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

Feb 1, 2016 – 02:10 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 2FRV |
| Title | : | CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE |
| Authors | : | Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C. |
| Deposited on | : | 1997-06-10 |
| 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

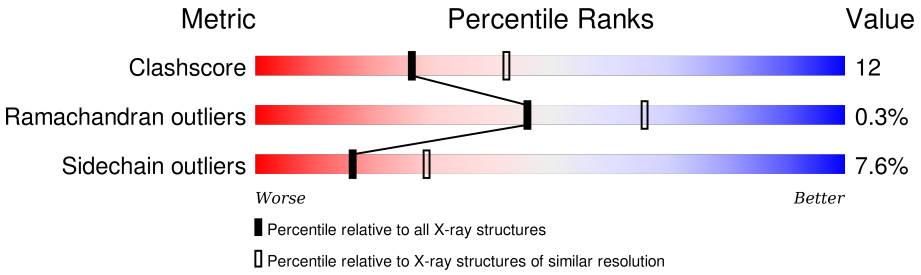
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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)) |
|---|---|---|
| Clashscore | 102246 | 5292 (2.58-2.50) |
| Ramachandran outliers | 100387 | 5194 (2.58-2.50) |
| Sidechain outliers | 100360 | 5196 (2.58-2.50) |

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. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 264 | 69% 26% • • |
| 1 | C | 264 | 70% 24% • • |
| 1 | E | 264 | 70% 24% 5% • |
| 1 | G | 264 | 70% 24% • • |
| 1 | I | 264 | 70% 23% 5% • |
| 1 | S | 264 | 70% 23% 5% • |
| 2 | B | 536 | 63% 31% • •• |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | D | 536 | 63% 30% |
| 2 | F | 536 | 62% 31% 5% |
| 2 | H | 536 | 63% 30% |
| 2 | J | 536 | 63% 30% 5% |
| 2 | L | 536 | 63% 30% 5% |

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 |
|---|---|---|---|---|---|---|---|
| 7 | FCO | B | 537 | - | - | X | - |
| 7 | FCO | D | 537 | - | - | X | - |
| 7 | FCO | F | 537 | - | - | X | - |
| 7 | FCO | H | 537 | - | - | X | - |
| 7 | FCO | J | 537 | - | - | X | - |
| 7 | FCO | L | 537 | - | - | X | - |

# 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 38040 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 PERIPLASMIC HYDROGENASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | S | 261 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1964 | 1249 | 329 | 367 | 19 | | | |
| 1 | A | 261 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1964 | 1249 | 329 | 367 | 19 | | | |
| 1 | C | 261 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1964 | 1249 | 329 | 367 | 19 | | | |
| 1 | E | 261 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1964 | 1249 | 329 | 367 | 19 | | | |
| 1 | G | 261 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1964 | 1249 | 329 | 367 | 19 | | | |
| 1 | I | 261 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1964 | 1249 | 329 | 367 | 19 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| S | 24 | VAL | LEU | CONFLICT | UNP P12943 |
| S | 89 | GLY | ARG | CONFLICT | UNP P12943 |
| A | 24 | VAL | LEU | CONFLICT | UNP P12943 |
| A | 89 | GLY | ARG | CONFLICT | UNP P12943 |
| C | 24 | VAL | LEU | CONFLICT | UNP P12943 |
| C | 89 | GLY | ARG | CONFLICT | UNP P12943 |
| E | 24 | VAL | LEU | CONFLICT | UNP P12943 |
| E | 89 | GLY | ARG | CONFLICT | UNP P12943 |
| G | 24 | VAL | LEU | CONFLICT | UNP P12943 |
| G | 89 | GLY | ARG | CONFLICT | UNP P12943 |
| I | 24 | VAL | LEU | CONFLICT | UNP P12943 |
| I | 89 | GLY | ARG | CONFLICT | UNP P12943 |

- Molecule 2 is a protein called PERIPLASMIC HYDROGENASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | L | 530 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4152 | 2653 | 725 | 757 | 17 | | | |
| 2 | B | 530 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4152 | 2653 | 725 | 757 | 17 | | | |
| 2 | D | 530 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4152 | 2653 | 725 | 757 | 17 | | | |
| 2 | F | 530 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4152 | 2653 | 725 | 757 | 17 | | | |
| 2 | H | 530 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4152 | 2653 | 725 | 757 | 17 | | | |
| 2 | J | 530 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4152 | 2653 | 725 | 757 | 17 | | | |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| L | 144 | LYS | ARG | CONFLICT | UNP P12944 |
| L | 332 | GLY | ASP | CONFLICT | UNP P12944 |
| L | 482 | LEU | HIS | CONFLICT | UNP P12944 |
| L | 497 | GLY | ARG | CONFLICT | UNP P12944 |
| B | 144 | LYS | ARG | CONFLICT | UNP P12944 |
| B | 332 | GLY | ASP | CONFLICT | UNP P12944 |
| B | 482 | LEU | HIS | CONFLICT | UNP P12944 |
| B | 497 | GLY | ARG | CONFLICT | UNP P12944 |
| D | 144 | LYS | ARG | CONFLICT | UNP P12944 |
| D | 332 | GLY | ASP | CONFLICT | UNP P12944 |
| D | 482 | LEU | HIS | CONFLICT | UNP P12944 |
| D | 497 | GLY | ARG | CONFLICT | UNP P12944 |
| F | 144 | LYS | ARG | CONFLICT | UNP P12944 |
| F | 332 | GLY | ASP | CONFLICT | UNP P12944 |
| F | 482 | LEU | HIS | CONFLICT | UNP P12944 |
| F | 497 | GLY | ARG | CONFLICT | UNP P12944 |
| H | 144 | LYS | ARG | CONFLICT | UNP P12944 |
| H | 332 | GLY | ASP | CONFLICT | UNP P12944 |
| H | 482 | LEU | HIS | CONFLICT | UNP P12944 |
| H | 497 | GLY | ARG | CONFLICT | UNP P12944 |
| J | 144 | LYS | ARG | CONFLICT | UNP P12944 |
| J | 332 | GLY | ASP | CONFLICT | UNP P12944 |
| J | 482 | LEU | HIS | CONFLICT | UNP P12944 |
| J | 497 | GLY | ARG | CONFLICT | UNP P12944 |

