# wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 04:58 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 3ZYV |
| Title | : | Crystal structure of the mouse liver Aldehyde Oxidase 3 (mAOX3) |
| Authors | : | Trincao, J.; Coelho, C.; Mahro, M.; Rodrigues, D.; Terao, M.; Garattini, E.; Leimkuehler, S.; Romao, M.J. |
| Deposited on | : | 2011-08-27 |
| Resolution | : | 2.54 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

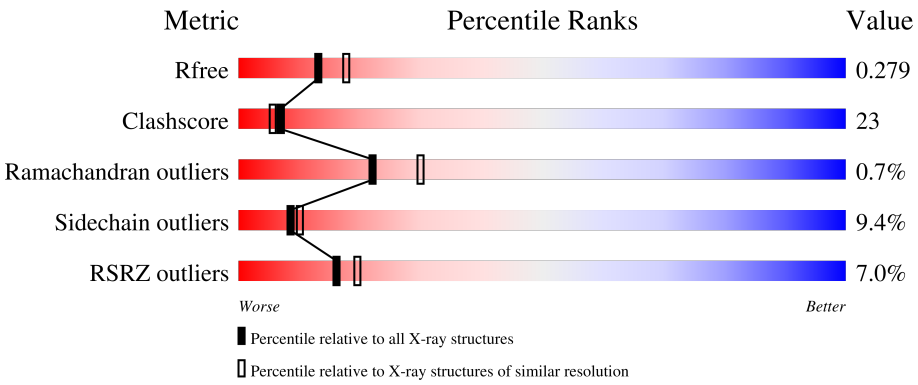
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1284 (2.56-2.52) |
| Clashscore | 141614 | 1332 (2.56-2.52) |
| Ramachandran outliers | 138981 | 1315 (2.56-2.52) |
| Sidechain outliers | 138945 | 1315 (2.56-2.52) |
| RSRZ outliers | 127900 | 1272 (2.56-2.52) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 1335 | 5% 58% 32% • 6% |
| 1 | B | 1335 | 5% 57% 33% 5% 5% |
| 1 | C | 1335 | 7% 59% 30% • 7% |
| 1 | D | 1335 | 9% 58% 32% • 6% |

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 |
|---|---|---|---|---|---|---|---|
| 3 | FES | D | 3002 | - | - | X | - |
| 5 | MOS | A | 3004 | - | - | X | - |
| 5 | MOS | B | 3004 | - | - | X | - |
| 5 | MOS | C | 3004 | - | - | X | - |
| 5 | MOS | D | 3004 | - | - | X | - |
| 6 | FAD | C | 3005 | - | - | X | - |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 38315 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.

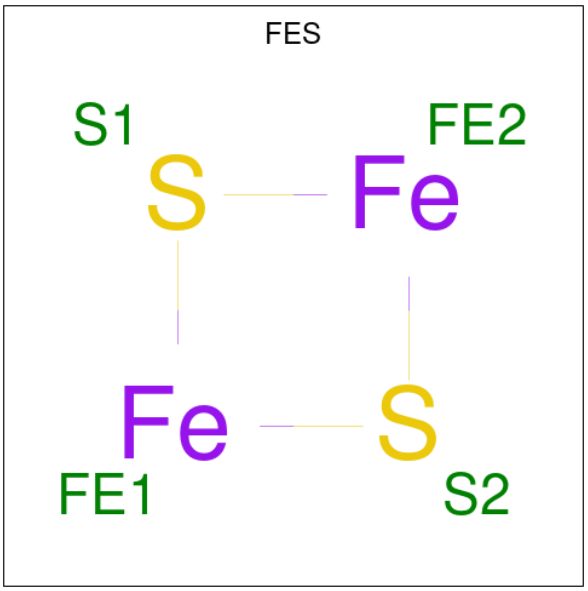
- Molecule 1 is a protein called AOX3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 1253 | 9314 | 5905 | 1602 | 1747 | 60 | 0 | 0 | 0 |
| 1 | B | 1262 | 9471 | 6016 | 1621 | 1774 | 60 | 0 | 0 | 0 |
| 1 | C | 1244 | 9231 | 5865 | 1579 | 1728 | 59 | 0 | 0 | 0 |
| 1 | D | 1257 | 9289 | 5892 | 1602 | 1739 | 56 | 0 | 0 | 0 |

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

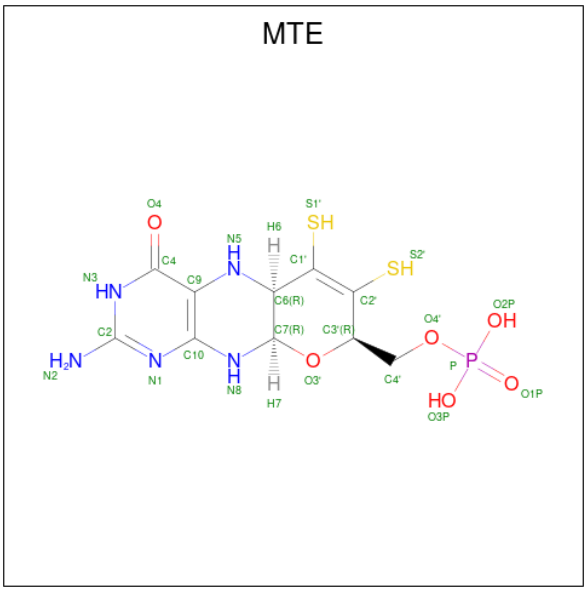
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Na | | |
| 2 | A | 1 | 1 | 1 | 0 | 0 |
| 2 | B | 1 | 1 | 1 | 0 | 0 |
| 2 | C | 1 | 1 | 1 | 0 | 0 |
| 2 | D | 1 | 1 | 1 | 0 | 0 |

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: $Fe_2S_2$).



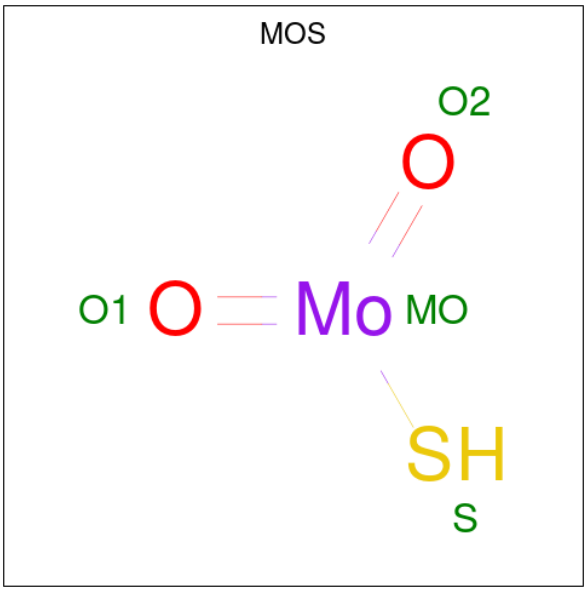

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | Fe | S | | |
| 3 | A | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | A | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | B | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | B | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | C | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | C | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | D | 1 | 4 | 2 | 2 | 0 | 0 |
| | | | Total | Fe | S | | |
| 3 | D | 1 | 4 | 2 | 2 | 0 | 0 |

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A,9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



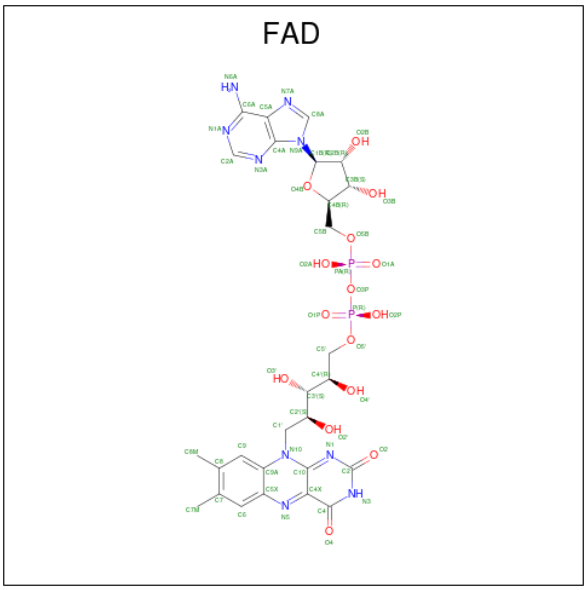

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | |
| 4 | A | 1 | 24 | 10 | 5 | 6 | 1 | 2 | 0 | 0 |
| 4 | B | 1 | 24 | 10 | 5 | 6 | 1 | 2 | 0 | 0 |
| 4 | C | 1 | 24 | 10 | 5 | 6 | 1 | 2 | 0 | 0 |
| 4 | D | 1 | 24 | 10 | 5 | 6 | 1 | 2 | 0 | 0 |

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | Mo | O | S | | |
| 5 | A | 1 | 4 | 1 | 2 | 1 | 0 | 0 |
| 5 | B | 1 | 4 | 1 | 2 | 1 | 0 | 0 |
| 5 | C | 1 | 4 | 1 | 2 | 1 | 0 | 0 |
| 5 | D | 1 | 4 | 1 | 2 | 1 | 0 | 0 |

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | A | 1 | 53 | 27 | 9 | 15 | 2 | 0 | 0 |
| 6 | B | 1 | 53 | 27 | 9 | 15 | 2 | 0 | 0 |
| 6 | C | 1 | 53 | 27 | 9 | 15 | 2 | 0 | 0 |
| 6 | D | 1 | 53 | 27 | 9 | 15 | 2 | 0 | 0 |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 7 | A | 182 | 182 | 182 | 0 | 0 |

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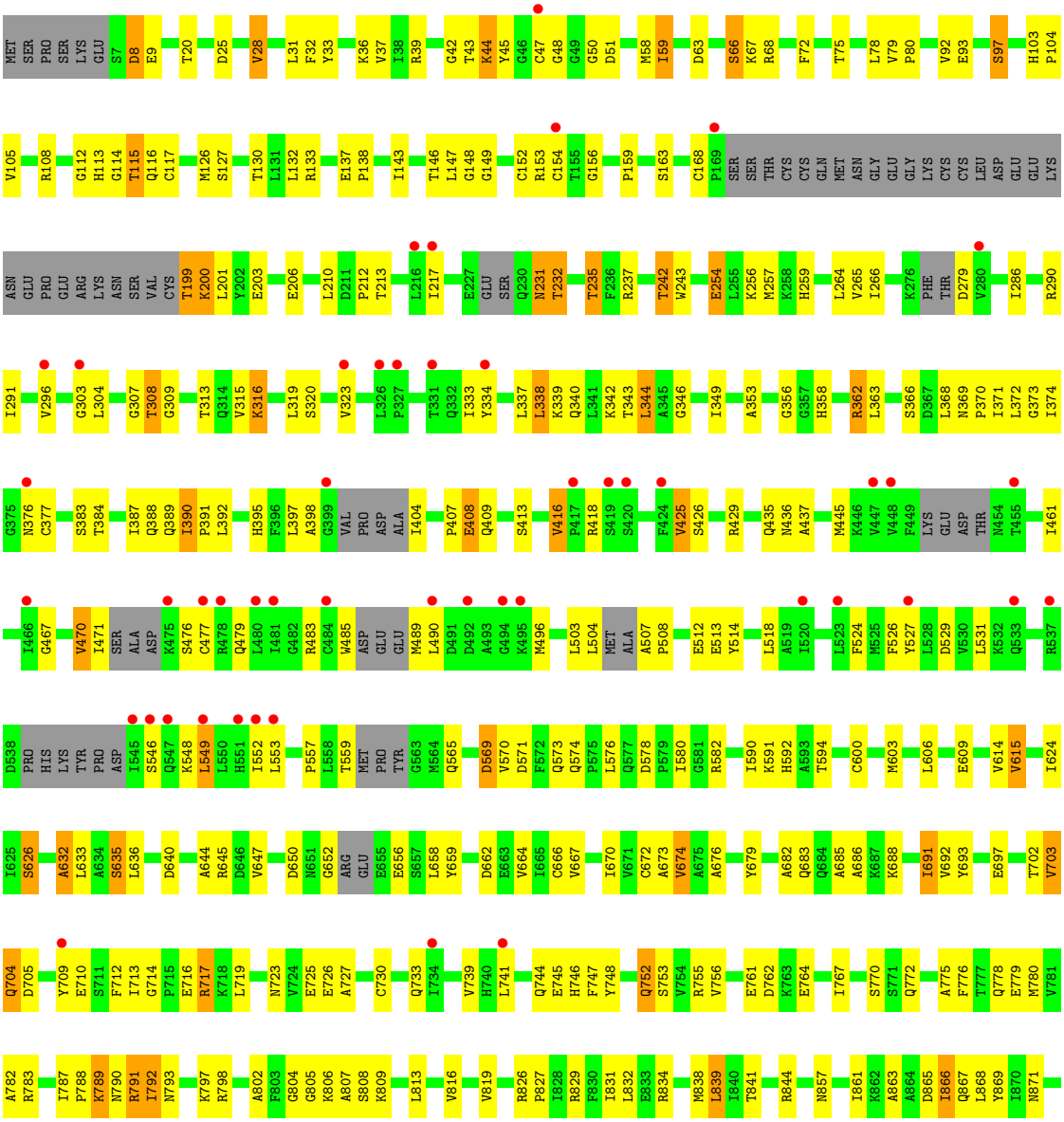
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 7 | B | 166 | 166 | 166 | 0 | 0 |
| | | | Total | O | | |
| 7 | C | 147 | 147 | 147 | 0 | 0 |
| | | | Total | O | | |
| 7 | D | 155 | 155 | 155 | 0 | 0 |

