# WORLDWIDE wwPDB PROTEIN DATA BANK

# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 04:08 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 4QRO |
| Title | : | CRYSTAL STRUCTURE of DIHYDROXYBENZOIC ACID DECARBOXYLASE BPRO_2061 (TARGET EFI-500288) FROM POLAROMONAS SP. JS666 WITH BOUND MANGANESE AND AN INHIBITOR, 2-NITRORESORCINOL |
| Authors | : | Patskovsky, Y.; Vladimirova, A.; Toro, R.; Bhosle, R.; Gerlt, J.A.; Raushel, M.; Almo, S.C. |
| Deposited on | : | 2014-07-01 |
| Resolution | : | 1.65 Å(reported) |

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

| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| 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) | : | 2.35.1 |

# 1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.65 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.
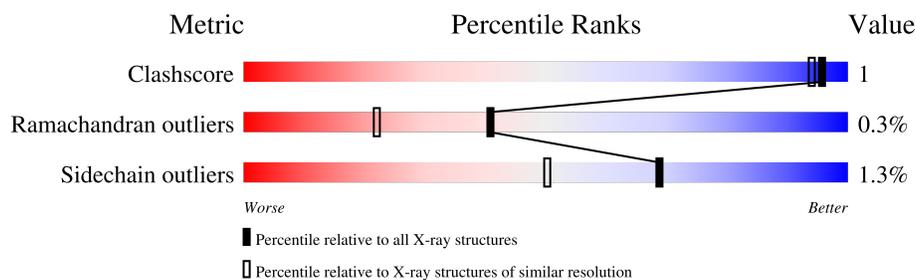


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 1931 (1.66-1.66) |
| Ramachandran outliers | 138981 | 1891 (1.66-1.66) |
| Sidechain outliers | 138945 | 1891 (1.66-1.66) |

# 2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 23784 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 Gamma-resorcylate decarboxylase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 332 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 2729 | 1745 | 481 | 493 | 10 | | | |
| 1 | B | 324 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 2655 | 1699 | 465 | 481 | 10 | | | |
| 1 | C | 325 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 2648 | 1692 | 463 | 483 | 10 | | | |
| 1 | D | 323 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 2628 | 1681 | 459 | 479 | 9 | | | |
| 1 | E | 324 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 2645 | 1691 | 461 | 484 | 9 | | | |
| 1 | F | 324 | Total | C | N | O | S | 0 | 5 | 0 |
| | | | 2660 | 1700 | 468 | 482 | 10 | | | |
| 1 | G | 327 | Total | C | N | O | S | 0 | 7 | 0 |
| | | | 2702 | 1732 | 469 | 491 | 10 | | | |
| 1 | H | 324 | Total | C | N | O | S | 0 | 8 | 0 |
| | | | 2671 | 1707 | 469 | 485 | 10 | | | |