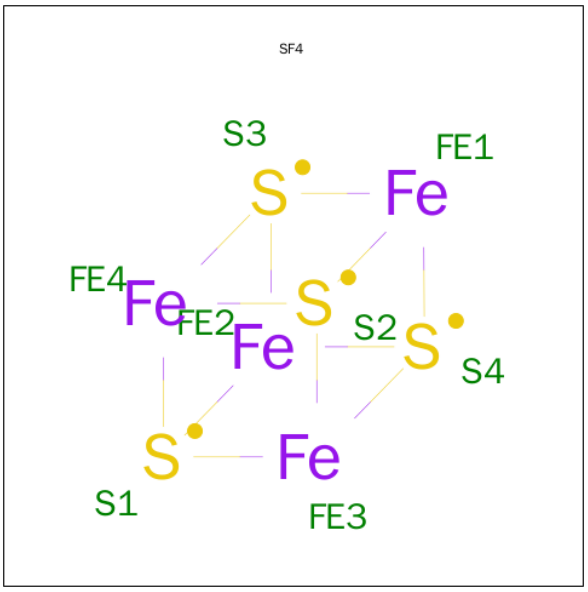
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | J | 1 | Total Ni<br>1 1 | 0 | 0 |
| 3 | D | 1 | Total Ni<br>1 1 | 0 | 0 |
| 3 | H | 1 | Total Ni<br>1 1 | 0 | 0 |
| 3 | B | 1 | Total Ni<br>1 1 | 0 | 0 |
| 3 | L | 1 | Total Ni<br>1 1 | 0 | 0 |
| 3 | F | 1 | Total Ni<br>1 1 | 0 | 0 |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

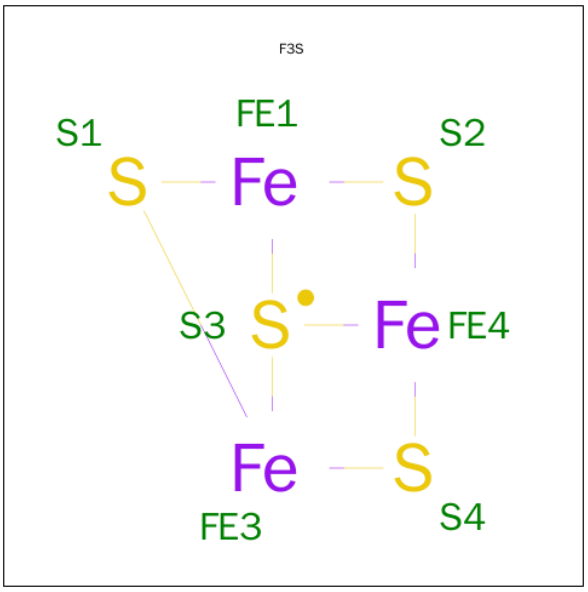
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | J | 1 | Total Mg<br>1 1 | 0 | 0 |
| 4 | D | 1 | Total Mg<br>1 1 | 0 | 0 |
| 4 | H | 1 | Total Mg<br>1 1 | 0 | 0 |
| 4 | B | 1 | Total Mg<br>1 1 | 0 | 0 |
| 4 | L | 1 | Total Mg<br>1 1 | 0 | 0 |
| 4 | F | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).



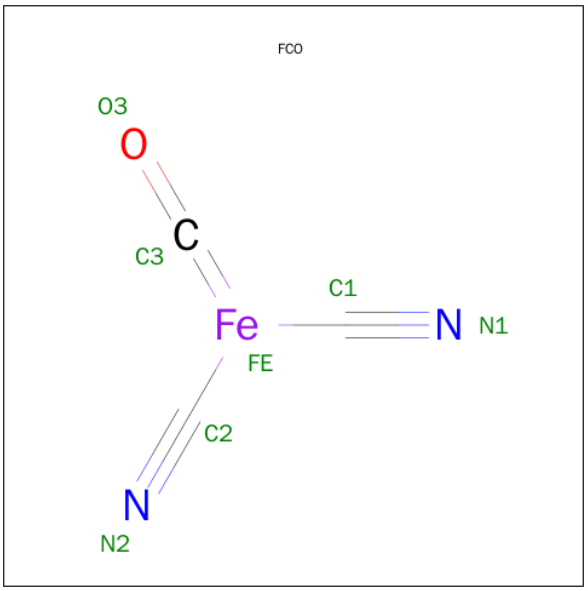

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | S | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | S | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | A | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | A | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | C | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | C | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | E | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | E | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | G | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | G | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | I | 1 | Total Fe S<br>8 4 4 | 0 | 0 |
| 5 | I | 1 | Total Fe S<br>8 4 4 | 0 | 0 |

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: $Fe_3S_4$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | S | 1 | Total Fe S<br>7 3 4 | 0 | 0 |
| 6 | A | 1 | Total Fe S<br>7 3 4 | 0 | 0 |
| 6 | C | 1 | Total Fe S<br>7 3 4 | 0 | 0 |
| 6 | E | 1 | Total Fe S<br>7 3 4 | 0 | 0 |
| 6 | G | 1 | Total Fe S<br>7 3 4 | 0 | 0 |
| 6 | I | 1 | Total Fe S<br>7 3 4 | 0 | 0 |

- Molecule 7 is CARBONMONOXIDE-(DICYANO) IRON (three-letter code: FCO) (formula: $C_3FeN_2O$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 7 | L | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 7 | 3 | 1 | 2 | 1 | | |
| 7 | B | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 7 | 3 | 1 | 2 | 1 | | |
| 7 | D | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 7 | 3 | 1 | 2 | 1 | | |
| 7 | F | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 7 | 3 | 1 | 2 | 1 | | |
| 7 | H | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 7 | 3 | 1 | 2 | 1 | | |
| 7 | J | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 7 | 3 | 1 | 2 | 1 | | |

- Molecule 8 is OXYGEN ATOM (three-letter code: O) (formula: O).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 8 | J | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 8 | D | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 8 | H | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 8 | B | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 8 | L | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 8 | F | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 9 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 9 | A | 78 | Total O<br>78 78 | 0 | 0 |
| 9 | B | 114 | Total O<br>114 114 | 0 | 0 |
| 9 | C | 76 | Total O<br>76 76 | 0 | 0 |
| 9 | D | 114 | Total O<br>114 114 | 0 | 0 |
| 9 | E | 81 | Total O<br>81 81 | 0 | 0 |
| 9 | F | 115 | Total O<br>115 115 | 0 | 0 |
| 9 | G | 76 | Total O<br>76 76 | 0 | 0 |
| 9 | H | 112 | Total O<br>112 112 | 0 | 0 |
| 9 | I | 80 | Total O<br>80 80 | 0 | 0 |
| 9 | J | 113 | Total O<br>113 113 | 0 | 0 |
| 9 | L | 110 | Total O<br>110 110 | 0 | 0 |
| 9 | S | 77 | Total O<br>77 77 | 0 | 0 |

