



## wwPDB EM Validation Summary Report ⓘ

Feb 20, 2025 – 06:09 pm GMT

PDB ID : 9H1L  
EMDB ID : EMD-51767  
Title : Methyl-coenzyme M reductase activation complex binding to the A2 component after incubation with ATP  
Authors : Ramirez-Amador, F.; Paul, S.; Kumar, A.; Schuller, J.M.  
Deposited on : 2024-10-09  
Resolution : 2.14 Å(reported)  
Based on initial model : .

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 : **FAILED**  
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 : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

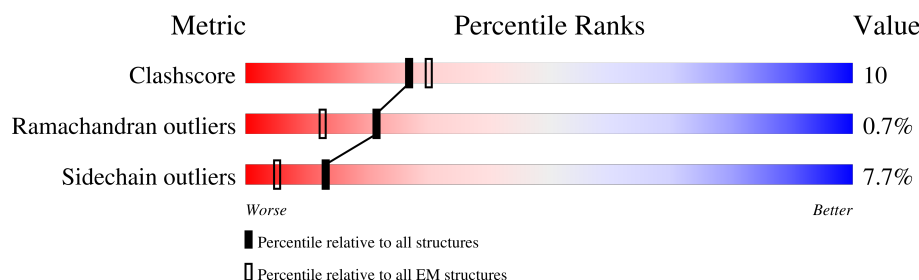
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.14 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.



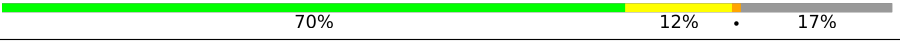

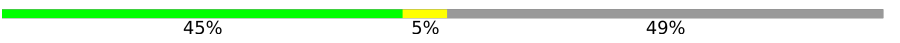
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 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   | J     | 501    | 58% 30% 9% .     |
| 2   | A     | 260    | 81% 18% .        |
| 2   | B     | 260    | 81% 18%          |
| 3   | D     | 443    | 84% 15% .        |
| 3   | E     | 443    | 84% 15%          |
| 4   | C     | 553    | 80% 18% ..       |
| 4   | F     | 553    | 80% 13% . 6%     |
| 5   | G     | 183    | 47% 15% 38%      |
| 6   | H     | 304    | 74% 22% . .      |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 7   | I     | 234    |  |
| 8   | K     | 531    |  |
| 9   | L     | 93     |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 13  | SHT  | F     | 602 | X         | -        | X       | -                |
| 4   | GL3  | C     | 448 | -         | -        | X       | -                |
| 4   | SMC  | C     | 455 | -         | -        | X       | -                |

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32524 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 UPF0288 protein MmarC6\_0796.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | J     | 499      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3962  | 2517 | 647 | 790 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| J     | 500     | SER      | LYS    | variant | UNP A9A8E0 |

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit gamma.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | A     | 259      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2071  | 1293 | 369 | 397 | 12 |         |       |
| 2   | B     | 259      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2071  | 1293 | 369 | 397 | 12 |         |       |

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | E     | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3263  | 2066 | 546 | 630 | 21 |         |       |
| 3   | D     | 442      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3263  | 2066 | 546 | 630 | 21 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| E     | 173     | GLY      | SER    | conflict | UNP A0A2L1CBB3 |
| D     | 173     | GLY      | SER    | conflict | UNP A0A2L1CBB3 |

- Molecule 4 is a protein called Methyl-coenzyme M reductase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | C     | 550      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4284  | 2707 | 731 | 826 | 20 |         |       |
| 4   | F     | 520      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4039  | 2556 | 684 | 779 | 20 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference      |
|-------|---------|----------|--------|---------|----------------|
| C     | 51      | SER      | ALA    | variant | UNP A0A2L1CBB0 |
| F     | 51      | SER      | ALA    | variant | UNP A0A2L1CBB0 |

- Molecule 5 is a protein called Methanogenesis marker protein 17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | G     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 931   | 600 | 152 | 172 | 7 |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| G     | 109     | VAL      | ILE    | variant | UNP G0H411 |
| G     | 129     | ILE      | VAL    | variant | UNP G0H411 |
| G     | 167     | GLU      | GLN    | variant | UNP G0H411 |
| G     | 168     | GLU      | ASP    | variant | UNP G0H411 |
| G     | 171     | ASN      | ASP    | variant | UNP G0H411 |

- Molecule 6 is a protein called Methanogenesis marker protein 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | H     | 296      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2393  | 1530 | 411 | 440 | 12 |         |       |

- Molecule 7 is a protein called Methyl-coenzyme M reductase operon protein C.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | I     | 194      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1469  | 929 | 261 | 271 | 8 |         |       |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| I     | -35     | MET      | -      | initiating methionine | UNP G0H3B1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | -34     | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -33     | ALA      | -      | expression tag | UNP G0H3B1 |
| I     | -32     | TRP      | -      | expression tag | UNP G0H3B1 |
| I     | -31     | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -30     | HIS      | -      | expression tag | UNP G0H3B1 |
| I     | -29     | PRO      | -      | expression tag | UNP G0H3B1 |
| I     | -28     | GLN      | -      | expression tag | UNP G0H3B1 |
| I     | -27     | PHE      | -      | expression tag | UNP G0H3B1 |
| I     | -26     | GLU      | -      | expression tag | UNP G0H3B1 |
| I     | -25     | LYS      | -      | expression tag | UNP G0H3B1 |
| I     | -24     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -23     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -22     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -21     | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -20     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -19     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -18     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -17     | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -16     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -15     | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -14     | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -13     | ALA      | -      | expression tag | UNP G0H3B1 |
| I     | -12     | TRP      | -      | expression tag | UNP G0H3B1 |
| I     | -11     | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -10     | HIS      | -      | expression tag | UNP G0H3B1 |
| I     | -9      | PRO      | -      | expression tag | UNP G0H3B1 |
| I     | -8      | GLN      | -      | expression tag | UNP G0H3B1 |
| I     | -7      | PHE      | -      | expression tag | UNP G0H3B1 |
| I     | -6      | GLU      | -      | expression tag | UNP G0H3B1 |
| I     | -5      | LYS      | -      | expression tag | UNP G0H3B1 |
| I     | -4      | SER      | -      | expression tag | UNP G0H3B1 |
| I     | -3      | ALA      | -      | expression tag | UNP G0H3B1 |
| I     | -2      | GLY      | -      | expression tag | UNP G0H3B1 |
| I     | -1      | SER      | -      | expression tag | UNP G0H3B1 |
| I     | 0       | GLY      | -      | expression tag | UNP G0H3B1 |

- Molecule 8 is a protein called Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA.

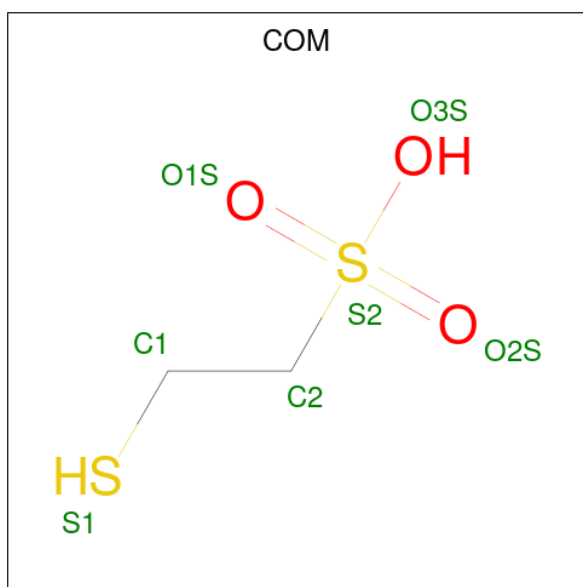
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | K     | 521      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4089  | 2598 | 693 | 774 | 24 |         |       |

- | Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | L     | 47       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 390   | 251 | 61 | 78 |         |       |

