# W O R L D W I D E

# wwPDB

## P R O T E I N  D A T A  B A N K

# wwPDB EM Validation Summary Report (i)

Mar 31, 2025 – 07:36 PM JST

|  |  |  |
| --- | --- | --- |
| PDB ID | : | 7DEG / pdb_00007deg |
| EMDB ID | : | EMD-30657 |
| Title | : | Cryo-EM structure of a heme-copper terminal oxidase dimer provides insights into its catalytic mechanism |
| Authors | : | Fei, S.; Hartmut, M.; Yun, Z.; Guoliang, Z.; Shuangbo, Z. |
| Deposited on | : | 2020-11-04 |
| Resolution | : | 3.40 Å(reported) |

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

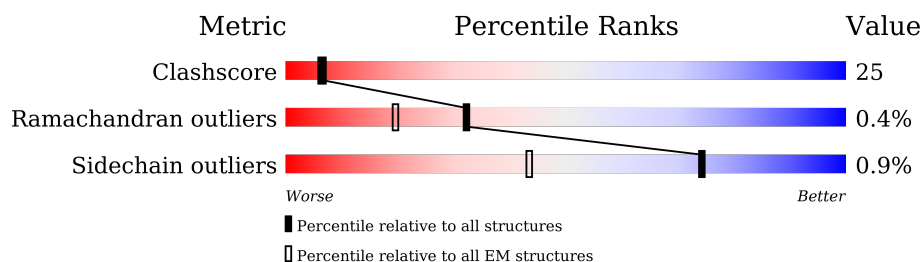|  |  |  |
| --- | --- | --- |
| EMDB validation analysis | : | 0.0.1.dev117 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.42 |

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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 | Percentile Ranks | Value |
|---|---|---|
| Clashscore | | 25 |
| Ramachandran outliers | | 0.4% |
| Sidechain outliers | | 0.9% |

*Worse* — *Better*

▋ Percentile relative to all structures
▯ Percentile relative to all EM structures

| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 587 | 55% 43% •• |
| 1 | D | 587 | 55% 42% •• |
| 2 | C | 32 | 50% 47% • |
| 2 | F | 32 | 50% 47% • |
| 3 | B | 147 | 61% 39% • |
| 3 | E | 147 | 61% 39% • |

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:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4 | HAS | A | 601 | X | - | - | - |
| 4 | HAS | D | 602 | X | - | - | - |
| 8 | PGV | A | 607 | - | - | X | - |
| 8 | PGV | D | 601 | - | - | X | - |
| 9 | 3PE | A | 606 | - | - | X | - |
| 9 | 3PE | D | 607 | - | - | X | - |

# 2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 12852 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytochrome c oxidase subunit I.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 1 | A | 581 | Total | C | N | O | S | 0 | 0 |
| | | | 4624 | 3131 | 715 | 762 | 16 | | |
| 1 | D | 581 | Total | C | N | O | S | 0 | 0 |
| | | | 4624 | 3131 | 715 | 762 | 16 | | |

- Molecule 2 is a protein called Cytochrome oxidase subunit IIa.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 2 | C | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 281 | 202 | 37 | 39 | 3 | | |
| 2 | F | 32 | Total | C | N | O | S | 0 | 0 |
| | | | 281 | 202 | 37 | 39 | 3 | | |

- Molecule 3 is a protein called Cytochrome oxidase subunit II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---------|-------|
| 3 | B | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1159 | 758 | 195 | 199 | 7 | | |
| 3 | E | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1159 | 758 | 195 | 199 | 7 | | |

- Molecule 4 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).

HAS
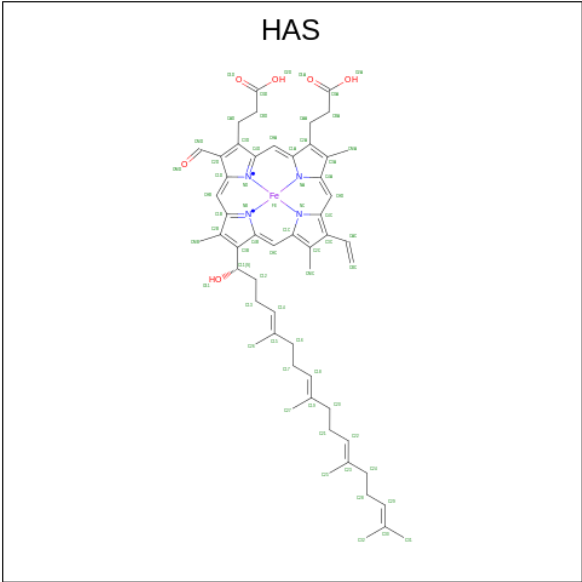
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 4 | A | 1 | Total | C | Fe | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |
| 4 | D | 1 | Total | C | Fe | N | O | 0 |
| | | | 65 | 54 | 1 | 4 | 6 | |

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
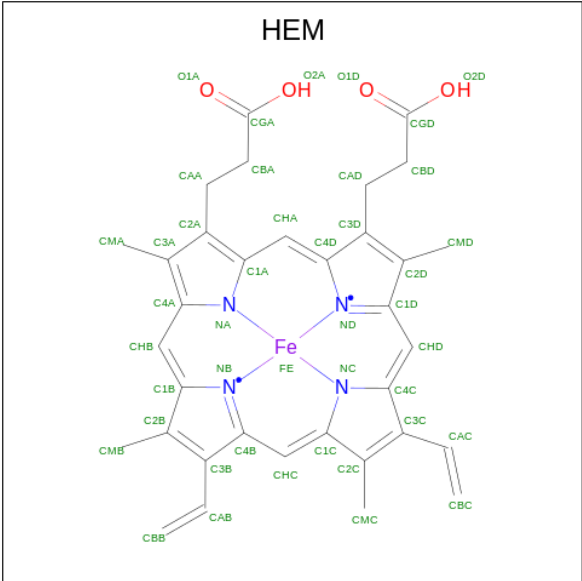
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 5 | A | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| | | | Total | C | Fe | N | O | |
| 5 | D | 1 | 43 | 34 | 1 | 4 | 4 | 0 |