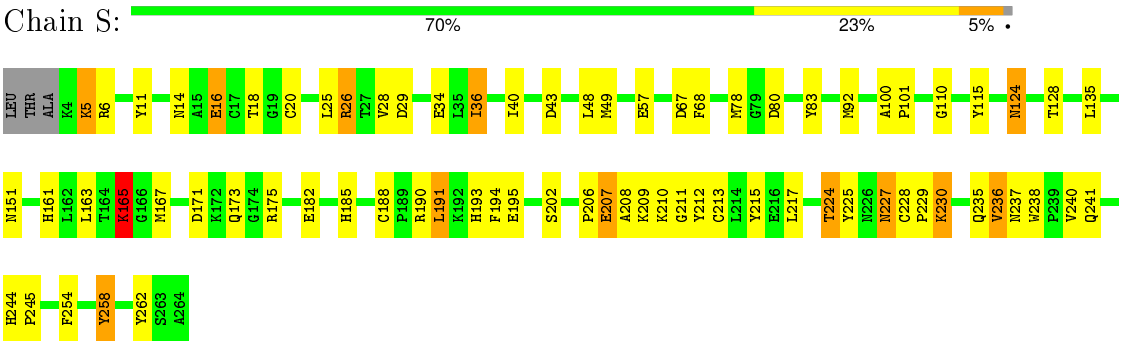
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

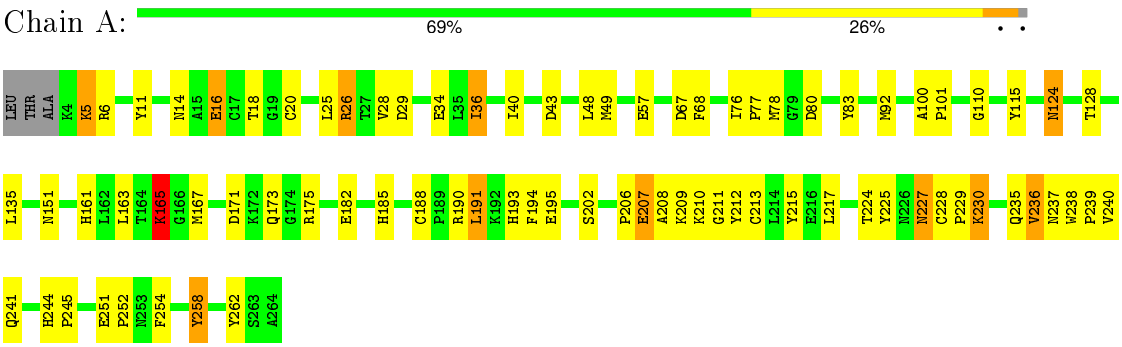
- Molecule 1: PERIPLASMIC HYDROGENASE

Chain S:



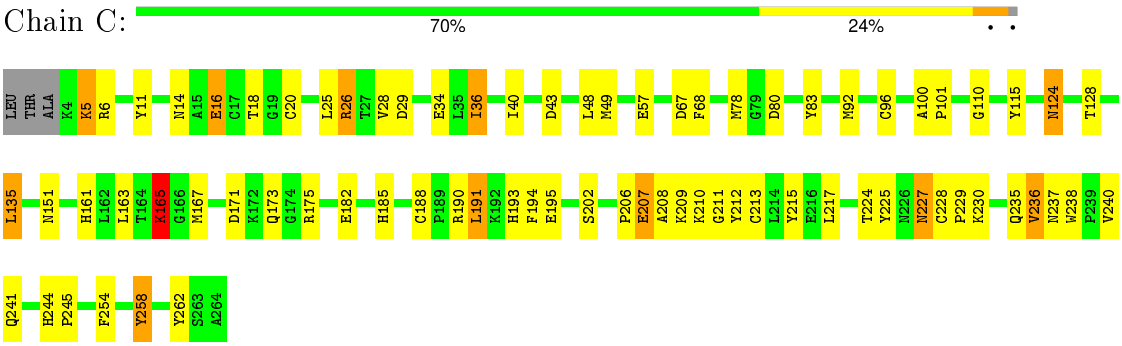

- Molecule 1: PERIPLASMIC HYDROGENASE

Chain A:



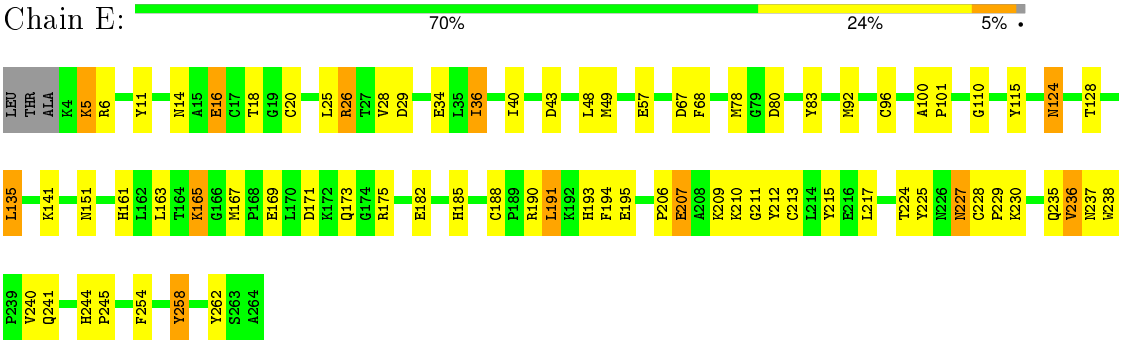

- Molecule 1: PERIPLASMIC HYDROGENASE

Chain C:



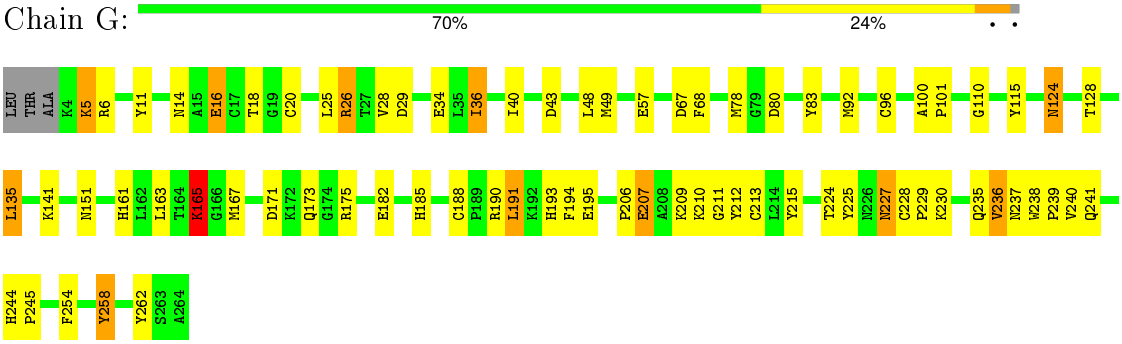
• Molecule 1: PERIPLASMIC HYDROGENASE

Chain E:



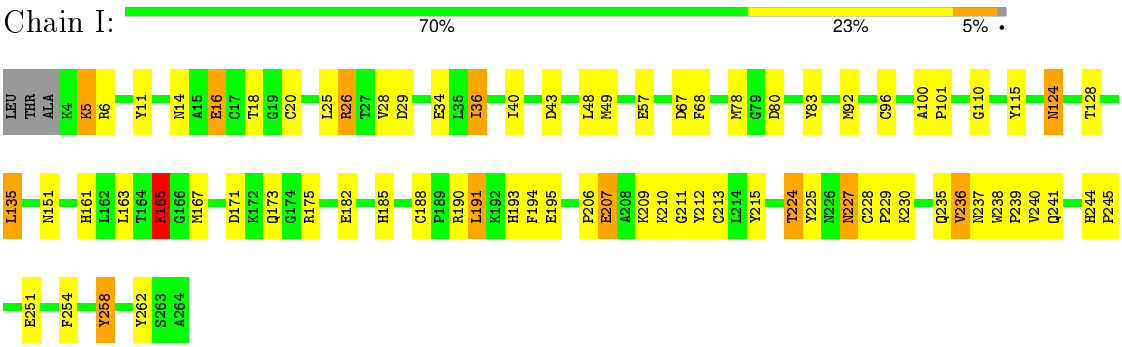

• Molecule 1: PERIPLASMIC HYDROGENASE

Chain G:



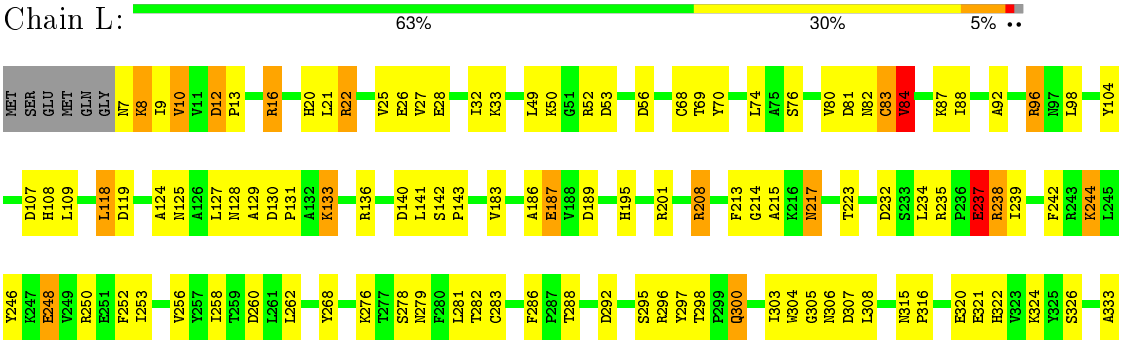

• Molecule 1: PERIPLASMIC HYDROGENASE

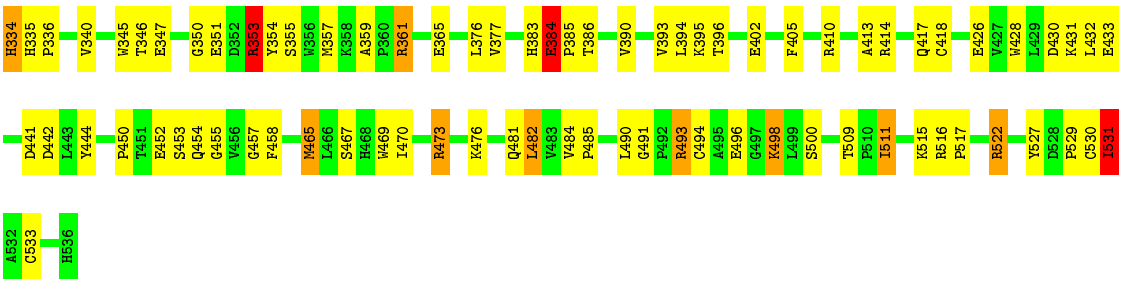
Chain I:




• Molecule 2: PERIPLASMIC HYDROGENASE

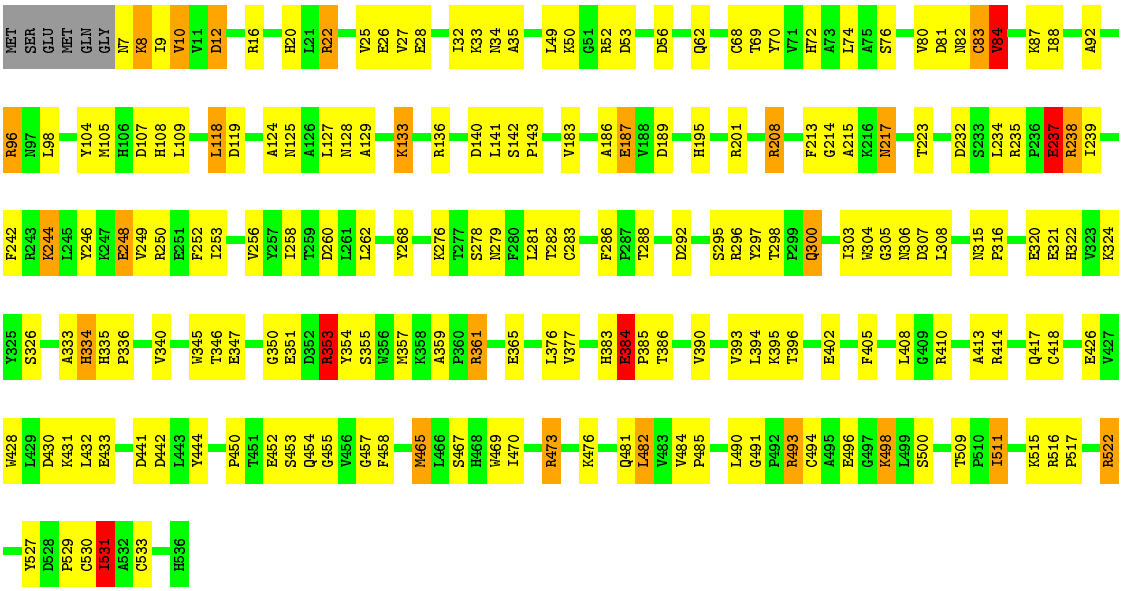
Chain L:





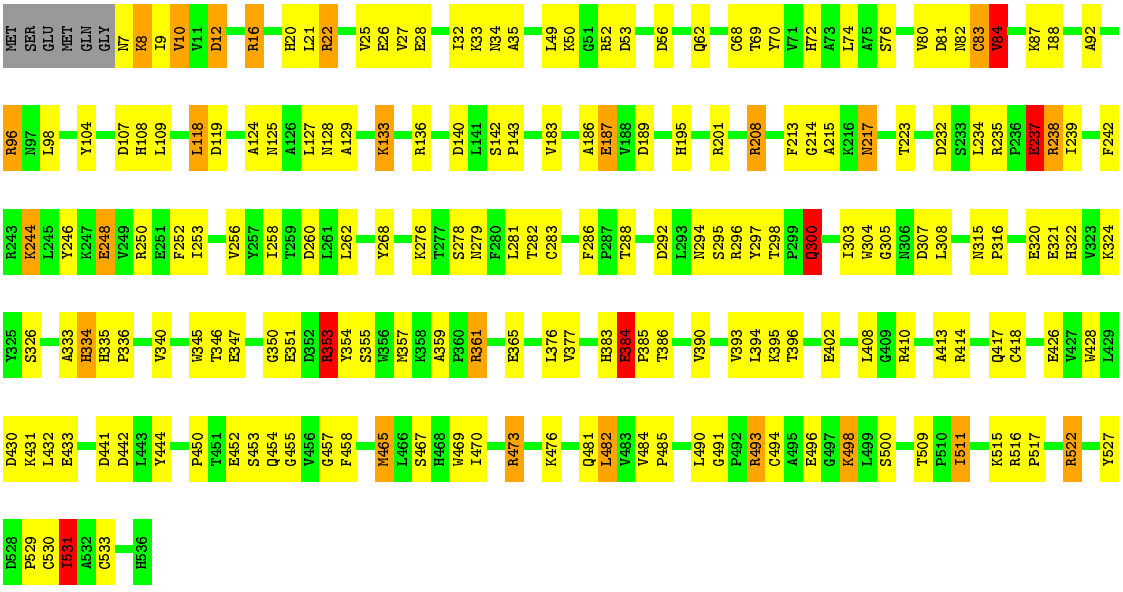

- Molecule 2: PERIPLASMIC HYDROGENASE

Chain B:



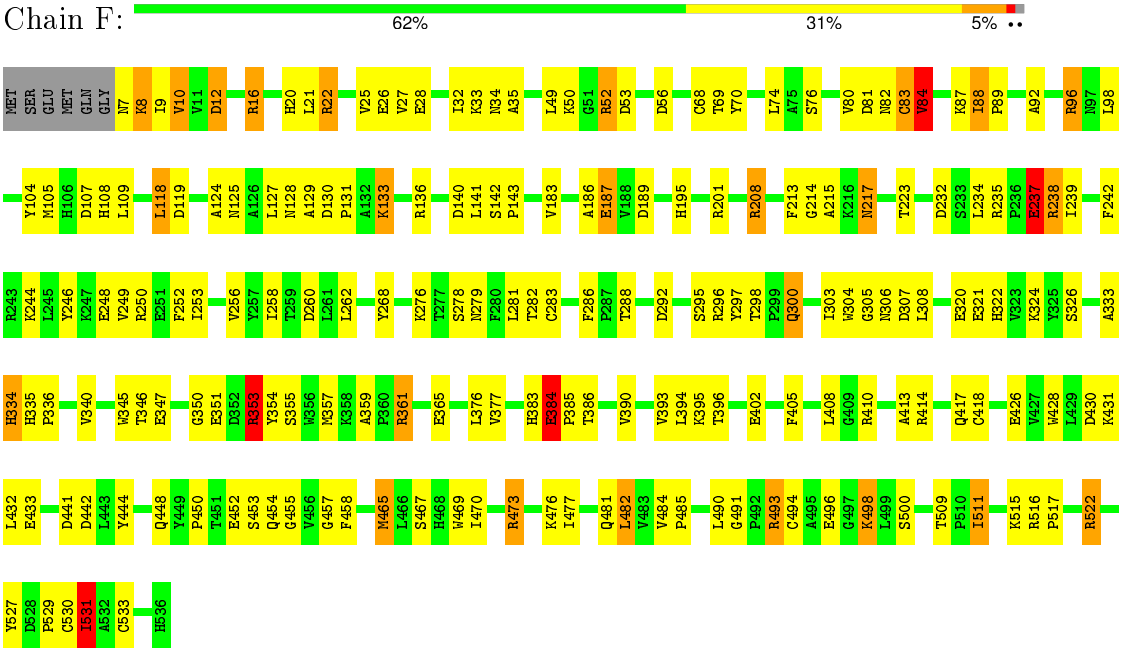

- Molecule 2: PERIPLASMIC HYDROGENASE

Chain D:



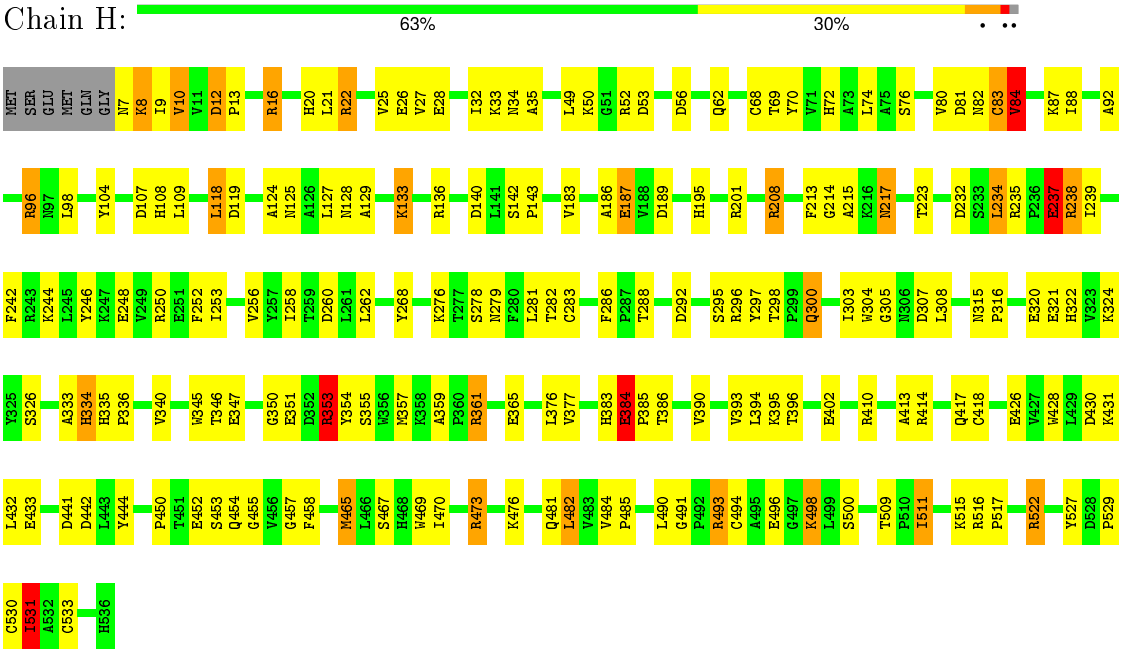
• Molecule 2: PERIPLASMIC HYDROGENASE

Chain F:



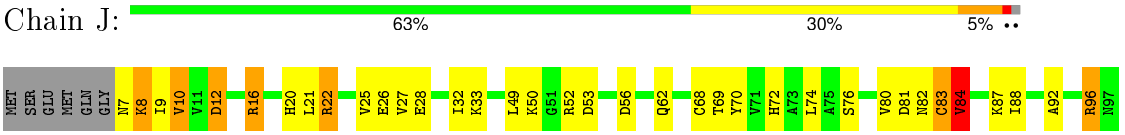

• Molecule 2: PERIPLASMIC HYDROGENASE

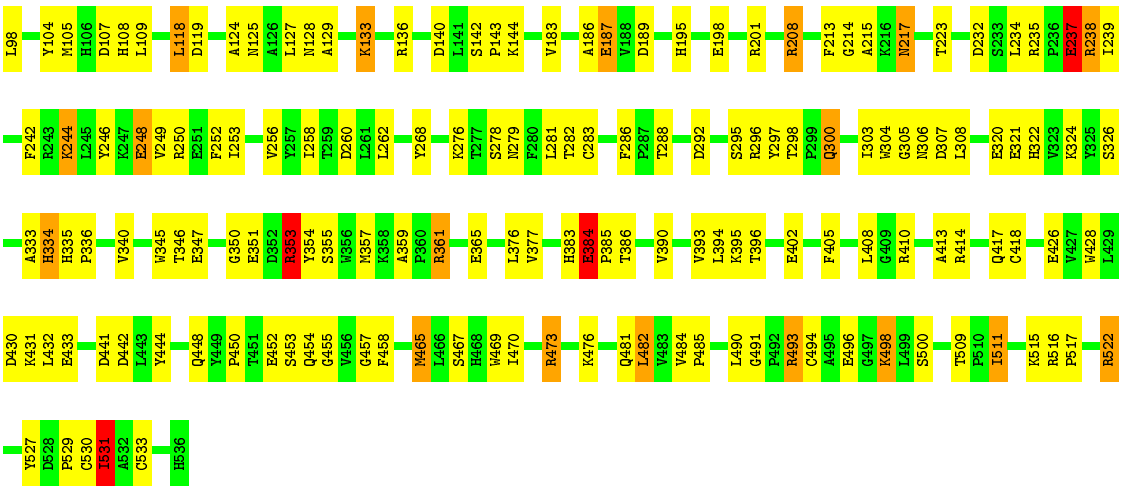
Chain H:




• Molecule 2: PERIPLASMIC HYDROGENASE

Chain J:




L98 Y104 M105 H106 D107 H108 L109 L118 D119 A124 N125 A126 L127 N128 A129 K133 R136 D140 L141 S142 P143 K144 V183 A186 E187 Y188 D189 H195 E198 R201 R208 F213 G214 A215 K216 N217 T223 D232 S233 L234 R235 P236 E237 R238 I239
F242 R243 K244 L245 Y246 K247 E248 V249 R250 E251 F252 I253 V256 Y257 I258 T259 D260 L261 L262 Y268 K276 T277 S278 N279 P280 L281 T282 C283 F286 P287 T288 D292 S295 R296 Y297 T298 P299 Q300 I303 W304 G305 N306 D307 L308 E320 E321 H322 V323 K324 Y325 S326
A333 H334 H335 P336 V340 W345 T346 E347 G350 E351 D352 R353 Y354 S355 W356 M357 K358 A359 P360 R361 E365 L376 V377 H383 E384 P385 T386 V390 V393 L394 K395 T396 E402 F405 L408 G409 R410 A413 R414 Q417 C418 E426 V427 W428 L429
D430 K431 L432 E433 D441 D442 L443 Y444 Q448 Y449 P450 T451 E452 S453 Q454 G455 V456 G457 F458 M465 L466 S467 H468 W469 I470 R473 K476 Q481 L482 V483 V484 P485 L490 G491 P492 R493 C494 A495 E496 G497 K498 L499 S500 T509 P510 I511 K515 R516 P517 R522
Y527 D528 P529 C530 I531 A532 C533 H536

# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 112.78Å 113.16Å 133.91Å<br>90.03° 90.02° 119.99° | Depositor |
| Resolution (Å) | 8.00 – 2.54 | Depositor |
| % Data completeness<br>(in resolution range) | 92.5 (8.00-2.54) | Depositor |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | PROLSQ | Depositor |
| R, $R_{free}$ | 0.201 , 0.219 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 38040 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 9.0 | wwPDB-VP |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, SF4, O, F3S, FCO

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 | 1.02 | 0/2017 | 1.83 | 44/2742 (1.6%) |
| 1 | C | 1.02 | 0/2017 | 1.83 | 44/2742 (1.6%) |
| 1 | E | 1.01 | 0/2017 | 1.83 | 43/2742 (1.6%) |
| 1 | G | 1.02 | 0/2017 | 1.83 | 44/2742 (1.6%) |
| 1 | I | 1.02 | 0/2017 | 1.83 | 45/2742 (1.6%) |
| 1 | S | 1.01 | 0/2017 | 1.83 | 44/2742 (1.6%) |
| 2 | B | 0.96 | 0/4257 | 1.90 | 81/5786 (1.4%) |
| 2 | D | 0.96 | 0/4257 | 1.90 | 81/5786 (1.4%) |
| 2 | F | 0.96 | 0/4257 | 1.90 | 81/5786 (1.4%) |
| 2 | H | 0.96 | 0/4257 | 1.90 | 81/5786 (1.4%) |
| 2 | J | 0.96 | 0/4257 | 1.90 | 80/5786 (1.4%) |
| 2 | L | 0.96 | 0/4257 | 1.90 | 81/5786 (1.4%) |
| All | All | 0.98 | 0/37644 | 1.88 | 749/51168 (1.5%) |

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 |
|---|---|---|---|
| 2 | B | 0 | 1 |
| 2 | D | 0 | 1 |
| 2 | F | 0 | 1 |
| 2 | H | 0 | 1 |
| 2 | J | 0 | 1 |
| 2 | L | 0 | 1 |
| All | All | 0 | 6 |

There are no bond length outliers.