- F43
- 
- The chemical structure of F43 is a complex macrocycle featuring a central core with two nickel (Ni) atoms coordinated by nitrogen atoms (N1A, N1B, N2A, N2B). The macrocycle is substituted with various side chains, including carboxylic acid groups (e.g., C6A, C6B, C6C, C6D, C6E, C6F, C6G, C6H, C6I, C6J, C6K, C6L, C6M, C6N, C6O, C6P, C6Q, C6R, C6S, C6T, C6U, C6V, C6W, C6X, C6Y, C6Z, C6AA, C6AB, C6AC, C6AD, C6AE, C6AF, C6AG, C6AH, C6AI, C6AJ, C6AK, C6AL, C6AM, C6AN, C6AO, C6AP, C6AQ, C6AR, C6AS, C6AT, C6AU, C6AV, C6AW, C6AX, C6AY, C6AZ, C6BA, C6BB, C6BC, C6BD, C6BE, C6BF, C6BG, C6BH, C6BI, C6BJ, C6BK, C6BL, C6BM, C6BN, C6BO, C6BP, C6BQ, C6BR, C6BS, C6BT, C6BU, C6BV, C6BW, C6BX, C6BY, C6BZ, C6CA, C6CB, C6CC, C6CD, C6CE, C6CF, C6CG, C6CH, C6CI, C6CJ, C6CK, C6CL, C6CM, C6CN, C6CO, C6CP, C6CQ, C6CR, C6CS, C6CT, C6CU, C6CV, C6CW, C6CX, C6CY, C6CZ, C6DA, C6DB, C6DC, C6DD, C6DE, C6DF, C6DG, C6DH, C6DI, C6DJ, C6DK, C6DL, C6DM, C6DN, C6DO, C6DP, C6DQ, C6DR, C6DS, C6DT, C6DU, C6DV, C6DW, C6DX, C6DY, C6DZ, C6EA, C6EB, C6EC, C6ED, C6EE, C6EF, C6EG, C6EH, C6EI, C6EJ, C6EK, C6EL, C6EM, C6EN, C6EO, C6EP, C6EQ, C6ER, C6ES, C6ET, C6EU, C6EV, C6EW, C6EX, C6EY, C6EZ, C6FA, C6FB, C6FC, C6FD, C6FE, C6FF, C6FG, C6FH, C6FI, C6FJ, C6FK, C6FL, C6FM, C6FN, C6FO, C6FP, C6FQ, C6FR, C6FS, C6FT, C6FU, C6FV, C6FW, C6FX, C6FY, C6FZ, C6GA, C6GB, C6GC, C6GD, C6GE, C6GF, C6GG, C6GH, C6GI, C6GJ, C6GK, C6GL, C6GM, C6GN, C6GO, C6GP, C6GQ, C6GR, C6GS, C6GT, C6GU, C6GV, C6GW, C6GX, C6GY, C6GZ, C6HA, C6HB, C6HC, C6HD, C6HE, C6HF, C6HG, C6HH, C6HI, C6HJ, C6HK, C6HL, C6HM, C6HN, C6HO, C6HP, C6HQ, C6HR, C6HS, C6HT, C6HU, C6HV, C6HW, C6HX, C6HY, C6HZ, C6IA, C6IB, C6IC, C6ID, C6IE, C6IF, C6IG, C6IH, C6II, C6IJ, C6IK, C6IL, C6IM, C6IN, C6IO, C6IP, C6IQ, C6IR, C6IS, C6IT, C6IU, C6IV, C6IW, C6IX, C6IY, C6IZ, C6JA, C6JB, C6JC, C6JD, C6JE, C6JF, C6JG, C6JH, C6JI, C6JJ, C6JK, C6JL, C6JM, C6JN, C6JO, C6JP, C6JQ, C6JR, C6JS, C6JT, C6JU, C6JV, C6JW, C6JX, C6JY, C6JZ, C6KA, C6KB, C6KC, C6KD, C6KE, C6KF, C6KG, C6KH, C6KI, C6KJ, C6KK, C6KL, C6KM, C6KN, C6KO, C6KP, C6KQ, C6KR, C6KS, C6KT, C6KU, C6KV, C6KW, C6KX, C6KY, C6KZ, C6LA, C6LB, C6LC, C6LD, C6LE, C6LF, C6LG, C6LH, C6LI, C6LJ, C6LK, C6LL, C6LM, C6LN, C6LO, C6LP, C6LQ, C6LR, C6LS, C6LT, C6LU, C6LV, C6LW, C6LX, C6LY, C6LZ, C6MA, C6MB, C6MC, C6MD, C6ME, C6MF, C6MG, C6MH, C6MI, C6MJ, C6MK, C6ML, C6MM, C6MN, C6MO, C6MP, C6MQ, C6MR, C6MS, C6MT, C6MU, C6MV, C6MW, C6MX, C6MY, C6MZ, C6NA, C6NB, C6NC, C6ND, C6NE, C6NF, C6NG, C6NH, C6NI, C6NJ, C6NK, C6NL, C6NM, C6NN, C6NO, C6NP, C6NQ, C6NR, C6NS, C6NT, C6NU, C6NV, C6NW, C6NX, C6NY, C6NZ, C6OA, C6OB, C6OC, C6OD, C6OE, C6OF, C6OG, C6OH, C6OI, C6OJ, C6OK, C6OL, C6OM, C6ON, C6OO, C6OP, C6OQ, C6OR, C6OS, C6OT, C6OU, C6OV, C6OW, C6OX, C6OY, C6OZ, C6PA, C6PB, C6PC, C6PD, C6PE, C6PF, C6PG, C6PH, C6PI, C6PJ, C6PK, C6PL, C6PM, C6PN, C6PO, C6PP, C6PQ, C6PR, C6PS, C6PT, C6PU, C6PV, C6PW, C6PX, C6PY, C6PZ, C6QA, C6QB, C6QC, C6QD, C6QE, C6QF, C6QG, C6QH, C6QI, C6QJ, C6QK, C6QL, C6QM, C6QN, C6QO, C6QP, C6QQ, C6QR, C6QS, C6QT, C6QU, C6QV, C6QW, C6QX, C6QY, C6QZ, C6RA, C6RB, C6RC, C6RD, C6RE, C6RF, C6RG, C6RH, C6RI, C6RJ, C6RK, C6RL, C6RM, C6RN, C6RO, C6RP, C6RQ, C6RR, C6RS, C6RT, C6RU, C6RV, C6RW, C6RX, C6RY, C6RZ, C6SA, C6SB, C6SC, C6SD, C6SE, C6SF, C6SG, C6SH, C6SI, C6SJ, C6SK, C6SL, C6SM, C6SN, C6SO, C6SP, C6SQ, C6SR, C6SS, C6ST, C6SU, C6SV, C6SW, C6SX, C6SY, C6SZ, C6TA, C6TB, C6TC, C6TD, C6TE, C6TF, C6TG, C6TH, C6TI, C6TJ, C6TK, C6TL, C6TM, C6TN, C6TO, C6TP, C6TQ, C6TR, C6TS, C6TT, C6TU, C6TV, C6TW, C6TX, C6TY, C6TZ, C6UA, C6UB, C6UC, C6UD, C6UE, C6UF, C6UG, C6UH, C6UI, C6UJ, C6UK, C6UL, C6UM, C6UN, C6UO, C6UP, C6UQ, C6UR, C6US, C6UT, C6UU, C6UV, C6UW, C6UX, C6UY, C6UZ, C6VA, C6VB, C6VC, C6VD, C6VE, C6VF, C6VG, C6VH, C6VI, C6VJ, C6VK, C6VL, C6VM, C6VN, C6VO, C6VP, C6VQ, C6VR, C6VS, C6VT, C6VU, C6VV, C6VW, C6VX, C6VY, C6VZ, C6WA, C6WB, C6WC, C6WD, C6WE, C6WF, C6WG, C6WH, C6WI, C6WJ, C6WK, C6WL, C6WM, C6WN, C6WO, C6WP, C6WQ, C6WR, C6WS, C6WT, C6WU, C6WV, C6WW, C6WX, C6WY, C6WZ, C6XA, C6XB, C6XC, C6XD, C6XE, C6XF, C6XG, C6XH, C6XI, C6XJ, C6XK, C6XL, C6XM, C6XN, C6XO, C6XP, C6XQ, C6XR, C6XS, C6XT, C6XU, C6XV, C6XW, C6XX, C6XY, C6XZ, C6YA, C6YB, C6YC, C6YD, C6YE, C6YF, C6YG, C6YH, C6YI, C6YJ, C6YK, C6YL, C6YM, C6YN, C6YO, C6YP, C6YQ, C6YR, C6YS, C6YT, C6YU, C6YV, C6YW, C6YX, C6YY, C6YZ, C6ZA, C6ZB, C6ZC, C6ZD, C6ZE, C6ZF, C6ZG, C6ZH, C6ZI, C6ZJ, C6ZK, C6ZL, C6ZM, C6ZN, C6ZO, C6ZP, C6ZQ, C6ZR, C6ZS, C6ZT, C6ZU, C6ZV, C6ZW, C6ZX, C6ZY, C6ZZ). The structure also includes several carboxylic acid groups (e.g., C6A, C6B, C6C, C6D, C6E, C6F, C6G, C6H, C6I, C6J, C6K, C6L, C6M, C6N, C6O, C6P, C6Q, C6R, C6S, C6T, C6U, C6V, C6W, C6X, C6Y, C6Z, C6AA, C6AB, C6AC, C6AD, C6AE, C6AF, C6AG, C6AH, C6AI, C6AJ, C6AK, C6AL, C6AM, C6AN, C6AO, C6AP, C6AQ, C6AR, C6AS, C6AT, C6AU, C6AV, C6AW, C6AX, C6AY, C6AZ, C6BA, C6BB, C6BC, C6BD, C6BE, C6BF, C6BG, C6BH, C6BI, C6BJ, C6BK, C6BL, C6BM, C6BN, C6BO, C6BP, C6BQ, C6BR, C6BS, C6BT, C6BU, C6BV, C6BW, C6BX, C6BY, C6BZ, C6CA, C6CB, C6CC, C6CD, C6CE, C6CF, C6CG, C6CH, C6CI, C6CJ, C6CK, C6CL, C6CM, C6CN, C6CO, C6CP, C6CQ, C6CR, C6CS, C6CT, C6CU, C6CV, C6CW, C6CX, C6CY, C6CZ, C6DA, C6DB, C6DC, C6DD, C6DE, C6DF, C6DG, C6DH, C6DI, C6DJ, C6DK, C6DL, C6DM, C6DN, C6DO, C6DP, C6DQ, C6DR, C6DS, C6DT, C6DU, C6DV, C6DW, C6DX, C6DY, C6DZ, C6EA, C6EB, C6EC, C6ED, C6EE, C6EF, C6EG, C6EH, C6EI, C6EJ, C6EK, C6EL, C6EM, C6EN, C6EO, C6EP, C6EQ, C6ER, C6ES, C6ET, C6EU, C6EV, C6EW, C6EX, C6EY, C6EZ, C6FA, C6FB, C6FC, C6FD, C6FE, C6FF, C6FG, C6FH, C6FI, C6FJ, C6FK, C6FL, C6FM, C6FN, C6FO, C6FP, C6FQ, C6FR, C6FS, C6FT, C6FU, C6FV, C6FW, C6FX, C6FY, C6FZ, C6GA, C6GB, C6GC, C6GD, C6GE, C6GF, C6GG, C6GH, C6GI, C6GJ, C6GK, C6GL, C6GM, C6GN, C6GO, C6GP, C6GQ, C6GR, C6GS, C6GT, C6GU, C6GV, C6GW, C6GX, C6GY, C6GZ, C6HA, C6HB, C6HC, C6HD, C6HE, C6HF, C6HG, C6HH, C6HI, C6HJ, C6HK, C6HL, C6HM, C6HN, C6HO, C6HP, C6HQ, C6HR, C6HS, C6HT, C6HU, C6HV, C6HW, C6HX, C6HY, C6HZ, C6IA, C6IB, C6IC, C6ID, C6IE, C6IF, C6IG, C6IH, C6II, C6IJ, C6IK, C6IL, C6IM, C6IN, C6IO, C6IP, C6IQ, C6IR, C6IS, C6IT, C6IU, C6IV, C6IW, C6IX, C6IY, C6IZ, C6JA

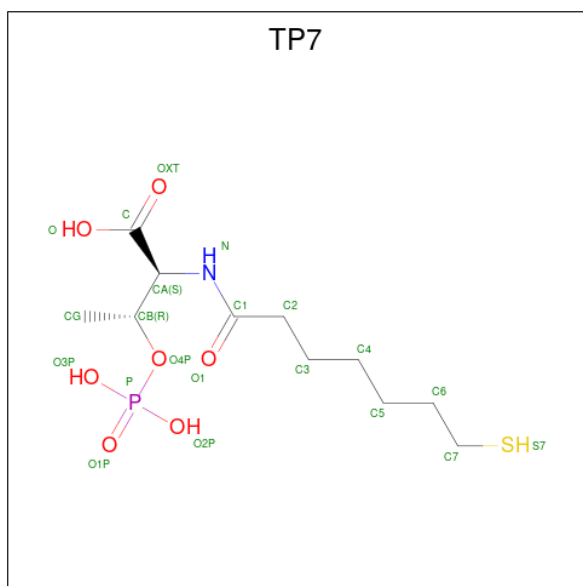
| Mol | Chain | Residues | Atoms       |         |        |         |         | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|
| 10  | A     | 1        | Total<br>62 | C<br>42 | N<br>6 | Ni<br>1 | O<br>13 | 0       |
| 10  | E     | 1        | Total<br>62 | C<br>42 | N<br>6 | Ni<br>1 | O<br>13 | 0       |

- 



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 11  | C     | 1        | Total | C | O | S | 0       |
|     |       |          | 7     | 2 | 3 | 2 |         |