There are 176 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 327 | ALA | - | expression tag | UNP Q12BV1 |
| A | 328 | GLU | - | expression tag | UNP Q12BV1 |
| A | 329 | ASN | - | expression tag | UNP Q12BV1 |
| A | 330 | LEU | - | expression tag | UNP Q12BV1 |
| A | 331 | TYR | - | expression tag | UNP Q12BV1 |
| A | 332 | PHE | - | expression tag | UNP Q12BV1 |
| A | 333 | GLN | - | expression tag | UNP Q12BV1 |
| A | 334 | SER | - | expression tag | UNP Q12BV1 |
| A | 335 | HIS | - | expression tag | UNP Q12BV1 |
| A | 336 | HIS | - | expression tag | UNP Q12BV1 |
| A | 337 | HIS | - | expression tag | UNP Q12BV1 |
| A | 338 | HIS | - | expression tag | UNP Q12BV1 |
| A | 339 | HIS | - | expression tag | UNP Q12BV1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 340 | HIS | - | expression tag | UNP Q12BV1 |
| A | 341 | TRP | - | expression tag | UNP Q12BV1 |
| A | 342 | SER | - | expression tag | UNP Q12BV1 |
| A | 343 | HIS | - | expression tag | UNP Q12BV1 |
| A | 344 | PRO | - | expression tag | UNP Q12BV1 |
| A | 345 | GLN | - | expression tag | UNP Q12BV1 |
| A | 346 | PHE | - | expression tag | UNP Q12BV1 |
| A | 347 | GLU | - | expression tag | UNP Q12BV1 |
| A | 348 | LYS | - | expression tag | UNP Q12BV1 |
| B | 327 | ALA | - | expression tag | UNP Q12BV1 |
| B | 328 | GLU | - | expression tag | UNP Q12BV1 |
| B | 329 | ASN | - | expression tag | UNP Q12BV1 |
| B | 330 | LEU | - | expression tag | UNP Q12BV1 |
| B | 331 | TYR | - | expression tag | UNP Q12BV1 |
| B | 332 | PHE | - | expression tag | UNP Q12BV1 |
| B | 333 | GLN | - | expression tag | UNP Q12BV1 |
| B | 334 | SER | - | expression tag | UNP Q12BV1 |
| B | 335 | HIS | - | expression tag | UNP Q12BV1 |
| B | 336 | HIS | - | expression tag | UNP Q12BV1 |
| B | 337 | HIS | - | expression tag | UNP Q12BV1 |
| B | 338 | HIS | - | expression tag | UNP Q12BV1 |
| B | 339 | HIS | - | expression tag | UNP Q12BV1 |
| B | 340 | HIS | - | expression tag | UNP Q12BV1 |
| B | 341 | TRP | - | expression tag | UNP Q12BV1 |
| B | 342 | SER | - | expression tag | UNP Q12BV1 |
| B | 343 | HIS | - | expression tag | UNP Q12BV1 |
| B | 344 | PRO | - | expression tag | UNP Q12BV1 |
| B | 345 | GLN | - | expression tag | UNP Q12BV1 |
| B | 346 | PHE | - | expression tag | UNP Q12BV1 |
| B | 347 | GLU | - | expression tag | UNP Q12BV1 |
| B | 348 | LYS | - | expression tag | UNP Q12BV1 |
| C | 327 | ALA | - | expression tag | UNP Q12BV1 |
| C | 328 | GLU | - | expression tag | UNP Q12BV1 |
| C | 329 | ASN | - | expression tag | UNP Q12BV1 |
| C | 330 | LEU | - | expression tag | UNP Q12BV1 |
| C | 331 | TYR | - | expression tag | UNP Q12BV1 |
| C | 332 | PHE | - | expression tag | UNP Q12BV1 |
| C | 333 | GLN | - | expression tag | UNP Q12BV1 |
| C | 334 | SER | - | expression tag | UNP Q12BV1 |
| C | 335 | HIS | - | expression tag | UNP Q12BV1 |
| C | 336 | HIS | - | expression tag | UNP Q12BV1 |
| C | 337 | HIS | - | expression tag | UNP Q12BV1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| C | 338 | HIS | - | expression tag | UNP Q12BV1 |
| C | 339 | HIS | - | expression tag | UNP Q12BV1 |
| C | 340 | HIS | - | expression tag | UNP Q12BV1 |
| C | 341 | TRP | - | expression tag | UNP Q12BV1 |
| C | 342 | SER | - | expression tag | UNP Q12BV1 |
| C | 343 | HIS | - | expression tag | UNP Q12BV1 |
| C | 344 | PRO | - | expression tag | UNP Q12BV1 |
| C | 345 | GLN | - | expression tag | UNP Q12BV1 |
| C | 346 | PHE | - | expression tag | UNP Q12BV1 |
| C | 347 | GLU | - | expression tag | UNP Q12BV1 |
| C | 348 | LYS | - | expression tag | UNP Q12BV1 |
| D | 327 | ALA | - | expression tag | UNP Q12BV1 |
| D | 328 | GLU | - | expression tag | UNP Q12BV1 |
| D | 329 | ASN | - | expression tag | UNP Q12BV1 |
| D | 330 | LEU | - | expression tag | UNP Q12BV1 |
| D | 331 | TYR | - | expression tag | UNP Q12BV1 |
| D | 332 | PHE | - | expression tag | UNP Q12BV1 |
| D | 333 | GLN | - | expression tag | UNP Q12BV1 |
| D | 334 | SER | - | expression tag | UNP Q12BV1 |
| D | 335 | HIS | - | expression tag | UNP Q12BV1 |
| D | 336 | HIS | - | expression tag | UNP Q12BV1 |
| D | 337 | HIS | - | expression tag | UNP Q12BV1 |
| D | 338 | HIS | - | expression tag | UNP Q12BV1 |
| D | 339 | HIS | - | expression tag | UNP Q12BV1 |
| D | 340 | HIS | - | expression tag | UNP Q12BV1 |
| D | 341 | TRP | - | expression tag | UNP Q12BV1 |
| D | 342 | SER | - | expression tag | UNP Q12BV1 |
| D | 343 | HIS | - | expression tag | UNP Q12BV1 |
| D | 344 | PRO | - | expression tag | UNP Q12BV1 |
| D | 345 | GLN | - | expression tag | UNP Q12BV1 |
| D | 346 | PHE | - | expression tag | UNP Q12BV1 |
| D | 347 | GLU | - | expression tag | UNP Q12BV1 |
| D | 348 | LYS | - | expression tag | UNP Q12BV1 |
| E | 327 | ALA | - | expression tag | UNP Q12BV1 |
| E | 328 | GLU | - | expression tag | UNP Q12BV1 |
| E | 329 | ASN | - | expression tag | UNP Q12BV1 |
| E | 330 | LEU | - | expression tag | UNP Q12BV1 |
| E | 331 | TYR | - | expression tag | UNP Q12BV1 |
| E | 332 | PHE | - | expression tag | UNP Q12BV1 |
| E | 333 | GLN | - | expression tag | UNP Q12BV1 |
| E | 334 | SER | - | expression tag | UNP Q12BV1 |
| E | 335 | HIS | - | expression tag | UNP Q12BV1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| E | 336 | HIS | - | expression tag | UNP Q12BV1 |
| E | 337 | HIS | - | expression tag | UNP Q12BV1 |
| E | 338 | HIS | - | expression tag | UNP Q12BV1 |
| E | 339 | HIS | - | expression tag | UNP Q12BV1 |
| E | 340 | HIS | - | expression tag | UNP Q12BV1 |
| E | 341 | TRP | - | expression tag | UNP Q12BV1 |
| E | 342 | SER | - | expression tag | UNP Q12BV1 |
| E | 343 | HIS | - | expression tag | UNP Q12BV1 |
| E | 344 | PRO | - | expression tag | UNP Q12BV1 |
| E | 345 | GLN | - | expression tag | UNP Q12BV1 |
| E | 346 | PHE | - | expression tag | UNP Q12BV1 |
| E | 347 | GLU | - | expression tag | UNP Q12BV1 |
| E | 348 | LYS | - | expression tag | UNP Q12BV1 |
| F | 327 | ALA | - | expression tag | UNP Q12BV1 |
| F | 328 | GLU | - | expression tag | UNP Q12BV1 |
| F | 329 | ASN | - | expression tag | UNP Q12BV1 |
| F | 330 | LEU | - | expression tag | UNP Q12BV1 |
| F | 331 | TYR | - | expression tag | UNP Q12BV1 |
| F | 332 | PHE | - | expression tag | UNP Q12BV1 |
| F | 333 | GLN | - | expression tag | UNP Q12BV1 |
| F | 334 | SER | - | expression tag | UNP Q12BV1 |
| F | 335 | HIS | - | expression tag | UNP Q12BV1 |
| F | 336 | HIS | - | expression tag | UNP Q12BV1 |
| F | 337 | HIS | - | expression tag | UNP Q12BV1 |
| F | 338 | HIS | - | expression tag | UNP Q12BV1 |
| F | 339 | HIS | - | expression tag | UNP Q12BV1 |
| F | 340 | HIS | - | expression tag | UNP Q12BV1 |
| F | 341 | TRP | - | expression tag | UNP Q12BV1 |
| F | 342 | SER | - | expression tag | UNP Q12BV1 |
| F | 343 | HIS | - | expression tag | UNP Q12BV1 |
| F | 344 | PRO | - | expression tag | UNP Q12BV1 |
| F | 345 | GLN | - | expression tag | UNP Q12BV1 |
| F | 346 | PHE | - | expression tag | UNP Q12BV1 |
| F | 347 | GLU | - | expression tag | UNP Q12BV1 |
| F | 348 | LYS | - | expression tag | UNP Q12BV1 |
| G | 327 | ALA | - | expression tag | UNP Q12BV1 |
| G | 328 | GLU | - | expression tag | UNP Q12BV1 |
| G | 329 | ASN | - | expression tag | UNP Q12BV1 |
| G | 330 | LEU | - | expression tag | UNP Q12BV1 |
| G | 331 | TYR | - | expression tag | UNP Q12BV1 |
| G | 332 | PHE | - | expression tag | UNP Q12BV1 |
| G | 333 | GLN | - | expression tag | UNP Q12BV1 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| G | 334 | SER | - | expression tag | UNP Q12BV1 |
| G | 335 | HIS | - | expression tag | UNP Q12BV1 |
| G | 336 | HIS | - | expression tag | UNP Q12BV1 |
| G | 337 | HIS | - | expression tag | UNP Q12BV1 |
| G | 338 | HIS | - | expression tag | UNP Q12BV1 |
| G | 339 | HIS | - | expression tag | UNP Q12BV1 |
| G | 340 | HIS | - | expression tag | UNP Q12BV1 |
| G | 341 | TRP | - | expression tag | UNP Q12BV1 |
| G | 342 | SER | - | expression tag | UNP Q12BV1 |
| G | 343 | HIS | - | expression tag | UNP Q12BV1 |
| G | 344 | PRO | - | expression tag | UNP Q12BV1 |
| G | 345 | GLN | - | expression tag | UNP Q12BV1 |
| G | 346 | PHE | - | expression tag | UNP Q12BV1 |
| G | 347 | GLU | - | expression tag | UNP Q12BV1 |
| G | 348 | LYS | - | expression tag | UNP Q12BV1 |
| H | 327 | ALA | - | expression tag | UNP Q12BV1 |
| H | 328 | GLU | - | expression tag | UNP Q12BV1 |
| H | 329 | ASN | - | expression tag | UNP Q12BV1 |
| H | 330 | LEU | - | expression tag | UNP Q12BV1 |
| H | 331 | TYR | - | expression tag | UNP Q12BV1 |
| H | 332 | PHE | - | expression tag | UNP Q12BV1 |
| H | 333 | GLN | - | expression tag | UNP Q12BV1 |
| H | 334 | SER | - | expression tag | UNP Q12BV1 |
| H | 335 | HIS | - | expression tag | UNP Q12BV1 |
| H | 336 | HIS | - | expression tag | UNP Q12BV1 |
| H | 337 | HIS | - | expression tag | UNP Q12BV1 |
| H | 338 | HIS | - | expression tag | UNP Q12BV1 |
| H | 339 | HIS | - | expression tag | UNP Q12BV1 |
| H | 340 | HIS | - | expression tag | UNP Q12BV1 |
| H | 341 | TRP | - | expression tag | UNP Q12BV1 |
| H | 342 | SER | - | expression tag | UNP Q12BV1 |
| H | 343 | HIS | - | expression tag | UNP Q12BV1 |
| H | 344 | PRO | - | expression tag | UNP Q12BV1 |
| H | 345 | GLN | - | expression tag | UNP Q12BV1 |
| H | 346 | PHE | - | expression tag | UNP Q12BV1 |
| H | 347 | GLU | - | expression tag | UNP Q12BV1 |
| H | 348 | LYS | - | expression tag | UNP Q12BV1 |