The worst 5 of 749 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 96 | ARG | NE-CZ-NH1 | 22.41 | 131.51 | 120.30 |
| 2 | H | 96 | ARG | NE-CZ-NH1 | 22.36 | 131.48 | 120.30 |
| 2 | F | 96 | ARG | NE-CZ-NH1 | 22.35 | 131.47 | 120.30 |
| 2 | L | 96 | ARG | NE-CZ-NH1 | 22.33 | 131.46 | 120.30 |
| 2 | D | 96 | ARG | NE-CZ-NH1 | 22.32 | 131.46 | 120.30 |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 353 | ARG | Sidechain |
| 2 | D | 353 | ARG | Sidechain |
| 2 | F | 353 | ARG | Sidechain |
| 2 | H | 353 | ARG | Sidechain |
| 2 | L | 353 | ARG | Sidechain |

## 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 | 1964 | 0 | 1895 | 44 | 0 |
| 1 | C | 1964 | 0 | 1895 | 38 | 0 |
| 1 | E | 1964 | 0 | 1895 | 42 | 0 |
| 1 | G | 1964 | 0 | 1895 | 41 | 0 |
| 1 | I | 1964 | 0 | 1895 | 40 | 0 |
| 1 | S | 1964 | 0 | 1895 | 42 | 0 |
| 2 | B | 4152 | 0 | 4114 | 118 | 0 |
| 2 | D | 4152 | 0 | 4114 | 114 | 0 |
| 2 | F | 4152 | 0 | 4114 | 117 | 0 |
| 2 | H | 4152 | 0 | 4114 | 113 | 0 |
| 2 | J | 4152 | 0 | 4114 | 117 | 0 |
| 2 | L | 4152 | 0 | 4114 | 113 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 3 | J | 1 | 0 | 0 | 0 | 0 |
| 3 | L | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 4 | L | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 16 | 0 | 0 | 0 | 0 |
| 5 | C | 16 | 0 | 0 | 0 | 0 |
| 5 | E | 16 | 0 | 0 | 0 | 0 |
| 5 | G | 16 | 0 | 0 | 0 | 0 |
| 5 | I | 16 | 0 | 0 | 0 | 0 |
| 5 | S | 16 | 0 | 0 | 0 | 0 |
| 6 | A | 7 | 0 | 0 | 0 | 0 |
| 6 | C | 7 | 0 | 0 | 0 | 0 |
| 6 | E | 7 | 0 | 0 | 0 | 0 |
| 6 | G | 7 | 0 | 0 | 0 | 0 |
| 6 | I | 7 | 0 | 0 | 1 | 0 |
| 6 | S | 7 | 0 | 0 | 1 | 0 |
| 7 | B | 7 | 0 | 0 | 2 | 0 |
| 7 | D | 7 | 0 | 0 | 2 | 0 |
| 7 | F | 7 | 0 | 0 | 2 | 0 |
| 7 | H | 7 | 0 | 0 | 2 | 0 |
| 7 | J | 7 | 0 | 0 | 2 | 0 |
| 7 | L | 7 | 0 | 0 | 2 | 0 |
| 8 | B | 1 | 0 | 0 | 0 | 0 |
| 8 | D | 1 | 0 | 0 | 0 | 0 |
| 8 | F | 1 | 0 | 0 | 0 | 0 |
| 8 | H | 1 | 0 | 0 | 0 | 0 |
| 8 | J | 1 | 0 | 0 | 0 | 0 |
| 8 | L | 1 | 0 | 0 | 0 | 0 |
| 9 | A | 78 | 0 | 0 | 0 | 2 |
| 9 | B | 114 | 0 | 0 | 0 | 0 |
| 9 | C | 76 | 0 | 0 | 0 | 1 |
| 9 | D | 114 | 0 | 0 | 0 | 0 |
| 9 | E | 81 | 0 | 0 | 0 | 1 |
| 9 | F | 115 | 0 | 0 | 0 | 0 |
| 9 | G | 76 | 0 | 0 | 0 | 0 |
| 9 | H | 112 | 0 | 0 | 0 | 0 |
| 9 | I | 80 | 0 | 0 | 0 | 1 |
| 9 | J | 113 | 0 | 0 | 0 | 0 |
| 9 | L | 110 | 0 | 0 | 0 | 0 |
| 9 | S | 77 | 0 | 0 | 0 | 1 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 38040 | 0 | 36054 | 878 | 3 |

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 12.

The worst 5 of 878 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:I:235:GLN:NE2 | 2:J:208:ARG:HH21 | 1.56 | 1.03 |
| 1:E:235:GLN:NE2 | 2:F:208:ARG:HH21 | 1.56 | 1.03 |
| 1:C:235:GLN:NE2 | 2:D:208:ARG:HH21 | 1.56 | 1.02 |
| 1:G:235:GLN:NE2 | 2:H:208:ARG:HH21 | 1.56 | 1.02 |
| 1:A:235:GLN:NE2 | 2:B:208:ARG:HH21 | 1.56 | 1.02 |

All (3) 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) |
|---|---|---|---|
| 9:A:340:HOH:O | 9:I:1015:HOH:O[1_445] | 1.32 | 0.88 |
| 9:A:341:HOH:O | 9:C:450:HOH:O[1_444] | 1.34 | 0.86 |
| 9:S:338:HOH:O | 9:E:639:HOH:O[1_556] | 1.41 | 0.79 |

## 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 | 259/264 (98%) | 244 (94%) | 14 (5%) | 1 (0%) | 39 | 60 |
| 1 | C | 259/264 (98%) | 244 (94%) | 14 (5%) | 1 (0%) | 39 | 60 |
| 1 | E | 259/264 (98%) | 244 (94%) | 14 (5%) | 1 (0%) | 39 | 60 |
| 1 | G | 259/264 (98%) | 244 (94%) | 14 (5%) | 1 (0%) | 39 | 60 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | I | 259/264 (98%) | 244 (94%) | 14 (5%) | 1 (0%) | 39 | 60 |
| 1 | S | 259/264 (98%) | 244 (94%) | 14 (5%) | 1 (0%) | 39 | 60 |
| 2 | B | 528/536 (98%) | 506 (96%) | 21 (4%) | 1 (0%) | 52 | 73 |
| 2 | D | 528/536 (98%) | 506 (96%) | 21 (4%) | 1 (0%) | 52 | 73 |
| 2 | F | 528/536 (98%) | 506 (96%) | 21 (4%) | 1 (0%) | 52 | 73 |
| 2 | H | 528/536 (98%) | 506 (96%) | 21 (4%) | 1 (0%) | 52 | 73 |
| 2 | J | 528/536 (98%) | 506 (96%) | 21 (4%) | 1 (0%) | 52 | 73 |
| 2 | L | 528/536 (98%) | 506 (96%) | 21 (4%) | 1 (0%) | 52 | 73 |
| All | All | 4722/4800 (98%) | 4500 (95%) | 210 (4%) | 12 (0%) | 46 | 66 |

