

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 02:47 AM EDT

| PDB ID | : | 7KB6 |
|--------------|---|---|
| Title | : | Co-crystal structure of alpha glucosidase with compound 7 |
| Authors | : | Karade, S.S.; Mariuzza, R.A. |
| Deposited on | : | 2020-10-01 |
| Resolution | : | 2.20 Å(reported) |
| | | |

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

| MolProbity | : | 4.02b-467 |
|--------------------------------|---|--|
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| buster-report | : | 1.1.7(2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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.



| Motric | Whole archive | Similar resolution | | |
|-----------------------|---------------------|---|--|--|
| WIEthte | $(\# { m Entries})$ | $(\# { m Entries}, { m resolution} { m range}({ m \AA}))$ | | |
| R_{free} | 130704 | 4898 (2.20-2.20) | | |
| Clashscore | 141614 | 5594 (2.20-2.20) | | |
| Ramachandran outliers | 138981 | 5503 (2.20-2.20) | | |
| Sidechain outliers | 138945 | 5504 (2.20-2.20) | | |
| RSRZ outliers | 127900 | 4800 (2.20-2.20) | | |

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

| Mol | Chain | Length | Quality of chain | |
|-----|-------|--------|------------------|----------|
| 1 | А | 977 | 2% 78% | 9% 13% |
| 1 | С | 977 | 6% 78% | 9% • 12% |
| 2 | В | 554 | 3% 14% • 85% | |
| 2 | D | 554 | 3% 14% • 85% | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4 | EDO | А | 1222 | - | - | Х | - |
| 7 | SO4 | А | 1240 | - | - | - | Х |
| 7 | SO4 | С | 1234 | - | - | - | Х |
| 7 | SO4 | С | 1235 | - | - | Х | - |

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 16287 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

| Mol | Chain | Residues | | Α | toms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|-----------|-----------|---------|---------|-------|---|
| 1 | А | 850 | Total 6878 | C 4405 | N 1188 | 0 1256 | S 29 | 0 | 8 | 0 |
| 1 | С | 856 | Total 6848 | C 4391 | N 1179 | 0 1249 | S 29 | 0 | 6 | 0 |

• Molecule 1 is a protein called Isoform 2 of Neutral alpha-glucosidase AB.

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|--------------|
| А | 2 | MET | - | initiating methionine | UNP Q8BHN3-2 |
| А | 3 | GLY | - | expression tag | UNP Q8BHN3-2 |
| А | 4 | ILE | - | expression tag | UNP Q8BHN3-2 |
| А | 5 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 6 | PRO | - | expression tag | UNP Q8BHN3-2 |
| А | 7 | SER | - | expression tag | UNP Q8BHN3-2 |
| А | 8 | PRO | - | expression tag | UNP Q8BHN3-2 |
| A | 9 | GLY | - | expression tag | UNP Q8BHN3-2 |
| А | 10 | MET | - | expression tag | UNP Q8BHN3-2 |
| А | 11 | PRO | - | expression tag | UNP Q8BHN3-2 |
| А | 12 | ALA | - | expression tag | UNP Q8BHN3-2 |
| А | 13 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 14 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 15 | SER | - | expression tag | UNP Q8BHN3-2 |
| A | 16 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 17 | VAL | - | expression tag | UNP Q8BHN3-2 |
| А | 18 | SER | - | expression tag | UNP Q8BHN3-2 |
| А | 19 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 20 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 21 | SER | - | expression tag | UNP Q8BHN3-2 |
| А | 22 | VAL | - | expression tag | UNP Q8BHN3-2 |
| А | 23 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 24 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 25 | MET | - | expression tag | UNP Q8BHN3-2 |
| А | 26 | GLY | - | expression tag | UNP Q8BHN3-2 |