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
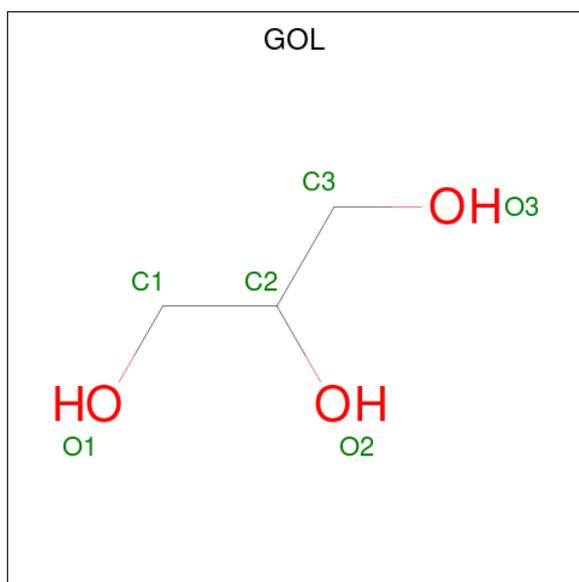


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 2 | A | 1 | Total 12 | C 6 | O 6 | 0 | 1 |
| 2 | B | 1 | Total 12 | C 6 | O 6 | 0 | 1 |
| 2 | C | 1 | Total 6 | C 3 | O 3 | 0 | 0 |
| 2 | F | 1 | Total 12 | C 6 | O 6 | 0 | 1 |
| 2 | H | 1 | Total 12 | C 6 | O 6 | 0 | 1 |

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | A | 1 | Total 1 | Mn 1 | 0 | 0 |
| 3 | B | 1 | Total 1 | Mn 1 | 0 | 0 |
| 3 | C | 1 | Total 1 | Mn 1 | 0 | 0 |
| 3 | D | 1 | Total 1 | Mn 1 | 0 | 0 |
| 3 | E | 1 | Total 1 | Mn 1 | 0 | 0 |
| 3 | F | 1 | Total 1 | Mn 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | G | 1 | Total Mn | | 0 | 0 |
| | | | 1 1 | | | |
| 3 | H | 1 | Total Mn | | 0 | 0 |
| | | | 1 1 | | | |