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| | | | Total | Cu | |
| 6 | A | 1 | 1 | 1 | 0 |
| | | | Total | Cu | |
| 6 | D | 1 | 1 | 1 | 0 |

- Molecule 7 is 2-[(2 {E},6 {E},10 {Z},14 {Z},18 {Z},23 {R})-3,7,11,15,19,23,27-heptamethylo ctacosa-2,6,10,14,18-pentaenyl]naphthalene-1,4-dione (CCD ID: DLX) (formula: $C_{45}H_{66}O_2$).



DLX
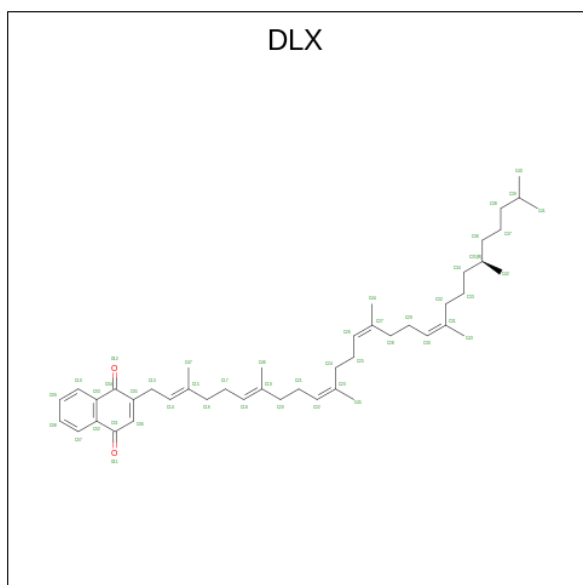
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| | | | Total | C | O | |
| 7 | A | 1 | 47 | 45 | 2 | 0 |
| | | | Total | C | O | |
| 7 | D | 1 | 47 | 45 | 2 | 0 |

- Molecule 8 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHO RYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).

PGV
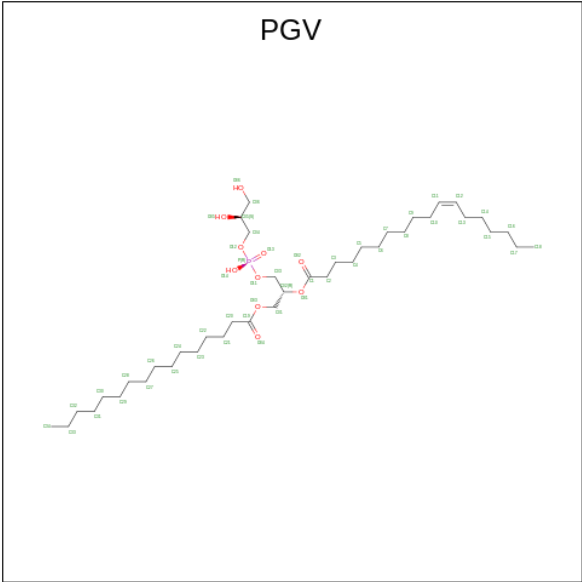
| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 8 | A | 1 | Total | C | O | P | 0 |
|   |   |   | 51 | 40 | 10 | 1 |   |
| 8 | A | 1 | Total | C | O | P | 0 |
|   |   |   | 51 | 40 | 10 | 1 |   |
| 8 | C | 1 | Total | C | O | P | 0 |
|   |   |   | 51 | 40 | 10 | 1 |   |
| 8 | D | 1 | Total | C | O | P | 0 |
|   |   |   | 51 | 40 | 10 | 1 |   |
| 8 | D | 1 | Total | C | O | P | 0 |
|   |   |   | 51 | 40 | 10 | 1 |   |
| 8 | F | 1 | Total | C | O | P | 0 |
|   |   |   | 51 | 40 | 10 | 1 |   |

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).

**3PE**
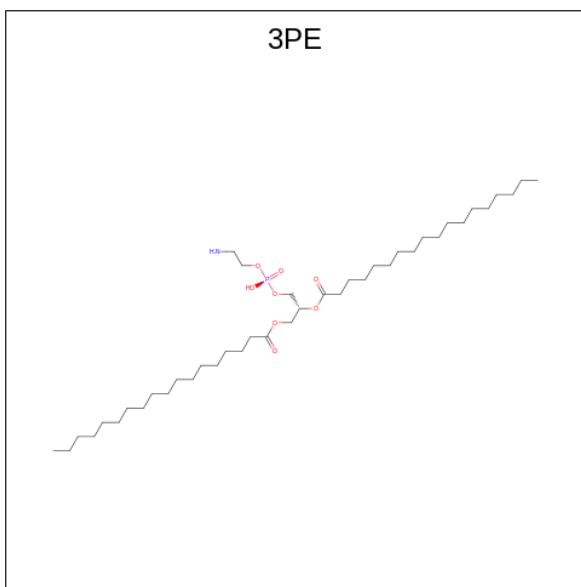
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 9 | A | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |
| 9 | D | 1 | Total | C | N | O | P | 0 |
| | | | 51 | 41 | 1 | 8 | 1 | |

- Molecule 10 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: $Cu_2$).

