

wwPDB X-ray Structure Validation Summary Report (i)

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| PDB ID | : | 1FFT |
|--------------|---|---|
| Title | : | The structure of ubiquinol oxidase from Escherichia coli |
| Authors | : | Abramson, J.; Riistama, S.; Larsson, G.; Jasaitis, A.; Svensson-Ek, M.; Pu- |
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| Deposited on | : | 2000-07-26 |
| Resolution | : | 3.50 Å(reported) |

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

| MolProbity | : | 4.02b-467 |
|--------------------------------|---|--|
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.50 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 | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$ | | |
|-----------------------|--|---|--|--|
| Clashscore | 141614 | 1036 (3.58-3.42) | | |
| Ramachandran outliers | 138981 | 1005 (3.58-3.42) | | |
| Sidechain outliers | 138945 | 1006 (3.58-3.42) | | |

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

Note EDS was not executed.

| Mol | Chain | Length | | Quality of chain | | | | | | | |
|-----|-------|--------|-----|------------------|-------|----------|--|--|--|--|--|
| 1 | А | 663 | 16% | 48% | 11% • | 24% | | | | | |
| 1 | F | 663 | 17% | 47% | 11% • | 24% | | | | | |
| 2 | В | 315 | 16% | 54% | 10% | • 18% | | | | | |
| 2 | G | 315 | 15% | 54% | 11% | • 18% | | | | | |
| 3 | С | 204 | 22% | 55% | | 12% • 9% | | | | | |
| 3 | Н | 204 | 19% | 58% | | 13% • 9% | | | | | |
| 4 | D | 109 | | 70% | | 30% | | | | | |
| 4 | Ι | 109 | | 70% | | 30% | | | | | |



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 | HEO | А | 1002 | X | - | - | - |
| 7 | HEO | F | 1002 | Х | - | - | - |



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16136 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 UBIQUINOL OXIDASE.

| Mol | Chain | Residues | | At | oms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|---|
| 1 | А | 501 | Total 3954 | C 2654 | N 630 | O 639 | S 31 | 312 | 0 | 0 |
| 1 | F | 501 | Total 3954 | C 2654 | N 630 | O 639 | S 31 | 312 | 0 | 0 |

• Molecule 2 is a protein called UBIQUINOL OXIDASE.

| Mol | Chain | Residues | | At | oms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|----|--------------|---------|-------|---|
| 2 | В | 257 | Total | С | Ν | Ο | \mathbf{S} | 155 | 0 | 0 |
| | 201 | 2015 | 1320 | 324 | 361 | 10 | 100 | 0 | 0 | |
| 0 | С | 257 | Total | С | Ν | Ο | \mathbf{S} | 155 | 0 | 0 |
| 2 G | 231 | 2015 | 1320 | 324 | 361 | 10 | 155 | 0 | 0 | |

• Molecule 3 is a protein called UBIQUINOL OXIDASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------|---------|---------|-------|
| 3 | С | 185 | Total 1451 | C 970 | N 229 | O 240 | S 12 | 157 | 0 | 0 |
| 3 | Н | 185 | Total 1451 | C 970 | N 229 | O 240 | S 12 | 157 | 0 | 0 |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| С | 1 | MET | - | cloning artifact | UNP P0ABJ3 |
| С | 2 | ALA | - | cloning artifact | UNP P0ABJ3 |
| С | 3 | THR | - | cloning artifact | UNP P0ABJ3 |
| С | 4 | ASP | - | cloning artifact | UNP P0ABJ3 |
| С | 5 | THR | - | cloning artifact | UNP P0ABJ3 |
| С | 6 | LEU | - | cloning artifact | UNP P0ABJ3 |
| С | 7 | THR | - | cloning artifact | UNP P0ABJ3 |
| С | 8 | HIS | - | cloning artifact | UNP P0ABJ3 |