- Molecule 12 is Coenzyme B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 12  | F     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 21    | 11 | 1 | 7 | 1 | 1 |         |

- Molecule 13 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (three-letter code: SHT) (formula:  $C_{13}H_{24}NO_{10}PS_3$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |   |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---|---------|
| 13  | F     | 1        | Total | C  | N | O  | P | S | 0       |
|     |       |          | 28    | 13 | 1 | 10 | 1 | 3 |         |

- Molecule 14 is FeFe cofactor (three-letter code: S5Q) (formula:  $\text{CFe}_8\text{S}_9$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |        |         |        | AltConf |
|-----|-------|----------|-------------|--------|---------|--------|---------|
| 14  | H     | 1        | Total<br>18 | C<br>1 | Fe<br>8 | S<br>9 | 0       |
| 14  | I     | 1        | Total<br>18 | C<br>1 | Fe<br>8 | S<br>9 | 0       |

*Continued on next page...*

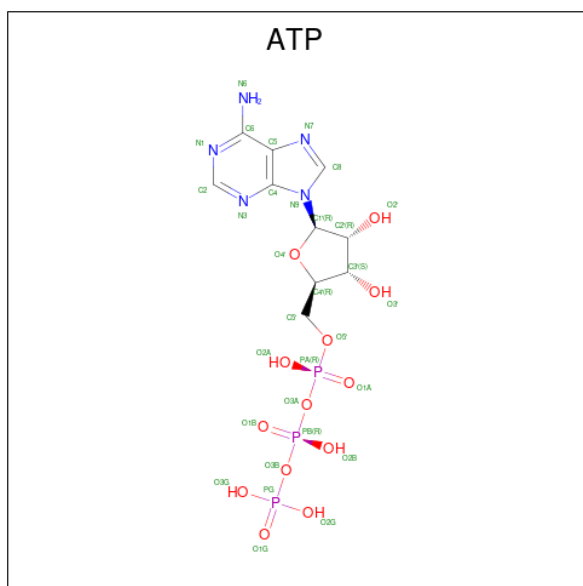
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |    |   | AltConf |
|-----|-------|----------|-------|---|----|---|---------|
| 14  | I     | 1        | Total | C | Fe | S | 0       |
|     |       |          | 18    | 1 | 8  | 9 |         |

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 15  | K     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 16  | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 16  | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

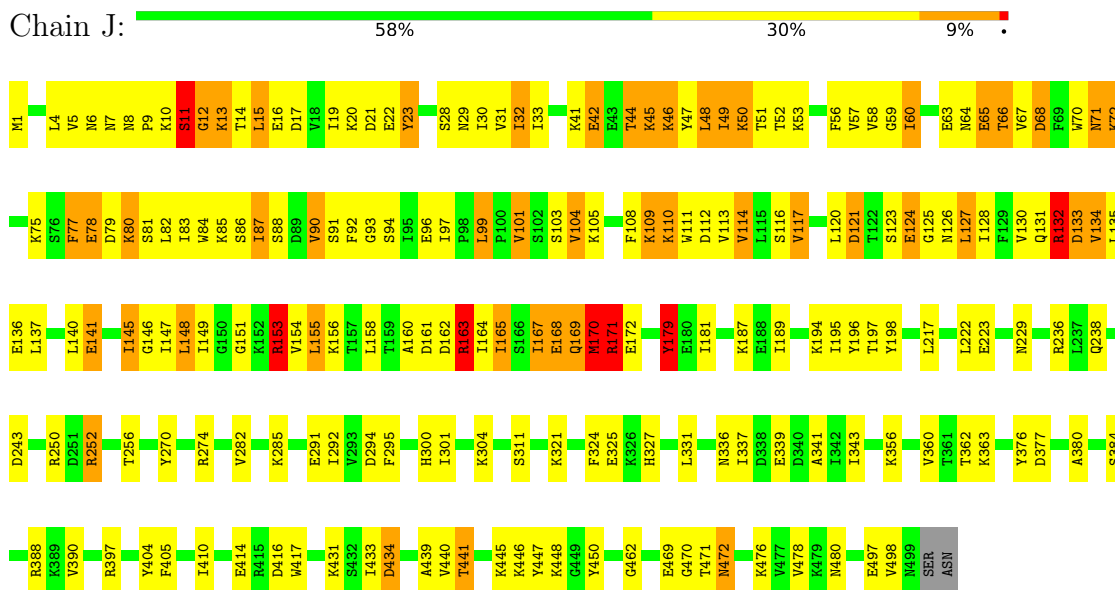
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | K     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

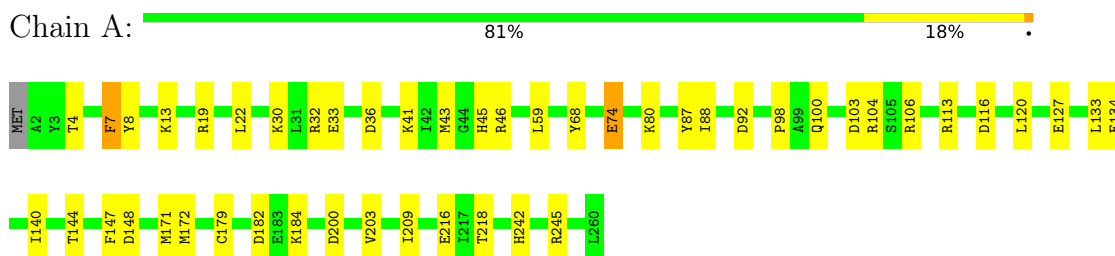
### 3 Residue-property plots

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.

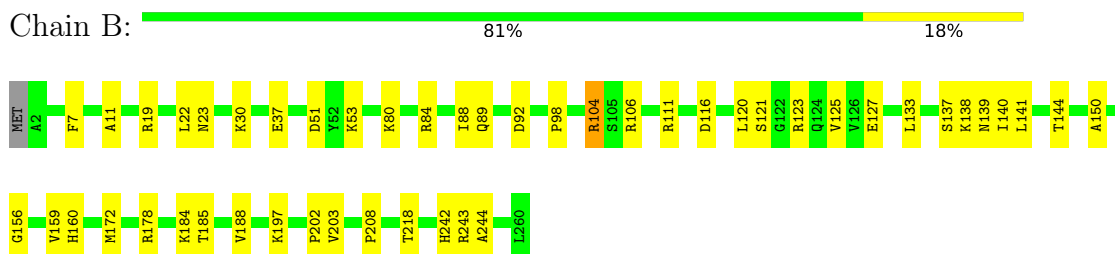
- Molecule 1: UPF0288 protein MmarC6\_0796



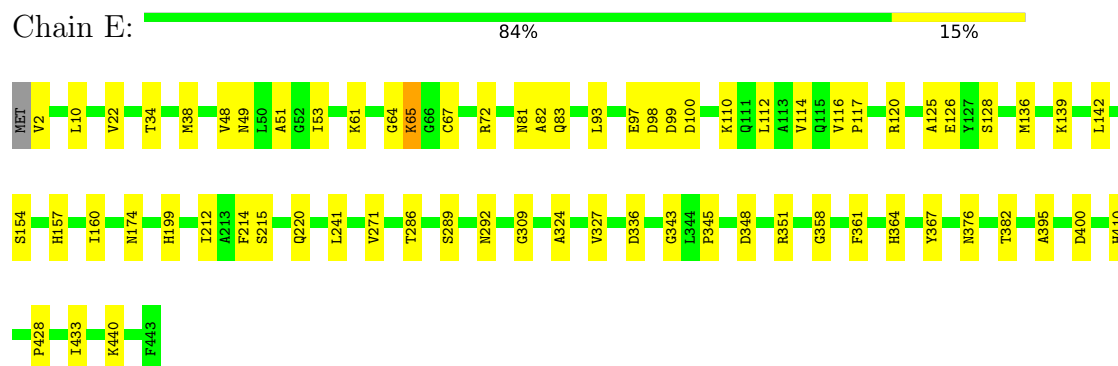
- Molecule 2: Methyl-coenzyme M reductase subunit gamma



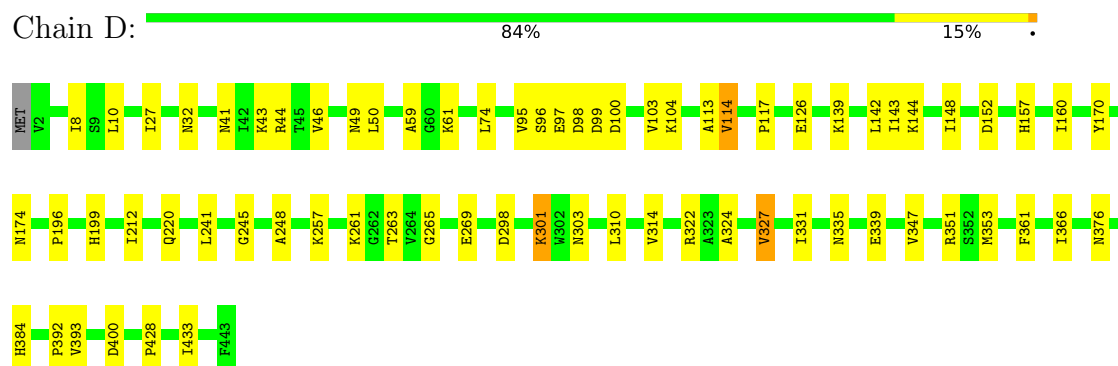
- Molecule 2: Methyl-coenzyme M reductase subunit gamma



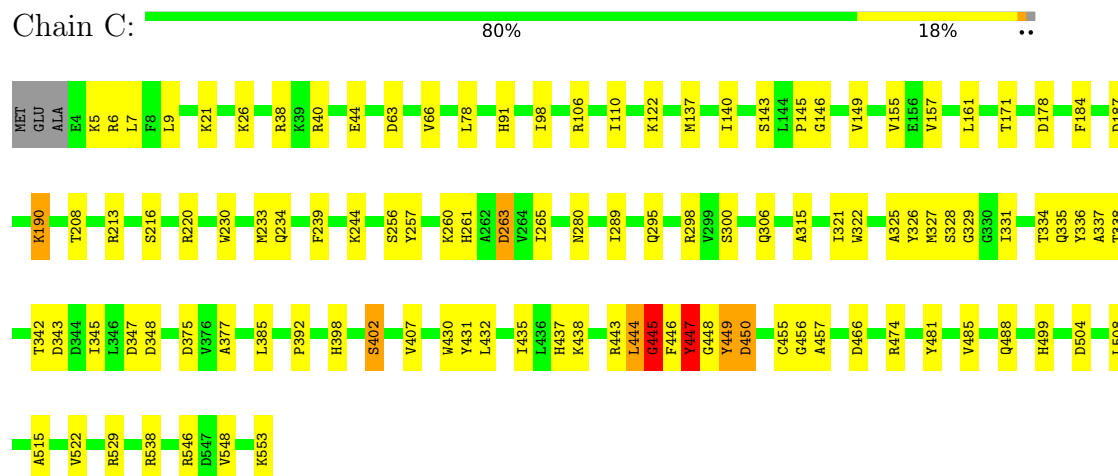
- Molecule 3: Methyl-coenzyme M reductase subunit beta



