# WORLDWIDE wwPDB PROTEIN DATA BANK

# Full wwPDB EM Validation Report ⓘ

Mar 5, 2024 – 01:22 AM EST

|  |  |  |
|---|---|---|
| PDB ID | : | 8V8D |
| EMDB ID | : | EMD-43035 |
| Title | : | Alpha7-nicotinic acetylcholine receptor time resolved bound to epibatidine and PNU-120596 asymmetric state 2 |
| Authors | : | Burke, S.M.; Noviello, C.M.; Hibbs, R.E. |
| Deposited on | : | 2023-12-05 |
| Resolution | : | 3.31 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

|  |  |  |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| 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 ⓘ

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

The reported resolution of this entry is 3.31 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 | | 4 |
| Ramachandran outliers | | 0 |
| Sidechain outliers | | 0 |

*Worse* ............................................................ *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures
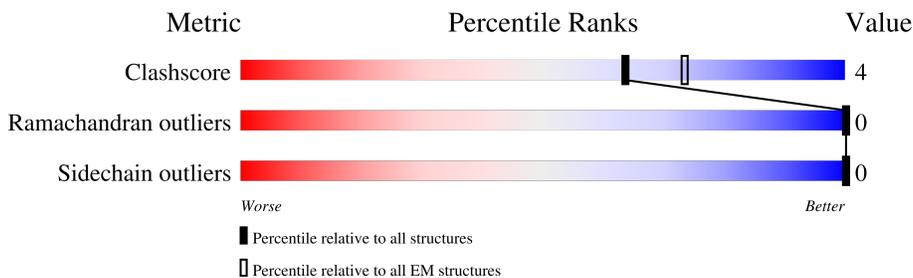
| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 599 | 58% · 5% 37% |
| 1 | B | 599 | 58% · 5% 37% |
| 1 | C | 599 | 56% · 7% 37% |
| 1 | D | 599 | 59% · · 37% |
| 1 | E | 599 | 60% · · 37% |
| 2 | F | 2 | 50% 50% |
| 2 | G | 2 | 50% 50% |
| 2 | H | 2 | 50% 50% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | I | 2 | 50%　　　　　　　　　50% |
| 2 | J | 2 | 50%　　　　　　　　　50% |

# 2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 31156 atoms, of which 15467 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 Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 1 | A | 377 | Total | C | H | N | O | S | 1 | 0 |
| | | | 6060 | 1987 | 3016 | 491 | 543 | 23 | | |
| 1 | B | 376 | Total | C | H | N | O | S | 1 | 0 |
| | | | 6036 | 1981 | 3003 | 487 | 542 | 23 | | |
| 1 | C | 377 | Total | C | H | N | O | S | 1 | 0 |
| | | | 6060 | 1987 | 3016 | 491 | 543 | 23 | | |
| 1 | D | 378 | Total | C | H | N | O | S | 1 | 0 |
| | | | 6080 | 1996 | 3025 | 492 | 544 | 23 | | |
| 1 | E | 378 | Total | C | H | N | O | S | 1 | 0 |
| | | | 6080 | 1996 | 3025 | 492 | 544 | 23 | | |