**CUA**

CU1 Cu — Cu CU2
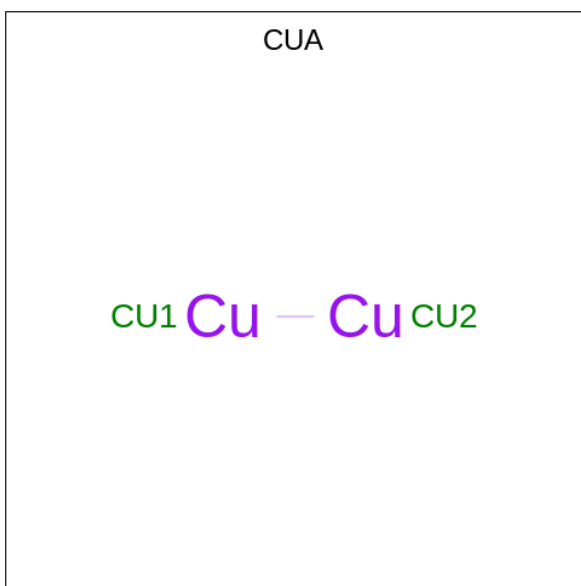
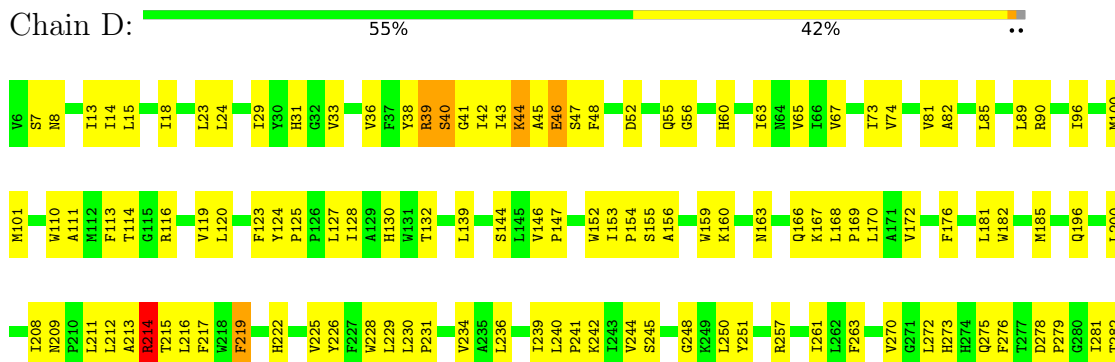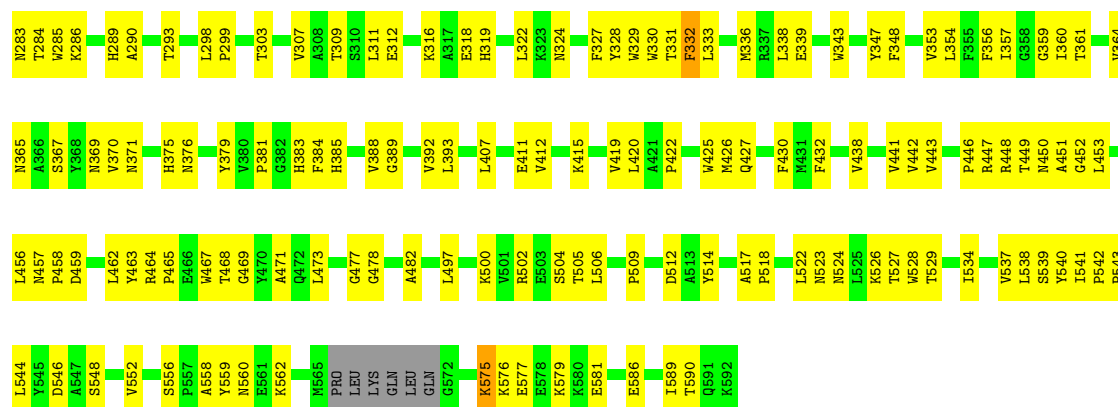| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 10 | B | 1 | Total | Cu | 0 |
| | | | 2 | 2 | |
| 10 | E | 1 | Total | Cu | 0 |
| | | | 2 | 2 | |

# 3   Residue-property plots ⓘ

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.
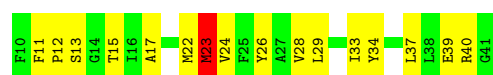
- Molecule 1: Cytochrome c oxidase subunit I



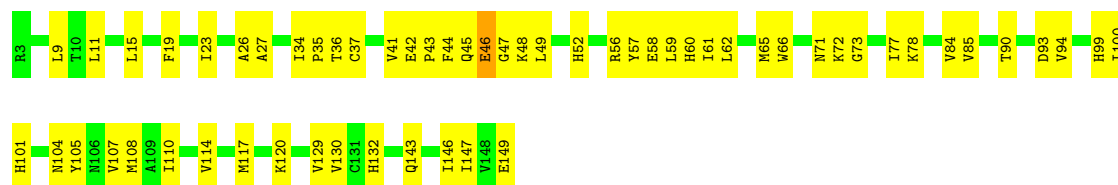- Molecule 1: Cytochrome c oxidase subunit I

N283 T284 W285 K286 H289 A290 T293 L298 P299 T303 V307 A308 T309 S310 L311 E312 K316 A317 E318 H319 L322 K323 N324 F327 Y328 W329 W330 T331 F332 L333 M336 R337 L338 E339 W343 Y347 F348 V353 L354 F355 F356 I357 G358 G359 I360 T361 V364

N365 A366 S367 Y368 N369 V370 N371 H375 N376 Y379 V380 P381 G382 H383 F384 H385 V388 G389 V392 L393 L407 E411 V412 K415 V419 L420 A421 P422 W425 M426 Q427 F430 M431 F432 V438 V441 V442 V443 P446 R447 R448 T449 N450 A451 G452 L453

