



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 12:22 pm BST

PDB ID : 4MVM  
Title : Structural Basis for Ca<sup>2+</sup> Selectivity of a Voltage-gated Calcium Channel  
Authors : Tang, L.; Gamal El-Din, T.M.; Payandeh, J.; Martinez, G.Q.; Heard, T.M.;  
Scheuer, T.; Zheng, N.; Catterall, W.A.  
Deposited on : 2013-09-24  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

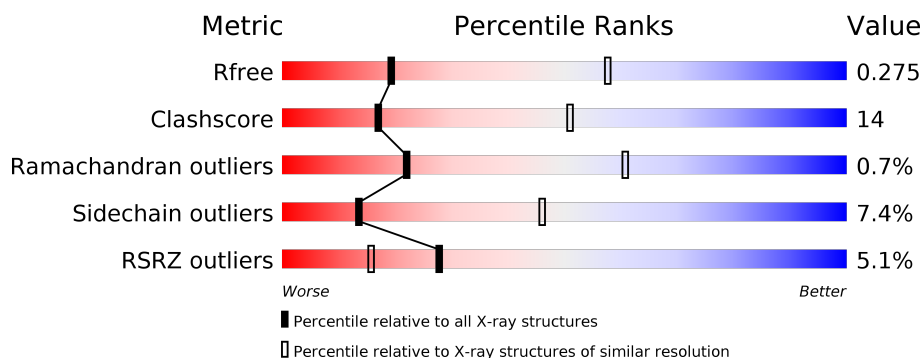
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1133 (3.20-3.20)                                      |
| Clashscore            | 141614                      | 1253 (3.20-3.20)                                      |
| Ramachandran outliers | 138981                      | 1234 (3.20-3.20)                                      |
| Sidechain outliers    | 138945                      | 1233 (3.20-3.20)                                      |
| RSRZ outliers         | 127900                      | 1095 (3.20-3.20)                                      |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 237    | <div> <div>5%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>•</div> <div>8%</div> </div> </div> |
| 1   | B     | 237    | <div> <div>4%</div> <div> <div></div> <div>54%</div> <div>36%</div> <div>•</div> <div>8%</div> </div> </div> |
| 1   | C     | 237    | <div> <div>5%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>•</div> <div>8%</div> </div> </div> |
| 1   | D     | 237    | <div> <div>4%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>•</div> <div>8%</div> </div> </div> |

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 crite-

ria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | PX4  | A     | 1302 | -         | -        | -       | X                |
| 3   | CA   | C     | 1307 | -         | -        | -       | X                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7407 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ion transport protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 219      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1798  | 1224 | 269 | 294 | 11 |         |         |       |
| 1   | B     | 219      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1798  | 1224 | 269 | 294 | 11 |         |         |       |
| 1   | C     | 219      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1798  | 1224 | 269 | 294 | 11 |         |         |       |
| 1   | D     | 219      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1798  | 1224 | 269 | 294 | 11 |         |         |       |

There are 88 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 983     | MET      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 984     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 985     | TYR      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 986     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 987     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 988     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 989     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 990     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 991     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 992     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 993     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 994     | LEU      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 995     | VAL      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 996     | PRO      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 997     | ARG      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 998     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 999     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 1000    | HIS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| A     | 1177    | ASP      | GLU    | CONFLICT       | UNP A8EVM5 |
| A     | 1178    | ASP      | SER    | CONFLICT       | UNP A8EVM5 |
| A     | 1181    | ASN      | MET    | CONFLICT       | UNP A8EVM5 |

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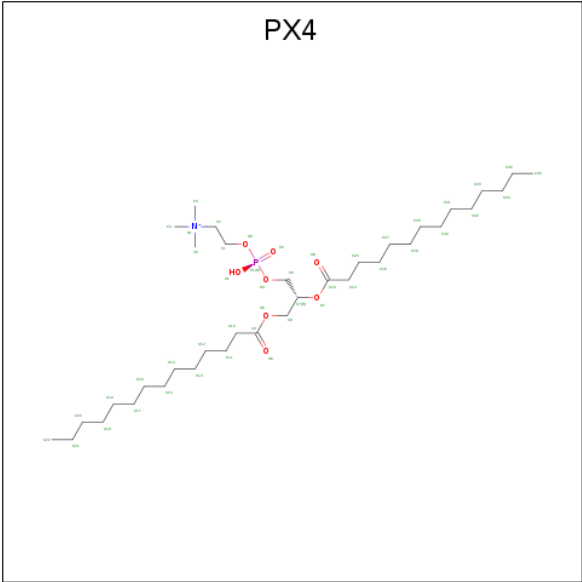
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1217    | CYS      | ILE    | CONFLICT       | UNP A8EVM5 |
| B     | 983     | MET      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 984     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 985     | TYR      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 986     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 987     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 988     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 989     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 990     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 991     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 992     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 993     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 994     | LEU      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 995     | VAL      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 996     | PRO      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 997     | ARG      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 998     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 999     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 1000    | HIS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| B     | 1177    | ASP      | GLU    | CONFLICT       | UNP A8EVM5 |
| B     | 1178    | ASP      | SER    | CONFLICT       | UNP A8EVM5 |
| B     | 1181    | ASN      | MET    | CONFLICT       | UNP A8EVM5 |
| B     | 1217    | CYS      | ILE    | CONFLICT       | UNP A8EVM5 |
| C     | 983     | MET      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 984     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 985     | TYR      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 986     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 987     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 988     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 989     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 990     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 991     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 992     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 993     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 994     | LEU      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 995     | VAL      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 996     | PRO      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 997     | ARG      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 998     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 999     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 1000    | HIS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| C     | 1177    | ASP      | GLU    | CONFLICT       | UNP A8EVM5 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 1178    | ASP      | SER    | CONFLICT       | UNP A8EVM5 |
| C     | 1181    | ASN      | MET    | CONFLICT       | UNP A8EVM5 |
| C     | 1217    | CYS      | ILE    | CONFLICT       | UNP A8EVM5 |
| D     | 983     | MET      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 984     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 985     | TYR      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 986     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 987     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 988     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 989     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 990     | ASP      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 991     | LYS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 992     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 993     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 994     | LEU      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 995     | VAL      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 996     | PRO      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 997     | ARG      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 998     | GLY      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 999     | SER      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 1000    | HIS      | -      | EXPRESSION TAG | UNP A8EVM5 |
| D     | 1177    | ASP      | GLU    | CONFLICT       | UNP A8EVM5 |
| D     | 1178    | ASP      | SER    | CONFLICT       | UNP A8EVM5 |
| D     | 1181    | ASN      | MET    | CONFLICT       | UNP A8EVM5 |
| D     | 1217    | CYS      | ILE    | CONFLICT       | UNP A8EVM5 |

- Molecule 2 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | A     | 1        | Total | C  |   |   | 0       | 0       |
|     |       |          | 6     | 6  |   |   |         |         |
| 2   | A     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | B     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | B     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 21    | 13 | 7 | 1 |         |         |
| 2   | B     | 1        | Total | C  |   |   | 0       | 0       |
|     |       |          | 6     | 6  |   |   |         |         |
| 2   | B     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | C     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | C     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 21    | 13 | 7 | 1 |         |         |
| 2   | C     | 1        | Total | C  |   |   | 0       | 0       |
|     |       |          | 6     | 6  |   |   |         |         |
| 2   | C     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 21    | 13 | 7 | 1 |         |         |
| 2   | C     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | D     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 10    | 3  | 6 | 1 |         |         |
| 2   | D     | 1        | Total | C  | O | P | 0       | 0       |
|     |       |          | 21    | 13 | 7 | 1 |         |         |

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| Mol | Chain | Residues | Atoms                   | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------|---------|---------|
| 2   | D     | 1        | Total C<br>6 6          | 0       | 0       |
| 2   | D     | 1        | Total C O P<br>10 3 6 1 | 0       | 0       |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 3        | Total Ca<br>3 3 | 0       | 0       |
| 3   | C     | 2        | Total Ca<br>2 2 | 0       | 0       |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4   | A     | 6        | Total O<br>6 6 | 0       | 0       |
| 4   | B     | 5        | Total O<br>5 5 | 0       | 0       |
| 4   | C     | 5        | Total O<br>5 5 | 0       | 0       |
| 4   | D     | 6        | Total O<br>6 6 | 0       | 0       |

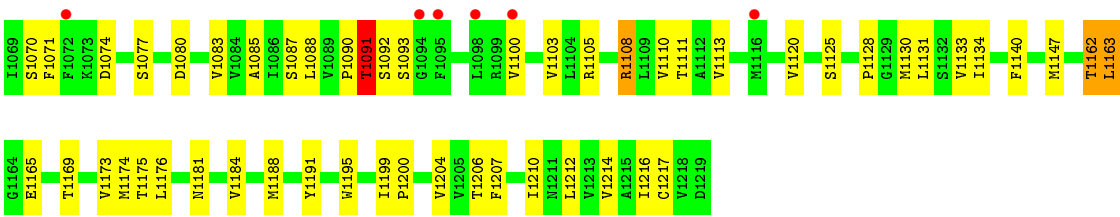


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

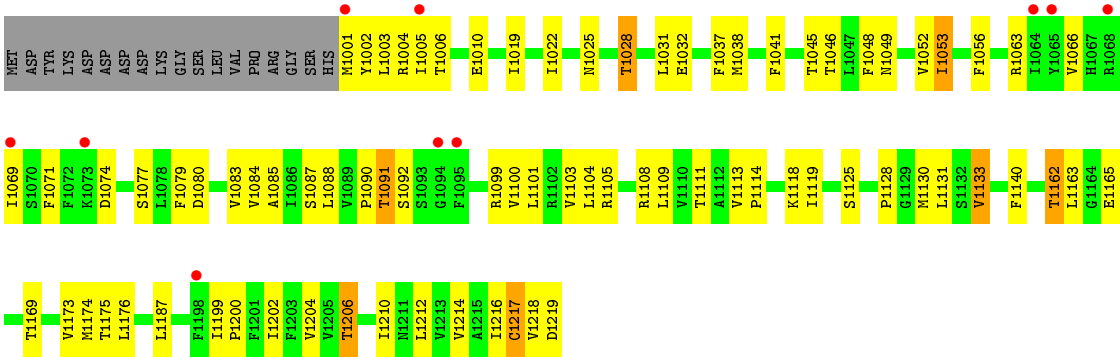
- Chain A:
- 
- 57% 32% 8%
- 5%
- Met ASP TSP TVR LYS ASP ASP ASP ASP ASP LYS GLY SER LEU VAL PRO ARG GLY SER HIS
- Y1001 Y1002 I1005 T1006 E1010 F1017 I1018 I1019 I1020 I1021 I1022 V1023 I1024 N1025 T1028 E1032 T1033 F1037 Q1038 Q1039 S1040 F1041 F1048 I1053 I1058 F1059 I1060 I1061 L1062 R1063 I1064 Y1065 V1066
- I1069 S1070 F1071 F1072 K1073 D1074 S1077 L1078 F1079 V1083 Y1084 A1085 L1086 S1087 L1088 Y1089 P1090 T1091 S1092 S1093 G1094 F1095 E1096 I1097 R1102 V1103 L1104 R1105 L1106 L1109 V1110 T1111 A1112 V1113 P1114 Q1115 M1116 R1117 K1118 L1119 V1120 S1121 A1122 S1125 P1128 F1129 M1130 V1133 I1134 M1137
- F1140 M1147 A1148 T1149 Q1150 F1160 G1161 T1162 L1163 G1164 E1165 T1169 L1170 V1173 M1174 T1175 N1181 V1184 M1188 Y1191 V1196 F1197 F1198 I1199 P1200 F1201 I1202 F1203 V1204 V1205 T1206 F1207 V1208 M1209 I1210 M1211 L1212 V1213 I1216 D1219