There are 88 discrepancies between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|--------------|
| А | 27 | CYS | - | expression tag | UNP Q8BHN3-2 |
| А | 28 | VAL | - | expression tag | UNP Q8BHN3-2 |
| А | 29 | ALA | - | expression tag | UNP Q8BHN3-2 |
| А | 30 | GLU | - | expression tag | UNP Q8BHN3-2 |
| А | 31 | THR | _ | expression tag | UNP Q8BHN3-2 |
| А | 32 | GLY | - | expression tag | UNP Q8BHN3-2 |
| А | 97 | ASP | ASN | engineered mutation | UNP Q8BHN3-2 |
| А | 967 | SER | - | expression tag | UNP Q8BHN3-2 |
| А | 968 | ALA | - | expression tag | UNP Q8BHN3-2 |
| А | 969 | TRP | - | expression tag | UNP Q8BHN3-2 |
| А | 970 | SER | - | expression tag | UNP Q8BHN3-2 |
| А | 971 | HIS | - | expression tag | UNP Q8BHN3-2 |
| А | 972 | PRO | - | expression tag | UNP Q8BHN3-2 |
| А | 973 | GLN | - | expression tag | UNP Q8BHN3-2 |
| А | 974 | PHE | - | expression tag | UNP Q8BHN3-2 |
| А | 975 | GLU | - | expression tag | UNP Q8BHN3-2 |
| А | 976 | LYS | - | expression tag | UNP Q8BHN3-2 |
| А | 977 | LEU | - | expression tag | UNP Q8BHN3-2 |
| А | 978 | GLU | - | expression tag | UNP Q8BHN3-2 |
| С | 2 | MET | - | initiating methionine | UNP Q8BHN3-2 |
| С | 3 | GLY | - | expression tag | UNP Q8BHN3-2 |
| С | 4 | ILE | - | expression tag | UNP Q8BHN3-2 |
| С | 5 | LEU | - | expression tag | UNP Q8BHN3-2 |
| С | 6 | PRO | - | expression tag | UNP Q8BHN3-2 |
| С | 7 | SER | - | expression tag | UNP Q8BHN3-2 |
| С | 8 | PRO | - | expression tag | UNP Q8BHN3-2 |
| C | 9 | GLY | - | expression tag | UNP Q8BHN3-2 |
| C | 10 | MET | - | expression tag | UNP Q8BHN3-2 |
| С | 11 | PRO | - | expression tag | UNP Q8BHN3-2 |
| С | 12 | ALA | - | expression tag | UNP Q8BHN3-2 |
| С | 13 | LEU | - | expression tag | UNP Q8BHN3-2 |
| С | 14 | LEU | - | expression tag | UNP Q8BHN3-2 |
| C | 15 | SER | _ | expression tag | UNP Q8BHN3-2 |
| C | 16 | LEU | - | expression tag | UNP Q8BHN3-2 |
| C | 17 | VAL | - | expression tag | UNP Q8BHN3-2 |
| C | 18 | SER | - | expression tag | UNP Q8BHN3-2 |
| C | 19 | | - | expression tag | UNP Q8BHN3-2 |
| C | 20 | LEU | - | expression tag | UNP Q8BHN3-2 |
| C | 21 | SER | - | expression tag | UNP Q8BHN3-2 |
| C | 22 | VAL | - | expression tag | UNP Q8BHN3-2 |
| C | 23 | | - | expression tag | UNP Q8BHN3-2 |
| C | 24 | LEU | - | expression tag | UNP Q8BHN3-2 |



| Chain | Residue | Modelled | Actual Comment | | Reference |
|-------|---------|----------|----------------|---------------------|--------------|
| С | 25 | MET | - | expression tag | UNP Q8BHN3-2 |
| С | 26 | GLY | - | expression tag | UNP Q8BHN3-2 |
| С | 27 | CYS | - | expression tag | UNP Q8BHN3-2 |
| С | 28 | VAL | - | expression tag | UNP Q8BHN3-2 |
| С | 29 | ALA | - | expression tag | UNP Q8BHN3-2 |
| С | 30 | GLU | - | expression tag | UNP Q8BHN3-2 |
| С | 31 | THR | - | expression tag | UNP Q8BHN3-2 |
| С | 32 | GLY | - | expression tag | UNP Q8BHN3-2 |
| С | 97 | ASP | ASN | engineered mutation | UNP Q8BHN3-2 |
| С | 967 | SER | - | expression tag | UNP Q8BHN3-2 |
| С | 968 | ALA | - | expression tag | UNP Q8BHN3-2 |
| С | 969 | TRP | - | expression tag | UNP Q8BHN3-2 |
| С | 970 | SER | - | expression tag | UNP Q8BHN3-2 |
| С | 971 | HIS | - | expression tag | UNP Q8BHN3-2 |
| С | 972 | PRO | - | expression tag | UNP Q8BHN3-2 |
| С | 973 | GLN | - | expression tag | UNP Q8BHN3-2 |
| С | 974 | PHE | - | expression tag | UNP Q8BHN3-2 |
| С | 975 | GLU | - | expression tag | UNP Q8BHN3-2 |
| С | 976 | LYS | - | expression tag | UNP Q8BHN3-2 |
| С | 977 | LEU | - | expression tag | UNP Q8BHN3-2 |
| С | 978 | GLU | - | expression tag | UNP Q8BHN3-2 |