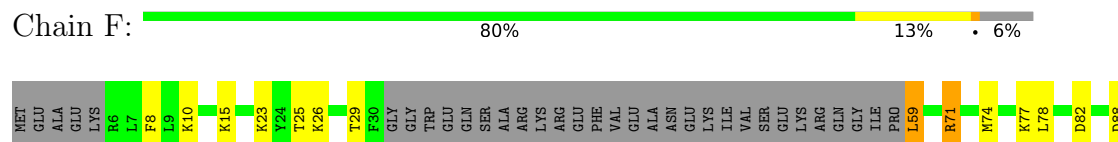
- Molecule 3: Methyl-coenzyme M reductase subunit beta

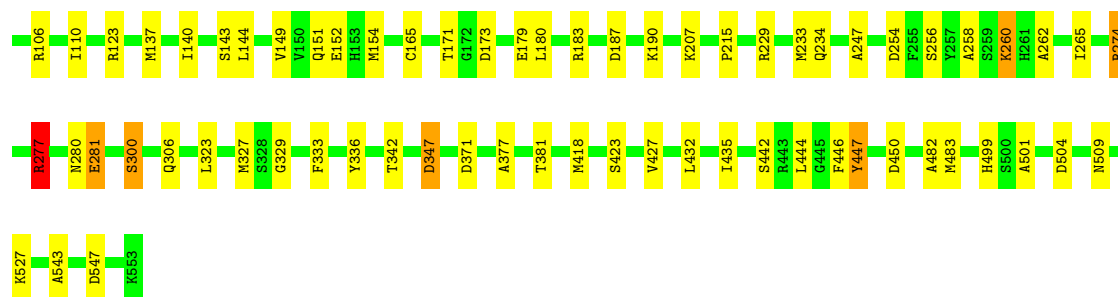


- Molecule 4: Methyl-coenzyme M reductase subunit alpha



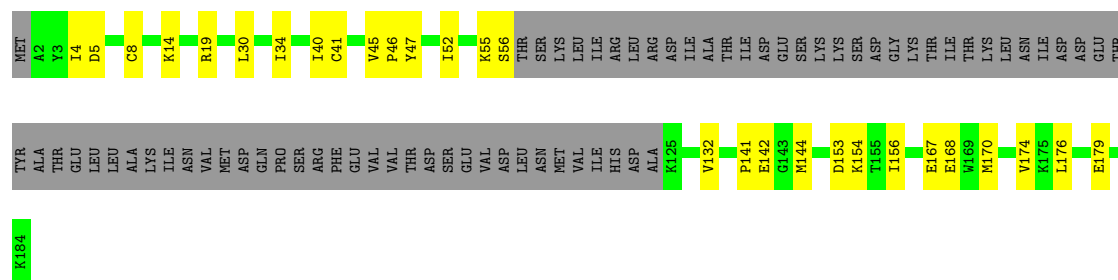
- Molecule 4: Methyl-coenzyme M reductase subunit alpha





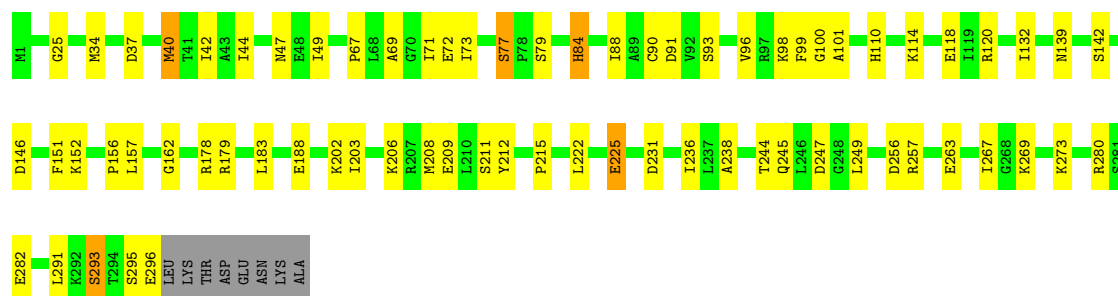
- Molecule 5: Methanogenesis marker protein 17

Chain G: 47% 15% 38%



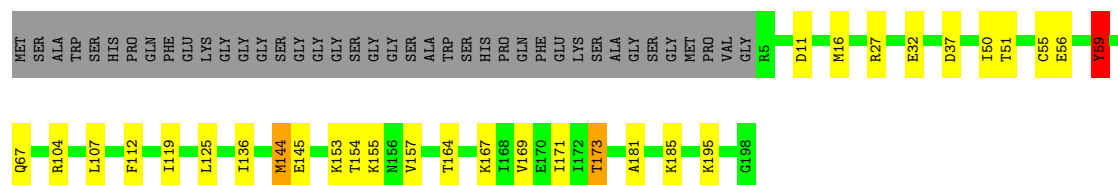
- Molecule 6: Methanogenesis marker protein 7

Chain H: 74% 22% ..



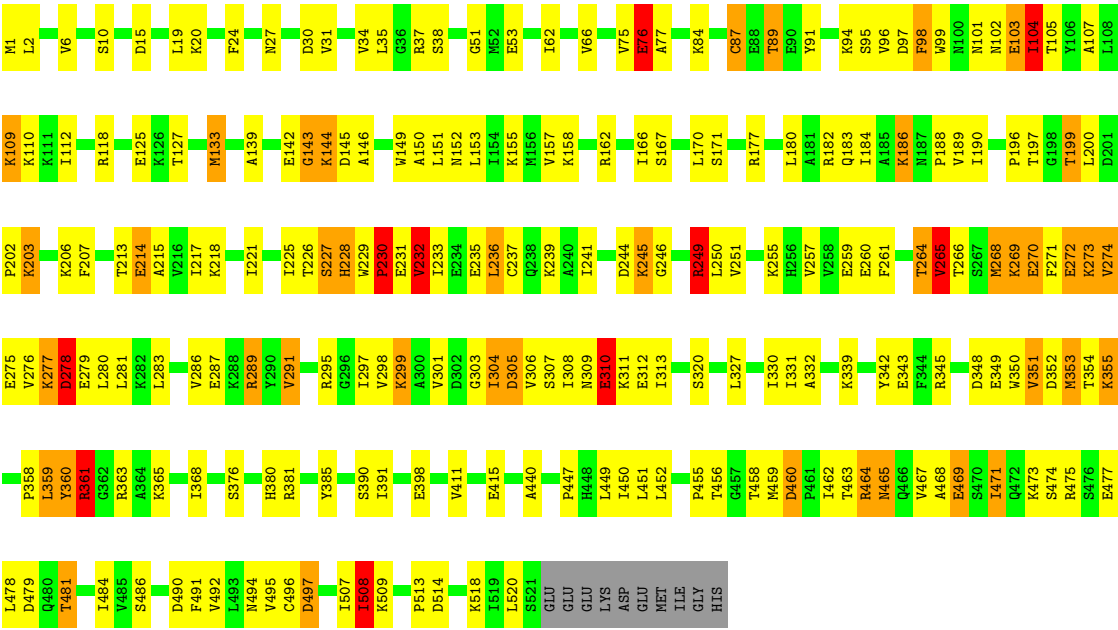
- Molecule 7: Methyl-coenzyme M reductase operon protein C

Chain I: 70% 12% 17%



- Molecule 8: Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA

Chain K: 56% 33% 8% ..



● Molecule 9: DUF2098 domain-containing protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 118247                                  | 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 ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k 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: AGM, SHT, MHS, TP7, MGN, GL3, MG, SMC, F43, ZN, S5Q, ATP, COM

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   | J     | 0.41         | 0/4026         | 0.74        | 6/5441 (0.1%)   |
| 2   | A     | 0.28         | 0/2116         | 0.57        | 2/2861 (0.1%)   |
| 2   | B     | 0.27         | 0/2116         | 0.54        | 0/2861          |
| 3   | D     | 0.29         | 0/3319         | 0.50        | 1/4499 (0.0%)   |
| 3   | E     | 0.29         | 0/3319         | 0.50        | 1/4499 (0.0%)   |
| 4   | C     | 0.28         | 0/4328         | 0.64        | 3/5856 (0.1%)   |
| 4   | F     | 0.28         | 0/4078         | 0.50        | 0/5522          |
| 5   | G     | 0.28         | 0/943          | 0.54        | 0/1262          |
| 6   | H     | 0.28         | 0/2435         | 0.52        | 0/3280          |
| 7   | I     | 0.27         | 0/1490         | 0.58        | 2/2006 (0.1%)   |
| 8   | K     | 0.52         | 1/4159 (0.0%)  | 0.94        | 28/5613 (0.5%)  |
| 9   | L     | 0.28         | 0/398          | 0.58        | 0/542           |
| All | All   | 0.34         | 1/32727 (0.0%) | 0.64        | 43/44242 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | J     | 0                   | 6                   |
| 2   | A     | 0                   | 1                   |
| 4   | F     | 0                   | 2                   |
| 6   | H     | 0                   | 1                   |
| 8   | K     | 0                   | 7                   |
| All | All   | 0                   | 17                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8   | K     | 230 | PRO  | N-CD  | 11.52 | 1.64        | 1.47     |



The worst 5 of 43 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4   | C     | 447 | TYR  | CB-CA-C | -26.05 | 58.31       | 110.40   |
| 1   | J     | 32  | ILE  | O-C-N   | 21.22  | 156.65      | 122.70   |
| 1   | J     | 32  | ILE  | CA-C-N  | -18.02 | 77.56       | 117.20   |
| 8   | K     | 354 | THR  | N-CA-CB | -14.10 | 83.50       | 110.30   |
| 4   | C     | 447 | TYR  | N-CA-C  | 13.90  | 148.54      | 111.00   |

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | J     | 132 | ARG  | Sidechain |
| 1   | J     | 153 | ARG  | Sidechain |
| 1   | J     | 163 | ARG  | Sidechain |
| 1   | J     | 171 | ARG  | Sidechain |
| 1   | J     | 42  | GLU  | Mainchain |

## 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   | J     | 3962  | 0        | 3996     | 179     | 0            |
| 2   | A     | 2071  | 0        | 2012     | 24      | 0            |
| 2   | B     | 2071  | 0        | 2012     | 32      | 0            |
| 3   | D     | 3263  | 0        | 3260     | 44      | 0            |
| 3   | E     | 3263  | 0        | 3259     | 33      | 0            |
| 4   | C     | 4284  | 0        | 4147     | 75      | 0            |
| 4   | F     | 4039  | 0        | 3904     | 64      | 0            |
| 5   | G     | 931   | 0        | 970      | 16      | 0            |
| 6   | H     | 2393  | 0        | 2475     | 45      | 0            |
| 7   | I     | 1469  | 0        | 1534     | 15      | 0            |
| 8   | K     | 4089  | 0        | 4163     | 156     | 0            |
| 9   | L     | 390   | 0        | 378      | 3       | 0            |
| 10  | A     | 62    | 0        | 43       | 7       | 0            |
| 10  | E     | 62    | 0        | 42       | 10      | 0            |
| 11  | C     | 7     | 0        | 5        | 3       | 0            |
| 12  | F     | 21    | 0        | 19       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | F     | 28    | 0        | 20       | 15      | 0            |
| 14  | H     | 18    | 0        | 0        | 0       | 0            |
| 14  | I     | 36    | 0        | 0        | 0       | 0            |
| 15  | K     | 1     | 0        | 0        | 0       | 0            |
| 16  | K     | 62    | 0        | 24       | 2       | 0            |
| 17  | K     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 32524 | 0        | 32263    | 631     | 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 10.