- Chain B:
- 
- | Token | Category |
|-------|----------|
| Si070 | Green    |
| F1071 | Green    |
| F1072 | Green    |
| K1073 | Green    |
| D1074 | Green    |
| Si077 | Green    |
| L1078 | Green    |
| F1079 | Green    |
| V1083 | Green    |
| V1084 | Green    |
| A1085 | Green    |
| L1086 | Green    |
| S1087 | Green    |
| L1088 | Green    |
| F1089 | Green    |
| P1090 | Green    |
| T1091 | Green    |
| S1092 | Green    |
| S1093 | Green    |
| G1094 | Green    |
| L1097 | Green    |
| V1100 | Green    |
| L1101 | Green    |
| R1102 | Green    |
| V1103 | Green    |
| L1104 | Green    |
| R1106 | Green    |
| F1107 | Green    |
| R1108 | Green    |
| L1109 | Green    |
| V1110 | Green    |
| T1111 | Green    |
| A1112 | Green    |
| V1113 | Green    |
| P1114 | Green    |
| R1117 | Green    |
| K1118 | Green    |
| L1119 | Green    |
| V1120 | Green    |
| S1121 | Green    |
| A1122 | Green    |
| L1123 | Green    |
| F1124 | Green    |
| S1125 | Green    |
| V1126 | Green    |
| L1127 | Green    |
| P1128 | Green    |
| G1129 | Green    |
| M1130 | Green    |
| L1131 | Green    |
| S1132 | Green    |
| V1133 | Green    |
| V1137 | Green    |
| F1140 | Green    |
| F1144 | Green    |
| M1147 | Green    |
| Q1150 | Green    |
| F1160 | Green    |
| G1161 | Green    |
| T1162 | Green    |
| L1163 | Green    |
| K1164 | Green    |
| E1165 | Green    |
| T1169 | Green    |
| V1173 | Green    |
| M1174 | Green    |
| L1175 | Green    |
| L1176 | Green    |
| D1177 | Green    |
| D1178 | Green    |
| V1184 | Green    |
| R1185 | Green    |
| P1186 | Green    |
| L1187 | Green    |
| M1188 | Green    |
| Y1191 | Green    |
| W1195 | Green    |
| L1199 | Green    |
| P1200 | Green    |
| F1201 | Green    |
| L1202 | Green    |
| F1203 | Green    |
| V1204 | Green    |
| V1205 | Green    |
| T1206 | Green    |
| M1209 | Green    |
| L1210 | Green    |
| M1211 | Green    |
| L1212 | Green    |
| L1213 | Green    |
| A1214 | Green    |
| A1215 | Green    |
| L1216 | Green    |
| G1217 | Green    |
| V1218 | Green    |
| D1219 | Green    |
| ME1   | Grey     |
| ASP   | Grey     |
| TVR   | Grey     |
| LVS   | Grey     |
| ASP   | Grey     |
| ASP   | Grey     |
| ASP   | Grey     |
| LVS   | Grey     |
| GLY   | Grey     |
| SER   | Grey     |
| LEU   | Grey     |
| VAL   | Grey     |
| PRQ   | Grey     |
| ARG   | Grey     |
| GLY   | Grey     |
| SER   | Grey     |
| HIS   | Grey     |
| F1001 | Grey     |
| V1002 | Grey     |
| R1003 | Grey     |
| L1004 | Grey     |
| I1005 | Yellow   |
| T1006 | Yellow   |
| V1009 | Yellow   |
| E1010 | Yellow   |
| T1015 | Yellow   |
| I1019 | Yellow   |
| V1020 | Yellow   |
| M1025 | Yellow   |
| T1028 | Yellow   |
| M1029 | Yellow   |
| G1030 | Yellow   |
| L1031 | Yellow   |
| E1032 | Yellow   |
| T1033 | Yellow   |
| M1038 | Yellow   |
| F1048 | Yellow   |
| V1052 | Yellow   |
| L1053 | Yellow   |
| I1058 | Yellow   |
| L1061 | Yellow   |
| L1062 | Yellow   |
| R1063 | Yellow   |
| L1064 | Yellow   |
| V1065 | Yellow   |
| V1066 | Yellow   |
| H1067 | Yellow   |
| R1068 | Yellow   |
| T1069 | Yellow   |

- Chain C:
- 
- 5% 61% 29% 8%
- MET ASP TYR LYS ASP ASP ASP ASP ASP GLY SER LEU VAL PRO ARG GLY SER HIS M1001 I1005 T1006 E1010 F1017 I1018 I1019 Y1020 L1021 L1022 M1025 T1028 L1031 E1032 K1035 M1038 Q1039 S1040 F1041 I1053 F1056 I1057 L1058 L1062 R1063 I1064 Y1065 V1066 H1067 L1068



● Molecule 1: Ion transport protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 177.46Å 177.89Å 130.89Å<br>90.00° 132.54° 90.00°                                      | Depositor        |
| Resolution (Å)  | 29.88 – 3.20<br>29.88 – 3.20  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.7 (29.88-3.20)<br>95.5 (29.88-3.20)  | Depositor<br>EDS |
| $R_{merge}$   | 0.90  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.84 (at 3.18Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.2_1309)  | Depositor        |
| R, $R_{free}$   | 0.254 , 0.275<br>0.254 , 0.275  | Depositor<br>DCC |
| $R_{free}$ test set   | 2404 reflections (5.06%)  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 97.6  | Xtriage          |
| Anisotropy  | 0.405   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 77.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$                           | Xtriage          |
| Estimated twinning fraction   | 0.438 for k,h,-1/2*h-1/2*k-l<br>0.427 for -k,-h,-1/2*h+1/2*k-l<br>0.427 for h,-k,-h-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 7407  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 103.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PX4

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     | 0.69         | 0/1849      | 0.77        | 1/2517 (0.0%)  |
| 1   | B     | 0.69         | 0/1849      | 0.76        | 0/2517         |
| 1   | C     | 0.71         | 0/1849      | 0.77        | 0/2517         |
| 1   | D     | 0.70         | 0/1849      | 0.74        | 0/2517         |
| All | All   | 0.70         | 0/7396      | 0.76        | 1/10068 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1   | A     | 1188 | MET  | CG-SD-CE | 5.16 | 108.45      | 100.20   |

There are no chirality outliers.

There are no planarity outliers.

### 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   | A     | 1798  | 0        | 1863     | 56      | 0            |
| 1   | B     | 1798  | 0        | 1863     | 58      | 0            |
| 1   | C     | 1798  | 0        | 1863     | 54      | 0            |
| 1   | D     | 1798  | 0        | 1863     | 49      | 0            |
| 2   | A     | 26    | 0        | 21       | 0       | 0            |
| 2   | B     | 47    | 0        | 40       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | C     | 68    | 0        | 59       | 4       | 0            |
| 2   | D     | 47    | 0        | 40       | 1       | 0            |
| 3   | A     | 3     | 0        | 0        | 0       | 0            |
| 3   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 6     | 0        | 0        | 2       | 0            |
| 4   | B     | 5     | 0        | 0        | 2       | 0            |
| 4   | C     | 5     | 0        | 0        | 1       | 0            |
| 4   | D     | 6     | 0        | 0        | 0       | 0            |
| All | All   | 7407  | 0        | 7612     | 210     | 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 14.

The worst 5 of 210 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:C:1162:THR:HG22 | 1:C:1165:GLU:H    | 1.38                     | 0.88              |
| 1:D:1133:VAL:HG11 | 1:D:1212:LEU:HD12 | 1.60                     | 0.83              |
| 1:D:1162:THR:HG22 | 1:D:1165:GLU:H    | 1.43                     | 0.82              |
| 1:C:1175:THR:HB   | 1:D:1176:LEU:HD13 | 1.60                     | 0.80              |
| 1:B:1162:THR:HG22 | 1:B:1165:GLU:H    | 1.46                     | 0.79              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 217/237 (92%) | 201 (93%) | 15 (7%) | 1 (0%)   | 29          | 67 |
| 1   | B     | 217/237 (92%) | 199 (92%) | 17 (8%) | 1 (0%)   | 29          | 67 |
| 1   | C     | 217/237 (92%) | 203 (94%) | 12 (6%) | 2 (1%)   | 17          | 56 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | D     | 217/237 (92%) | 195 (90%) | 20 (9%) | 2 (1%)   | 17          | 56 |
| All | All   | 868/948 (92%) | 798 (92%) | 64 (7%) | 6 (1%)   | 22          | 61 |

5 of 6 Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1091 | THR  |
| 1   | B     | 1091 | THR  |
| 1   | C     | 1091 | THR  |
| 1   | C     | 1093 | SER  |
| 1   | D     | 1091 | THR  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 202/218 (93%) | 187 (93%) | 15 (7%)  | 13          | 46 |
| 1   | B     | 202/218 (93%) | 185 (92%) | 17 (8%)  | 11          | 39 |
| 1   | C     | 202/218 (93%) | 190 (94%) | 12 (6%)  | 19          | 54 |
| 1   | D     | 202/218 (93%) | 186 (92%) | 16 (8%)  | 12          | 43 |
| All | All   | 808/872 (93%) | 748 (93%) | 60 (7%)  | 13          | 46 |

5 of 60 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1162 | THR  |
| 1   | C     | 1028 | THR  |
| 1   | D     | 1162 | THR  |
| 1   | B     | 1206 | THR  |
| 1   | C     | 1035 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1150 | GLN  |
| 1   | D     | 1150 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 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$ |
| 2   | PX4  | B     | 1304 | -    | 9,9,45       | 0.58 | 0           | 11,12,53    | 1.45 | 2 (18%)     |
| 2   | PX4  | C     | 1302 | -    | 20,20,45     | 1.34 | 2 (10%)     | 22,24,53    | 1.91 | 2 (9%)      |
| 2   | PX4  | D     | 1304 | -    | 9,9,45       | 0.59 | 0           | 11,12,53    | 1.39 | 2 (18%)     |
| 2   | PX4  | A     | 1302 | -    | 5,5,45       | 0.43 | 0           | 4,4,53      | 0.50 | 0           |
| 2   | PX4  | D     | 1301 | -    | 9,9,45       | 0.66 | 0           | 11,12,53    | 1.34 | 1 (9%)      |
| 2   | PX4  | C     | 1305 | -    | 9,9,45       | 0.59 | 0           | 11,12,53    | 1.55 | 3 (27%)     |
| 2   | PX4  | A     | 1301 | -    | 9,9,45       | 0.59 | 0           | 11,12,53    | 1.19 | 1 (9%)      |
| 2   | PX4  | B     | 1301 | -    | 9,9,45       | 0.45 | 0           | 11,12,53    | 1.29 | 1 (9%)      |
| 2   | PX4  | C     | 1301 | -    | 9,9,45       | 0.73 | 0           | 11,12,53    | 1.55 | 2 (18%)     |
| 2   | PX4  | C     | 1304 | -    | 20,20,45     | 1.29 | 2 (10%)     | 22,24,53    | 1.92 | 3 (13%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | PX4  | D     | 1302 | -    | 20,20,45     | 1.26 | 2 (10%)  | 22,24,53    | 2.02 | 2 (9%)   |
| 2   | PX4  | B     | 1302 | -    | 20,20,45     | 1.36 | 3 (15%)  | 22,24,53    | 1.92 | 2 (9%)   |
| 2   | PX4  | D     | 1303 | -    | 5,5,45       | 0.49 | 0        | 4,4,53      | 0.53 | 0        |
| 2   | PX4  | B     | 1303 | -    | 5,5,45       | 0.45 | 0        | 4,4,53      | 0.42 | 0        |
| 2   | PX4  | C     | 1303 | -    | 5,5,45       | 0.38 | 0        | 4,4,53      | 0.20 | 0        |
| 2   | PX4  | A     | 1303 | -    | 9,9,45       | 0.75 | 0        | 11,12,53    | 1.24 | 2 (18%)  |