5 of 12 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 5 | LYS |
| 2 | L | 118 | LEU |
| 1 | A | 5 | LYS |
| 2 | B | 118 | LEU |
| 1 | C | 5 | LYS |

### 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 | 208/210 (99%) | 194 (93%) | 14 (7%) | 20 | 35 |
| 1 | C | 208/210 (99%) | 194 (93%) | 14 (7%) | 20 | 35 |
| 1 | E | 208/210 (99%) | 194 (93%) | 14 (7%) | 20 | 35 |
| 1 | G | 208/210 (99%) | 194 (93%) | 14 (7%) | 20 | 35 |
| 1 | I | 208/210 (99%) | 194 (93%) | 14 (7%) | 20 | 35 |
| 1 | S | 208/210 (99%) | 194 (93%) | 14 (7%) | 20 | 35 |
| 2 | B | 434/439 (99%) | 399 (92%) | 35 (8%) | 15 | 26 |
| 2 | D | 434/439 (99%) | 399 (92%) | 35 (8%) | 15 | 26 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 2 | F | 434/439 (99%) | 399 (92%) | 35 (8%) | 15 | 26 |
| 2 | H | 434/439 (99%) | 399 (92%) | 35 (8%) | 15 | 26 |
| 2 | J | 434/439 (99%) | 399 (92%) | 35 (8%) | 15 | 26 |
| 2 | L | 434/439 (99%) | 399 (92%) | 35 (8%) | 15 | 26 |
| All | All | 3852/3894 (99%) | 3558 (92%) | 294 (8%) | 16 | 29 |

5 of 294 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 353 | ARG |
| 2 | F | 28 | GLU |
| 2 | J | 109 | LEU |
| 2 | D | 402 | GLU |
| 1 | E | 25 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 334 | HIS |
| 1 | E | 235 | GLN |
| 2 | J | 217 | ASN |
| 2 | D | 448 | GLN |
| 1 | E | 124 | ASN |

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 18 are monoatomic - leaving 24 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 | $\#\|Z\| > 2$ |
| 5 | SF4 | A | 265 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 6 | F3S | A | 266 | 1 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 5 | SF4 | A | 267 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 7 | FCO | B | 537 | 8,2 | 0,6,6 | 0.00 | - | 0,6,6 | 0.00 | - |
| 5 | SF4 | C | 265 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 6 | F3S | C | 266 | 1 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 5 | SF4 | C | 267 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 7 | FCO | D | 537 | 8,2 | 0,6,6 | 0.00 | - | 0,6,6 | 0.00 | - |
| 5 | SF4 | E | 265 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 6 | F3S | E | 266 | 1 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 5 | SF4 | E | 267 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 7 | FCO | F | 537 | 8,2 | 0,6,6 | 0.00 | - | 0,6,6 | 0.00 | - |
| 5 | SF4 | G | 265 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 6 | F3S | G | 266 | 1 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 5 | SF4 | G | 267 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 7 | FCO | H | 537 | 8,2 | 0,6,6 | 0.00 | - | 0,6,6 | 0.00 | - |
| 5 | SF4 | I | 265 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 6 | F3S | I | 266 | 1 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 5 | SF4 | I | 267 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 7 | FCO | J | 537 | 8,2 | 0,6,6 | 0.00 | - | 0,6,6 | 0.00 | - |
| 7 | FCO | L | 537 | 8,2 | 0,6,6 | 0.00 | - | 0,6,6 | 0.00 | - |
| 5 | SF4 | S | 265 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |
| 6 | F3S | S | 266 | 1 | 0,9,9 | 0.00 | - | 0,15,15 | 0.00 | - |
| 5 | SF4 | S | 267 | 1 | 0,12,12 | 0.00 | - | 0,24,24 | 0.00 | - |

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 |
|---|---|---|---|---|---|---|---|
| 5 | SF4 | A | 265 | 1 | - | 0/0/48/48 | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 6 | F3S | A | 266 | 1 | - | 0/0/24/24 | 0/0/3/3 |
| 5 | SF4 | A | 267 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 7 | FCO | B | 537 | 8,2 | - | 0/0/6/6 | 0/0/0/0 |
| 5 | SF4 | C | 265 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 6 | F3S | C | 266 | 1 | - | 0/0/24/24 | 0/0/3/3 |
| 5 | SF4 | C | 267 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 7 | FCO | D | 537 | 8,2 | - | 0/0/6/6 | 0/0/0/0 |
| 5 | SF4 | E | 265 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 6 | F3S | E | 266 | 1 | - | 0/0/24/24 | 0/0/3/3 |
| 5 | SF4 | E | 267 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 7 | FCO | F | 537 | 8,2 | - | 0/0/6/6 | 0/0/0/0 |
| 5 | SF4 | G | 265 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 6 | F3S | G | 266 | 1 | - | 0/0/24/24 | 0/0/3/3 |
| 5 | SF4 | G | 267 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 7 | FCO | H | 537 | 8,2 | - | 0/0/6/6 | 0/0/0/0 |
| 5 | SF4 | I | 265 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 6 | F3S | I | 266 | 1 | - | 0/0/24/24 | 0/0/3/3 |
| 5 | SF4 | I | 267 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 7 | FCO | J | 537 | 8,2 | - | 0/0/6/6 | 0/0/0/0 |
| 7 | FCO | L | 537 | 8,2 | - | 0/0/6/6 | 0/0/0/0 |
| 5 | SF4 | S | 265 | 1 | - | 0/0/48/48 | 0/6/5/5 |
| 6 | F3S | S | 266 | 1 | - | 0/0/24/24 | 0/0/3/3 |
| 5 | SF4 | S | 267 | 1 | - | 0/0/48/48 | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | B | 537 | FCO | 2 | 0 |
| 7 | D | 537 | FCO | 2 | 0 |
| 7 | F | 537 | FCO | 2 | 0 |
| 7 | H | 537 | FCO | 2 | 0 |
| 6 | I | 266 | F3S | 1 | 0 |
| 7 | J | 537 | FCO | 2 | 0 |
| 7 | L | 537 | FCO | 2 | 0 |
| 6 | S | 266 | F3S | 1 | 0 |

## 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

EDS was not executed - this section will therefore be empty.

## 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

## 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

## 6.4 Ligands

EDS was not executed - this section will therefore be empty.

## 6.5 Other polymers

EDS was not executed - this section will therefore be empty.