There are 475 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| A | ? | - | SER | deletion | UNP P36544 |
| A | ? | - | VAL | deletion | UNP P36544 |
| A | ? | - | GLU | deletion | UNP P36544 |
| A | ? | - | MET | deletion | UNP P36544 |
| A | ? | - | SER | deletion | UNP P36544 |
| A | ? | - | ALA | deletion | UNP P36544 |
| A | ? | - | VAL | deletion | UNP P36544 |
| A | ? | - | ALA | deletion | UNP P36544 |
| A | ? | - | PRO | deletion | UNP P36544 |
| A | ? | - | PRO | deletion | UNP P36544 |
| A | ? | - | PRO | deletion | UNP P36544 |
| A | ? | - | ALA | deletion | UNP P36544 |
| A | ? | - | SER | deletion | UNP P36544 |
| A | ? | - | ASN | deletion | UNP P36544 |
| A | ? | - | GLY | deletion | UNP P36544 |
| A | ? | - | ASN | deletion | UNP P36544 |
| A | ? | - | LEU | deletion | UNP P36544 |
| A | ? | - | LEU | deletion | UNP P36544 |
| A | ? | - | TYR | deletion | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | ? | - | ILE | deletion | UNP P36544 |
| A | ? | - | GLY | deletion | UNP P36544 |
| A | ? | - | PHE | deletion | UNP P36544 |
| A | ? | - | ARG | deletion | UNP P36544 |
| A | ? | - | GLY | deletion | UNP P36544 |
| A | ? | - | LEU | deletion | UNP P36544 |
| A | ? | - | ASP | deletion | UNP P36544 |
| A | ? | - | GLY | deletion | UNP P36544 |
| A | ? | - | VAL | deletion | UNP P36544 |
| A | ? | - | HIS | deletion | UNP P36544 |
| A | ? | - | CYS | deletion | UNP P36544 |
| A | ? | - | VAL | deletion | UNP P36544 |
| A | ? | - | PRO | deletion | UNP P36544 |
| A | ? | - | THR | deletion | UNP P36544 |
| A | ? | - | PRO | deletion | UNP P36544 |
| A | ? | - | ASP | deletion | UNP P36544 |
| A | ? | - | SER | deletion | UNP P36544 |
| A | ? | - | GLY | deletion | UNP P36544 |
| A | ? | - | VAL | deletion | UNP P36544 |
| A | ? | - | VAL | deletion | UNP P36544 |
| A | 324B | ALA | - | linker | UNP P36544 |
| A | 324C | GLY | - | linker | UNP P36544 |
| A | 324D | ALA | - | linker | UNP P36544 |
| A | 324E | MET | - | linker | UNP P36544 |
| A | 324L | TRP | MET | conflict | UNP P0ABE7 |
| A | 328C | ILE | HIS | conflict | UNP P0ABE7 |
| A | 328G | LEU | ARG | conflict | UNP P0ABE7 |
| A | 480 | TRP | - | expression tag | UNP P36544 |
| A | 481 | SER | - | expression tag | UNP P36544 |
| A | 482 | HIS | - | expression tag | UNP P36544 |
| A | 483 | PRO | - | expression tag | UNP P36544 |
| A | 484 | GLN | - | expression tag | UNP P36544 |
| A | 485 | PHE | - | expression tag | UNP P36544 |
| A | 486 | GLU | - | expression tag | UNP P36544 |
| A | 487 | LYS | - | expression tag | UNP P36544 |
| A | 488 | GLY | - | linker | UNP P36544 |
| A | 489 | GLY | - | linker | UNP P36544 |
| A | 490 | GLY | - | linker | UNP P36544 |
| A | 491 | SER | - | linker | UNP P36544 |
| A | 492 | GLY | - | linker | UNP P36544 |
| A | 493 | GLY | - | linker | UNP P36544 |
| A | 494 | GLY | - | linker | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| A | 495 | SER | - | linker | UNP P36544 |
| A | 496 | GLY | - | linker | UNP P36544 |
| A | 497 | GLY | - | linker | UNP P36544 |
| A | 498 | SER | - | linker | UNP P36544 |
| A | 499 | SER | - | linker | UNP P36544 |
| A | 500 | ALA | - | linker | UNP P36544 |
| A | 501 | TRP | - | expression tag | UNP P36544 |
| A | 502 | SER | - | expression tag | UNP P36544 |
| A | 503 | HIS | - | expression tag | UNP P36544 |
| A | 504 | PRO | - | expression tag | UNP P36544 |
| A | 505 | GLN | - | expression tag | UNP P36544 |
| A | 506 | PHE | - | expression tag | UNP P36544 |
| A | 507 | GLU | - | expression tag | UNP P36544 |
| A | 508 | LYS | - | expression tag | UNP P36544 |
| A | 509 | GLY | - | linker | UNP P36544 |
| A | 510 | SER | - | linker | UNP P36544 |
| A | 511 | GLY | - | linker | UNP P36544 |
| A | 512 | GLU | - | linker | UNP P36544 |
| A | 513 | GLY | - | linker | UNP P36544 |
| A | 514 | ARG | - | linker | UNP P36544 |
| A | 515 | GLY | - | linker | UNP P36544 |
| A | 516 | SER | - | linker | UNP P36544 |
| A | 517 | LEU | - | linker | UNP P36544 |
| A | 518 | LEU | - | linker | UNP P36544 |
| A | 519 | THR | - | linker | UNP P36544 |
| A | 520 | CYS | - | linker | UNP P36544 |
| A | 521 | GLY | - | linker | UNP P36544 |
| A | 522 | ASP | - | linker | UNP P36544 |
| A | 523 | VAL | - | linker | UNP P36544 |
| A | 524 | GLU | - | linker | UNP P36544 |
| A | 525 | GLU | - | linker | UNP P36544 |
| A | 526 | ASN | - | linker | UNP P36544 |
| A | 527 | PRO | - | linker | UNP P36544 |
| A | 528 | GLY | - | linker | UNP P36544 |
| B | ? | - | SER | deletion | UNP P36544 |
| B | ? | - | VAL | deletion | UNP P36544 |
| B | ? | - | GLU | deletion | UNP P36544 |
| B | ? | - | MET | deletion | UNP P36544 |
| B | ? | - | SER | deletion | UNP P36544 |
| B | ? | - | ALA | deletion | UNP P36544 |
| B | ? | - | VAL | deletion | UNP P36544 |
| B | ? | - | ALA | deletion | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-:|:-:|:-:|:-:|:-:|:-:|
| B | ? | - | PRO | deletion | UNP P36544 |
| B | ? | - | PRO | deletion | UNP P36544 |
| B | ? | - | PRO | deletion | UNP P36544 |
| B | ? | - | ALA | deletion | UNP P36544 |
| B | ? | - | SER | deletion | UNP P36544 |
| B | ? | - | ASN | deletion | UNP P36544 |
| B | ? | - | GLY | deletion | UNP P36544 |
| B | ? | - | ASN | deletion | UNP P36544 |
| B | ? | - | LEU | deletion | UNP P36544 |
| B | ? | - | LEU | deletion | UNP P36544 |
| B | ? | - | TYR | deletion | UNP P36544 |
| B | ? | - | ILE | deletion | UNP P36544 |
| B | ? | - | GLY | deletion | UNP P36544 |
| B | ? | - | PHE | deletion | UNP P36544 |
| B | ? | - | ARG | deletion | UNP P36544 |
| B | ? | - | GLY | deletion | UNP P36544 |
| B | ? | - | LEU | deletion | UNP P36544 |
| B | ? | - | ASP | deletion | UNP P36544 |
| B | ? | - | GLY | deletion | UNP P36544 |
| B | ? | - | VAL | deletion | UNP P36544 |
| B | ? | - | HIS | deletion | UNP P36544 |
| B | ? | - | CYS | deletion | UNP P36544 |
| B | ? | - | VAL | deletion | UNP P36544 |
| B | ? | - | PRO | deletion | UNP P36544 |
| B | ? | - | THR | deletion | UNP P36544 |
| B | ? | - | PRO | deletion | UNP P36544 |
| B | ? | - | ASP | deletion | UNP P36544 |
| B | ? | - | SER | deletion | UNP P36544 |
| B | ? | - | GLY | deletion | UNP P36544 |
| B | ? | - | VAL | deletion | UNP P36544 |
| B | ? | - | VAL | deletion | UNP P36544 |
| B | 324B | ALA | - | linker | UNP P36544 |
| B | 324C | GLY | - | linker | UNP P36544 |
| B | 324D | ALA | - | linker | UNP P36544 |
| B | 324E | MET | - | linker | UNP P36544 |
| B | 324L | TRP | MET | conflict | UNP P0ABE7 |
| B | 328C | ILE | HIS | conflict | UNP P0ABE7 |
| B | 328G | LEU | ARG | conflict | UNP P0ABE7 |
| B | 480 | TRP | - | expression tag | UNP P36544 |
| B | 481 | SER | - | expression tag | UNP P36544 |
| B | 482 | HIS | - | expression tag | UNP P36544 |
| B | 483 | PRO | - | expression tag | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| B | 484 | GLN | - | expression tag | UNP P36544 |
| B | 485 | PHE | - | expression tag | UNP P36544 |
| B | 486 | GLU | - | expression tag | UNP P36544 |
| B | 487 | LYS | - | expression tag | UNP P36544 |
| B | 488 | GLY | - | linker | UNP P36544 |
| B | 489 | GLY | - | linker | UNP P36544 |
| B | 490 | GLY | - | linker | UNP P36544 |
| B | 491 | SER | - | linker | UNP P36544 |
| B | 492 | GLY | - | linker | UNP P36544 |
| B | 493 | GLY | - | linker | UNP P36544 |
| B | 494 | GLY | - | linker | UNP P36544 |
| B | 495 | SER | - | linker | UNP P36544 |
| B | 496 | GLY | - | linker | UNP P36544 |
| B | 497 | GLY | - | linker | UNP P36544 |
| B | 498 | SER | - | linker | UNP P36544 |
| B | 499 | SER | - | linker | UNP P36544 |
| B | 500 | ALA | - | linker | UNP P36544 |
| B | 501 | TRP | - | expression tag | UNP P36544 |
| B | 502 | SER | - | expression tag | UNP P36544 |
| B | 503 | HIS | - | expression tag | UNP P36544 |
| B | 504 | PRO | - | expression tag | UNP P36544 |
| B | 505 | GLN | - | expression tag | UNP P36544 |
| B | 506 | PHE | - | expression tag | UNP P36544 |
| B | 507 | GLU | - | expression tag | UNP P36544 |
| B | 508 | LYS | - | expression tag | UNP P36544 |
| B | 509 | GLY | - | linker | UNP P36544 |
| B | 510 | SER | - | linker | UNP P36544 |
| B | 511 | GLY | - | linker | UNP P36544 |
| B | 512 | GLU | - | linker | UNP P36544 |
| B | 513 | GLY | - | linker | UNP P36544 |
| B | 514 | ARG | - | linker | UNP P36544 |
| B | 515 | GLY | - | linker | UNP P36544 |
| B | 516 | SER | - | linker | UNP P36544 |
| B | 517 | LEU | - | linker | UNP P36544 |
| B | 518 | LEU | - | linker | UNP P36544 |
| B | 519 | THR | - | linker | UNP P36544 |
| B | 520 | CYS | - | linker | UNP P36544 |
| B | 521 | GLY | - | linker | UNP P36544 |
| B | 522 | ASP | - | linker | UNP P36544 |
| B | 523 | VAL | - | linker | UNP P36544 |
| B | 524 | GLU | - | linker | UNP P36544 |
| B | 525 | GLU | - | linker | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| B | 526 | ASN | - | linker | UNP P36544 |
| B | 527 | PRO | - | linker | UNP P36544 |
| B | 528 | GLY | - | linker | UNP P36544 |
| C | ? | - | SER | deletion | UNP P36544 |
| C | ? | - | VAL | deletion | UNP P36544 |
| C | ? | - | GLU | deletion | UNP P36544 |
| C | ? | - | MET | deletion | UNP P36544 |
| C | ? | - | SER | deletion | UNP P36544 |
| C | ? | - | ALA | deletion | UNP P36544 |
| C | ? | - | VAL | deletion | UNP P36544 |
| C | ? | - | ALA | deletion | UNP P36544 |
| C | ? | - | PRO | deletion | UNP P36544 |
| C | ? | - | PRO | deletion | UNP P36544 |
| C | ? | - | PRO | deletion | UNP P36544 |
| C | ? | - | ALA | deletion | UNP P36544 |
| C | ? | - | SER | deletion | UNP P36544 |
| C | ? | - | ASN | deletion | UNP P36544 |
| C | ? | - | GLY | deletion | UNP P36544 |
| C | ? | - | ASN | deletion | UNP P36544 |
| C | ? | - | LEU | deletion | UNP P36544 |
| C | ? | - | LEU | deletion | UNP P36544 |
| C | ? | - | TYR | deletion | UNP P36544 |
| C | ? | - | ILE | deletion | UNP P36544 |
| C | ? | - | GLY | deletion | UNP P36544 |
| C | ? | - | PHE | deletion | UNP P36544 |
| C | ? | - | ARG | deletion | UNP P36544 |
| C | ? | - | GLY | deletion | UNP P36544 |
| C | ? | - | LEU | deletion | UNP P36544 |
| C | ? | - | ASP | deletion | UNP P36544 |
| C | ? | - | GLY | deletion | UNP P36544 |
| C | ? | - | VAL | deletion | UNP P36544 |
| C | ? | - | HIS | deletion | UNP P36544 |
| C | ? | - | CYS | deletion | UNP P36544 |
| C | ? | - | VAL | deletion | UNP P36544 |
| C | ? | - | PRO | deletion | UNP P36544 |
| C | ? | - | THR | deletion | UNP P36544 |
| C | ? | - | PRO | deletion | UNP P36544 |
| C | ? | - | ASP | deletion | UNP P36544 |
| C | ? | - | SER | deletion | UNP P36544 |
| C | ? | - | GLY | deletion | UNP P36544 |
| C | ? | - | VAL | deletion | UNP P36544 |
| C | ? | - | VAL | deletion | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| C | 324B | ALA | - | linker | UNP P36544 |
| C | 324C | GLY | - | linker | UNP P36544 |
| C | 324D | ALA | - | linker | UNP P36544 |
| C | 324E | MET | - | linker | UNP P36544 |
| C | 324L | TRP | MET | conflict | UNP P0ABE7 |
| C | 328C | ILE | HIS | conflict | UNP P0ABE7 |
| C | 328G | LEU | ARG | conflict | UNP P0ABE7 |
| C | 480 | TRP | - | expression tag | UNP P36544 |
| C | 481 | SER | - | expression tag | UNP P36544 |
| C | 482 | HIS | - | expression tag | UNP P36544 |
| C | 483 | PRO | - | expression tag | UNP P36544 |
| C | 484 | GLN | - | expression tag | UNP P36544 |
| C | 485 | PHE | - | expression tag | UNP P36544 |
| C | 486 | GLU | - | expression tag | UNP P36544 |
| C | 487 | LYS | - | expression tag | UNP P36544 |
| C | 488 | GLY | - | linker | UNP P36544 |
| C | 489 | GLY | - | linker | UNP P36544 |
| C | 490 | GLY | - | linker | UNP P36544 |
| C | 491 | SER | - | linker | UNP P36544 |
| C | 492 | GLY | - | linker | UNP P36544 |
| C | 493 | GLY | - | linker | UNP P36544 |
| C | 494 | GLY | - | linker | UNP P36544 |
| C | 495 | SER | - | linker | UNP P36544 |
| C | 496 | GLY | - | linker | UNP P36544 |
| C | 497 | GLY | - | linker | UNP P36544 |
| C | 498 | SER | - | linker | UNP P36544 |
| C | 499 | SER | - | linker | UNP P36544 |
| C | 500 | ALA | - | linker | UNP P36544 |
| C | 501 | TRP | - | expression tag | UNP P36544 |
| C | 502 | SER | - | expression tag | UNP P36544 |
| C | 503 | HIS | - | expression tag | UNP P36544 |
| C | 504 | PRO | - | expression tag | UNP P36544 |
| C | 505 | GLN | - | expression tag | UNP P36544 |
| C | 506 | PHE | - | expression tag | UNP P36544 |
| C | 507 | GLU | - | expression tag | UNP P36544 |
| C | 508 | LYS | - | expression tag | UNP P36544 |
| C | 509 | GLY | - | linker | UNP P36544 |
| C | 510 | SER | - | linker | UNP P36544 |
| C | 511 | GLY | - | linker | UNP P36544 |
| C | 512 | GLU | - | linker | UNP P36544 |
| C | 513 | GLY | - | linker | UNP P36544 |
| C | 514 | ARG | - | linker | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| C | 515 | GLY | - | linker | UNP P36544 |
| C | 516 | SER | - | linker | UNP P36544 |
| C | 517 | LEU | - | linker | UNP P36544 |
| C | 518 | LEU | - | linker | UNP P36544 |
| C | 519 | THR | - | linker | UNP P36544 |
| C | 520 | CYS | - | linker | UNP P36544 |
| C | 521 | GLY | - | linker | UNP P36544 |
| C | 522 | ASP | - | linker | UNP P36544 |
| C | 523 | VAL | - | linker | UNP P36544 |
| C | 524 | GLU | - | linker | UNP P36544 |
| C | 525 | GLU | - | linker | UNP P36544 |
| C | 526 | ASN | - | linker | UNP P36544 |
| C | 527 | PRO | - | linker | UNP P36544 |
| C | 528 | GLY | - | linker | UNP P36544 |
| D | ? | - | SER | deletion | UNP P36544 |
| D | ? | - | VAL | deletion | UNP P36544 |
| D | ? | - | GLU | deletion | UNP P36544 |
| D | ? | - | MET | deletion | UNP P36544 |
| D | ? | - | SER | deletion | UNP P36544 |
| D | ? | - | ALA | deletion | UNP P36544 |
| D | ? | - | VAL | deletion | UNP P36544 |
| D | ? | - | ALA | deletion | UNP P36544 |
| D | ? | - | PRO | deletion | UNP P36544 |
| D | ? | - | PRO | deletion | UNP P36544 |
| D | ? | - | PRO | deletion | UNP P36544 |
| D | ? | - | ALA | deletion | UNP P36544 |
| D | ? | - | SER | deletion | UNP P36544 |
| D | ? | - | ASN | deletion | UNP P36544 |
| D | ? | - | GLY | deletion | UNP P36544 |
| D | ? | - | ASN | deletion | UNP P36544 |
| D | ? | - | LEU | deletion | UNP P36544 |
| D | ? | - | LEU | deletion | UNP P36544 |
| D | ? | - | TYR | deletion | UNP P36544 |
| D | ? | - | ILE | deletion | UNP P36544 |
| D | ? | - | GLY | deletion | UNP P36544 |
| D | ? | - | PHE | deletion | UNP P36544 |
| D | ? | - | ARG | deletion | UNP P36544 |
| D | ? | - | GLY | deletion | UNP P36544 |
| D | ? | - | LEU | deletion | UNP P36544 |
| D | ? | - | ASP | deletion | UNP P36544 |
| D | ? | - | GLY | deletion | UNP P36544 |
| D | ? | - | VAL | deletion | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| D | ? | - | HIS | deletion | UNP P36544 |
| D | ? | - | CYS | deletion | UNP P36544 |
| D | ? | - | VAL | deletion | UNP P36544 |
| D | ? | - | PRO | deletion | UNP P36544 |
| D | ? | - | THR | deletion | UNP P36544 |
| D | ? | - | PRO | deletion | UNP P36544 |
| D | ? | - | ASP | deletion | UNP P36544 |
| D | ? | - | SER | deletion | UNP P36544 |
| D | ? | - | GLY | deletion | UNP P36544 |
| D | ? | - | VAL | deletion | UNP P36544 |
| D | ? | - | VAL | deletion | UNP P36544 |
| D | 324B | ALA | - | linker | UNP P36544 |
| D | 324C | GLY | - | linker | UNP P36544 |
| D | 324D | ALA | - | linker | UNP P36544 |
| D | 324E | MET | - | linker | UNP P36544 |
| D | 324L | TRP | MET | conflict | UNP P0ABE7 |
| D | 328C | ILE | HIS | conflict | UNP P0ABE7 |
| D | 328G | LEU | ARG | conflict | UNP P0ABE7 |
| D | 480 | TRP | - | expression tag | UNP P36544 |
| D | 481 | SER | - | expression tag | UNP P36544 |
| D | 482 | HIS | - | expression tag | UNP P36544 |
| D | 483 | PRO | - | expression tag | UNP P36544 |
| D | 484 | GLN | - | expression tag | UNP P36544 |
| D | 485 | PHE | - | expression tag | UNP P36544 |
| D | 486 | GLU | - | expression tag | UNP P36544 |
| D | 487 | LYS | - | expression tag | UNP P36544 |
| D | 488 | GLY | - | linker | UNP P36544 |
| D | 489 | GLY | - | linker | UNP P36544 |
| D | 490 | GLY | - | linker | UNP P36544 |
| D | 491 | SER | - | linker | UNP P36544 |
| D | 492 | GLY | - | linker | UNP P36544 |
| D | 493 | GLY | - | linker | UNP P36544 |
| D | 494 | GLY | - | linker | UNP P36544 |
| D | 495 | SER | - | linker | UNP P36544 |
| D | 496 | GLY | - | linker | UNP P36544 |
| D | 497 | GLY | - | linker | UNP P36544 |
| D | 498 | SER | - | linker | UNP P36544 |
| D | 499 | SER | - | linker | UNP P36544 |
| D | 500 | ALA | - | linker | UNP P36544 |
| D | 501 | TRP | - | expression tag | UNP P36544 |
| D | 502 | SER | - | expression tag | UNP P36544 |
| D | 503 | HIS | - | expression tag | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-----:|:-------:|:--------:|:------:|:-------:|:---------:|
| D | 504 | PRO | - | expression tag | UNP P36544 |
| D | 505 | GLN | - | expression tag | UNP P36544 |
| D | 506 | PHE | - | expression tag | UNP P36544 |
| D | 507 | GLU | - | expression tag | UNP P36544 |
| D | 508 | LYS | - | expression tag | UNP P36544 |
| D | 509 | GLY | - | linker | UNP P36544 |
| D | 510 | SER | - | linker | UNP P36544 |
| D | 511 | GLY | - | linker | UNP P36544 |
| D | 512 | GLU | - | linker | UNP P36544 |
| D | 513 | GLY | - | linker | UNP P36544 |
| D | 514 | ARG | - | linker | UNP P36544 |
| D | 515 | GLY | - | linker | UNP P36544 |
| D | 516 | SER | - | linker | UNP P36544 |
| D | 517 | LEU | - | linker | UNP P36544 |
| D | 518 | LEU | - | linker | UNP P36544 |
| D | 519 | THR | - | linker | UNP P36544 |
| D | 520 | CYS | - | linker | UNP P36544 |
| D | 521 | GLY | - | linker | UNP P36544 |
| D | 522 | ASP | - | linker | UNP P36544 |
| D | 523 | VAL | - | linker | UNP P36544 |
| D | 524 | GLU | - | linker | UNP P36544 |
| D | 525 | GLU | - | linker | UNP P36544 |
| D | 526 | ASN | - | linker | UNP P36544 |
| D | 527 | PRO | - | linker | UNP P36544 |
| D | 528 | GLY | - | linker | UNP P36544 |
| E | ? | - | SER | deletion | UNP P36544 |
| E | ? | - | VAL | deletion | UNP P36544 |
| E | ? | - | GLU | deletion | UNP P36544 |
| E | ? | - | MET | deletion | UNP P36544 |
| E | ? | - | SER | deletion | UNP P36544 |
| E | ? | - | ALA | deletion | UNP P36544 |
| E | ? | - | VAL | deletion | UNP P36544 |
| E | ? | - | ALA | deletion | UNP P36544 |
| E | ? | - | PRO | deletion | UNP P36544 |
| E | ? | - | PRO | deletion | UNP P36544 |
| E | ? | - | PRO | deletion | UNP P36544 |
| E | ? | - | ALA | deletion | UNP P36544 |
| E | ? | - | SER | deletion | UNP P36544 |
| E | ? | - | ASN | deletion | UNP P36544 |
| E | ? | - | GLY | deletion | UNP P36544 |
| E | ? | - | ASN | deletion | UNP P36544 |
| E | ? | - | LEU | deletion | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-:|:-:|:-:|:-:|:-:|:-:|
| E | ? | - | LEU | deletion | UNP P36544 |
| E | ? | - | TYR | deletion | UNP P36544 |
| E | ? | - | ILE | deletion | UNP P36544 |
| E | ? | - | GLY | deletion | UNP P36544 |
| E | ? | - | PHE | deletion | UNP P36544 |
| E | ? | - | ARG | deletion | UNP P36544 |
| E | ? | - | GLY | deletion | UNP P36544 |
| E | ? | - | LEU | deletion | UNP P36544 |
| E | ? | - | ASP | deletion | UNP P36544 |
| E | ? | - | GLY | deletion | UNP P36544 |
| E | ? | - | VAL | deletion | UNP P36544 |
| E | ? | - | HIS | deletion | UNP P36544 |
| E | ? | - | CYS | deletion | UNP P36544 |
| E | ? | - | VAL | deletion | UNP P36544 |
| E | ? | - | PRO | deletion | UNP P36544 |
| E | ? | - | THR | deletion | UNP P36544 |
| E | ? | - | PRO | deletion | UNP P36544 |
| E | ? | - | ASP | deletion | UNP P36544 |
| E | ? | - | SER | deletion | UNP P36544 |
| E | ? | - | GLY | deletion | UNP P36544 |
| E | ? | - | VAL | deletion | UNP P36544 |
| E | ? | - | VAL | deletion | UNP P36544 |
| E | 324B | ALA | - | linker | UNP P36544 |
| E | 324C | GLY | - | linker | UNP P36544 |
| E | 324D | ALA | - | linker | UNP P36544 |
| E | 324E | MET | - | linker | UNP P36544 |
| E | 324L | TRP | MET | conflict | UNP P0ABE7 |
| E | 328C | ILE | HIS | conflict | UNP P0ABE7 |
| E | 328G | LEU | ARG | conflict | UNP P0ABE7 |
| E | 480 | TRP | - | expression tag | UNP P36544 |
| E | 481 | SER | - | expression tag | UNP P36544 |
| E | 482 | HIS | - | expression tag | UNP P36544 |
| E | 483 | PRO | - | expression tag | UNP P36544 |
| E | 484 | GLN | - | expression tag | UNP P36544 |
| E | 485 | PHE | - | expression tag | UNP P36544 |
| E | 486 | GLU | - | expression tag | UNP P36544 |
| E | 487 | LYS | - | expression tag | UNP P36544 |
| E | 488 | GLY | - | linker | UNP P36544 |
| E | 489 | GLY | - | linker | UNP P36544 |
| E | 490 | GLY | - | linker | UNP P36544 |
| E | 491 | SER | - | linker | UNP P36544 |
| E | 492 | GLY | - | linker | UNP P36544 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| E | 493 | GLY | - | linker | UNP P36544 |
| E | 494 | GLY | - | linker | UNP P36544 |
| E | 495 | SER | - | linker | UNP P36544 |
| E | 496 | GLY | - | linker | UNP P36544 |
| E | 497 | GLY | - | linker | UNP P36544 |
| E | 498 | SER | - | linker | UNP P36544 |
| E | 499 | SER | - | linker | UNP P36544 |
| E | 500 | ALA | - | linker | UNP P36544 |
| E | 501 | TRP | - | expression tag | UNP P36544 |
| E | 502 | SER | - | expression tag | UNP P36544 |
| E | 503 | HIS | - | expression tag | UNP P36544 |
| E | 504 | PRO | - | expression tag | UNP P36544 |
| E | 505 | GLN | - | expression tag | UNP P36544 |
| E | 506 | PHE | - | expression tag | UNP P36544 |
| E | 507 | GLU | - | expression tag | UNP P36544 |
| E | 508 | LYS | - | expression tag | UNP P36544 |
| E | 509 | GLY | - | linker | UNP P36544 |
| E | 510 | SER | - | linker | UNP P36544 |
| E | 511 | GLY | - | linker | UNP P36544 |
| E | 512 | GLU | - | linker | UNP P36544 |
| E | 513 | GLY | - | linker | UNP P36544 |
| E | 514 | ARG | - | linker | UNP P36544 |
| E | 515 | GLY | - | linker | UNP P36544 |
| E | 516 | SER | - | linker | UNP P36544 |
| E | 517 | LEU | - | linker | UNP P36544 |
| E | 518 | LEU | - | linker | UNP P36544 |
| E | 519 | THR | - | linker | UNP P36544 |
| E | 520 | CYS | - | linker | UNP P36544 |
| E | 521 | GLY | - | linker | UNP P36544 |
| E | 522 | ASP | - | linker | UNP P36544 |
| E | 523 | VAL | - | linker | UNP P36544 |
| E | 524 | GLU | - | linker | UNP P36544 |
| E | 525 | GLU | - | linker | UNP P36544 |
| E | 526 | ASN | - | linker | UNP P36544 |
| E | 527 | PRO | - | linker | UNP P36544 |
| E | 528 | GLY | - | linker | UNP P36544 |

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
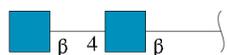
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|---|----|---------|-------|
| 2 | F | 2 | Total | C | H | N | O | 0 | 0 |
|   |   |   | 53 | 16 | 25 | 2 | 10 |   |   |
| 2 | G | 2 | Total | C | H | N | O | 0 | 0 |
|   |   |   | 52 | 16 | 24 | 2 | 10 |   |   |
| 2 | H | 2 | Total | C | H | N | O | 0 | 0 |
|   |   |   | 52 | 16 | 24 | 2 | 10 |   |   |
| 2 | I | 2 | Total | C | H | N | O | 0 | 0 |
|   |   |   | 52 | 16 | 24 | 2 | 10 |   |   |
| 2 | J | 2 | Total | C | H | N | O | 0 | 0 |
|   |   |   | 52 | 16 | 24 | 2 | 10 |   |   |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
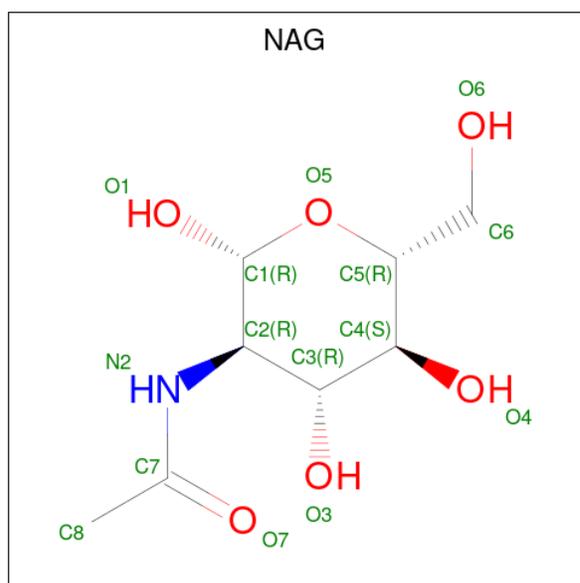


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|
| 3 | A | 1 | Total | C | H | N | O | 0 |
|   |   |   | 27 | 8 | 13 | 1 | 5 |   |
| 3 | A | 1 | Total | C | H | N | O | 0 |
|   |   |   | 27 | 8 | 13 | 1 | 5 |   |
| 3 | B | 1 | Total | C | H | N | O | 0 |
|   |   |   | 27 | 8 | 13 | 1 | 5 |   |
| 3 | B | 1 | Total | C | H | N | O | 0 |
|   |   |   | 26 | 8 | 12 | 1 | 5 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 1 | Total | C | H | N | O | | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | | |
| 3 | C | 1 | Total | C | H | N | O | | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | | |
| 3 | D | 1 | Total | C | H | N | O | | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | | |
| 3 | D | 1 | Total | C | H | N | O | | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | | |
| 3 | E | 1 | Total | C | H | N | O | | 0 |
| | | | 27 | 8 | 13 | 1 | 5 | | |
| 3 | E | 1 | Total | C | H | N | O | | 0 |
| | | | 26 | 8 | 12 | 1 | 5 | | |

- Molecule 4 is EPIBATIDINE (three-letter code: EPJ) (formula: $C_{11}H_{13}ClN_2$) (labeled as "Ligand of Interest" by depositor).