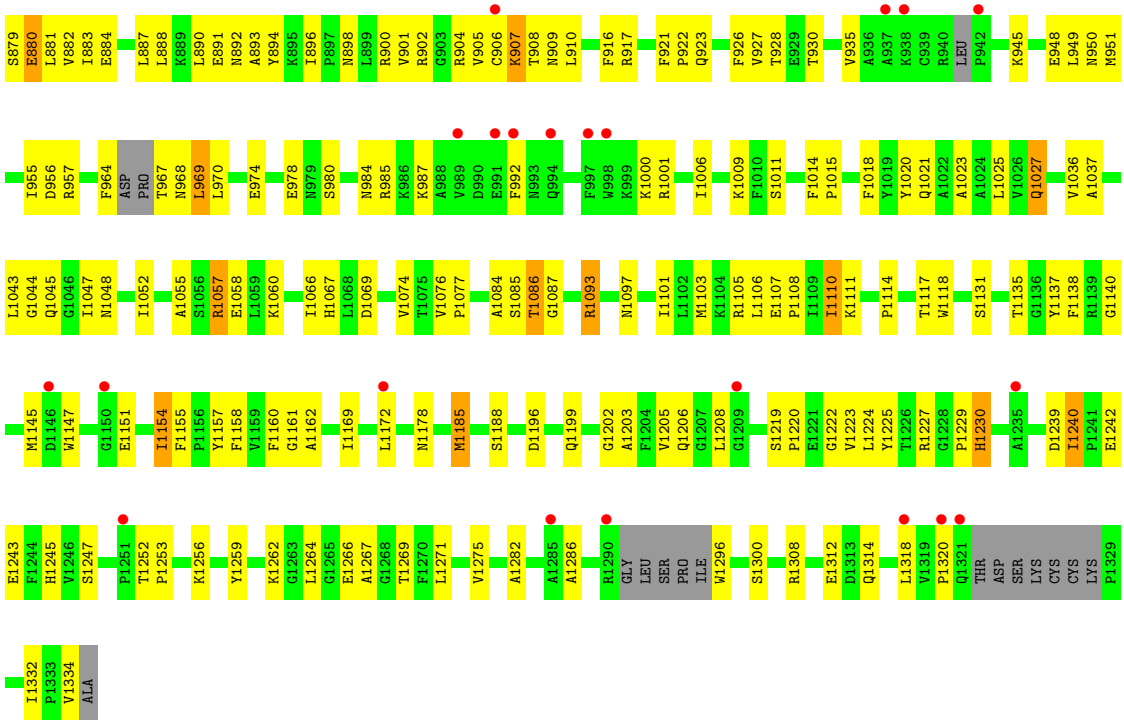
# 3 Residue-property plots (i)

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

- Molecule 1: AOX3

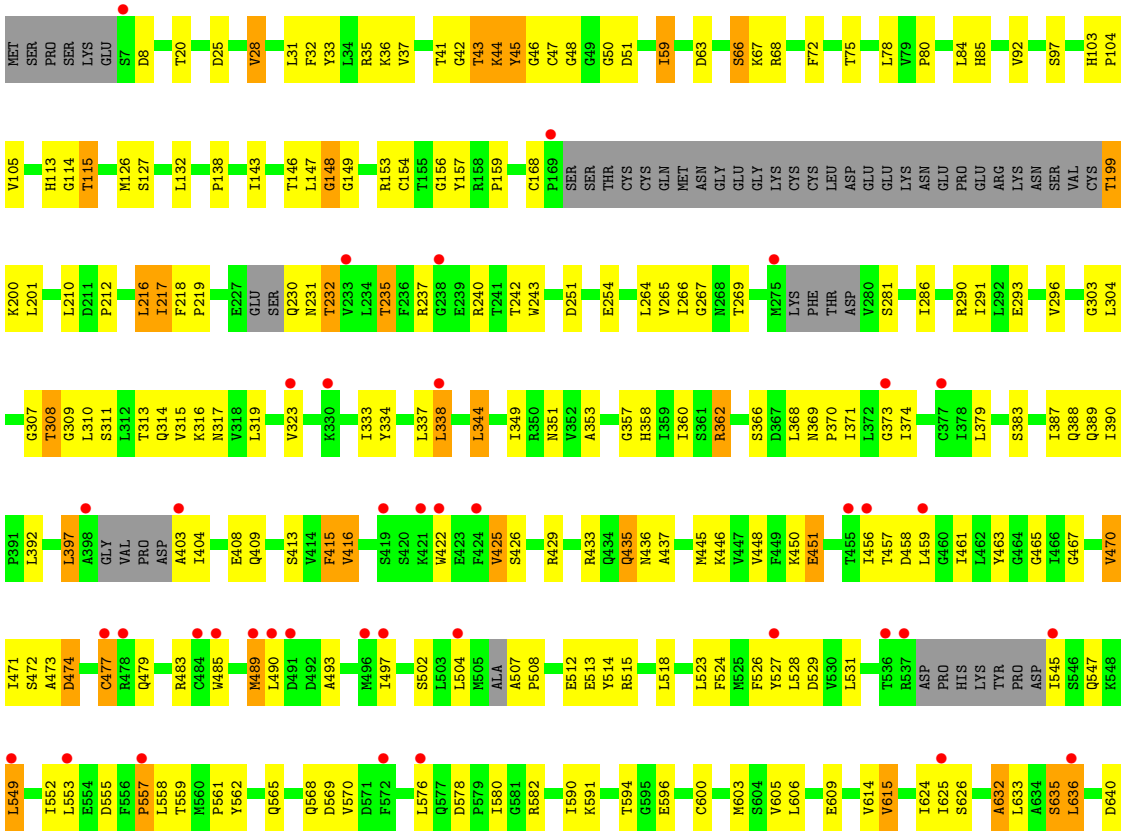
Chain A:

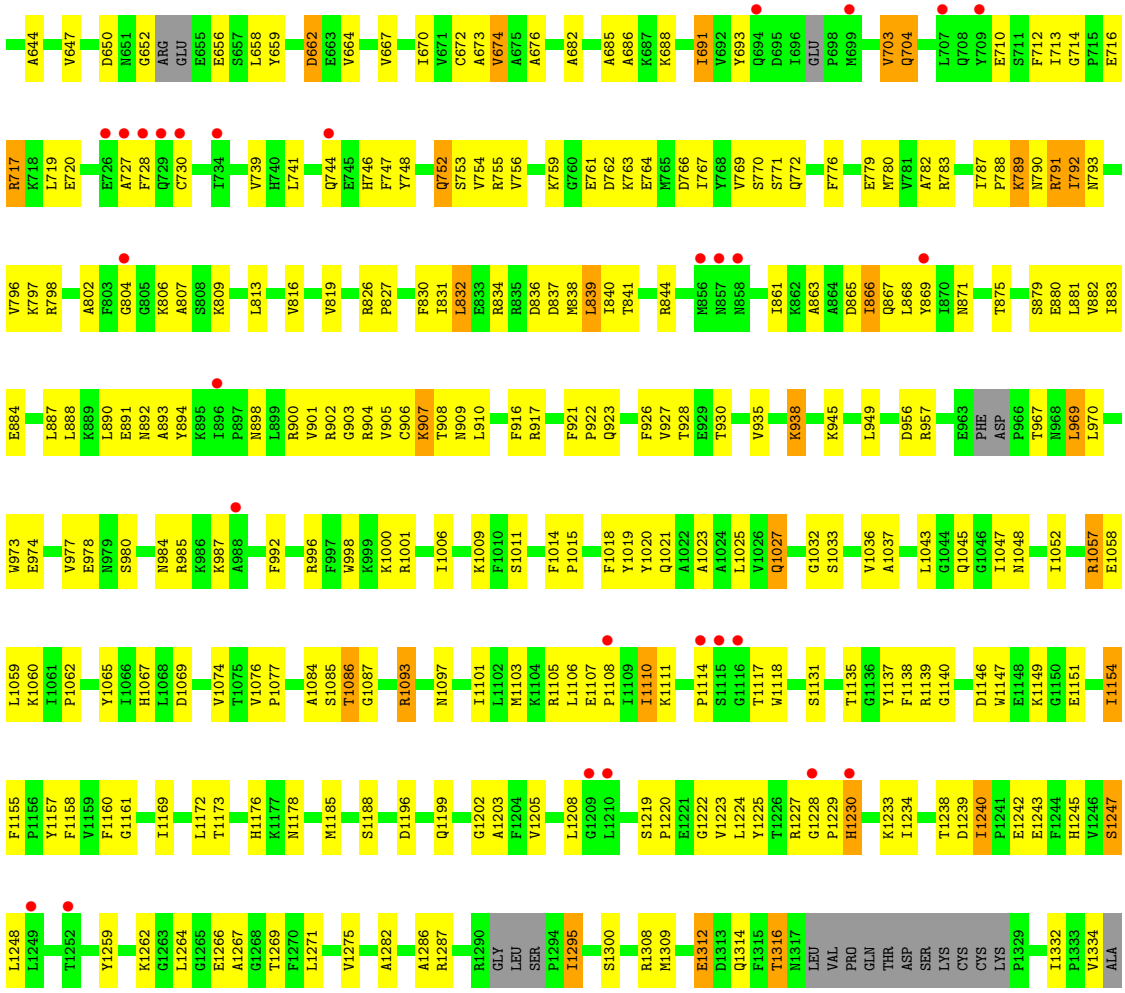






- Molecule 1: AOX3

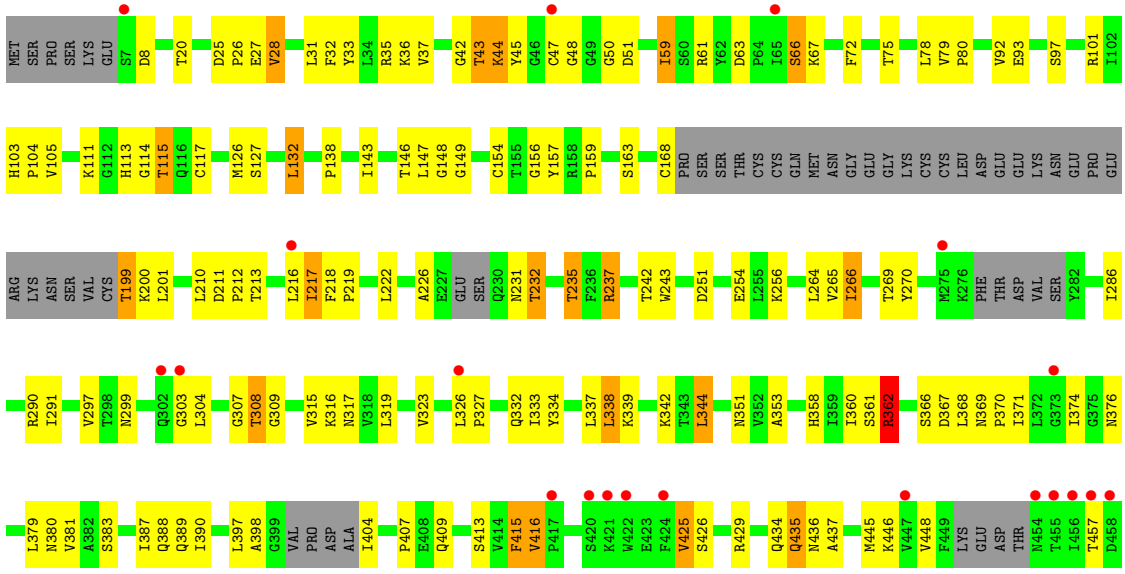
Chain B:





- Molecule 1: AOX3

Chain C:



L459 G460 I461 L462 Y463 G467 A468 T469 V470 I471 S472 A473 D474 C477 R478 Q479 L480 I481 G482 R483 C484 W485 D486 M489 L490 D491 D492 A493 G494 K495 M496 I497 C498 E499 L504 M505 A506 A507 P508 G509 E512 E513 Y514 L518 F524 M525 F526 Y527 V530 L531 K532 Q533

L534 K535 T536 R537 D538 PRO HIS LYS TYR PRO ASP ILE S546 Q547 K548 L549 I552 LEU E554 P557 LEU THR MET PRO TYR G563 M564 Q565 Q568 D569 V570 D571 F572 L576 G577 D578 P579 I580 G581 R582 I590 K591 H592 A593 T594 G595 E596 C600 M603 L606 E609

V614 V615 K619 I624 I625 S626 L627 A632 L633 A634 S635 L636 D640 T643 A644 V647 D650 N651 G652 ARG GLU E655 E656 S657 L658 Y659 D662 E663 V664 I665 C666 V667 I670 V671 C672 A673 V674 A675 A676 A682 Q683 Q684 A685 A686 K687 K688 I691 V692

Y693 I696 GLU P698 V701 T702 V703 Q704 Q708 Y709 E710 S711 F712 I713 R717 K718 L719 E720 Q721 G722 N723 V724 E725 E726 A727 F728 Q729 C730 A731 V739 H740 L741 H746 F747 Y748 Q752 S753 V754 R755 V756 E761 D762 K763 E764 I767 S770 S771 Q772 A775

Q778 E779 A782 R783 I787 P788 K789 N790 R791 I792 N793 V796 K797 R798 A802 F803 G804 G805 K806 A807 S808 K809 L813 V816 V819 R826 P827 I828 R829 F830 I831 L832 E833 R834 M838 L839 I840 T841 R844 L848 G854 F855 M856 N857 N858 G859 K860

I861 K862 A863 I866 Q867 L868 N871 S879 E880 L881 V882 I883 E884 L887 L888 K889 L890 E891 N892 A893 Y894 LYS ILE PRO N898 V901 V905 C906 K907 T908 N909 L910 F916 R917 F921 P922 Q923 G924 A925 F926 V927 T928 E929 T930 S933 A934 V935 A936 A937 R940

LEU P942 K945 L949 D956 R957 Q962 GLU PHE ASP PRO T967 N968 L969 L970 W973 E974 V977 E978 N979 S980 S981 Y982 Y983 N984 R985 K986 K987 D990 E991 F992 N993 Q994 Q995 R996 F997 K1000 R1001 I1005 I1006 K1009 F1010 S1011 V1012 P1015 F1018 Q1021

A1022 A1023 A1024 L1025 V1026 Q1027 V1036 A1037 V1041 E1042 L1043 G1044 Q1045 G1046 I1047 N1048 I1052 A1055 S1056 R1057 E1058 P1062 Y1065 I1066 H1067 L1068 D1069 V1074 T1075 V1076 P1077 N1078 A1084 S1085 T1086 G1087 R1093 A1094 N1097 I1101 L1102 M1103 K1104 R1105 L1106 E1107 P1108 I1109 I1110

K1111 P1114 S1115 G1116 T1117 W1118 S1131 T1135 G1136 Y1137 F1138 R1139 G1140 Y1141 Q1142 A1143 D1144 W1147 E1148 E1151 I1154 F1155 P1156 Y1157 F1158 V1159 F1160 G1161 I1169 D1170 C1171 L1172 N1178 M1185 S1188 D1196 G1202 A1203 L1208 S1219 G1222 V1223 L1224 Y1225 T1226

R1227 GLY PRO H1230 D1239 I1240 E1243 F1244 H1245 V1246 S1247 T1252 P1253 K1256 Y1259 K1262 G1263 L1264 A1267 L1271 V1275 A1282 A1285 A1286 R1290 GLY LEU SER P1294 I1295 S1300 R1308 C1311 Q1314 F1315 T1316 N1317 L1318 VAL PRO GLN THR ASP SER

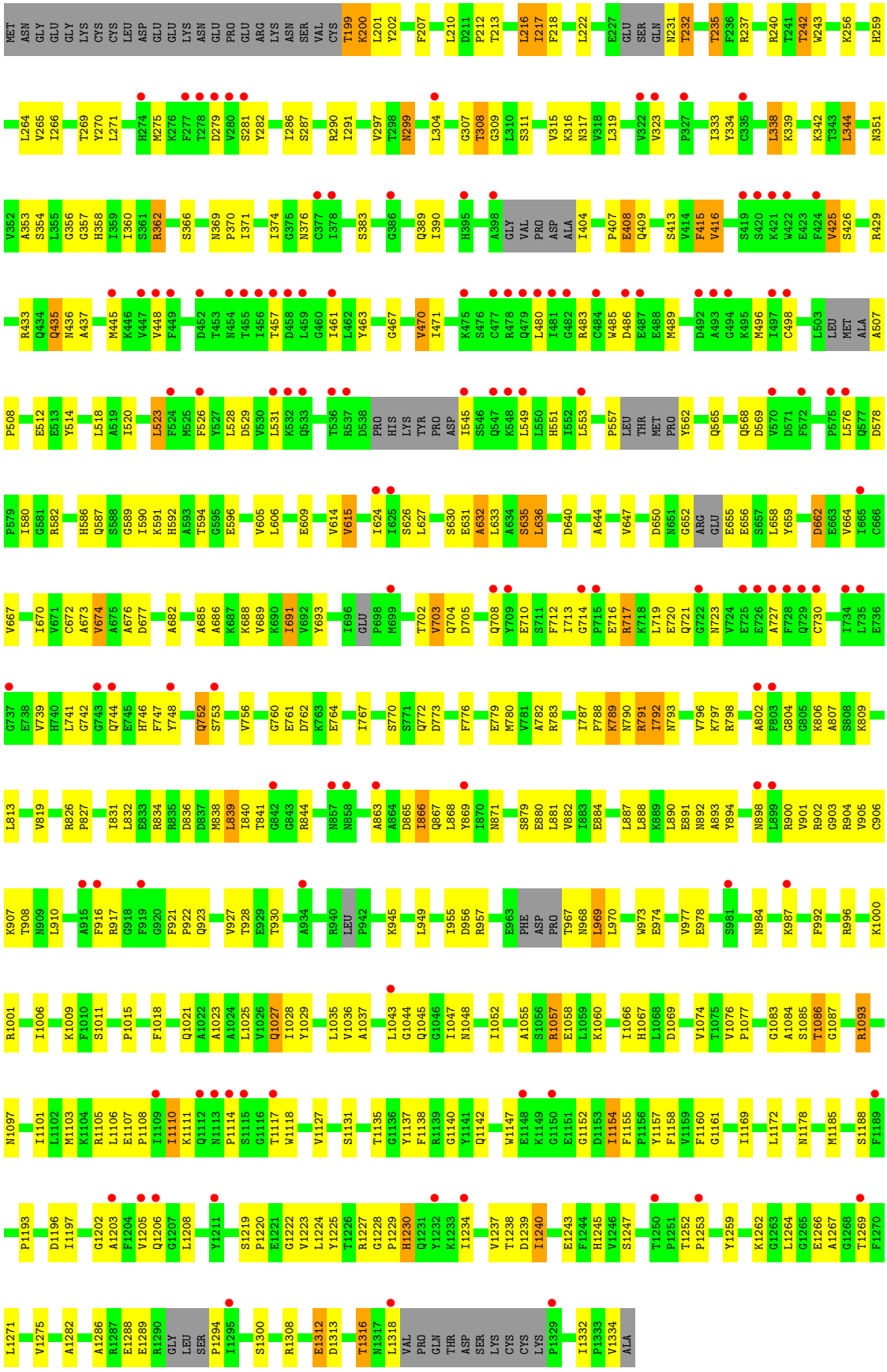
LYS CYS CYS LYS P1329 V1334 ALA

- Molecule 1: AOX3

Chain D: 9% 58% 32% 6%

MET SER PRO SER LYS GLU S7 D8 E9 L10 I11 F12 N15 G16 T20 A24 D25 P26 E27 V28 L31 F32 Y33 L34 R35 K36 V37 I38 R39 G42 T43 K44 Y45 G46 C47 G48 G49 G50 D51 C52 G53 A54 M58 I59 D63 S66 K67 R68 F72 T75

L78 V79 P80 H85 G86 T90 T91 V92 E93 G94 I95 G96 S97 H103 P104 V105 H113 G114 T115 Q116 C117 C120 M126 S127 L132 E137 I143 T146 L147 G148 G149 C152 R153 C154 T155 G156 Y157 R158 P159 C168 PRO SER SER THR CYS CYS GLN