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 |
|-----|------|-------|------|------|---------|-------------|-------|
| 2   | PX4  | B     | 1304 | -    | -       | 7/8/8/49    | -     |
| 2   | PX4  | C     | 1302 | -    | -       | 10/22/22/49 | -     |
| 2   | PX4  | D     | 1304 | -    | -       | 7/8/8/49    | -     |
| 2   | PX4  | A     | 1302 | -    | -       | 1/3/3/49    | -     |
| 2   | PX4  | D     | 1301 | -    | -       | 5/8/8/49    | -     |
| 2   | PX4  | C     | 1305 | -    | -       | 4/8/8/49    | -     |
| 2   | PX4  | A     | 1301 | -    | -       | 5/8/8/49    | -     |
| 2   | PX4  | B     | 1301 | -    | -       | 5/8/8/49    | -     |
| 2   | PX4  | C     | 1301 | -    | -       | 5/8/8/49    | -     |
| 2   | PX4  | C     | 1304 | -    | -       | 9/22/22/49  | -     |
| 2   | PX4  | D     | 1302 | -    | -       | 8/22/22/49  | -     |
| 2   | PX4  | B     | 1302 | -    | -       | 7/22/22/49  | -     |
| 2   | PX4  | D     | 1303 | -    | -       | 1/3/3/49    | -     |
| 2   | PX4  | B     | 1303 | -    | -       | 0/3/3/49    | -     |
| 2   | PX4  | C     | 1303 | -    | -       | 3/3/3/49    | -     |
| 2   | PX4  | A     | 1303 | -    | -       | 4/8/8/49    | -     |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | B     | 1302 | PX4  | O6-C9 | 4.68 | 1.36        | 1.22     |
| 2   | C     | 1302 | PX4  | O6-C9 | 4.51 | 1.35        | 1.22     |
| 2   | C     | 1304 | PX4  | O6-C9 | 4.49 | 1.35        | 1.22     |
| 2   | D     | 1302 | PX4  | O6-C9 | 4.33 | 1.35        | 1.22     |
| 2   | C     | 1302 | PX4  | O5-C9 | 2.58 | 1.40        | 1.33     |



The worst 5 of 23 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | D     | 1302 | PX4  | O5-C9-O6  | -7.79 | 103.93      | 123.59   |
| 2   | C     | 1302 | PX4  | O5-C9-O6  | -7.13 | 105.59      | 123.59   |
| 2   | B     | 1302 | PX4  | O5-C9-O6  | -7.08 | 105.73      | 123.59   |
| 2   | C     | 1304 | PX4  | O5-C9-O6  | -6.95 | 106.05      | 123.59   |
| 2   | B     | 1302 | PX4  | O6-C9-C10 | -4.43 | 106.45      | 123.73   |

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

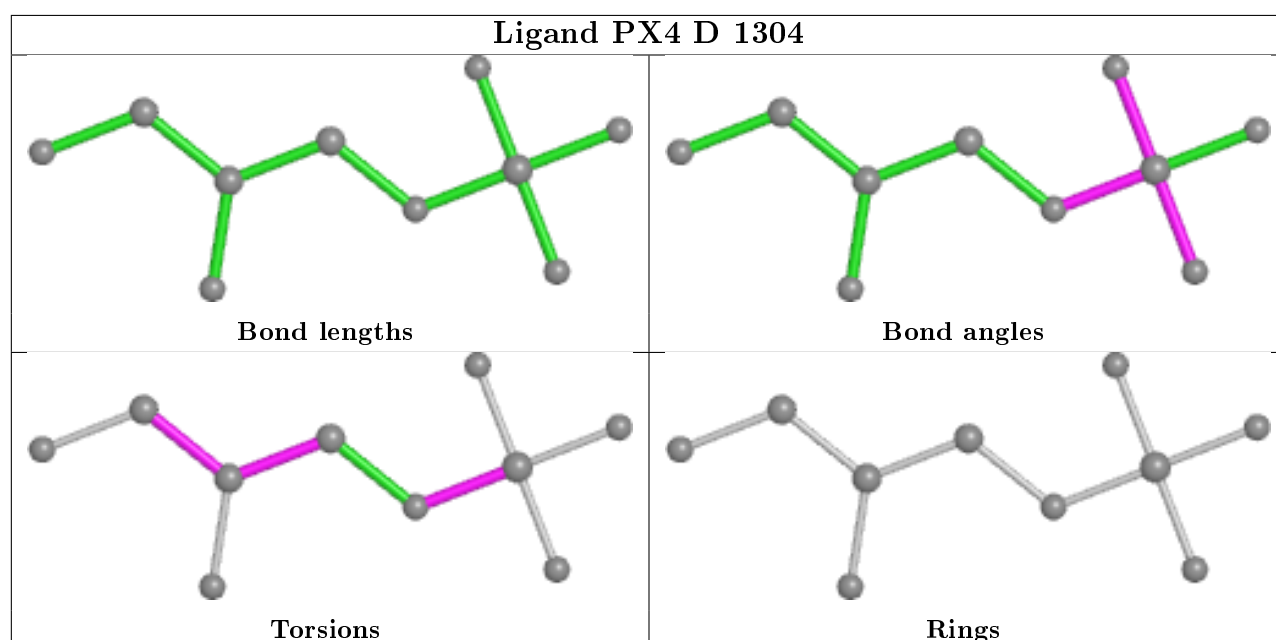
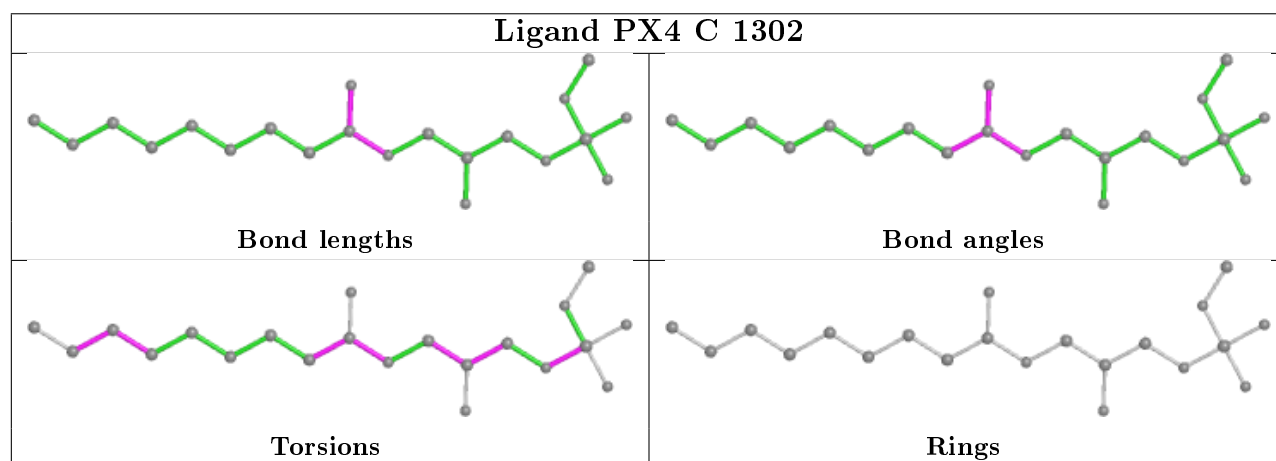
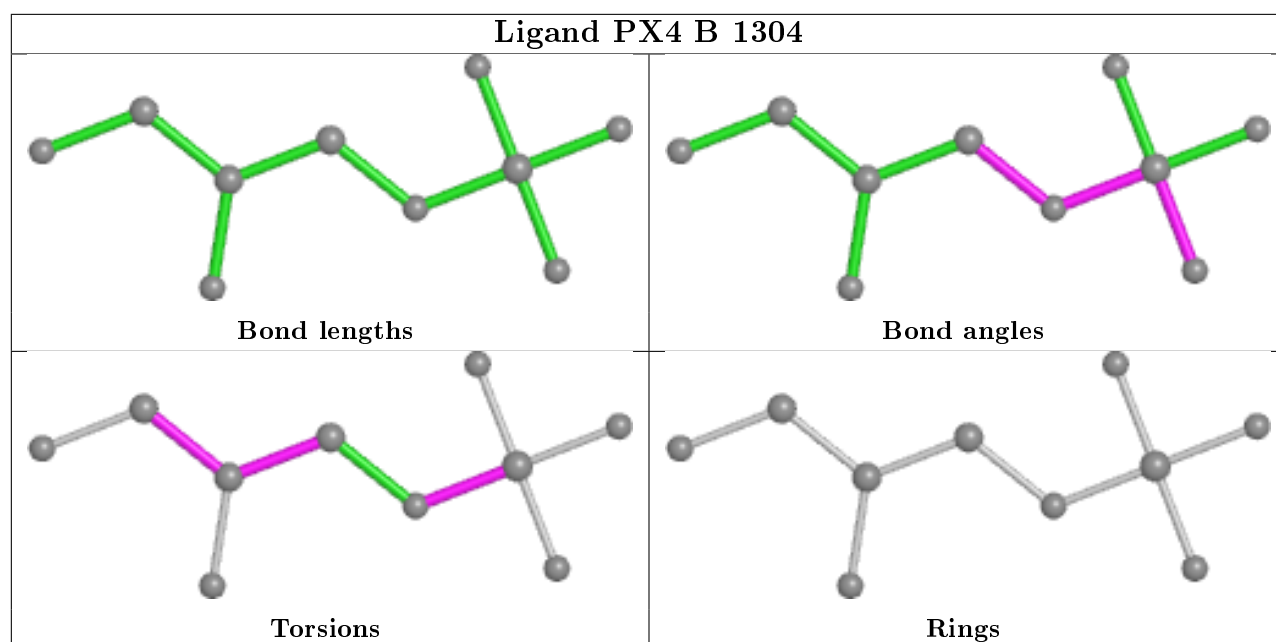
| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 2   | B     | 1304 | PX4  | C6-O4-P1-O1 |
| 2   | B     | 1304 | PX4  | C6-O4-P1-O2 |
| 2   | B     | 1304 | PX4  | C6-O4-P1-O3 |
| 2   | B     | 1304 | PX4  | C6-C7-C8-O5 |
| 2   | C     | 1302 | PX4  | C6-O4-P1-O1 |

