# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2020 – 02:56 PM BST

| | | |
|---|---|---|
| PDB ID | : | 6DVH |
| Title | : | Lactate Monooxygenase from Mycobacterium smegmatis - C203A mutant |
| Authors | : | Kean, K.M.; Karplus, P.A. |
| Deposited on | : | 2018-06-23 |
| Resolution | : | 1.70 Å(reported) |

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

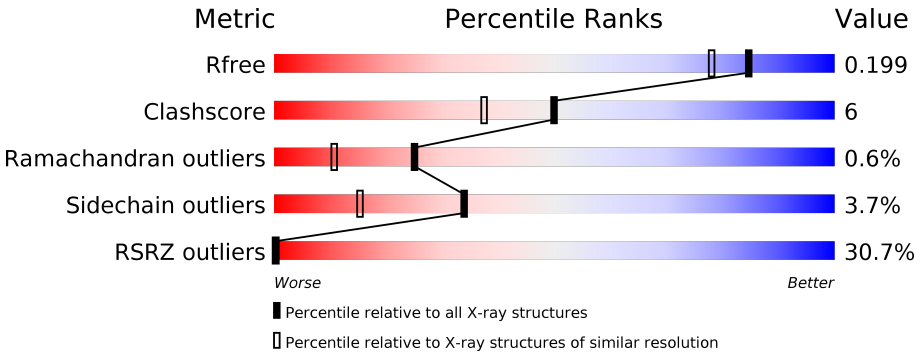
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.14.3.dev2 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 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) | : | 2.14.3.dev2 |

# 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 1.70 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 | 4298 (1.70-1.70) |
| Clashscore | 141614 | 4695 (1.70-1.70) |
| Ramachandran outliers | 138981 | 4610 (1.70-1.70) |
| Sidechain outliers | 138945 | 4610 (1.70-1.70) |
| RSRZ outliers | 127900 | 4222 (1.70-1.70) |

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 >=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 | 394 | 5% 91% 8% · |
| 1 | B | 394 | 13% 89% 9% ·· |
| 1 | C | 394 | 11% 92% 6% · |
| 1 | D | 394 | 22% 86% 13% · |
| 1 | E | 394 | 61% 85% 13% · |
| 1 | F | 394 | 72% 85% 13% · |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20104 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.

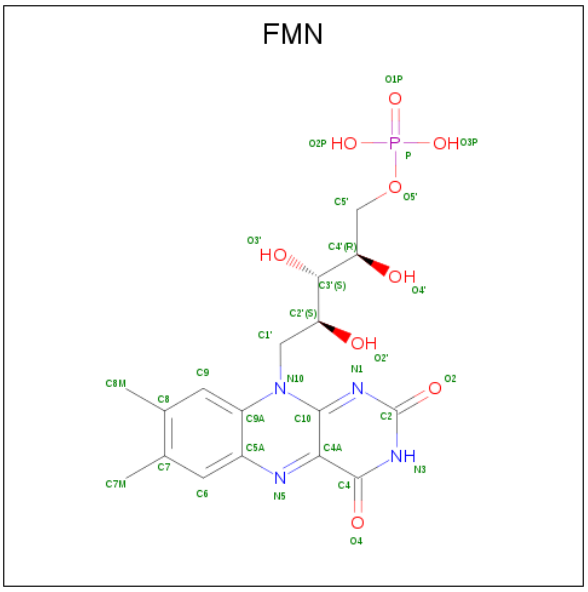
- Molecule 1 is a protein called Lactate 2-monooxygenase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 394 | Total | C | N | O | S | 0 | 12 | 0 |
| | | | 3080 | 1964 | 533 | 571 | 12 | | | |
| 1 | B | 394 | Total | C | N | O | S | 0 | 22 | 0 |
| | | | 3166 | 2020 | 548 | 586 | 12 | | | |
| 1 | C | 394 | Total | C | N | O | S | 0 | 7 | 0 |
| | | | 3066 | 1949 | 540 | 565 | 12 | | | |
| 1 | D | 394 | Total | C | N | O | S | 0 | 7 | 0 |
| | | | 3062 | 1949 | 535 | 566 | 12 | | | |
| 1 | E | 394 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 3043 | 1935 | 530 | 566 | 12 | | | |
| 1 | F | 393 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 3037 | 1933 | 529 | 564 | 11 | | | |

There are 6 discrepancies between the modelled and reference sequences:

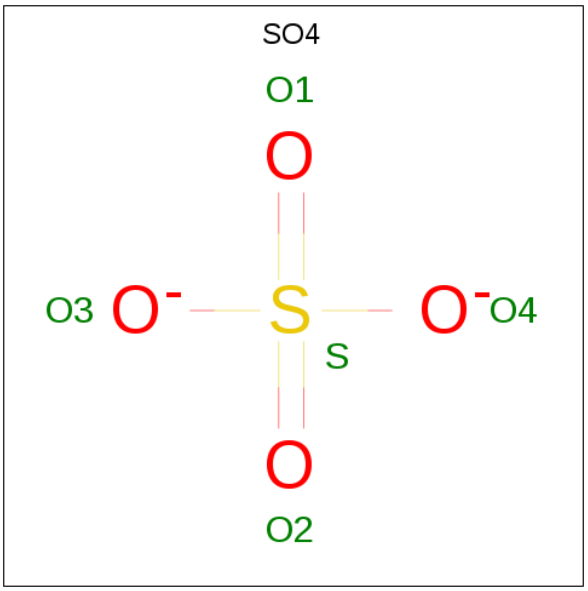
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 203 | ALA | CYS | engineered mutation | UNP P21795 |
| B | 203 | ALA | CYS | engineered mutation | UNP P21795 |
| C | 203 | ALA | CYS | engineered mutation | UNP P21795 |
| D | 203 | ALA | CYS | engineered mutation | UNP P21795 |
| E | 203 | ALA | CYS | engineered mutation | UNP P21795 |
| F | 203 | ALA | CYS | engineered mutation | UNP P21795 |

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 2 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: $O_4S$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | A | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | A | 1 | Total O S<br>5 4 1 | 0 | 1 |
| 3 | A | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | B | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | B | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | B | 1 | Total O S<br>5 4 1 | 0 | 1 |
| 3 | B | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | B | 1 | Total O S<br>5 4 1 | 0 | 1 |
| 3 | C | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | C | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | C | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | D | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | D | 1 | Total O S<br>5 4 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | E | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | E | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | F | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | F | 1 | Total O S<br>5 4 1 | 0 | 0 |

- Molecule 4 is water.

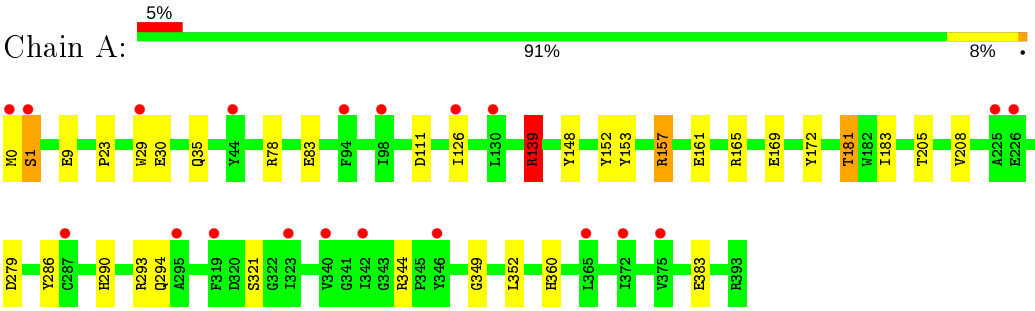
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 499 | Total O<br>499 499 | 0 | 4 |
| 4 | B | 358 | Total O<br>358 358 | 0 | 4 |
| 4 | C | 313 | Total O<br>313 313 | 0 | 2 |
| 4 | D | 182 | Total O<br>182 182 | 0 | 2 |
| 4 | E | 13 | Total O<br>13 13 | 0 | 0 |
| 4 | F | 9 | Total O<br>9 9 | 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.

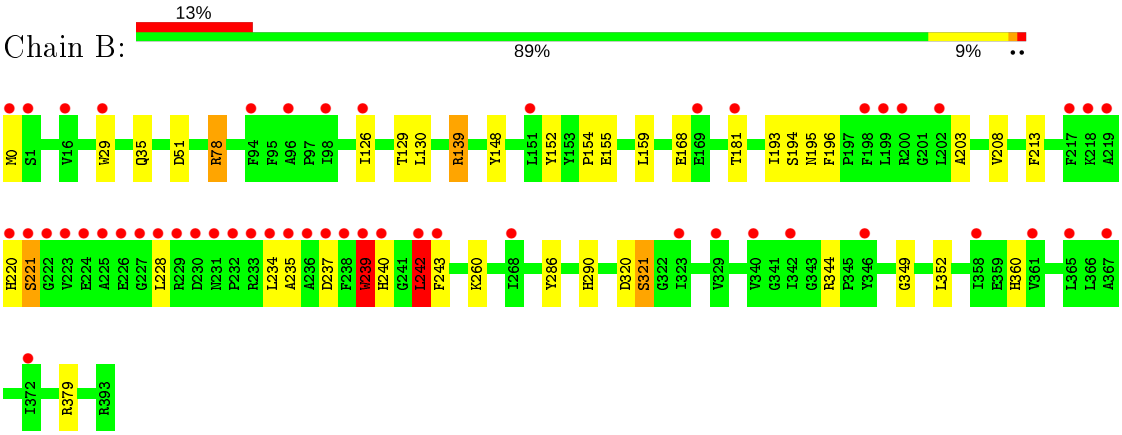
- Molecule 1: Lactate 2-monooxygenase

Chain A:



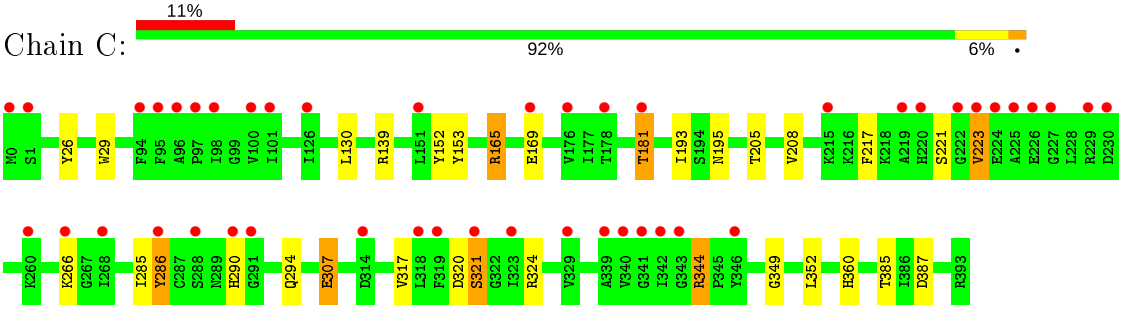

- Molecule 1: Lactate 2-monooxygenase

Chain B:



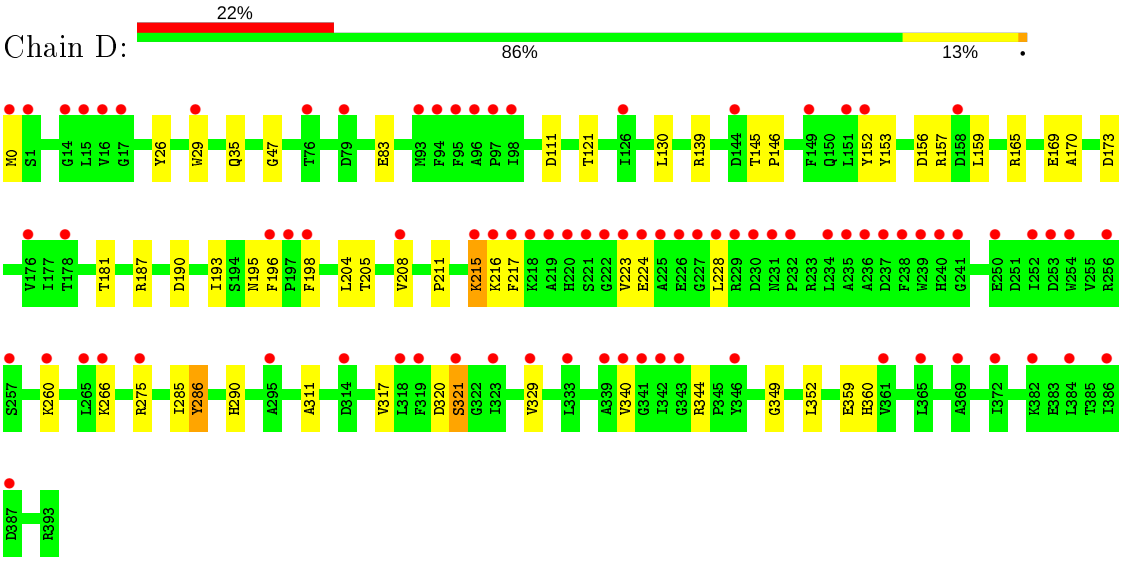

- Molecule 1: Lactate 2-monooxygenase

Chain C:



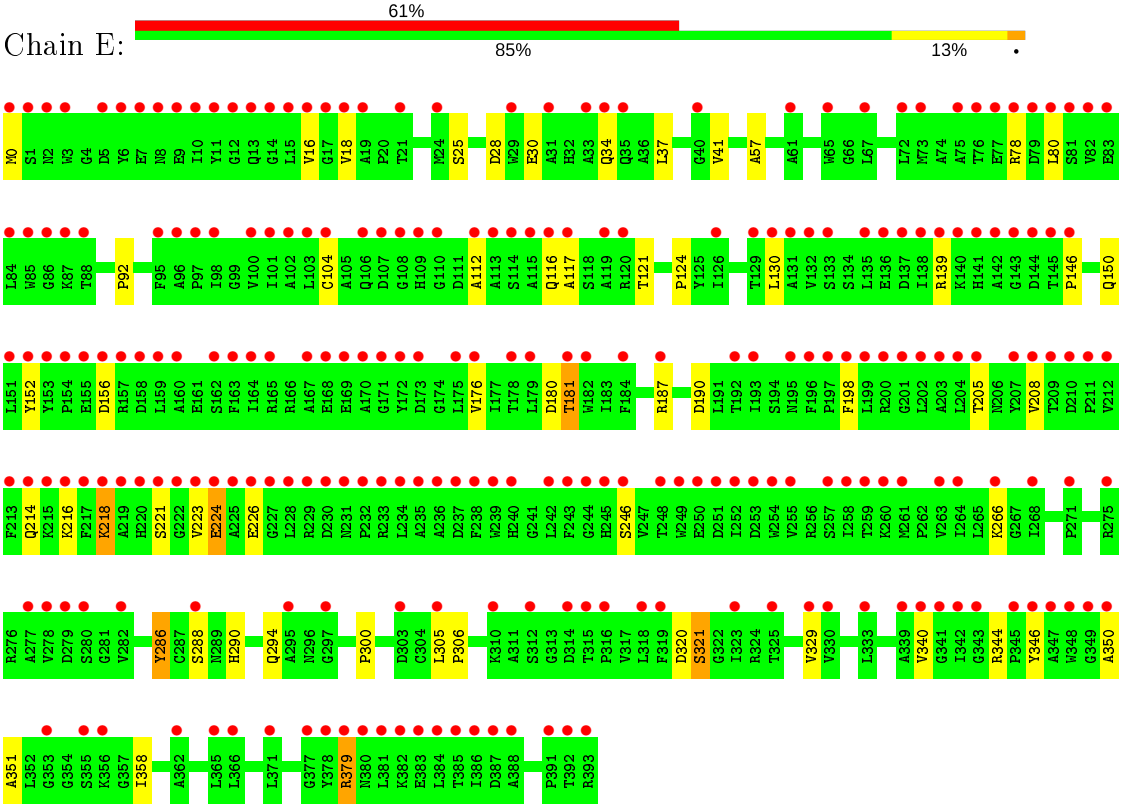

- Molecule 1: Lactate 2-monooxygenase

Chain D:



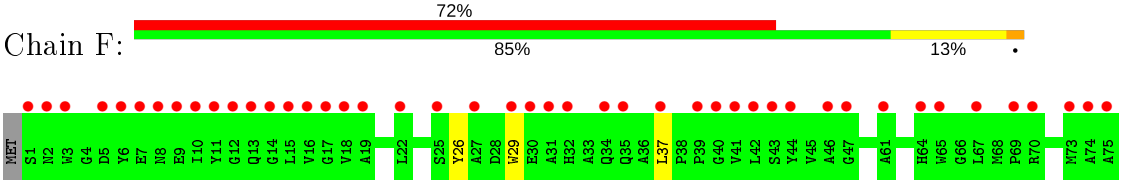

- Molecule 1: Lactate 2-monooxygenase

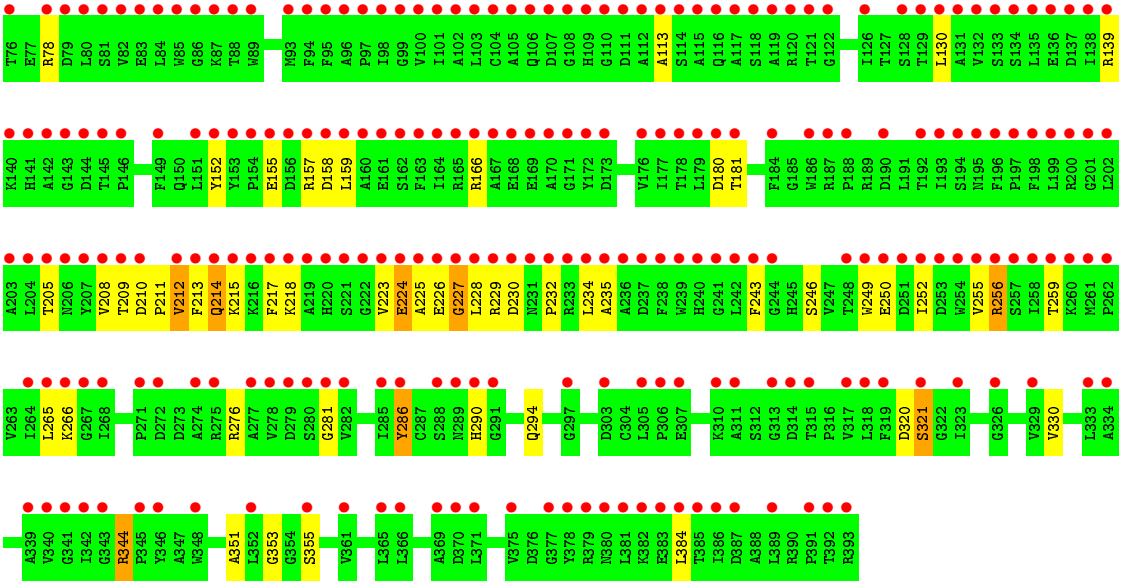
Chain E:




- Molecule 1: Lactate 2-monooxygenase

Chain F:




T76 E77 R78 D79 L80 S81 V82 E83 L84 W85 G86 K87 T88 W89
M93 F94 F95 A96 P97 I98 G99 V100 I101 A102 L103 C104 A105 Q106 D107 G108 H109 G110 D111 A112 A113 S114 A115 Q116 A117 S118 A119 R120 T121 G122
I126 T127 S128 T129 L130 A131 V132 S133 S134 L135 E136 D137 I138 R139
K140 H141 A142 G143 D144 T145 P146
F149 Q150 L151 Y152 Y153 P154 E155 D156 R157 D158 L159 A160 E161 S162 F163 I164 R165 R166 A167 E168 E169 A170 G171 Y172 D173
V176 I177 T178 L179 D180 T181
F184 G185 W186 R187 P188 R189 D190 L191 T192 I193 S194 N195 F196 P197 F198 L199 R200 G201 L202
A203 L204 T205 N206 Y207 V208 T209 D210 P211 V212 F213 Q214 K215 K216 F217 K218 A219 H220 S221 G222 V223 E224 A225 E226 G227 L228 R229 D230 N231 P232 R233 L234 A235 A236 D237 F238 W239 H240 G241 L242 F243 G244 H245 S246 V247 T248 W249 E250 D251 I252 D253 W254 V255 R256 S257 I258 T259 K260 M261 P262
V263 I264 L265 K266 G267 I268
P271 D272 D273 A274 R275 R276
A277 V278 D279 S280 G281 V282
I285 Y286 C287 S288 N289 H290 G291
Q294
G297
D303 C304 L305 P306 E307
K310 A311 S312 G313 D314 T315 P316 V317 L318 F319 D320 S321 G322 I323
G326
V329 V330
L333 A334
A339 Y340 G341 I342 G343 R344 P345 Y346 A347 W348
A351 L352 G353 G354 S355
V361
L365 L366
A369 D370 I371
V375 D376 G377 Y378 R379 N380 L381 K382 E383 L384 T385 I386 D387 A388 L389 R390 P391 T392 R393

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 4 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 149.62Å 149.62Å 274.25Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.90 – 1.70<br>30.90 – 1.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.9 (30.90-1.70)<br>100.0 (30.90-1.70) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.48 (at 1.70Å) | Xtriage |
| Refinement program | PHENIX (1.13_2998: ???) | Depositor |
| R, $R_{free}$ | 0.169 , 0.194<br>0.176 , 0.199 | Depositor<br>DCC |
| $R_{free}$ test set | 34003 reflections (10.06%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 30.5 | Xtriage |
| Anisotropy | 0.223 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 58.3 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.97 | EDS |
| Total number of atoms | 20104 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 68.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.64% 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

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SO4

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 | 0.84 | 1/3197 (0.0%) | 0.86 | 3/4353 (0.1%) |
| 1 | B | 0.70 | 1/3286 (0.0%) | 0.80 | 6/4473 (0.1%) |
| 1 | C | 0.63 | 0/3168 | 0.71 | 1/4311 (0.0%) |
| 1 | D | 0.51 | 0/3164 | 0.60 | 0/4306 |
| 1 | E | 0.36 | 0/3140 | 0.49 | 0/4275 |
| 1 | F | 0.34 | 0/3134 | 0.51 | 0/4268 |
| All | All | 0.60 | 2/19089 (0.0%) | 0.68 | 10/25986 (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 | B | 0 | 2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 30 | GLU | CD-OE2 | -8.02 | 1.16 | 1.25 |
| 1 | B | 78 | ARG | CG-CD | -5.07 | 1.39 | 1.51 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 78 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 1 | B | 78 | ARG | NE-CZ-NH2 | -6.41 | 117.10 | 120.30 |
| 1 | A | 139 | ARG | NE-CZ-NH1 | -6.09 | 117.25 | 120.30 |
| 1 | A | 111 | ASP | CB-CG-OD1 | 6.04 | 123.74 | 118.30 |
| 1 | B | 78 | ARG | CA-CB-CG | -5.82 | 100.59 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 344 | ARG | NE-CZ-NH2 | 5.26 | 122.93 | 120.30 |
| 1 | B | 51 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 1 | B | 242[A] | LEU | CB-CG-CD2 | 5.20 | 119.84 | 111.00 |
| 1 | B | 242[B] | LEU | CB-CG-CD2 | 5.20 | 119.84 | 111.00 |
| 1 | A | 293 | ARG | NE-CZ-NH1 | -5.08 | 117.76 | 120.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 239[A] | TRP | Peptide |
| 1 | B | 242[A] | LEU | 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 | 3080 | 0 | 3026 | 24 | 0 |
| 1 | B | 3166 | 0 | 3083 | 44 | 0 |
| 1 | C | 3066 | 0 | 3002 | 28 | 0 |
| 1 | D | 3062 | 0 | 2997 | 38 | 0 |
| 1 | E | 3043 | 0 | 2978 | 33 | 0 |
| 1 | F | 3037 | 0 | 2975 | 45 | 0 |
| 2 | A | 31 | 0 | 19 | 0 | 0 |
| 2 | B | 31 | 0 | 19 | 0 | 0 |
| 2 | C | 31 | 0 | 19 | 1 | 0 |
| 2 | D | 31 | 0 | 19 | 1 | 0 |
| 2 | E | 31 | 0 | 19 | 0 | 0 |
| 2 | F | 31 | 0 | 19 | 1 | 0 |
| 3 | A | 20 | 0 | 0 | 0 | 0 |
| 3 | B | 25 | 0 | 0 | 0 | 0 |
| 3 | C | 15 | 0 | 0 | 0 | 0 |
| 3 | D | 10 | 0 | 0 | 0 | 0 |
| 3 | E | 10 | 0 | 0 | 0 | 0 |
| 3 | F | 10 | 0 | 0 | 0 | 0 |
| 4 | A | 499 | 0 | 0 | 5 | 2 |
| 4 | B | 358 | 0 | 0 | 6 | 1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | C | 313 | 0 | 0 | 1 | 1 |
| 4 | D | 182 | 0 | 0 | 5 | 0 |
| 4 | E | 13 | 0 | 0 | 0 | 0 |
| 4 | F | 9 | 0 | 0 | 0 | 0 |
| All | All | 20104 | 0 | 18175 | 213 | 2 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (213) 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:A:383:GLU:OE2 | 4:A:501:HOH:O | 1.82 | 0.97 |
| 1:A:139:ARG:NH1 | 4:A:502:HOH:O | 1.97 | 0.96 |
| 1:B:240[A]:HIS:O | 1:B:243[A]:PHE:N | 2.02 | 0.93 |
| 1:C:181[B]:THR:HG22 | 1:C:294:GLN:HG3 | 1.55 | 0.89 |
| 1:B:237[A]:ASP:O | 1:B:239[A]:TRP:N | 2.06 | 0.88 |
| 1:D:145:THR:O | 4:D:501:HOH:O | 1.93 | 0.85 |
| 1:D:139[A]:ARG:NH1 | 4:D:501:HOH:O | 2.03 | 0.84 |
| 1:D:329:VAL:HG13 | 1:D:340[B]:VAL:HG21 | 1.64 | 0.79 |
| 1:B:155:GLU:H | 1:B:242[A]:LEU:CD1 | 1.96 | 0.78 |
| 1:F:205:THR:O | 1:F:209:THR:HG23 | 1.84 | 0.78 |
| 1:B:154:PRO:HB2 | 1:B:242[A]:LEU:HD11 | 1.66 | 0.78 |
| 1:F:256:ARG:NH2 | 1:F:281:GLY:O | 2.17 | 0.78 |
| 1:E:181[B]:THR:HG22 | 1:E:294:GLN:HG3 | 1.64 | 0.77 |
| 1:F:225:ALA:HA | 1:F:228:LEU:HB3 | 1.71 | 0.73 |
| 1:E:181[B]:THR:HG21 | 1:E:290:HIS:CE1 | 2.24 | 0.72 |
| 1:F:212:VAL:O | 1:F:215:LYS:N | 2.21 | 0.72 |
| 1:A:152:TYR:HE1 | 1:A:181[A]:THR:HG23 | 1.54 | 0.72 |
| 1:C:181[B]:THR:HG21 | 1:C:290:HIS:CE1 | 2.24 | 0.72 |
| 1:E:112:ALA:O | 1:E:116:GLN:HG3 | 1.92 | 0.70 |
| 1:B:29[B]:TRP:CE3 | 1:B:352:LEU:HD12 | 2.25 | 0.70 |
| 1:B:168:GLU:OE1 | 4:B:501:HOH:O | 2.09 | 0.70 |
| 1:A:279[A]:ASP:OD2 | 4:A:503:HOH:O | 2.10 | 0.69 |
| 1:B:29[B]:TRP:HZ2 | 1:B:360:HIS:HD2 | 1.38 | 0.69 |
| 1:A:29[B]:TRP:CE3 | 1:A:352:LEU:HD12 | 2.29 | 0.67 |
| 1:F:181[B]:THR:HG22 | 1:F:294:GLN:HG3 | 1.76 | 0.67 |
| 1:B:155:GLU:N | 1:B:242[A]:LEU:CD1 | 2.58 | 0.66 |
| 1:C:205:THR:HA | 1:C:208[A]:VAL:HG22 | 1.79 | 0.65 |
| 1:B:234:LEU:HD11 | 4:B:648:HOH:O | 1.97 | 0.64 |
| 1:F:226:GLU:O | 1:F:230:ASP:N | 2.29 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:29[B]:TRP:HZ2 | 1:A:360:HIS:HD2 | 1.46 | 0.64 |
| 1:C:152:TYR:HE1 | 1:C:181[A]:THR:HG23 | 1.63 | 0.63 |
| 1:F:208[B]:VAL:HG22 | 1:F:228:LEU:HG | 1.79 | 0.63 |
| 1:A:35[A]:GLN:NE2 | 4:A:504:HOH:O | 2.11 | 0.63 |
| 1:E:221:SER:OG | 1:E:223:VAL:HG13 | 1.99 | 0.62 |
| 1:B:237[B]:ASP:OD1 | 1:B:237[B]:ASP:N | 2.33 | 0.62 |
| 1:B:29[B]:TRP:CZ3 | 1:B:352:LEU:HD12 | 2.37 | 0.60 |
| 1:B:155:GLU:N | 1:B:242[A]:LEU:HD11 | 2.17 | 0.60 |
| 1:A:181[A]:THR:HG21 | 1:A:290:HIS:CE1 | 2.36 | 0.60 |
| 1:A:294:GLN:OE1 | 4:A:505[B]:HOH:O | 2.17 | 0.60 |
| 1:D:266:LYS:HA | 1:D:286:TYR:HB3 | 1.83 | 0.60 |
| 1:F:249:TRP:CH2 | 1:F:276:ARG:HG2 | 2.37 | 0.60 |
| 1:C:29[B]:TRP:HZ2 | 1:C:360:HIS:HD2 | 1.50 | 0.59 |
| 1:F:225:ALA:HA | 1:F:228:LEU:CB | 2.31 | 0.59 |
| 1:C:181[B]:THR:HG22 | 1:C:294:GLN:CG | 2.32 | 0.58 |
| 1:C:181[B]:THR:CG2 | 1:C:294:GLN:HG3 | 2.30 | 0.58 |
| 1:A:205:THR:HA | 1:A:208[A]:VAL:HG22 | 1.84 | 0.58 |
| 1:D:139[B]:ARG:HG2 | 1:D:170:ALA:O | 2.04 | 0.58 |
| 1:B:193:ILE:HG13 | 1:B:195:ASN:HB2 | 1.85 | 0.58 |
| 1:D:211:PRO:O | 1:D:215:LYS:HG2 | 2.03 | 0.58 |
| 1:E:266:LYS:HA | 1:E:286:TYR:HB3 | 1.86 | 0.58 |
| 1:F:255:VAL:O | 1:F:259:THR:HG22 | 2.04 | 0.57 |
| 1:B:155:GLU:H | 1:B:242[A]:LEU:HD13 | 1.68 | 0.57 |
| 1:A:139:ARG:HG2 | 1:A:172:TYR:CZ | 2.41 | 0.56 |
| 1:D:208:VAL:HG12 | 1:D:228:LEU:HG | 1.86 | 0.56 |
| 1:C:165:ARG:O | 1:C:169:GLU:HG3 | 2.06 | 0.55 |
| 1:D:29[A]:TRP:HZ2 | 1:D:360:HIS:HD2 | 1.53 | 0.55 |
| 1:E:180:ASP:OD1 | 1:E:181[B]:THR:HG23 | 2.06 | 0.55 |
| 1:A:152:TYR:CE1 | 1:A:181[A]:THR:HG23 | 2.39 | 0.55 |
| 1:A:29[B]:TRP:CZ3 | 1:A:352:LEU:HD12 | 2.43 | 0.54 |
| 1:B:239[A]:TRP:CE3 | 1:B:239[A]:TRP:HA | 2.43 | 0.54 |
| 1:D:139[A]:ARG:HG2 | 1:D:170:ALA:O | 2.08 | 0.54 |
| 1:D:29[A]:TRP:CE3 | 1:D:352:LEU:HD12 | 2.43 | 0.54 |
| 1:C:29[B]:TRP:CE3 | 1:C:352:LEU:HD12 | 2.43 | 0.54 |
| 1:D:130:LEU:HD13 | 1:D:198:PHE:CE1 | 2.43 | 0.54 |
| 1:E:130[B]:LEU:HD13 | 1:E:198:PHE:CZ | 2.43 | 0.54 |
| 1:C:29[B]:TRP:CZ3 | 1:C:349:GLY:HA2 | 2.43 | 0.53 |
| 1:B:239[A]:TRP:HB3 | 1:B:242[A]:LEU:H | 1.73 | 0.53 |
| 1:D:320:ASP:O | 1:D:321:SER:HB2 | 2.08 | 0.53 |
| 1:B:155:GLU:HB2 | 1:B:242[A]:LEU:HD13 | 1.90 | 0.53 |
| 1:F:205:THR:HA | 1:F:208[A]:VAL:HG22 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:29[B]:TRP:CZ2 | 1:A:360:HIS:HD2 | 2.27 | 0.53 |
| 1:E:187[B]:ARG:NE | 1:E:190:ASP:OD2 | 2.37 | 0.53 |
| 1:C:152:TYR:CE1 | 1:C:181[A]:THR:HG23 | 2.43 | 0.53 |
| 1:B:154:PRO:CB | 1:B:242[A]:LEU:HD11 | 2.36 | 0.52 |
| 1:F:266:LYS:HA | 1:F:286:TYR:HB3 | 1.91 | 0.52 |
| 1:C:266:LYS:HA | 1:C:286:TYR:HB3 | 1.90 | 0.52 |
| 1:C:152:TYR:CE1 | 1:C:181[B]:THR:OG1 | 2.62 | 0.52 |
| 1:D:205:THR:HA | 1:D:208:VAL:CG2 | 2.40 | 0.52 |
| 1:C:152:TYR:HE1 | 1:C:181[B]:THR:OG1 | 1.91 | 0.52 |
| 1:A:126:ILE:HG12 | 1:A:148:TYR:HB2 | 1.92 | 0.52 |
| 1:B:220:HIS:O | 1:B:221:SER:HB3 | 2.10 | 0.52 |
| 1:F:211:PRO:O | 1:F:214:GLN:C | 2.48 | 0.52 |
| 1:F:227:GLY:CA | 1:F:234:LEU:HD12 | 2.40 | 0.51 |
| 1:E:130[B]:LEU:HD13 | 1:E:198:PHE:CE1 | 2.45 | 0.51 |
| 1:F:26:TYR:HA | 1:F:29:TRP:CE3 | 2.45 | 0.51 |
| 1:D:187[B]:ARG:NH2 | 1:D:190:ASP:OD2 | 2.41 | 0.51 |
| 1:F:159:LEU:CA | 1:F:212:VAL:HG11 | 2.41 | 0.51 |
| 1:D:29[A]:TRP:CZ2 | 1:D:360:HIS:HD2 | 2.29 | 0.51 |
| 1:F:226:GLU:C | 1:F:228:LEU:N | 2.64 | 0.51 |
| 1:B:213:PHE:HE1 | 1:B:242[B]:LEU:HD21 | 1.77 | 0.50 |
| 1:B:239[A]:TRP:HA | 1:B:239[A]:TRP:HE3 | 1.75 | 0.50 |
| 1:F:250:GLU:N | 1:F:250:GLU:OE1 | 2.44 | 0.50 |
| 1:A:181[A]:THR:HG21 | 1:A:290:HIS:HE1 | 1.76 | 0.50 |
| 1:A:165:ARG:O | 1:A:169:GLU:HG3 | 2.12 | 0.50 |
| 1:A:29[B]:TRP:CZ3 | 1:A:349:GLY:HA2 | 2.47 | 0.50 |
| 1:F:210:ASP:O | 1:F:214:GLN:HB2 | 2.11 | 0.50 |
| 1:F:223:VAL:O | 1:F:223:VAL:HG12 | 2.11 | 0.50 |
| 1:B:242[A]:LEU:O | 1:B:242[A]:LEU:HD12 | 2.12 | 0.49 |
| 1:D:29[A]:TRP:HZ2 | 1:D:360:HIS:CD2 | 2.30 | 0.49 |
| 1:B:152:TYR:OH | 4:B:502:HOH:O | 2.19 | 0.49 |
| 1:B:220:HIS:O | 1:B:221:SER:CB | 2.61 | 0.49 |
| 1:E:350:ALA:HB2 | 1:E:358:ILE:HD11 | 1.93 | 0.49 |
| 1:B:242[A]:LEU:C | 1:B:242[A]:LEU:HD12 | 2.32 | 0.49 |
| 1:F:218:LYS:HD3 | 1:F:224:GLU:HG3 | 1.95 | 0.49 |
| 1:B:193:ILE:HG13 | 1:B:195:ASN:CB | 2.43 | 0.49 |
| 1:F:218:LYS:NZ | 1:F:224:GLU:OE1 | 2.45 | 0.49 |
| 1:F:130[A]:LEU:HD21 | 1:F:243:PHE:HE1 | 1.77 | 0.49 |
| 1:E:288:SER:OG | 1:E:320:ASP:OD1 | 2.27 | 0.48 |
| 1:E:205:THR:HA | 1:E:208[A]:VAL:HG22 | 1.95 | 0.48 |
| 1:E:218:LYS:HD2 | 1:E:224:GLU:HA | 1.94 | 0.48 |
| 1:E:329:VAL:HG13 | 1:E:340[A]:VAL:HG21 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:29[B]:TRP:CZ2 | 1:C:360:HIS:HD2 | 2.31 | 0.48 |
| 1:E:16:VAL:HG23 | 1:E:18:VAL:HG23 | 1.94 | 0.48 |
| 1:B:139:ARG:HD3 | 1:B:139:ARG:O | 2.14 | 0.48 |
| 1:F:180:ASP:OD1 | 1:F:181[B]:THR:HG23 | 2.14 | 0.48 |
| 1:B:320:ASP:O | 1:B:321:SER:HB2 | 2.14 | 0.48 |
| 1:C:307:GLU:HG3 | 4:C:566:HOH:O | 2.13 | 0.48 |
| 1:F:208[A]:VAL:HG12 | 1:F:228:LEU:HG | 1.95 | 0.48 |
| 1:F:223:VAL:HG11 | 1:F:234:LEU:HD13 | 1.96 | 0.47 |
| 1:A:157:ARG:HG2 | 1:A:254:TRP:CH2 | 2.49 | 0.47 |
| 1:B:193:ILE:O | 1:B:194:SER:C | 2.51 | 0.47 |
| 1:F:212:VAL:HG12 | 1:F:213:PHE:N | 2.28 | 0.47 |
| 1:B:228:LEU:HD13 | 1:B:235[B]:ALA:HB2 | 1.96 | 0.47 |
| 1:C:181[B]:THR:CG2 | 1:C:290:HIS:CE1 | 2.98 | 0.47 |
| 1:D:152:TYR:HE1 | 1:D:181:THR:HG1 | 1.62 | 0.47 |
| 1:F:227:GLY:O | 1:F:234:LEU:HD12 | 2.15 | 0.47 |
| 1:E:187[B]:ARG:NH2 | 1:E:190:ASP:OD2 | 2.48 | 0.47 |
| 1:F:227:GLY:HA3 | 1:F:234:LEU:HD12 | 1.97 | 0.47 |
| 1:F:228:LEU:O | 1:F:232:PRO:HA | 2.14 | 0.47 |
| 1:B:237[B]:ASP:HB2 | 4:B:507:HOH:O | 2.14 | 0.47 |
| 1:C:217:PHE:CE2 | 1:C:223:VAL:HG13 | 2.50 | 0.46 |
| 1:D:139[B]:ARG:NH1 | 4:D:501:HOH:O | 2.47 | 0.46 |
| 1:B:129:THR:HB | 1:B:152:TYR:HD2 | 1.80 | 0.46 |
| 1:D:111:ASP:OD1 | 1:D:111:ASP:N | 2.48 | 0.46 |
| 1:F:320:ASP:O | 1:F:321:SER:HB2 | 2.14 | 0.46 |
| 1:F:166:ARG:NH1 | 1:F:210:ASP:HB2 | 2.30 | 0.46 |
| 1:C:181[A]:THR:HG21 | 1:C:290:HIS:CE1 | 2.51 | 0.46 |
| 1:A:139:ARG:HG2 | 1:A:172:TYR:CE2 | 2.51 | 0.45 |
| 1:B:29[B]:TRP:CZ3 | 1:B:349:GLY:HA2 | 2.51 | 0.45 |
| 1:E:124:PRO:HB3 | 1:E:146:PRO:O | 2.16 | 0.45 |
| 1:F:37:LEU:HD21 | 1:F:351:ALA:HB2 | 1.98 | 0.45 |
| 1:D:121:THR:CG2 | 1:D:359:GLU:HG3 | 2.46 | 0.45 |
| 1:E:80:LEU:HB3 | 1:E:92:PRO:HD3 | 1.98 | 0.45 |
| 1:F:252:ILE:HD12 | 1:F:265:LEU:HD21 | 1.99 | 0.45 |
| 1:D:329:VAL:HG13 | 1:D:340[B]:VAL:CG2 | 2.39 | 0.45 |
| 1:E:320:ASP:OD1 | 1:E:320:ASP:C | 2.56 | 0.45 |
| 1:D:139[A]:ARG:CZ | 4:D:501:HOH:O | 2.58 | 0.45 |
| 1:B:213:PHE:CE1 | 1:B:242[B]:LEU:HD21 | 2.52 | 0.44 |
| 1:D:156:ASP:OD2 | 1:D:216:LYS:HD3 | 2.17 | 0.44 |
| 1:D:193:ILE:HG13 | 1:D:195:ASN:HB2 | 1.99 | 0.44 |
| 1:B:35[A]:GLN:HG3 | 1:D:35:GLN:HG3 | 2.00 | 0.44 |
| 1:E:104:CYS:O | 1:E:351:ALA:HA | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:159:LEU:HB2 | 1:F:212:VAL:HG11 | 1.99 | 0.44 |
| 1:D:217:PHE:CE2 | 1:D:223:VAL:HB | 2.53 | 0.44 |
| 1:E:117:ALA:O | 1:E:121:THR:HG23 | 2.18 | 0.43 |
| 1:E:37:LEU:HD22 | 1:E:41:VAL:HG11 | 2.00 | 0.43 |
| 1:A:205:THR:HA | 1:A:208[A]:VAL:CG2 | 2.48 | 0.43 |
| 1:D:152:TYR:HE1 | 1:D:181:THR:OG1 | 2.02 | 0.43 |
| 1:E:30:GLU:O | 1:E:34:GLN:HG3 | 2.19 | 0.43 |
| 1:F:252:ILE:O | 1:F:256:ARG:HG2 | 2.18 | 0.43 |
| 1:D:146:PRO:HA | 1:D:173:ASP:OD2 | 2.18 | 0.43 |
| 1:F:159:LEU:HB2 | 1:F:212:VAL:CG1 | 2.49 | 0.43 |
| 1:D:156:ASP:OD2 | 1:D:216:LYS:CD | 2.66 | 0.43 |
| 1:D:275:ARG:HG3 | 1:D:311:ALA:HB1 | 1.99 | 0.43 |
| 1:A:183:ILE:HG21 | 1:A:183:ILE:HD13 | 1.79 | 0.43 |
| 1:B:237[B]:ASP:HA | 1:B:239[B]:TRP:HE1 | 1.83 | 0.43 |
| 1:C:385:THR:OG1 | 1:C:387:ASP:OD1 | 2.27 | 0.42 |
| 1:E:156:ASP:OD2 | 1:E:216:LYS:HE3 | 2.18 | 0.42 |
| 1:A:23:PRO:HB2 | 1:A:29[A]:TRP:CD1 | 2.53 | 0.42 |
| 1:D:29[A]:TRP:CZ3 | 1:D:352:LEU:HD12 | 2.54 | 0.42 |
| 1:D:29[A]:TRP:CZ3 | 1:D:349:GLY:HA2 | 2.54 | 0.42 |
| 1:F:217:PHE:CE2 | 1:F:235:ALA:HB2 | 2.55 | 0.42 |
| 1:A:161:GLU:HG2 | 1:A:165:ARG:NH1 | 2.34 | 0.42 |
| 1:E:214:GLN:O | 1:E:218:LYS:HB2 | 2.19 | 0.42 |
| 2:D:401:FMN:H9 | 2:D:401:FMN:O4' | 2.20 | 0.42 |
| 1:F:113:ALA:HB1 | 1:F:355:SER:HB2 | 2.02 | 0.42 |
| 1:D:26:TYR:HA | 1:D:29[B]:TRP:CE3 | 2.55 | 0.42 |
| 1:E:150:GLN:HA | 1:E:176:VAL:O | 2.19 | 0.42 |
| 1:E:320:ASP:O | 1:E:321:SER:HB2 | 2.19 | 0.42 |
| 1:B:181[A]:THR:HG21 | 4:B:502:HOH:O | 2.20 | 0.42 |
| 1:C:285:ILE:O | 1:C:317:VAL:HA | 2.20 | 0.42 |
| 1:B:239[B]:TRP:N | 1:B:239[B]:TRP:CD1 | 2.87 | 0.42 |
| 1:B:78:ARG:HA | 1:B:379:ARG:O | 2.20 | 0.42 |
| 1:C:320:ASP:O | 1:C:321:SER:HB2 | 2.19 | 0.42 |
| 1:E:25:SER:OG | 1:E:28:ASP:OD2 | 2.37 | 0.42 |
| 1:B:181[A]:THR:CG2 | 1:B:290:HIS:CE1 | 3.03 | 0.41 |
| 1:D:320:ASP:C | 1:D:320:ASP:OD1 | 2.59 | 0.41 |
| 1:E:57:ALA:HB1 | 1:E:300:PRO:HG3 | 2.03 | 0.41 |
| 1:B:242[B]:LEU:N | 1:B:242[B]:LEU:HD13 | 2.35 | 0.41 |
| 1:C:26:TYR:HA | 1:C:29[A]:TRP:CE3 | 2.55 | 0.41 |
| 1:F:159:LEU:N | 1:F:212:VAL:HG11 | 2.36 | 0.41 |
| 1:C:26:TYR:CZ | 1:C:324:ARG:HD2 | 2.55 | 0.41 |
| 1:B:181[B]:THR:HG21 | 4:B:502:HOH:O | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:181[B]:THR:HG21 | 1:F:290:HIS:CE1 | 2.55 | 0.41 |
| 1:D:224:GLU:H | 1:D:224:GLU:CD | 2.24 | 0.41 |
| 1:B:126:ILE:HG12 | 1:B:148:TYR:HB2 | 2.03 | 0.41 |
| 1:B:130:LEU:HD21 | 1:B:243[A]:PHE:CZ | 2.55 | 0.41 |
| 1:C:29[B]:TRP:HZ2 | 1:C:360:HIS:CD2 | 2.35 | 0.41 |
| 1:E:305:LEU:HB3 | 1:E:306:PRO:HD3 | 2.02 | 0.41 |
| 1:E:379:ARG:HB2 | 1:E:379:ARG:CZ | 2.51 | 0.41 |
| 1:D:181:THR:HG21 | 1:D:290:HIS:CE1 | 2.56 | 0.41 |
| 1:E:218:LYS:HE3 | 1:E:224:GLU:CD | 2.42 | 0.41 |
| 1:F:330:VAL:HG13 | 1:F:384:LEU:HD21 | 2.03 | 0.41 |
| 1:F:344:ARG:HD3 | 2:F:401:FMN:C8M | 2.52 | 0.41 |
| 1:C:320:ASP:OD1 | 1:C:320:ASP:C | 2.59 | 0.40 |
| 1:D:285:ILE:O | 1:D:317:VAL:HA | 2.21 | 0.40 |
| 1:C:221:SER:OG | 1:C:223:VAL:HG12 | 2.21 | 0.40 |
| 2:C:401:FMN:O4' | 2:C:401:FMN:H9 | 2.22 | 0.40 |
| 1:D:47:GLY:HA3 | 4:D:617:HOH:O | 2.21 | 0.40 |
| 1:C:193:ILE:HG13 | 1:C:195:ASN:HB2 | 2.04 | 0.40 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:A:584:HOH:O | 4:B:604:HOH:O[7_555] | 2.13 | 0.07 |
| 4:A:992:HOH:O | 4:C:813:HOH:O[3_545] | 2.19 | 0.01 |