L456 N457 P458 D459 L462 Y463 R464 P465 E466 W467 T468 G469 Y470 A471 Q472 L473 G477 G478 A482 L497 K500 V501 R502 E503 S504 T505 L506 P509 D512 Y514 A517 P518 L522 N523 N524 L525 K526 T527 W528 T529 I534 V537 L538 S539 Y540 I541 P542 P543

L544 Y545 D546 A547 S548 V552 S556 P557 A558 Y559 N560 E561 K562 M565 PRO LEU LYS GLN LEU GLN G572 K575 K576 E577 E578 K579 K580 E581 E586 I589 T590 Q591 K592

- Molecule 2: Cytochrome oxidase subunit IIa

Chain C:



F10 F11 P12 S13 G14 T15 I16 A17 M22 M23 V24 F25 Y26 A27 V28 L29 I33 Y34 L37 L38 E39 R40 G41

- Molecule 2: Cytochrome oxidase subunit IIa

Chain F:



F10 F11 P12 S13 G14 T15 I16 A17 M22 M23 V24 F25 Y26 A27 V28 L29 I33 Y34 L37 L38 E39 R40 G41

- Molecule 3: Cytochrome oxidase subunit II

Chain B:



R3 L9 T10 L11 L15 F19 I23 A26 A27 I34 P35 T36 C37 V41 E42 P43 F44 Q45 E46 G47 K48 L49 H52 R56 Y57 E58 L59 H60 I61 L62 M65 W66 N71 K72 G73 I77 K78 V84 V85 T90 D93 V94 H99 I100

H101 N104 Y105 N106 V107 M108 A109 I110 V114 M117 K120 V129 V130 C131 H132 Q143 I146 I147 V148 E149

- Molecule 3: Cytochrome oxidase subunit II

Chain E:



R3 L11 L15 F19 I23 A26 A27 I34 P35 T36 C37 V41 E42 P43 F44 Q45 E46 G47 K48 L49 H52 R56 Y57 E58 L59 H60 I61 L62 M65 W66 N71 K72 G73 I77 K78 V84 V85 T90 D93 V94 H99 I100 H101

N104 Y105 N106 V107 M108 A109 I110 V114 M117 K120 V129 V130 C131 H132 Q143 I146 I147 V148 E149

# 4 Experimental information ⓘ

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 32982 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 60 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGV, DLX, 3PE, CU, HAS, HEM, CUA

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 | 0.81 | 1/4777 (0.0%) | 0.65 | 0/6521 |
| 1 | D | 0.81 | 1/4777 (0.0%) | 0.65 | 0/6521 |
| 2 | C | 0.74 | 0/294 | 0.60 | 0/397 |
| 2 | F | 0.74 | 0/294 | 0.60 | 0/397 |
| 3 | B | 0.72 | 0/1188 | 0.63 | 0/1607 |
| 3 | E | 0.72 | 0/1188 | 0.63 | 0/1607 |
| All | All | 0.79 | 2/12518 (0.0%) | 0.65 | 0/17050 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 2 |
| 1 | D | 0 | 2 |
| 2 | C | 0 | 1 |
| 2 | F | 0 | 1 |
| 3 | B | 0 | 1 |
| 3 | E | 0 | 1 |
| All | All | 0 | 8 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | D | 332 | PHE | C-N | -5.09 | 1.22 | 1.34 |
| 1 | A | 332 | PHE | C-N | -5.08 | 1.22 | 1.34 |

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1 | A | 214 | ARG | Peptide |
| 1 | A | 512 | ASP | Peptide |
| 3 | B | 46 | GLU | Peptide |
| 2 | C | 23 | MET | Peptide |
| 1 | D | 214 | ARG | Peptide |

## 5.2   Too-close contacts ⓘ

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 | 4624 | 0 | 4725 | 238 | 0 |
| 1 | D | 4624 | 0 | 4725 | 238 | 0 |
| 2 | C | 281 | 0 | 274 | 24 | 0 |
| 2 | F | 281 | 0 | 274 | 23 | 0 |
| 3 | B | 1159 | 0 | 1184 | 54 | 0 |
| 3 | E | 1159 | 0 | 1184 | 53 | 0 |
| 4 | A | 65 | 0 | 62 | 11 | 0 |
| 4 | D | 65 | 0 | 62 | 11 | 0 |
| 5 | A | 43 | 0 | 30 | 8 | 0 |
| 5 | D | 43 | 0 | 30 | 8 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| 7 | A | 47 | 0 | 0 | 3 | 0 |
| 7 | D | 47 | 0 | 0 | 3 | 0 |
| 8 | A | 102 | 0 | 151 | 30 | 0 |
| 8 | C | 51 | 0 | 76 | 4 | 0 |
| 8 | D | 102 | 0 | 151 | 29 | 0 |
| 8 | F | 51 | 0 | 76 | 4 | 0 |
| 9 | A | 51 | 0 | 80 | 36 | 0 |
| 9 | D | 51 | 0 | 80 | 34 | 0 |
| 10 | B | 2 | 0 | 0 | 0 | 0 |
| 10 | E | 2 | 0 | 0 | 0 | 0 |
| All | All | 12852 | 0 | 13164 | 653 | 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 25.