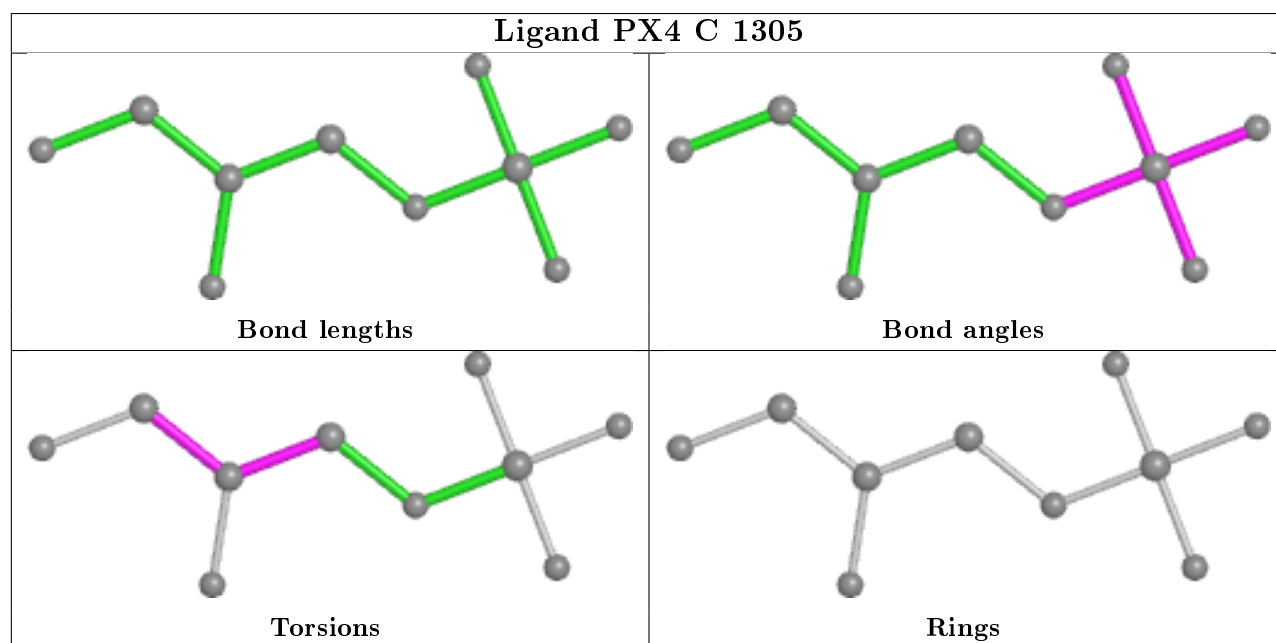
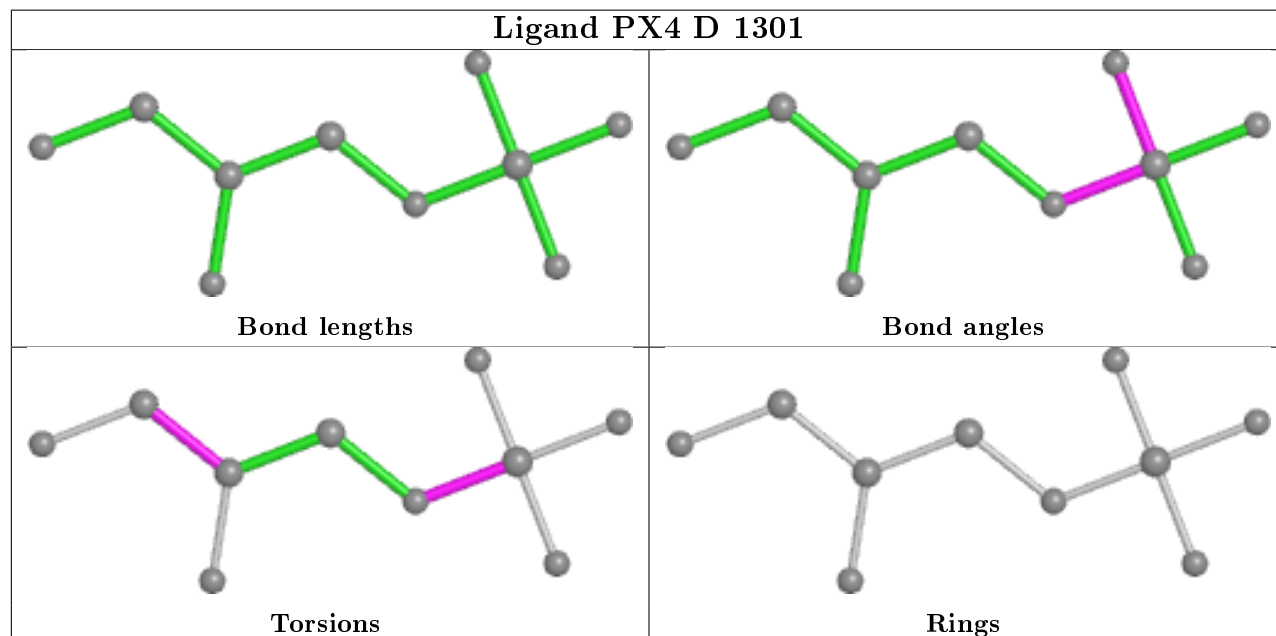
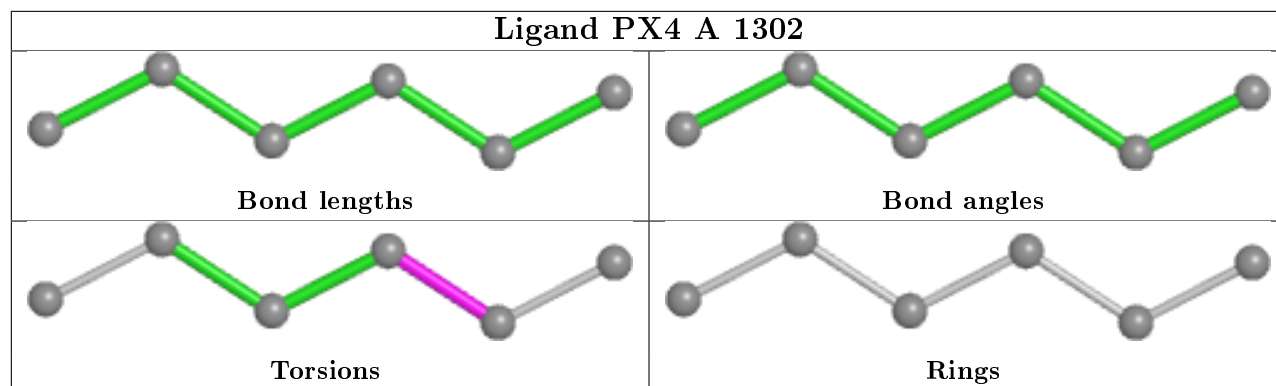
There are no ring outliers.

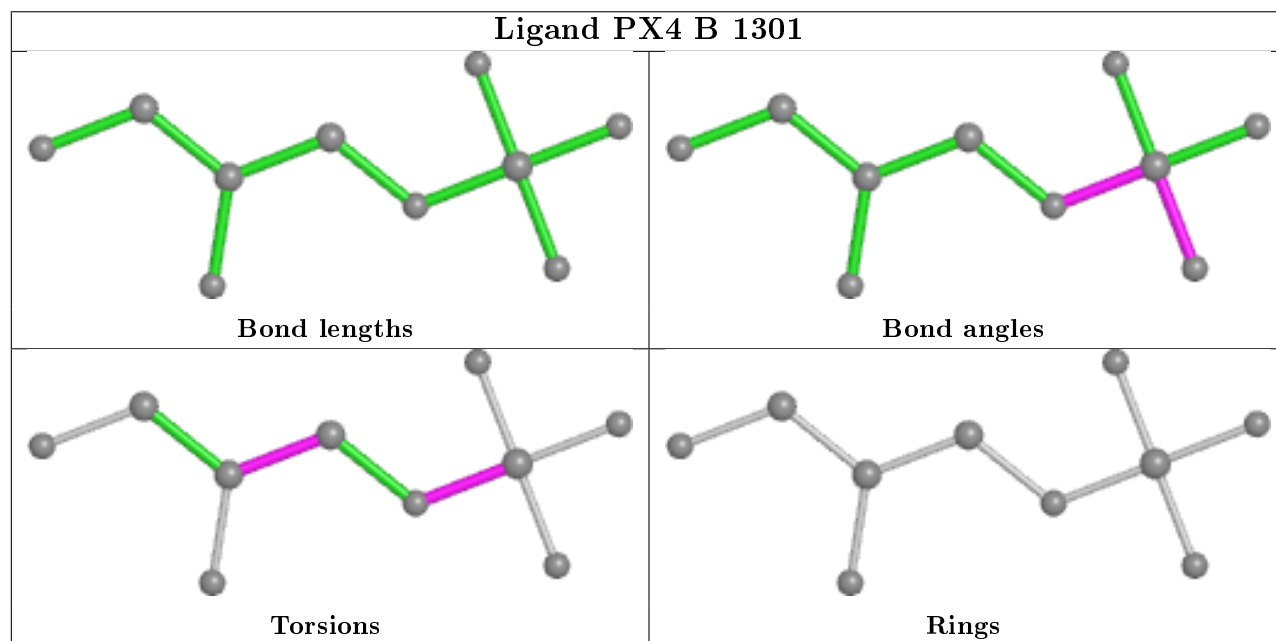
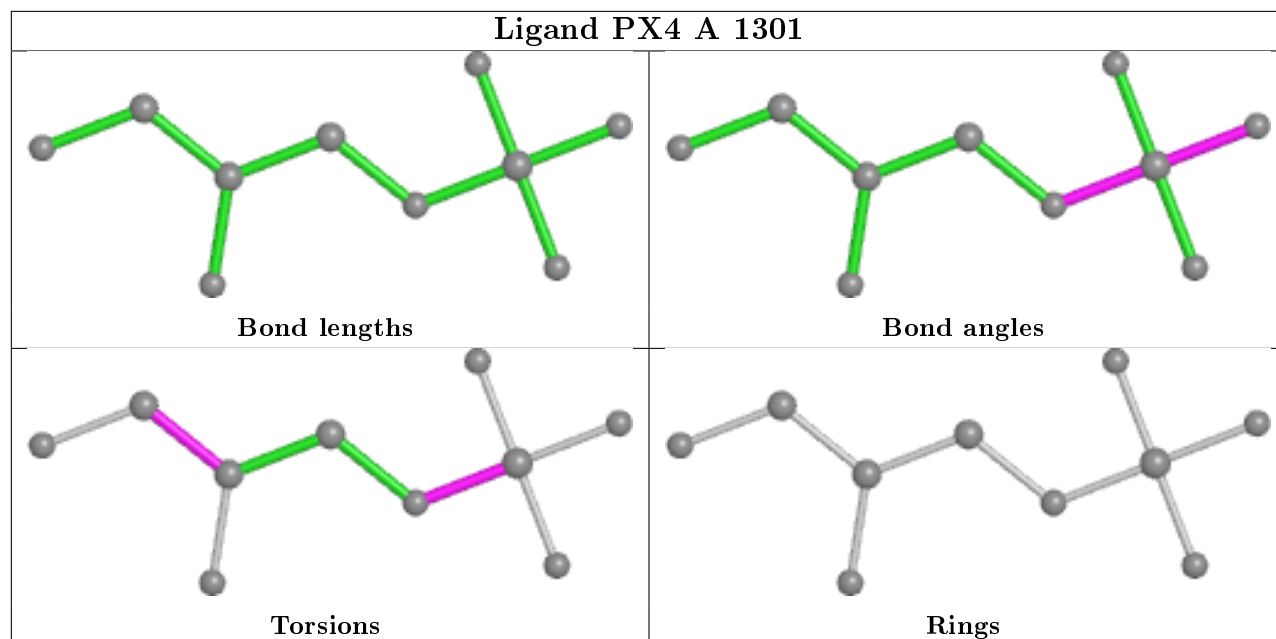
4 monomers are involved in 8 short contacts:

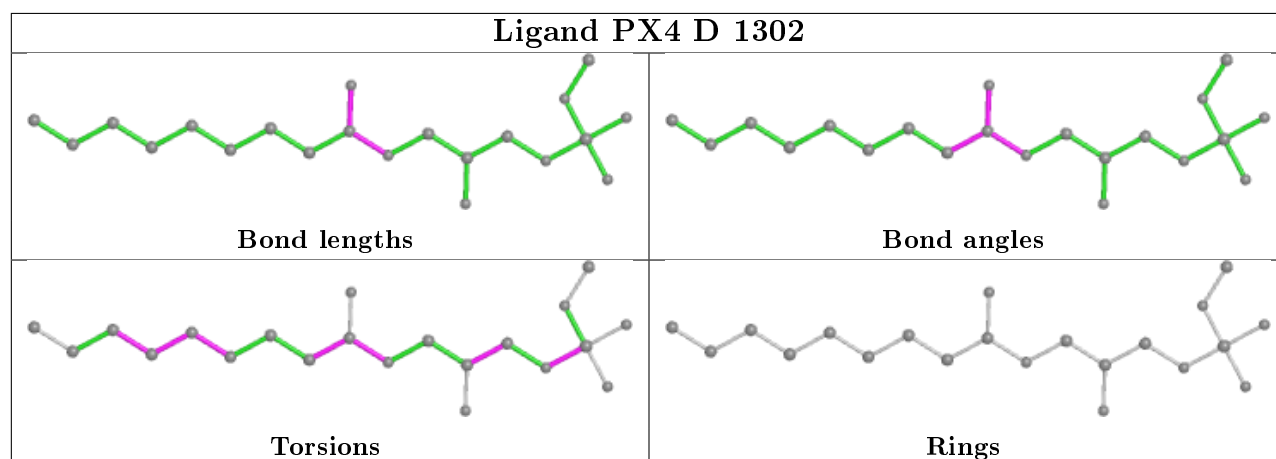
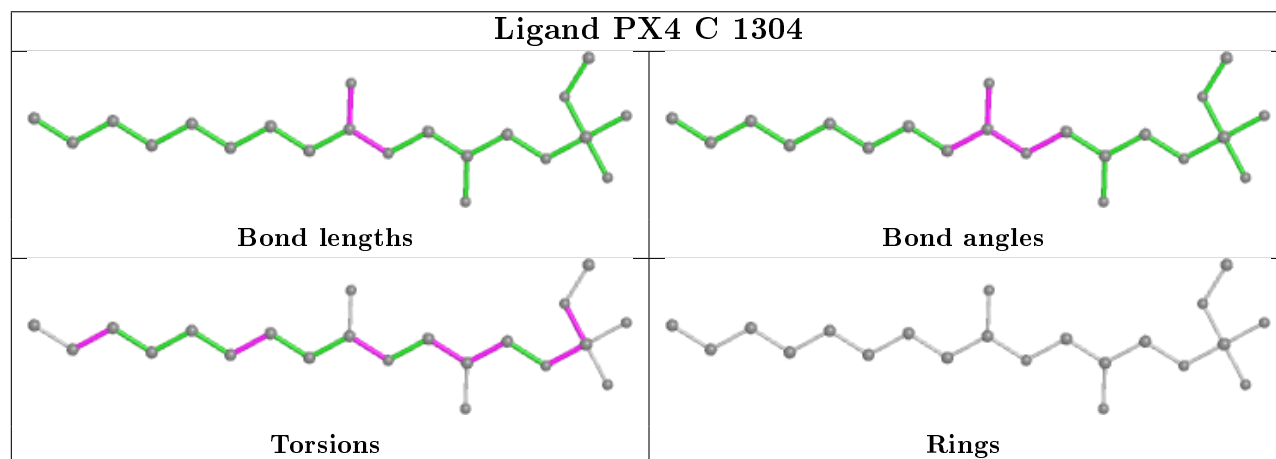
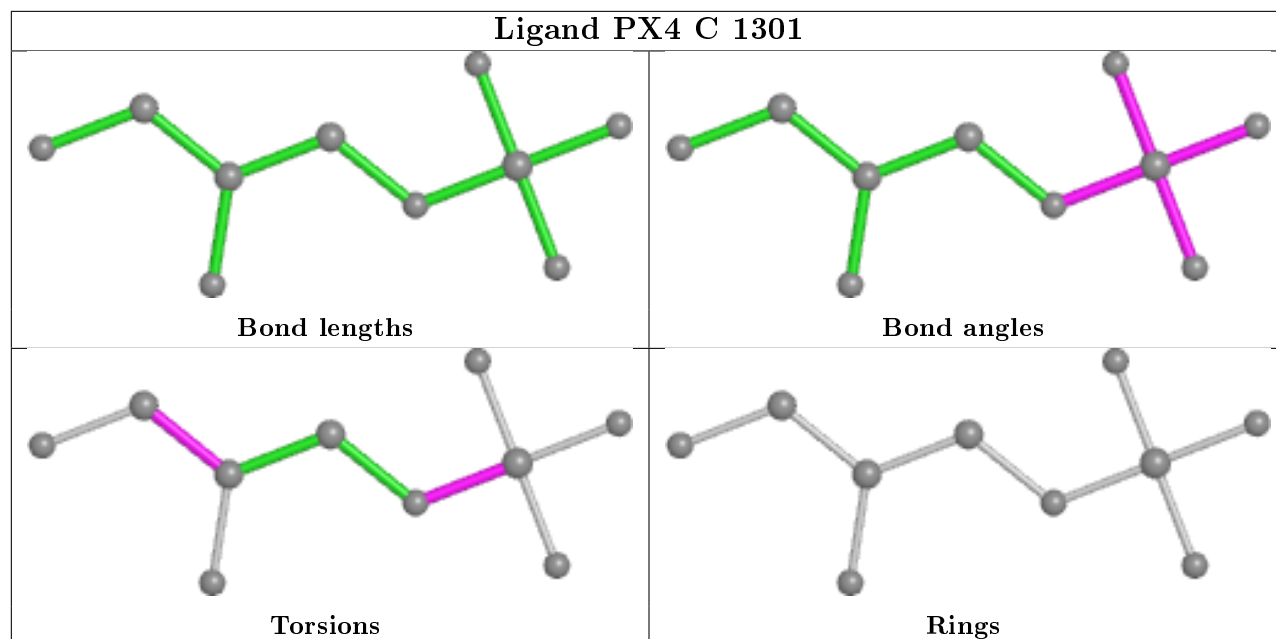
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | C     | 1302 | PX4  | 2       | 0            |
| 2   | C     | 1304 | PX4  | 2       | 0            |
| 2   | D     | 1302 | PX4  | 1       | 0            |
| 2   | B     | 1302 | PX4  | 3       | 0            |

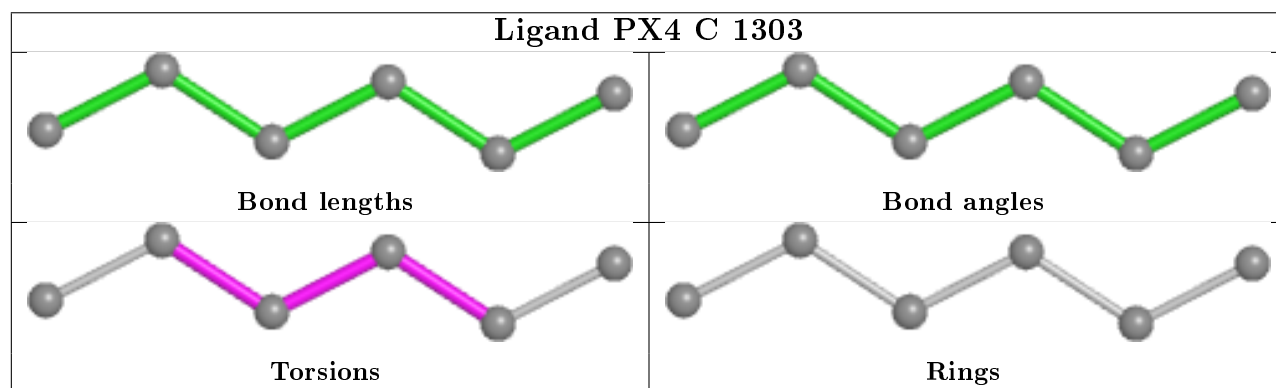
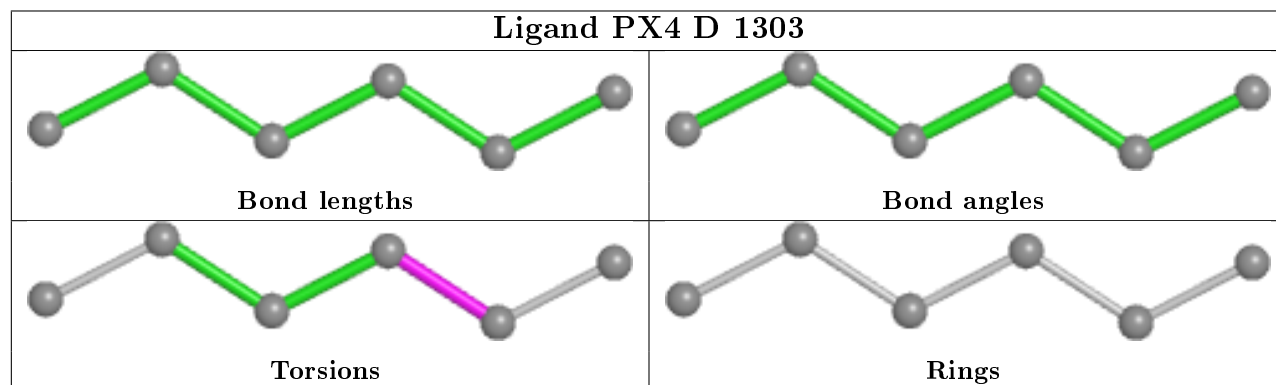
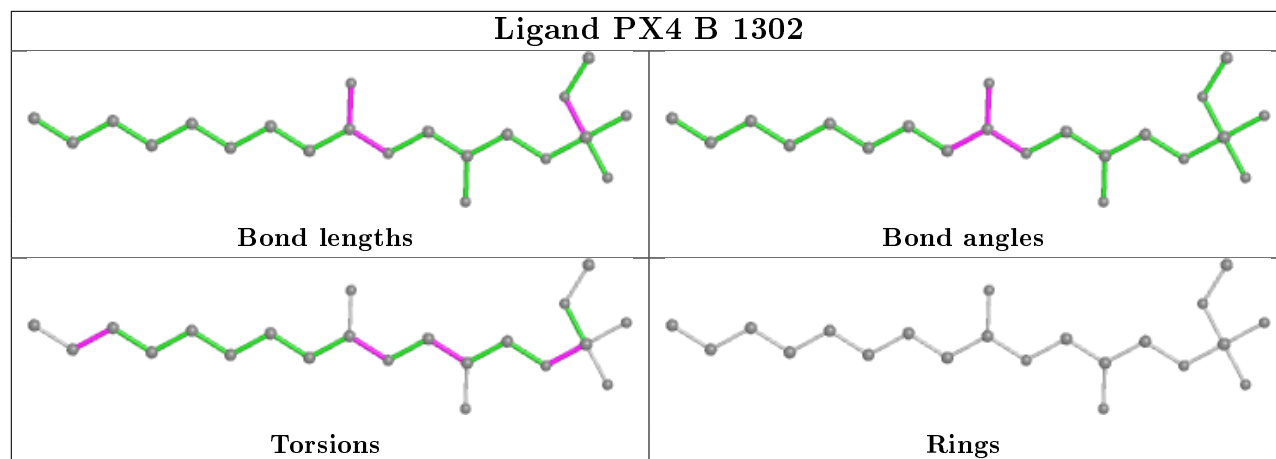
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