EPJ
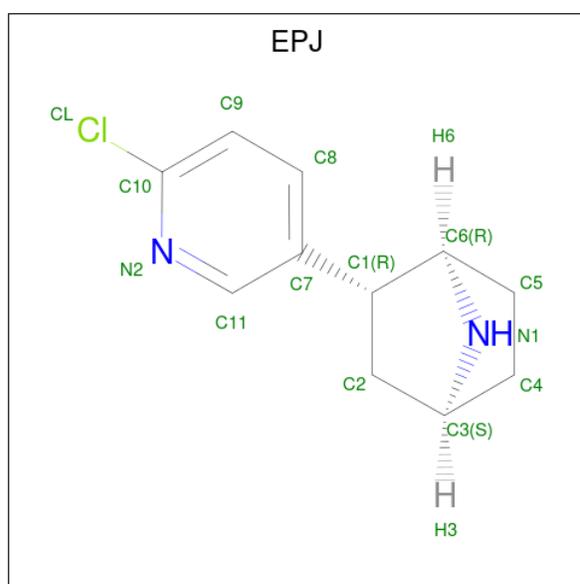
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | C | Cl | H | N | 0 |
| | | | 27 | 11 | 1 | 13 | 2 | |
| 4 | B | 1 | Total | C | Cl | H | N | 0 |
| | | | 27 | 11 | 1 | 13 | 2 | |
| 4 | C | 1 | Total | C | Cl | H | N | 0 |
| | | | 27 | 11 | 1 | 13 | 2 | |
| 4 | D | 1 | Total | C | Cl | H | N | 0 |
| | | | 27 | 11 | 1 | 13 | 2 | |
| 4 | E | 1 | Total | C | Cl | H | N | 0 |
| | | | 27 | 11 | 1 | 13 | 2 | |

- Molecule 5 is N-(5-Chloro-2,4-dimethoxyphenyl)-N'-(5-methyl-3-isoxazolyl)-urea (three-letter code: I34) (formula: $C_{13}H_{14}ClN_3O_4$) (labeled as "Ligand of Interest" by depositor).
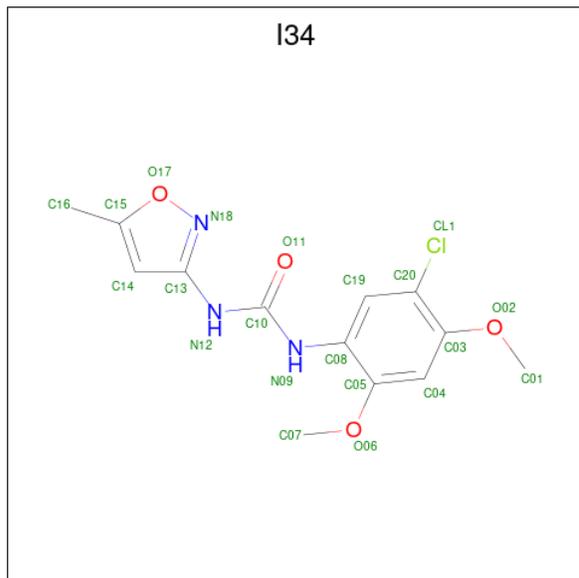


| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|----|----|----|---|---|---------|
| 5 | A | 1 | Total | C | Cl | H | N | O | 0 |
|   |   |   | 35 | 13 | 1 | 14 | 3 | 4 | |
| 5 | B | 1 | Total | C | Cl | H | N | O | 0 |
|   |   |   | 35 | 13 | 1 | 14 | 3 | 4 | |
| 5 | C | 1 | Total | C | Cl | H | N | O | 0 |
|   |   |   | 35 | 13 | 1 | 14 | 3 | 4 | |
| 5 | D | 1 | Total | C | Cl | H | N | O | 0 |
|   |   |   | 35 | 13 | 1 | 14 | 3 | 4 | |
| 5 | D | 1 | Total | C | Cl | H | N | O | 0 |
|   |   |   | 35 | 13 | 1 | 14 | 3 | 4 | |

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 6 | B | 1 | Total | Ca | 0 |
|   |   |   | 1 | 1 | |
| 6 | C | 1 | Total | Ca | 0 |
|   |   |   | 1 | 1 | |
| 6 | D | 1 | Total | Ca | 0 |
|   |   |   | 1 | 1 | |

# 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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562



• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562

• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562

Chain C:

56%    7%    37%

E1 S33 L34 L37 Q38 I39 E44 W54 D96 E97 R98 S111 H114 C115 Q116 I129 D130 V131 F134 N170 E188 C189 C190 K191 E192 Y209 Y210 N213 S222 A223 L224 A225 L226 V245 S248 F252 M253 M260 P268 F274

H295 W307 W315 F319 L320 R321 M322 K323 ARG PRO GLY GLU ASP LYS VAL ARG PRO ALA CYS GLN HIS LYS GLN ARG ARG CYS SER LEU ALA CYS GLY ARG MET ALA ALA GLY ALA GLN LYS SER ALA THR PRO PRO LYS GLU LEU ASP LYS SER PRO ASP ASN TRP GLU THR LEU ASN ASP LEU LYS VAL ILE

GLU LYS ALA ASP ASN ALA ALA GLN VAL LYS ASP ALA LEU THR LYS MET ARG ALA ALA ALA LEU ASP ALA GLN LYS ALA ALA GLU GLN LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU SER PRO THR HIS ASP HIS HIS LEU HIS GLY GLN PRO GLU GLY ASP ASP ASP LEU LYS LEU LEU GLU ILE ASP ALA LEU LYS

LEU ALA ASN GLY LYS LYS GLU GLU ALA GLN GLU ALA LEU LEU LYS THR THR ARG ASN ALA TYR ILE GLN LYS TYR LEU SER PRO THR HIS ASP HIS HIS LEU HIS GLY GLN PRO GLU GLY ASP ASP ASP LEU LYS LEU LEU GLU ILE ASP ALA LEU LYS

ALA ASN ARG PHE R425 C426 Q427 A432 S435 K438 C459 T460 F478 ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS SER GLY GLY ARG GLY SER LEU GLU THR CYS

GLY ASP VAL GLU GLU ASN PRO GLY

• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562

Chain D:

59%    •    37%

E1 E18 I39 E44 Q47 H114 C115 Q116 E161 N170 D174 L175 V176 G177 I178 C190 K191 T202 M203 R204 A225 V245 L246 L247 M253 A275 V291 W307 I311 C316 L320 R321 M322 K323 ARG PRO GLY GLU ASP LYS VAL

ARG PRO ALA CYS GLN HIS LYS GLN ARG ARG CYS SER LEU ALA CYS GLY ARG MET ALA ALA GLY ALA GLN LYS SER ALA THR PRO PRO LYS GLU LEU ASP LYS SER PRO ASP ASN TRP GLU THR LEU ASN ASP LEU LYS MET ARG ALA ALA ALA

ALA LEU ASP ALA GLN LYS ALA THR PRO PRO LYS GLU LEU ASP LYS SER PRO ASP SER PRO GLU MET LYS ASP PHE ARG HIS GLY PHE ASP ILE LEU VAL GLY GLN ILE ASP ASP ALA LEU LYS LEU ALA ASN ALA ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA ALA GLU GLN LEU LYS THR

THR ARG ASN ALA TYR ILE GLN LYS TYR LEU SER PRO THR HIS ASP HIS LEU HIS GLY PHE ASP ILE LEU VAL GLY GLN ILE ASP ASP ALA LEU LYS LEU ALA ASN ALA ASN ARG F424 R425 A441 D445 F478 ALA TRP SER HIS PRO GLN PHE GLU

LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS SER GLY GLY ARG GLY SER LEU GLU THR CYS GLY ASP VAL GLU GLU ASN PRO GLY

• Molecule 1: Neuronal acetylcholine receptor subunit alpha-7,Soluble cytochrome b562

Chain E:

60%    •    37%

E1 R4 E18 S33 L34 I39 Y63 H114 C115 Q116 E161 N170 E188 K191 L247 S248 L254 E258 D265 V289 L292 Q293 Y294 H295 P305 K306 W307 R321 M322 K323 ARG PRO GLY GLU ASP LYS VAL ARG PRO ALA CYS GLN

HIS LYS GLN ARG ARG CYS SER LEU ALA CYS GLY ARG MET ALA CYS ALA GLY ALA MET ALA ASP GLU LEU ASP ASN TRP GLU THR LEU ASN ASP LEU LYS VAL ILE GLU LYS ALA ASP ASN ALA ALA GLN VAL LYS ASP ALA LEU THR LYS MET ARG ALA ALA ALA LEU ASP ASP ALA GLN

LYS ALA THR PRO LYS LEU GLU ASP LYS SER PRO ASP SER PRO GLU MET LYS ASP PHE ARG HIS GLY PHE ASP ILE LEU VAL GLY ILE ASP ASP ALA LEU LYS LEU ALA ASN ASN GLU GLY LYS VAL LYS GLU ALA GLN ALA ALA ALA GLU GLN GLU LEU LYS THR THR ARG ASN ALA TYR

ILE GLN LYS TYR LEU SER PRO THR HIS ASP GLU HIS LEU LEU HIS GLY GLY GLN PRO PRO GLU GLU ASP PRO ASP LEU ALA LYS ILE LEU GLU GLU VAL ARG TYR ILE ALA ASN ARG **F424** GLU GLY LYS VAL LYS **D428** **E431** GLU ALA GLN ALA **S435** ALA ALA GLU GLU **K438** GLU LEU LYS THR THR ARG ASN ALA TYR **F478** ALA TRP SER HIS PRO GLN PHE GLU LYS GLY

GLY GLY SER GLY GLY GLY SER GLY GLY SER SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLU GLY ARG GLY SER LEU LEU THR CYS GLY ASP VAL GLU GLU ASN PRO GLY

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

50%  50%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

50%  50%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

50%  50%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

50%  50%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

50%  50%

NAG1 NAG2

# 4   Experimental information  ⓘ

| Property | Value | Source |
| --- | --- | --- |
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 33508 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $(e^-/\text{Å}^2)$ | 40 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 1.034 | Depositor |
| Minimum map value | -0.190 | Depositor |
| Average map value | 0.006 | Depositor |
| Map value standard deviation | 0.021 | Depositor |
| Recommended contour level | 0.097 | Depositor |
| Map size (Å) | 277.19998, 277.19998, 277.19998 | wwPDB |
| Map dimensions | 336, 336, 336 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8249999, 0.8249999, 0.8249999 | Depositor |

# 5   Model quality ⓘ

## 5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I34, EPJ, NAG, CA

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     | 0.34 | 0/3133  | 0.65 | 0/4269  |
| 1   | B     | 0.35 | 0/3122  | 0.64 | 0/4255  |
| 1   | C     | 0.35 | 0/3133  | 0.66 | 0/4269  |
| 1   | D     | 0.35 | 0/3145  | 0.63 | 0/4285  |
| 1   | E     | 0.32 | 0/3145  | 0.60 | 0/4285  |
| All | All   | 0.34 | 0/15678 | 0.64 | 0/21363 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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     | 3044  | 3016     | 3021     | 27      | 0            |
| 1   | B     | 3033  | 3003     | 3008     | 33      | 0            |
| 1   | C     | 3044  | 3016     | 3021     | 45      | 0            |
| 1   | D     | 3055  | 3025     | 3030     | 21      | 0            |
| 1   | E     | 3055  | 3025     | 3030     | 25      | 0            |
| 2   | F     | 28    | 25       | 25       | 2       | 0            |
| 2   | G     | 28    | 24       | 25       | 2       | 0            |
| 2   | H     | 28    | 24       | 25       | 2       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | I | 28 | 24 | 25 | 2 | 0 |
| 2 | J | 28 | 24 | 25 | 3 | 0 |
| 3 | A | 28 | 26 | 26 | 0 | 0 |
| 3 | B | 28 | 25 | 26 | 0 | 0 |
| 3 | C | 28 | 25 | 26 | 0 | 0 |
| 3 | D | 28 | 25 | 26 | 0 | 0 |
| 3 | E | 28 | 25 | 26 | 0 | 0 |
| 4 | A | 14 | 13 | 13 | 0 | 0 |
| 4 | B | 14 | 13 | 13 | 0 | 0 |
| 4 | C | 14 | 13 | 13 | 0 | 0 |
| 4 | D | 14 | 13 | 13 | 0 | 0 |
| 4 | E | 14 | 13 | 13 | 0 | 0 |
| 5 | A | 21 | 14 | 0 | 0 | 0 |
| 5 | B | 21 | 14 | 0 | 0 | 0 |
| 5 | C | 21 | 14 | 0 | 4 | 0 |
| 5 | D | 42 | 28 | 0 | 4 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 6 | C | 1 | 0 | 0 | 0 | 0 |
| 6 | D | 1 | 0 | 0 | 0 | 0 |
| All | All | 15689 | 15467 | 15430 | 133 | 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 4.