The worst 5 of 631 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:179:TYR:CE1 | 1:J:295:PHE:HB3  | 1.36                     | 1.59              |
| 3:E:367:TYR:OH  | 10:E:601:F43:C5A | 1.67                     | 1.40              |
| 1:J:179:TYR:CD1 | 1:J:295:PHE:HB3  | 1.61                     | 1.33              |
| 1:J:179:TYR:CE1 | 1:J:295:PHE:CB   | 2.16                     | 1.26              |
| 1:J:42:GLU:HA   | 1:J:172:GLU:HB3  | 1.24                     | 1.13              |

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   | J     | 493/501 (98%) | 435 (88%) | 47 (10%) | 11 (2%)  | 5 1         |
| 2   | A     | 257/260 (99%) | 253 (98%) | 4 (2%)   | 0        | 100 100     |
| 2   | B     | 257/260 (99%) | 252 (98%) | 5 (2%)   | 0        | 100 100     |
| 3   | D     | 440/443 (99%) | 422 (96%) | 18 (4%)  | 0        | 100 100     |
| 3   | E     | 440/443 (99%) | 422 (96%) | 17 (4%)  | 1 (0%)   | 44 43       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | C     | 539/553 (98%)   | 515 (96%)  | 22 (4%)  | 2 (0%)   | 30          | 26  |
| 4   | F     | 511/553 (92%)   | 490 (96%)  | 20 (4%)  | 1 (0%)   | 44          | 43  |
| 5   | G     | 110/183 (60%)   | 107 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 6   | H     | 294/304 (97%)   | 283 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 7   | I     | 192/234 (82%)   | 183 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 8   | K     | 519/531 (98%)   | 450 (87%)  | 57 (11%) | 12 (2%)  | 5           | 1   |
| 9   | L     | 45/93 (48%)     | 45 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 4097/4358 (94%) | 3857 (94%) | 213 (5%) | 27 (1%)  | 21          | 13  |

5 of 27 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 445 | GLY  |
| 8   | K     | 103 | GLU  |
| 8   | K     | 231 | GLU  |
| 8   | K     | 265 | VAL  |
| 8   | K     | 270 | GLU  |

### 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   | J     | 452/454 (100%) | 377 (83%) | 75 (17%) | 2           | 0  |
| 2   | A     | 223/224 (100%) | 212 (95%) | 11 (5%)  | 21          | 17 |
| 2   | B     | 223/224 (100%) | 219 (98%) | 4 (2%)   | 54          | 57 |
| 3   | D     | 341/342 (100%) | 332 (97%) | 9 (3%)   | 41          | 41 |
| 3   | E     | 341/342 (100%) | 327 (96%) | 14 (4%)  | 26          | 23 |
| 4   | C     | 437/439 (100%) | 415 (95%) | 22 (5%)  | 20          | 16 |
| 4   | F     | 412/439 (94%)  | 389 (94%) | 23 (6%)  | 17          | 13 |
| 5   | G     | 104/168 (62%)  | 95 (91%)  | 9 (9%)   | 8           | 4  |
| 6   | H     | 264/271 (97%)  | 248 (94%) | 16 (6%)  | 15          | 11 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 7   | I     | 160/186 (86%)   | 149 (93%)  | 11 (7%)  | 13          | 8  |
| 8   | K     | 449/458 (98%)   | 378 (84%)  | 71 (16%) | 2           | 0  |
| 9   | L     | 43/81 (53%)     | 41 (95%)   | 2 (5%)   | 22          | 18 |
| All | All   | 3449/3628 (95%) | 3182 (92%) | 267 (8%) | 13          | 5  |

5 of 267 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | K     | 269 | LYS  |
| 8   | K     | 291 | VAL  |
| 8   | K     | 471 | ILE  |
| 3   | E     | 114 | VAL  |
| 3   | E     | 98  | ASP  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 459 | ASN  |
| 8   | K     | 102 | ASN  |
| 8   | K     | 210 | ASN  |
| 8   | K     | 228 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | MHS  | C     | 261 | 4    | 7,11,12      | 0.78 | 0        | 6,14,16     | 1.00 | 0        |
| 4   | MHS  | F     | 261 | 4    | 7,11,12      | 0.78 | 0        | 6,14,16     | 0.87 | 0        |
| 4   | MGN  | C     | 403 | -    | 6,9,10       | 0.69 | 0        | 5,12,14     | 0.74 | 0        |
| 4   | AGM  | F     | 275 | 4    | 10,11,12     | 0.45 | 0        | 6,13,15     | 0.26 | 0        |
| 4   | MGN  | F     | 403 | 4    | 6,9,10       | 0.68 | 0        | 5,12,14     | 0.76 | 0        |
| 4   | GL3  | F     | 448 | 4    | 2,3,4        | 0.48 | 0        | 1,2,4       | 0.35 | 0        |
| 4   | SMC  | F     | 455 | 4    | 5,6,7        | 0.71 | 0        | 2,6,8       | 0.81 | 0        |
| 4   | GL3  | C     | 448 | -    | 2,3,4        | 1.40 | 0        | 1,2,4       | 0.17 | 0        |
| 4   | AGM  | C     | 275 | 3,4  | 10,11,12     | 0.36 | 0        | 6,13,15     | 0.69 | 0        |
| 4   | SMC  | C     | 455 | 4    | 5,6,7        | 0.80 | 0        | 2,6,8       | 1.69 | 0        |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 4   | MHS  | C     | 261 | 4    | -       | 2/5/6/8    | 0/1/1/1 |
| 4   | MHS  | F     | 261 | 4    | -       | 2/5/6/8    | 0/1/1/1 |
| 4   | MGN  | C     | 403 | -    | -       | 1/7/9/12   | -       |
| 4   | AGM  | F     | 275 | 4    | -       | 6/10/11/13 | -       |
| 4   | MGN  | F     | 403 | 4    | -       | 0/7/9/12   | -       |
| 4   | GL3  | F     | 448 | 4    | -       | 1/1/1/2    | -       |
| 4   | SMC  | F     | 455 | 4    | -       | 2/3/5/7    | -       |
| 4   | GL3  | C     | 448 | -    | -       | 1/1/1/2    | -       |
| 4   | AGM  | C     | 275 | 3,4  | -       | 1/10/11/13 | -       |
| 4   | SMC  | C     | 455 | 4    | -       | 2/3/5/7    | -       |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | C     | 261 | MHS  | O-C-CA-CB   |
| 4   | C     | 448 | GL3  | S-C-CA-N    |
| 4   | C     | 455 | SMC  | N-CA-CB-SG  |
| 4   | C     | 455 | SMC  | CA-CB-SG-CS |
| 4   | F     | 261 | MHS  | N-CA-CB-CG  |

There are no ring outliers.

3 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | C     | 261 | MHS  | 1       | 0            |
| 4   | C     | 448 | GL3  | 12      | 0            |
| 4   | C     | 455 | SMC  | 4       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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 | $\# Z  > 2$ |
| 14  | S5Q  | I     | 202 | 7    | 18,30,30     | 2.61 | 11 (61%)    | -           |      |             |
| 11  | COM  | C     | 601 | 10   | 6,6,6        | 1.81 | 3 (50%)     | 7,8,8       | 2.81 | 4 (57%)     |
| 16  | ATP  | K     | 603 | 17   | 26,33,33     | 0.88 | 0           | 31,52,52    | 0.81 | 1 (3%)      |
| 10  | F43  | A     | 601 | 11,4 | 61,71,71     | 2.04 | 4 (6%)      | 64,118,118  | 1.11 | 4 (6%)      |
| 13  | SHT  | F     | 602 | -    | 26,27,27     | 2.04 | 7 (26%)     | 30,36,36    | 2.00 | 6 (20%)     |
| 12  | TP7  | F     | 601 | -    | 19,20,20     | 0.68 | 0           | 24,26,26    | 0.58 | 0           |
| 14  | S5Q  | H     | 401 | 6    | 18,30,30     | 2.60 | 12 (66%)    | -           |      |             |
| 16  | ATP  | K     | 602 | 17   | 26,33,33     | 0.97 | 2 (7%)      | 31,52,52    | 0.75 | 1 (3%)      |
| 10  | F43  | E     | 601 | -    | 61,71,71     | 1.96 | 4 (6%)      | 64,118,118  | 1.03 | 5 (7%)      |
| 14  | S5Q  | I     | 201 | 7    | 18,30,30     | 2.59 | 11 (61%)    | -           |      |             |

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   |
|-----|------|-------|-----|------|---------|---------------|---------|
| 11  | COM  | C     | 601 | 10   | -       | 0/4/4/4       | -       |
| 16  | ATP  | K     | 603 | 17   | -       | 4/18/38/38    | 0/3/3/3 |
| 10  | F43  | A     | 601 | 11,4 | -       | 14/28/185/185 | -       |
| 13  | SHT  | F     | 602 | -    | 1/1/6/9 | 17/31/31/31   | -       |
| 12  | TP7  | F     | 601 | -    | -       | 5/24/24/24    | -       |
| 16  | ATP  | K     | 602 | 17   | -       | 3/18/38/38    | 0/3/3/3 |
| 10  | F43  | E     | 601 | -    | -       | 9/28/185/185  | -       |

The worst 5 of 54 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 10  | A     | 601 | F43  | NI-NA | 9.76 | 2.10        | 1.89     |
| 10  | E     | 601 | F43  | NI-NA | 9.38 | 2.09        | 1.89     |
| 10  | A     | 601 | F43  | NI-NB | 9.21 | 2.09        | 1.89     |
| 10  | E     | 601 | F43  | NI-NB | 9.08 | 2.09        | 1.89     |
| 10  | A     | 601 | F43  | NI-ND | 7.16 | 2.04        | 1.89     |