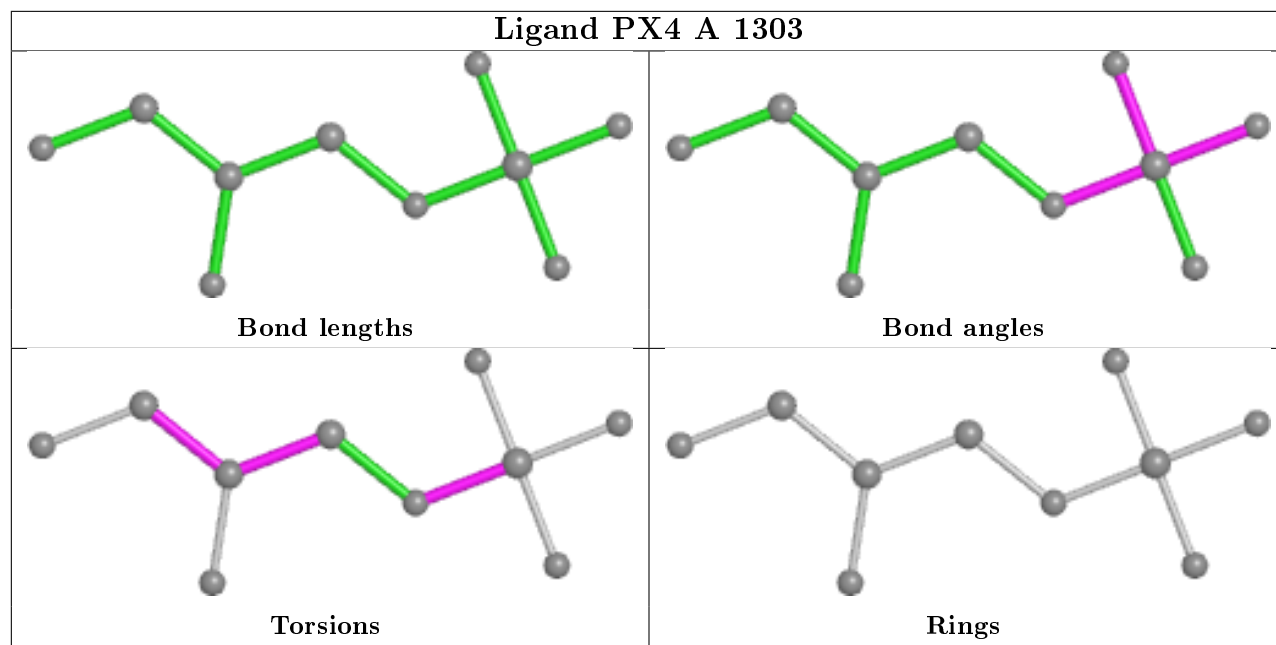












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 219/237 (92%) | 0.59   | 13 (5%) | 22 13 | 48, 105, 147, 170     | 0     |
| 1   | B     | 219/237 (92%) | 0.55   | 10 (4%) | 32 20 | 50, 107, 143, 166     | 0     |
| 1   | C     | 219/237 (92%) | 0.60   | 12 (5%) | 25 14 | 49, 108, 146, 168     | 0     |
| 1   | D     | 219/237 (92%) | 0.64   | 10 (4%) | 32 20 | 49, 111, 150, 168     | 0     |
| All | All   | 876/948 (92%) | 0.59   | 45 (5%) | 28 16 | 48, 108, 147, 170     | 0     |

The worst 5 of 45 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 1094 | GLY  | 7.1  |
| 1   | D     | 1095 | PHE  | 6.6  |
| 1   | C     | 1065 | TYR  | 4.6  |
| 1   | B     | 1065 | TYR  | 3.9  |
| 1   | A     | 1095 | PHE  | 3.4  |

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

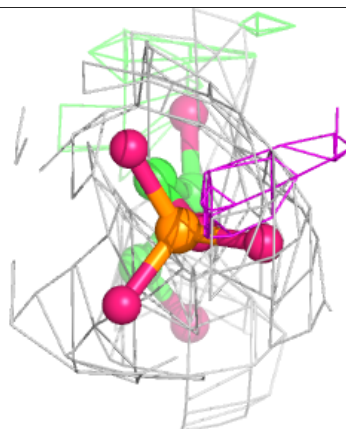
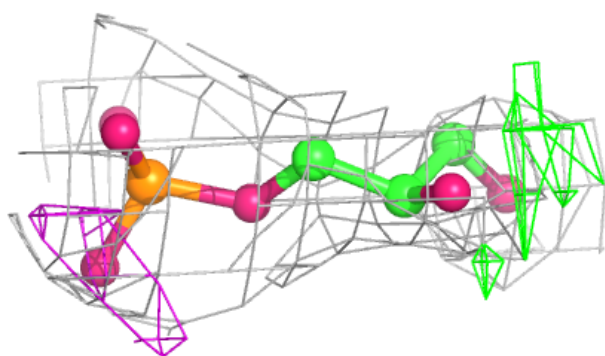
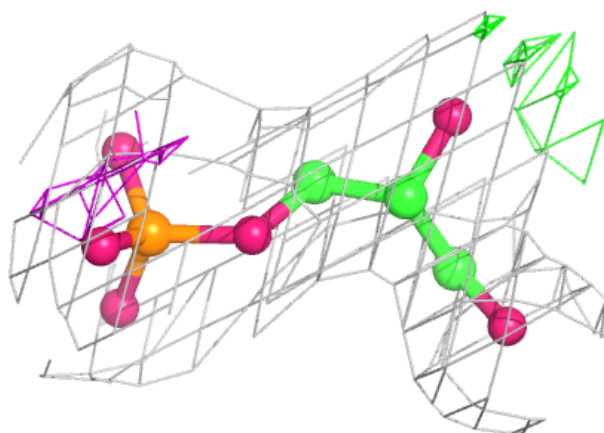


| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | CA   | A     | 1305 | 1/1   | 0.27 | 0.29 | 111,111,111,111             | 0     |
| 3   | CA   | A     | 1306 | 1/1   | 0.34 | 0.33 | 120,120,120,120             | 0     |
| 2   | PX4  | D     | 1304 | 10/46 | 0.74 | 0.24 | 92,114,125,128              | 0     |
| 2   | PX4  | C     | 1301 | 10/46 | 0.75 | 0.20 | 67,90,109,128               | 0     |
| 2   | PX4  | C     | 1305 | 10/46 | 0.77 | 0.21 | 80,105,123,125              | 0     |
| 2   | PX4  | C     | 1304 | 21/46 | 0.77 | 0.27 | 70,82,102,109               | 0     |
| 2   | PX4  | A     | 1302 | 6/46  | 0.78 | 0.45 | 56,63,64,70                 | 0     |
| 2   | PX4  | B     | 1304 | 10/46 | 0.79 | 0.22 | 92,106,120,124              | 0     |
| 2   | PX4  | A     | 1301 | 10/46 | 0.79 | 0.23 | 69,84,118,135               | 0     |
| 3   | CA   | C     | 1307 | 1/1   | 0.79 | 0.45 | 136,136,136,136             | 0     |
| 2   | PX4  | C     | 1303 | 6/46  | 0.79 | 0.34 | 58,63,71,74                 | 0     |
| 2   | PX4  | D     | 1301 | 10/46 | 0.79 | 0.19 | 72,89,113,134               | 0     |
| 2   | PX4  | B     | 1301 | 10/46 | 0.81 | 0.19 | 62,87,114,130               | 0     |
| 2   | PX4  | A     | 1303 | 10/46 | 0.82 | 0.20 | 90,104,126,126              | 0     |
| 2   | PX4  | D     | 1302 | 21/46 | 0.82 | 0.27 | 66,80,92,99                 | 0     |
| 2   | PX4  | B     | 1302 | 21/46 | 0.84 | 0.29 | 67,79,97,102                | 0     |
| 2   | PX4  | C     | 1302 | 21/46 | 0.84 | 0.25 | 70,80,100,106               | 0     |
| 2   | PX4  | B     | 1303 | 6/46  | 0.88 | 0.31 | 51,65,69,71                 | 0     |
| 2   | PX4  | D     | 1303 | 6/46  | 0.88 | 0.37 | 58,62,66,71                 | 0     |
| 3   | CA   | C     | 1306 | 1/1   | 0.91 | 0.17 | 78,78,78,78                 | 0     |
| 3   | CA   | A     | 1304 | 1/1   | 0.95 | 0.09 | 80,80,80,80                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

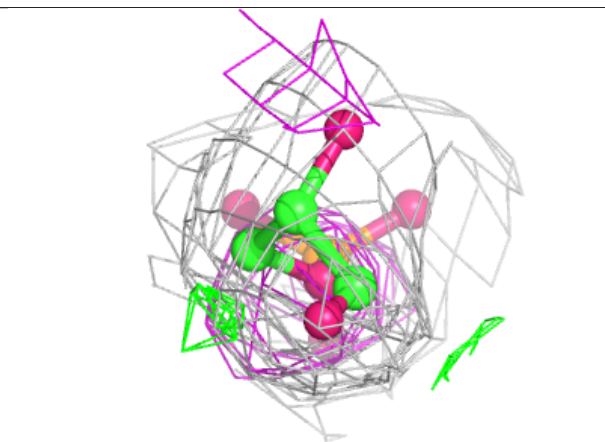
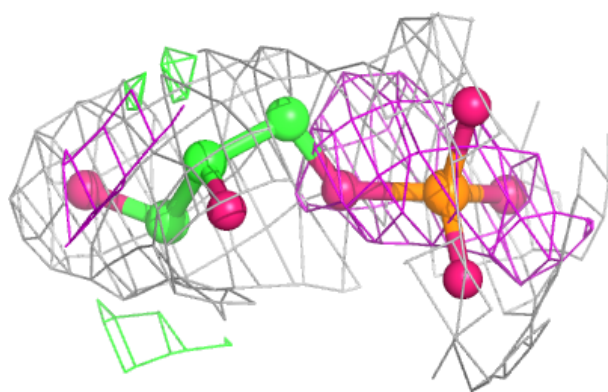
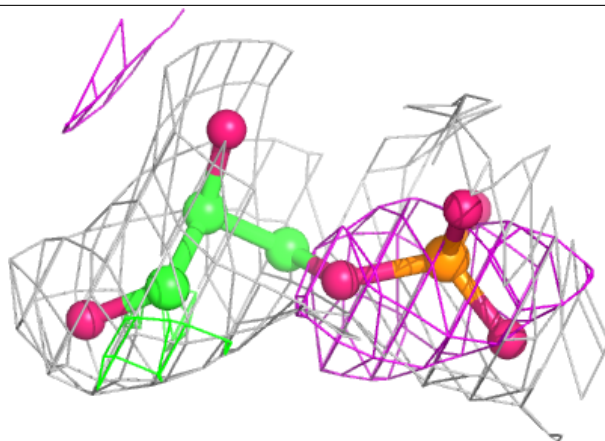
**Electron density around PX4 D 1304:**

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

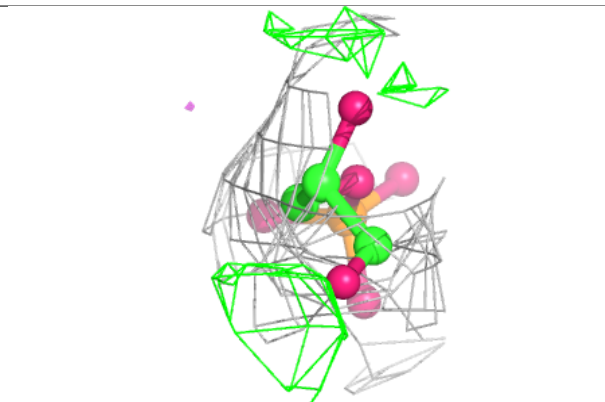
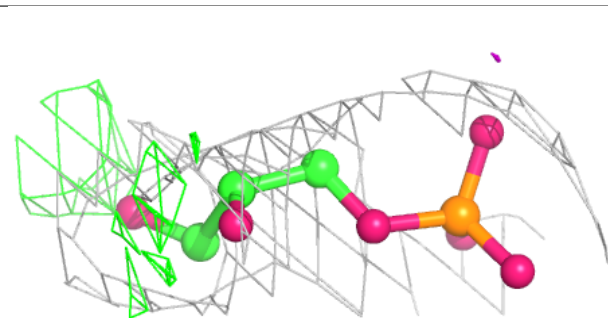
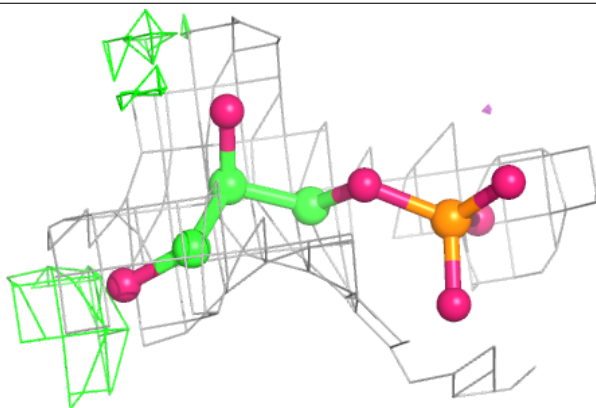