## 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 | 404/394 (102%) | 392 (97%) | 10 (2%) | 2 (0%) | 29 13 |
| 1 | B | 414/394 (105%) | 397 (96%) | 12 (3%) | 5 (1%) | 13 3 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | C | 399/394 (101%) | 389 (98%) | 9 (2%) | 1 (0%) | 41 24 |
| 1 | D | 399/394 (101%) | 388 (97%) | 10 (2%) | 1 (0%) | 41 24 |
| 1 | E | 398/394 (101%) | 384 (96%) | 13 (3%) | 1 (0%) | 41 24 |
| 1 | F | 397/394 (101%) | 373 (94%) | 20 (5%) | 4 (1%) | 15 4 |
| All | All | 2411/2364 (102%) | 2323 (96%) | 74 (3%) | 14 (1%) | 25 11 |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1 | SER |
| 1 | B | 321 | SER |
| 1 | C | 321 | SER |
| 1 | D | 321 | SER |
| 1 | A | 321 | SER |
| 1 | B | 221 | SER |
| 1 | E | 321 | SER |
| 1 | F | 227 | GLY |
| 1 | B | 203 | ALA |
| 1 | B | 239[A] | TRP |
| 1 | B | 239[B] | TRP |
| 1 | F | 224 | GLU |
| 1 | F | 321 | SER |
| 1 | F | 353 | GLY |

### 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 | 316/304 (104%) | 304 (96%) | 12 (4%) | 33 14 |
| 1 | B | 322/304 (106%) | 312 (97%) | 10 (3%) | 40 21 |
| 1 | C | 311/304 (102%) | 300 (96%) | 11 (4%) | 36 17 |
| 1 | D | 311/304 (102%) | 298 (96%) | 13 (4%) | 30 12 |
| 1 | E | 310/304 (102%) | 296 (96%) | 14 (4%) | 27 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | F | 309/304 (102%) | 296 (96%) | 13 (4%) | 30 12 |
| All | All | 1879/1824 (103%) | 1806 (96%) | 73 (4%) | 34 13 |

All (73) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 0 | MET |
| 1 | A | 1 | SER |
| 1 | A | 9 | GLU |
| 1 | A | 78 | ARG |
| 1 | A | 83 | GLU |
| 1 | A | 139 | ARG |
| 1 | A | 153 | TYR |
| 1 | A | 157 | ARG |
| 1 | A | 181[A] | THR |
| 1 | A | 181[B] | THR |
| 1 | A | 286 | TYR |
| 1 | A | 344 | ARG |
| 1 | B | 0 | MET |
| 1 | B | 139 | ARG |
| 1 | B | 159 | LEU |
| 1 | B | 196 | PHE |
| 1 | B | 208 | VAL |
| 1 | B | 242[A] | LEU |
| 1 | B | 242[B] | LEU |
| 1 | B | 260 | LYS |
| 1 | B | 286 | TYR |
| 1 | B | 344 | ARG |
| 1 | C | 130 | LEU |
| 1 | C | 139[A] | ARG |
| 1 | C | 139[B] | ARG |
| 1 | C | 153 | TYR |
| 1 | C | 165 | ARG |
| 1 | C | 181[A] | THR |
| 1 | C | 181[B] | THR |
| 1 | C | 223 | VAL |
| 1 | C | 286 | TYR |
| 1 | C | 307 | GLU |
| 1 | C | 344 | ARG |
| 1 | D | 0 | MET |
| 1 | D | 83 | GLU |
| 1 | D | 153 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 157 | ARG |
| 1 | D | 159 | LEU |
| 1 | D | 165 | ARG |
| 1 | D | 169 | GLU |
| 1 | D | 196 | PHE |
| 1 | D | 204 | LEU |
| 1 | D | 215 | LYS |
| 1 | D | 260 | LYS |
| 1 | D | 286 | TYR |
| 1 | D | 344 | ARG |
| 1 | E | 0 | MET |
| 1 | E | 78 | ARG |
| 1 | E | 139 | ARG |
| 1 | E | 152 | TYR |
| 1 | E | 181[A] | THR |
| 1 | E | 181[B] | THR |
| 1 | E | 218 | LYS |
| 1 | E | 224 | GLU |
| 1 | E | 226 | GLU |
| 1 | E | 246 | SER |
| 1 | E | 286 | TYR |
| 1 | E | 344 | ARG |
| 1 | E | 346 | TYR |
| 1 | E | 379 | ARG |
| 1 | F | 78 | ARG |
| 1 | F | 139 | ARG |
| 1 | F | 152 | TYR |
| 1 | F | 155 | GLU |
| 1 | F | 157 | ARG |
| 1 | F | 158 | ASP |
| 1 | F | 212 | VAL |
| 1 | F | 214 | GLN |
| 1 | F | 229 | ARG |
| 1 | F | 246 | SER |
| 1 | F | 256 | ARG |
| 1 | F | 286 | TYR |
| 1 | F | 344 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

24 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | SO4 | A | 403 | - | 4,4,4 | 0.56 | 0 | 6,6,6 | 0.70 | 0 |
| 3 | SO4 | E | 403 | - | 4,4,4 | 0.12 | 0 | 6,6,6 | 0.21 | 0 |
| 2 | FMN | E | 401 | - | 31,33,33 | 2.51 | 5 (16%) | 40,50,50 | 2.12 | 8 (20%) |
| 3 | SO4 | B | 404[A] | - | 4,4,4 | 0.20 | 0 | 6,6,6 | 0.12 | 0 |
| 3 | SO4 | D | 402 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.69 | 0 |
| 2 | FMN | A | 401 | - | 31,33,33 | 2.56 | 8 (25%) | 40,50,50 | 2.92 | 10 (25%) |
| 3 | SO4 | A | 402 | - | 4,4,4 | 0.54 | 0 | 6,6,6 | 0.83 | 0 |
| 3 | SO4 | C | 402 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.74 | 0 |
| 2 | FMN | B | 401 | - | 31,33,33 | 2.70 | 10 (32%) | 40,50,50 | 2.44 | 11 (27%) |
| 3 | SO4 | B | 403 | - | 4,4,4 | 0.20 | 0 | 6,6,6 | 0.38 | 0 |
| 3 | SO4 | B | 405 | - | 4,4,4 | 0.08 | 0 | 6,6,6 | 0.14 | 0 |
| 2 | FMN | D | 401 | - | 31,33,33 | 2.60 | 8 (25%) | 40,50,50 | 2.29 | 9 (22%) |
| 3 | SO4 | B | 406[B] | - | 4,4,4 | 0.42 | 0 | 6,6,6 | 0.36 | 0 |
| 3 | SO4 | F | 403 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.26 | 0 |
| 3 | SO4 | C | 404 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.16 | 0 |
| 3 | SO4 | C | 403 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 1.00 | 0 |
| 3 | SO4 | A | 405 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.14 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | FMN | F | 401 | - | 31,33,33 | 2.43 | 5 (16%) | 40,50,50 | 2.35 | 10 (25%) |
| 3 | SO4 | D | 403 | - | 4,4,4 | 0.41 | 0 | 6,6,6 | 0.42 | 0 |
| 3 | SO4 | F | 402 | - | 4,4,4 | 0.11 | 0 | 6,6,6 | 0.19 | 0 |
| 2 | FMN | C | 401 | - | 31,33,33 | 2.73 | 9 (29%) | 40,50,50 | 2.32 | 10 (25%) |
| 3 | SO4 | B | 402 | - | 4,4,4 | 0.55 | 0 | 6,6,6 | 0.47 | 0 |
| 3 | SO4 | E | 402 | - | 4,4,4 | 0.21 | 0 | 6,6,6 | 0.30 | 0 |
| 3 | SO4 | A | 404[A] | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.59 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | FMN | E | 401 | - | - | 3/18/18/18 | 0/3/3/3 |
| 2 | FMN | C | 401 | - | - | 1/18/18/18 | 0/3/3/3 |
| 2 | FMN | A | 401 | - | - | 1/18/18/18 | 0/3/3/3 |
| 2 | FMN | F | 401 | - | - | 5/18/18/18 | 0/3/3/3 |
| 2 | FMN | D | 401 | - | - | 1/18/18/18 | 0/3/3/3 |
| 2 | FMN | B | 401 | - | - | 1/18/18/18 | 0/3/3/3 |