All (133) 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:C:37:LEU:HD21 | 1:C:54:TRP:CZ2 | 1.83 | 1.13 |
| 1:C:44:GLU:HA | 1:C:129:ILE:CD1 | 2.01 | 0.90 |
| 1:C:44:GLU:HA | 1:C:129:ILE:HD12 | 1.57 | 0.86 |
| 1:B:44:GLU:HA | 1:B:129:ILE:CD1 | 2.07 | 0.85 |
| 1:A:243:ILE:O | 1:A:247:LEU:HD13 | 1.80 | 0.81 |
| 1:B:253:MET:HE2 | 5:C:601:I34:C10 | 2.12 | 0.79 |
| 1:E:305:PRO:CB | 1:E:307:TRP:NE1 | 2.45 | 0.79 |
| 1:B:308:THR:CG2 | 1:B:312:LEU:HD12 | 2.13 | 0.78 |
| 1:B:246:LEU:HD23 | 1:C:224:LEU:HD21 | 1.67 | 0.77 |
| 1:B:308:THR:HG23 | 1:B:312:LEU:HD12 | 1.67 | 0.76 |
| 1:B:190:CYS:SG | 1:C:116:GLN:NE2 | 2.60 | 0.74 |
| 1:A:137:ASP:OD2 | 1:A:139:GLN:NE2 | 2.20 | 0.74 |
| 1:C:37:LEU:CD2 | 1:C:54:TRP:CZ2 | 2.67 | 0.74 |
| 1:C:253:MET:SD | 1:C:274:PHE:HB3 | 2.29 | 0.73 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:37:LEU:HD21 | 1:C:54:TRP:CE2 | 2.24 | 0.72 |
| 1:B:44:GLU:HA | 1:B:129:ILE:HD13 | 1.74 | 0.70 |
| 1:B:253:MET:SD | 1:B:274:PHE:HB3 | 2.32 | 0.70 |
| 1:C:44:GLU:CB | 1:C:129:ILE:HD13 | 2.22 | 0.70 |
| 1:B:253:MET:SD | 1:B:274:PHE:CB | 2.81 | 0.69 |
| 1:E:305:PRO:HB3 | 1:E:307:TRP:NE1 | 2.07 | 0.68 |
| 1:A:178:ILE:HD12 | 1:A:201:VAL:HG22 | 1.76 | 0.68 |
| 1:C:190:CYS:SG | 1:D:116:GLN:NE2 | 2.67 | 0.67 |
| 1:D:253:MET:SD | 5:D:606:I34:C10 | 2.83 | 0.67 |
| 1:A:228:VAL:HG22 | 1:A:241:LEU:HD23 | 1.77 | 0.66 |
| 1:B:253:MET:CE | 5:C:601:I34:C10 | 2.75 | 0.65 |
| 1:D:178:ILE:HG23 | 1:D:178:ILE:O | 1.96 | 0.64 |
| 1:E:305:PRO:HB2 | 1:E:307:TRP:NE1 | 2.10 | 0.64 |
| 1:C:222:SER:O | 1:C:226:LEU:HD13 | 1.97 | 0.64 |
| 1:C:253:MET:SD | 1:C:274:PHE:CB | 2.86 | 0.64 |
| 1:D:176:VAL:HB | 1:D:202:THR:HG22 | 1.80 | 0.62 |
| 1:C:44:GLU:HB3 | 1:C:129:ILE:HD13 | 1.82 | 0.61 |
| 1:A:244:THR:HG22 | 1:E:247:LEU:CD1 | 2.30 | 0.61 |
| 1:B:262:ALA:HB1 | 1:C:209:TYR:CE2 | 2.35 | 0.61 |
| 1:C:37:LEU:CD2 | 1:C:54:TRP:CE2 | 2.83 | 0.60 |
| 1:B:129:ILE:HG22 | 1:B:131:VAL:HG13 | 1.84 | 0.59 |
| 1:E:39:ILE:O | 1:E:170:ASN:ND2 | 2.34 | 0.59 |
| 1:C:39:ILE:O | 1:C:170:ASN:ND2 | 2.36 | 0.59 |
| 1:C:44:GLU:CA | 1:C:129:ILE:CD1 | 2.78 | 0.58 |
| 1:D:174:ASP:OD2 | 1:D:204:ARG:NH2 | 2.35 | 0.58 |
| 1:B:212:LEU:HD23 | 1:B:216:ILE:HD12 | 1.85 | 0.57 |
| 1:A:178:ILE:HG23 | 1:A:178:ILE:O | 2.04 | 0.57 |
| 1:C:222:SER:O | 1:C:226:LEU:CD1 | 2.52 | 0.57 |
| 1:A:137:ASP:OD1 | 1:A:137:ASP:N | 2.37 | 0.56 |
| 1:B:114[A]:HIS:ND1 | 2:G:1:NAG:H5 | 2.19 | 0.56 |
| 1:C:114[A]:HIS:ND1 | 2:H:1:NAG:H5 | 2.19 | 0.56 |
| 1:E:265:ASP:O | 1:E:265:ASP:OD1 | 2.23 | 0.56 |
| 1:B:97:GLU:OE2 | 1:C:98:ARG:CZ | 2.54 | 0.56 |
| 1:C:432:ALA:O | 1:C:435:SER:OG | 2.20 | 0.56 |
| 1:D:247:LEU:HD13 | 1:E:248:SER:HB2 | 1.88 | 0.56 |
| 1:E:305:PRO:CB | 1:E:307:TRP:CD1 | 2.89 | 0.55 |
| 1:A:42:VAL:HG22 | 1:A:49:LEU:CD1 | 2.37 | 0.55 |
| 1:E:305:PRO:HB3 | 1:E:307:TRP:HE1 | 1.71 | 0.55 |
| 1:B:253:MET:CE | 5:C:601:I34:N12 | 2.70 | 0.55 |
| 1:D:321:ARG:HG3 | 1:D:321:ARG:O | 2.08 | 0.54 |
| 1:A:178:ILE:CD1 | 1:A:201:VAL:HG22 | 2.38 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:246:LEU:HD12 | 1:B:278:MET:HG3 | 1.89 | 0.54 |
| 1:E:305:PRO:HB2 | 1:E:307:TRP:CD1 | 2.43 | 0.54 |
| 1:A:100:ASP:CG | 1:A:102:THR:HG22 | 2.29 | 0.53 |
| 1:B:308:THR:HG23 | 1:B:312:LEU:CD1 | 2.37 | 0.53 |
| 1:A:114[A]:HIS:ND1 | 2:F:1:NAG:H5 | 2.24 | 0.53 |
| 1:B:39:ILE:O | 1:B:170:ASN:ND2 | 2.41 | 0.53 |
| 1:D:253:MET:SD | 5:D:606:I34:N09 | 2.81 | 0.53 |
| 1:B:253:MET:SD | 1:B:274:PHE:HB2 | 2.47 | 0.53 |
| 1:D:176:VAL:HB | 1:D:202:THR:CG2 | 2.38 | 0.52 |
| 1:C:44:GLU:CA | 1:C:129:ILE:HD12 | 2.36 | 0.52 |
| 1:B:262:ALA:CB | 1:C:209:TYR:CE2 | 2.92 | 0.52 |
| 1:C:37:LEU:HD21 | 1:C:54:TRP:CH2 | 2.40 | 0.52 |
| 1:B:97:GLU:OE2 | 1:C:98:ARG:NE | 2.43 | 0.52 |
| 1:A:262:ALA:O | 1:B:172:GLU:HB2 | 2.11 | 0.51 |
| 1:C:44:GLU:CB | 1:C:129:ILE:CD1 | 2.88 | 0.51 |
| 1:D:291:VAL:HG13 | 1:D:441:ALA:HB1 | 1.93 | 0.51 |
| 1:E:114[B]:HIS:CE1 | 2:J:1:NAG:H62 | 2.46 | 0.51 |
| 1:E:295:HIS:CD2 | 1:E:438:LYS:HG2 | 2.46 | 0.50 |
| 1:D:291:VAL:CG1 | 1:D:441:ALA:HB1 | 2.41 | 0.50 |
| 1:A:431:GLU:O | 1:A:435:SER:N | 2.41 | 0.50 |
| 1:C:111:SER:OG | 2:H:1:NAG:H82 | 2.12 | 0.50 |
| 1:C:427:GLN:OE1 | 1:C:427:GLN:N | 2.43 | 0.50 |
| 1:C:320:LEU:O | 1:C:321:ARG:HG2 | 2.12 | 0.50 |
| 1:B:111:SER:OG | 2:G:1:NAG:H82 | 2.12 | 0.49 |
| 1:D:114[A]:HIS:ND1 | 2:I:1:NAG:H5 | 2.28 | 0.49 |
| 1:E:305:PRO:HB3 | 1:E:307:TRP:CD1 | 2.47 | 0.49 |
| 1:B:246:LEU:HD23 | 1:C:224:LEU:CD2 | 2.41 | 0.49 |
| 1:D:114[B]:HIS:CE1 | 2:I:1:NAG:H62 | 2.48 | 0.49 |
| 1:B:44:GLU:HA | 1:B:129:ILE:HD12 | 1.93 | 0.48 |
| 1:C:253:MET:HE2 | 5:D:601:I34:C10 | 2.43 | 0.48 |
| 1:A:132:ARG:O | 1:A:132:ARG:NH1 | 2.42 | 0.48 |
| 1:A:243:ILE:O | 1:A:247:LEU:CD1 | 2.57 | 0.48 |
| 1:B:262:ALA:HB1 | 1:C:209:TYR:CD2 | 2.48 | 0.48 |
| 1:B:238:LYS:HB3 | 1:B:288:THR:HG21 | 1.95 | 0.47 |
| 1:E:114[B]:HIS:ND1 | 2:J:1:NAG:H62 | 2.28 | 0.47 |
| 1:C:260:MET:HE2 | 1:C:268:PRO:HG2 | 1.96 | 0.47 |
| 1:E:114[A]:HIS:ND1 | 2:J:1:NAG:H5 | 2.30 | 0.47 |
| 1:C:245:VAL:O | 1:C:248:SER:OG | 2.28 | 0.46 |
| 1:E:305:PRO:CB | 1:E:307:TRP:HE1 | 2.27 | 0.46 |
| 1:A:230:LEU:O | 1:E:293:GLN:NE2 | 2.48 | 0.46 |
| 1:E:431:GLU:O | 1:E:435:SER:N | 2.45 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:33:SER:OG | 1:B:34:LEU:N | 2.48 | 0.46 |
| 1:C:323:LYS:N | 1:C:323:LYS:HD2 | 2.31 | 0.45 |
| 1:B:322:MET:O | 1:B:323:LYS:HB3 | 2.16 | 0.45 |
| 1:C:131:VAL:HB | 1:C:260:MET:HE3 | 1.98 | 0.45 |
| 1:C:33:SER:OG | 1:C:34:LEU:N | 2.50 | 0.45 |
| 1:E:33:SER:OG | 1:E:34:LEU:N | 2.50 | 0.45 |
| 1:D:316:CYS:O | 1:D:320:LEU:HD13 | 2.17 | 0.45 |
| 1:E:18:GLU:OE2 | 1:E:63:TYR:OH | 2.25 | 0.44 |
| 1:C:131:VAL:HB | 1:C:260:MET:CE | 2.48 | 0.44 |
| 1:D:39:ILE:O | 1:D:170:ASN:ND2 | 2.51 | 0.44 |
| 1:D:291:VAL:HG13 | 1:D:441:ALA:CB | 2.47 | 0.43 |
| 1:A:323:LYS:N | 1:A:323:LYS:HD2 | 2.32 | 0.43 |
| 1:C:134:PHE:CZ | 1:C:210:TYR:CE2 | 3.07 | 0.43 |
| 1:B:308:THR:HG22 | 1:B:312:LEU:HD12 | 1.94 | 0.43 |
| 1:D:18:GLU:OE1 | 1:E:4:ARG:NE | 2.50 | 0.43 |
| 1:A:244:THR:HG22 | 1:E:247:LEU:HD12 | 2.01 | 0.43 |
| 1:D:275:ALA:HB2 | 5:D:606:I34:C14 | 2.49 | 0.43 |
| 1:D:190:CYS:SG | 1:E:116:GLN:NE2 | 2.92 | 0.42 |
| 1:B:129:ILE:HG22 | 1:B:131:VAL:CG1 | 2.47 | 0.42 |
| 1:C:295:HIS:CE1 | 1:C:438:LYS:HE2 | 2.55 | 0.42 |
| 1:D:44:GLU:O | 1:D:47:GLN:NE2 | 2.50 | 0.42 |
| 1:A:34:LEU:HD11 | 1:A:178:ILE:CD1 | 2.50 | 0.42 |
| 1:A:231:LEU:HA | 1:E:289:VAL:HG13 | 2.01 | 0.42 |
| 1:C:459:CYS:SG | 1:C:460:THR:N | 2.93 | 0.41 |
| 1:A:132:ARG:HD3 | 1:A:266:SER:HB2 | 2.02 | 0.41 |
| 1:C:209:TYR:O | 1:C:213:ASN:ND2 | 2.50 | 0.41 |
| 1:A:114[B]:HIS:CD2 | 2:F:1:NAG:H62 | 2.55 | 0.41 |
| 1:C:260:MET:HE2 | 1:C:268:PRO:CG | 2.51 | 0.41 |
| 1:A:9:GLU:OE1 | 1:A:71:TYR:OH | 2.39 | 0.41 |
| 1:A:232:PRO:HG3 | 1:E:292:LEU:O | 2.21 | 0.41 |
| 1:B:309:ARG:NH1 | 1:B:436:GLU:OE2 | 2.53 | 0.41 |
| 1:C:96:ASP:OD1 | 1:C:97:GLU:N | 2.54 | 0.41 |
| 1:C:252:PHE:HZ | 5:C:601:I34:CL1 | 2.41 | 0.41 |
| 1:A:100:ASP:OD2 | 1:A:102:THR:HG22 | 2.20 | 0.41 |
| 1:D:225:ALA:HB2 | 1:D:245:VAL:HG11 | 2.02 | 0.40 |
| 1:A:307:TRP:HE3 | 1:A:311:ILE:HD12 | 1.86 | 0.40 |
| 1:A:46:ASN:O | 1:A:48:VAL:HG23 | 2.22 | 0.40 |

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 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 | 374/599 (62%) | 358 (96%) | 16 (4%) | 0 | 100 | 100 |
| 1 | B | 373/599 (62%) | 362 (97%) | 11 (3%) | 0 | 100 | 100 |
| 1 | C | 374/599 (62%) | 359 (96%) | 15 (4%) | 0 | 100 | 100 |
| 1 | D | 375/599 (63%) | 365 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | E | 375/599 (63%) | 363 (97%) | 12 (3%) | 0 | 100 | 100 |
| All | All | 1871/2995 (62%) | 1807 (97%) | 64 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 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 | 342/514 (66%) | 342 (100%) | 0 | 100 | 100 |
| 1 | B | 341/514 (66%) | 341 (100%) | 0 | 100 | 100 |
| 1 | C | 342/514 (66%) | 342 (100%) | 0 | 100 | 100 |
| 1 | D | 343/514 (67%) | 343 (100%) | 0 | 100 | 100 |
| 1 | E | 343/514 (67%) | 343 (100%) | 0 | 100 | 100 |
| All | All | 1711/2570 (67%) | 1711 (100%) | 0 | 100 | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
| --- | --- | --- | --- |
| 1 | B | 213 | ASN |
| 1 | C | 272 | GLN |
| 1 | D | 272 | GLN |

### 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 ⓘ

10 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| | | | | | Counts | RMSZ | $\#|Z| > 2$ | Counts | RMSZ | $\#|Z| > 2$ |
| 2 | NAG | F | 1 | 2,1 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | F | 2 | 2 | 14,14,15 | 0.17 | 0 | 17,19,21 | 0.40 | 0 |
| 2 | NAG | G | 1 | 2,1 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | G | 2 | 2 | 14,14,15 | 0.17 | 0 | 17,19,21 | 0.40 | 0 |
| 2 | NAG | H | 1 | 2,1 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.39 | 0 |
| 2 | NAG | H | 2 | 2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | I | 1 | 2,1 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | I | 2 | 2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.42 | 0 |
| 2 | NAG | J | 1 | 2,1 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | J | 2 | 2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.40 | 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 | NAG | F | 1 | 2,1 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | F | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | G | 1 | 2,1 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | G | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | H | 1 | 2,1 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | H | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | I | 1 | 2,1 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | I | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | J | 1 | 2,1 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | J | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 2 | J | 2 | NAG | C4-C5-C6-O6 |
| 2 | G | 2 | NAG | C4-C5-C6-O6 |
| 2 | H | 1 | NAG | O5-C5-C6-O6 |
| 2 | H | 1 | NAG | C4-C5-C6-O6 |
| 2 | J | 2 | NAG | O5-C5-C6-O6 |
| 2 | I | 1 | NAG | O5-C5-C6-O6 |
| 2 | G | 2 | NAG | O5-C5-C6-O6 |
| 2 | I | 1 | NAG | C4-C5-C6-O6 |
| 2 | I | 2 | NAG | O5-C5-C6-O6 |
| 2 | I | 2 | NAG | C4-C5-C6-O6 |
| 2 | G | 1 | NAG | C4-C5-C6-O6 |
| 2 | G | 1 | NAG | O5-C5-C6-O6 |

There are no ring outliers.

5 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | J | 1 | NAG | 3 | 0 |
| 2 | I | 1 | NAG | 2 | 0 |
| 2 | H | 1 | NAG | 2 | 0 |
| 2 | G | 1 | NAG | 2 | 0 |
| 2 | F | 1 | NAG | 2 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