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
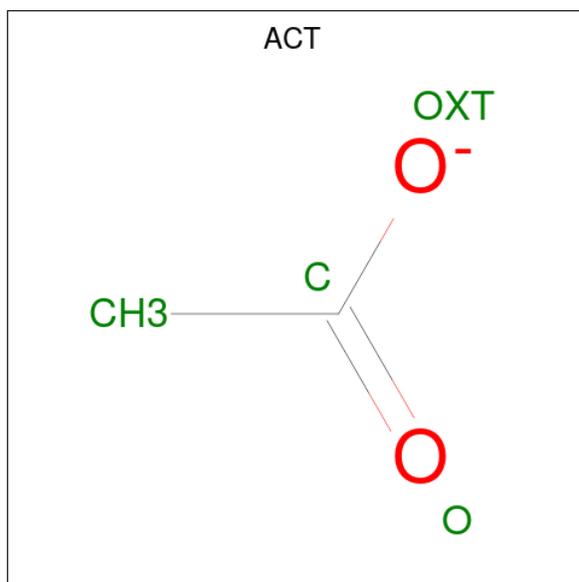


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | D | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | F | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | G | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | H | 1 | Total<br>4 | C<br>2 | O<br>2 | 0 | 0 |
| 4 | H | 1 | Total<br>4 | C<br>2 | O<br>2 | 0 | 0 |

- Molecule 5 is 2-nitrobenzene-1,3-diol (three-letter code: 38L) (formula: $C_6H_5NO_4$).
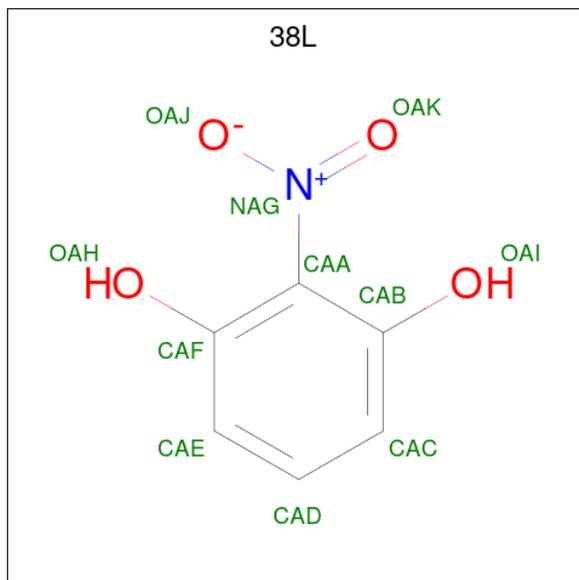


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5 | A | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | B | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | C | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | D | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | E | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | F | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | G | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |
| 5 | H | 1 | Total<br>11 | C<br>6 | N<br>1 | O<br>4 | 0 | 0 |

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula: $CHO_3$).
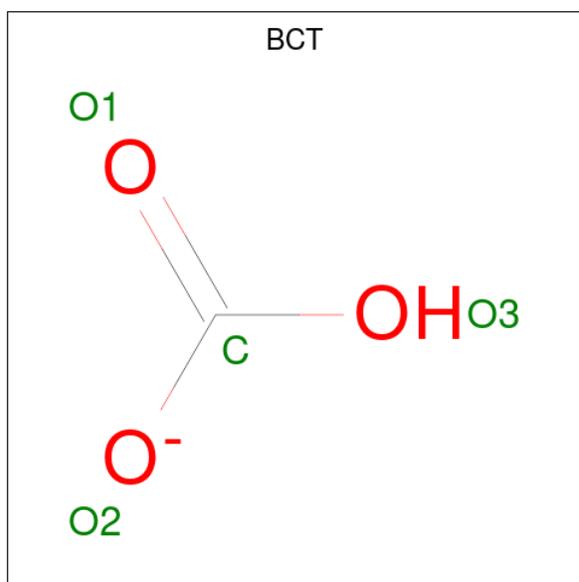
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6 | G | 1 | Total<br>4 | C<br>1 | O<br>3 | 0 | 0 |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 7 | A | 287 | Total<br>288 | O<br>288 | 0 | 1 |
| 7 | B | 245 | Total<br>245 | O<br>245 | 0 | 0 |
| 7 | C | 273 | Total<br>273 | O<br>273 | 0 | 0 |
| 7 | D | 240 | Total<br>240 | O<br>240 | 0 | 0 |
| 7 | E | 312 | Total<br>312 | O<br>312 | 0 | 0 |
| 7 | F | 290 | Total<br>290 | O<br>290 | 0 | 0 |
| 7 | G | 310 | Total<br>310 | O<br>310 | 0 | 0 |
| 7 | H | 284 | Total<br>284 | O<br>284 | 0 | 0 |

SEQUENCE-PLOTS INFOmissingINFO

# 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, $\alpha$, $\beta$, $\gamma$ | 80.96Å    151.06Å    143.83Å <br> 90.00°    92.15°    90.00° | Depositor |
| Resolution (Å) | 50.00    –    1.65 | Depositor |
| % Data completeness (in resolution range) | 99.8 (50.00-1.65) | Depositor |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | 0.10 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.95 (at 1.65Å) | Xtriage |
| Refinement program | REFMAC 5.8.0071 | Depositor |
| R, $R_{free}$ | 0.189    ,    0.223 | Depositor |
| Wilson B-factor (Å²) | 17.9 | Xtriage |
| Anisotropy | 0.807 | Xtriage |
| L-test for twinning [2] | $< |L| > = 0.51, < L^2 > = 0.34$ | Xtriage |
| Estimated twinning fraction | 0.105 for h,-k,-l | Xtriage |
| Total number of atoms | 23784 | wwPDB-VP |
| Average B, all atoms (Å²) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3262e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 4   Model quality ⓘ