All (45) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | E | 401 | FMN | C4A-C10 | 10.73 | 1.49 | 1.38 |
| 2 | F | 401 | FMN | C4A-C10 | 10.29 | 1.49 | 1.38 |
| 2 | B | 401 | FMN | C4A-C10 | 10.17 | 1.49 | 1.38 |
| 2 | D | 401 | FMN | C4A-C10 | 9.86 | 1.48 | 1.38 |
| 2 | A | 401 | FMN | C4A-C10 | 9.11 | 1.47 | 1.38 |
| 2 | C | 401 | FMN | C4A-C10 | 8.83 | 1.47 | 1.38 |
| 2 | C | 401 | FMN | C9A-N10 | 6.16 | 1.46 | 1.38 |
| 2 | C | 401 | FMN | C4A-N5 | 5.46 | 1.41 | 1.33 |
| 2 | D | 401 | FMN | C9A-N10 | 5.32 | 1.45 | 1.38 |
| 2 | A | 401 | FMN | C4-C4A | 5.01 | 1.50 | 1.41 |
| 2 | C | 401 | FMN | C10-N1 | 4.84 | 1.39 | 1.33 |
| 2 | A | 401 | FMN | C5'-C4' | 4.76 | 1.58 | 1.51 |
| 2 | E | 401 | FMN | C4-C4A | 4.36 | 1.48 | 1.41 |
| 2 | B | 401 | FMN | C5'-C4' | 4.30 | 1.57 | 1.51 |
| 2 | F | 401 | FMN | C4-C4A | 4.27 | 1.48 | 1.41 |
| 2 | B | 401 | FMN | C4A-N5 | 4.09 | 1.39 | 1.33 |
| 2 | C | 401 | FMN | C4-C4A | 4.05 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 401 | FMN | C9A-C5A | 3.95 | 1.50 | 1.42 |
| 2 | D | 401 | FMN | C4A-N5 | 3.93 | 1.38 | 1.33 |
| 2 | F | 401 | FMN | C9A-C5A | 3.92 | 1.50 | 1.42 |
| 2 | E | 401 | FMN | C9A-C5A | 3.85 | 1.50 | 1.42 |
| 2 | A | 401 | FMN | C1'-N10 | -3.79 | 1.44 | 1.48 |
| 2 | E | 401 | FMN | C9A-N10 | 3.77 | 1.43 | 1.38 |
| 2 | F | 401 | FMN | C8-C7 | 3.73 | 1.50 | 1.40 |
| 2 | D | 401 | FMN | C4-C4A | 3.72 | 1.47 | 1.41 |
| 2 | A | 401 | FMN | C8-C7 | 3.54 | 1.49 | 1.40 |
| 2 | F | 401 | FMN | C9A-N10 | 3.50 | 1.43 | 1.38 |
| 2 | D | 401 | FMN | C9A-C5A | 3.47 | 1.49 | 1.42 |
| 2 | B | 401 | FMN | C4-C4A | 3.47 | 1.47 | 1.41 |
| 2 | B | 401 | FMN | C10-N1 | 3.38 | 1.37 | 1.33 |
| 2 | A | 401 | FMN | C5A-N5 | 3.33 | 1.40 | 1.35 |
| 2 | E | 401 | FMN | C8-C7 | 3.28 | 1.49 | 1.40 |
| 2 | D | 401 | FMN | C4-N3 | 3.03 | 1.38 | 1.33 |
| 2 | B | 401 | FMN | C9A-N10 | 2.88 | 1.42 | 1.38 |
| 2 | A | 401 | FMN | C6-C5A | -2.73 | 1.37 | 1.41 |
| 2 | B | 401 | FMN | C1'-N10 | -2.67 | 1.45 | 1.48 |
| 2 | D | 401 | FMN | C10-N1 | 2.37 | 1.36 | 1.33 |
| 2 | D | 401 | FMN | C8-C7 | 2.30 | 1.46 | 1.40 |
| 2 | A | 401 | FMN | C9A-C5A | 2.29 | 1.47 | 1.42 |
| 2 | B | 401 | FMN | C8-C7 | 2.26 | 1.46 | 1.40 |
| 2 | B | 401 | FMN | O4-C4 | 2.25 | 1.30 | 1.24 |
| 2 | C | 401 | FMN | C2-N3 | -2.24 | 1.33 | 1.38 |
| 2 | C | 401 | FMN | C4-N3 | 2.13 | 1.36 | 1.33 |
| 2 | C | 401 | FMN | C8-C7 | 2.10 | 1.46 | 1.40 |
| 2 | C | 401 | FMN | C9A-C5A | 2.09 | 1.46 | 1.42 |

All (58) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 401 | FMN | C4-N3-C2 | 9.18 | 122.89 | 115.14 |
| 2 | A | 401 | FMN | C4-N3-C2 | 8.99 | 122.73 | 115.14 |
| 2 | A | 401 | FMN | C4-C4A-C10 | -8.63 | 114.24 | 119.95 |
| 2 | F | 401 | FMN | C4-N3-C2 | 8.63 | 122.43 | 115.14 |
| 2 | B | 401 | FMN | C4-N3-C2 | 8.32 | 122.17 | 115.14 |
| 2 | D | 401 | FMN | C4-N3-C2 | 8.27 | 122.12 | 115.14 |
| 2 | B | 401 | FMN | C4-C4A-C10 | -8.23 | 114.50 | 119.95 |
| 2 | A | 401 | FMN | C1'-N10-C9A | 8.15 | 124.71 | 118.29 |
| 2 | E | 401 | FMN | C4-N3-C2 | 8.06 | 121.95 | 115.14 |
| 2 | D | 401 | FMN | C4-C4A-C10 | -6.95 | 115.35 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 401 | FMN | C4-C4A-C10 | -6.20 | 115.85 | 119.95 |
| 2 | F | 401 | FMN | C1'-N10-C9A | 6.13 | 123.12 | 118.29 |
| 2 | F | 401 | FMN | C4-C4A-C10 | -4.85 | 116.74 | 119.95 |
| 2 | A | 401 | FMN | C5A-C9A-N10 | 4.78 | 121.18 | 117.72 |
| 2 | E | 401 | FMN | C4-C4A-C10 | -4.39 | 117.05 | 119.95 |
| 2 | A | 401 | FMN | C4A-C10-N10 | -4.35 | 115.83 | 120.30 |
| 2 | E | 401 | FMN | C1'-N10-C9A | 4.25 | 121.64 | 118.29 |
| 2 | C | 401 | FMN | C1'-N10-C9A | 4.04 | 121.47 | 118.29 |
| 2 | B | 401 | FMN | C4-C4A-N5 | 3.99 | 123.16 | 118.60 |
| 2 | F | 401 | FMN | C9A-N10-C10 | -3.95 | 116.74 | 121.91 |
| 2 | D | 401 | FMN | C1'-N10-C9A | 3.81 | 121.30 | 118.29 |
| 2 | E | 401 | FMN | C4A-N5-C5A | 3.79 | 120.56 | 116.77 |
| 2 | F | 401 | FMN | C4A-C4-N3 | -3.79 | 118.25 | 123.43 |
| 2 | C | 401 | FMN | C9A-N10-C10 | -3.74 | 117.01 | 121.91 |
| 2 | A | 401 | FMN | C4-C4A-N5 | 3.62 | 122.73 | 118.60 |
| 2 | F | 401 | FMN | C4A-N5-C5A | 3.62 | 120.39 | 116.77 |
| 2 | C | 401 | FMN | C4A-C4-N3 | -3.57 | 118.56 | 123.43 |
| 2 | E | 401 | FMN | C4A-C4-N3 | -3.52 | 118.61 | 123.43 |
| 2 | D | 401 | FMN | C4-C4A-N5 | 3.52 | 122.62 | 118.60 |
| 2 | D | 401 | FMN | C9A-N10-C10 | -3.45 | 117.39 | 121.91 |
| 2 | E | 401 | FMN | C9A-N10-C10 | -3.41 | 117.44 | 121.91 |
| 2 | B | 401 | FMN | P-O5'-C5' | 3.41 | 127.69 | 118.30 |
| 2 | D | 401 | FMN | C4A-C4-N3 | -3.30 | 118.92 | 123.43 |
| 2 | D | 401 | FMN | C1'-N10-C10 | 3.25 | 121.32 | 118.41 |
| 2 | B | 401 | FMN | C1'-N10-C9A | 3.15 | 120.78 | 118.29 |
| 2 | A | 401 | FMN | C1'-N10-C10 | -3.12 | 115.62 | 118.41 |
| 2 | F | 401 | FMN | C4-C4A-N5 | 3.01 | 122.03 | 118.60 |
| 2 | B | 401 | FMN | C9A-N10-C10 | -2.85 | 118.17 | 121.91 |
| 2 | A | 401 | FMN | O3P-P-O5' | -2.71 | 99.53 | 106.73 |
| 2 | E | 401 | FMN | C4-C4A-N5 | 2.61 | 121.58 | 118.60 |
| 2 | C | 401 | FMN | C1'-N10-C10 | 2.53 | 120.67 | 118.41 |
| 2 | C | 401 | FMN | O5'-P-O1P | -2.52 | 99.41 | 106.47 |
| 2 | B | 401 | FMN | C1'-N10-C10 | 2.49 | 120.64 | 118.41 |
| 2 | C | 401 | FMN | C4-C4A-N5 | 2.49 | 121.44 | 118.60 |
| 2 | D | 401 | FMN | O5'-P-O1P | -2.48 | 99.52 | 106.47 |
| 2 | D | 401 | FMN | O3P-P-O2P | 2.41 | 116.86 | 107.64 |
| 2 | A | 401 | FMN | C9A-C5A-N5 | -2.37 | 118.66 | 122.36 |
| 2 | B | 401 | FMN | C5A-C9A-N10 | 2.32 | 119.40 | 117.72 |
| 2 | B | 401 | FMN | O3'-C3'-C4' | -2.28 | 103.30 | 108.81 |
| 2 | B | 401 | FMN | C4A-C4-N3 | -2.27 | 120.33 | 123.43 |
| 2 | B | 401 | FMN | O2'-C2'-C3' | -2.26 | 103.60 | 109.10 |
| 2 | E | 401 | FMN | O3P-P-O2P | 2.16 | 115.89 | 107.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 401 | FMN | C6-C5A-N5 | -2.15 | 116.68 | 119.05 |
| 2 | F | 401 | FMN | O2P-P-O5' | -2.13 | 101.06 | 106.73 |
| 2 | A | 401 | FMN | C10-C4A-N5 | 2.11 | 122.72 | 121.26 |
| 2 | F | 401 | FMN | O3P-P-O2P | 2.06 | 115.52 | 107.64 |
| 2 | C | 401 | FMN | C10-C4A-N5 | 2.05 | 122.67 | 121.26 |
| 2 | F | 401 | FMN | O5'-P-O1P | -2.04 | 100.76 | 106.47 |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | E | 401 | FMN | C2'-C3'-C4'-O4' |
| 2 | F | 401 | FMN | C2'-C3'-C4'-O4' |
| 2 | F | 401 | FMN | C2'-C3'-C4'-C5' |
| 2 | E | 401 | FMN | C4'-C5'-O5'-P |
| 2 | B | 401 | FMN | C4'-C5'-O5'-P |
| 2 | C | 401 | FMN | C4'-C5'-O5'-P |
| 2 | A | 401 | FMN | C4'-C5'-O5'-P |
| 2 | D | 401 | FMN | C4'-C5'-O5'-P |
| 2 | F | 401 | FMN | O3'-C3'-C4'-C5' |
| 2 | F | 401 | FMN | C4'-C5'-O5'-P |
| 2 | E | 401 | FMN | C2'-C3'-C4'-C5' |
| 2 | F | 401 | FMN | O3'-C3'-C4'-O4' |

There are no ring outliers.

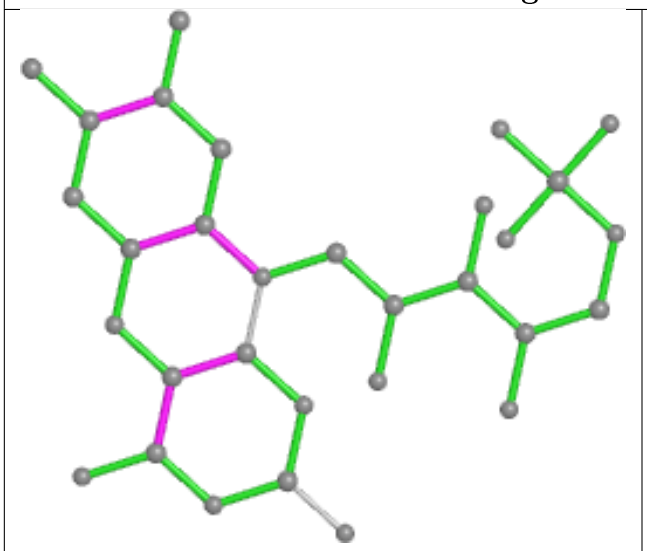
3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | D | 401 | FMN | 1 | 0 |
| 2 | F | 401 | FMN | 1 | 0 |
| 2 | C | 401 | FMN | 1 | 0 |

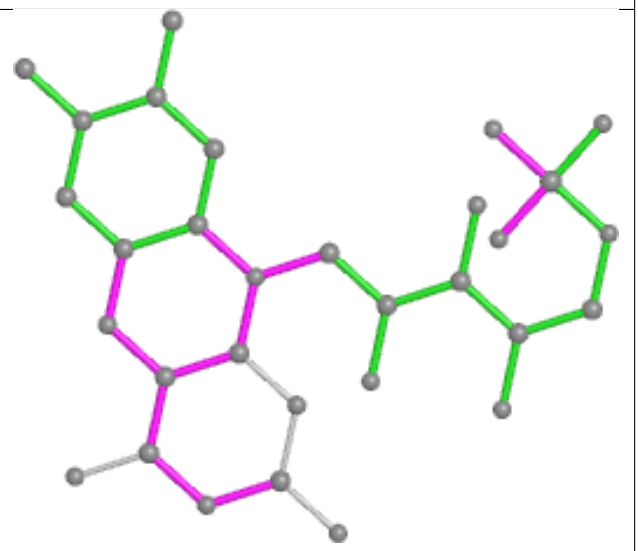
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