## Oligosaccharide Chain G


Bond lengths


Bond angles


Torsions


Rings

## Oligosaccharide Chain H



Bond lengths



Bond angles



Torsions



Rings

## Oligosaccharide Chain I



Bond lengths



Bond angles



Torsions



Rings

**Oligosaccharide Chain J**



Bond lengths



Bond angles



Torsions



Rings
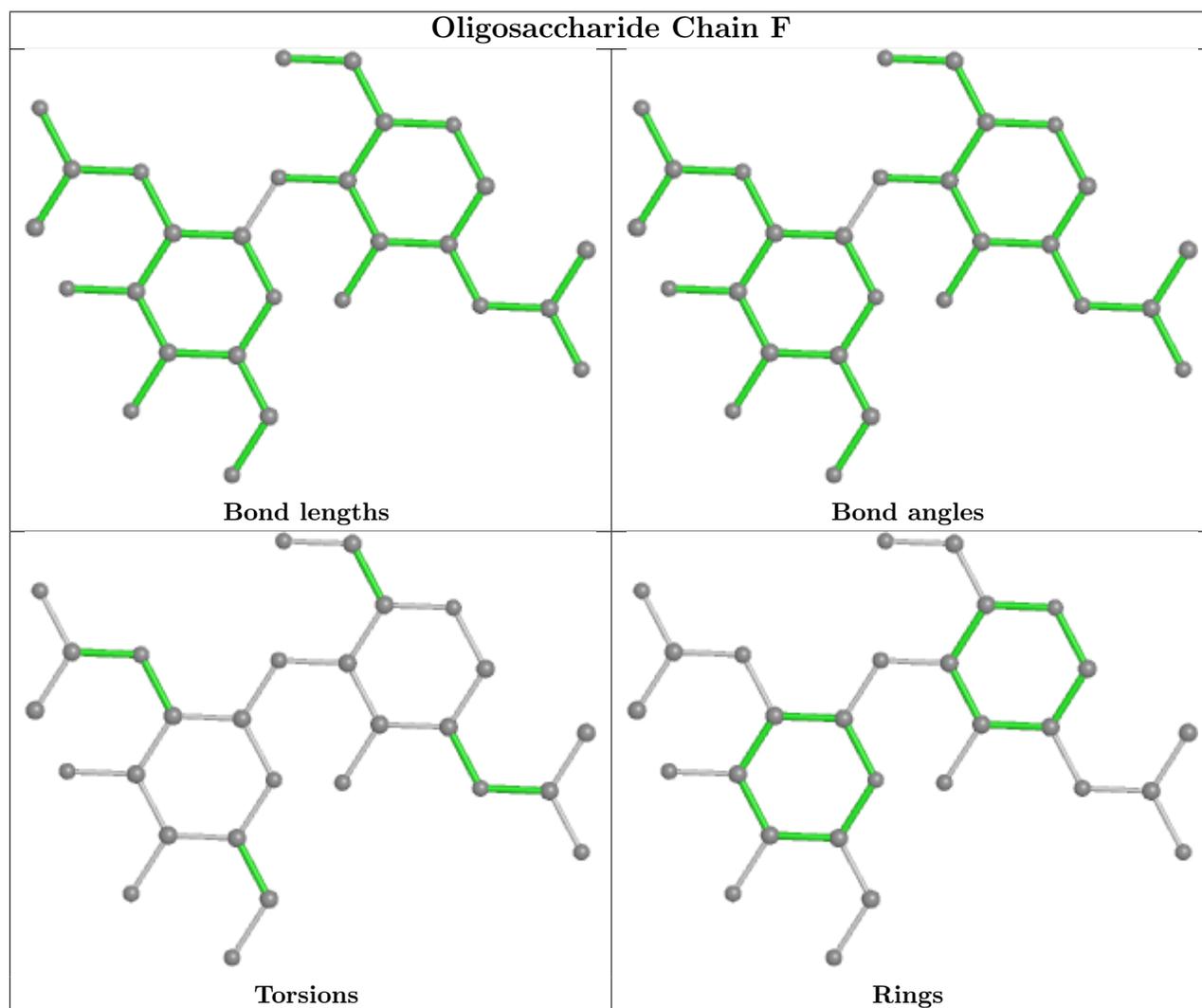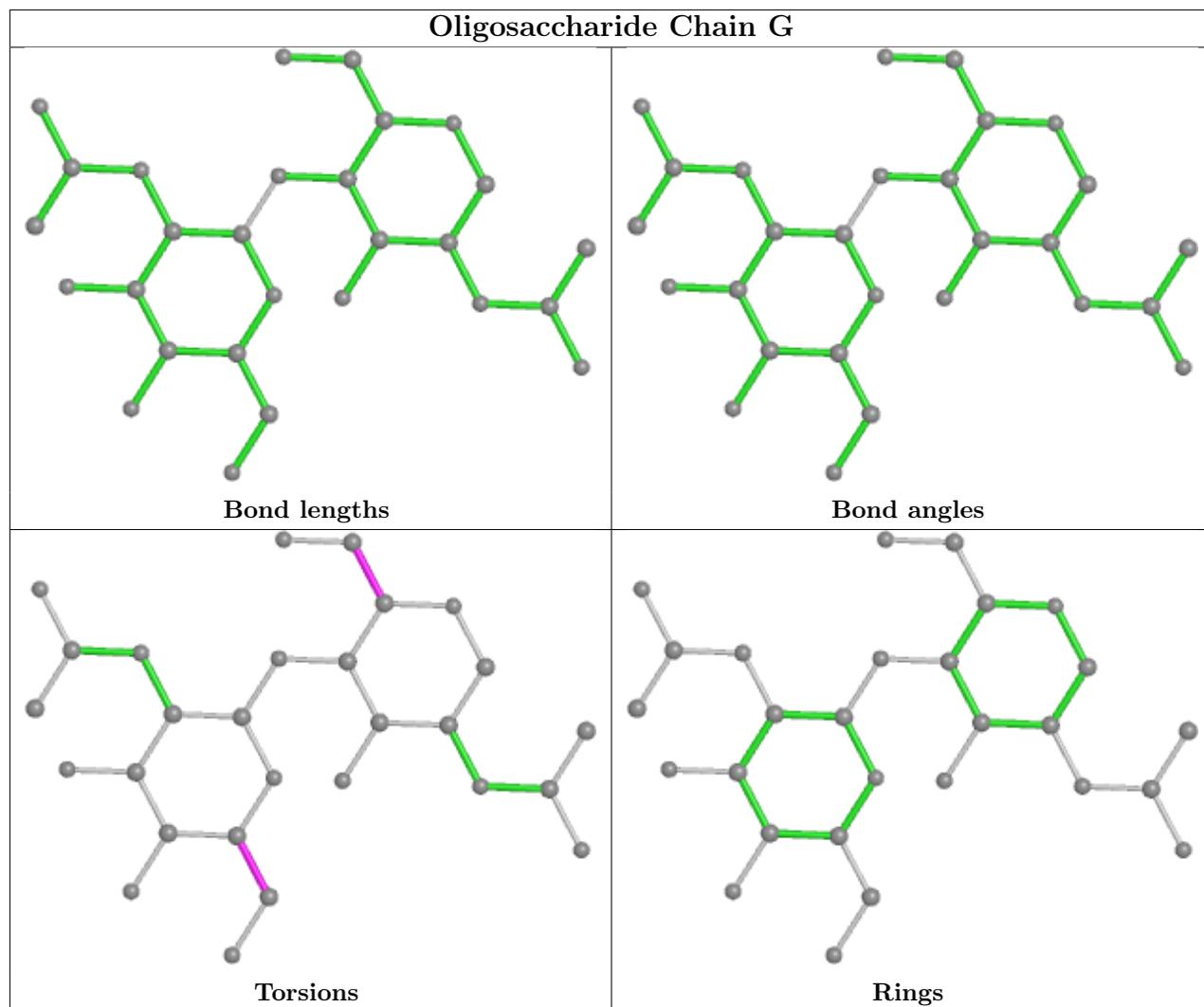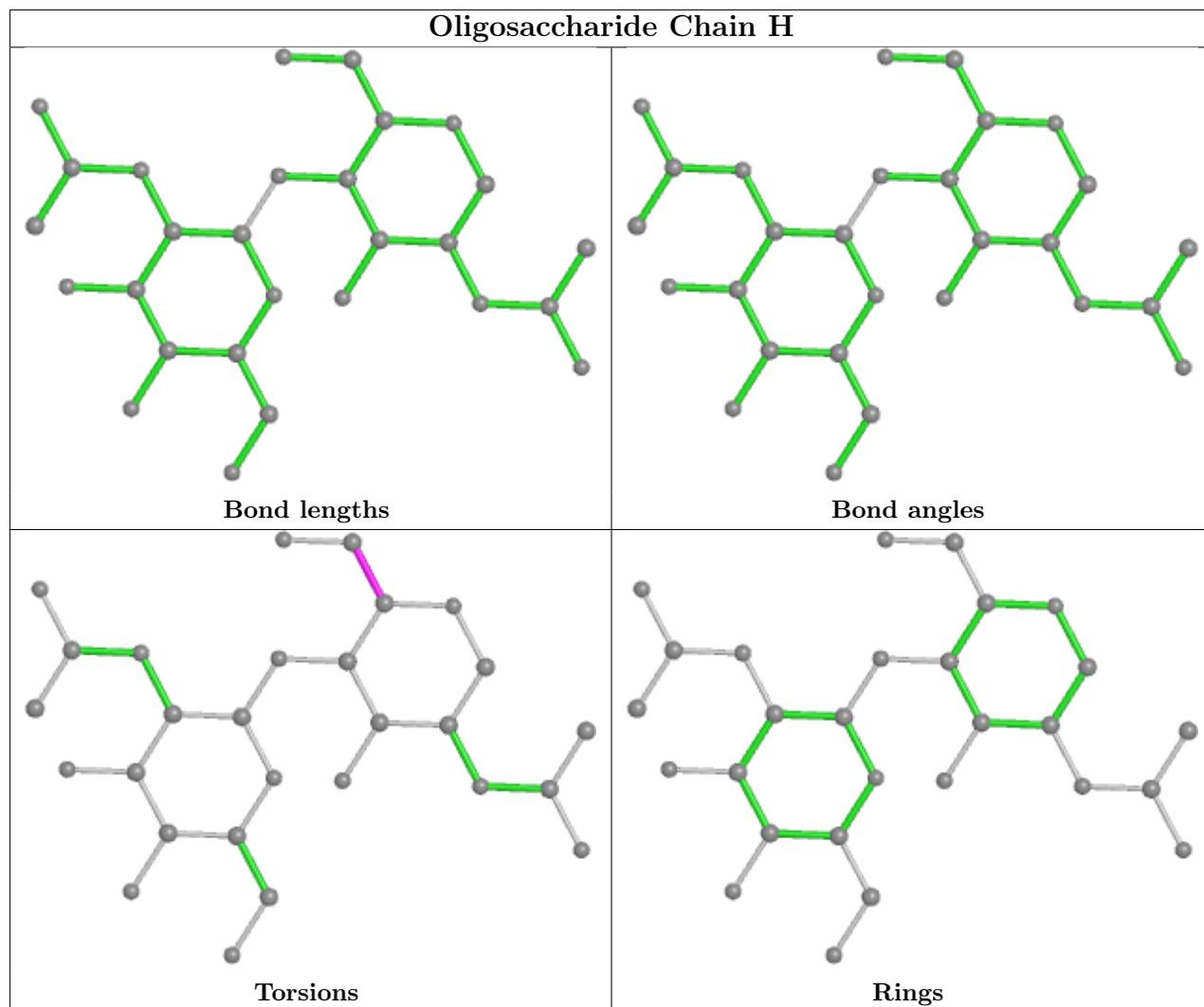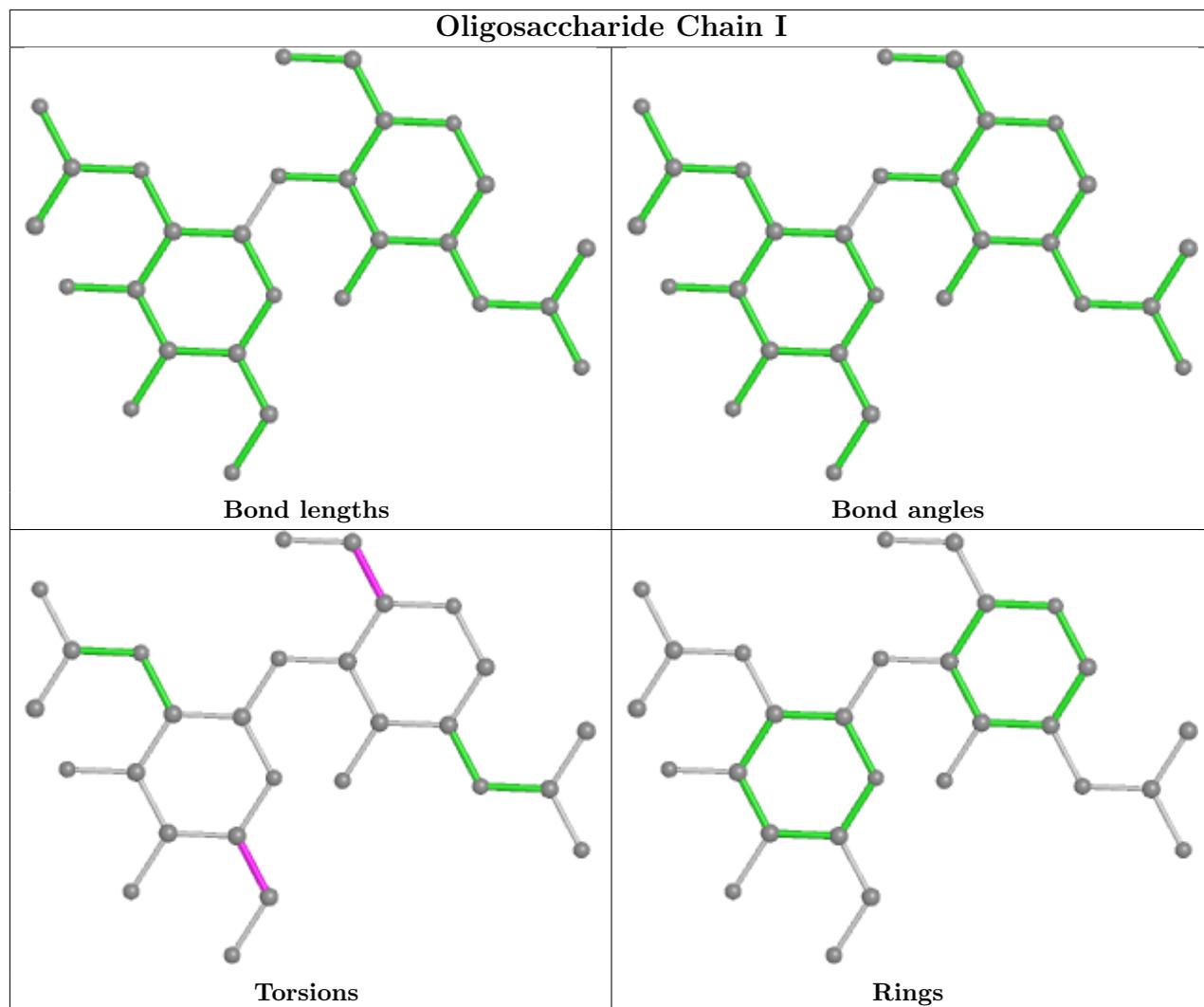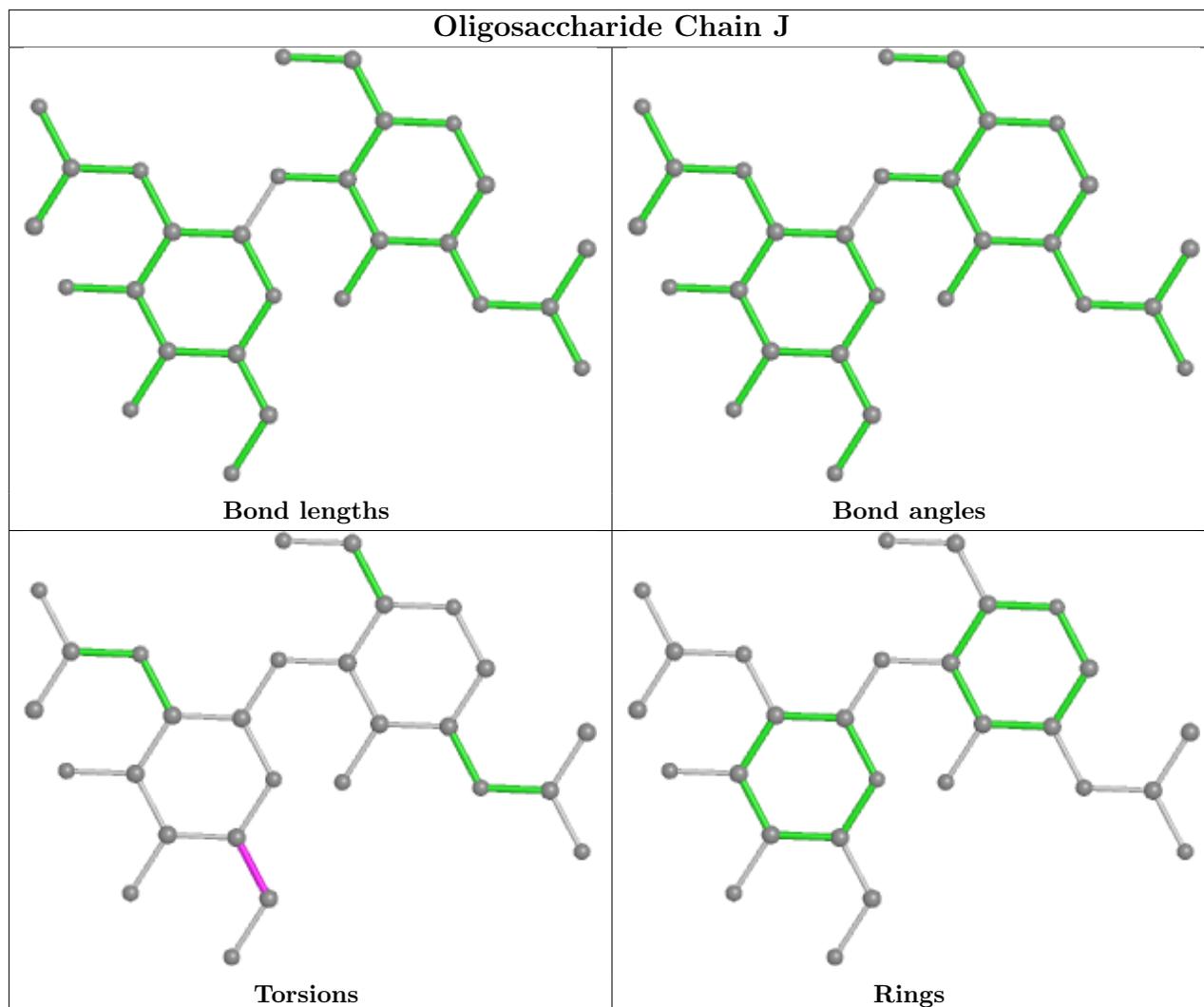
## 5.6   Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|-----------|--------|------|-----------|
| | | | | | Counts | RMSZ | $\#|Z| > 2$ | Counts | RMSZ | $\#|Z| > 2$ |
| 5 | I34 | D | 606 | - | 19,22,22 | 1.00 | 1 (5%) | 23,30,30 | 0.85 | 1 (4%) |
| 5 | I34 | A | 604 | - | 19,22,22 | 0.96 | 1 (5%) | 23,30,30 | 0.98 | 2 (8%) |
| 3 | NAG | C | 603 | 1 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.50 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 3 | NAG | D | 604 | 1 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.37 | 0 |
| 4 | EPJ | C | 605 | - | 16,16,16 | 0.18 | 0 | 20,23,23 | 0.66 | 0 |
| 3 | NAG | A | 601 | 1 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.54 | 0 |
| 3 | NAG | E | 601 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.52 | 0 |
| 3 | NAG | B | 603 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.54 | 0 |
| 3 | NAG | A | 602 | 1 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.37 | 0 |
| 3 | NAG | D | 603 | 1 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | NAG | B | 604 | 1 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.37 | 0 |
| 4 | EPJ | E | 603 | - | 16,16,16 | 0.19 | 0 | 20,23,23 | 0.66 | 0 |
| 3 | NAG | E | 602 | 1 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.36 | 0 |
| 4 | EPJ | A | 603 | - | 16,16,16 | 0.20 | 0 | 20,23,23 | 0.65 | 0 |
| 3 | NAG | C | 604 | 1 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.37 | 0 |
| 5 | I34 | B | 601 | - | 19,22,22 | 1.01 | 1 (5%) | 23,30,30 | 0.84 | 1 (4%) |
| 5 | I34 | D | 601 | - | 19,22,22 | 0.93 | 1 (5%) | 23,30,30 | 0.81 | 1 (4%) |
| 4 | EPJ | B | 605 | - | 16,16,16 | 0.19 | 0 | 20,23,23 | 0.66 | 0 |
| 4 | EPJ | D | 605 | - | 16,16,16 | 0.18 | 0 | 20,23,23 | 0.66 | 0 |
| 5 | I34 | C | 601 | - | 19,22,22 | 0.93 | 1 (5%) | 23,30,30 | 0.80 | 1 (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 |
|---|---|---|---|---|---|---|---|
| 5 | I34 | D | 606 | - | - | 2/10/12/12 | 0/2/2/2 |
| 5 | I34 | A | 604 | - | - | 2/10/12/12 | 0/2/2/2 |
| 3 | NAG | C | 603 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | D | 604 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | EPJ | C | 605 | - | - | 2/4/21/21 | 0/4/3/3 |
| 3 | NAG | A | 601 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | E | 601 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | B | 603 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | A | 602 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | D | 603 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | B | 604 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | EPJ | E | 603 | - | - | 2/4/21/21 | 0/4/3/3 |
| 3 | NAG | E | 602 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | EPJ | A | 603 | - | - | 2/4/21/21 | 0/4/3/3 |
| 3 | NAG | C | 604 | 1 | - | 1/6/23/26 | 0/1/1/1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 5 | I34 | B | 601 | - | - | 2/10/12/12 | 0/2/2/2 |
| 5 | I34 | D | 601 | - | - | 2/10/12/12 | 0/2/2/2 |
| 4 | EPJ | B | 605 | - | - | 2/4/21/21 | 0/4/3/3 |
| 4 | EPJ | D | 605 | - | - | 2/4/21/21 | 0/4/3/3 |
| 5 | I34 | C | 601 | - | - | 2/10/12/12 | 0/2/2/2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 5 | B | 601 | I34 | C14-C15 | -4.25 | 1.33 | 1.39 |
| 5 | D | 606 | I34 | C14-C15 | -4.20 | 1.33 | 1.39 |
| 5 | A | 604 | I34 | C14-C15 | -3.99 | 1.34 | 1.39 |
| 5 | C | 601 | I34 | C14-C15 | -3.85 | 1.34 | 1.39 |
| 5 | D | 601 | I34 | C14-C15 | -3.85 | 1.34 | 1.39 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 5 | C | 601 | I34 | C15-C14-C13 | -2.36 | 104.79 | 107.23 |
| 5 | D | 601 | I34 | C15-C14-C13 | -2.33 | 104.83 | 107.23 |
| 5 | A | 604 | I34 | C15-C14-C13 | -2.32 | 104.84 | 107.23 |
| 5 | D | 606 | I34 | C15-C14-C13 | -2.30 | 104.86 | 107.23 |
| 5 | B | 601 | I34 | C15-C14-C13 | -2.23 | 104.93 | 107.23 |
| 5 | A | 604 | I34 | O11-C10-N12 | -2.04 | 120.17 | 123.62 |