## 4.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GOL, ACT, BCT, 38L

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 | 0.56 | 0/2813 | 0.70 | 4/3819 (0.1%) |
| 1 | B | 0.54 | 0/2740 | 0.65 | 0/3720 |
| 1 | C | 0.55 | 0/2721 | 0.69 | 0/3696 |
| 1 | D | 0.58 | 2/2704 (0.1%) | 0.69 | 0/3674 |
| 1 | E | 0.74 | 0/2727 | 0.75 | 2/3705 (0.1%) |
| 1 | F | 0.69 | 1/2742 (0.0%) | 0.73 | 1/3723 (0.0%) |
| 1 | G | 0.73 | 0/2788 | 0.80 | 5/3783 (0.1%) |
| 1 | H | 0.70 | 0/2759 | 0.72 | 0/3746 |
| All | All | 0.64 | 3/21994 (0.0%) | 0.72 | 12/29866 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | F | 148 | TRP | CB-CG | 5.93 | 1.60 | 1.50 |
| 1 | D | 45[A] | ARG | N-CA | 5.14 | 1.56 | 1.46 |
| 1 | D | 45[B] | ARG | N-CA | 5.14 | 1.56 | 1.46 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | G | 45 | ARG | NE-CZ-NH2 | 8.92 | 124.76 | 120.30 |
| 1 | A | 174 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 1 | G | 45 | ARG | NE-CZ-NH1 | -5.60 | 117.50 | 120.30 |
| 1 | A | 133 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | F | 247 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 1 | G | 174 | ARG | NE-CZ-NH2 | 5.32 | 122.96 | 120.30 |
| 1 | A | 310 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 1 | E | 72 | ARG | NE-CZ-NH2 | 5.19 | 122.90 | 120.30 |
| 1 | E | 45 | ARG | NE-CZ-NH2 | 5.19 | 122.89 | 120.30 |
| 1 | A | 174 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | G | 174 | ARG | NE-CZ-NH1 | -5.08 | 117.76 | 120.30 |
| 1 | G | 35 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

## 4.2 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 | 2729 | 0 | 2654 | 9 | 0 |
| 1 | B | 2655 | 0 | 2592 | 5 | 0 |
| 1 | C | 2648 | 0 | 2567 | 1 | 0 |
| 1 | D | 2628 | 0 | 2548 | 1 | 0 |
| 1 | E | 2645 | 0 | 2565 | 4 | 0 |
| 1 | F | 2660 | 0 | 2591 | 7 | 0 |
| 1 | G | 2702 | 0 | 2630 | 8 | 0 |
| 1 | H | 2671 | 0 | 2603 | 8 | 0 |
| 2 | A | 18 | 0 | 24 | 4 | 0 |
| 2 | B | 12 | 0 | 16 | 0 | 0 |
| 2 | C | 6 | 0 | 8 | 0 | 0 |
| 2 | F | 12 | 0 | 16 | 1 | 0 |
| 2 | H | 12 | 0 | 16 | 3 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 4 | 0 | 3 | 1 | 0 |
| 4 | B | 4 | 0 | 3 | 0 | 0 |
| 4 | C | 8 | 0 | 6 | 0 | 0 |
| 4 | D | 4 | 0 | 3 | 0 | 0 |
| 4 | E | 8 | 0 | 6 | 0 | 0 |
| 4 | F | 4 | 0 | 3 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | G | 4 | 0 | 3 | 0 | 0 |
| 4 | H | 8 | 0 | 6 | 0 | 0 |
| 5 | A | 11 | 0 | 3 | 0 | 0 |
| 5 | B | 11 | 0 | 4 | 0 | 0 |
| 5 | C | 11 | 0 | 3 | 0 | 0 |
| 5 | D | 11 | 0 | 3 | 0 | 0 |
| 5 | E | 11 | 0 | 3 | 0 | 0 |
| 5 | F | 11 | 0 | 3 | 0 | 0 |
| 5 | G | 11 | 0 | 3 | 0 | 0 |
| 5 | H | 11 | 0 | 3 | 0 | 0 |
| 6 | G | 4 | 0 | 0 | 0 | 0 |
| 7 | A | 288 | 0 | 0 | 5 | 0 |
| 7 | B | 245 | 0 | 0 | 1 | 0 |
| 7 | C | 273 | 0 | 0 | 1 | 0 |
| 7 | D | 240 | 0 | 0 | 0 | 0 |
| 7 | E | 312 | 0 | 0 | 1 | 0 |
| 7 | F | 290 | 0 | 0 | 2 | 0 |
| 7 | G | 310 | 0 | 0 | 2 | 0 |
| 7 | H | 284 | 0 | 0 | 2 | 0 |
| All | All | 23784 | 0 | 20888 | 46 | 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 1.