MET ASN GLY GLU GLY LYS CYS CYS LEU ASP GLU GLU LYS ASN GLU PRO GLU ARG LYS ASN SER VAL CYS T199 K200 L201 Y202 F207 L210 D211 P212 T213 L216 I217 F218 L222 E227 GLU SER GLN N231 T232 T235 F236 R237 R240 T241 T242 W243 K256 H259
L264 V265 I266 T269 Y270 L271 H274 M275 K276 F277 T278 D279 V280 S281 Y282 I286 S287 R290 I291 V297 T298 N299 L304 G307 T308 G309 L310 S311 V315 K316 N317 V318 L319 V322 V323 P327 I333 Y334 C335 L338 K339 K342 T343 L344 N351
V352 A353 S354 L355 G356 G357 H358 I359 I360 S361 R362 S366 N369 P370 I371 I374 G375 N376 C377 I378 S383 G386 Q389 I390 H395 A398 GLY VAL PRO ASP ALA I404 P407 E408 Q409 S413 V414 F415 V416 S419 S420 K421 W422 E423 F424 V425 S426 R429
R433 Q434 Q435 N436 A437 M445 K446 V447 V448 F449 D452 T453 N454 T455 I456 T457 D458 L459 G460 I461 L462 Y463 G467 V470 I471 K475 S476 C477 R478 Q479 L480 I481 G482 R483 C484 W485 D486 E487 E488 M489 D492 A493 G494 K495 M496 I497 C498 L503 LEU MET ALA A507
P508 E512 E513 Y514 L518 A519 I520 L523 F524 M525 F526 Y527 L528 D529 V530 L531 K532 Q533 T536 R537 D538 PRO HIS LYS TYR PRO ASP I545 S546 Q547 K548 L549 L550 H551 I552 L553 P557 LEU THR MET PRO Y562 Q565 Q568 D569 V570 D571 F572 P575 L576 Q577 D578
P579 I580 G581 R582 H586 Q587 S588 G589 I590 K591 H592 A593 T594 G595 E596 V605 L606 E609 V614 V615 I624 I625 S626 L627 S630 E631 A632 L633 A634 S635 L636 D640 A644 V647 D650 N651 G652 ARG GLU E655 E656 S657 L658 Y659 D662 E663 V664 I665 C666
V667 I670 V671 C672 A673 V674 A675 A676 D677 A682 A685 A686 K687 K688 V689 K690 I691 V692 Y693 L696 GLU P698 M699 T702 V703 Q704 D705 Q708 Y709 E710 S711 F712 I713 G714 P715 E716 R717 K718 L719 E720 Q721 G722 N723 V724 E725 E726 A727 F728 Q729 C730 I734 L735 E736
G737 E738 V739 H740 L741 G742 G743 Q744 E745 H746 F747 Y748 Q752 S753 V756 G760 E761 D762 K763 E764 I767 S770 S771 Q772 D773 F776 E779 M780 V781 A782 R783 I787 P788 K789 R790 R791 I792 N793 V796 K797 R798 A802 F803 G804 G805 K806 A807 S808 K809
L813 V819 R826 P827 I831 L832 E833 R834 R835 D836 D837 M838 L839 I840 T841 G842 G843 R844 N857 N858 A863 A864 D865 I866 Q867 L868 Y869 I870 N871 S879 E880 L881 V882 I883 E884 L887 L888 K889 L890 E891 N892 A893 Y894 N898 L899 R900 V901 R902 G903 R904 V905 C906
K907 T908 N909 L910 A915 F916 R917 G918 F919 G920 F921 P922 Q923 V927 T928 E929 T930 A934 R940 LEU P942 K945 L949 I955 D956 R957 E963 PHE ASP PRO T967 N968 L969 L970 W973 E974 V977 E978 S981 N984 K987 F992 R996 K1000
R1001 I1006 K1009 F1010 S1011 P1015 F1018 Q1021 A1022 A1023 A1024 L1025 V1026 Q1027 I1028 Y1029 L1035 V1036 A1037 L1043 G1044 Q1045 G1046 I1047 N1048 I1052 A1055 S1056 R1057 E1058 L1059 K1060 I1066 H1067 L1068 D1069 V1074 T1075 V1076 P1077 G1083 A1084 S1085 T1086 G1087 R1093
N1097 I1101 L1102 M1103 K1104 R1105 L1106 E1107 P1108 I1109 I1110 K1111 Q1112 N1113 P1114 S1115 G1116 T1117 W1118 V1127 S1131 T1135 G1136 Y1137 F1138 R1139 G1140 Y1141 Q1142 W1147 E1148 K1149 G1150 E1151 G1152 D1153 I1154 F1155 P1156 Y1157 F1158 V1159 F1160 G1161 I1169 L1172 N1178 M1185 S1188 F1189
P1193 D1196 I1197 G1202 A1203 F1204 V1205 Q1206 G1207 L1208 Y1211 S1219 P1220 E1221 G1222 V1223 L1224 Y1225 T1226 R1227 G1228 P1229 H1230 Q1231 Y1232 K1233 I1234 V1237 T1238 D1239 I1240 E1243 F1244 H1245 V1246 S1247 T1250 P1251 T1252 P1253 Y1259 K1262 G1263 L1264 G1265 E1266 A1267 G1268 T1269 F1270
L1271 V1275 A1282 A1286 R1287 E1288 E1289 R1290 GLY LEU SER P1294 I1295 S1300 R1308 E1312 D1313 T1316 N1317 L1318 VAL PRO GLN THR ASP SER LYS CYS CYS LYS P1329 I1332 P1333 V1334 ALA

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 90.88Å 135.27Å 147.37Å<br>78.16° 77.72° 89.90° | Depositor |
| Resolution (Å) | 49.91 – 2.54<br>49.91 – 2.55 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 75.0 (49.91-2.54)<br>75.0 (49.91-2.55) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.82 (at 2.54Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, $R_{free}$ | 0.256 , 0.285<br>0.250 , 0.279 | Depositor<br>DCC |
| $R_{free}$ test set | 8336 reflections (5.05%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 35.6 | Xtriage |
| Anisotropy | 0.770 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 66.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.35$, $< L^2 > = 0.18$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.86 | EDS |
| Total number of atoms | 38315 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 43.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FES, MTE, MOS, NA, FAD

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 | 0.31 | 0/9482 | 0.50 | 1/12869 (0.0%) |
| 1 | B | 0.32 | 0/9650 | 0.50 | 2/13097 (0.0%) |
| 1 | C | 0.31 | 0/9398 | 0.51 | 1/12757 (0.0%) |
| 1 | D | 0.31 | 0/9460 | 0.49 | 0/12852 |
| All | All | 0.31 | 0/37990 | 0.50 | 4/51575 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | B | 0 | 1 |
| 1 | C | 0 | 1 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 619 | LYS | CB-CG-CD | 7.44 | 130.95 | 111.60 |
| 1 | A | 697 | GLU | C-N-CD | -6.60 | 106.07 | 120.60 |
| 1 | B | 558 | LEU | N-CA-C | -6.30 | 93.99 | 111.00 |
| 1 | B | 561 | PRO | N-CA-CB | 5.06 | 109.37 | 103.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 557 | PRO | Peptide |
| 1 | B | 557 | PRO | Peptide |
| 1 | C | 226 | ALA | Peptide |

## 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 | 9314 | 0 | 9046 | 438 | 0 |
| 1 | B | 9471 | 0 | 9271 | 446 | 0 |
| 1 | C | 9231 | 0 | 8962 | 414 | 0 |
| 1 | D | 9289 | 0 | 8958 | 438 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 8 | 0 | 0 | 1 | 0 |
| 3 | B | 8 | 0 | 0 | 1 | 0 |
| 3 | C | 8 | 0 | 0 | 1 | 0 |
| 3 | D | 8 | 0 | 0 | 2 | 0 |
| 4 | A | 24 | 0 | 10 | 4 | 0 |
| 4 | B | 24 | 0 | 10 | 1 | 0 |
| 4 | C | 24 | 0 | 10 | 3 | 0 |
| 4 | D | 24 | 0 | 10 | 3 | 0 |
| 5 | A | 4 | 0 | 0 | 2 | 0 |
| 5 | B | 4 | 0 | 0 | 2 | 0 |
| 5 | C | 4 | 0 | 0 | 2 | 0 |
| 5 | D | 4 | 0 | 0 | 2 | 0 |
| 6 | A | 53 | 0 | 31 | 8 | 0 |
| 6 | B | 53 | 0 | 31 | 14 | 0 |
| 6 | C | 53 | 0 | 31 | 21 | 0 |
| 6 | D | 53 | 0 | 31 | 15 | 0 |
| 7 | A | 182 | 0 | 0 | 93 | 0 |
| 7 | B | 166 | 0 | 0 | 65 | 0 |
| 7 | C | 147 | 0 | 0 | 57 | 0 |
| 7 | D | 155 | 0 | 0 | 90 | 0 |
| All | All | 38315 | 0 | 36401 | 1701 | 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 23.

The worst 5 of 1701 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:B:3005:FAD:H9 | 6:B:3005:FAD:O2' | 1.48 | 1.12 |
| 1:A:308:THR:HG21 | 6:A:3005:FAD:N6A | 1.62 | 1.11 |
| 1:B:308:THR:HG21 | 6:B:3005:FAD:N6A | 1.67 | 1.09 |
| 1:A:496:MET:SD | 7:A:2076:HOH:O | 2.12 | 1.07 |
| 1:D:12:PHE:HB3 | 7:D:2002:HOH:O | 1.55 | 1.06 |

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 | 1221/1335 (92%) | 1123 (92%) | 89 (7%) | 9 (1%) | 22 | 30 |
| 1 | B | 1238/1335 (93%) | 1137 (92%) | 93 (8%) | 8 (1%) | 25 | 34 |
| 1 | C | 1210/1335 (91%) | 1111 (92%) | 88 (7%) | 11 (1%) | 17 | 24 |
| 1 | D | 1231/1335 (92%) | 1120 (91%) | 104 (8%) | 7 (1%) | 25 | 34 |
| All | All | 4900/5340 (92%) | 4491 (92%) | 374 (8%) | 35 (1%) | 22 | 30 |

5 of 35 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 398 | ALA |
| 1 | B | 762 | ASP |
| 1 | C | 398 | ALA |
| 1 | C | 474 | ASP |
| 1 | A | 762 | ASP |

### 5.3.2 Protein sidechains (i)

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 | 958/1129 (85%) | 869 (91%) | 89 (9%) | 9 10 |
| 1 | B | 988/1129 (88%) | 891 (90%) | 97 (10%) | 8 9 |
| 1 | C | 948/1129 (84%) | 862 (91%) | 86 (9%) | 9 11 |
| 1 | D | 941/1129 (83%) | 854 (91%) | 87 (9%) | 9 11 |
| All | All | 3835/4516 (85%) | 3476 (91%) | 359 (9%) | 8 10 |

5 of 359 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 635 | SER |
| 1 | D | 199 | THR |
| 1 | C | 691 | ILE |
| 1 | C | 1110 | ILE |
| 1 | D | 316 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 867 | GLN |
| 1 | D | 708 | GLN |
| 1 | C | 1067 | HIS |
| 1 | D | 208 | GLN |
| 1 | D | 1100 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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 | $\#\|Z\| > 2$ |
| 3 | FES | A | 3001 | 1 | 0,4,4 | - | - | - | | |
| 3 | FES | A | 3002 | 1 | 0,4,4 | - | - | - | | |
| 6 | FAD | A | 3005 | - | 53,58,58 | 1.26 | 6 (11%) | 68,89,89 | 1.31 | 10 (14%) |
| 6 | FAD | B | 3005 | - | 53,58,58 | 1.27 | 5 (9%) | 68,89,89 | 1.50 | 14 (20%) |
| 3 | FES | D | 3002 | 1 | 0,4,4 | - | - | - | | |
| 6 | FAD | D | 3005 | - | 53,58,58 | 1.27 | 5 (9%) | 68,89,89 | 1.30 | 10 (14%) |
| 5 | MOS | A | 3004 | 4 | 0,3,3 | - | - | - | | |
| 4 | MTE | B | 3003 | 5 | 21,26,26 | 1.35 | 2 (9%) | 21,40,40 | 2.15 | 8 (38%) |
| 5 | MOS | B | 3004 | 4 | 0,3,3 | - | - | - | | |
| 5 | MOS | D | 3004 | 4 | 0,3,3 | - | - | - | | |
| 5 | MOS | C | 3004 | 4 | 0,3,3 | - | - | - | | |
| 3 | FES | B | 3002 | 1 | 0,4,4 | - | - | - | | |
| 3 | FES | D | 3001 | 1 | 0,4,4 | - | - | - | | |
| 4 | MTE | C | 3003 | 5 | 21,26,26 | 1.43 | 2 (9%) | 21,40,40 | 2.54 | 7 (33%) |
| 6 | FAD | C | 3005 | - | 53,58,58 | 1.27 | 6 (11%) | 68,89,89 | 1.29 | 10 (14%) |
| 3 | FES | C | 3001 | 1 | 0,4,4 | - | - | - | | |
| 3 | FES | B | 3001 | 1 | 0,4,4 | - | - | - | | |
| 3 | FES | C | 3002 | 1 | 0,4,4 | - | - | - | | |
| 4 | MTE | D | 3003 | 5 | 21,26,26 | 1.37 | 2 (9%) | 21,40,40 | 2.17 | 6 (28%) |
| 4 | MTE | A | 3003 | 5 | 21,26,26 | 1.30 | 2 (9%) | 21,40,40 | 2.18 | 7 (33%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | FES | C | 3001 | 1 | - | - | 0/1/1/1 |
| 3 | FES | B | 3001 | 1 | - | - | 0/1/1/1 |
| 3 | FES | A | 3001 | 1 | - | - | 0/1/1/1 |
| 3 | FES | A | 3002 | 1 | - | - | 0/1/1/1 |
| 6 | FAD | A | 3005 | - | - | 8/30/50/50 | 0/6/6/6 |
| 4 | MTE | B | 3003 | 5 | - | 2/6/34/34 | 0/3/3/3 |
| 3 | FES | C | 3002 | 1 | - | - | 0/1/1/1 |
| 4 | MTE | D | 3003 | 5 | - | 4/6/34/34 | 0/3/3/3 |
| 6 | FAD | B | 3005 | - | - | 16/30/50/50 | 0/6/6/6 |
| 3 | FES | B | 3002 | 1 | - | - | 0/1/1/1 |
| 4 | MTE | A | 3003 | 5 | - | 0/6/34/34 | 0/3/3/3 |
| 4 | MTE | C | 3003 | 5 | - | 0/6/34/34 | 0/3/3/3 |
| 6 | FAD | C | 3005 | - | - | 17/30/50/50 | 0/6/6/6 |
| 3 | FES | D | 3001 | 1 | - | - | 0/1/1/1 |
| 3 | FES | D | 3002 | 1 | - | - | 0/1/1/1 |
| 6 | FAD | D | 3005 | - | - | 12/30/50/50 | 0/6/6/6 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | B | 3005 | FAD | C9A-C5X | 5.13 | 1.49 | 1.41 |
| 6 | C | 3005 | FAD | C9A-C5X | 5.08 | 1.49 | 1.41 |
| 6 | D | 3005 | FAD | C9A-C5X | 4.88 | 1.49 | 1.41 |
| 6 | A | 3005 | FAD | C9A-C5X | 4.86 | 1.49 | 1.41 |
| 4 | C | 3003 | MTE | C9-C4 | 4.68 | 1.47 | 1.41 |

