#  wwPDB EM Validation Summary Report (i) 

## Nov 7, 2023-12:54 am GMT

PDB ID : 7QTQ<br>EMDB ID : EMD-14145<br>Title : Structure of Native, iodinated bovine thyroglobulin solved on strepavidin affinity grids.<br>Authors : Marechal, N.; Weitz, J.C.; Serrano, B.P.; Zhang, X.<br>Deposited on : 2022-01-15<br>Resolution : $3.30 \AA$ (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

```
    EMDB validation analysis : 0.0.1.dev70
                            Mogul : 1.8.4, CSD as541be (2020)
                            MolProbity : 4.02b-467
    Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
                            MapQ : FAILED
    Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36
```


## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is $3.30 \AA$.
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 <br> (\#Entries) | EM structures <br> (\#Entries) |
| :---: | :---: | :---: |
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 55234 atoms, of which 27101 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 Thyroglobulin.

| Mol | Chain | Residues | Atoms |  |  |  |  |  |  | AltConf | Trace |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | A | 1790 | $\begin{gathered} \hline \text { Total } \\ 27329 \end{gathered}$ | $\begin{gathered} \mathrm{C} \\ 8768 \end{gathered}$ | $\begin{gathered} \mathrm{H} \\ 13410 \end{gathered}$ | I | $\begin{gathered} \mathrm{N} \\ 2459 \end{gathered}$ | $\begin{gathered} \mathrm{O} \\ 2587 \end{gathered}$ | $\begin{gathered} \hline \mathrm{S} \\ 101 \end{gathered}$ | 0 | 0 |
| 1 | B | 1789 | $\begin{gathered} \text { Total } \\ 27329 \end{gathered}$ | $\begin{gathered} \mathrm{C} \\ 8768 \end{gathered}$ | $\begin{gathered} \mathrm{H} \\ 13417 \end{gathered}$ | I | $\begin{gathered} \mathrm{N} \\ 2455 \end{gathered}$ | $\begin{gathered} \mathrm{O} \\ 2584 \end{gathered}$ | $\begin{gathered} \mathrm{S} \\ 101 \end{gathered}$ | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
| :---: | :---: | :---: | :---: | :---: | :---: |
| A | 196 | PHE | LEU | variant | UNP P01267 |
| A | 2540 | DHA | TYR | modified residue | UNP P01267 |
| A | 2573 | T44 | TYR | modified residue | UNP P01267 |
| B | 196 | PHE | LEU | variant | UNP P01267 |
| B | 2540 | DHA | TYR | modified residue | UNP P01267 |
| B | 2573 | T44 | TYR | modified residue | UNP P01267 |

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.


| Mol | Chain | Residues | Atoms |  |  |  |  | AltConf | Trace |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | C | 3 | Total <br> 73 | C <br> 22 | H <br> 34 | N | O | 15 | 0 |$⿻ 0.0$

- Molecule 3 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 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | D | 2 | $\begin{array}{c}\text { Total } \\ 53\end{array}$ | $\begin{array}{c}\mathrm{C} \\ 16\end{array}$ | $\begin{array}{c}\text { H }\end{array}$ | N | O | 2 | 10 |$) 0$| 0 |
| :---: |
| 3 |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\mathrm{C}_{8} \mathrm{H}_{15} \mathrm{NO}_{6}$ ).


| Mol | Chain | Residues | Atoms |  |  |  |  | AltConf |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | A | 1 | $\begin{array}{c}\text { Total } \\ 27\end{array}$ | $\begin{array}{c}\mathrm{C} \\ 8\end{array}$ | $\begin{array}{c}\mathrm{H} \\ 13\end{array}$ | $\begin{array}{c}\mathrm{N} \\ \hline\end{array}$ | O | 5 |$) 0$

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| Mol | Chain | Residues | Atoms |  |  |  |  | AltConf |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | B | 1 | $\begin{array}{c}\text { Total } \\ 27\end{array}$ | $\begin{array}{c}\text { C } \\ 8\end{array}$ | $\begin{array}{c}\text { H } \\ 13\end{array}$ | N | O | 5 |$) 0$

SEQUENCE-PLOTS INFOmissingINFO

## 3 Experimental information (i)

| Property | Value | Source |
| :--- | :--- | :--- |
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 242813 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE <br> CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose $\left(e^{-} / \AA^{2}\right)$ | 54 | Depositor |
| Minimum defocus $(\mathrm{nm})$ | 500 | Depositor |
| Maximum defocus $(\mathrm{nm})$ | 3500 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |

## 4 Model quality (i)

### 4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, DHA, T44, NAG

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 | 0.41 | $0 / 14211$ | 0.52 | $3 / 19249(0.0 \%)$ |
| 1 | B | 0.41 | $0 / 14204$ | 0.51 | $0 / 19241$ |
| All | All | 0.41 | $0 / 28415$ | 0.51 | $3 / 38490(0.0 \%)$ |

There are no bond length outliers.
All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed $\left({ }^{\circ}\right)$ | Ideal $\left({ }^{\circ}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | A | 965 | LEU | CB-CG-CD1 | -5.95 | 100.88 | 111.00 |
| 1 | A | 965 | LEU | CB-CA-C | 5.36 | 120.38 | 110.20 |
| 1 | A | 313 | HIS | CB-CA-C | 5.33 | 121.05 | 110.40 |

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 | 13919 | 13410 | 13428 | 247 | 0 |
| 1 | B | 13912 | 13417 | 13430 | 266 | 0 |
| 2 | C | 39 | 34 | 34 | 3 | 0 |
| 2 | E | 39 | 34 | 34 | 3 | 0 |
| 3 | D | 28 | 25 | 25 | 0 | 0 |
| 3 | F | 28 | 25 | 25 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | A | 84 | 78 | 78 | 3 | 0 |
| 4 | B | 84 | 78 | 78 | 5 | 0 |
| All | All | 28133 | 27101 | 27132 | 513 | 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 9 .

The worst 5 of 513 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic <br> distance $(\AA)$ | Clash <br> overlap $(\AA)$ |
| :---: | :---: | :---: | :---: |
| 2:C:2:NAG:O7 | 2:C:2:NAG:O3 | 2.05 | 0.74 |
| 1:B:296:ARG:NH1 | 1:B:321:PRO:O | 2.20 | 0.74 |
| 1:A:1977:ILE:HD12 | 1:A:1979:ILE:HD11 | 1.70 | 0.74 |
| 4:B:2804:NAG:O7 | 4:B:2804:NAG:O3 | 2.05 | 0.74 |
| 4:A:2802:NAG:O7 | 4:A:2802:NAG:O3 | 2.05 | 0.73 |

There are no symmetry-related clashes.

### 4.3 Torsion angles (i)

### 4.3.1 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 | $1726 / 2769(62 \%)$ | $1548(90 \%)$ | $178(10 \%)$ | 0 | 100 | 100 |
| 1 | B | $1725 / 2769(62 \%)$ | $1539(89 \%)$ | $186(11 \%)$ | 0 | 100 | 100 |
| All | All | $3451 / 5538(62 \%)$ | $3087(90 \%)$ | $364(10 \%)$ | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 4.3.2 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 | $1509 / 2312(65 \%)$ | $1505(100 \%)$ | $4(0 \%)$ | 92 | 96 |
| 1 | B | $1509 / 2312(65 \%)$ | $1505(100 \%)$ | $4(0 \%)$ | 92 | 96 |
| All | All | $3018 / 4624(65 \%)$ | $3010(100 \%)$ | $8(0 \%)$ | 92 | 96 |

5 of 8 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
| :---: | :---: | :---: | :---: |
| 1 | B | 2353 | ASN |
| 1 | B | 1244 | ARG |
| 1 | B | 214 | PHE |
| 1 | A | 979 | ARG |
| 1 | B | 495 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
| :---: | :---: | :---: | :---: |
| 1 | A | 605 | GLN |
| 1 | A | 2137 | HIS |

### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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 | $\#\|Z\|>2$ |
| 1 | DHA | B | 2540 | 1 | $4,4,5$ | 4.43 | $2(50 \%)$ | $2,4,6$ | 3.37 | $1(50 \%)$ |
| 1 | DHA | A | 2540 | 1 | $4,4,5$ | 4.50 | $2(50 \%)$ | $2,4,6$ | 3.31 | $1(50 \%)$ |

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 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | DHA | B | 2540 | 1 | - | $0 / 0 / 2 / 4$ | - |
| 1 | DHA | A | 2540 | 1 | - | $0 / 0 / 2 / 4$ | - |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed $(\AA)$ | Ideal $(\AA)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | A | 2540 | DHA | C-CA | 7.61 | 1.57 | 1.45 |
| 1 | B | 2540 | DHA | C-CA | 7.45 | 1.57 | 1.45 |
| 1 | B | 2540 | DHA | CA-N | 4.55 | 1.46 | 1.35 |
| 1 | A | 2540 | DHA | CA-N | 4.48 | 1.46 | 1.35 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed $\left({ }^{\circ}\right)$ | Ideal $\left({ }^{\circ}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | B | 2540 | DHA | O-C-CA | -4.70 | 116.78 | 125.54 |
| 1 | A | 2540 | DHA | O-C-CA | -4.46 | 117.22 | 125.54 |

There are no chirality outliers.
There are no torsion outliers.
There are no ring outliers.
No monomer is involved in short contacts.