All (46) 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) |
|--------|--------|--------------------------|-------------------|
| 4:A:404:ACT:H1 | 7:A:783:HOH:O | 1.80 | 0.79 |
| 2:F:401[A]:GOL:H32 | 1:G:267:THR:OG1 | 1.84 | 0.78 |
| 1:H:267:THR:OG1 | 2:H:401[A]:GOL:H32 | 1.83 | 0.78 |
| 1:A:41:ASP:OD1 | 1:A:45[A]:ARG:NH1 | 2.20 | 0.74 |
| 1:H:146:GLN:HE21 | 1:H:146:GLN:H | 1.36 | 0.73 |
| 1:E:267:THR:OG1 | 2:H:401[B]:GOL:H11 | 1.90 | 0.69 |
| 1:H:219:MET:HE1 | 1:H:270:LEU:HD13 | 1.74 | 0.68 |
| 1:F:219:MET:HE1 | 1:F:270:LEU:HD13 | 1.81 | 0.63 |
| 1:A:219:MET:HE1 | 1:A:270:LEU:HD13 | 1.82 | 0.62 |
| 1:A:248:LYS:NZ | 7:A:743:HOH:O | 2.34 | 0.60 |
| 1:G:219:MET:HE1 | 1:G:270:LEU:HD13 | 1.85 | 0.57 |
| 1:G:144:MET:HE2 | 7:G:716:HOH:O | 2.05 | 0.56 |
| 2:A:402[B]:GOL:H32 | 1:D:267:THR:OG1 | 2.05 | 0.55 |
| 1:H:33[A]:ARG:HH21 | 1:H:33[A]:ARG:HG3 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:9:GLU:OE2 | 1:A:286:THR:OG1 | 2.22 | 0.53 |
| 1:E:174:ARG:NE | 7:E:790:HOH:O | 2.34 | 0.53 |
| 1:A:21[B]:ALA:O | 7:A:744:HOH:O | 2.20 | 0.47 |
| 2:A:402[A]:GOL:H12 | 7:A:782:HOH:O | 2.14 | 0.47 |
| 1:A:10:HIS:HA | 1:A:58:SER:O | 2.14 | 0.47 |
| 1:H:42:ARG:HD3 | 7:H:721:HOH:O | 2.14 | 0.47 |
| 2:A:402[A]:GOL:C1 | 7:A:782:HOH:O | 2.62 | 0.47 |
| 1:G:93:THR:HG22 | 1:G:330:LEU:HD21 | 1.97 | 0.47 |
| 1:G:93:THR:HG22 | 1:G:330:LEU:CD2 | 2.46 | 0.45 |
| 1:G:144:MET:CE | 7:G:716:HOH:O | 2.63 | 0.45 |
| 1:B:227:MET:HA | 1:B:230:ILE:HD12 | 1.98 | 0.45 |
| 1:H:134[A]:ASN:ND2 | 7:H:674:HOH:O | 2.24 | 0.45 |
| 1:A:267:THR:OG1 | 2:A:402[A]:GOL:H11 | 2.17 | 0.44 |
| 1:E:72:ARG:CG | 1:E:72:ARG:HH21 | 2.30 | 0.44 |
| 1:B:292:ASN:HB3 | 1:B:294:ASP:OD1 | 2.18 | 0.44 |
| 1:H:9:GLU:OE2 | 1:H:286:THR:OG1 | 2.30 | 0.44 |
| 1:F:96:ARG:NH1 | 7:F:727:HOH:O | 2.51 | 0.43 |
| 1:B:35:ARG:HB3 | 1:B:289:PRO:HB3 | 2.00 | 0.43 |
| 1:B:116:CYS:HB3 | 1:B:122:PHE:CD2 | 2.54 | 0.42 |
| 1:F:10:HIS:HA | 1:F:58:SER:O | 2.20 | 0.42 |
| 1:F:160:PRO:HG2 | 1:F:322:PHE:CE1 | 2.55 | 0.42 |
| 1:G:218:HIS:HA | 1:G:262:SER:O | 2.20 | 0.42 |
| 1:F:281[B]:ARG:HA | 1:F:281[B]:ARG:HD3 | 1.83 | 0.42 |
| 1:E:267:THR:OG1 | 2:H:401[B]:GOL:C1 | 2.64 | 0.41 |
| 1:F:174[A]:ARG:HG2 | 7:F:610:HOH:O | 2.20 | 0.41 |
| 1:A:218:HIS:O | 1:A:219:MET:HB2 | 2.21 | 0.41 |
| 1:F:292:ASN:HB3 | 1:F:294:ASP:OD1 | 2.21 | 0.41 |
| 1:H:35:ARG:HB3 | 1:H:289:PRO:HB3 | 2.03 | 0.41 |
| 1:C:238:LYS:HE2 | 7:C:601:HOH:O | 2.21 | 0.41 |
| 1:G:280:ASP:OD1 | 1:G:312[A]:LYS:CE | 2.69 | 0.41 |
| 1:B:179:HIS:CE1 | 7:B:729:HOH:O | 2.73 | 0.40 |
| 1:A:280:ASP:OD1 | 1:A:312:LYS:CE | 2.70 | 0.40 |

There are no symmetry-related clashes.

## 4.3　Torsion angles　ⓘ

### 4.3.1　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 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 | 336/348 (97%) | 328 (98%) | 7 (2%) | 1 (0%) | 41 | 22 |
| 1 | B | 327/348 (94%) | 317 (97%) | 9 (3%) | 1 (0%) | 41 | 22 |
| 1 | C | 326/348 (94%) | 317 (97%) | 8 (2%) | 1 (0%) | 41 | 22 |
| 1 | D | 323/348 (93%) | 314 (97%) | 8 (2%) | 1 (0%) | 41 | 22 |
| 1 | E | 327/348 (94%) | 318 (97%) | 8 (2%) | 1 (0%) | 41 | 22 |
| 1 | F | 327/348 (94%) | 319 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | G | 330/348 (95%) | 321 (97%) | 8 (2%) | 1 (0%) | 41 | 22 |
| 1 | H | 330/348 (95%) | 322 (98%) | 7 (2%) | 1 (0%) | 41 | 22 |
| All | All | 2626/2784 (94%) | 2556 (97%) | 63 (2%) | 7 (0%) | 41 | 22 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 187 | TRP |
| 1 | A | 187 | TRP |
| 1 | B | 187 | TRP |
| 1 | C | 187 | TRP |
| 1 | E | 187 | TRP |
| 1 | G | 187 | TRP |
| 1 | H | 187 | TRP |

### 4.3.2 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 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 | 281/294 (96%) | 278 (99%) | 3 (1%) | 73 | 57 |
| 1 | B | 276/294 (94%) | 272 (99%) | 4 (1%) | 67 | 46 |
| 1 | C | 273/294 (93%) | 269 (98%) | 4 (2%) | 65 | 44 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------------|---|
| 1 | D | 272/294 (92%) | 269 (99%) | 3 (1%) | 73 | 57 |
| 1 | E | 274/294 (93%) | 270 (98%) | 4 (2%) | 65 | 44 |
| 1 | F | 276/294 (94%) | 272 (99%) | 4 (1%) | 67 | 46 |
| 1 | G | 281/294 (96%) | 277 (99%) | 4 (1%) | 67 | 46 |
| 1 | H | 277/294 (94%) | 273 (99%) | 4 (1%) | 67 | 46 |
| All | All | 2210/2352 (94%) | 2180 (99%) | 30 (1%) | 69 | 46 |