The worst 5 of 21 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | F     | 602 | SHT  | CK3-CK2-CK1 | -6.48 | 111.95      | 125.85   |
| 13  | F     | 602 | SHT  | OS1-SG2-CD  | 4.10  | 111.85      | 106.92   |
| 11  | C     | 601 | COM  | O2S-S2-C2   | 3.90  | 111.61      | 106.92   |
| 11  | C     | 601 | COM  | O1S-S2-C2   | 3.80  | 111.49      | 106.92   |
| 11  | C     | 601 | COM  | O2S-S2-O1S  | -3.77 | 100.91      | 113.95   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 13  | F     | 602 | SHT  | CB   |

5 of 52 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 10  | A     | 601 | F43  | C2A-C3A-CAA-CBA |
| 10  | A     | 601 | F43  | C4A-C3A-CAA-CBA |
| 10  | E     | 601 | F43  | C1A-C2A-C5A-C6A |
| 10  | E     | 601 | F43  | C9A-C2A-C5A-C6A |
| 10  | E     | 601 | F43  | C2A-C3A-CAA-CBA |

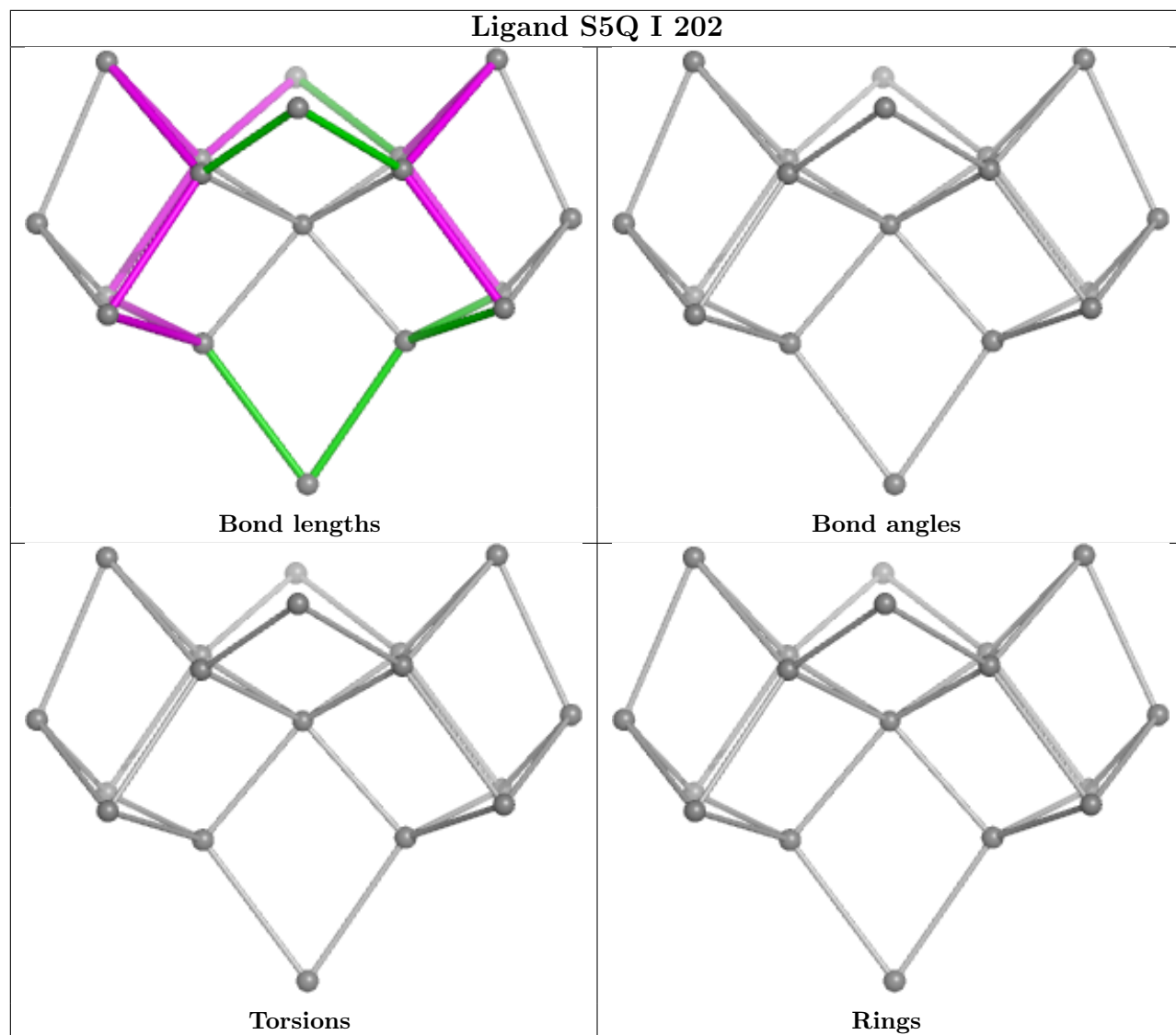
There are no ring outliers.

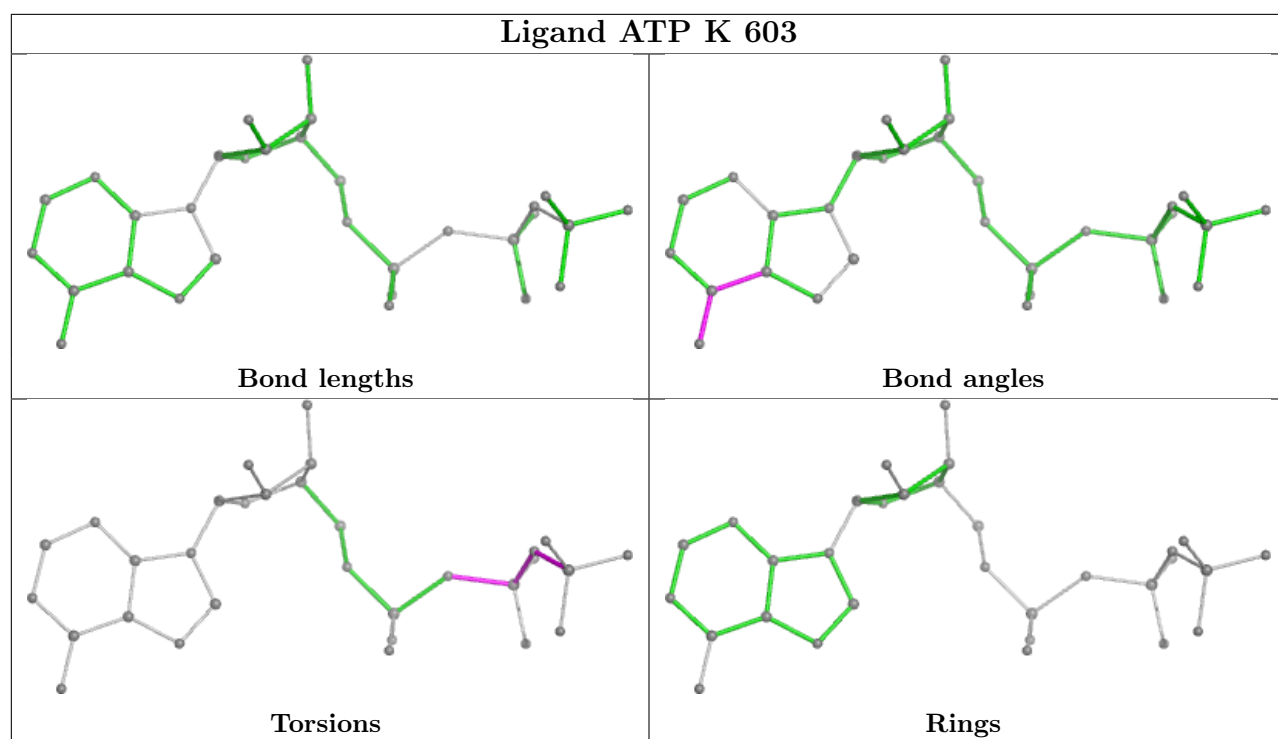
6 monomers are involved in 37 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | C     | 601 | COM  | 3       | 0            |
| 16  | K     | 603 | ATP  | 2       | 0            |
| 10  | A     | 601 | F43  | 7       | 0            |
| 13  | F     | 602 | SHT  | 15      | 0            |
| 12  | F     | 601 | TP7  | 3       | 0            |
| 10  | E     | 601 | F43  | 10      | 0            |

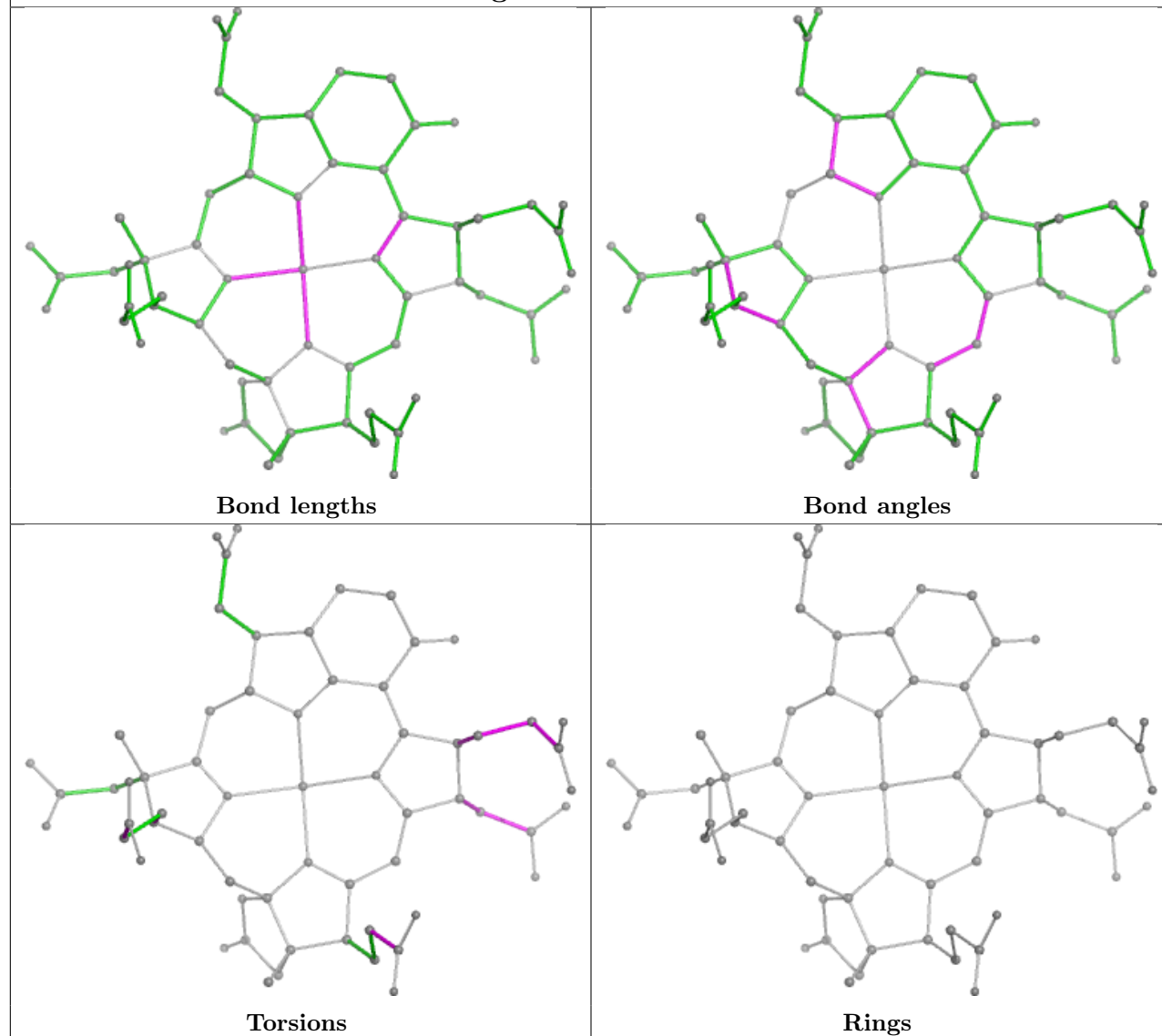
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