### 4.5 Carbohydrates (i)

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 | C | 1 | 1,2 | $14,14,15$ | 0.60 | 0 | $17,19,21$ | 2.74 | $7(41 \%)$ |
| 2 | NAG | C | 2 | 2 | $14,14,15$ | 0.38 | 0 | $17,19,21$ | 0.98 | $1(5 \%)$ |
| 2 | MAN | C | 3 | 2 | $11,11,12$ | 0.26 | 0 | $15,15,17$ | 0.96 | $1(6 \%)$ |
| 3 | NAG | D | 1 | 1,3 | $14,14,15$ | 0.56 | 0 | $17,19,21$ | 0.81 | 0 |
| 3 | NAG | D | 2 | 3 | $14,14,15$ | 0.35 | 0 | $17,19,21$ | 1.20 | $2(11 \%)$ |
| 2 | NAG | E | 1 | 1,2 | $14,14,15$ | 0.94 | $1(7 \%)$ | $17,19,21$ | 1.13 | $1(5 \%)$ |
| 2 | NAG | E | 2 | 2 | $14,14,15$ | 0.27 | 0 | $17,19,21$ | 1.35 | $3(17 \%)$ |
| 2 | MAN | E | 3 | 2 | $11,11,12$ | 0.37 | 0 | $15,15,17$ | 1.34 | $1(6 \%)$ |
| 3 | NAG | F | 1 | 1,3 | $14,14,15$ | 0.29 | 0 | $17,19,21$ | 0.72 | 0 |
| 3 | NAG | F | 2 | 3 | $14,14,15$ | 0.28 | 0 | $17,19,21$ | 0.56 | 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 | C | 1 | 1,2 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 2 | NAG | C | 2 | 2 | - | $3 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 2 | MAN | C | 3 | 2 | - | $1 / 2 / 19 / 22$ | $0 / 1 / 1 / 1$ |
| 3 | NAG | D | 1 | 1,3 | - | $4 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 3 | NAG | D | 2 | 3 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 2 | NAG | E | 1 | 1,2 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 2 | NAG | E | 2 | 2 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 2 | MAN | E | 3 | 2 | - | $1 / 2 / 19 / 22$ | $0 / 1 / 1 / 1$ |
| 3 | NAG | F | 1 | 1,3 | - | $1 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 3 | NAG | F | 2 | 3 | - | $0 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $\operatorname{Observed}(\AA)$ | Ideal $(\AA)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | E | 1 | NAG | C1-C2 | 3.18 | 1.57 | 1.52 |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed $\left({ }^{\circ}\right)$ | Ideal $\left({ }^{\circ}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | C | 1 | NAG | O5-C1-C2 | -7.58 | 99.31 | 111.29 |
| 2 | C | 1 | NAG | C1-O5-C5 | -3.94 | 106.85 | 112.19 |
| 2 | E | 2 | NAG | O5-C1-C2 | -3.55 | 105.69 | 111.29 |
| 2 | C | 1 | NAG | C2-N2-C7 | -3.49 | 117.94 | 122.90 |
| 2 | E | 3 | MAN | O5-C5-C6 | 3.41 | 112.54 | 107.20 |

There are no chirality outliers.
5 of 18 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
| :---: | :---: | :---: | :---: | :---: |
| 2 | E | 2 | NAG | C1-C2-N2-C7 |
| 2 | C | 2 | NAG | C1-C2-N2-C7 |
| 3 | D | 2 | NAG | O5-C5-C6-O6 |
| 2 | C | 1 | NAG | O5-C5-C6-O6 |
| 3 | D | 2 | NAG | C4-C5-C6-O6 |

There are no ring outliers.
4 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 2 | C | 2 | NAG | 2 | 0 |
| 2 | E | 2 | NAG | 2 | 0 |
| 2 | C | 1 | NAG | 1 | 0 |
| 2 | E | 3 | MAN | 1 | 0 |