• Molecule 2 is a protein called Glucosidase 2 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--------------|---------|---------|-------|
| 2 | В | B 83 | Total | С | Ν | 0 | S | 0 | 0 | 0 |
| _ | | | 575 | 338 | 95 | 132 | 10 | 0 | Ŭ | Ŭ |
| 2 | | 02 | Total | С | Ν | Ο | \mathbf{S} | 0 | 0 | 0 |
| 2 D | 00 | 591 | 353 | 95 | 133 | 10 | 0 | | 0 | |

There are 102 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| В | -16 | MET | - | initiating methionine | UNP 008795 |
| В | -15 | GLY | - | expression tag | UNP 008795 |
| В | -14 | ILE | - | expression tag | UNP 008795 |
| В | -13 | LEU | - | expression tag | UNP 008795 |
| В | -12 | PRO | - | expression tag | UNP 008795 |
| В | -11 | SER | - | expression tag | UNP 008795 |
| В | -10 | PRO | - | expression tag | UNP 008795 |
| В | -9 | GLY | - | expression tag | UNP 008795 |
| В | -8 | MET | - | expression tag | UNP 008795 |



| Comment | Reference |
|---------------|------------|
| xpression tag | UNP 008795 |
| | |

Continued from previous page... Chain Residue Modelled Actual

| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | -7 | PRO | - | expression tag | UNP 008795 |
|--|---|-----|-----|---|----------------|------------|
| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | -6 | ALA | - | expression tag | UNP 008795 |
| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | -5 | LEU | - | expression tag | UNP 008795 |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$ | В | -4 | LEU | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | -3 | SER | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | -2 | LEU | - | expression tag | UNP 008795 |
| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | -1 | VAL | - | expression tag | UNP 008795 |
| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 0 | SER | - | expression tag | UNP 008795 |
| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 1 | LEU | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 2 | LEU | - | expression tag | UNP 008795 |
| $ \begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 3 | SER | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 4 | VAL | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 5 | LEU | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 6 | LEU | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 7 | MET | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 8 | GLY | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 9 | CYS | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 10 | VAL | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 11 | ALA | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 12 | GLU | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 13 | THR | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 14 | GLY | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 518 | SER | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 519 | ALA | - | expression tag | UNP 008795 |
| $\begin{array}{c c c c c c c c c c c c c c c c c c c $ | В | 520 | TRP | - | expression tag | UNP 008795 |
| B 522 HIS-expression tagUNP 008795B 523 PRO-expression tagUNP 008795B 524 GLN-expression tagUNP 008795B 525 PHE-expression tagUNP 008795B 526 GLU-expression tagUNP 008795B 526 GLU-expression tagUNP 008795B 527 LYS-expression tagUNP 008795B 528 LEU-expression tagUNP 008795B 529 GLU-expression tagUNP 008795B 530 THR-expression tagUNP 008795B 531 LYS-expression tagUNP 008795B 532 HIS-expression tagUNP 008795B 533 HIS-expression tagUNP 008795B 534 HIS-expression tagUNP 008795B 536 HIS-expression tagUNP 008795B 536 HIS-expression tagUNP 008795B 537 HIS-expression tagUNP 008795 | В | 521 | SER | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 522 | HIS | - | expression tag | UNP 008795 |
| $\begin{array}{ c c c c c c c c c c c c c c c c c c c$ | В | 523 | PRO | - | expression tag | UNP 008795 |
| B525PHE-expression tagUNP 008795B526GLU-expression tagUNP 008795B527LYS-expression tagUNP 008795B528LEU-expression tagUNP 008795B529GLU-expression tagUNP 008795B530THR-expression tagUNP 008795B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 524 | GLN | - | expression tag | UNP 008795 |