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| С | 9 | ALA | - | cloning artifact | UNP P0ABJ3 |
| С | 10 | THR | _ | cloning artifact | UNP P0ABJ3 |
| С | 11 | ALA | - | cloning artifact | UNP P0ABJ3 |
| С | 12 | HIS | - | cloning artifact | UNP P0ABJ3 |
| С | 13 | ALA | - | cloning artifact | UNP P0ABJ3 |
| С | 14 | HIS | - | cloning artifact | UNP P0ABJ3 |
| С | 15 | GLU | - | cloning artifact | UNP P0ABJ3 |
| С | 16 | HIS | - | cloning artifact | UNP P0ABJ3 |
| С | 17 | GLY | - | cloning artifact | UNP P0ABJ3 |
| С | 18 | HIS | - | cloning artifact | UNP P0ABJ3 |
| С | 19 | HIS | - | cloning artifact | UNP P0ABJ3 |
| С | 20 | ASP | - | cloning artifact | UNP P0ABJ3 |
| С | 21 | ALA | - | cloning artifact | UNP P0ABJ3 |
| С | 22 | GLY | - | cloning artifact | UNP P0ABJ3 |
| С | 23 | GLY | - | cloning artifact | UNP P0ABJ3 |
| С | 24 | THR | - | cloning artifact | UNP P0ABJ3 |
| Н | 1 | MET | - | cloning artifact | UNP P0ABJ3 |
| Н | 2 | ALA | - | cloning artifact | UNP P0ABJ3 |
| Н | 3 | THR | - | cloning artifact | UNP P0ABJ3 |
| Н | 4 | ASP | - | cloning artifact | UNP P0ABJ3 |
| Н | 5 | THR | - | cloning artifact | UNP P0ABJ3 |
| Н | 6 | LEU | - | cloning artifact | UNP P0ABJ3 |
| Н | 7 | THR | - | cloning artifact | UNP P0ABJ3 |
| Н | 8 | HIS | - | cloning artifact | UNP P0ABJ3 |
| Н | 9 | ALA | - | cloning artifact | UNP P0ABJ3 |
| Н | 10 | THR | - | cloning artifact | UNP P0ABJ3 |
| H | 11 | ALA | - | cloning artifact | UNP P0ABJ3 |
| H | 12 | HIS | - | cloning artifact | UNP P0ABJ3 |
| H | 13 | ALA | - | cloning artifact | UNP P0ABJ3 |
| H | 14 | HIS | - | cloning artifact | UNP P0ABJ3 |
| H | 15 | GLU | - | cloning artifact | UNP P0ABJ3 |
| H | 16 | HIS | - | cloning artifact | UNP P0ABJ3 |
| H | 17 | GLY | - | cloning artifact | UNP P0ABJ3 |
| H | 18 | HIS | - | cloning artifact | UNP P0ABJ3 |
| H | 19 | HIS | - | cloning artifact | UNP P0ABJ3 |
| H | 20 | ASP | - | cloning artifact | UNP P0ABJ3 |
| H | 21 | ALA | - | cloning artifact | UNP P0ABJ3 |
| H | 22 | GLY | - | cloning artifact | UNP P0ABJ3 |
| H | 23 | GLY | - | cloning artifact | UNP P0ABJ3 |
| H | 24 | THR | - | cloning artifact | UNP P0ABJ3 |

Continued from previous page...

• Molecule 4 is a protein called UBIQUINOL OXIDASE.



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 4 | П | 109 | Total | С | Ν | Ο | 0 | 0 | 0 |
| 4 D | D | | 545 | 327 | 109 | 109 | 0 | 0 | |
| 4 | т | 100 | Total | С | Ν | Ο | 0 | 0 | 0 |
| 4 1 | 109 | 545 | 327 | 109 | 109 | 0 | 0 | 0 | |

• Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | А | 1 | Total Cu 1 1 | 0 | 0 |
| 5 | F | 1 | Total Cu 1 1 | 0 | 0 |

• Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|----|---|---|---------|---------|--|
| 6 | Λ | 1 | Total | С | Fe | Ν | Ο | 0 | 0 | |
| 0 | 0 A | L | 43 | 34 | 1 | 4 | 4 | 0 | 0 | |
| 6 | Б | 1 | Total | С | Fe | Ν | Ο | 0 | 0 | |
| 0 | Г | | 43 | 34 | 1 | 4 | 4 | 0 | 0 | |

• Molecule 7 is HEME O (three-letter code: HEO) (formula: $C_{49}H_{58}FeN_4O_5$).





| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | |
|----------|-------|----------|-------|----|----|---|---|---------|---------|--|
| 7 | Δ | 1 | Total | С | Fe | Ν | 0 | 0 | 0 | |
| 1 | | I | 59 | 49 | 1 | 4 | 5 | 0 | 0 | |
| 7 | Б | 1 | Total | С | Fe | Ν | 0 | 0 | 0 | |
| <i>'</i> | Г | L | 59 | 49 | 1 | 4 | 5 | 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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: UBIQUINOL OXIDASE



• Molecule 1: UBIQUINOL OXIDASE







wiw

K 2552 K 2552 K 2553 K 2554 K 2556 K

GLU SER ALA HIS



• Molecule 3: UBIQUINOL OXIDASE







L200 M201 G202 A203 MET

• Molecule 4: UBIQUINOL OXIDASE

| Chain D | nain D: 70% | | | | | | 30% | | | | | | | | | | | | | | | | | | | | | | | | | |
|----------------------------|-------------|------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|--------------|-----|------|-----|------------|--|-----|-----|-----|-----|--------------------|-----|--|------|------|------|------|------|------|
| X1 X2 X3 X4 X7 | X11 | X14 X15 | X20 | X25 | X29 | X41 | X42 | X53 | X57 | X61 | X62 | X63 | | X 66 X 67 | X68 | X 69 | X70 | X71 X72 | | X75 | X79 | X86 | X87 | 0 <mark>6 X</mark> | 26X | | X103 | X105 | X106 | X107 | X108 | X109 |

• Molecule 4: UBIQUINOL OXIDASE

| Chain I: | | 30% | | | |
|--|---------------------------------|-------------------|---------------------------------|---|--|
| X1 X2 X3 X3 X4 X5 X5 X6 X7 | X10 X11 X14 X15 X15 | X21 X25 X29 | X41 X42 X57 X57 X63 | X66 X67 X68 X71 X71 X72 X72 X72 X75 X75 X77 X79 X79 | X90 X97 X103 X104 X104 X106 X107 X108 X109 X109 |



4 Data and refinement statistics (i)

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

| Property | Value | Source | |
|--|---|-----------|--|
| Space group | C 2 2 21 | Depositor | |
| Cell constants | 92.10Å 372.50Å 232.70Å | Depositor | |
| a, b, c, α , β , γ | 90.00° 90.00° 90.00° | Depositor | |
| Resolution (Å) | 40.00 - 3.50 | Depositor | |
| % Data completeness | (Not available) $(40.00-3.50)$ | Depositor | |
| (in resolution range) | (100 available) (40.00-5.50) | Depositor | |
| R_{merge} | 0.12 | Depositor | |
| R_{sym} | (Not available) | Depositor | |
| Refinement program | | Depositor | |
| R, R_{free} | (Not available) , (Not available) | Depositor | |
| Estimated twinning fraction | No twinning to report. | Xtriage | |
| Total number of atoms | 16136 | wwPDB-VP | |
| Average B, all atoms $(Å^2)$ | 29.0 | wwPDB-VP | |



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HEO, CU

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).

| Mal | Chain | Bo | nd lengths | Bond angles | | | | |
|-------|-------|------|----------------|-------------|----------------|--|--|--|
| INIOI | Unain | RMSZ | # Z > 5 | RMSZ | # Z > 5 | | | |
| 1 | А | 0.46 | 1/4086~(0.0%) | 0.71 | 4/5573~(0.1%) | | | |
| 1 | F | 0.44 | 0/4086 | 0.68 | 2/5573~(0.0%) | | | |
| 2 | В | 0.43 | 0/2074 | 0.65 | 0/2825 | | | |
| 2 | G | 0.43 | 0/2074 | 0.67 | 0/2825 | | | |
| 3 | С | 0.47 | 0/1494 | 0.66 | 0/2030 | | | |
| 3 | Н | 0.43 | 0/1494 | 0.65 | 0/2030 | | | |
| All | All | 0.45 | 1/15308~(0.0%) | 0.68 | 6/20856~(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 | А | 0 | 1 |
| 1 | F | 0 | 1 |
| All | All | 0 | 2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | А | 174 | PRO | C-N | -9.24 | 1.16 | 1.34 |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|---------|--------|------------------|---------------|
| 1 | А | 174 | PRO | C-N-CD | -12.28 | 93.59 | 120.60 |
| 1 | А | 175 | PRO | CB-CA-C | 7.79 | 131.48 | 112.00 |
| 1 | F | 175 | PRO | CB-CA-C | 7.42 | 130.56 | 112.00 |
| 1 | F | 174 | PRO | C-N-CD | -6.30 | 106.74 | 120.60 |