There are no chirality outliers.

All (31) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | C | 603 | NAG | C4-C5-C6-O6 |
| 3 | A | 601 | NAG | C4-C5-C6-O6 |
| 3 | B | 603 | NAG | C4-C5-C6-O6 |
| 3 | C | 603 | NAG | O5-C5-C6-O6 |
| 3 | A | 601 | NAG | O5-C5-C6-O6 |
| 3 | B | 603 | NAG | O5-C5-C6-O6 |
| 3 | D | 604 | NAG | O5-C5-C6-O6 |
| 3 | D | 604 | NAG | C4-C5-C6-O6 |
| 3 | E | 602 | NAG | C4-C5-C6-O6 |
| 3 | E | 602 | NAG | O5-C5-C6-O6 |
| 4 | A | 603 | EPJ | C6-C1-C7-C11 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 4 | B | 605 | EPJ | C6-C1-C7-C11 |
| 4 | C | 605 | EPJ | C6-C1-C7-C11 |
| 4 | D | 605 | EPJ | C6-C1-C7-C11 |
| 4 | E | 603 | EPJ | C6-C1-C7-C11 |
| 4 | A | 603 | EPJ | C6-C1-C7-C8 |
| 4 | B | 605 | EPJ | C6-C1-C7-C8 |
| 4 | C | 605 | EPJ | C6-C1-C7-C8 |
| 4 | D | 605 | EPJ | C6-C1-C7-C8 |
| 4 | E | 603 | EPJ | C6-C1-C7-C8 |
| 5 | C | 601 | I34 | C08-C05-O06-C07 |
| 5 | D | 601 | I34 | C08-C05-O06-C07 |
| 3 | C | 604 | NAG | O5-C5-C6-O6 |
| 5 | A | 604 | I34 | C08-C05-O06-C07 |
| 5 | A | 604 | I34 | C04-C05-O06-C07 |
| 5 | D | 601 | I34 | C04-C05-O06-C07 |
| 5 | D | 606 | I34 | C04-C05-O06-C07 |
| 5 | C | 601 | I34 | C04-C05-O06-C07 |
| 5 | B | 601 | I34 | C04-C05-O06-C07 |
| 5 | B | 601 | I34 | C08-C05-O06-C07 |
| 5 | D | 606 | I34 | C08-C05-O06-C07 |

There are no ring outliers.

3 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | D | 606 | I34 | 3 | 0 |
| 5 | D | 601 | I34 | 1 | 0 |
| 5 | C | 601 | I34 | 4 | 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 I34 D 606**


Bond lengths


Bond angles


Torsions


Rings

**Ligand I34 A 604**


Bond lengths


Bond angles


Torsions


Rings

## Ligand EPJ C 605



Bond lengths



Bond angles



Torsions



Rings

## Ligand EPJ E 603



Bond lengths



Bond angles



Torsions



Rings

## Ligand EPJ A 603



Bond lengths



Bond angles



Torsions



Rings

## Ligand I34 B 601



Bond lengths



Bond angles



Torsions



Rings

## Ligand I34 D 601



Bond lengths



Bond angles



Torsions



Rings

## Ligand EPJ B 605



Bond lengths



Bond angles



Torsions



Rings

## Ligand EPJ D 605



Bond lengths



Bond angles



Torsions



Rings

**Ligand I34 C 601**

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-43035. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1   Orthogonal projections ⓘ

### 6.1.1   Primary map



X      Y      Z

### 6.1.2   Raw map



X      Y      Z
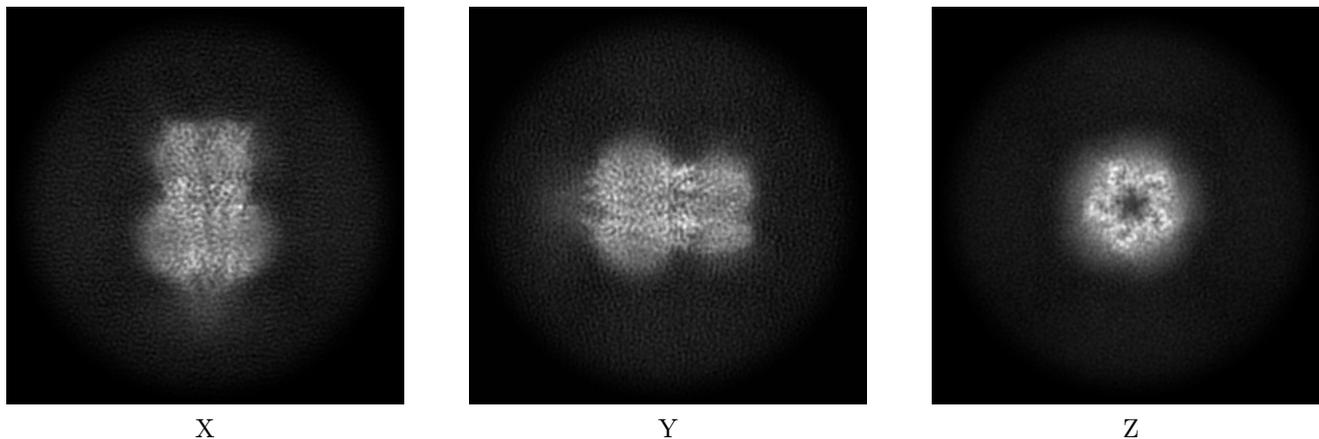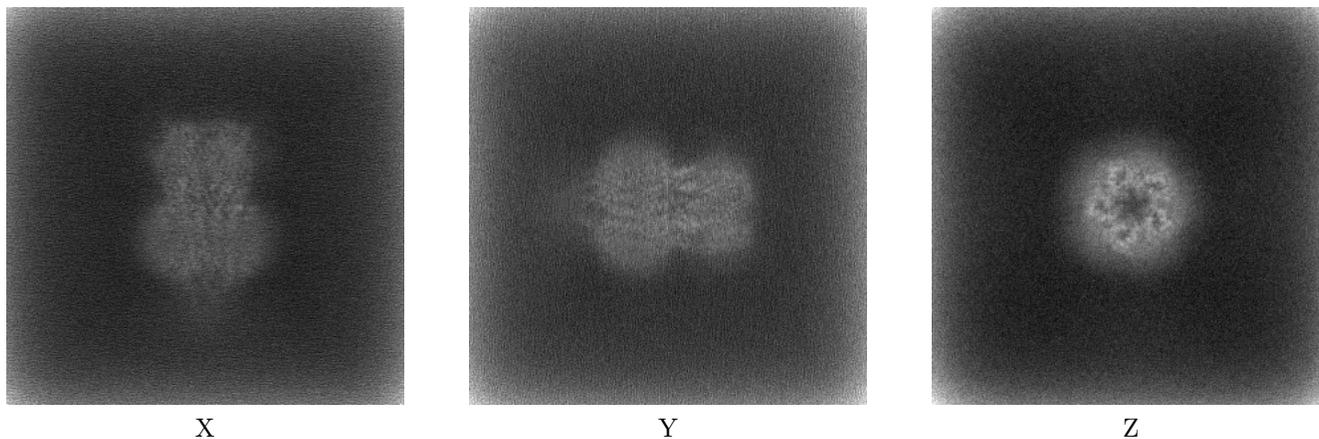
The images above show the map projected in three orthogonal directions.

## 6.2　Central slices ⓘ
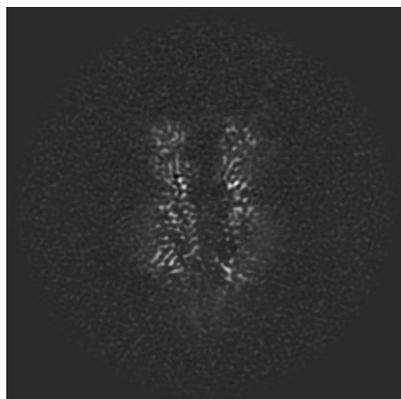
### 6.2.1　Primary map
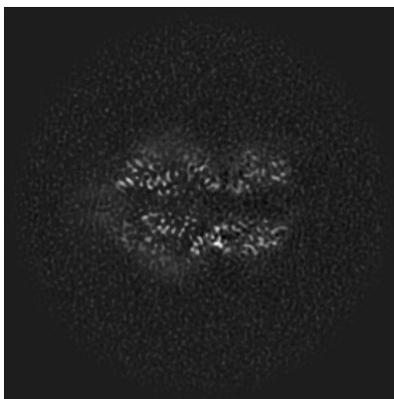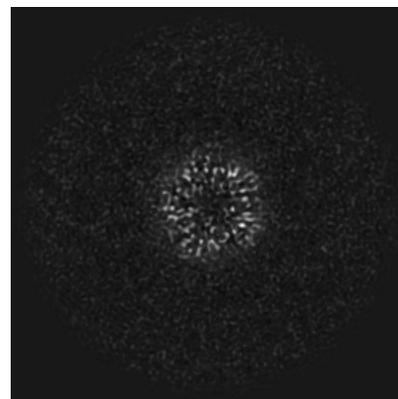


X Index: 168　　　　Y Index: 168　　　　Z Index: 168

### 6.2.2　Raw map
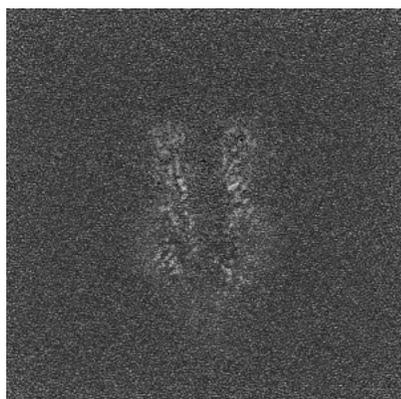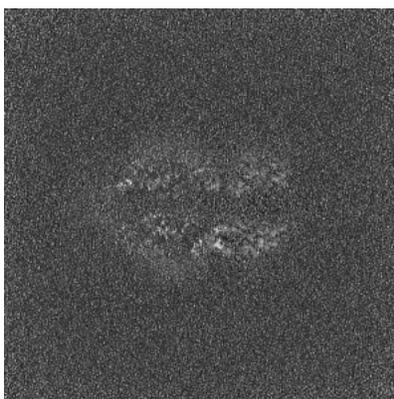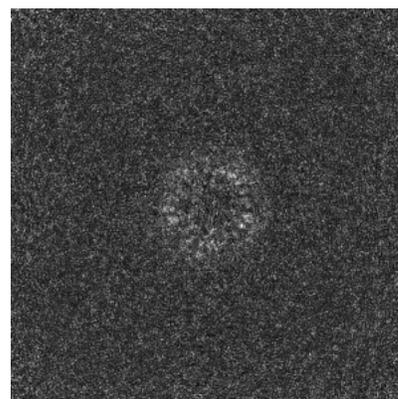


X Index: 168　　　　Y Index: 168　　　　Z Index: 168

The images above show central slices of the map in three orthogonal directions.