The worst 5 of 72 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | C | 3003 | MTE | O3'-C7-C6 | -7.24 | 104.14 | 108.96 |
| 6 | B | 3005 | FAD | C1'-N10-C9A | 5.51 | 129.70 | 120.51 |
| 4 | B | 3003 | MTE | O3'-C7-C6 | -4.32 | 106.08 | 108.96 |
| 4 | D | 3003 | MTE | C10-N8-C7 | -4.30 | 115.24 | 123.67 |
| 4 | C | 3003 | MTE | C4-C9-N5 | 4.23 | 122.67 | 119.12 |

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | D | 3003 | MTE | C4'-O4'-P-O1P |
| 4 | D | 3003 | MTE | C4'-O4'-P-O2P |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | D | 3003 | MTE | C4'-O4'-P-O3P |
| 6 | A | 3005 | FAD | C5B-O5B-PA-O2A |
| 6 | A | 3005 | FAD | C5B-O5B-PA-O3P |

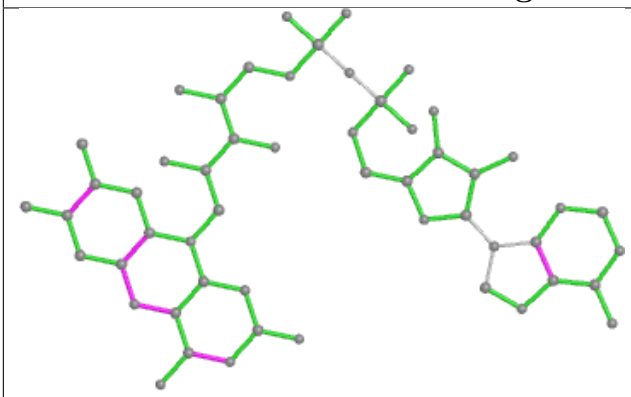
There are no ring outliers.

16 monomers are involved in 82 short contacts:

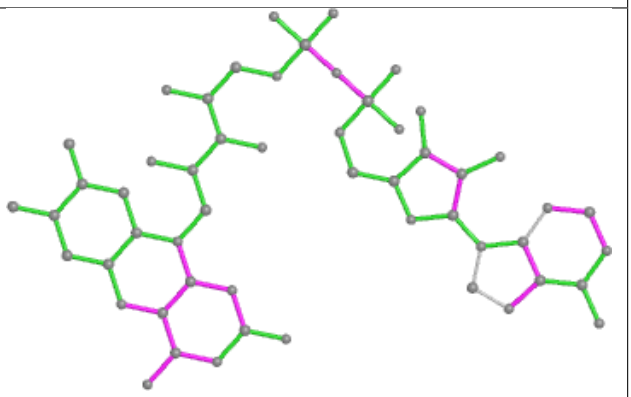
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 3002 | FES | 1 | 0 |
| 6 | A | 3005 | FAD | 8 | 0 |
| 6 | B | 3005 | FAD | 14 | 0 |
| 3 | D | 3002 | FES | 2 | 0 |
| 6 | D | 3005 | FAD | 15 | 0 |
| 5 | A | 3004 | MOS | 2 | 0 |
| 4 | B | 3003 | MTE | 1 | 0 |
| 5 | B | 3004 | MOS | 2 | 0 |
| 5 | D | 3004 | MOS | 2 | 0 |
| 5 | C | 3004 | MOS | 2 | 0 |
| 3 | B | 3002 | FES | 1 | 0 |
| 4 | C | 3003 | MTE | 3 | 0 |
| 6 | C | 3005 | FAD | 21 | 0 |
| 3 | C | 3002 | FES | 1 | 0 |
| 4 | D | 3003 | MTE | 3 | 0 |
| 4 | A | 3003 | MTE | 4 | 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 then 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.

