chirality outliers.

5 of 173 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 22  | H     | 401 | UQ9  | C9-C11-C12-C13 |
| 22  | H     | 401 | UQ9  | C1-C6-C7-C8    |
| 22  | H     | 401 | UQ9  | C5-C6-C7-C8    |
| 23  | H     | 402 | PTY  | C5-O14-P1-O13  |
| 23  | N     | 501 | PTY  | C5-C6-O7-C8    |

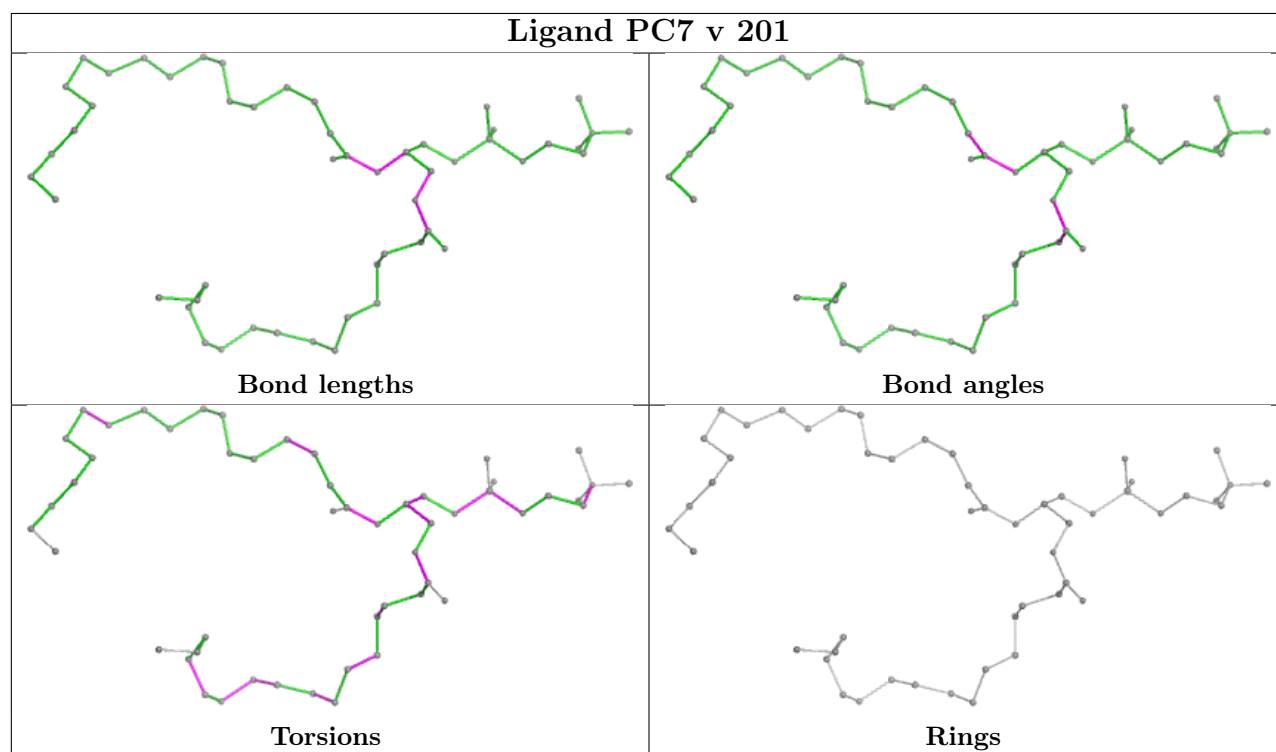
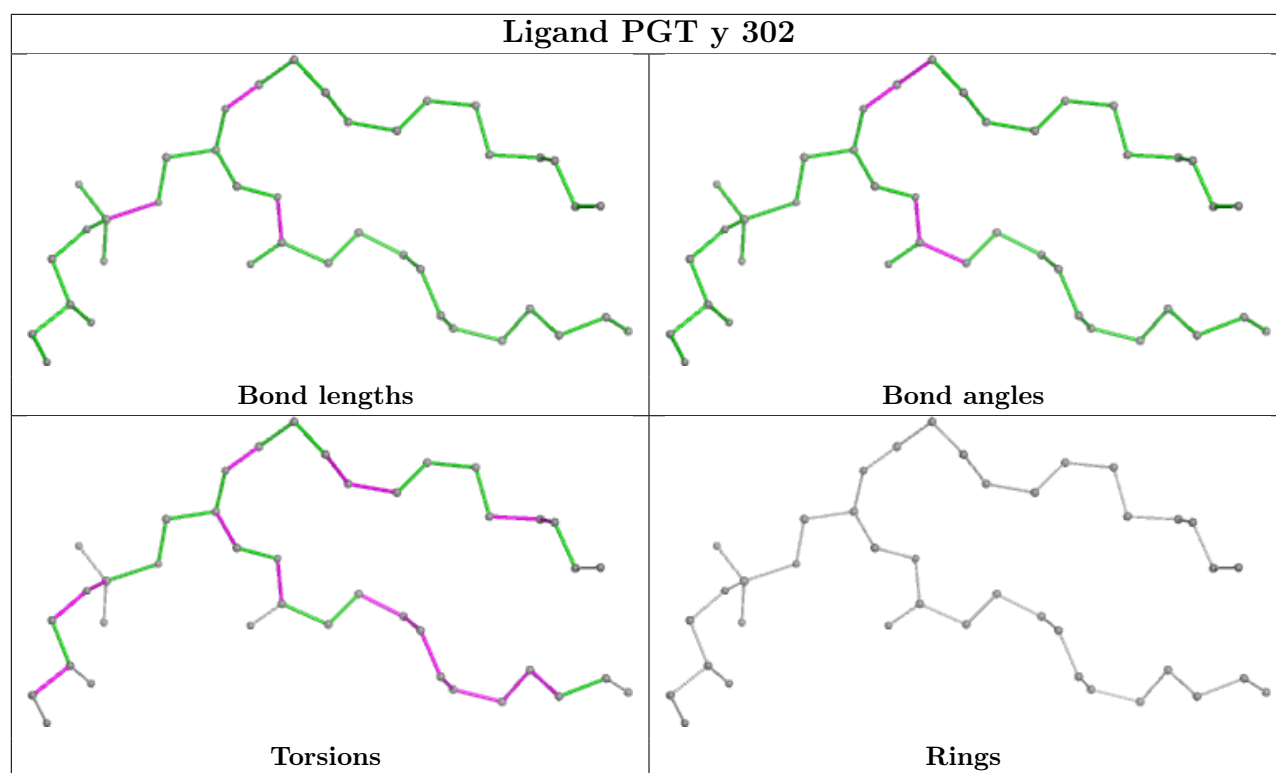