## 6.3　Largest variance slices ⓘ
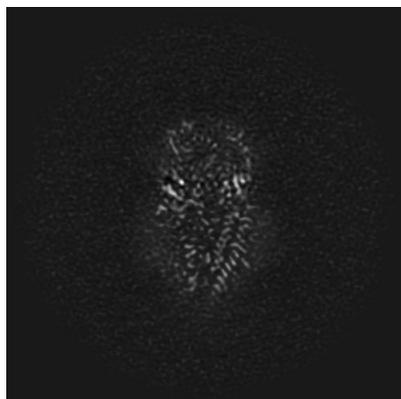
### 6.3.1　Primary map
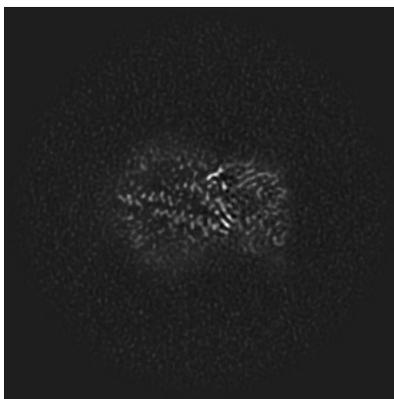


X Index: 152　　　　　　　Y Index: 148　　　　　　　Z Index: 183
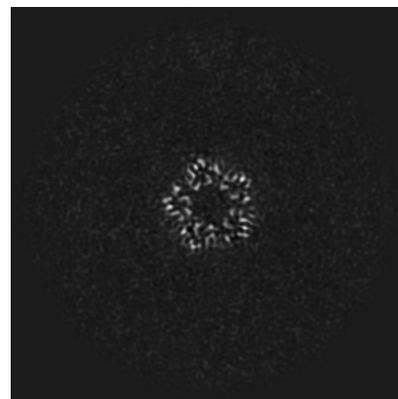
### 6.3.2　Raw map
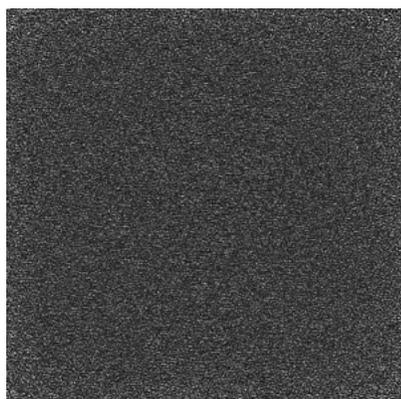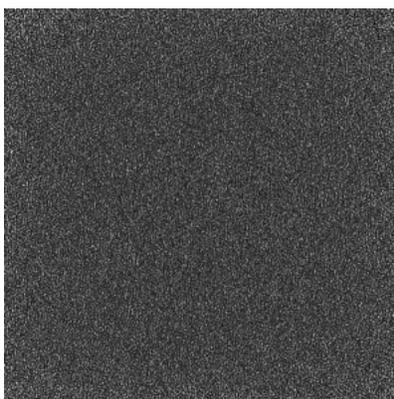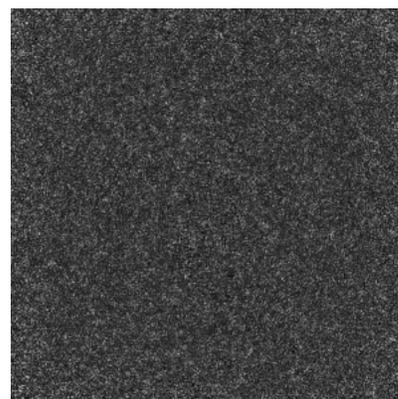


X Index: 1　　　　　　　Y Index: 0　　　　　　　Z Index: 335

The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



| X | Y | Z |

### 6.4.2 Raw map



| X | Y | Z |
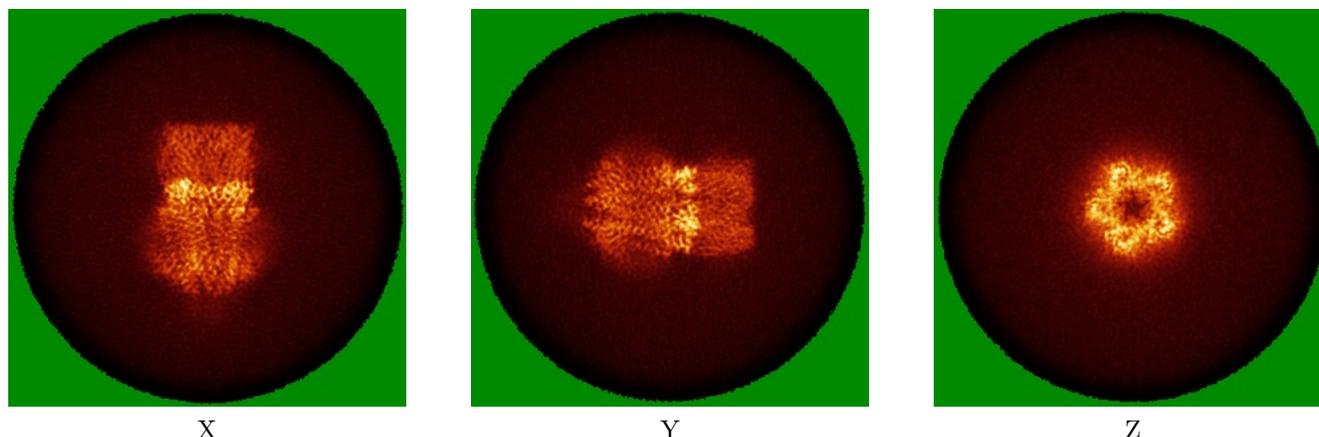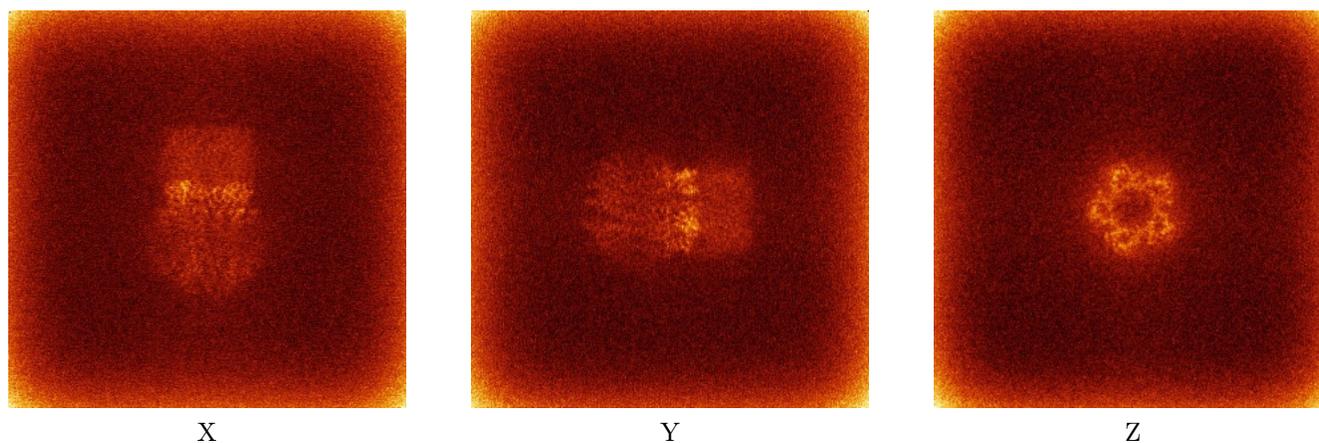
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X　　　　　　　　　　Y　　　　　　　　　　Z
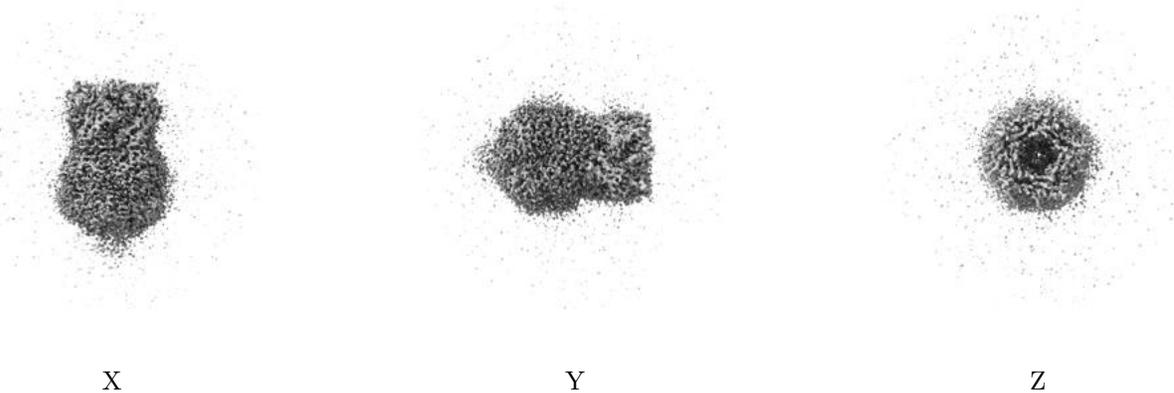
The images above show the 3D surface view of the map at the recommended contour level 0.097. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X　　　　　　　　　　Y　　　　　　　　　　Z
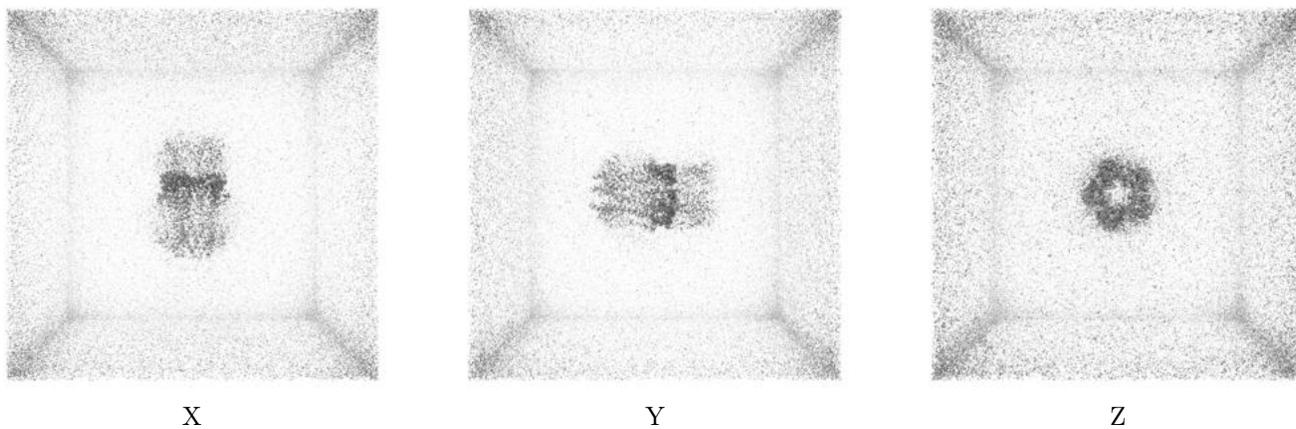
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation (i)

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 ⓘ
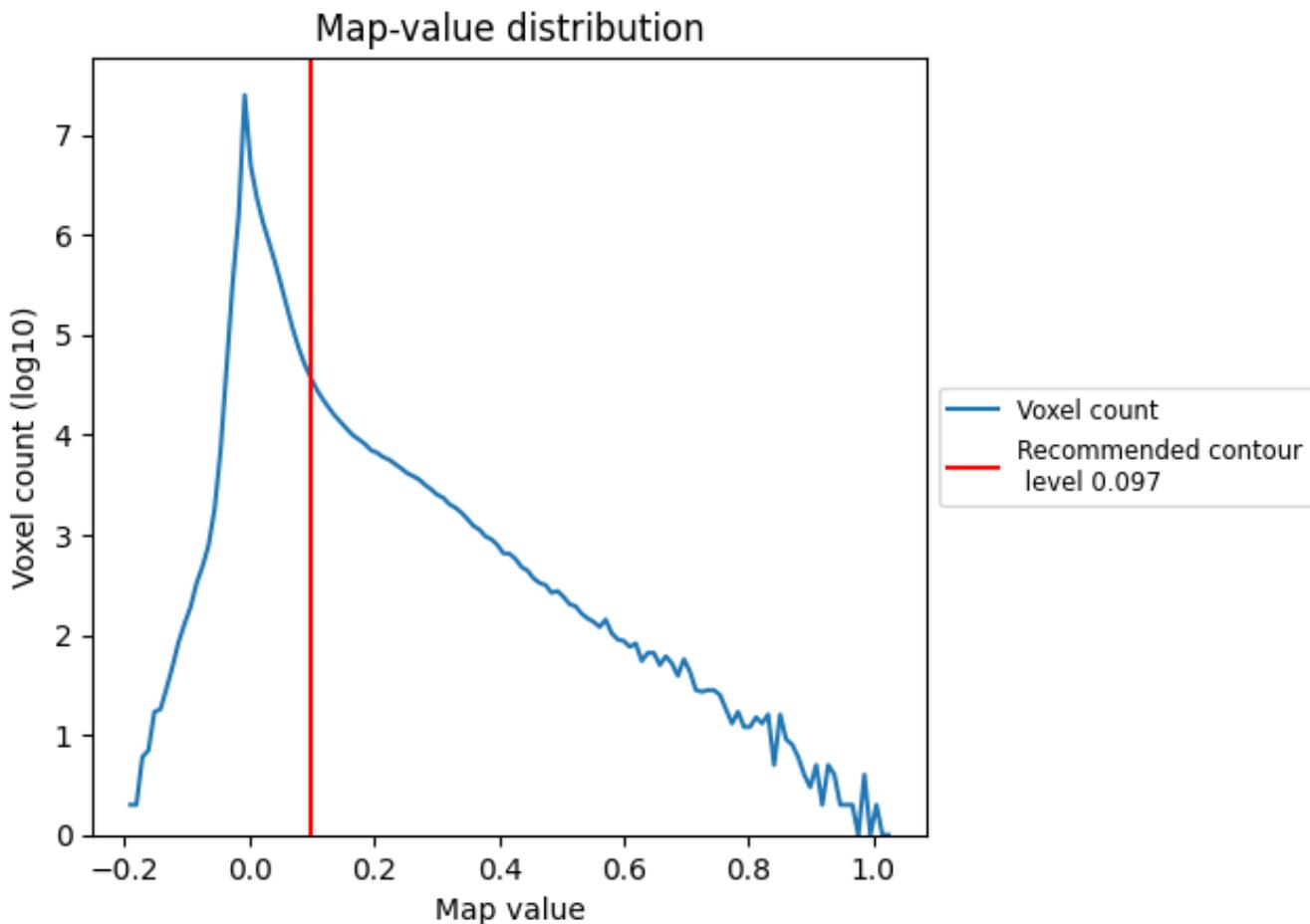


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2　Volume estimate ⓘ
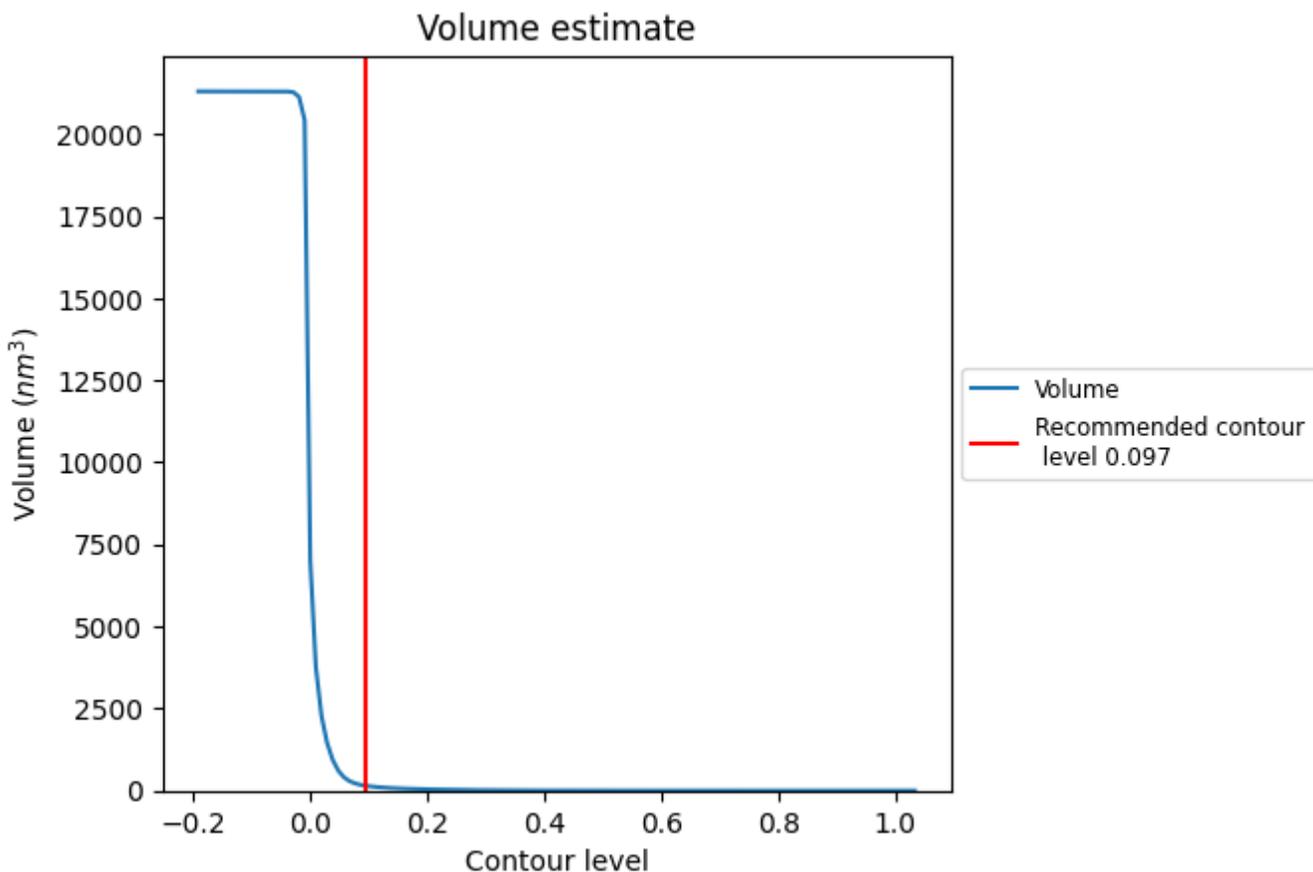