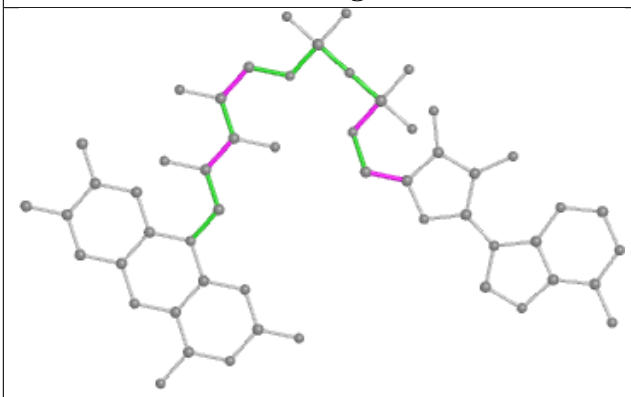
**Ligand FAD A 3005**



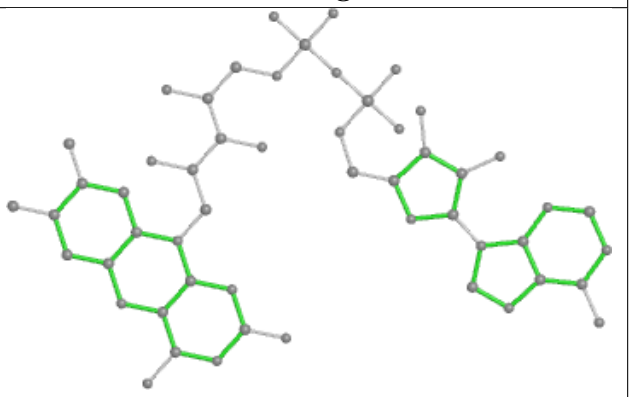
**Bond lengths**



**Bond angles**

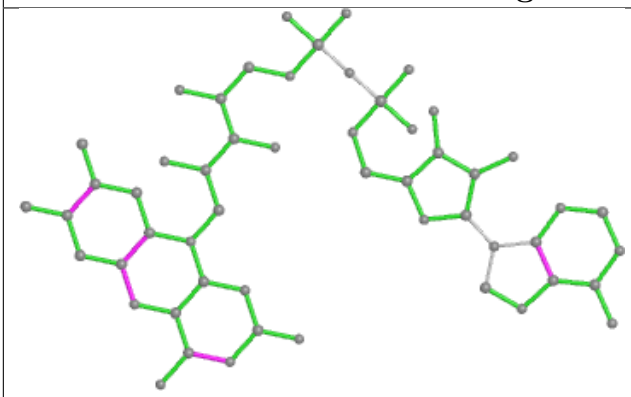


**Torsions**

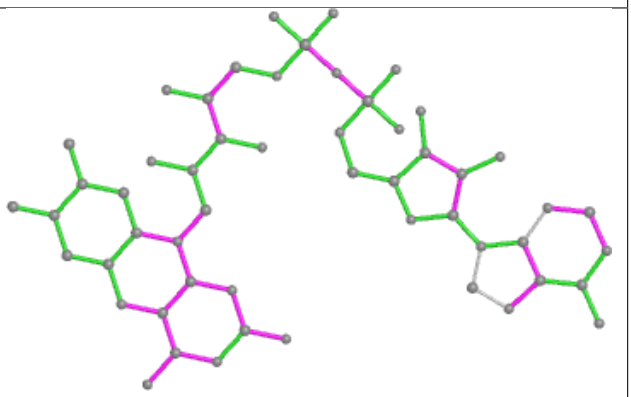


**Rings**

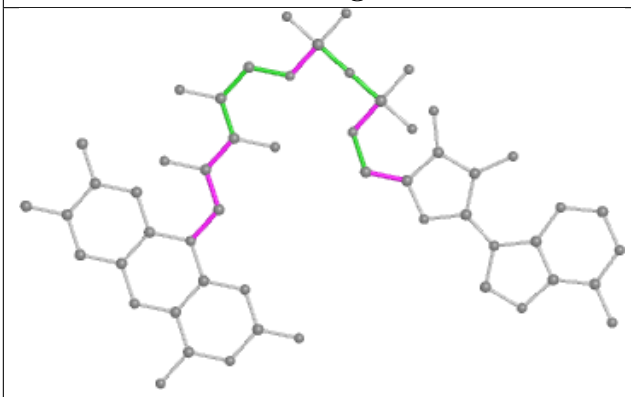
**Ligand FAD B 3005**



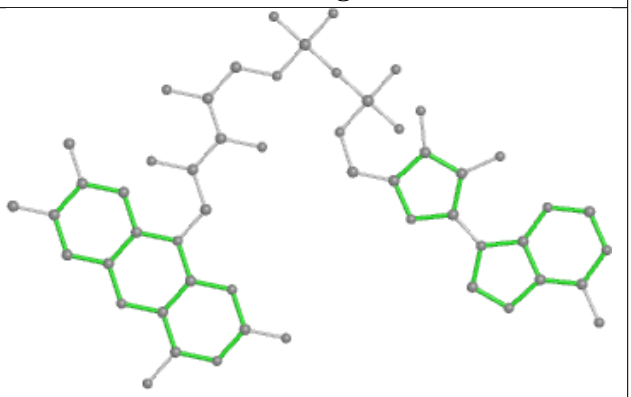
**Bond lengths**



**Bond angles**

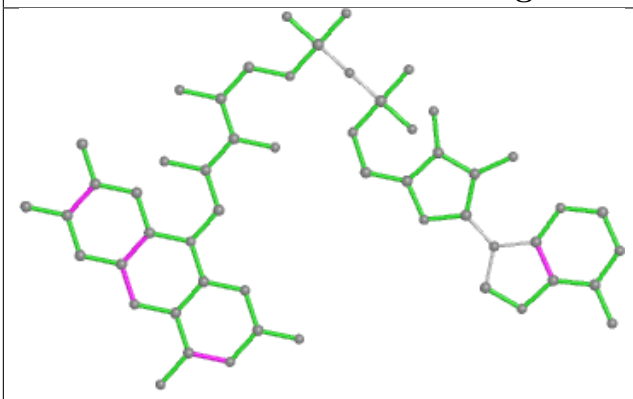


**Torsions**

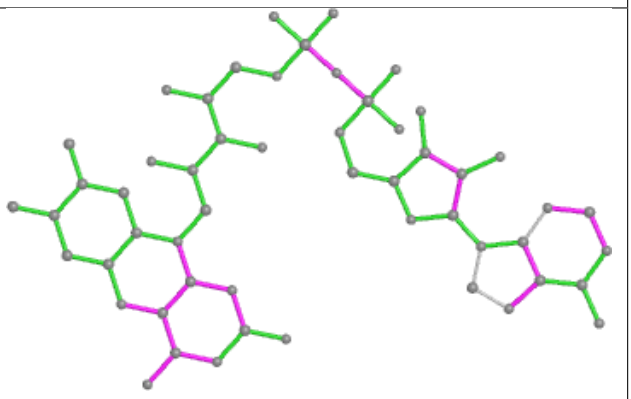


**Rings**

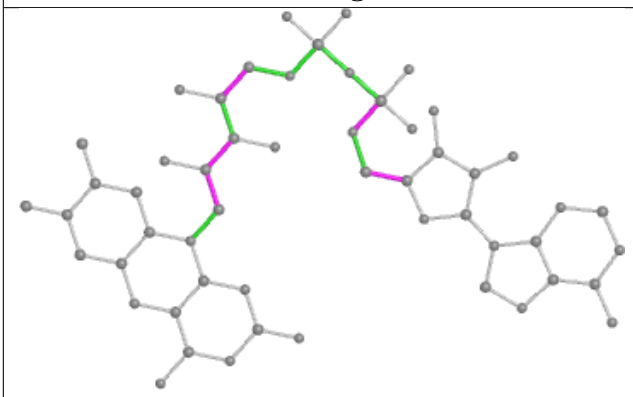
## Ligand FAD D 3005



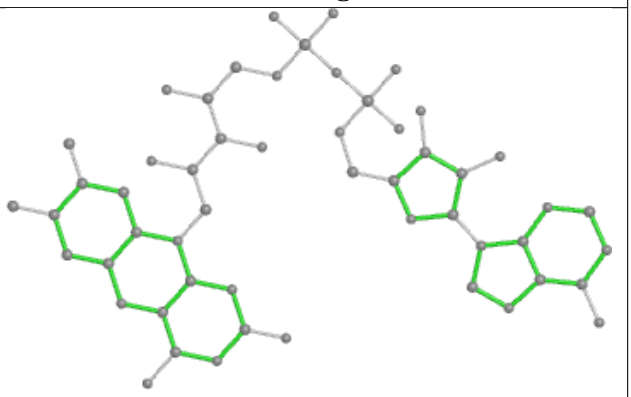
Bond lengths



Bond angles

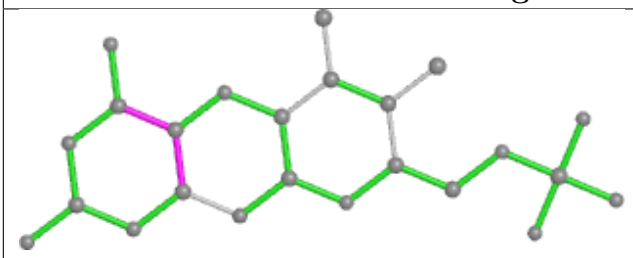


Torsions

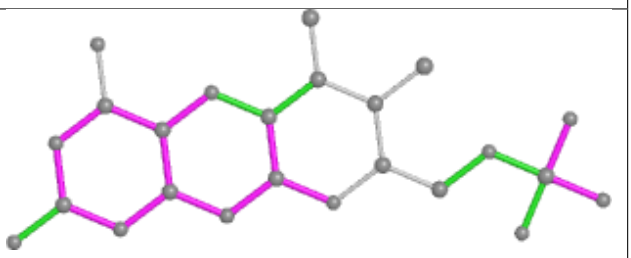


Rings

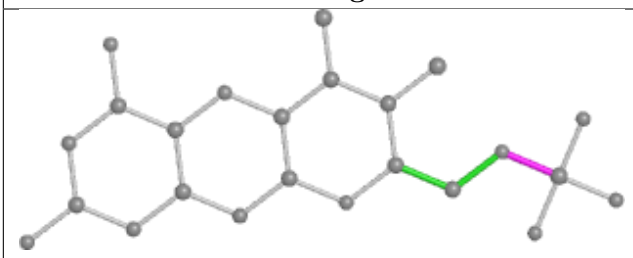
## Ligand MTE B 3003



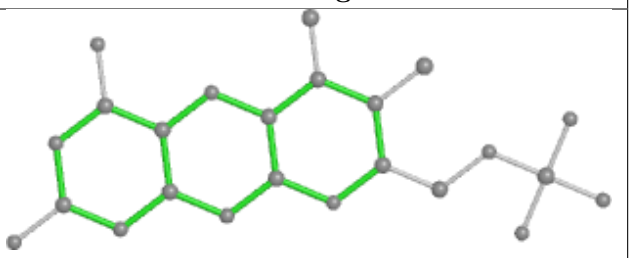
Bond lengths



Bond angles

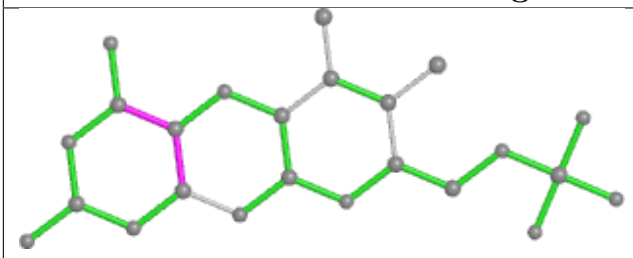


Torsions

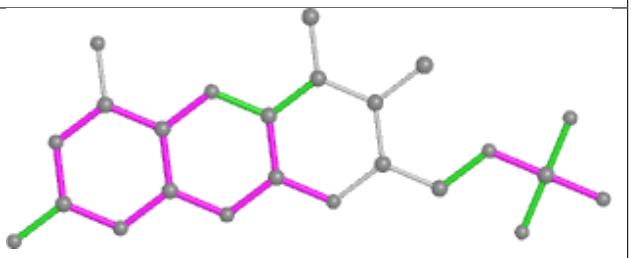


Rings

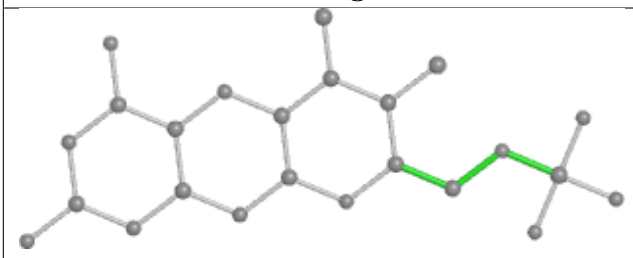
## Ligand MTE C 3003



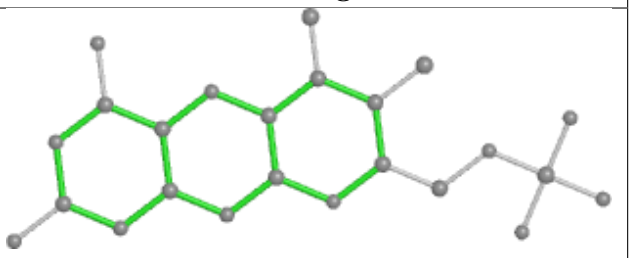
Bond lengths



Bond angles

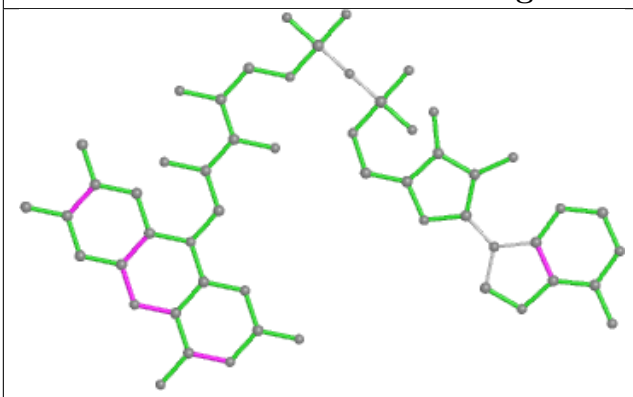


Torsions

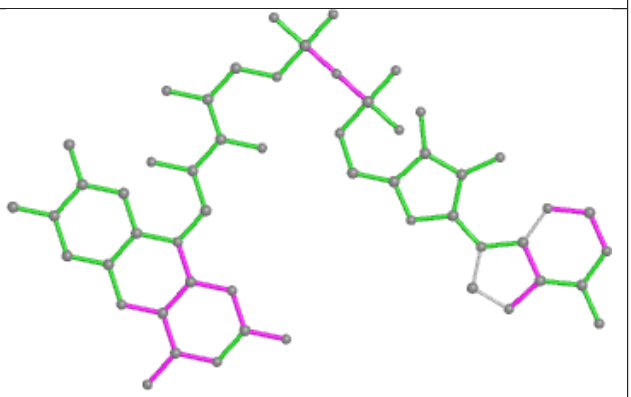


Rings

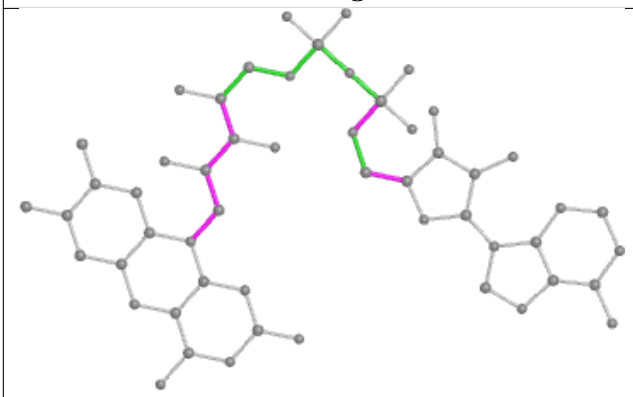
## Ligand FAD C 3005



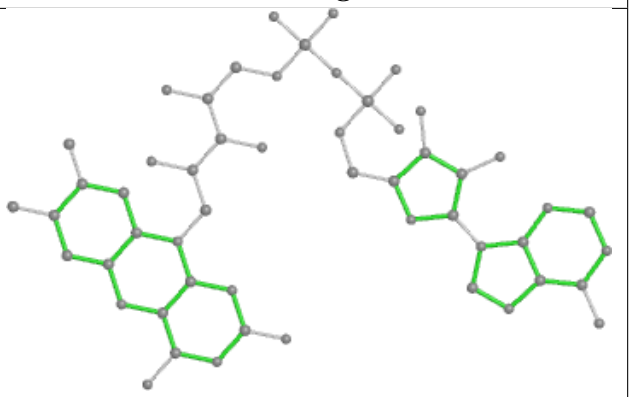
Bond lengths



Bond angles

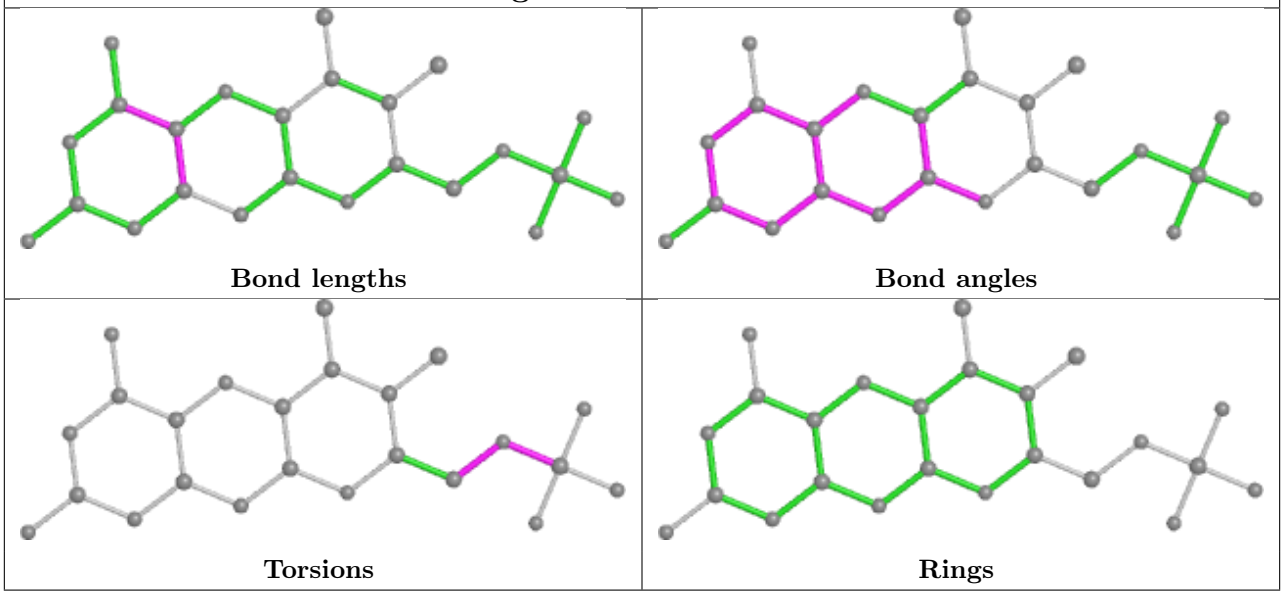


Torsions

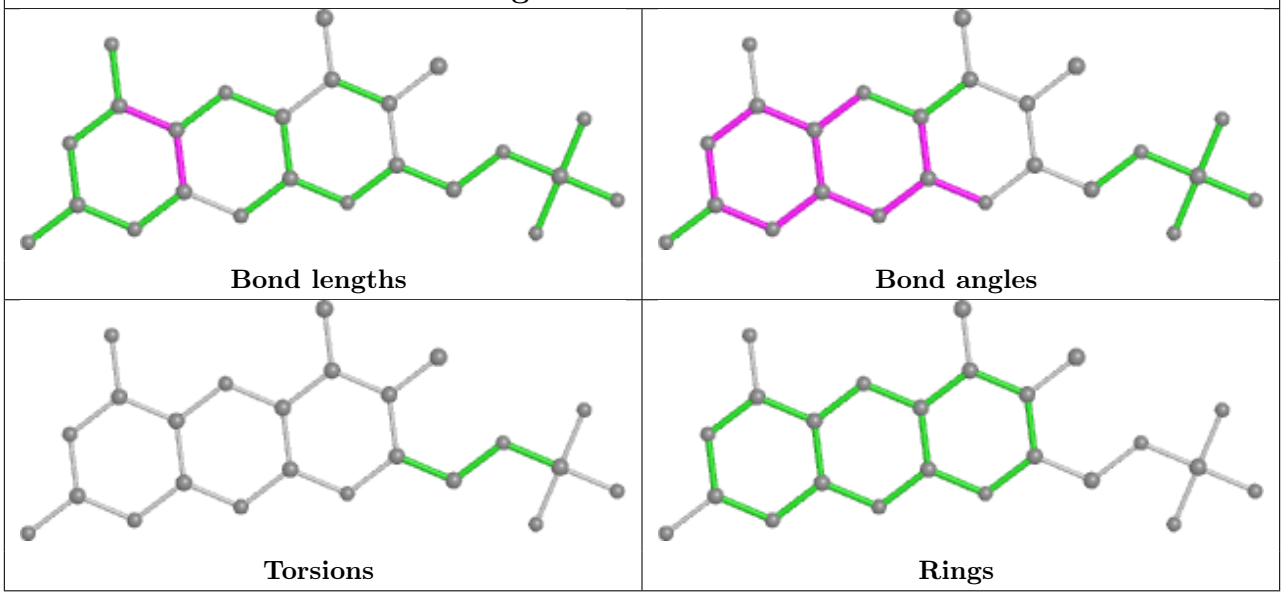


Rings

**Ligand MTE D 3003**




**Ligand MTE A 3003**




## 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, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 1253/1335 (93%) | 0.43 | 69 (5%) | 25 | 30 | 12, 40, 70, 88 | 0 |
| 1 | B | 1262/1335 (94%) | 0.44 | 68 (5%) | 25 | 30 | 10, 39, 67, 87 | 0 |
| 1 | C | 1244/1335 (93%) | 0.48 | 88 (7%) | 16 | 19 | 18, 43, 73, 99 | 0 |
| 1 | D | 1257/1335 (94%) | 0.66 | 125 (9%) | 7 | 9 | 20, 45, 79, 97 | 0 |
| All | All | 5016/5340 (93%) | 0.50 | 350 (6%) | 16 | 19 | 10, 42, 73, 99 | 0 |

The worst 5 of 350 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 477 | CYS | 7.0 |
| 1 | C | 937 | ALA | 6.1 |
| 1 | D | 492 | ASP | 5.3 |
| 1 | B | 728 | PHE | 5.1 |
| 1 | D | 278 | THR | 5.0 |