### 4.6 Ligand geometry (i)

12 ligands 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 | $\#\|Z\|>2$ |
| 4 | NAG | A | 2805 | 1 | $14,14,15$ | 0.43 | 0 | $17,19,21$ | 1.28 | $1(5 \%)$ |
| 4 | NAG | B | 2806 | 1 | $14,14,15$ | 0.43 | 0 | $17,19,21$ | 1.19 | $1(5 \%)$ |
| 4 | NAG | A | 2804 | 1 | $14,14,15$ | 0.35 | 0 | $17,19,21$ | 1.29 | $1(5 \%)$ |


| Mol | Type | Chain | Res | Link | Bond lengths |  |  | Bond angles |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 4 | NAG | A | 2802 | 1 | $14,14,15$ | 0.64 | 0 | $17,19,21$ | 1.97 | $4(23 \%)$ |
| 4 | NAG | A | 2801 | 1 | $14,14,15$ | 0.45 | 0 | $17,19,21$ | 0.72 | 0 |
| 4 | NAG | A | 2806 | 1 | $14,14,15$ | 0.40 | 0 | $17,19,21$ | 1.37 | $1(5 \%)$ |
| 4 | NAG | B | 2801 | 1 | $14,14,15$ | 0.46 | 0 | $17,19,21$ | 1.03 | $1(5 \%)$ |
| 4 | NAG | A | 2803 | 1 | $14,14,15$ | 0.48 | 0 | $17,19,21$ | 1.16 | $2(11 \%)$ |
| 4 | NAG | B | 2803 | 1 | $14,14,15$ | 0.42 | 0 | $17,19,21$ | 1.27 | $3(17 \%)$ |
| 4 | NAG | B | 2804 | 1 | $14,14,15$ | 0.62 | 0 | $17,19,21$ | 1.92 | $4(23 \%)$ |
| 4 | NAG | B | 2805 | 1 | $14,14,15$ | 0.63 | 0 | $17,19,21$ | 1.14 | $1(5 \%)$ |
| 4 | NAG | B | 2802 | 1 | $14,14,15$ | 0.44 | 0 | $17,19,21$ | 0.66 | 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 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | NAG | A | 2805 | 1 | - | $3 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | B | 2806 | 1 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | A | 2804 | 1 | - | $1 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | A | 2802 | 1 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | A | 2801 | 1 | - | $0 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | A | 2806 | 1 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | B | 2801 | 1 | - | $4 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | A | 2803 | 1 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | B | 2803 | 1 | - | $0 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | B | 2804 | 1 | - | $2 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | B | 2805 | 1 | - | $0 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |
| 4 | NAG | B | 2802 | 1 | - | $0 / 6 / 23 / 26$ | $0 / 1 / 1 / 1$ |

There are no bond length outliers.
The worst 5 of 19 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed $\left({ }^{\circ}\right)$ | Ideal $\left({ }^{\circ}\right)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | A | 2802 | NAG | C1-O5-C5 | 5.32 | 119.41 | 112.19 |
| 4 | B | 2804 | NAG | C1-O5-C5 | 5.23 | 119.27 | 112.19 |
| 4 | A | 2806 | NAG | C1-O5-C5 | 4.82 | 118.72 | 112.19 |
| 4 | A | 2804 | NAG | C1-O5-C5 | 4.45 | 118.22 | 112.19 |
| 4 | A | 2805 | NAG | C1-O5-C5 | 3.90 | 117.48 | 112.19 |

There are no chirality outliers.
5 of 18 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
| :---: | :---: | :---: | :---: | :---: |
| 4 | B | 2801 | NAG | C1-C2-N2-C7 |
| 4 | A | 2805 | NAG | C1-C2-N2-C7 |
| 4 | A | 2806 | NAG | O5-C5-C6-O6 |
| 4 | A | 2803 | NAG | O5-C5-C6-O6 |
| 4 | B | 2801 | NAG | O5-C5-C6-O6 |

There are no ring outliers.
5 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 4 | A | 2805 | NAG | 2 | 0 |
| 4 | B | 2806 | NAG | 2 | 0 |
| 4 | A | 2802 | NAG | 1 | 0 |
| 4 | B | 2801 | NAG | 2 | 0 |
| 4 | B | 2804 | NAG | 1 | 0 |

### 4.7 Other polymers (i)

There are no such residues in this entry.

### 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

## 5 Map visualisation

This section contains visualisations of the EMDB entry EMD-14145. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 5.1 Orthogonal projections (i)

This section was not generated.

### 5.2 Central slices (i)

This section was not generated.

### 5.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

### 5.5 Orthogonal surface views (i)

This section was not generated.

### 5.6 Mask visualisation (i)

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

## 6 Map analysis (i)

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

### 6.1 Map-value distribution (i)

This section was not generated.

### 6.2 Volume estimate versus contour level (i)

This section was not generated.

### 6.3 Rotationally averaged power spectrum (i)

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

## 7 Fourier-Shell correlation (i)

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

## 8 Map-model fit (i)

This section was not generated.