| B526GLU-expression tagUNP 008795B527LYS-expression tagUNP 008795B528LEU-expression tagUNP 008795B529GLU-expression tagUNP 008795B530THR-expression tagUNP 008795B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 525 | PHE | - | expression tag | UNP 008795 |
| B527LYS-expression tagUNP 008795B528LEU-expression tagUNP 008795B529GLU-expression tagUNP 008795B530THR-expression tagUNP 008795B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 526 | GLU | - | expression tag | UNP 008795 |
| B528LEU-expression tagUNP 008795B529GLU-expression tagUNP 008795B530THR-expression tagUNP 008795B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 527 | LYS | - | expression tag | UNP 008795 |
| B529GLU-expression tagUNP 008795B530THR-expression tagUNP 008795B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 528 | LEU | - | expression tag | UNP 008795 |
| B530THR-expression tagUNP 008795B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 529 | GLU | - | expression tag | UNP 008795 |
| B531LYS-expression tagUNP 008795B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 530 | THR | - | expression tag | UNP 008795 |
| B532HIS-expression tagUNP 008795B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 531 | LYS | - | expression tag | UNP 008795 |
| B533HIS-expression tagUNP 008795B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 532 | HIS | - | expression tag | UNP 008795 |
| B534HIS-expression tagUNP 008795B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 533 | HIS | - | expression tag | UNP 008795 |
| B535HIS-expression tagUNP 008795B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 534 | HIS | - | expression tag | UNP 008795 |
| B536HIS-expression tagUNP 008795B537HIS-expression tagUNP 008795 | В | 535 | HIS | - | expression tag | UNP 008795 |
| B537HIS-expression tagUNP 008795 | В | 536 | HIS | - | expression tag | UNP 008795 |
| | В | 537 | HIS | - | expression tag | UNP 008795 |



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| D | -16 | MET | - | initiating methionine | UNP 008795 |
| D | -15 | GLY | - | expression tag | UNP 008795 |
| D | -14 | ILE | - | expression tag | UNP 008795 |
| D | -13 | LEU | - | expression tag | UNP 008795 |
| D | -12 | PRO | - | expression tag | UNP 008795 |
| D | -11 | SER | - | expression tag | UNP 008795 |
| D | -10 | PRO | - | expression tag | UNP 008795 |
| D | -9 | GLY | - | expression tag | UNP 008795 |
| D | -8 | MET | - | expression tag | UNP 008795 |
| D | -7 | PRO | - | expression tag | UNP 008795 |
| D | -6 | ALA | - | expression tag | UNP 008795 |
| D | -5 | LEU | - | expression tag | UNP 008795 |
| D | -4 | LEU | - | expression tag | UNP 008795 |
| D | -3 | SER | - | expression tag | UNP 008795 |
| D | -2 | LEU | - | expression tag | UNP 008795 |
| D | -1 | VAL | - | expression tag | UNP 008795 |
| D | 0 | SER | - | expression tag | UNP 008795 |
| D | 1 | LEU | - | expression tag | UNP 008795 |
| D | 2 | LEU | - | expression tag | UNP 008795 |
| D | 3 | SER | - | expression tag | UNP 008795 |
| D | 4 | VAL | - | expression tag | UNP 008795 |
| D | 5 | LEU | - | expression tag | UNP 008795 |
| D | 6 | LEU | - | expression tag | UNP 008795 |
| D | 7 | MET | - | expression tag | UNP 008795 |
| D | 8 | GLY | - | expression tag | UNP 008795 |
| D | 9 | CYS | - | expression tag | UNP 008795 |
| D | 10 | VAL | - | expression tag | UNP 008795 |
| D | 11 | ALA | - | expression tag | UNP 008795 |
| D | 12 | GLU | - | expression tag | UNP 008795 |
| D | 13 | THR | - | expression tag | UNP 008795 |
| D | 14 | GLY | - | expression tag | UNP 008795 |
| D | 518 | SER | - | expression tag | UNP 008795 |
| D | 519 | ALA | - | expression tag | UNP 008795 |
| D | 520 | TRP | - | expression tag | UNP 008795 |
| D | 521 | SER | - | expression tag | UNP 008795 |
| D | 522 | HIS | - | expression tag | UNP 008795 |
| D | 523 | PRO | - | expression tag | UNP 008795 |
| D | 524 | GLN | - | expression tag | UNP 008795 |
| D | 525 | PHE | - | expression tag | UNP 008795 |
| D | 526 | GLU | - | expression tag | UNP 008795 |
| D | 527 | LYS | - | expression tag | UNP 008795 |
| D | 528 | LEU | - | expression tag | UNP 008795 |