## 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 monosaccharides in this entry.

## 6.4 Ligands (i)

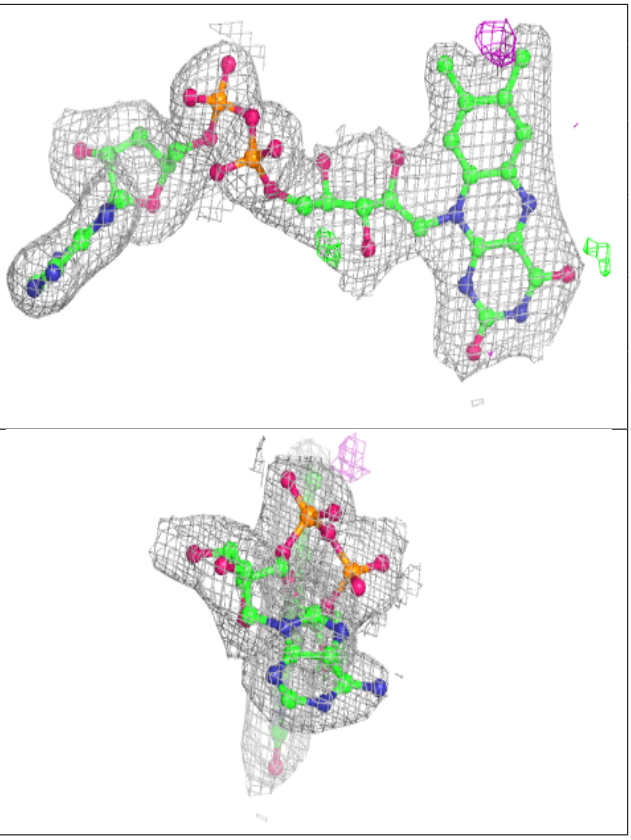
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

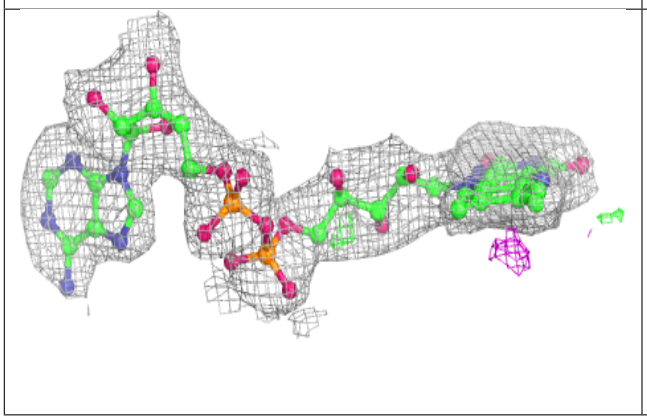
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | NA | C | 2337 | 1/1 | 0.89 | 0.16 | 50,50,50,50 | 0 |
| 2 | NA | A | 2337 | 1/1 | 0.90 | 0.14 | 26,26,26,26 | 0 |
| 6 | FAD | B | 3005 | 53/53 | 0.94 | 0.16 | 7,31,43,51 | 0 |
| 6 | FAD | C | 3005 | 53/53 | 0.94 | 0.15 | 9,31,49,50 | 0 |
| 6 | FAD | D | 3005 | 53/53 | 0.94 | 0.15 | 6,33,46,53 | 0 |
| 2 | NA | B | 2337 | 1/1 | 0.96 | 0.16 | 12,12,12,12 | 0 |
| 4 | MTE | B | 3003 | 24/24 | 0.96 | 0.17 | 15,35,49,67 | 0 |
| 6 | FAD | A | 3005 | 53/53 | 0.96 | 0.14 | 9,28,45,49 | 0 |
| 4 | MTE | A | 3003 | 24/24 | 0.97 | 0.17 | 12,27,37,42 | 0 |
| 3 | FES | C | 3002 | 4/4 | 0.97 | 0.08 | 29,33,36,38 | 0 |
| 4 | MTE | C | 3003 | 24/24 | 0.97 | 0.16 | 7,32,46,61 | 0 |
| 4 | MTE | D | 3003 | 24/24 | 0.97 | 0.18 | 13,33,49,53 | 0 |
| 5 | MOS | B | 3004 | 4/4 | 0.98 | 0.15 | 42,55,69,77 | 0 |
| 5 | MOS | D | 3004 | 4/4 | 0.98 | 0.16 | 42,55,69,77 | 0 |
| 3 | FES | A | 3002 | 4/4 | 0.98 | 0.09 | 16,23,33,38 | 0 |
| 3 | FES | B | 3002 | 4/4 | 0.98 | 0.11 | 20,21,34,38 | 0 |
| 3 | FES | C | 3001 | 4/4 | 0.98 | 0.12 | 24,24,31,39 | 0 |
| 2 | NA | D | 2337 | 1/1 | 0.98 | 0.17 | 17,17,17,17 | 0 |
| 5 | MOS | C | 3004 | 4/4 | 0.99 | 0.09 | 42,55,69,77 | 0 |
| 3 | FES | A | 3001 | 4/4 | 0.99 | 0.14 | 19,20,23,26 | 0 |
| 3 | FES | D | 3001 | 4/4 | 0.99 | 0.13 | 15,23,23,26 | 0 |
| 3 | FES | D | 3002 | 4/4 | 0.99 | 0.10 | 15,24,25,41 | 0 |
| 5 | MOS | A | 3004 | 4/4 | 0.99 | 0.12 | 42,55,69,77 | 0 |
| 3 | FES | B | 3001 | 4/4 | 0.99 | 0.14 | 7,20,22,26 | 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 FAD B 3005:**

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

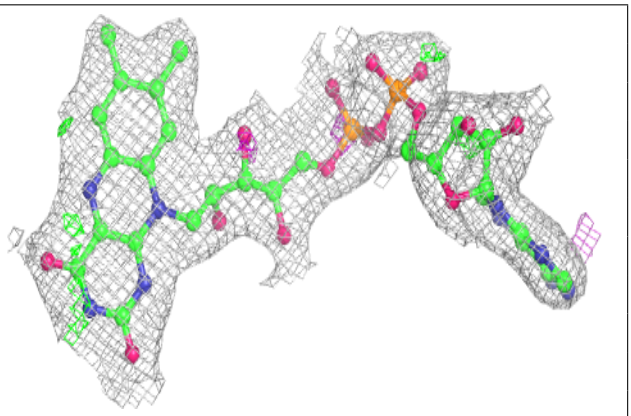


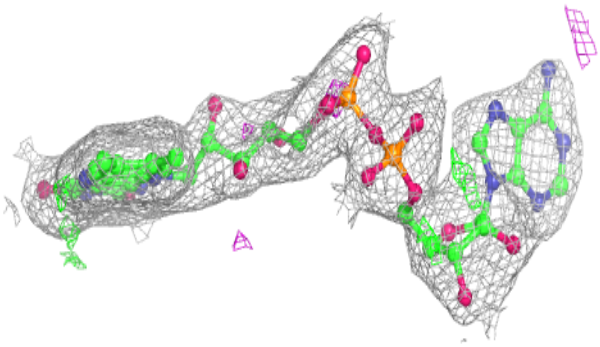


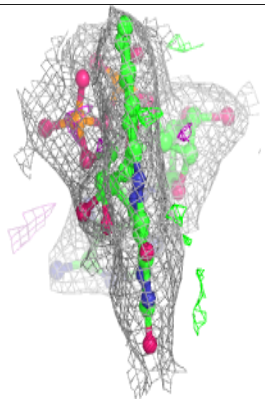


**Electron density around FAD C 3005:**

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







**Electron density around FAD D 3005:**

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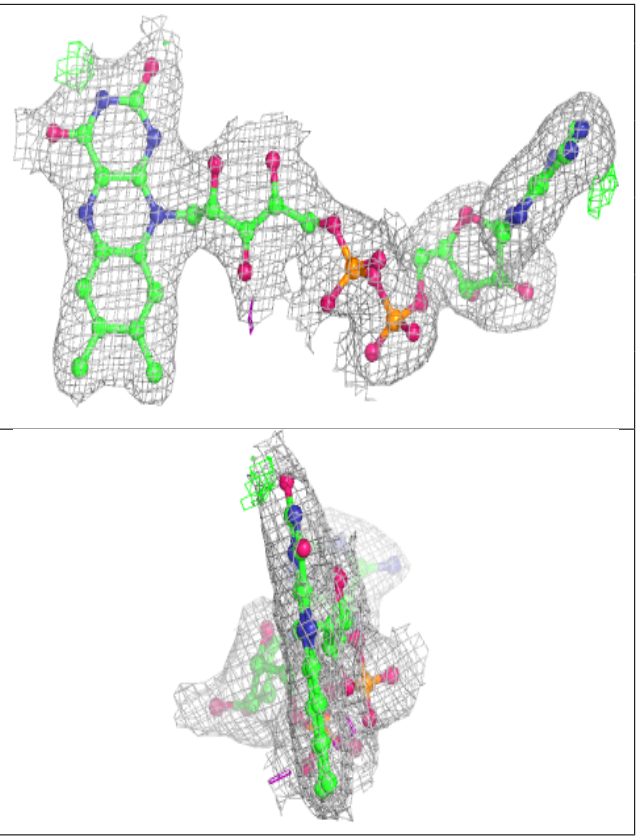
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