**Electron density around PX4 C 1301:**

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

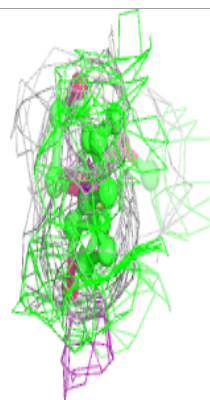
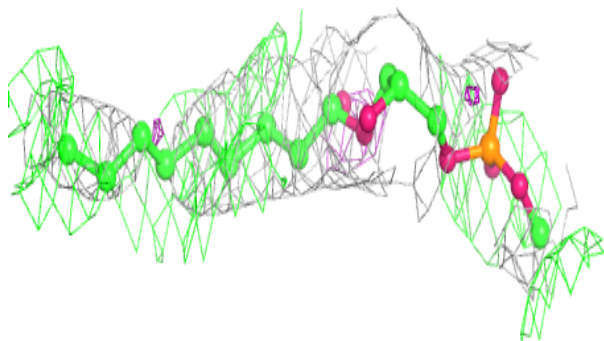
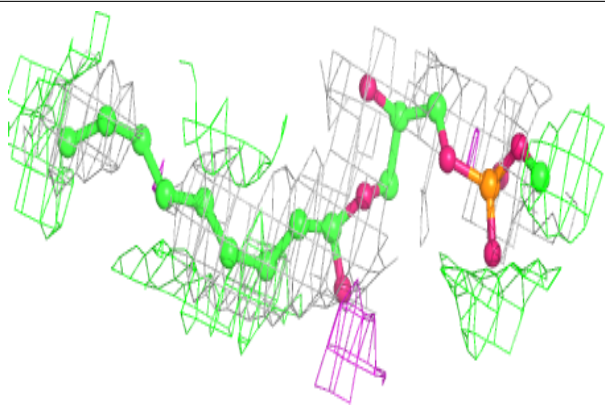
**Electron density around PX4 C 1305:**

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

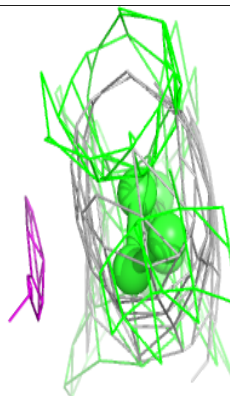
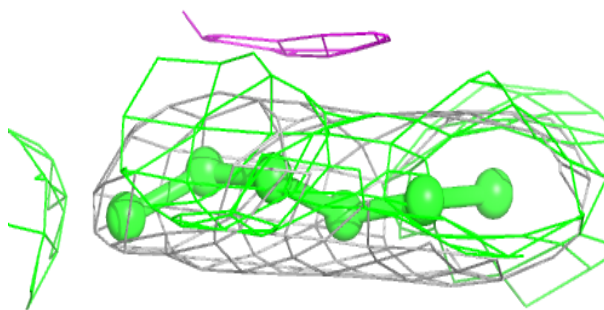
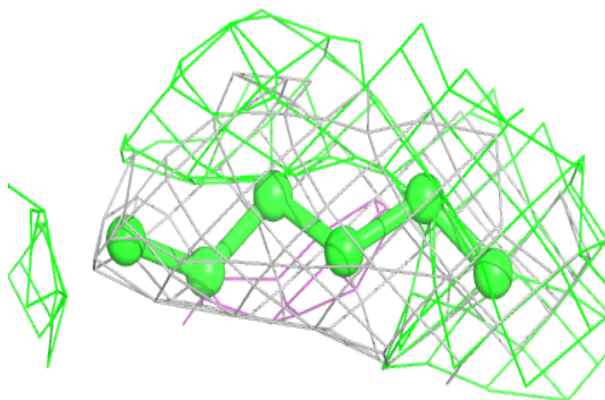


**Electron density around PX4 C 1304:**

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

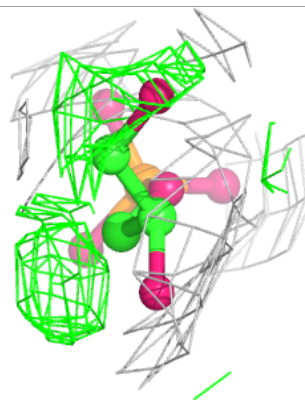
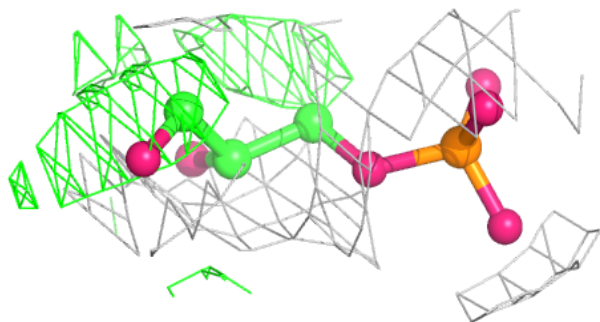
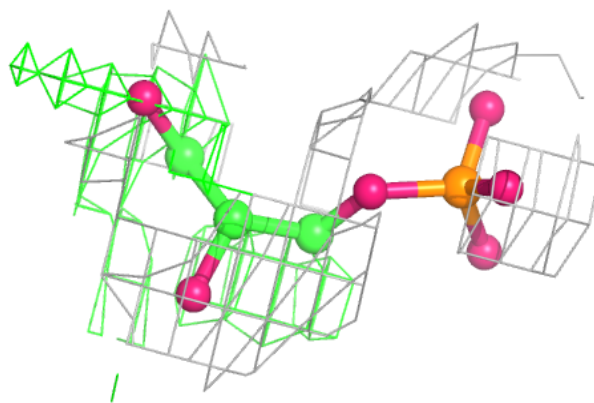
**Electron density around PX4 A 1302:**

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

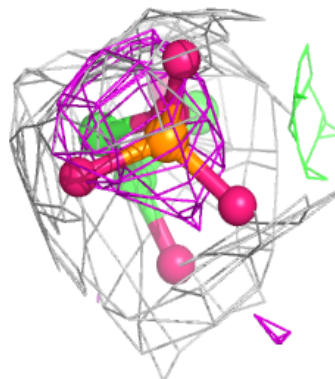
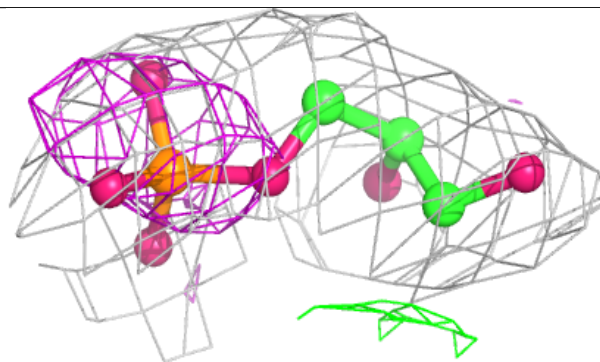
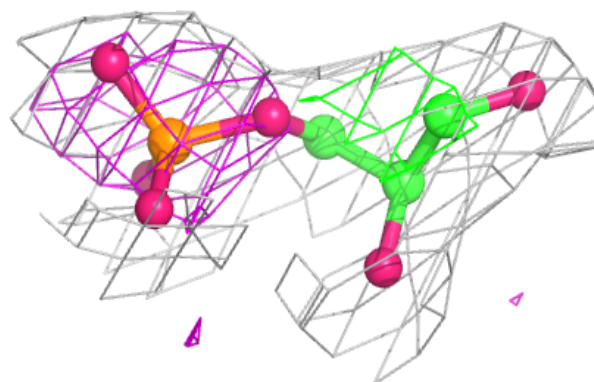


**Electron density around PX4 B 1304:**

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

**Electron density around PX4 A 1301:**

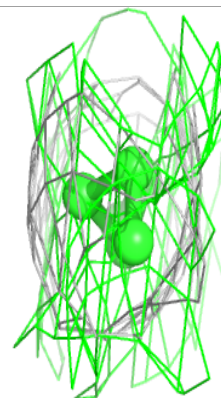
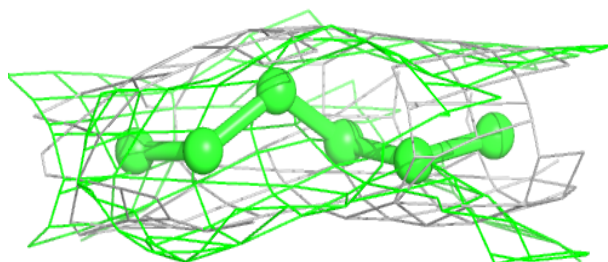
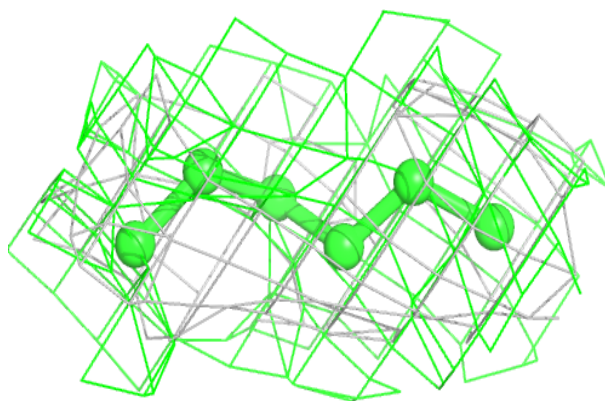
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



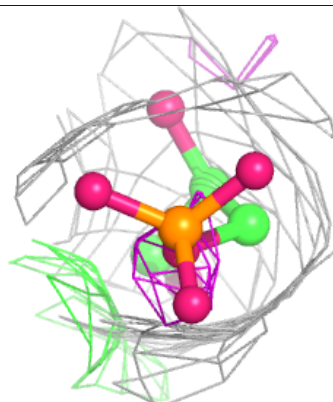
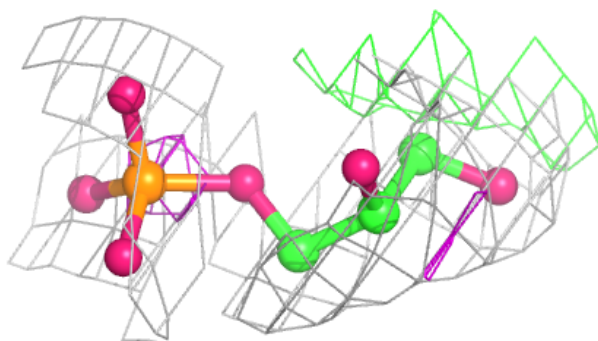
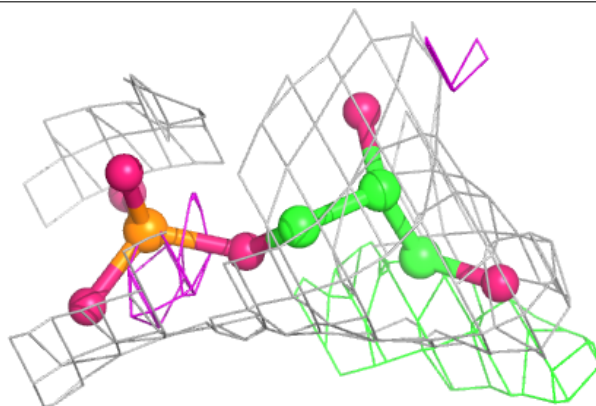