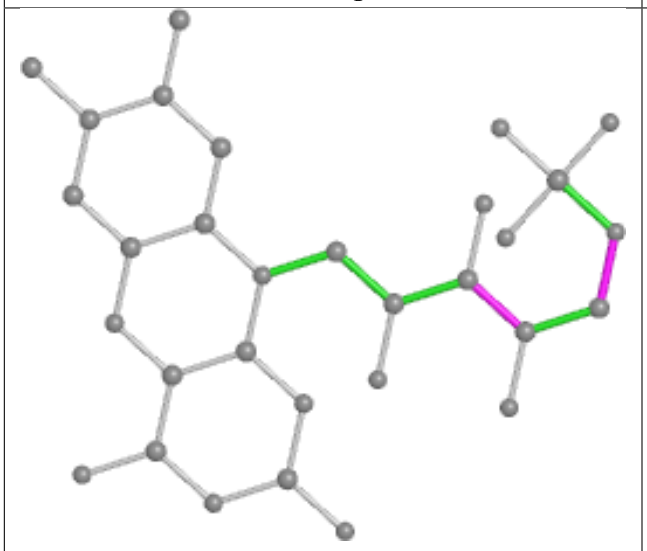
**Ligand FMN E 401**



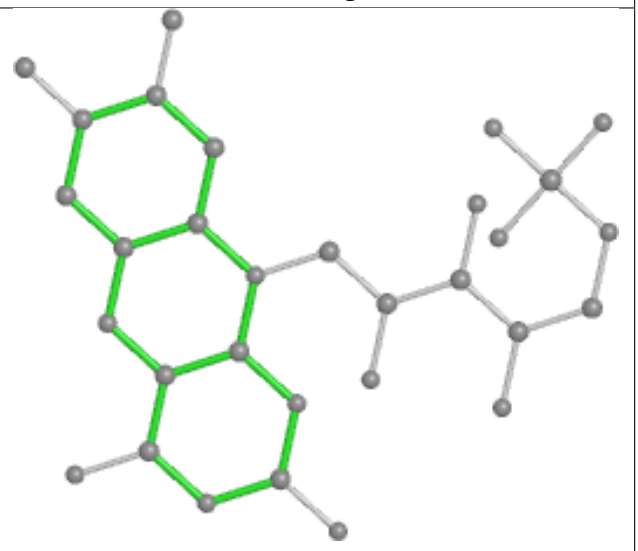
**Bond lengths**



**Bond angles**

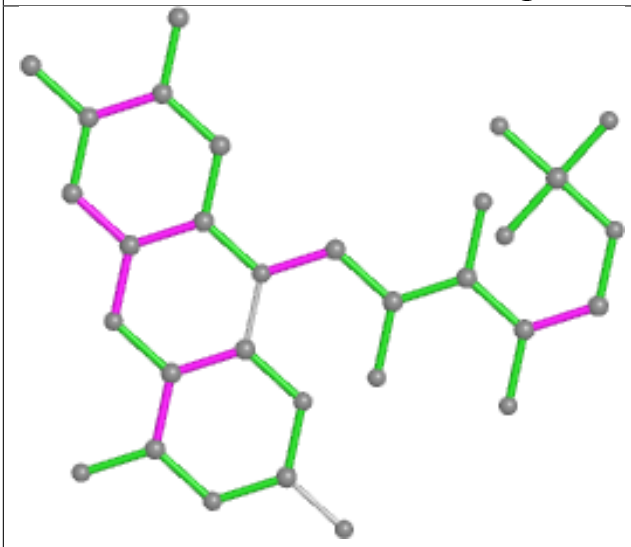


**Torsions**

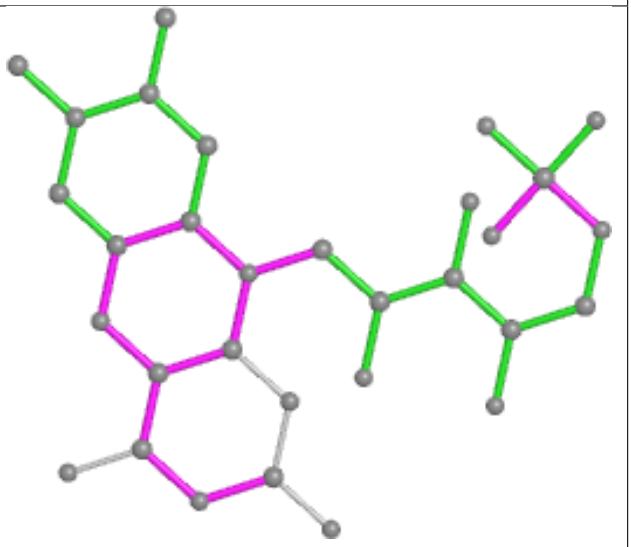


**Rings**

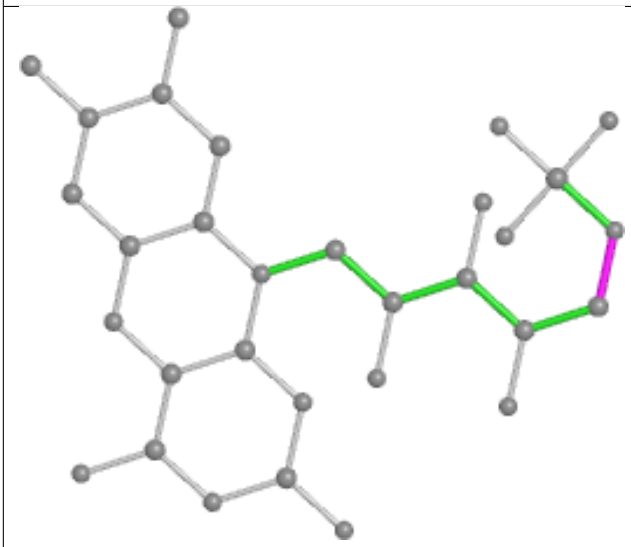
**Ligand FMN A 401**



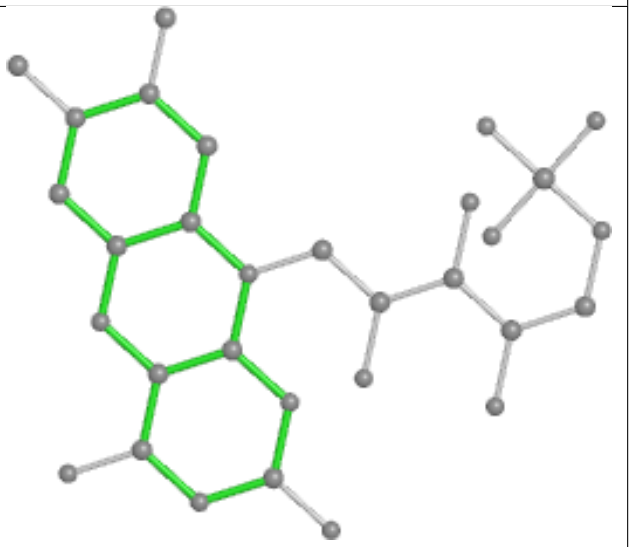
**Bond lengths**



**Bond angles**

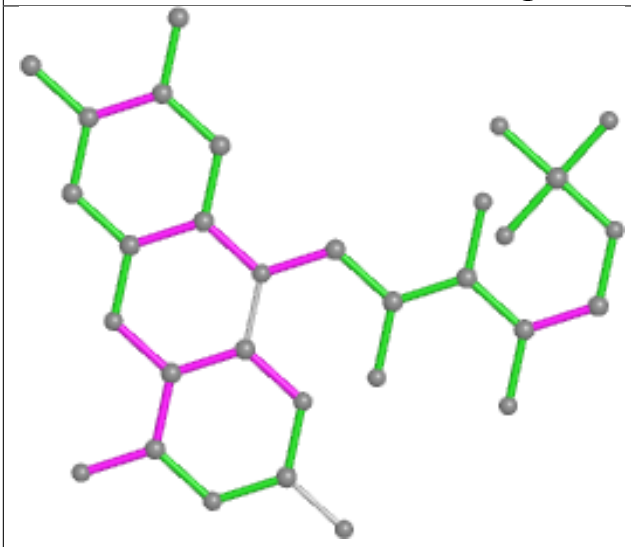


**Torsions**

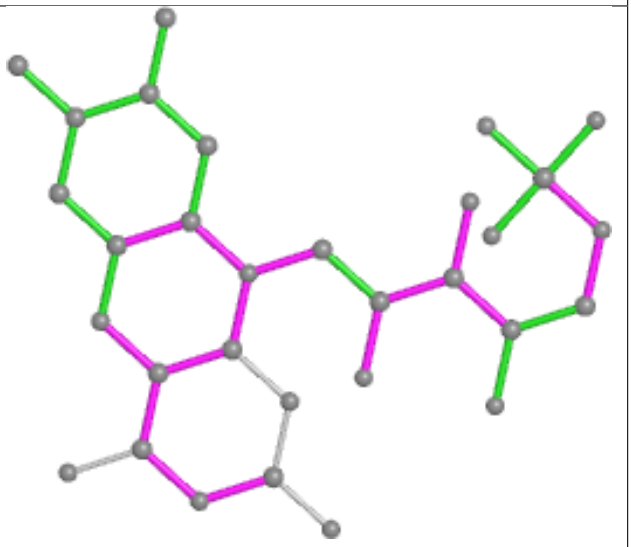


**Rings**

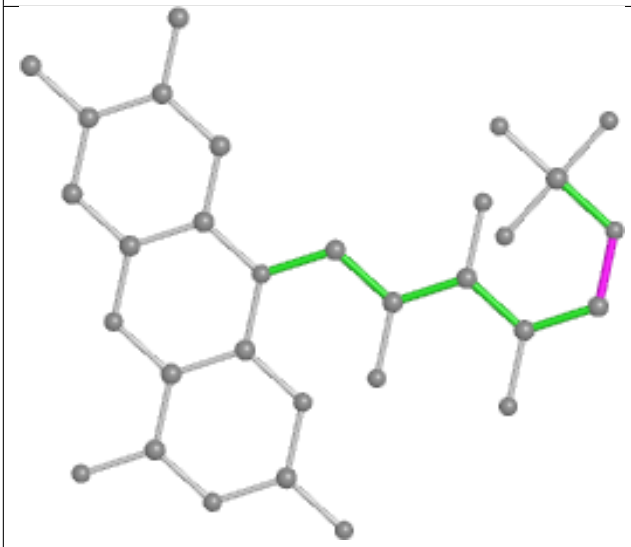
**Ligand FMN B 401**



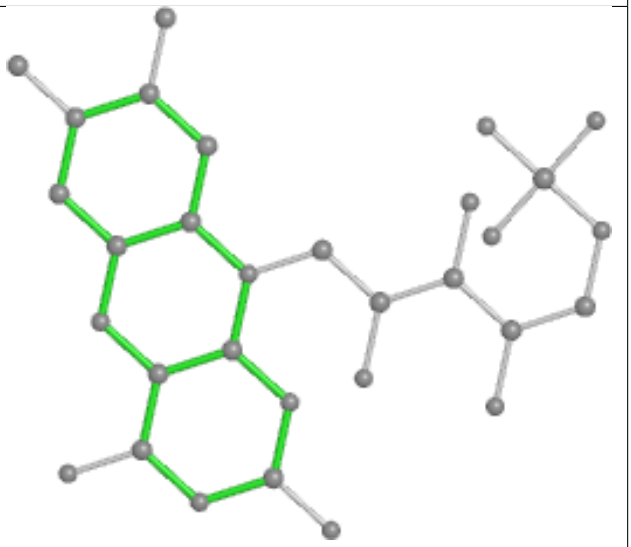
**Bond lengths**



**Bond angles**

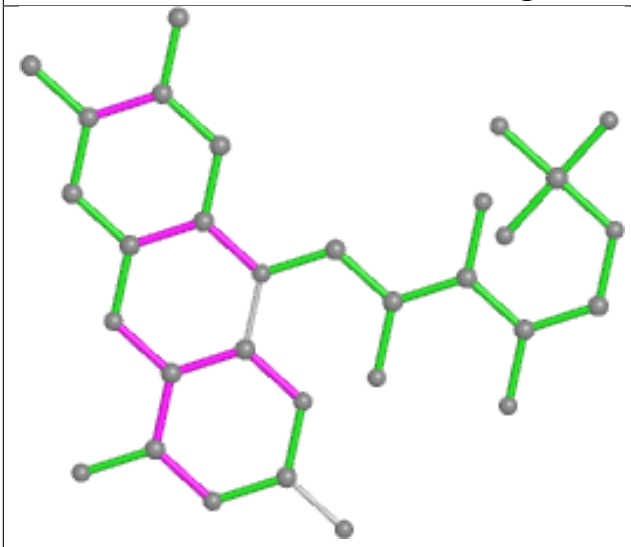


**Torsions**

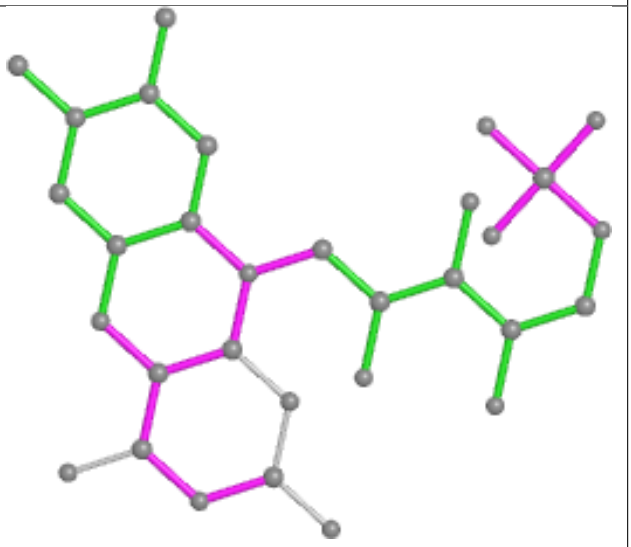


**Rings**

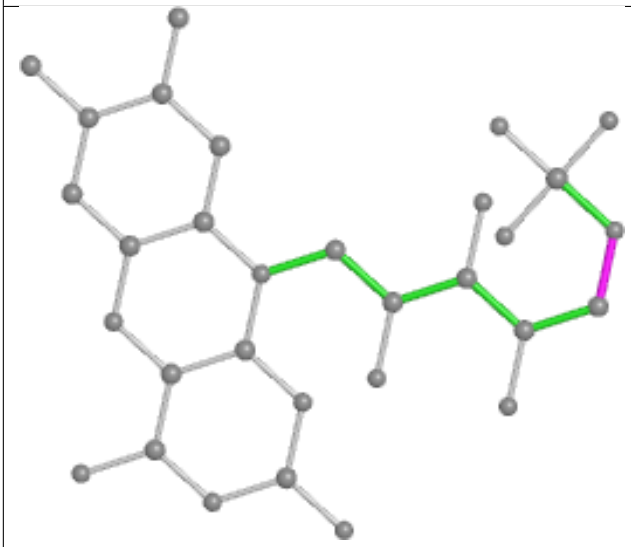
**Ligand FMN D 401**



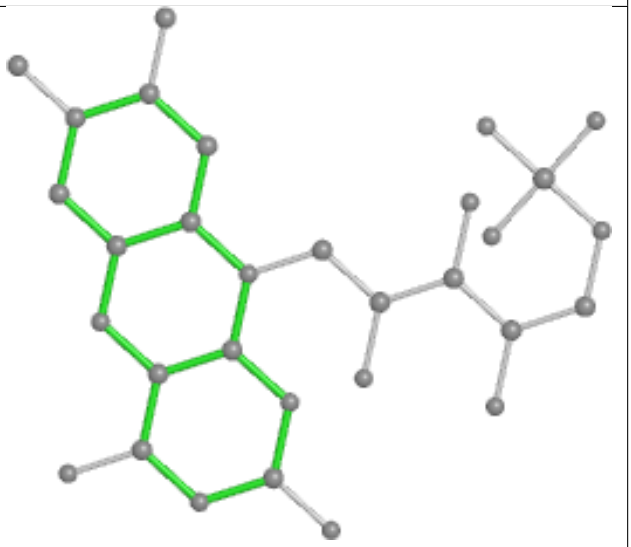
**Bond lengths**



**Bond angles**

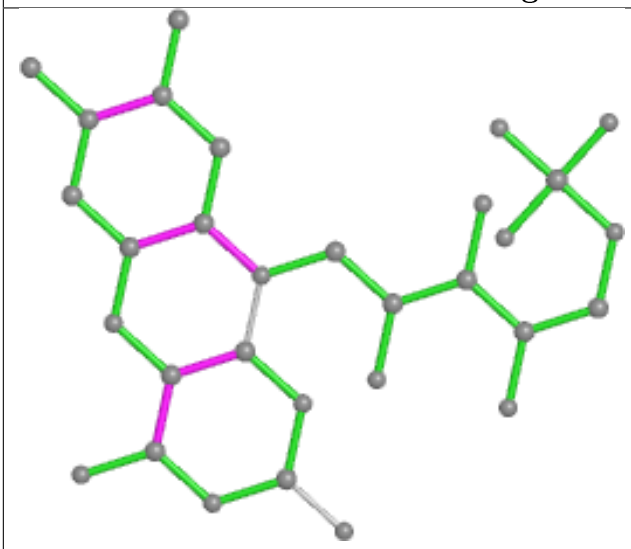


**Torsions**

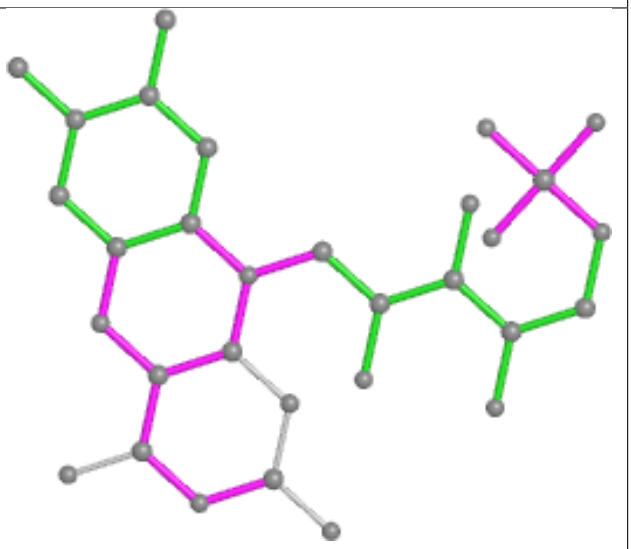


**Rings**

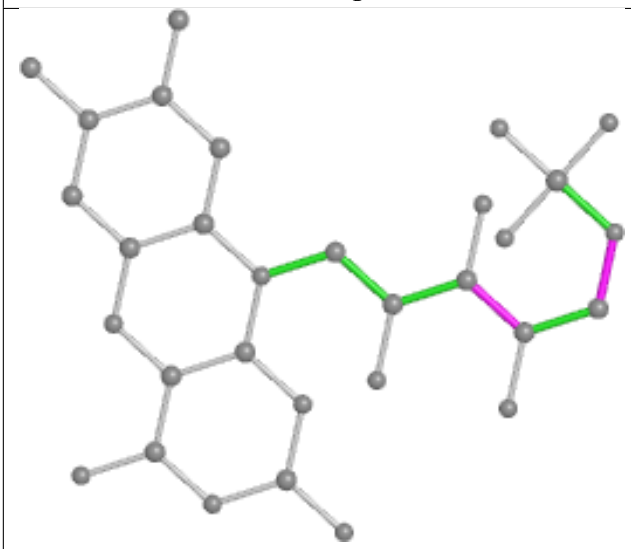
**Ligand FMN F 401**



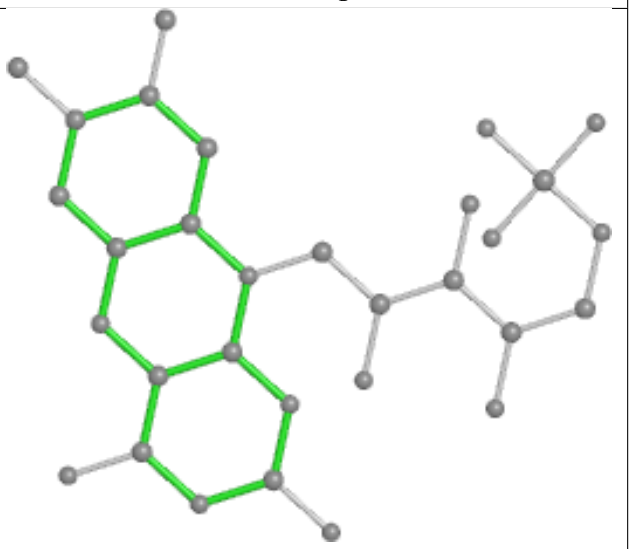
**Bond lengths**



**Bond angles**

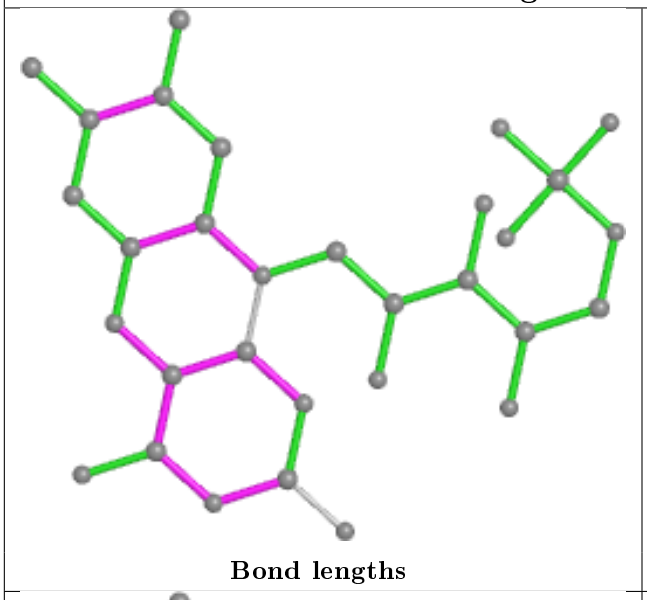


**Torsions**

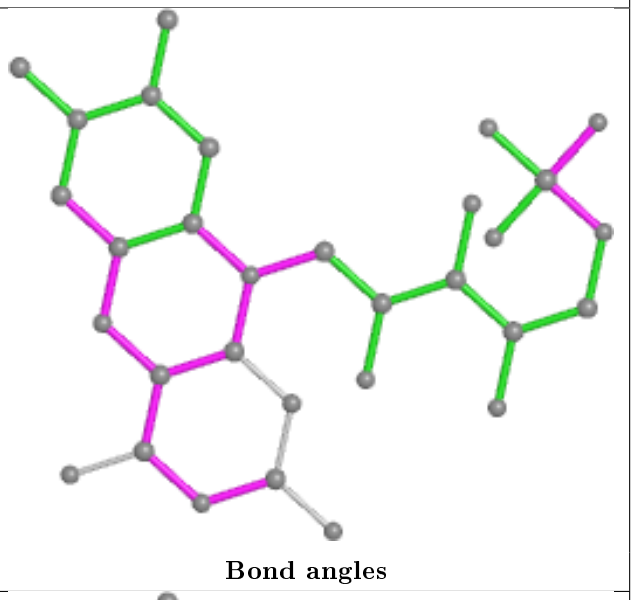


**Rings**

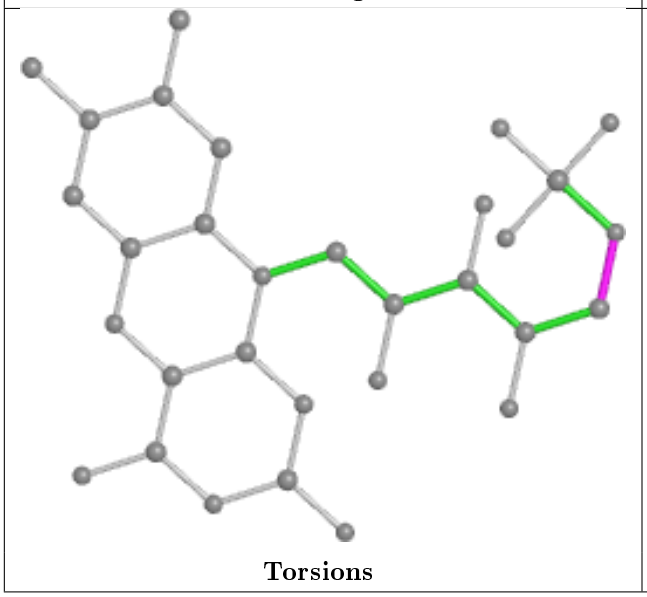
**Ligand FMN C 401**



Bond lengths



Bond angles



Torsions

Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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 | 394/394 (100%) | 0.28 | 21 (5%) 26 29 | 19, 30, 49, 77 | 0 |
| 1 | B | 394/394 (100%) | 0.66 | 52 (13%) 3 3 | 25, 38, 88, 131 | 0 |
| 1 | C | 394/394 (100%) | 0.47 | 45 (11%) 5 5 | 30, 43, 70, 100 | 0 |
| 1 | D | 394/394 (100%) | 1.16 | 85 (21%) 0 0 | 46, 62, 103, 160 | 0 |
| 1 | E | 394/394 (100%) | 3.40 | 241 (61%) 0 0 | 72, 103, 158, 190 | 394 (100%) |
| 1 | F | 393/394 (99%) | 4.05 | 282 (71%) 0 0 | 87, 113, 169, 204 | 393 (100%) |
| All | All | 2363/2364 (99%) | 1.67 | 726 (30%) 0 0 | 19, 57, 137, 204 | 787 (33%) |