The worst 5 of 653 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:D:327:PHE:O | 9:D:607:3PE:C22 | 1.68 | 1.41 |
| 1:A:327:PHE:O | 9:A:606:3PE:C22 | 1.68 | 1.39 |
| 1:D:40:SER:HB2 | 1:D:471:ALA:O | 1.31 | 1.27 |
| 1:A:40:SER:HB2 | 1:A:471:ALA:O | 1.31 | 1.22 |
| 3:B:48:LYS:HD2 | 3:B:77:ILE:HD11 | 1.48 | 0.96 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 577/587 (98%) | 482 (84%) | 93 (16%) | 2 (0%) | 37 | 66 |
| 1 | D | 577/587 (98%) | 481 (83%) | 94 (16%) | 2 (0%) | 37 | 66 |
| 2 | C | 30/32 (94%) | 25 (83%) | 4 (13%) | 1 (3%) | 3 | 18 |
| 2 | F | 30/32 (94%) | 25 (83%) | 4 (13%) | 1 (3%) | 3 | 18 |
| 3 | B | 145/147 (99%) | 118 (81%) | 27 (19%) | 0 | 100 | 100 |
| 3 | E | 145/147 (99%) | 118 (81%) | 27 (19%) | 0 | 100 | 100 |
| All | All | 1504/1532 (98%) | 1249 (83%) | 249 (17%) | 6 (0%) | 32 | 60 |

5 of 6 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 44 | LYS |
| 1 | D | 44 | LYS |
| 1 | A | 46 | GLU |
| 1 | D | 46 | GLU |
| 2 | C | 23 | MET |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 486/492 (99%) | 480 (99%) | 6 (1%) | 67 | 80 |
| 1 | D | 486/492 (99%) | 480 (99%) | 6 (1%) | 67 | 80 |
| 2 | C | 28/28 (100%) | 28 (100%) | 0 | 100 | 100 |
| 2 | F | 28/28 (100%) | 28 (100%) | 0 | 100 | 100 |
| 3 | B | 125/125 (100%) | 125 (100%) | 0 | 100 | 100 |
| 3 | E | 125/125 (100%) | 125 (100%) | 0 | 100 | 100 |
| All | All | 1278/1290 (99%) | 1266 (99%) | 12 (1%) | 74 | 86 |

5 of 12 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 40 | SER |
| 1 | D | 42 | ILE |
| 1 | D | 575 | LYS |
| 1 | D | 214 | ARG |
| 1 | A | 214 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 375 | HIS |
| 1 | D | 524 | ASN |
| 1 | D | 560 | ASN |
| 1 | D | 472 | GLN |
| 1 | A | 524 | ASN |

### 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 oligosaccharides in this entry.

## 5.6   Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|------------|--------|------|------------|
| | | | | | Counts | RMSZ | #$|Z| > 2$ | Counts | RMSZ | #$|Z| > 2$ |
| 4 | HAS | D | 602 | 2,1 | 69,72,72 | 3.18 | 26 (37%) | 73,109,109 | 3.59 | 41 (56%) |
| 4 | HAS | A | 601 | 2,1 | 69,72,72 | 3.18 | 26 (37%) | 73,109,109 | 3.59 | 41 (56%) |
| 5 | HEM | D | 603 | 1 | 41,50,50 | 1.60 | 6 (14%) | 45,82,82 | 1.46 | 6 (13%) |
| 8 | PGV | A | 605 | - | 50,50,50 | 0.87 | 2 (4%) | 53,56,56 | 1.10 | 5 (9%) |
| 8 | PGV | C | 101 | - | 50,50,50 | 0.91 | 2 (4%) | 53,56,56 | 1.09 | 4 (7%) |
| 8 | PGV | D | 606 | - | 50,50,50 | 0.87 | 2 (4%) | 53,56,56 | 1.10 | 5 (9%) |
| 8 | PGV | A | 607 | 8 | 50,50,50 | 0.94 | 2 (4%) | 53,56,56 | 1.15 | 3 (5%) |
| 8 | PGV | D | 601 | 8 | 50,50,50 | 0.94 | 2 (4%) | 53,56,56 | 1.15 | 3 (5%) |
| 8 | PGV | F | 101 | - | 50,50,50 | 0.91 | 2 (4%) | 53,56,56 | 1.09 | 4 (7%) |
| 9 | 3PE | A | 606 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.30 | 0 |
| 9 | 3PE | D | 607 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.31 | 0 |
| 10 | CUA | E | 600 | 3 | 0,1,1 | - | - | - | | |
| 10 | CUA | B | 600 | 3 | 0,1,1 | - | - | - | | |
| 5 | HEM | A | 602 | 1 | 41,50,50 | 1.60 | 6 (14%) | 45,82,82 | 1.47 | 6 (13%) |
| 7 | DLX | D | 605 | 2,1 | 48,48,48 | 3.23 | 12 (25%) | 59,61,61 | 3.24 | 22 (37%) |
| 7 | DLX | A | 604 | 2,1 | 48,48,48 | 3.24 | 12 (25%) | 59,61,61 | 3.24 | 22 (37%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 4 | HAS | D | 602 | 2,1 | 1/1/8/18 | 23/40/82/82 | - |
| 4 | HAS | A | 601 | 2,1 | 1/1/8/18 | 23/40/82/82 | - |
| 5 | HEM | D | 603 | 1 | - | 2/12/54/54 | - |
| 8 | PGV | A | 605 | - | - | 16/55/55/55 | - |
| 8 | PGV | C | 101 | - | - | 21/55/55/55 | - |
| 8 | PGV | D | 606 | - | - | 16/55/55/55 | - |
| 8 | PGV | A | 607 | 8 | - | 28/55/55/55 | - |
| 8 | PGV | D | 601 | 8 | - | 28/55/55/55 | - |
| 8 | PGV | F | 101 | - | - | 21/55/55/55 | - |
| 9 | 3PE | A | 606 | - | - | 28/54/54/54 | - |
| 9 | 3PE | D | 607 | - | - | 28/54/54/54 | - |
| 5 | HEM | A | 602 | 1 | - | 2/12/54/54 | - |
| 7 | DLX | D | 605 | 2,1 | - | 28/41/57/57 | 0/2/2/2 |
| 7 | DLX | A | 604 | 2,1 | - | 28/41/57/57 | 0/2/2/2 |