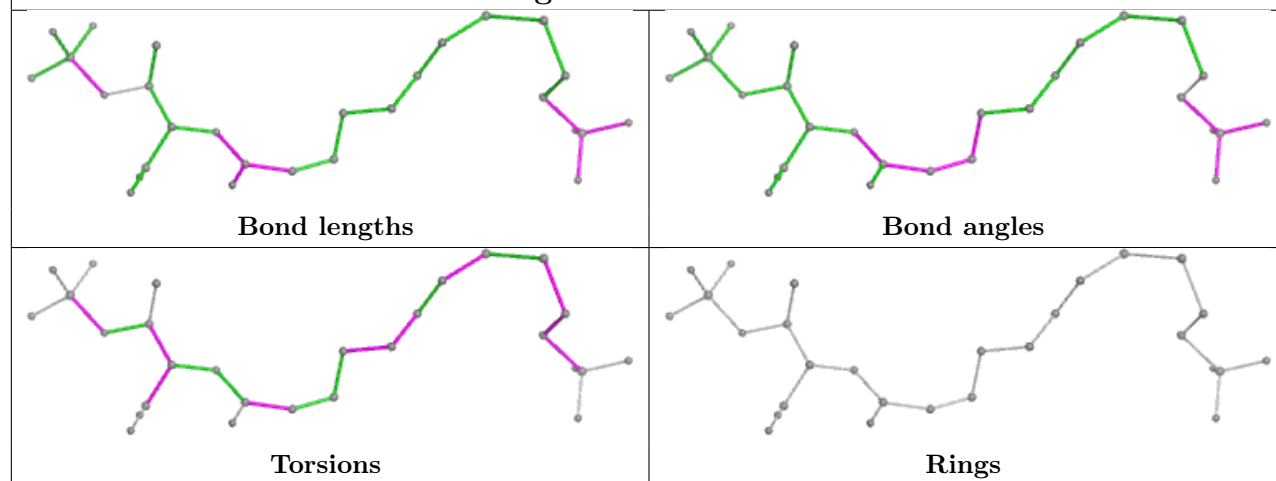


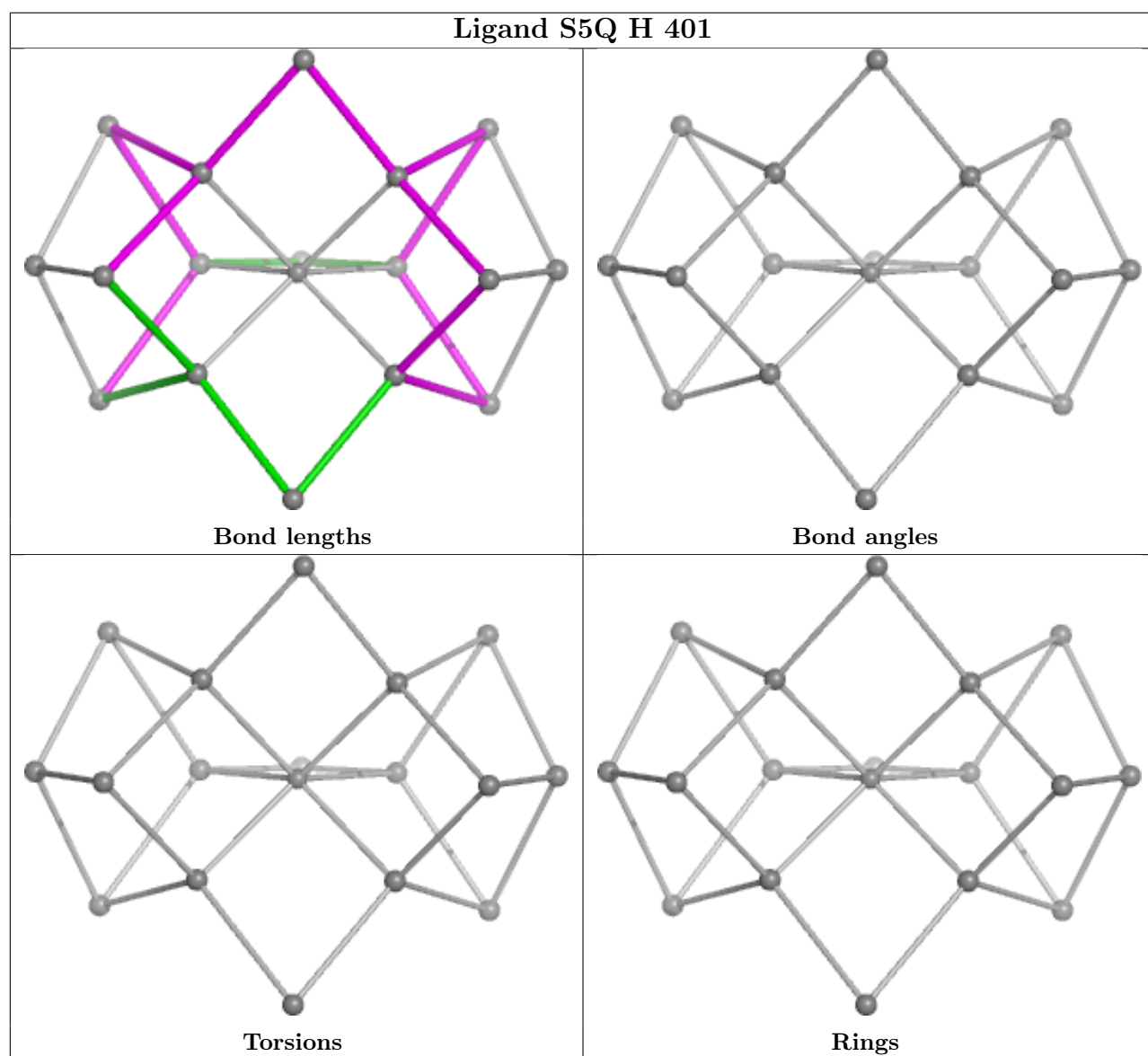
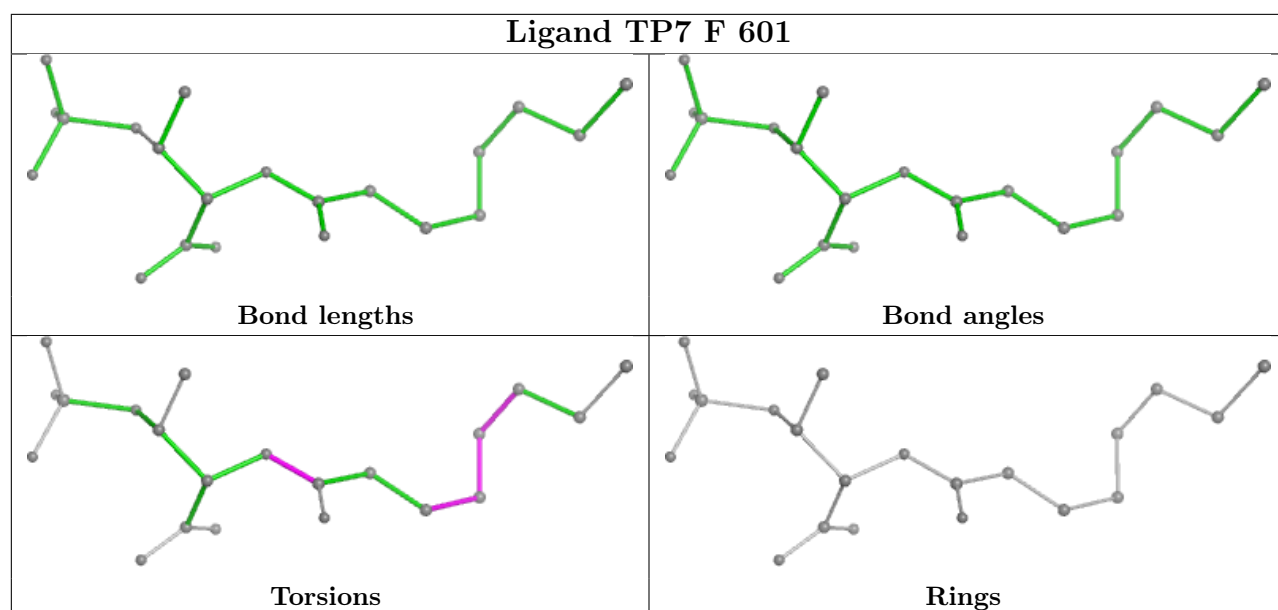