The volume at the recommended contour level is 145 nm$^3$; this corresponds to an approximate mass of 131 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum ⓘ
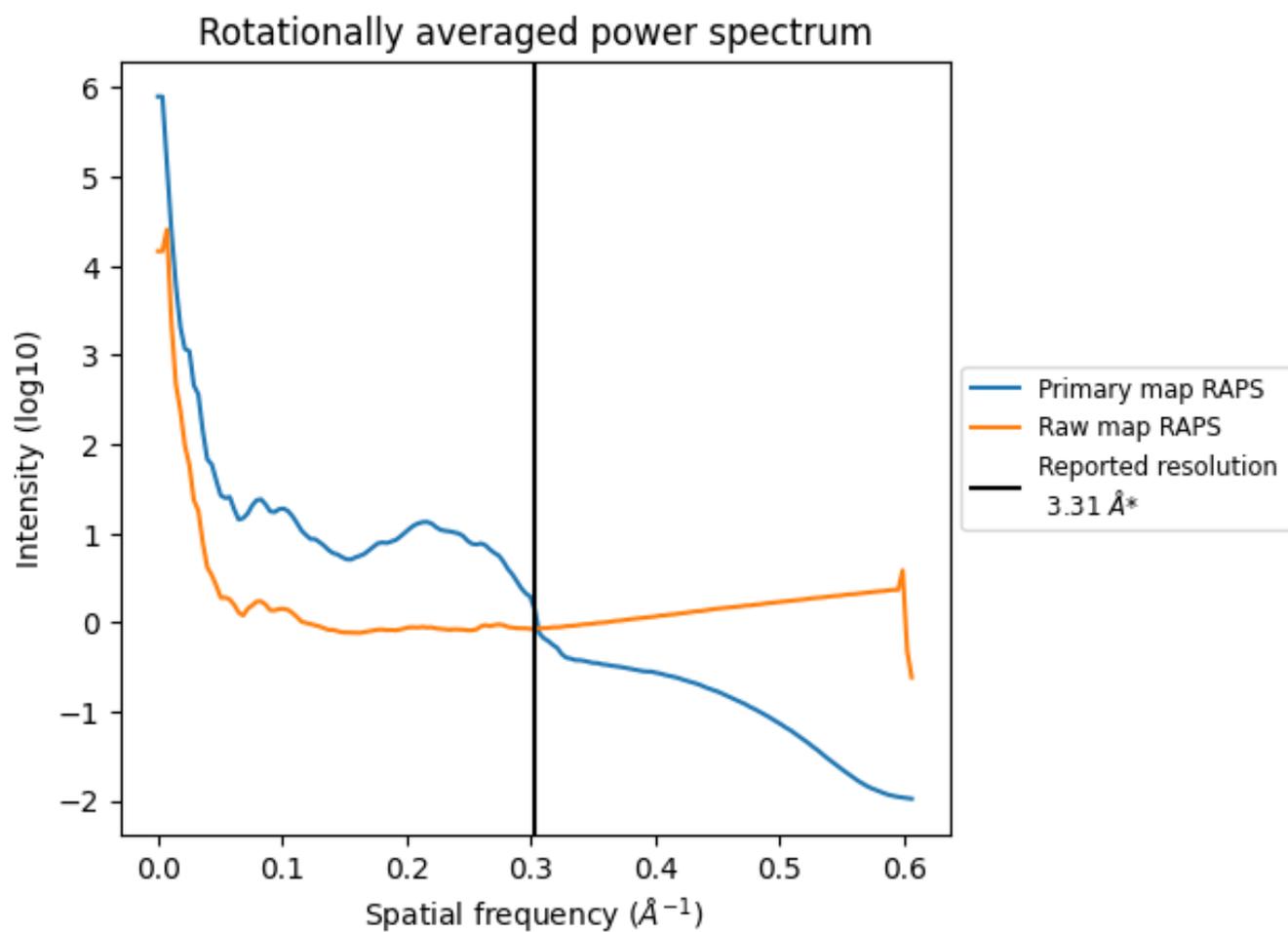


*Reported resolution corresponds to spatial frequency of 0.302 Å$^{-1}$

# 8    Fourier-Shell correlation  ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1    FSC  ⓘ
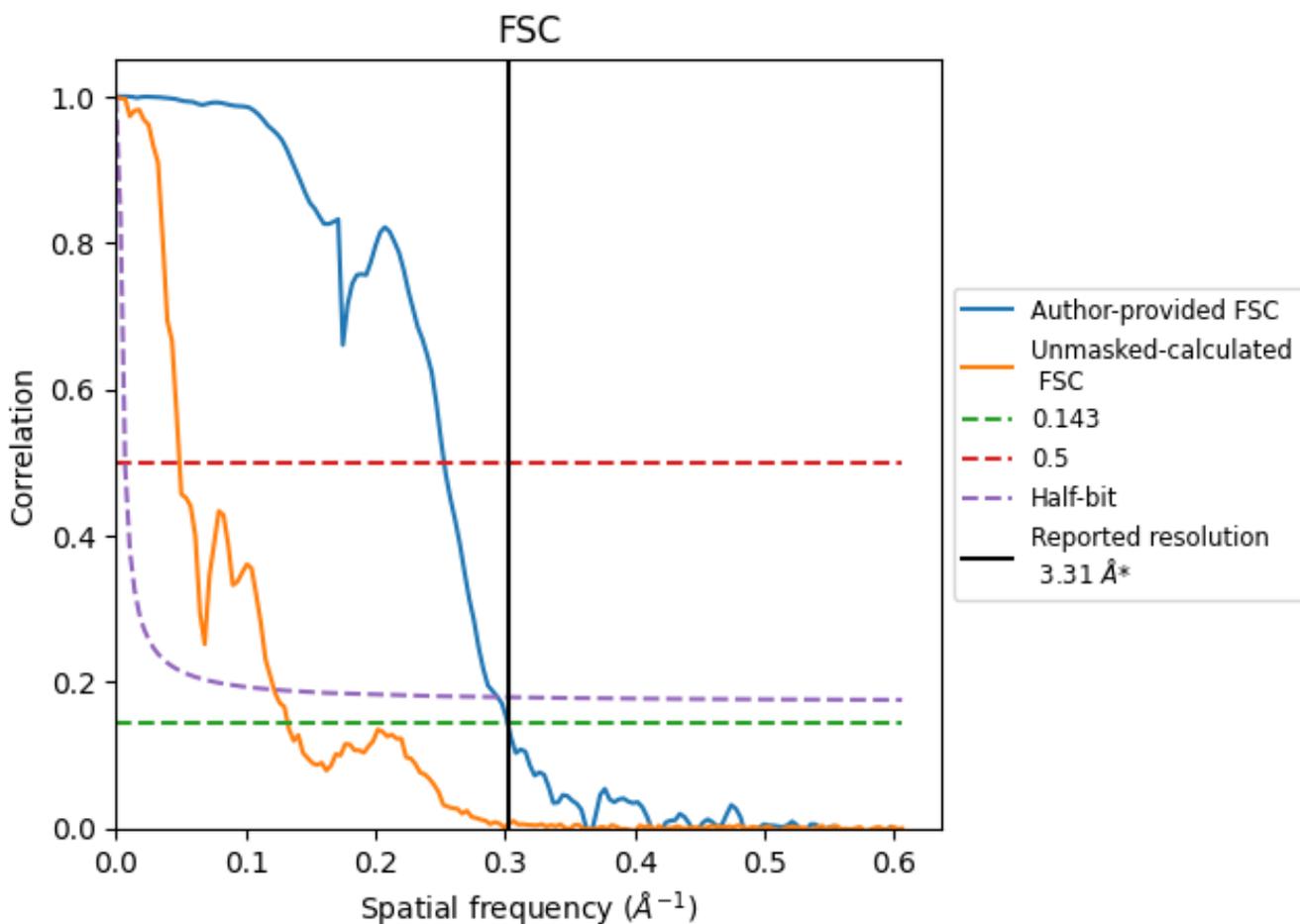


*Reported resolution corresponds to spatial frequency of 0.302 $\text{Å}^{-1}$

## 8.2　Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.31 | - | - |
| Author-provided FSC curve | 3.31 | 3.95 | 3.40 |
| Unmasked-calculated* | 7.55 | 20.37 | 8.20 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.55 differs from the reported value 3.31 by more than 10 %

# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-43035 and PDB model 8V8D. Per-residue inclusion information can be found in section 3 on page 19.

## 9.1 Map-model overlay (i)



| X | Y | Z |
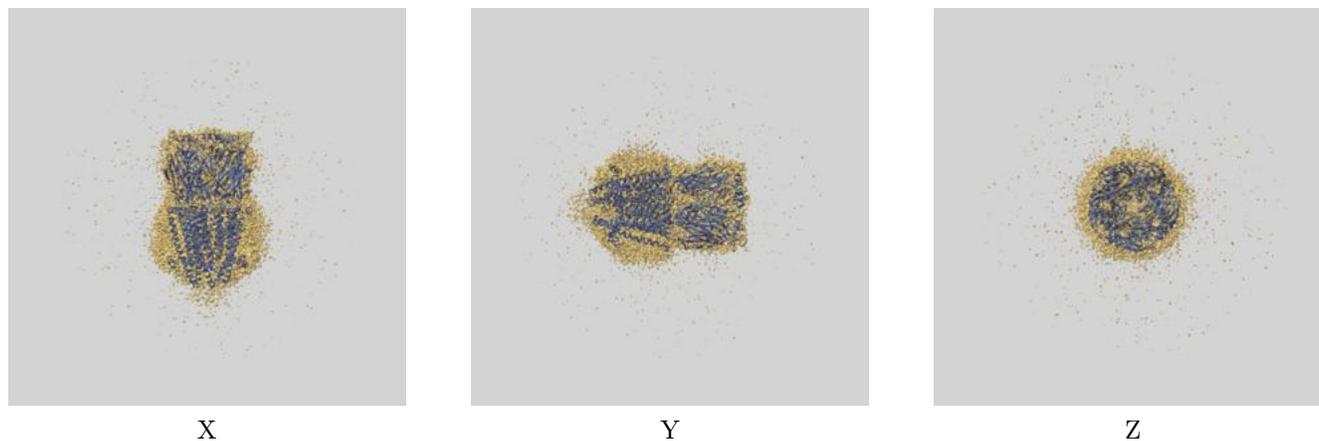
The images above show the 3D surface view of the map at the recommended contour level 0.097 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model (i)



X          Y          Z
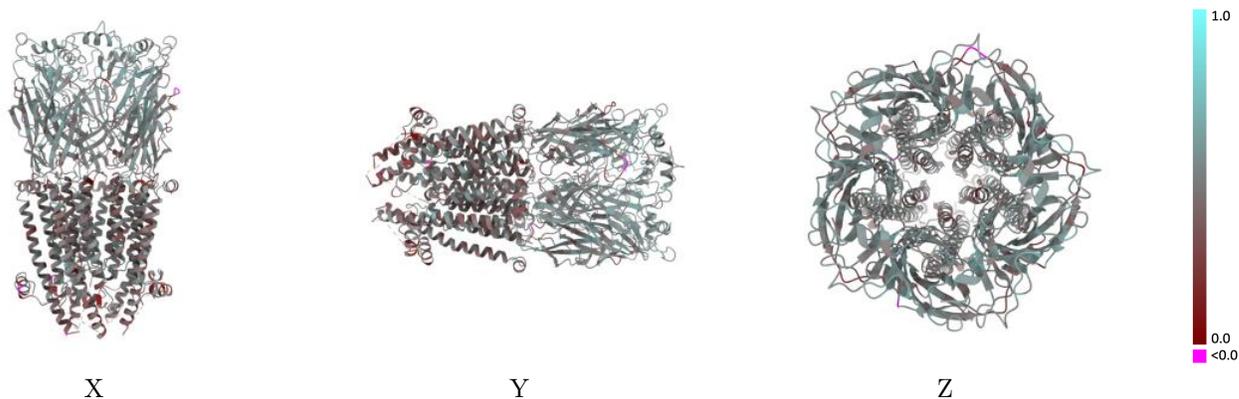
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model (i)



X          Y          Z
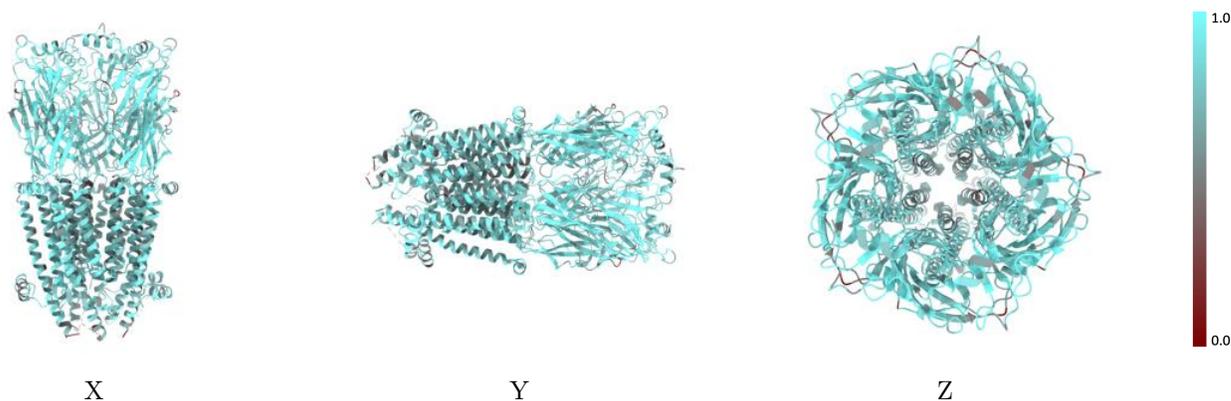
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.097).

## 9.4　Atom inclusion ⓘ
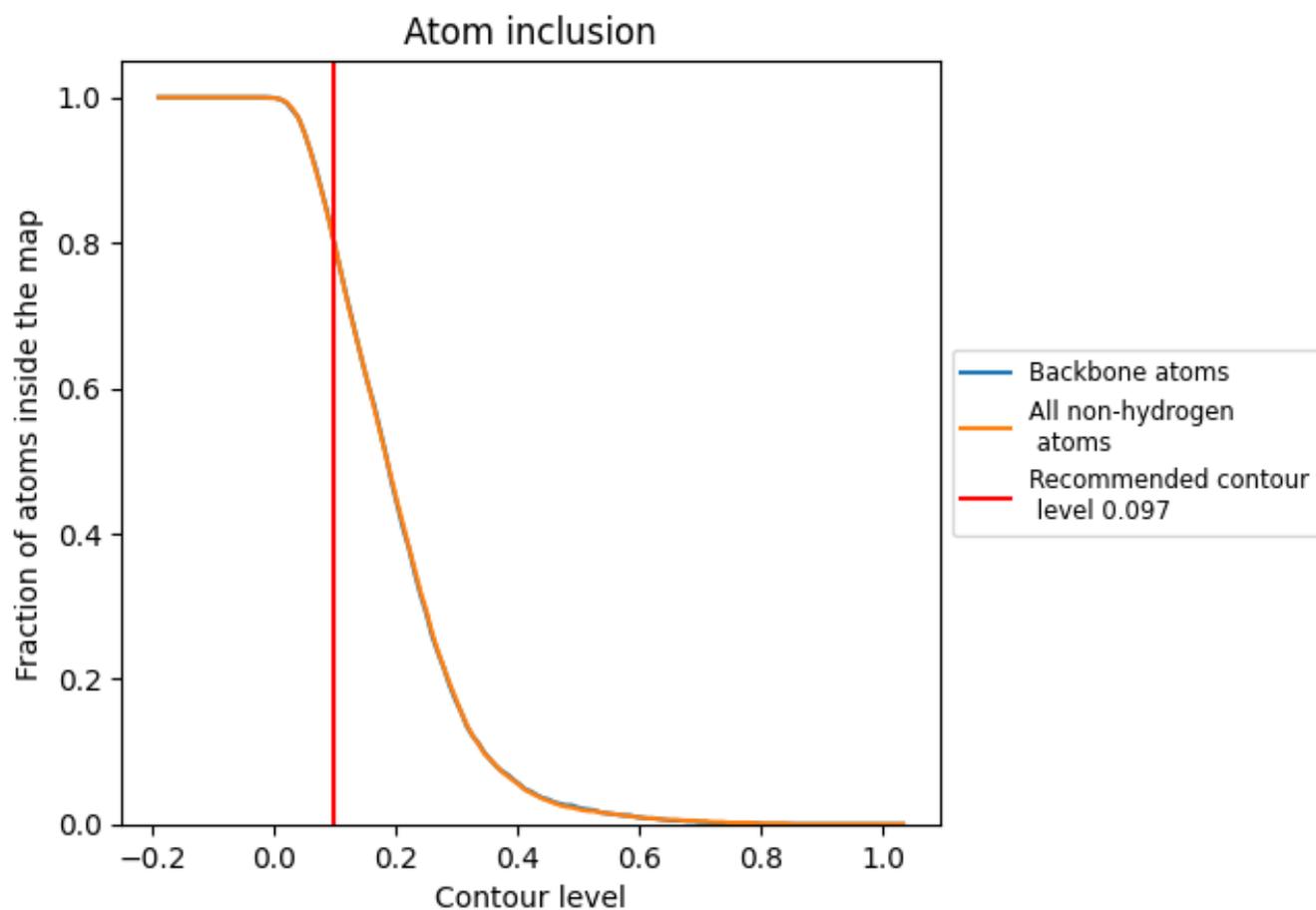


At the recommended contour level, 80% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.097) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.8030 | 0.4670 |
| A | 0.7900 | 0.4600 |
| B | 0.8130 | 0.4700 |
| C | 0.8110 | 0.4660 |
| D | 0.8170 | 0.4680 |
| E | 0.8140 | 0.4710 |
| F | 0.7860 | 0.4820 |
| G | 0.6790 | 0.4430 |
| H | 0.6070 | 0.3890 |
| I | 0.7860 | 0.4860 |
| J | 0.7140 | 0.4580 |

1.0

0.0
<0.0