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| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|---------|-------|------------------|---------------|
| 1 | А | 547 | PRO | CA-N-CD | -6.28 | 102.72 | 111.50 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | А | 174 | PRO | Mainchain |
| 1 | F | 174 | PRO | Mainchain |

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | А | 3954 | 0 | 3975 | 658 | 0 |
| 1 | F | 3954 | 0 | 3975 | 661 | 0 |
| 2 | В | 2015 | 0 | 2016 | 317 | 0 |
| 2 | G | 2015 | 0 | 2016 | 348 | 0 |
| 3 | С | 1451 | 0 | 1458 | 254 | 0 |
| 3 | Н | 1451 | 0 | 1458 | 265 | 0 |
| 4 | D | 545 | 0 | 114 | 57 | 0 |
| 4 | Ι | 545 | 0 | 115 | 55 | 0 |
| 5 | А | 1 | 0 | 0 | 0 | 0 |
| 5 | F | 1 | 0 | 0 | 0 | 0 |
| 6 | А | 43 | 0 | 30 | 18 | 0 |
| 6 | F | 43 | 0 | 30 | 17 | 0 |
| 7 | А | 59 | 0 | 56 | 16 | 0 |
| 7 | F | 59 | 0 | 56 | 14 | 0 |
| All | All | 16136 | 0 | 15299 | 2417 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 83.

The worst 5 of 2417 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-1 Atom-2 | | Clash overlap (Å) | |
|----------------|----------------|------|----------------------|--|
| 3:H:86:ALA:HB1 | 3:H:91:TYR:CD1 | 1.43 | 1.53 | |



| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|-----------------------------|----------------------|
| 3:C:78:PHE:HZ | 4:D:57:UNK:CB | 1.44 | 1.30 |
| 3:H:83:TYR:HE1 | 4:I:14:UNK:CB | 1.44 | 1.30 |
| 1:A:55:LYS:NZ | 1:A:551:ASN:HA | 1.44 | 1.29 |
| 3:C:78:PHE:CZ | 4:D:57:UNK:CB | 2.20 | 1.24 |

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There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|-----------|-------------|
| 1 | А | 499/663~(75%) | 331~(66%) | 110 (22%) | 58 (12%) | 0 5 |
| 1 | F | 499/663~(75%) | 333~(67%) | 108 (22%) | 58 (12%) | 0 5 |
| 2 | В | 255/315~(81%) | 162 (64%) | 66 (26%) | 27 (11%) | 0 7 |
| 2 | G | 255/315~(81%) | 167~(66%) | 58 (23%) | 30 (12%) | 0 5 |
| 3 | С | 183/204~(90%) | 112 (61%) | 52 (28%) | 19 (10%) | 0 7 |
| 3 | Н | 183/204 (90%) | 107 (58%) | 56 (31%) | 20 (11%) | 0 6 |
| All | All | 1874/2364 (79%) | 1212 (65%) | 450 (24%) | 212 (11%) | 0 6 |

5 of 212 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 96 | PRO |
| 1 | А | 102 | ILE |
| 1 | А | 106 | HIS |
| 1 | А | 135 | ASP |
| 1 | А | 175 | PRO |



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 side chain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Perce | ntiles |
|-----|-------|-----------------|------------|-----------|-------|--------|
| 1 | А | 413/547~(76%) | 373~(90%) | 40 (10%) | 8 | 33 |
| 1 | F | 413/547~(76%) | 373~(90%) | 40 (10%) | 8 | 33 |
| 2 | В | 215/262~(82%) | 188 (87%) | 27~(13%) | 4 | 22 |
| 2 | G | 215/262~(82%) | 187 (87%) | 28 (13%) | 4 | 21 |
| 3 | С | 152/166~(92%) | 133 (88%) | 19 (12%) | 4 | 23 |
| 3 | Н | 152/166~(92%) | 134 (88%) | 18 (12%) | 5 | 25 |
| All | All | 1560/1950~(80%) | 1388 (89%) | 172 (11%) | 6 | 29 |