**Electron density around PX4 C 1303:**

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

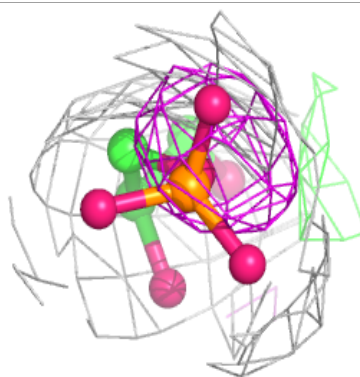
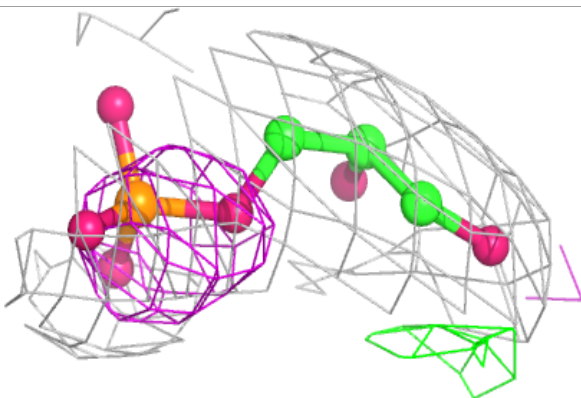
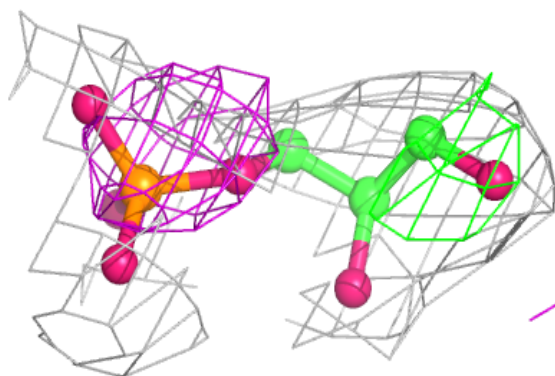
**Electron density around PX4 D 1301:**

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

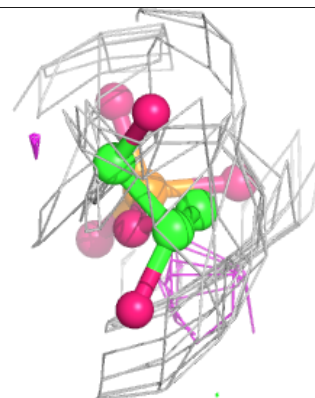
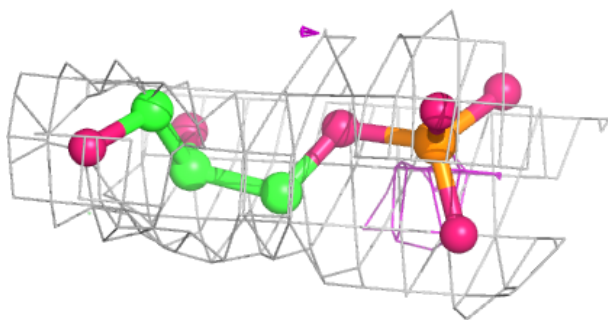
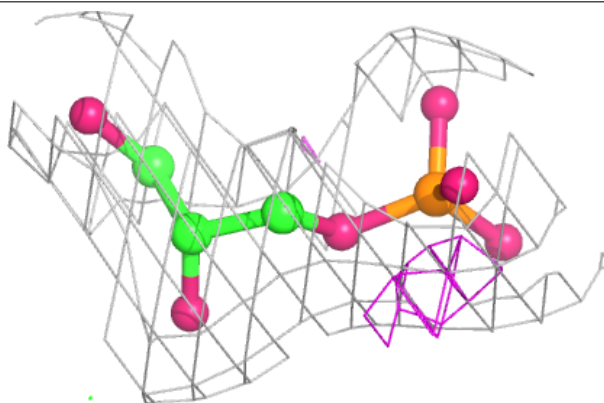


**Electron density around PX4 B 1301:**

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

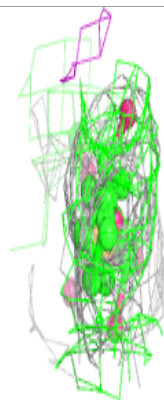
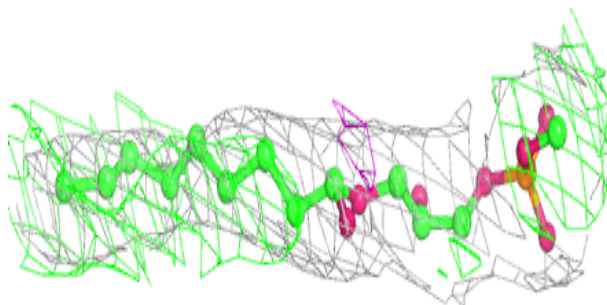
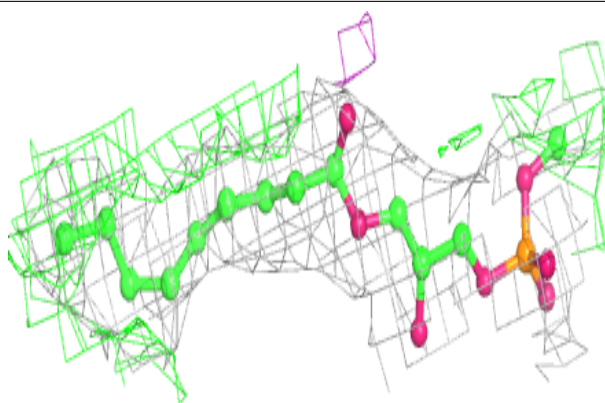
**Electron density around PX4 A 1303:**

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

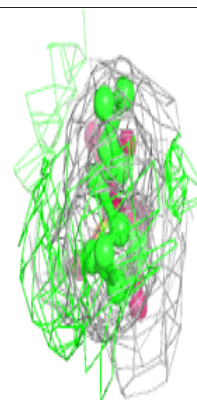
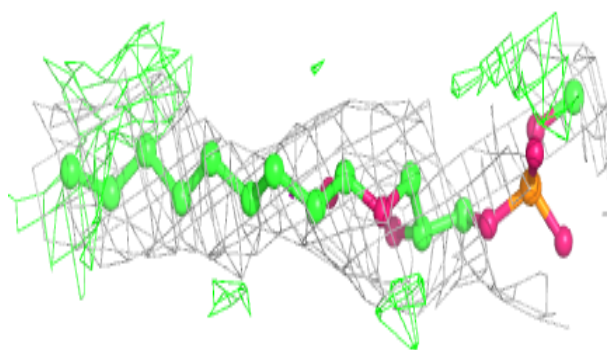
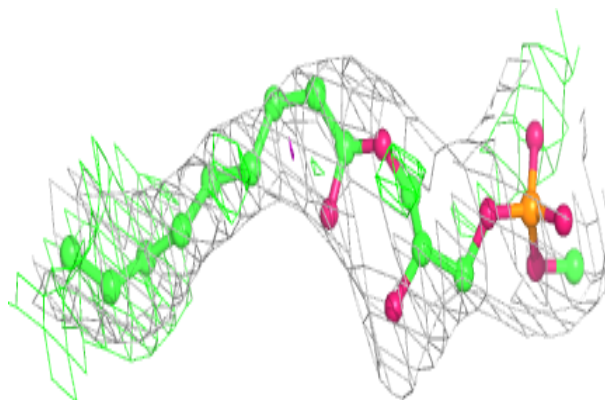


**Electron density around PX4 D 1302:**

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

**Electron density around PX4 B 1302:**

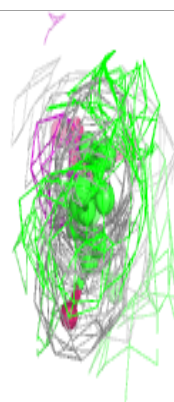
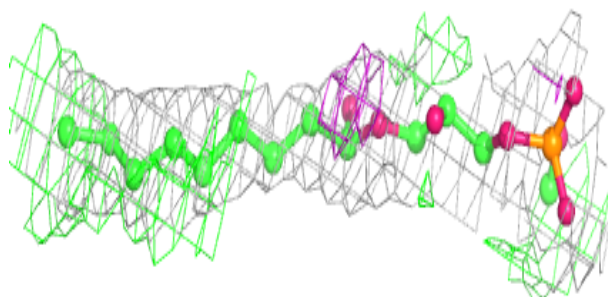
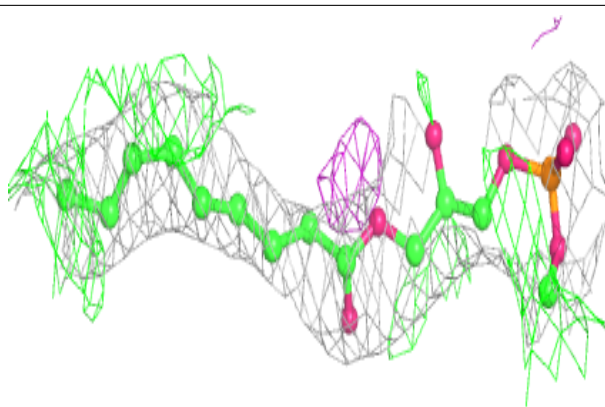
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



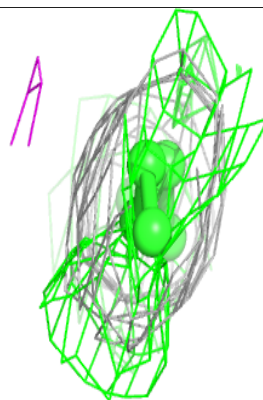
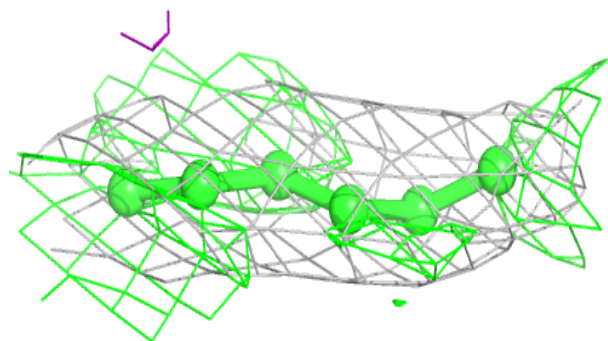
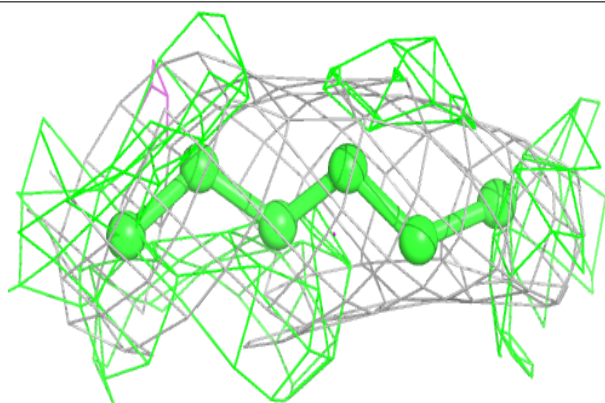


**Electron density around PX4 C 1302:**

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

**Electron density around PX4 D 1303:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.