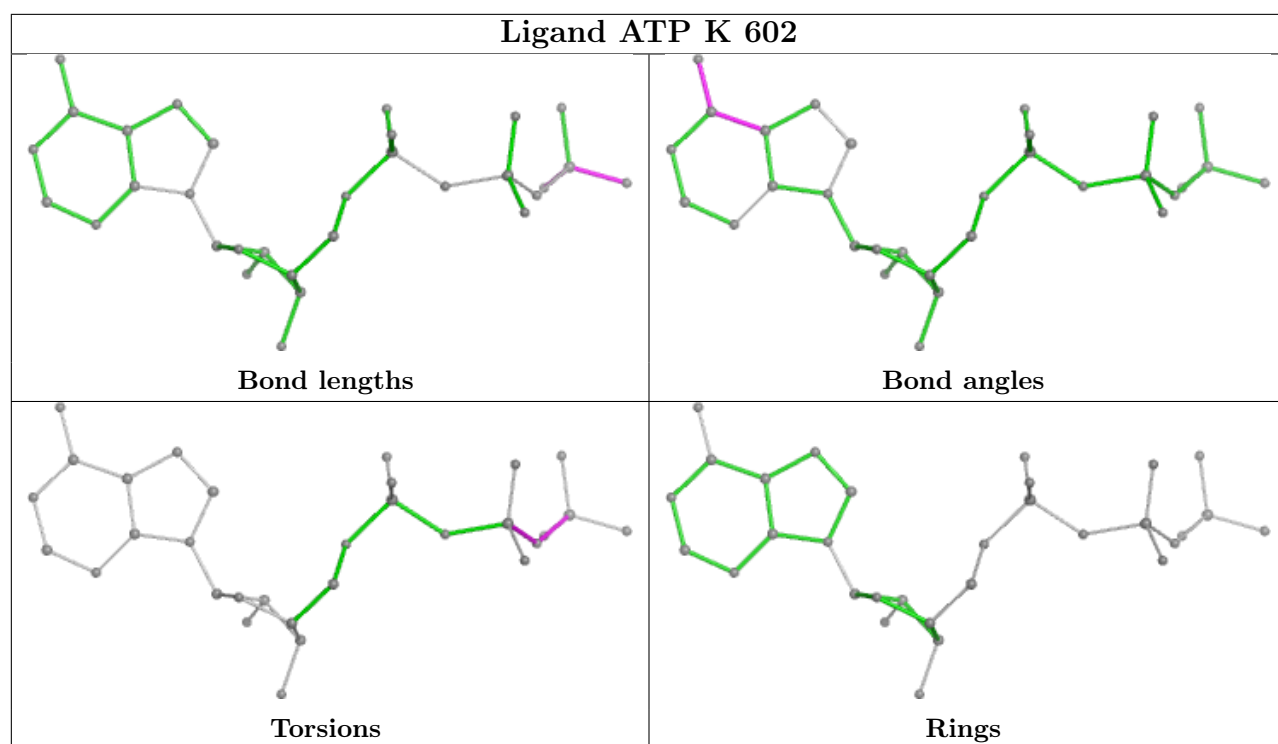
## Ligand F43 A 601



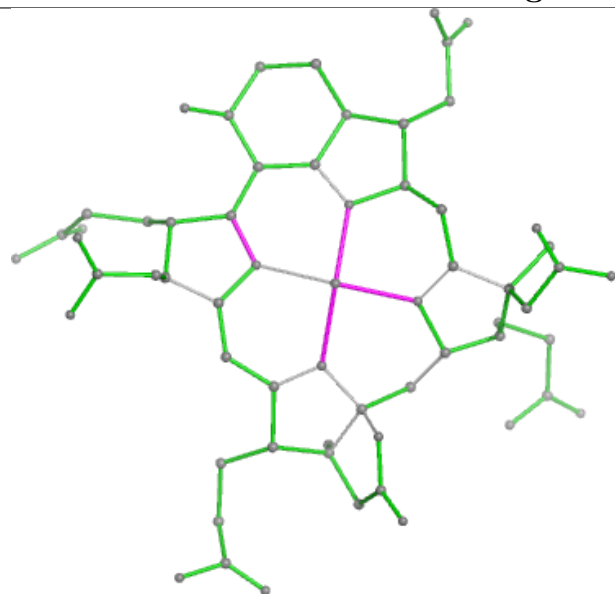
## Ligand SHT F 602



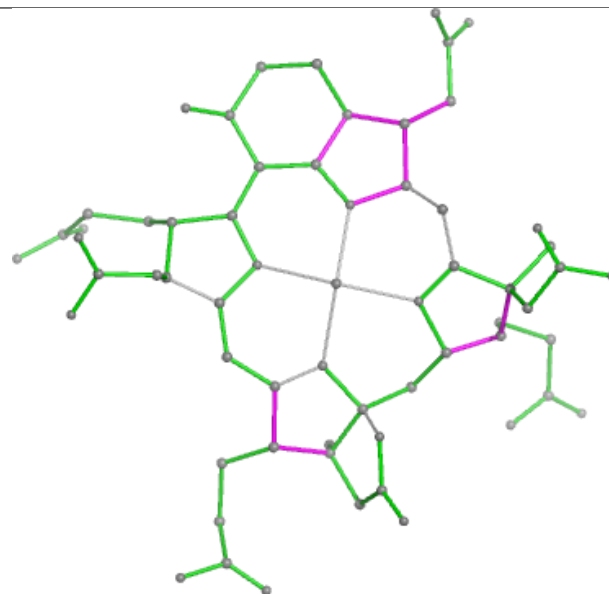




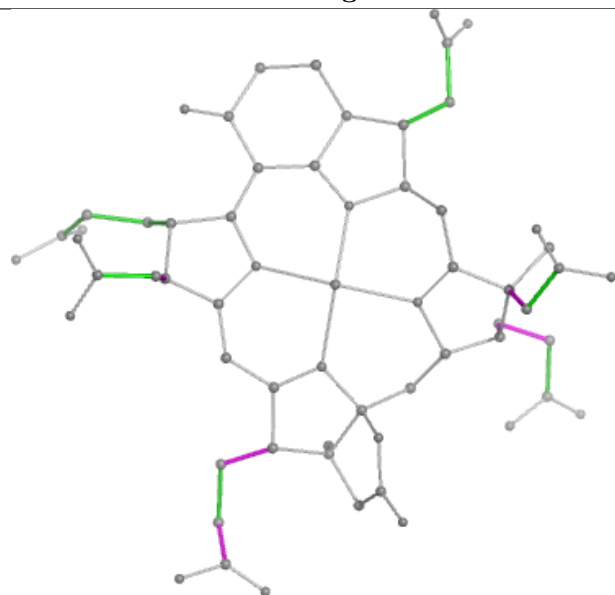
## Ligand F43 E 601



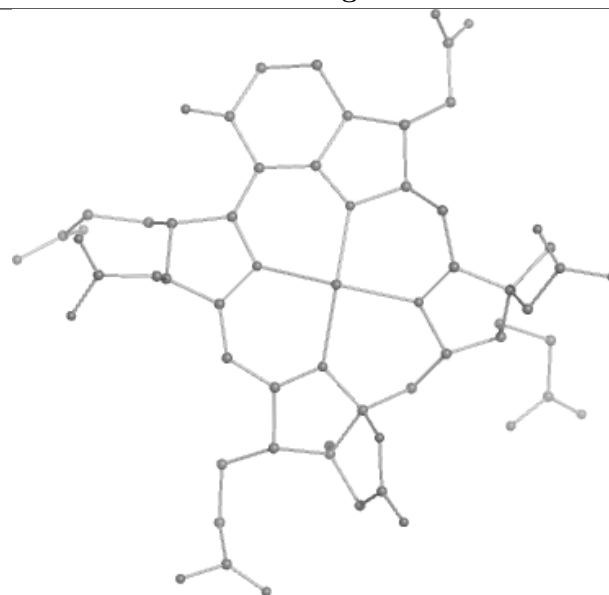
Bond lengths



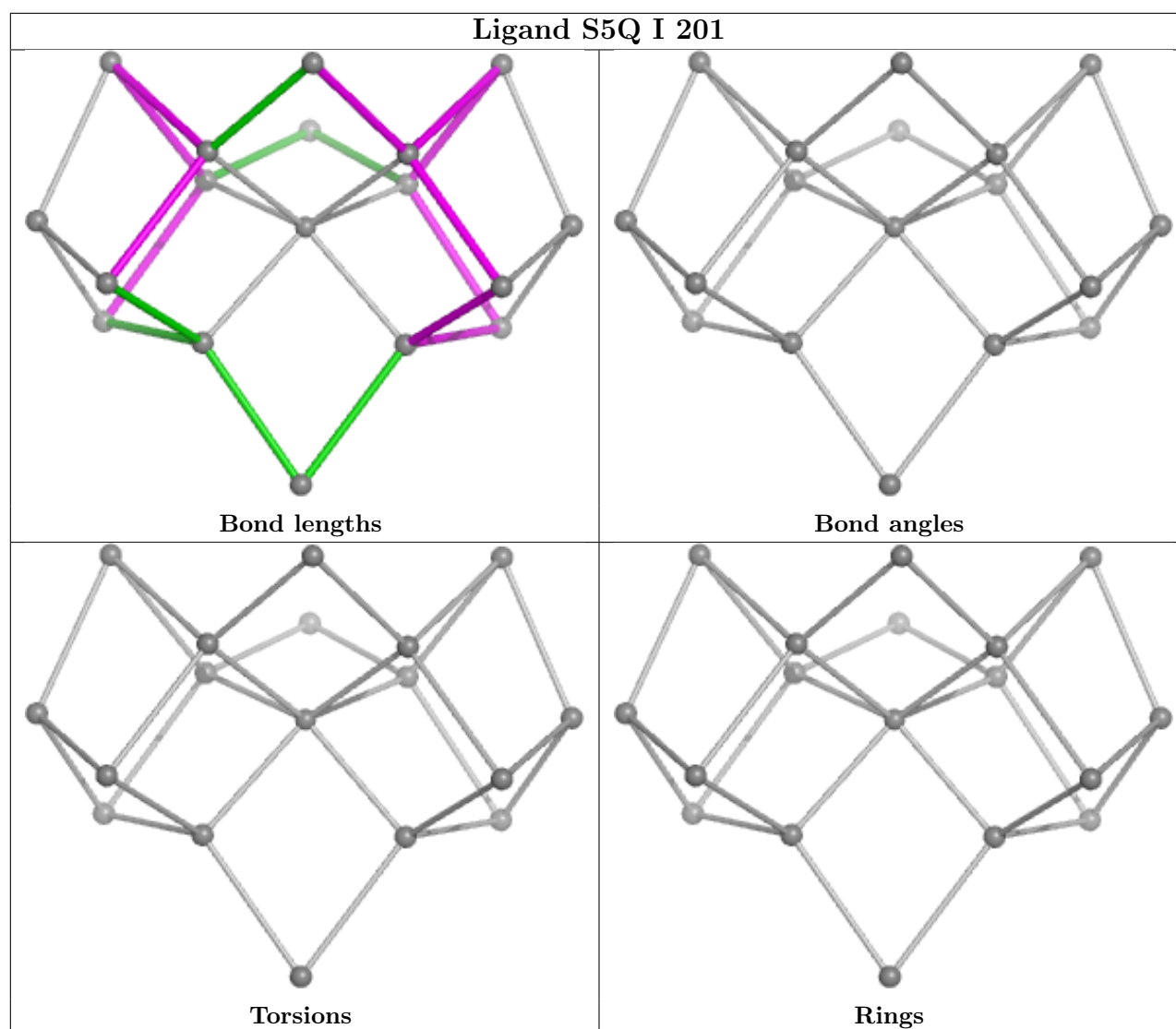
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 4   | C     | 4                |
| 1   | J     | 2                |

The worst 5 of 6 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | J     | 183:THR   | C      | 184:ASN   | N      | 3.52         |
| 1     | C     | 402:SER   | C      | 403:MGN   | N      | 3.12         |
| 1     | C     | 403:MGN   | C      | 404:ARG   | N      | 3.07         |
| 1     | C     | 447:TYR   | C      | 448:GL3   | N      | 3.00         |
| 1     | J     | 22:GLU    | C      | 23:TYR    | N      | 2.59         |