The worst 5 of 100 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 4 | D | 602 | HAS | CHD-C4A | 9.83 | 1.49 | 1.35 |
| 4 | A | 601 | HAS | CHD-C4A | 9.83 | 1.48 | 1.35 |
| 7 | A | 604 | DLX | C26-C27 | 8.47 | 1.53 | 1.33 |
| 7 | A | 604 | DLX | C30-C31 | 8.45 | 1.53 | 1.33 |
| 7 | D | 605 | DLX | C30-C31 | 8.45 | 1.53 | 1.33 |

The worst 5 of 162 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 7 | D | 605 | DLX | C13-C14-C15 | -10.03 | 110.10 | 126.79 |
| 7 | A | 604 | DLX | C13-C14-C15 | -10.02 | 110.10 | 126.79 |
| 7 | A | 604 | DLX | C16-C15-C14 | -7.09 | 106.78 | 121.12 |
| 4 | D | 602 | HAS | C17-C18-C19 | -7.08 | 110.61 | 127.66 |
| 7 | D | 605 | DLX | C16-C15-C14 | -7.08 | 106.80 | 121.12 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 4 | A | 601 | HAS | NA |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 4 | D | 602 | HAS | NA |

5 of 292 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 4 | A | 601 | HAS | C3A-C2A-CAA-CBA |
| 4 | A | 601 | HAS | C1D-C2D-CMD-OMD |
| 4 | A | 601 | HAS | C13-C14-C15-C26 |
| 4 | A | 601 | HAS | C14-C15-C16-C17 |
| 4 | A | 601 | HAS | C17-C18-C19-C20 |

There are no ring outliers.
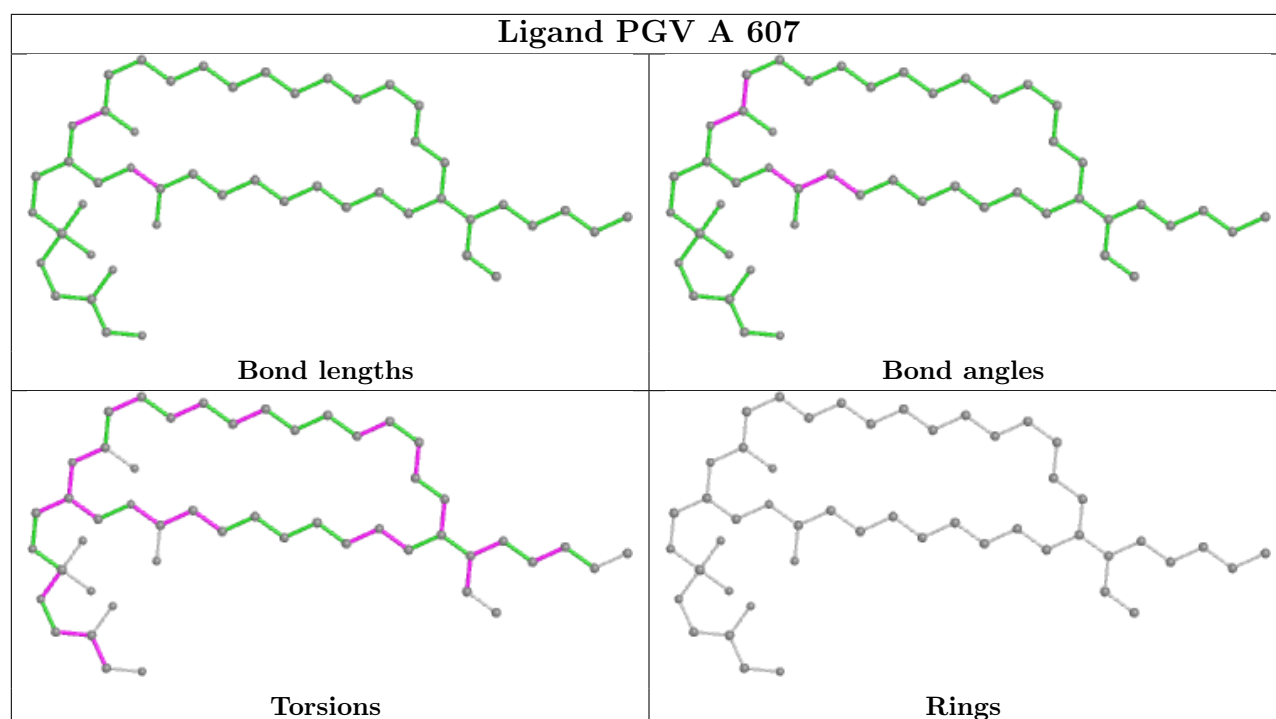
14 monomers are involved in 133 short contacts:

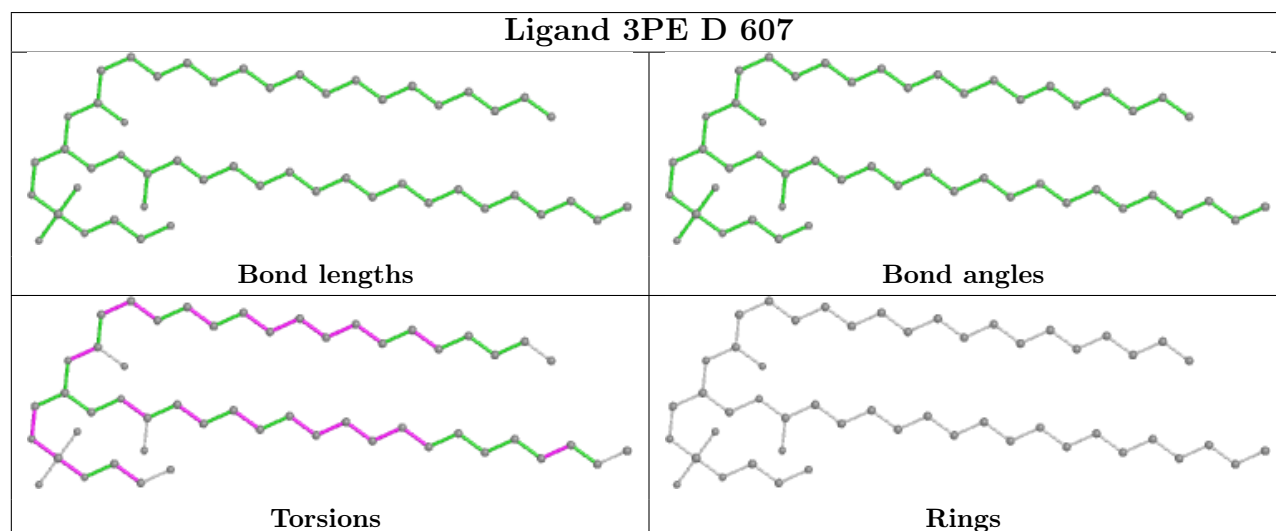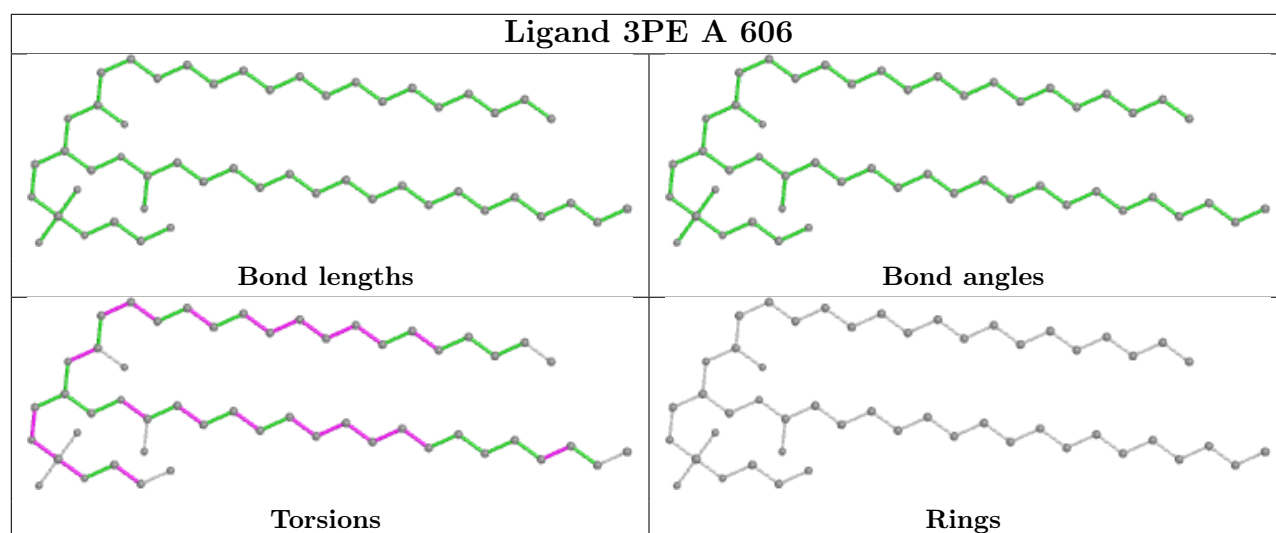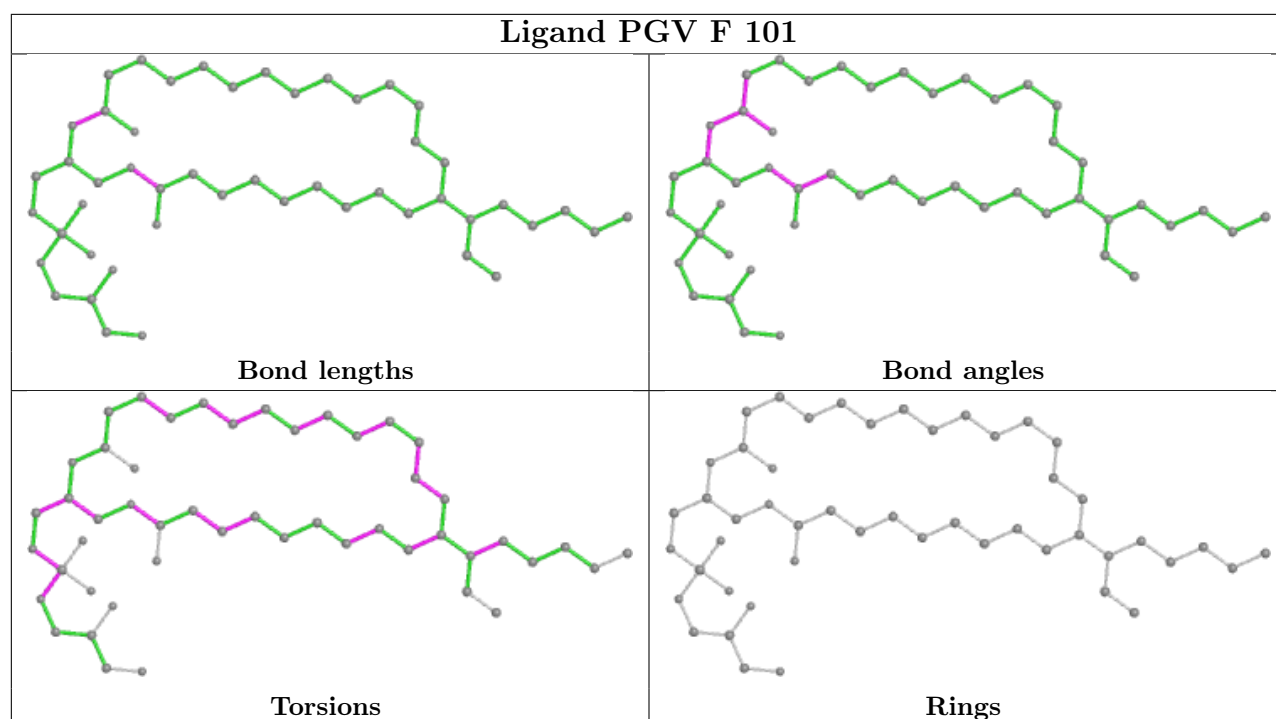| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | D | 602 | HAS | 11 | 0 |
| 4 | A | 601 | HAS | 11 | 0 |
| 5 | D | 603 | HEM | 8 | 0 |
| 8 | A | 605 | PGV | 3 | 0 |
| 8 | C | 101 | PGV | 4 | 0 |
| 8 | D | 606 | PGV | 2 | 0 |
| 8 | A | 607 | PGV | 27 | 0 |
| 8 | D | 601 | PGV | 27 | 0 |
| 8 | F | 101 | PGV | 4 | 0 |
| 9 | A | 606 | 3PE | 36 | 0 |
| 9 | D | 607 | 3PE | 34 | 0 |
| 5 | A | 602 | HEM | 8 | 0 |
| 7 | D | 605 | DLX | 3 | 0 |
| 7 | A | 604 | DLX | 3 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 HAS D 602