All (30) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 7 | LEU |
| 1 | A | 107 | GLU |
| 1 | A | 233 | ARG |
| 1 | B | 7 | LEU |
| 1 | B | 72 | ARG |
| 1 | B | 111 | ARG |
| 1 | B | 233 | ARG |
| 1 | C | 7 | LEU |
| 1 | C | 72 | ARG |
| 1 | C | 233 | ARG |
| 1 | C | 242 | LYS |
| 1 | D | 7 | LEU |
| 1 | D | 72 | ARG |
| 1 | D | 233 | ARG |
| 1 | E | 7 | LEU |
| 1 | E | 72 | ARG |
| 1 | E | 233 | ARG |
| 1 | E | 307 | GLU |
| 1 | F | 7 | LEU |
| 1 | F | 45[A] | ARG |
| 1 | F | 45[B] | ARG |
| 1 | F | 233 | ARG |
| 1 | G | 7 | LEU |
| 1 | G | 233 | ARG |
| 1 | G | 307[A] | GLU |
| 1 | G | 307[B] | GLU |
| 1 | H | 7 | LEU |
| 1 | H | 146 | GLN |
| 1 | H | 162 | TYR |
| 1 | H | 233 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 179 | HIS |
| 1 | A | 254 | ASN |
| 1 | B | 254 | ASN |
| 1 | C | 2 | ASN |
| 1 | C | 134 | ASN |
| 1 | C | 254 | ASN |
| 1 | D | 179 | HIS |
| 1 | D | 254 | ASN |
| 1 | E | 2 | ASN |
| 1 | E | 134 | ASN |
| 1 | E | 254 | ASN |
| 1 | F | 254 | ASN |
| 1 | G | 179 | HIS |
| 1 | G | 254 | ASN |
| 1 | H | 132 | GLN |
| 1 | H | 146 | GLN |
| 1 | H | 254 | ASN |

### 4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 4.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 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 | ACT | G | 402 | - | 3,3,3 | 0.93 | 0 | 3,3,3 | 1.26 | 0 |
| 4 | ACT | B | 403 | - | 3,3,3 | 0.96 | 0 | 3,3,3 | 0.28 | 0 |
| 4 | ACT | E | 403 | - | 3,3,3 | 0.90 | 0 | 3,3,3 | 1.34 | 0 |
| 2 | GOL | A | 402[A] | - | 5,5,5 | 0.47 | 0 | 5,5,5 | 0.30 | 0 |
| 2 | GOL | H | 401[A] | - | 5,5,5 | 0.46 | 0 | 5,5,5 | 0.46 | 0 |
| 5 | 38L | H | 405 | 3 | 10,11,11 | 1.02 | 1 (10%) | 11,15,15 | 1.01 | 1 (9%) |
| 4 | ACT | F | 403 | - | 3,3,3 | 0.82 | 0 | 3,3,3 | 1.09 | 0 |
| 2 | GOL | B | 401[A] | - | 5,5,5 | 0.31 | 0 | 5,5,5 | 0.37 | 0 |
| 6 | BCT | G | 404 | - | 2,3,3 | 0.57 | 0 | 2,3,3 | 0.61 | 0 |
| 5 | 38L | F | 404 | 3 | 10,11,11 | 1.22 | 2 (20%) | 11,15,15 | 0.94 | 1 (9%) |
| 4 | ACT | C | 404 | - | 3,3,3 | 0.73 | 0 | 3,3,3 | 0.61 | 0 |
| 4 | ACT | D | 402 | - | 3,3,3 | 0.87 | 0 | 3,3,3 | 0.30 | 0 |
| 5 | 38L | B | 404 | 3 | 10,11,11 | 1.16 | 1 (10%) | 11,15,15 | 0.87 | 0 |
| 2 | GOL | A | 402[B] | - | 5,5,5 | 0.28 | 0 | 5,5,5 | 0.65 | 0 |
| 2 | GOL | H | 401[B] | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.89 | 0 |
| 4 | ACT | H | 403 | - | 3,3,3 | 0.95 | 0 | 3,3,3 | 0.56 | 0 |
| 5 | 38L | A | 405 | 3 | 10,11,11 | 0.88 | 1 (10%) | 11,15,15 | 1.22 | 2 (18%) |
| 4 | ACT | E | 402 | - | 3,3,3 | 0.80 | 0 | 3,3,3 | 1.04 | 0 |
| 2 | GOL | B | 401[B] | - | 5,5,5 | 0.43 | 0 | 5,5,5 | 0.34 | 0 |
| 2 | GOL | F | 401[A] | - | 5,5,5 | 0.47 | 0 | 5,5,5 | 0.86 | 0 |
| 5 | 38L | D | 403 | 3 | 10,11,11 | 0.94 | 1 (10%) | 11,15,15 | 1.32 | 1 (9%) |
| 4 | ACT | A | 404 | - | 3,3,3 | 0.73 | 0 | 3,3,3 | 1.04 | 0 |
| 5 | 38L | E | 404 | 3 | 10,11,11 | 1.13 | 1 (10%) | 11,15,15 | 1.21 | 2 (18%) |
| 5 | 38L | C | 405 | 3 | 10,11,11 | 0.61 | 0 | 11,15,15 | 1.21 | 2 (18%) |
| 5 | 38L | G | 403 | 3 | 10,11,11 | 1.59 | 1 (10%) | 11,15,15 | 1.03 | 2 (18%) |
| 2 | GOL | A | 401 | - | 5,5,5 | 0.27 | 0 | 5,5,5 | 0.41 | 0 |
| 4 | ACT | H | 404 | - | 3,3,3 | 0.73 | 0 | 3,3,3 | 0.90 | 0 |
| 2 | GOL | F | 401[B] | - | 5,5,5 | 0.24 | 0 | 5,5,5 | 0.38 | 0 |
| 4 | ACT | C | 403 | - | 3,3,3 | 0.85 | 0 | 3,3,3 | 0.50 | 0 |
| 2 | GOL | C | 401 | - | 5,5,5 | 0.31 | 0 | 5,5,5 | 0.21 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2 | GOL | H | 401[A] | - | - | 4/4/4/4 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 5 | 38L | C | 405 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 5 | 38L | G | 403 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 5 | 38L | H | 405 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 5 | 38L | E | 404 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 5 | 38L | A | 405 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 2 | GOL | B | 401[A] | - | - | 4/4/4/4 | - |
| 2 | GOL | B | 401[B] | - | - | 4/4/4/4 | - |
| 2 | GOL | A | 401 | - | - | 0/4/4/4 | - |
| 2 | GOL | F | 401[A] | - | - | 4/4/4/4 | - |
| 5 | 38L | D | 403 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 2 | GOL | F | 401[B] | - | - | 4/4/4/4 | - |
| 5 | 38L | F | 404 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 5 | 38L | B | 404 | 3 | - | 0/2/4/4 | 0/1/1/1 |
| 2 | GOL | A | 402[B] | - | - | 3/4/4/4 | - |
| 2 | GOL | H | 401[B] | - | - | 2/4/4/4 | - |
| 2 | GOL | C | 401 | - | - | 4/4/4/4 | - |
| 2 | GOL | A | 402[A] | - | - | 4/4/4/4 | - |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 5 | G | 403 | 38L | CAA-NAG | -4.00 | 1.38 | 1.45 |
| 5 | B | 404 | 38L | CAA-NAG | -2.84 | 1.40 | 1.45 |
| 5 | E | 404 | 38L | CAA-NAG | -2.72 | 1.40 | 1.45 |
| 5 | D | 403 | 38L | CAA-NAG | -2.56 | 1.41 | 1.45 |
| 5 | F | 404 | 38L | CAA-NAG | -2.45 | 1.41 | 1.45 |
| 5 | H | 405 | 38L | CAA-NAG | -2.31 | 1.41 | 1.45 |
| 5 | F | 404 | 38L | OAK-NAG | -2.14 | 1.19 | 1.22 |
| 5 | A | 405 | 38L | CAA-NAG | -2.05 | 1.42 | 1.45 |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 5 | D | 403 | 38L | CAC-CAB-CAA | 2.65 | 120.47 | 118.30 |
| 5 | C | 405 | 38L | CAE-CAF-CAA | 2.64 | 120.46 | 118.30 |
| 5 | A | 405 | 38L | CAE-CAF-CAA | 2.59 | 120.42 | 118.30 |
| 5 | A | 405 | 38L | CAC-CAB-CAA | 2.44 | 120.30 | 118.30 |
| 5 | E | 404 | 38L | CAE-CAF-CAA | 2.39 | 120.26 | 118.30 |
| 5 | F | 404 | 38L | CAE-CAF-CAA | 2.32 | 120.20 | 118.30 |
| 5 | C | 405 | 38L | CAC-CAB-CAA | 2.27 | 120.16 | 118.30 |