There are no ring outliers.

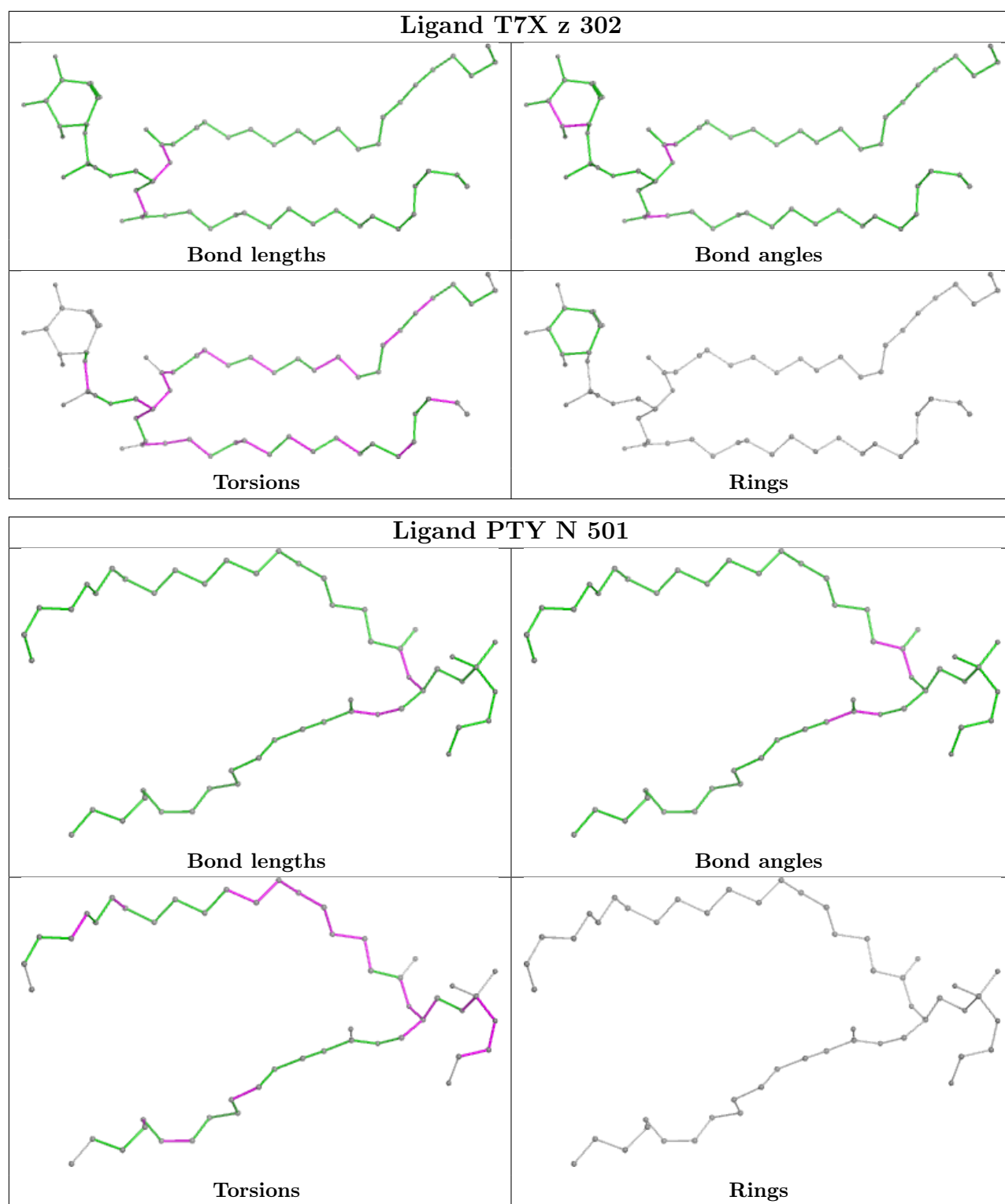
4 monomers are involved in 12 short contacts:

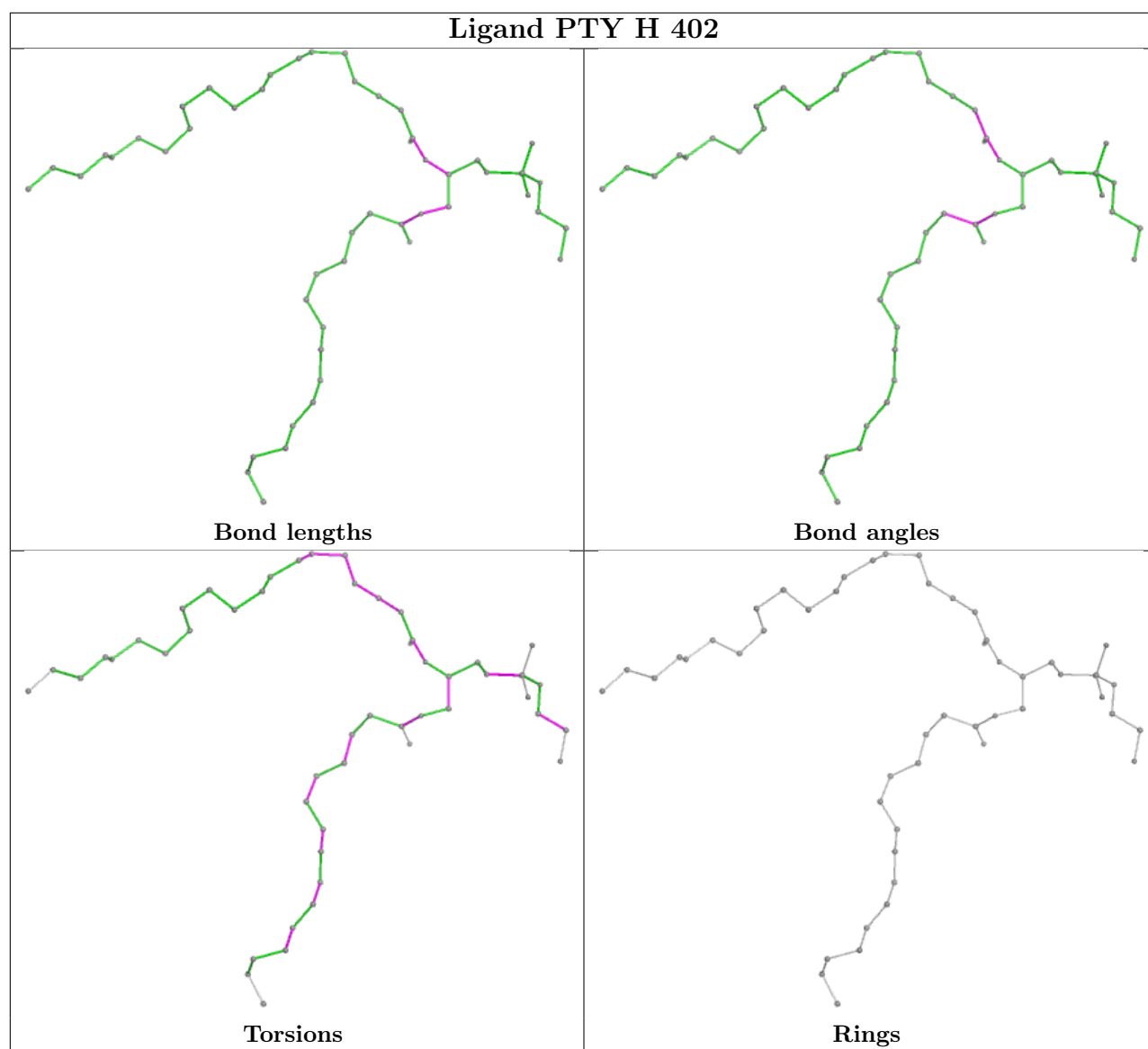
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | N     | 501 | PTY  | 5       | 0            |
| 23  | H     | 402 | PTY  | 4       | 0            |
| 24  | M     | 501 | LMN  | 1       | 0            |
| 22  | H     | 401 | UQ9  | 2       | 0            |

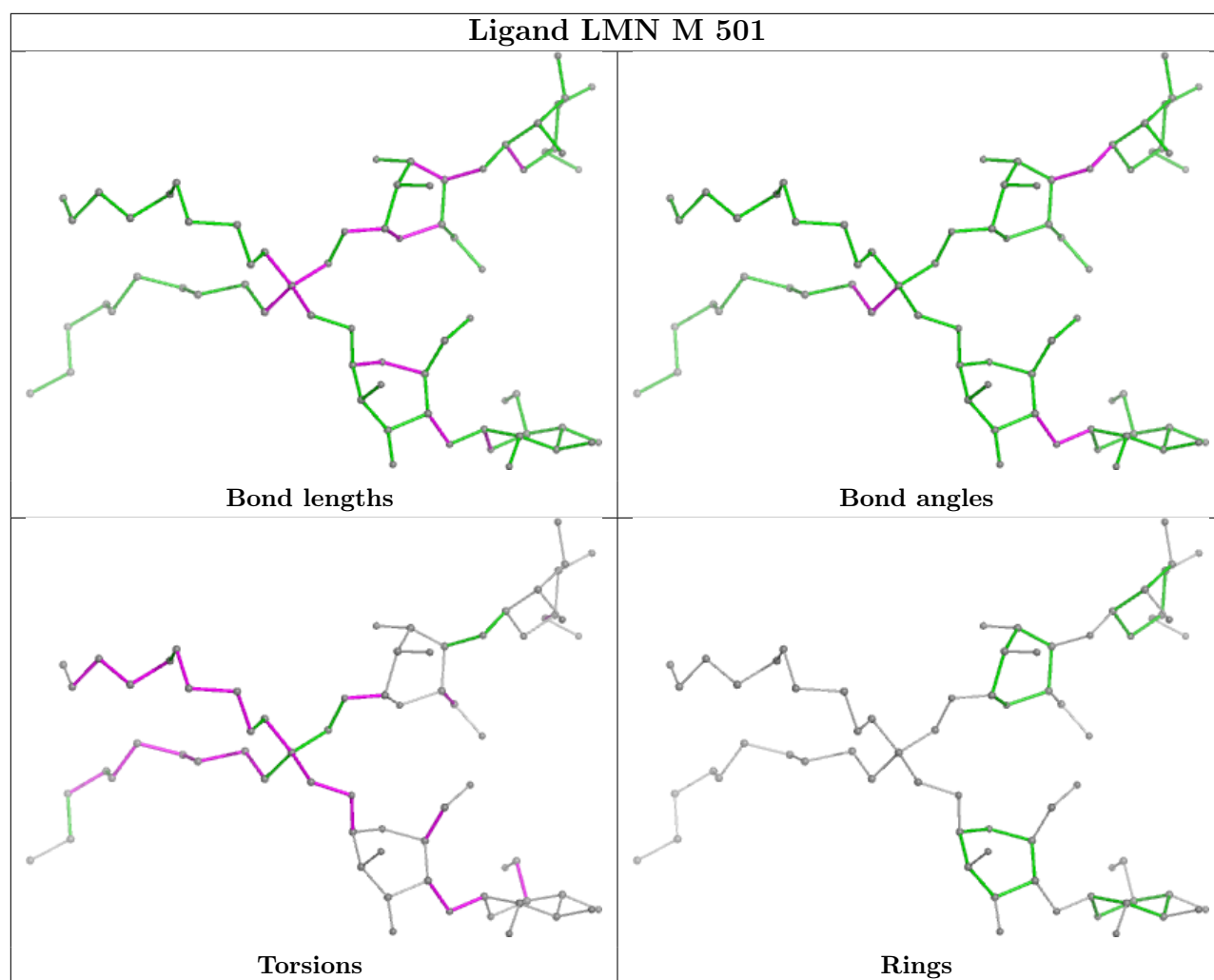
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

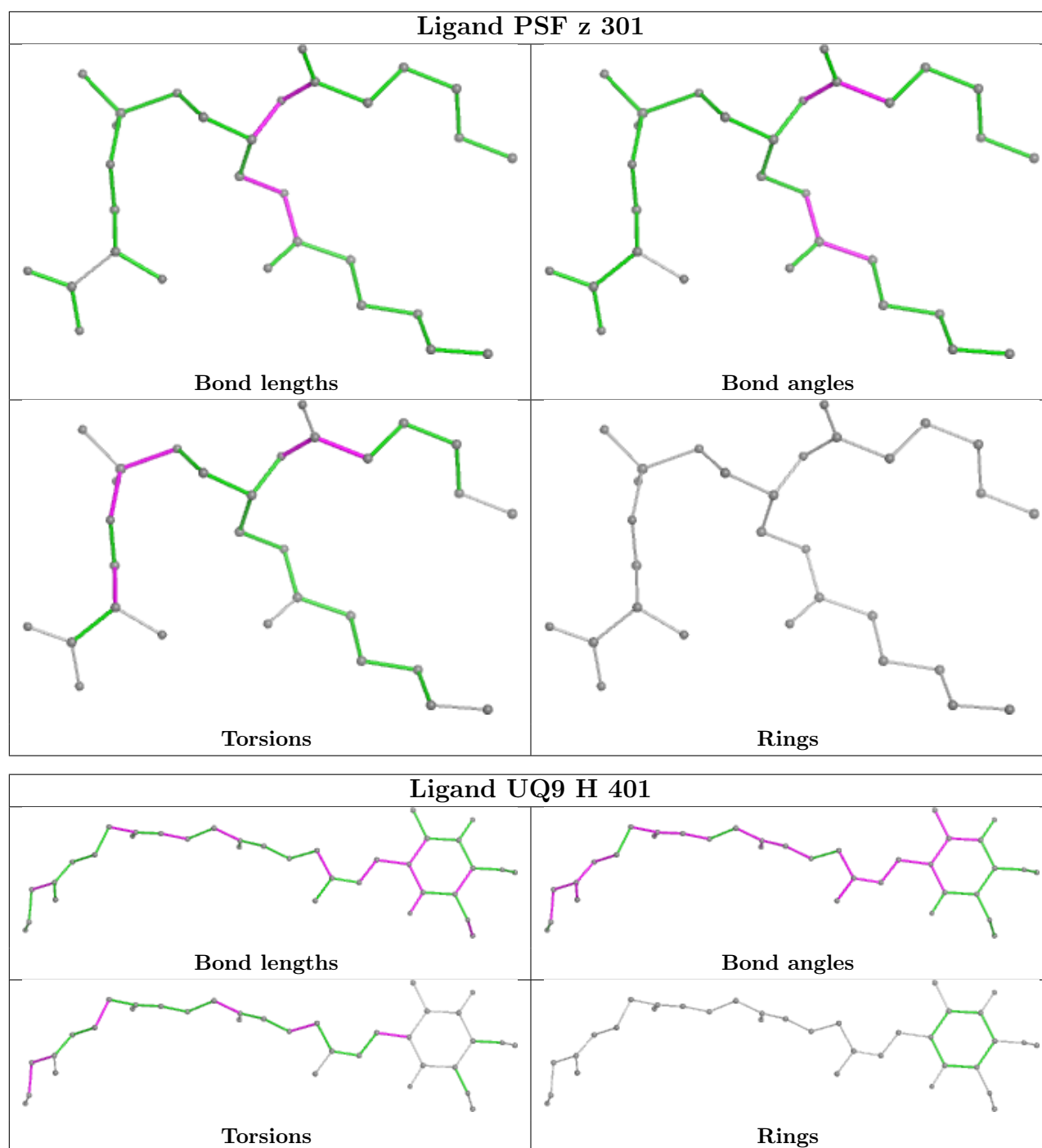












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.