Bond lengths



Bond angles



Torsions



Rings

## Ligand HAS A 601



Bond lengths



Bond angles



Torsions



Rings

**Ligand HEM D 603**



Bond lengths



Bond angles



Torsions



Rings

**Ligand PGV A 605**



Bond lengths



Bond angles



Torsions



Rings

**Ligand PGV C 101**


Bond lengths


Bond angles


Torsions


Rings

**Ligand PGV D 606**


Bond lengths


Bond angles


Torsions


Rings

**Ligand PGV A 607**



Bond lengths



Bond angles



Torsions



Rings

**Ligand PGV D 601**



Bond lengths



Bond angles



Torsions



Rings

**Ligand PGV F 101**



Bond lengths



Bond angles



Torsions



Rings

**Ligand 3PE A 606**



Bond lengths



Bond angles



Torsions



Rings

**Ligand 3PE D 607**



Bond lengths



Bond angles



Torsions



Rings

**Ligand HEM A 602**

Bond lengths

Bond angles

Torsions

Rings

**Ligand DLX D 605**

Bond lengths

Bond angles

Torsions

Rings

**Ligand DLX A 604**
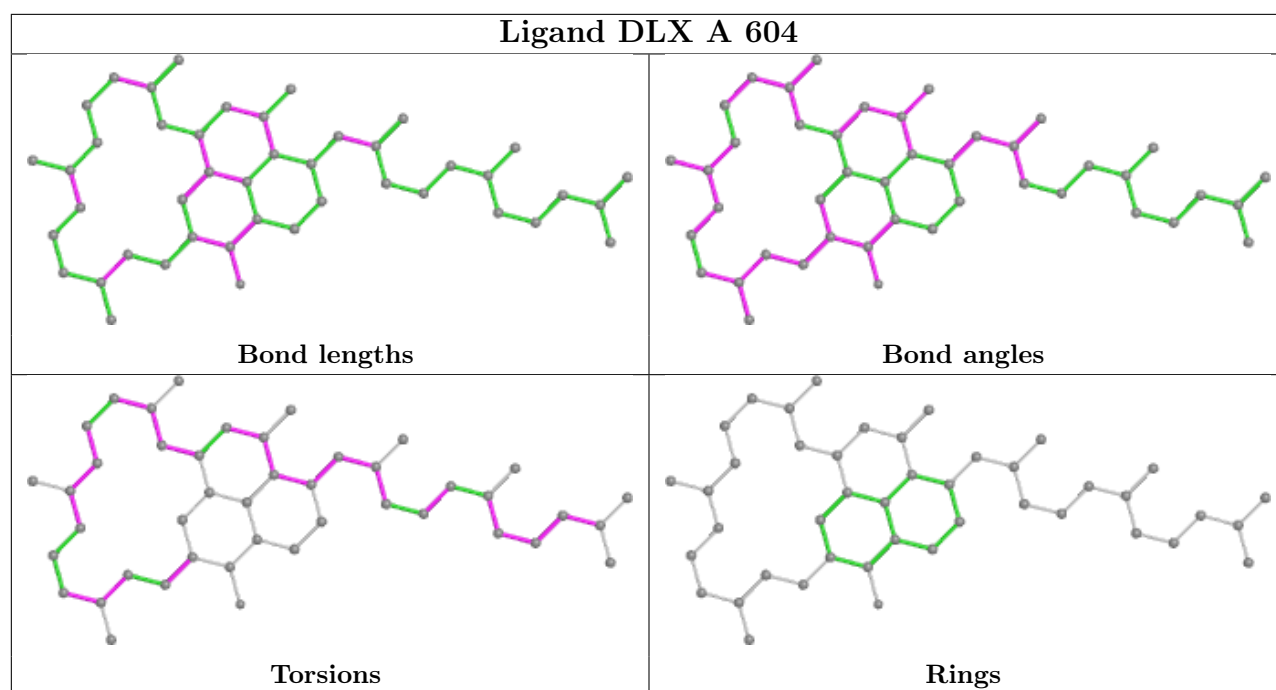


Bond lengths

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 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-30657. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections ⓘ

This section was not generated.

## 6.2 Central slices ⓘ

This section was not generated.

## 6.3 Largest variance slices ⓘ

This section was not generated.

## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

## 6.5 Orthogonal surface views ⓘ

This section was not generated.

## 6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution ⓘ

This section was not generated.

## 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

## 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 8   Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit (i)

This section was not generated.