 $5~{\rm of}~172$ residues with a non-rotameric side chain are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 1 | F | 359 | THR |
| 2 | G | 144 | GLU |
| 1 | F | 416 | LEU |
| 2 | G | 67 | TRP |
| 2 | G | 189 | MET |

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such side chains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 190 | GLN |
| 3 | Н | 185 | HIS |
| 2 | G | 198 | ASN |
| 2 | G | 268 | ASN |
| 2 | В | 190 | GLN |

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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 | Dec | Dec | Bos | Tiple | Bo | ond leng | $_{\rm ths}$ | Bo | nd angl | es | |
|----------------|------|------|------|-------|----------|----------|--------------|------------|---------|--------|----------|
| IVIOI | туре | Type | Unam | nes | LIIIK | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 7 | HEO | F | 1002 | 1 | 63,66,66 | 1.09 | 3 (4%) | 71,102,102 | 1.22 | 7 (9%) | |
| 6 | HEM | F | 1001 | 1 | 41,50,50 | 1.47 | 3 (7%) | 45,82,82 | 1.16 | 2 (4%) | |
| 7 | HEO | А | 1002 | 1 | 63,66,66 | 1.08 | 2 (3%) | 71,102,102 | 1.21 | 7 (9%) | |
| 6 | HEM | А | 1001 | 1 | 41,50,50 | 1.44 | 3 (7%) | 45,82,82 | 1.12 | 2 (4%) | |

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 |
|-----|------|-------|------|------|-----------|--------------|-------|
| 7 | HEO | F | 1002 | 1 | 2/2/17/25 | 7/32/114/114 | - |
| 7 | HEO | А | 1002 | 1 | 2/2/17/25 | 6/32/114/114 | - |
| 6 | HEM | А | 1001 | 1 | - | 6/12/54/54 | - |
| 6 | HEM | F | 1001 | 1 | - | 6/12/54/54 | - |

The worst 5 of 11 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 6 | А | 1001 | HEM | CBB-CAB | 4.68 | 1.53 | 1.30 |



| Mol | Chain | Res | Type | Atoms | Ζ | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | F | 1001 | HEM | CBB-CAB | 4.58 | 1.53 | 1.30 |
| 7 | А | 1002 | HEO | C3C-CAC | -4.12 | 1.39 | 1.47 |
| 7 | F | 1002 | HEO | C3C-CAC | -4.07 | 1.39 | 1.47 |
| 6 | F | 1001 | HEM | C3C-CAC | -3.90 | 1.39 | 1.47 |

Continued from previous page...

The worst 5 of 18 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|-------------|-------|------------------|---------------|
| 6 | А | 1001 | HEM | CBB-CAB-C3B | -3.59 | 109.76 | 127.62 |
| 6 | F | 1001 | HEM | CBB-CAB-C3B | -3.55 | 109.95 | 127.62 |
| 7 | А | 1002 | HEO | C1D-ND-C4D | -2.94 | 102.03 | 105.07 |
| 7 | F | 1002 | HEO | C1D-ND-C4D | -2.86 | 102.12 | 105.07 |
| 7 | А | 1002 | HEO | C3C-C4C-NC | 2.52 | 112.47 | 109.21 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 7 | А | 1002 | HEO | ND |
| 7 | А | 1002 | HEO | NB |
| 7 | F | 1002 | HEO | ND |
| 7 | F | 1002 | HEO | NB |

5 of 25 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 6 | А | 1001 | HEM | C2B-C3B-CAB-CBB |
| 6 | F | 1001 | HEM | C2B-C3B-CAB-CBB |
| 7 | А | 1002 | HEO | C15-C16-C17-C18 |
| 7 | F | 1002 | HEO | C15-C16-C17-C18 |
| 6 | А | 1001 | HEM | C4B-C3B-CAB-CBB |

There are no ring outliers.

4 monomers are involved in 65 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 7 | F | 1002 | HEO | 14 | 0 |
| 6 | F | 1001 | HEM | 17 | 0 |
| 7 | А | 1002 | HEO | 16 | 0 |
| 6 | А | 1001 | HEM | 18 | 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.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | А | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | А | 174:PRO | С | 175:PRO | Ν | 1.16 |

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