All (726) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 223 | VAL | 28.1 |
| 1 | E | 238 | PHE | 23.5 |
| 1 | E | 234 | LEU | 21.9 |
| 1 | F | 222 | GLY | 19.6 |
| 1 | F | 226 | GLU | 18.9 |
| 1 | E | 236 | ALA | 18.9 |
| 1 | F | 239 | TRP | 17.2 |
| 1 | E | 239 | TRP | 16.9 |
| 1 | F | 228 | LEU | 16.8 |
| 1 | E | 235 | ALA | 15.5 |
| 1 | E | 229 | ARG | 15.4 |
| 1 | F | 213 | PHE | 15.2 |
| 1 | F | 230 | ASP | 14.8 |
| 1 | F | 236 | ALA | 14.6 |
| 1 | F | 235 | ALA | 14.4 |
| 1 | E | 223 | VAL | 13.3 |
| 1 | F | 234 | LEU | 13.2 |
| 1 | F | 238 | PHE | 12.7 |
| 1 | F | 225 | ALA | 12.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 217 | PHE | 12.0 |
| 1 | E | 198 | PHE | 12.0 |
| 1 | F | 227 | GLY | 11.9 |
| 1 | F | 172 | TYR | 11.8 |
| 1 | E | 16 | VAL | 11.8 |
| 1 | D | 225 | ALA | 11.4 |
| 1 | F | 15 | LEU | 11.4 |
| 1 | F | 159 | LEU | 11.3 |
| 1 | E | 227 | GLY | 11.3 |
| 1 | E | 0 | MET | 10.9 |
| 1 | F | 219 | ALA | 10.7 |
| 1 | F | 221 | SER | 10.5 |
| 1 | F | 258 | ILE | 10.5 |
| 1 | E | 222 | GLY | 10.5 |
| 1 | E | 224 | GLU | 10.1 |
| 1 | E | 230 | ASP | 9.9 |
| 1 | E | 225 | ALA | 9.9 |
| 1 | F | 212 | VAL | 9.9 |
| 1 | E | 172 | TYR | 9.8 |
| 1 | E | 228 | LEU | 9.8 |
| 1 | E | 254 | TRP | 9.8 |
| 1 | F | 229 | ARG | 9.8 |
| 1 | F | 19 | ALA | 9.6 |
| 1 | F | 254 | TRP | 9.5 |
| 1 | D | 220 | HIS | 9.5 |
| 1 | E | 212 | VAL | 9.4 |
| 1 | E | 231 | ASN | 9.3 |
| 1 | F | 142 | ALA | 9.2 |
| 1 | F | 163 | PHE | 9.2 |
| 1 | F | 220 | HIS | 9.1 |
| 1 | E | 1 | SER | 9.1 |
| 1 | F | 199 | LEU | 9.1 |
| 1 | F | 16 | VAL | 9.0 |
| 1 | F | 231 | ASN | 8.8 |
| 1 | D | 239 | TRP | 8.8 |
| 1 | E | 240 | HIS | 8.8 |
| 1 | E | 219 | ALA | 8.8 |
| 1 | E | 226 | GLU | 8.8 |
| 1 | E | 15 | LEU | 8.7 |
| 1 | F | 217 | PHE | 8.6 |
| 1 | F | 18 | VAL | 8.6 |
| 1 | E | 12 | GLY | 8.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 259 | THR | 8.5 |
| 1 | F | 17 | GLY | 8.4 |
| 1 | F | 99 | GLY | 8.4 |
| 1 | D | 226 | GLU | 8.3 |
| 1 | E | 132 | VAL | 8.3 |
| 1 | D | 0 | MET | 8.3 |
| 1 | F | 14 | GLY | 8.3 |
| 1 | F | 37 | LEU | 8.2 |
| 1 | E | 10 | ILE | 8.2 |
| 1 | F | 198 | PHE | 8.2 |
| 1 | B | 220 | HIS | 8.1 |
| 1 | F | 88 | THR | 8.1 |
| 1 | E | 17 | GLY | 8.0 |
| 1 | F | 12 | GLY | 8.0 |
| 1 | E | 220 | HIS | 8.0 |
| 1 | D | 217 | PHE | 7.9 |
| 1 | E | 18 | VAL | 7.9 |
| 1 | B | 234 | LEU | 7.9 |
| 1 | B | 235[A] | ALA | 7.8 |
| 1 | F | 196 | PHE | 7.8 |
| 1 | E | 130[A] | LEU | 7.8 |
| 1 | F | 76 | THR | 7.8 |
| 1 | E | 221 | SER | 7.8 |
| 1 | F | 143 | GLY | 7.8 |
| 1 | D | 238 | PHE | 7.8 |
| 1 | F | 257 | SER | 7.6 |
| 1 | F | 164 | ILE | 7.6 |
| 1 | F | 286 | TYR | 7.6 |
| 1 | D | 219 | ALA | 7.5 |
| 1 | E | 208[A] | VAL | 7.5 |
| 1 | F | 260 | LYS | 7.4 |
| 1 | F | 195 | ASN | 7.4 |
| 1 | D | 236 | ALA | 7.4 |
| 1 | E | 201 | GLY | 7.3 |
| 1 | F | 65 | TRP | 7.2 |
| 1 | F | 266 | LYS | 7.2 |
| 1 | E | 213 | PHE | 7.2 |
| 1 | F | 97 | PRO | 7.2 |
| 1 | F | 318 | LEU | 7.2 |
| 1 | F | 170 | ALA | 7.2 |
| 1 | E | 165 | ARG | 7.1 |
| 1 | B | 0 | MET | 7.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 14 | GLY | 6.9 |
| 1 | F | 140 | LYS | 6.9 |
| 1 | E | 210 | ASP | 6.9 |
| 1 | D | 234 | LEU | 6.9 |
| 1 | D | 221 | SER | 6.8 |
| 1 | F | 208[A] | VAL | 6.8 |
| 1 | E | 193 | ILE | 6.8 |
| 1 | F | 138 | ILE | 6.8 |
| 1 | E | 199 | LEU | 6.8 |
| 1 | E | 237 | ASP | 6.7 |
| 1 | D | 227 | GLY | 6.7 |
| 1 | F | 79 | ASP | 6.6 |
| 1 | E | 131 | ALA | 6.6 |
| 1 | E | 377 | GLY | 6.6 |
| 1 | B | 230 | ASP | 6.6 |
| 1 | D | 230 | ASP | 6.6 |
| 1 | F | 342 | ILE | 6.6 |
| 1 | F | 207 | TYR | 6.6 |
| 1 | F | 8 | ASN | 6.6 |
| 1 | F | 144 | ASP | 6.6 |
| 1 | F | 386 | ILE | 6.5 |
| 1 | E | 260 | LYS | 6.5 |
| 1 | F | 261 | MET | 6.5 |
| 1 | B | 221 | SER | 6.5 |
| 1 | F | 265 | LEU | 6.5 |
| 1 | F | 42 | LEU | 6.5 |
| 1 | D | 340[A] | VAL | 6.4 |
| 1 | A | 0 | MET | 6.4 |
| 1 | E | 98 | ILE | 6.4 |
| 1 | F | 98 | ILE | 6.4 |
| 1 | F | 11 | TYR | 6.4 |
| 1 | F | 85 | TRP | 6.4 |
| 1 | E | 255 | VAL | 6.4 |
| 1 | E | 101 | ILE | 6.4 |
| 1 | B | 239[A] | TRP | 6.3 |
| 1 | F | 153 | TYR | 6.3 |
| 1 | E | 144 | ASP | 6.3 |
| 1 | E | 135 | LEU | 6.3 |
| 1 | D | 235 | ALA | 6.3 |
| 1 | E | 232 | PRO | 6.3 |
| 1 | F | 218 | LYS | 6.2 |
| 1 | B | 227 | GLY | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 209 | THR | 6.2 |
| 1 | F | 70 | ARG | 6.2 |
| 1 | B | 225 | ALA | 6.2 |
| 1 | F | 253 | ASP | 6.2 |
| 1 | F | 365 | LEU | 6.2 |
| 1 | D | 224 | GLU | 6.2 |
| 1 | E | 83 | GLU | 6.2 |
| 1 | F | 131 | ALA | 6.2 |
| 1 | F | 224 | GLU | 6.2 |
| 1 | E | 382 | LYS | 6.1 |
| 1 | F | 197 | PRO | 6.1 |
| 1 | B | 238[A] | PHE | 6.1 |
| 1 | E | 250 | GLU | 6.1 |
| 1 | F | 41 | VAL | 6.1 |
| 1 | F | 169 | GLU | 6.1 |
| 1 | F | 156 | ASP | 6.1 |
| 1 | F | 237 | ASP | 6.0 |
| 1 | F | 10 | ILE | 6.0 |
| 1 | F | 75 | ALA | 6.0 |
| 1 | F | 152 | TYR | 6.0 |
| 1 | F | 101 | ILE | 6.0 |
| 1 | F | 250 | GLU | 6.0 |
| 1 | F | 340[A] | VAL | 6.0 |
| 1 | F | 244 | GLY | 6.0 |
| 1 | F | 381 | LEU | 5.9 |
| 1 | B | 228 | LEU | 5.9 |
| 1 | E | 145 | THR | 5.9 |
| 1 | F | 233 | ARG | 5.9 |
| 1 | E | 138 | ILE | 5.9 |
| 1 | F | 86 | GLY | 5.8 |
| 1 | F | 200 | ARG | 5.8 |
| 1 | F | 178 | THR | 5.8 |
| 1 | E | 323 | ILE | 5.8 |
| 1 | D | 228 | LEU | 5.8 |
| 1 | F | 135 | LEU | 5.8 |
| 1 | F | 385 | THR | 5.8 |
| 1 | E | 86 | GLY | 5.8 |
| 1 | F | 341 | GLY | 5.8 |
| 1 | F | 40 | GLY | 5.7 |
| 1 | B | 243[A] | PHE | 5.7 |
| 1 | F | 343 | GLY | 5.7 |
| 1 | B | 236[A] | ALA | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 380 | ASN | 5.6 |
| 1 | E | 340[A] | VAL | 5.6 |
| 1 | D | 342 | ILE | 5.6 |
| 1 | B | 223 | VAL | 5.6 |
| 1 | E | 233 | ARG | 5.6 |
| 1 | B | 217 | PHE | 5.6 |
| 1 | F | 305 | LEU | 5.5 |
| 1 | E | 257 | SER | 5.5 |
| 1 | F | 393 | ARG | 5.5 |
| 1 | C | 0 | MET | 5.5 |
| 1 | F | 112 | ALA | 5.5 |
| 1 | F | 215 | LYS | 5.5 |
| 1 | E | 211 | PRO | 5.5 |
| 1 | E | 142 | ALA | 5.4 |
| 1 | F | 202 | LEU | 5.4 |
| 1 | E | 13 | GLN | 5.4 |
| 1 | F | 141 | HIS | 5.4 |
| 1 | F | 78 | ARG | 5.4 |
| 1 | E | 196 | PHE | 5.4 |
| 1 | B | 222 | GLY | 5.4 |
| 1 | E | 140 | LYS | 5.4 |
| 1 | E | 353 | GLY | 5.3 |
| 1 | D | 94 | PHE | 5.3 |
| 1 | E | 143 | GLY | 5.3 |
| 1 | F | 203 | ALA | 5.3 |
| 1 | F | 130[A] | LEU | 5.3 |
| 1 | F | 82 | VAL | 5.3 |
| 1 | F | 94 | PHE | 5.3 |
| 1 | F | 184 | PHE | 5.3 |
| 1 | E | 342 | ILE | 5.2 |
| 1 | F | 243 | PHE | 5.2 |
| 1 | E | 141 | HIS | 5.2 |
| 1 | E | 216 | LYS | 5.2 |
| 1 | E | 85 | TRP | 5.2 |
| 1 | B | 229 | ARG | 5.2 |
| 1 | F | 122 | GLY | 5.2 |
| 1 | E | 169 | GLU | 5.2 |
| 1 | E | 88 | THR | 5.2 |
| 1 | F | 242 | LEU | 5.1 |
| 1 | E | 11 | TYR | 5.1 |
| 1 | F | 1 | SER | 5.1 |
| 1 | E | 151 | LEU | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 381 | LEU | 5.1 |
| 1 | E | 76 | THR | 5.1 |
| 1 | E | 379 | ARG | 5.0 |
| 1 | F | 181[A] | THR | 5.0 |
| 1 | E | 386 | ILE | 5.0 |
| 1 | C | 226 | GLU | 5.0 |
| 1 | F | 391 | PRO | 5.0 |
| 1 | B | 237[A] | ASP | 5.0 |
| 1 | E | 258 | ILE | 5.0 |
| 1 | F | 256 | ARG | 5.0 |
| 1 | F | 102 | ALA | 5.0 |
| 1 | B | 226 | GLU | 5.0 |
| 1 | D | 176 | VAL | 5.0 |
| 1 | F | 187[A] | ARG | 5.0 |
| 1 | F | 87 | LYS | 5.0 |
| 1 | F | 366 | LEU | 4.9 |
| 1 | F | 176 | VAL | 4.9 |
| 1 | F | 382 | LYS | 4.9 |
| 1 | E | 195 | ASN | 4.9 |
| 1 | D | 237 | ASP | 4.9 |
| 1 | E | 9 | GLU | 4.8 |
| 1 | D | 223 | VAL | 4.8 |
| 1 | F | 232 | PRO | 4.8 |
| 1 | D | 229 | ARG | 4.8 |
| 1 | E | 242 | LEU | 4.8 |
| 1 | F | 104 | CYS | 4.8 |
| 1 | F | 74 | ALA | 4.8 |
| 1 | E | 109 | HIS | 4.8 |
| 1 | E | 253 | ASP | 4.8 |
| 1 | E | 152 | TYR | 4.8 |
| 1 | E | 348 | TRP | 4.7 |
| 1 | E | 176 | VAL | 4.7 |
| 1 | F | 9 | GLU | 4.7 |
| 1 | F | 210 | ASP | 4.7 |
| 1 | D | 222 | GLY | 4.7 |
| 1 | E | 82 | VAL | 4.7 |
| 1 | F | 7 | GLU | 4.7 |
| 1 | F | 378 | TYR | 4.7 |
| 1 | D | 231 | ASN | 4.6 |
| 1 | F | 165 | ARG | 4.6 |
| 1 | F | 105 | ALA | 4.6 |
| 1 | E | 384 | LEU | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 329 | VAL | 4.6 |
| 1 | B | 231 | ASN | 4.6 |
| 1 | D | 16 | VAL | 4.6 |
| 1 | C | 98 | ILE | 4.6 |
| 1 | E | 346 | TYR | 4.6 |
| 1 | C | 229 | ARG | 4.5 |
| 1 | F | 168 | GLU | 4.5 |
| 1 | B | 98 | ILE | 4.5 |
| 1 | E | 218 | LYS | 4.5 |
| 1 | F | 107 | ASP | 4.5 |
| 1 | E | 116 | GLN | 4.5 |
| 1 | F | 84 | LEU | 4.5 |
| 1 | D | 126 | ILE | 4.5 |
| 1 | E | 261 | MET | 4.5 |
| 1 | F | 193 | ILE | 4.5 |
| 1 | C | 225 | ALA | 4.5 |
| 1 | F | 379 | ARG | 4.4 |
| 1 | E | 343 | GLY | 4.4 |
| 1 | E | 385 | THR | 4.4 |
| 1 | C | 126 | ILE | 4.4 |
| 1 | F | 119 | ALA | 4.4 |
| 1 | E | 207 | TYR | 4.4 |
| 1 | F | 329 | VAL | 4.4 |
| 1 | E | 266 | LYS | 4.4 |
| 1 | F | 96 | ALA | 4.4 |
| 1 | F | 137 | ASP | 4.4 |
| 1 | E | 215 | LYS | 4.3 |
| 1 | D | 365 | LEU | 4.3 |
| 1 | E | 259 | THR | 4.3 |
| 1 | F | 157 | ARG | 4.3 |
| 1 | E | 200 | ARG | 4.3 |
| 1 | D | 29[A] | TRP | 4.3 |
| 1 | E | 110 | GLY | 4.3 |
| 1 | B | 219 | ALA | 4.3 |
| 1 | E | 119 | ALA | 4.3 |
| 1 | F | 113 | ALA | 4.3 |
| 1 | F | 13 | GLN | 4.3 |
| 1 | F | 392 | THR | 4.3 |
| 1 | F | 285 | ILE | 4.2 |
| 1 | F | 288 | SER | 4.2 |
| 1 | F | 255 | VAL | 4.2 |
| 1 | C | 219 | ALA | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 319 | PHE | 4.2 |
| 1 | B | 232 | PRO | 4.2 |
| 1 | F | 201 | GLY | 4.2 |
| 1 | E | 168 | GLU | 4.2 |
| 1 | E | 356 | LYS | 4.2 |
| 1 | C | 340 | VAL | 4.2 |
| 1 | E | 120 | ARG | 4.2 |
| 1 | E | 171 | GLY | 4.2 |
| 1 | E | 6 | TYR | 4.2 |
| 1 | F | 132 | VAL | 4.2 |
| 1 | E | 3 | TRP | 4.2 |
| 1 | D | 323 | ILE | 4.1 |
| 1 | E | 391 | PRO | 4.1 |
| 1 | F | 29 | TRP | 4.1 |
| 1 | F | 333 | LEU | 4.1 |
| 1 | E | 96 | ALA | 4.1 |
| 1 | D | 198 | PHE | 4.1 |
| 1 | F | 34 | GLN | 4.1 |
| 1 | E | 197 | PRO | 4.1 |
| 1 | F | 262 | PRO | 4.1 |
| 1 | F | 307 | GLU | 4.1 |
| 1 | E | 137 | ASP | 4.1 |
| 1 | E | 387 | ASP | 4.1 |
| 1 | F | 5 | ASP | 4.1 |
| 1 | F | 290 | HIS | 4.1 |
| 1 | E | 87 | LYS | 4.1 |
| 1 | D | 95 | PHE | 4.1 |
| 1 | E | 159 | LEU | 4.0 |
| 1 | F | 173 | ASP | 4.0 |
| 1 | F | 64 | HIS | 4.0 |
| 1 | C | 319 | PHE | 4.0 |
| 1 | E | 365 | LEU | 4.0 |
| 1 | E | 248 | THR | 4.0 |
| 1 | E | 392 | THR | 4.0 |
| 1 | E | 170 | ALA | 4.0 |
| 1 | E | 277 | ALA | 4.0 |
| 1 | F | 311 | ALA | 4.0 |
| 1 | D | 15 | LEU | 3.9 |
| 1 | B | 198 | PHE | 3.9 |
| 1 | E | 187[A] | ARG | 3.9 |
| 1 | E | 314 | ASP | 3.9 |
| 1 | E | 157 | ARG | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 260 | LYS | 3.9 |
| 1 | F | 387 | ASP | 3.9 |
| 1 | E | 355 | SER | 3.9 |
| 1 | B | 224 | GLU | 3.9 |
| 1 | F | 81 | SER | 3.9 |