**Electron density around MTE B 3003:**

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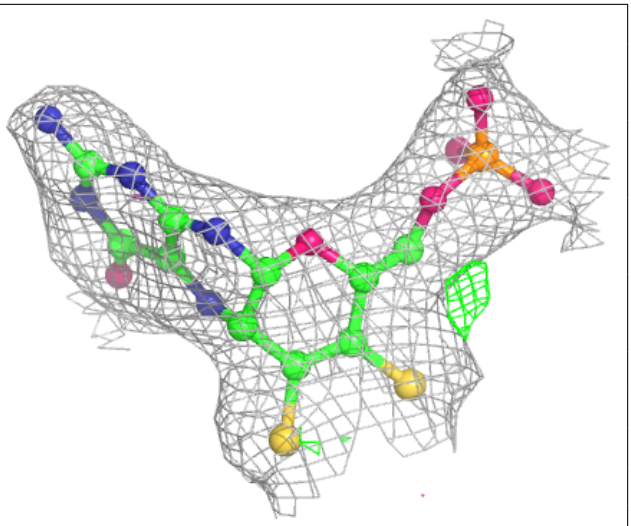
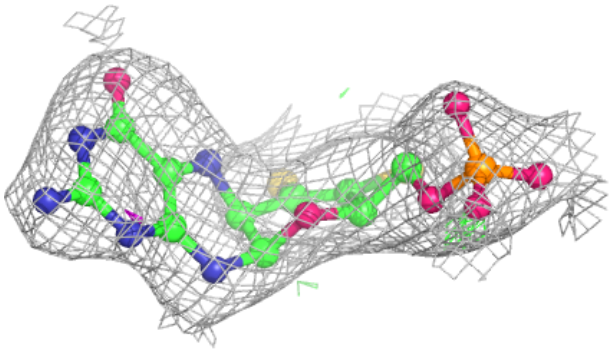
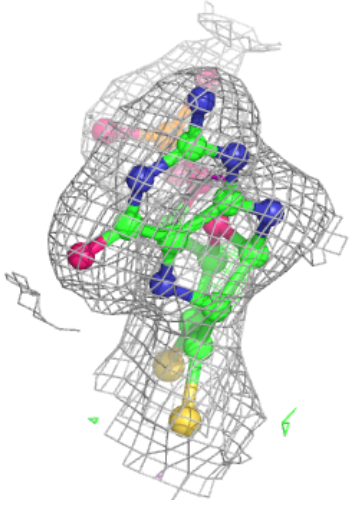
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)







**Electron density around FAD A 3005:**

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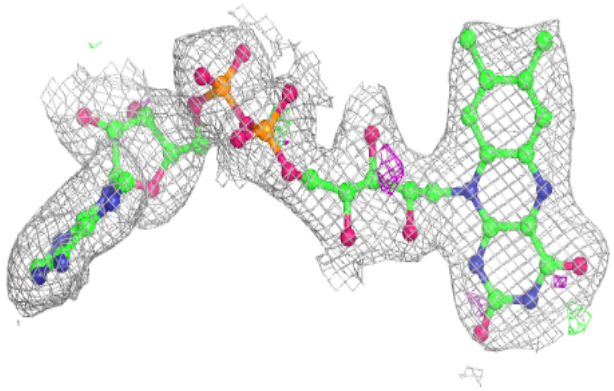
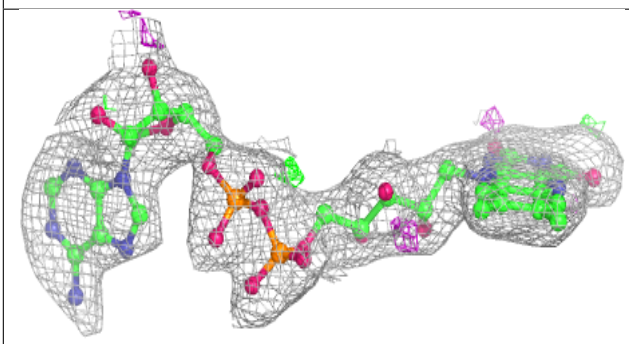
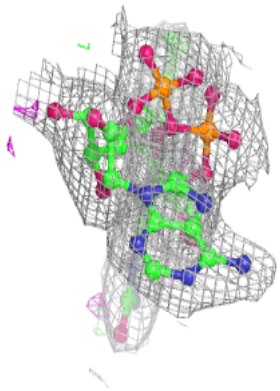
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)







**Electron density around MTE A 3003:**

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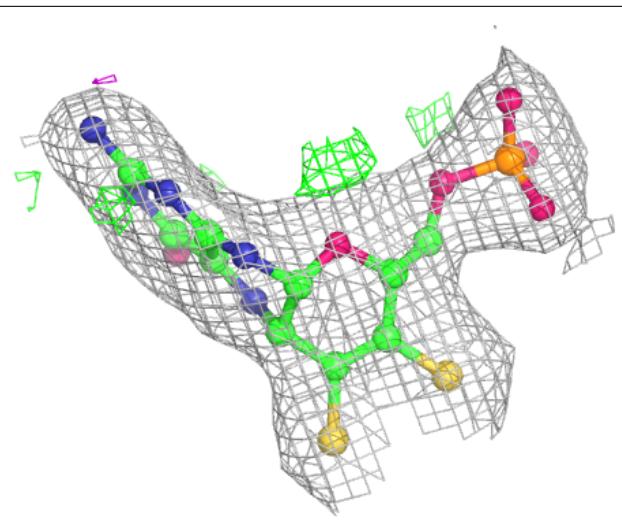
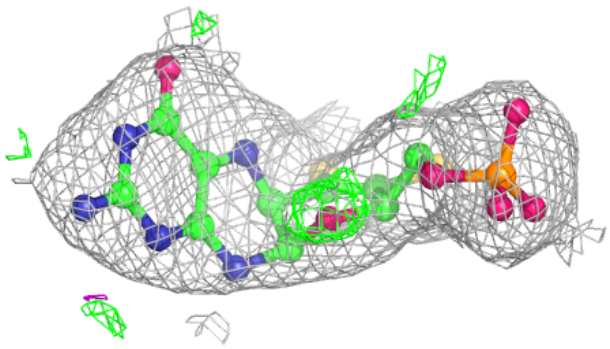
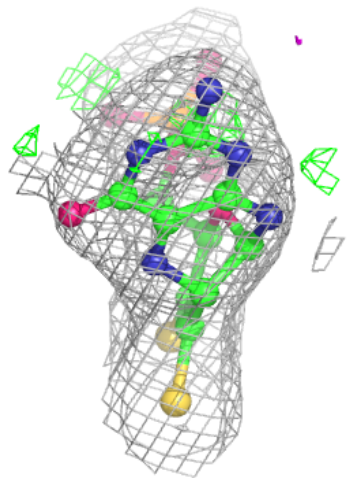
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

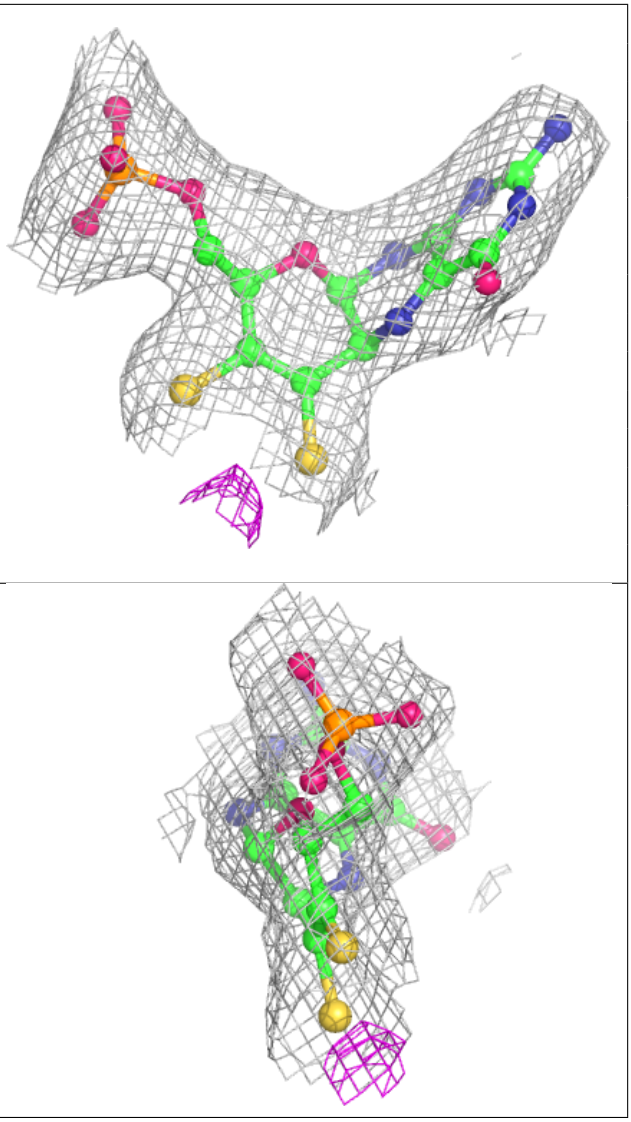






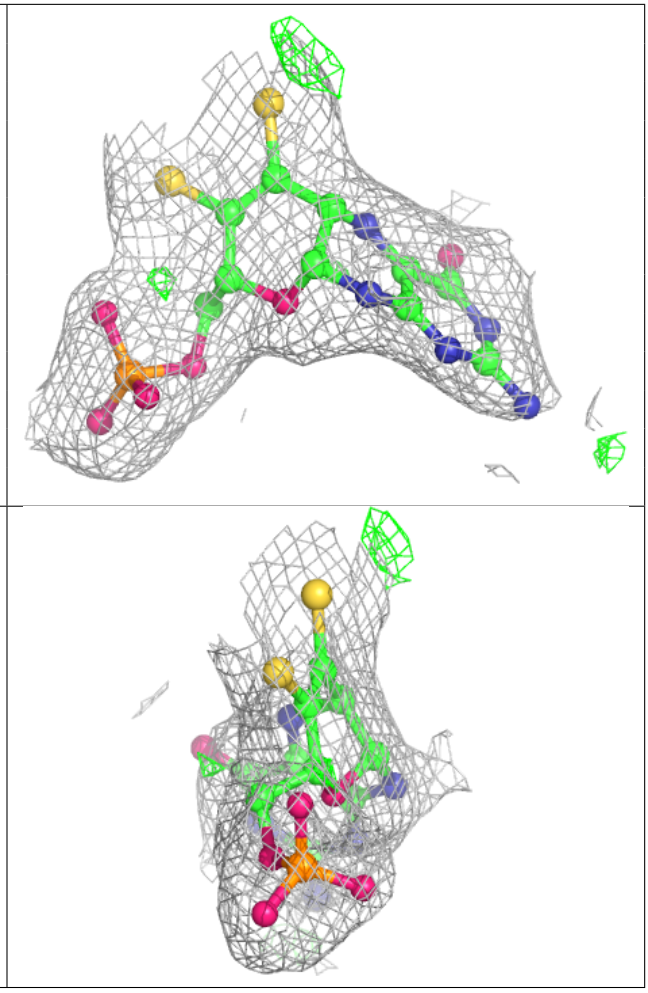
**Electron density around MTE C 3003:**

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



**Electron density around MTE D 3003:**

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



## 6.5 Other polymers (i)

There are no such residues in this entry.