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 5 | G | 403 | 38L | CAC-CAB-CAA | 2.18 | 120.09 | 118.30 |
| 5 | H | 405 | 38L | CAE-CAF-CAA | 2.11 | 120.03 | 118.30 |
| 5 | G | 403 | 38L | CAE-CAF-CAA | 2.09 | 120.02 | 118.30 |
| 5 | E | 404 | 38L | CAC-CAB-CAA | 2.01 | 119.95 | 118.30 |

There are no chirality outliers.

All (33) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 2 | A | 402[A] | GOL | O1-C1-C2-C3 |
| 2 | A | 402[B] | GOL | O1-C1-C2-C3 |
| 2 | B | 401[A] | GOL | O1-C1-C2-C3 |
| 2 | B | 401[A] | GOL | C1-C2-C3-O3 |
| 2 | B | 401[B] | GOL | O1-C1-C2-C3 |
| 2 | B | 401[B] | GOL | C1-C2-C3-O3 |
| 2 | F | 401[A] | GOL | O2-C2-C3-O3 |
| 2 | F | 401[B] | GOL | O1-C1-C2-C3 |
| 2 | F | 401[B] | GOL | C1-C2-C3-O3 |
| 2 | H | 401[B] | GOL | C1-C2-C3-O3 |
| 2 | B | 401[B] | GOL | O1-C1-C2-O2 |
| 2 | B | 401[B] | GOL | O2-C2-C3-O3 |
| 2 | F | 401[B] | GOL | O1-C1-C2-O2 |
| 2 | A | 402[A] | GOL | C1-C2-C3-O3 |
| 2 | A | 402[B] | GOL | C1-C2-C3-O3 |
| 2 | C | 401 | GOL | O1-C1-C2-C3 |
| 2 | C | 401 | GOL | C1-C2-C3-O3 |
| 2 | F | 401[A] | GOL | C1-C2-C3-O3 |
| 2 | H | 401[A] | GOL | O1-C1-C2-C3 |
| 2 | H | 401[A] | GOL | C1-C2-C3-O3 |
| 2 | A | 402[A] | GOL | O1-C1-C2-O2 |
| 2 | B | 401[A] | GOL | O1-C1-C2-O2 |
| 2 | B | 401[A] | GOL | O2-C2-C3-O3 |
| 2 | F | 401[B] | GOL | O2-C2-C3-O3 |
| 2 | H | 401[A] | GOL | O1-C1-C2-O2 |
| 2 | H | 401[A] | GOL | O2-C2-C3-O3 |
| 2 | A | 402[A] | GOL | O2-C2-C3-O3 |
| 2 | A | 402[B] | GOL | O1-C1-C2-O2 |
| 2 | H | 401[B] | GOL | O2-C2-C3-O3 |
| 2 | F | 401[A] | GOL | O1-C1-C2-O2 |
| 2 | F | 401[A] | GOL | O1-C1-C2-C3 |
| 2 | C | 401 | GOL | O1-C1-C2-O2 |
| 2 | C | 401 | GOL | O2-C2-C3-O3 |

There are no ring outliers.

6 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 402[A] | GOL | 3 | 0 |
| 2 | H | 401[A] | GOL | 1 | 0 |
| 2 | A | 402[B] | GOL | 1 | 0 |
| 2 | H | 401[B] | GOL | 2 | 0 |
| 2 | F | 401[A] | GOL | 1 | 0 |
| 4 | A | 404 | ACT | 1 | 0 |

## 4.7 Other polymers ⓘ

There are no such residues in this entry.

## 4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 5 Fit of model and data ⓘ

## 5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

## 5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

## 5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

## 5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

## 5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.