| 1 | F | 314 | ASP | 3.9 |
| 1 | F | 241 | GLY | 3.9 |
| 1 | F | 145 | THR | 3.9 |
| 1 | F | 109 | HIS | 3.8 |
| 1 | E | 158 | ASP | 3.8 |
| 1 | C | 181[A] | THR | 3.8 |
| 1 | E | 214 | GLN | 3.8 |
| 1 | E | 2 | ASN | 3.8 |
| 1 | E | 310 | LYS | 3.8 |
| 1 | F | 214 | GLN | 3.7 |
| 1 | F | 151 | LEU | 3.7 |
| 1 | E | 303 | ASP | 3.7 |
| 1 | F | 352 | LEU | 3.7 |
| 1 | C | 286 | TYR | 3.7 |
| 1 | E | 249 | TRP | 3.7 |
| 1 | F | 216 | LYS | 3.7 |
| 1 | E | 81 | SER | 3.7 |
| 1 | E | 114 | SER | 3.7 |
| 1 | E | 173 | ASP | 3.7 |
| 1 | D | 98 | ILE | 3.7 |
| 1 | E | 315 | THR | 3.7 |
| 1 | F | 375 | VAL | 3.7 |
| 1 | F | 149 | PHE | 3.6 |
| 1 | B | 342 | ILE | 3.6 |
| 1 | D | 386 | ILE | 3.6 |
| 1 | E | 278 | VAL | 3.6 |
| 1 | F | 278 | VAL | 3.6 |
| 1 | D | 387 | ASP | 3.6 |
| 1 | F | 83 | GLU | 3.6 |
| 1 | F | 251 | ASP | 3.6 |
| 1 | E | 167 | ALA | 3.6 |
| 1 | F | 133 | SER | 3.6 |
| 1 | F | 315 | THR | 3.6 |
| 1 | F | 291 | GLY | 3.6 |
| 1 | D | 215 | LYS | 3.6 |
| 1 | E | 126 | ILE | 3.6 |
| 1 | E | 8 | ASN | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 102 | ALA | 3.5 |
| 1 | F | 306 | PRO | 3.5 |
| 1 | C | 96 | ALA | 3.5 |
| 1 | A | 226 | GLU | 3.5 |
| 1 | C | 230 | ASP | 3.5 |
| 1 | E | 245 | HIS | 3.5 |
| 1 | E | 75 | ALA | 3.5 |
| 1 | E | 318 | LEU | 3.5 |
| 1 | E | 251 | ASP | 3.5 |
| 1 | F | 268 | ILE | 3.5 |
| 1 | D | 240 | HIS | 3.5 |
| 1 | E | 244 | GLY | 3.5 |
| 1 | F | 194 | SER | 3.5 |
| 1 | E | 252 | ILE | 3.5 |
| 1 | E | 113 | ALA | 3.5 |
| 1 | F | 6 | TYR | 3.4 |
| 1 | B | 218 | LYS | 3.4 |
| 1 | E | 155 | GLU | 3.4 |
| 1 | D | 17 | GLY | 3.4 |
| 1 | C | 342 | ILE | 3.4 |
| 1 | D | 1 | SER | 3.4 |
| 1 | B | 329 | VAL | 3.4 |
| 1 | E | 84 | LEU | 3.4 |
| 1 | E | 330 | VAL | 3.4 |
| 1 | D | 372 | ILE | 3.4 |
| 1 | E | 156 | ASP | 3.4 |
| 1 | F | 166 | ARG | 3.4 |
| 1 | F | 129 | THR | 3.4 |
| 1 | E | 388 | ALA | 3.3 |
| 1 | F | 120 | ARG | 3.3 |
| 1 | F | 310 | LYS | 3.3 |
| 1 | C | 94 | PHE | 3.3 |
| 1 | E | 117 | ALA | 3.3 |
| 1 | B | 181[A] | THR | 3.3 |
| 1 | F | 160 | ALA | 3.3 |
| 1 | F | 339 | ALA | 3.3 |
| 1 | F | 370 | ASP | 3.3 |
| 1 | E | 371 | LEU | 3.3 |
| 1 | E | 164 | ILE | 3.3 |
| 1 | F | 139 | ARG | 3.3 |
| 1 | E | 112 | ALA | 3.3 |
| 1 | F | 118 | SER | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 134 | SER | 3.3 |
| 1 | F | 240 | HIS | 3.3 |
| 1 | D | 329 | VAL | 3.3 |
| 1 | F | 69 | PRO | 3.3 |
| 1 | F | 95 | PHE | 3.2 |
| 1 | B | 340[A] | VAL | 3.2 |
| 1 | C | 1 | SER | 3.2 |
| 1 | E | 162 | SER | 3.2 |
| 1 | F | 171 | GLY | 3.2 |
| 1 | D | 382 | LYS | 3.2 |
| 1 | F | 3 | TRP | 3.2 |
| 1 | F | 209 | THR | 3.2 |
| 1 | F | 111 | ASP | 3.2 |
| 1 | E | 77 | GLU | 3.2 |
| 1 | D | 218 | LYS | 3.2 |
| 1 | F | 282 | VAL | 3.2 |
| 1 | E | 264 | ILE | 3.2 |
| 1 | F | 177 | ILE | 3.2 |
| 1 | E | 362 | ALA | 3.2 |
| 1 | A | 1 | SER | 3.2 |
| 1 | F | 89 | TRP | 3.1 |
| 1 | B | 240[A] | HIS | 3.1 |
| 1 | C | 314 | ASP | 3.1 |
| 1 | F | 100 | VAL | 3.1 |
| 1 | E | 154 | PRO | 3.1 |
| 1 | E | 205 | THR | 3.1 |
| 1 | F | 383 | GLU | 3.1 |
| 1 | B | 242[A] | LEU | 3.1 |
| 1 | E | 350 | ALA | 3.1 |
| 1 | F | 281 | GLY | 3.1 |
| 1 | A | 94 | PHE | 3.1 |
| 1 | A | 342 | ILE | 3.1 |
| 1 | F | 35 | GLN | 3.1 |
| 1 | A | 229 | ARG | 3.1 |
| 1 | D | 97 | PRO | 3.1 |
| 1 | E | 97 | PRO | 3.1 |
| 1 | F | 326 | GLY | 3.1 |
| 1 | B | 1 | SER | 3.1 |
| 1 | F | 146 | PRO | 3.0 |
| 1 | E | 108 | GLY | 3.0 |
| 1 | E | 136 | GLU | 3.0 |
| 1 | E | 40 | GLY | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 250 | GLU | 3.0 |
| 1 | E | 5 | ASP | 3.0 |
| 1 | E | 80 | LEU | 3.0 |
| 1 | E | 163 | PHE | 3.0 |
| 1 | F | 116 | GLN | 3.0 |
| 1 | F | 248 | THR | 3.0 |
| 1 | C | 227 | GLY | 3.0 |
| 1 | F | 154 | PRO | 3.0 |
| 1 | C | 223 | VAL | 3.0 |
| 1 | C | 260 | LYS | 3.0 |
| 1 | F | 369 | ALA | 3.0 |
| 1 | F | 348 | TRP | 3.0 |
| 1 | D | 343 | GLY | 3.0 |
| 1 | F | 297 | GLY | 3.0 |
| 1 | C | 318 | LEU | 3.0 |
| 1 | E | 115 | ALA | 2.9 |
| 1 | E | 29 | TRP | 2.9 |
| 1 | E | 107 | ASP | 2.9 |
| 1 | E | 366 | LEU | 2.9 |
| 1 | F | 162 | SER | 2.9 |
| 1 | E | 279 | ASP | 2.9 |
| 1 | F | 323 | ILE | 2.9 |
| 1 | B | 199 | LEU | 2.9 |
| 1 | E | 282 | VAL | 2.9 |
| 1 | C | 97 | PRO | 2.9 |
| 1 | F | 277 | ALA | 2.9 |
| 1 | F | 180 | ASP | 2.9 |
| 1 | F | 252 | ILE | 2.9 |
| 1 | D | 197 | PRO | 2.9 |
| 1 | B | 96 | ALA | 2.9 |
| 1 | E | 181[A] | THR | 2.9 |
| 1 | F | 115 | ALA | 2.9 |
| 1 | F | 361 | VAL | 2.9 |
| 1 | D | 384[A] | LEU | 2.8 |
| 1 | F | 289 | ASN | 2.8 |
| 1 | D | 266 | LYS | 2.8 |
| 1 | D | 339 | ALA | 2.8 |
| 1 | E | 19 | ALA | 2.8 |
| 1 | C | 346 | TYR | 2.8 |
| 1 | D | 253 | ASP | 2.8 |
| 1 | A | 372 | ILE | 2.8 |
| 1 | C | 222 | GLY | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 241 | GLY | 2.8 |
| 1 | F | 39 | PRO | 2.8 |
| 1 | B | 151 | LEU | 2.8 |
| 1 | C | 95 | PHE | 2.8 |
| 1 | E | 79 | ASP | 2.8 |
| 1 | E | 184 | PHE | 2.8 |
| 1 | E | 192 | THR | 2.8 |
| 1 | C | 341 | GLY | 2.8 |
| 1 | F | 110 | GLY | 2.8 |
| 1 | C | 323 | ILE | 2.8 |
| 1 | C | 266 | LYS | 2.8 |
| 1 | F | 179 | LEU | 2.8 |
| 1 | D | 257 | SER | 2.8 |
| 1 | E | 393 | ARG | 2.8 |
| 1 | F | 279 | ASP | 2.8 |
| 1 | E | 133 | SER | 2.7 |
| 1 | A | 365 | LEU | 2.7 |
| 1 | D | 144 | ASP | 2.7 |
| 1 | D | 333 | LEU | 2.7 |
| 1 | E | 175 | LEU | 2.7 |
| 1 | B | 94 | PHE | 2.7 |
| 1 | D | 79 | ASP | 2.7 |
| 1 | F | 46 | ALA | 2.7 |
| 1 | F | 167 | ALA | 2.7 |
| 1 | D | 361 | VAL | 2.7 |
| 1 | F | 204[A] | LEU | 2.7 |
| 1 | F | 106 | GLN | 2.7 |
| 1 | F | 121 | THR | 2.7 |
| 1 | C | 224 | GLU | 2.7 |
| 1 | A | 98 | ILE | 2.7 |
| 1 | E | 106 | GLN | 2.7 |
| 1 | A | 130[A] | LEU | 2.7 |
| 1 | B | 29[A] | TRP | 2.7 |
| 1 | E | 179 | LEU | 2.7 |
| 1 | E | 178 | THR | 2.7 |
| 1 | E | 288 | SER | 2.7 |
| 1 | D | 96 | ALA | 2.6 |
| 1 | B | 126 | ILE | 2.6 |
| 1 | F | 303 | ASP | 2.6 |
| 1 | E | 153 | TYR | 2.6 |
| 1 | B | 200 | ARG | 2.6 |
| 1 | D | 149 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 108 | GLY | 2.6 |
| 1 | E | 339 | ALA | 2.6 |
| 1 | E | 312 | SER | 2.6 |
| 1 | A | 126 | ILE | 2.6 |
| 1 | A | 340[A] | VAL | 2.6 |
| 1 | C | 151 | LEU | 2.6 |
| 1 | E | 202 | LEU | 2.6 |
| 1 | E | 305 | LEU | 2.6 |
| 1 | F | 206 | ASN | 2.6 |
| 1 | E | 65 | TRP | 2.6 |
| 1 | D | 76 | THR | 2.6 |
| 1 | B | 16 | VAL | 2.6 |
| 1 | D | 275 | ARG | 2.5 |
| 1 | E | 297 | GLY | 2.5 |
| 1 | F | 205 | THR | 2.5 |
| 1 | F | 334 | ALA | 2.5 |
| 1 | C | 101 | ILE | 2.5 |
| 1 | C | 176 | VAL | 2.5 |
| 1 | E | 78 | ARG | 2.5 |
| 1 | F | 44 | TYR | 2.5 |
| 1 | F | 267 | GLY | 2.5 |
| 1 | E | 139 | ARG | 2.5 |
| 1 | D | 319 | PHE | 2.5 |
| 1 | D | 341 | GLY | 2.5 |
| 1 | F | 190 | ASP | 2.5 |
| 1 | C | 178 | THR | 2.5 |
| 1 | F | 22 | LEU | 2.5 |
| 1 | B | 233 | ARG | 2.5 |
| 1 | F | 158 | ASP | 2.5 |
| 1 | E | 383 | GLU | 2.5 |
| 1 | F | 136 | GLU | 2.5 |
| 1 | E | 21 | THR | 2.5 |
| 1 | D | 152 | TYR | 2.5 |
| 1 | E | 24 | MET | 2.5 |
| 1 | E | 61 | ALA | 2.5 |
| 1 | E | 35 | GLN | 2.5 |
| 1 | F | 2 | ASN | 2.5 |
| 1 | E | 243 | PHE | 2.5 |
| 1 | F | 249 | TRP | 2.5 |
| 1 | B | 346 | TYR | 2.4 |
| 1 | D | 295 | ALA | 2.4 |
| 1 | D | 369 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 274 | ALA | 2.4 |
| 1 | F | 155 | GLU | 2.4 |
| 1 | D | 216 | LYS | 2.4 |
| 1 | E | 246 | SER | 2.4 |
| 1 | F | 321 | SER | 2.4 |
| 1 | F | 355 | SER | 2.4 |
| 1 | B | 365 | LEU | 2.4 |
| 1 | E | 72 | LEU | 2.4 |
| 1 | F | 384 | LEU | 2.4 |
| 1 | E | 31 | ALA | 2.4 |
| 1 | E | 380 | ASN | 2.4 |
| 1 | C | 220 | HIS | 2.4 |
| 1 | E | 73 | MET | 2.4 |
| 1 | C | 329 | VAL | 2.4 |
| 1 | D | 151 | LEU | 2.4 |
| 1 | F | 27 | ALA | 2.4 |
| 1 | F | 80 | LEU | 2.4 |
| 1 | C | 343 | GLY | 2.4 |
| 1 | D | 232 | PRO | 2.4 |
| 1 | E | 275 | ARG | 2.4 |
| 1 | E | 104 | CYS | 2.4 |
| 1 | C | 215 | LYS | 2.4 |
| 1 | F | 186 | TRP | 2.4 |
| 1 | C | 100 | VAL | 2.3 |
| 1 | A | 323 | ILE | 2.3 |
| 1 | D | 252 | ILE | 2.3 |
| 1 | E | 204 | LEU | 2.3 |
| 1 | F | 67 | LEU | 2.3 |
| 1 | E | 203 | ALA | 2.3 |
| 1 | D | 314[A] | ASP | 2.3 |
| 1 | F | 128 | SER | 2.3 |
| 1 | E | 347 | ALA | 2.3 |
| 1 | F | 61 | ALA | 2.3 |
| 1 | F | 117 | ALA | 2.3 |
| 1 | F | 25 | SER | 2.3 |
| 1 | E | 333 | LEU | 2.3 |
| 1 | F | 103 | LEU | 2.3 |
| 1 | F | 126 | ILE | 2.3 |
| 1 | D | 178 | THR | 2.3 |
| 1 | D | 318 | LEU | 2.3 |
| 1 | F | 114 | SER | 2.2 |
| 1 | B | 202 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 268 | ILE | 2.2 |
| 1 | E | 341 | GLY | 2.2 |
| 1 | F | 313 | GLY | 2.2 |
| 1 | C | 321 | SER | 2.2 |
| 1 | A | 295 | ALA | 2.2 |
| 1 | F | 31 | ALA | 2.2 |
| 1 | D | 208 | VAL | 2.2 |
| 1 | E | 100 | VAL | 2.2 |
| 1 | B | 372 | ILE | 2.2 |
| 1 | A | 29[A] | TRP | 2.2 |
| 1 | E | 182 | TRP | 2.2 |
| 1 | F | 280 | SER | 2.2 |
| 1 | E | 263 | VAL | 2.2 |
| 1 | F | 30 | GLU | 2.2 |
| 1 | F | 272 | ASP | 2.2 |
| 1 | D | 254 | TRP | 2.2 |
| 1 | E | 325 | THR | 2.2 |
| 1 | A | 225 | ALA | 2.2 |
| 1 | E | 33 | ALA | 2.2 |
| 1 | E | 378 | TYR | 2.2 |
| 1 | C | 290 | HIS | 2.2 |
| 1 | F | 32 | HIS | 2.2 |
| 1 | B | 358 | ILE | 2.2 |
| 1 | C | 339 | ALA | 2.2 |
| 1 | D | 196 | PHE | 2.1 |
| 1 | E | 319 | PHE | 2.1 |
| 1 | C | 169 | GLU | 2.1 |
| 1 | E | 7 | GLU | 2.1 |
| 1 | F | 188 | PRO | 2.1 |
| 1 | F | 271 | PRO | 2.1 |
| 1 | F | 345 | PRO | 2.1 |
| 1 | E | 103 | LEU | 2.1 |
| 1 | A | 44 | TYR | 2.1 |
| 1 | D | 158 | ASP | 2.1 |
| 1 | A | 287 | CYS | 2.1 |
| 1 | D | 265 | LEU | 2.1 |
| 1 | E | 129 | THR | 2.1 |
| 1 | C | 288 | SER | 2.1 |
| 1 | E | 280[A] | SER | 2.1 |
| 1 | F | 73 | MET | 2.1 |
| 1 | B | 169 | GLU | 2.1 |
| 1 | E | 349 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 346 | TYR | 2.1 |
| 1 | A | 319 | PHE | 2.1 |
| 1 | E | 95 | PHE | 2.1 |
| 1 | F | 43 | SER | 2.1 |
| 1 | A | 375 | VAL | 2.1 |
| 1 | F | 317 | VAL | 2.1 |
| 1 | E | 295 | ALA | 2.1 |
| 1 | E | 146 | PRO | 2.1 |
| 1 | E | 345 | PRO | 2.1 |
| 1 | C | 268 | ILE | 2.1 |
| 1 | F | 47 | GLY | 2.1 |
| 1 | F | 264 | ILE | 2.1 |
| 1 | F | 377 | GLY | 2.1 |
| 1 | B | 367 | ALA | 2.1 |
| 1 | E | 160 | ALA | 2.1 |
| 1 | F | 389 | LEU | 2.1 |
| 1 | B | 268 | ILE | 2.1 |
| 1 | B | 323 | ILE | 2.1 |
| 1 | E | 34 | GLN | 2.0 |
| 1 | F | 192 | THR | 2.0 |
| 1 | E | 271 | PRO | 2.0 |
| 1 | F | 161 | GLU | 2.0 |
| 1 | A | 346 | TYR | 2.0 |
| 1 | C | 291 | GLY | 2.0 |
| 1 | F | 346 | TYR | 2.0 |
| 1 | D | 256 | ARG | 2.0 |
| 1 | F | 371 | LEU | 2.0 |
| 1 | D | 93 | MET | 2.0 |
| 1 | F | 93 | MET | 2.0 |
| 1 | F | 275 | ARG | 2.0 |
| 1 | D | 321 | SER | 2.0 |
| 1 | B | 361 | VAL | 2.0 |
| 1 | E | 67 | LEU | 2.0 |
| 1 | D | 14 | GLY | 2.0 |
| 1 | E | 316 | PRO | 2.0 |

## 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)

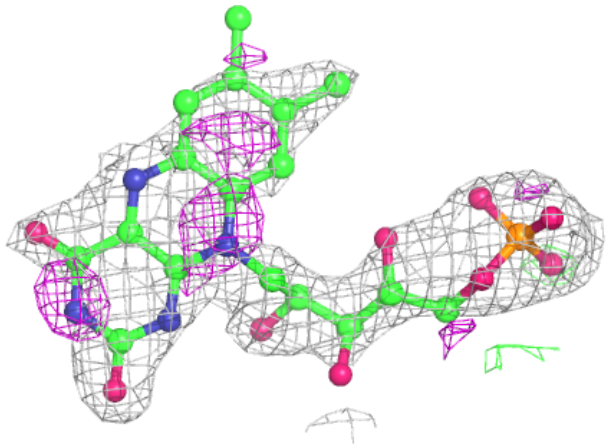
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

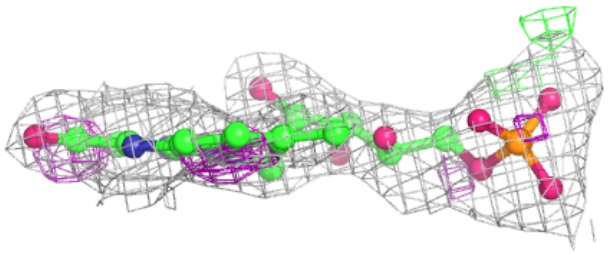
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | SO4 | B | 406[B] | 5/5 | 0.71 | 0.23 | 50,56,56,59 | 5 |
| 3 | SO4 | A | 404[A] | 5/5 | 0.78 | 0.31 | 50,56,58,59 | 5 |
| 2 | FMN | F | 401 | 31/31 | 0.81 | 0.18 | 74,79,82,82 | 31 |
| 3 | SO4 | F | 402 | 5/5 | 0.84 | 0.14 | 88,89,89,90 | 5 |
| 3 | SO4 | E | 403 | 5/5 | 0.85 | 0.14 | 94,95,95,96 | 5 |
| 2 | FMN | E | 401 | 31/31 | 0.86 | 0.20 | 74,78,81,81 | 31 |
| 3 | SO4 | B | 404[A] | 5/5 | 0.87 | 0.22 | 67,67,68,70 | 5 |
| 3 | SO4 | C | 404 | 5/5 | 0.90 | 0.24 | 66,66,67,68 | 5 |
| 3 | SO4 | F | 403 | 5/5 | 0.93 | 0.23 | 72,72,74,74 | 5 |
| 3 | SO4 | A | 405 | 5/5 | 0.94 | 0.19 | 63,64,64,65 | 5 |
| 3 | SO4 | B | 405 | 5/5 | 0.94 | 0.26 | 99,99,101,104 | 0 |
| 2 | FMN | C | 401 | 31/31 | 0.96 | 0.16 | 29,33,37,39 | 0 |
| 3 | SO4 | E | 402 | 5/5 | 0.96 | 0.26 | 98,98,99,99 | 0 |
| 2 | FMN | D | 401 | 31/31 | 0.96 | 0.10 | 39,46,51,52 | 0 |
| 2 | FMN | B | 401 | 31/31 | 0.97 | 0.12 | 23,29,33,36 | 0 |
| 2 | FMN | A | 401 | 31/31 | 0.98 | 0.15 | 19,23,26,30 | 0 |
| 3 | SO4 | D | 403 | 5/5 | 0.98 | 0.11 | 64,64,69,71 | 0 |
| 3 | SO4 | C | 403 | 5/5 | 0.99 | 0.08 | 36,42,43,45 | 0 |
| 3 | SO4 | B | 403 | 5/5 | 0.99 | 0.09 | 38,40,44,45 | 0 |
| 3 | SO4 | B | 402 | 5/5 | 0.99 | 0.08 | 38,39,43,43 | 0 |
| 3 | SO4 | A | 403 | 5/5 | 0.99 | 0.12 | 35,35,39,39 | 0 |
| 3 | SO4 | D | 402 | 5/5 | 0.99 | 0.11 | 51,51,55,56 | 0 |
| 3 | SO4 | A | 402 | 5/5 | 1.00 | 0.06 | 30,34,35,37 | 0 |
| 3 | SO4 | C | 402 | 5/5 | 1.00 | 0.08 | 39,44,46,49 | 0 |

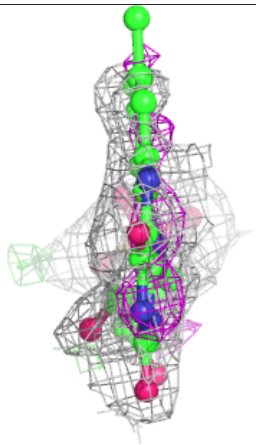
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FMN F 401:**

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

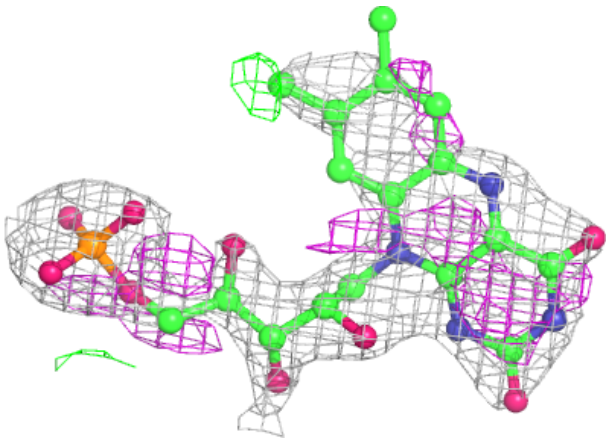


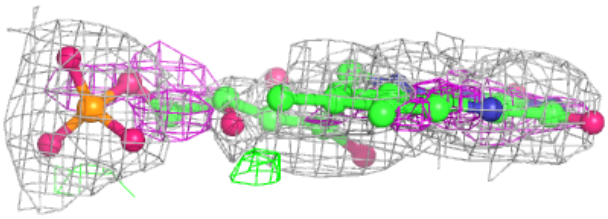


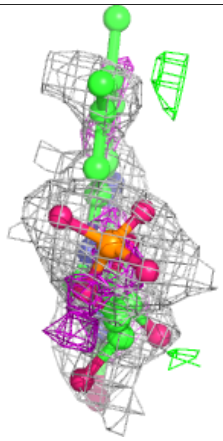


**Electron density around FMN E 401:**

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

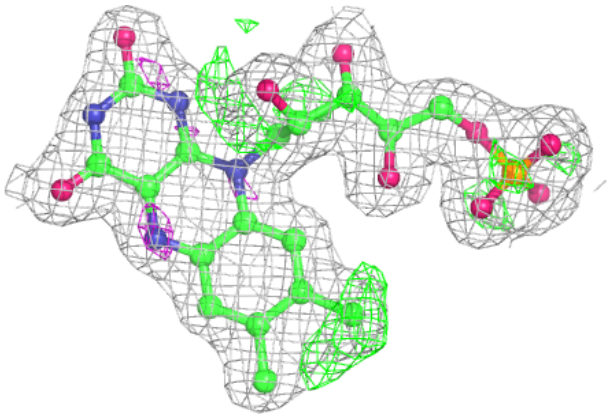


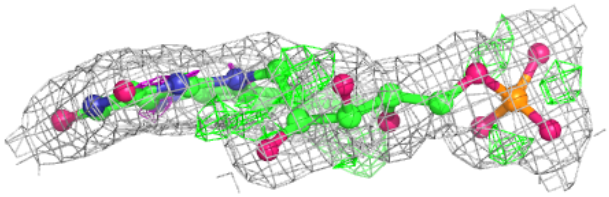


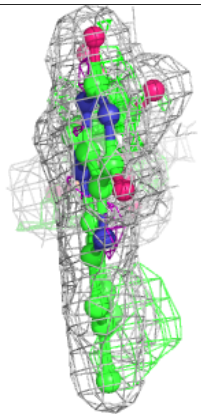


**Electron density around FMN C 401:**

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

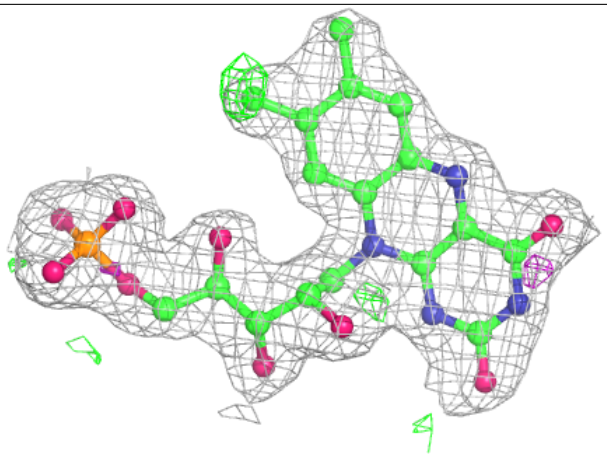


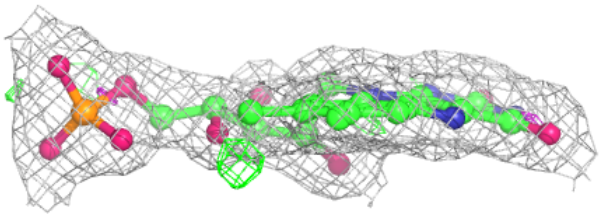


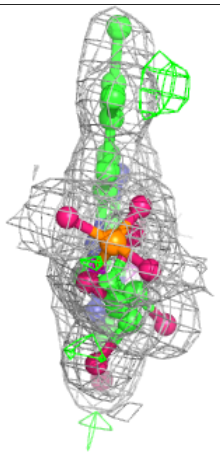


**Electron density around FMN D 401:**

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

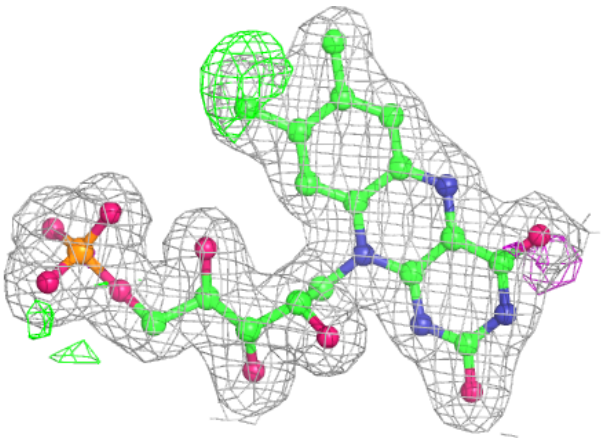


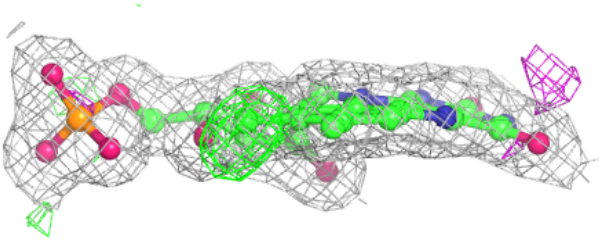


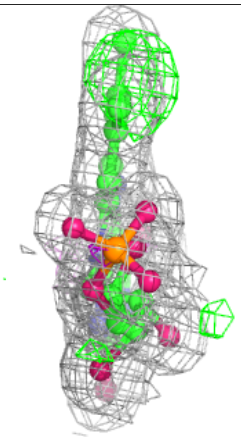


**Electron density around FMN B 401:**

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

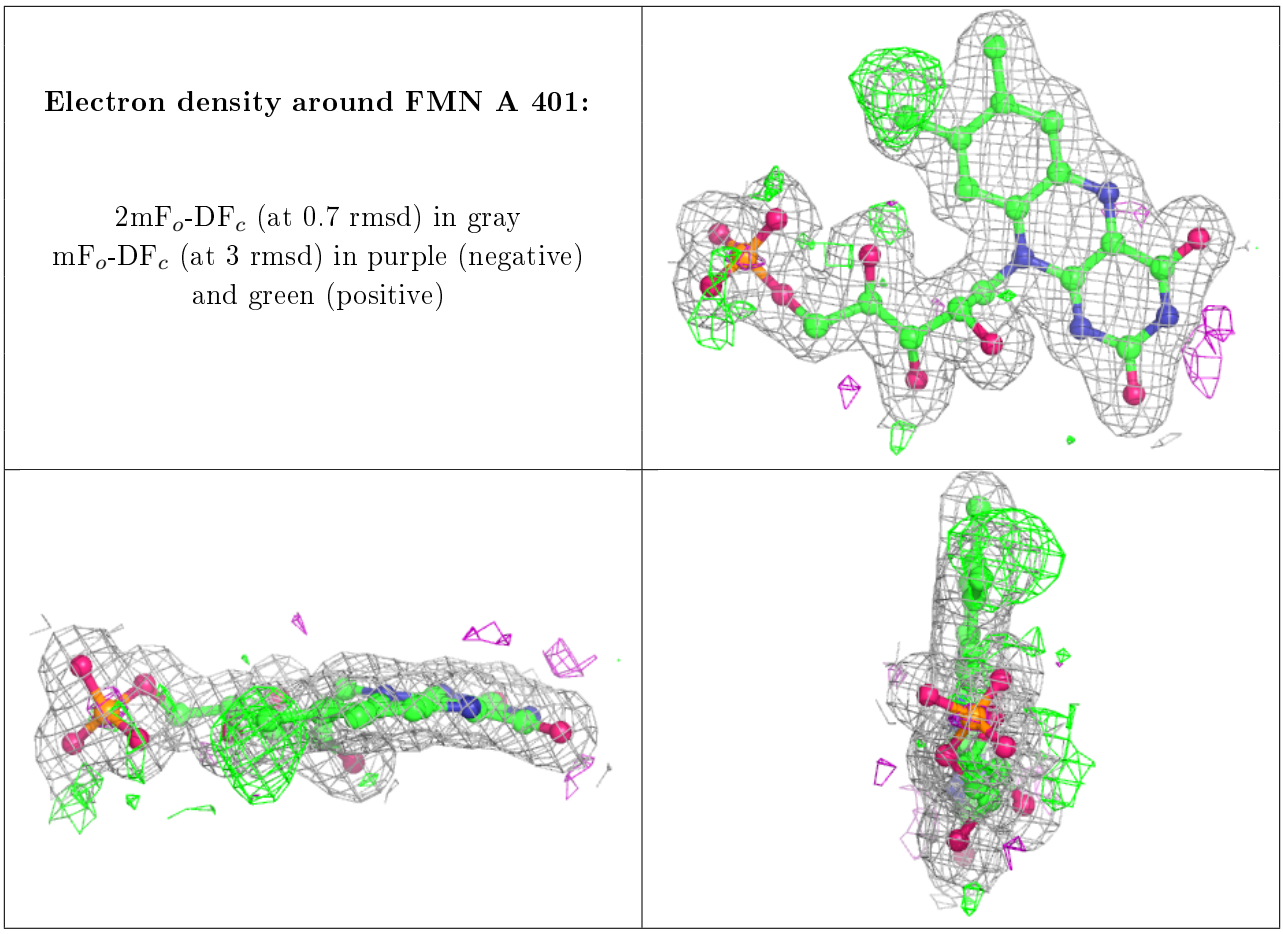






**Electron density around FMN A 401:**

$2mF_o$-$DF_c$ (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.