| 7KB6 | |
|------|--|
|------|--|

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| D | 529 | GLU | - | expression tag | UNP 008795 |
| D | 530 | THR | - | expression tag | UNP 008795 |
| D | 531 | LYS | - | expression tag | UNP 008795 |
| D | 532 | HIS | - | expression tag | UNP 008795 |
| D | 533 | HIS | - | expression tag | UNP 008795 |
| D | 534 | HIS | - | expression tag | UNP 008795 |
| D | 535 | HIS | - | expression tag | UNP 008795 |
| D | 536 | HIS | - | expression tag | UNP 008795 |
| D | 537 | HIS | - | expression tag | UNP 008795 |

• Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 3 | А | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | А | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | А | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | А | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | А | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | С | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | С | 1 | Total C O 10 6 4 | 0 | 0 |



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 3 | С | 1 | Total C O 10 6 4 | 0 | 0 |
| 3 | D | 1 | Total C O 10 6 4 | 0 | 0 |

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |



Continued from previous page...

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | А | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | В | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{c ccc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 4 & 2 & 2 \end{array}$ | 0 | 0 |



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---|---------|---------|
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | С | 1 | $\begin{array}{ccc} \overline{\text{Total}} & \mathrm{C} & \mathrm{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |
| 4 | D | 1 | $\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$ | 0 | 0 |

• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | А | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | В | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |
| 5 | С | 1 | $\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$ | 0 | 0 |



• Molecule 6 is (1S,2S,3R,4S,5S)-1-(hydroxymethyl)-5-[(6-{[2-nitro-4-(pyrimidin-2-yl)p henyl]amino}hexyl)amino]cyclohexane-1,2,3,4-tetrol (three-letter code: XOD) (formula: C₂₃H₃₃N₅O₇) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|---------|
| 6 | А | 1 | Total 35 | C 23 | N 5 | O 7 | 0 | 0 |
| 6 | С | 1 | Total 35 | C 23 | N 5 | 0 7 | 0 | 0 |

• Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





| Mol | Chain | Residues | Ato | \mathbf{ms} | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------------------|------------------|---------|---------|
| 7 | А | 1 | Total | 0 | S 1 | 0 | 0 |
| - | • | 1 | D Total | $\frac{4}{0}$ | $\frac{1}{S}$ | 0 | 0 |
| (| А | 1 | 5 | 4 | 1 | 0 | 0 |
| 7 | А | 1 | Total 5 | O 4 | ${ m S}$ | 0 | 0 |
| 7 | А | 1 | Total 5 | 0 4 | S 1 | 0 | 0 |
| 7 | В | 1 | Total 5 | 0 4 | S 1 | 0 | 0 |
| 7 | С | 1 | Total 5 | 0 4 | S 1 | 0 | 0 |
| 7 | С | 1 | Total 5 | \overline{O} 4 | \overline{S} 1 | 0 | 0 |
| 7 | С | 1 | Total 5 | \overline{O} 4 | S 1 | 0 | 0 |
| 7 | С | 1 | Total 5 | 0 4 | S 1 | 0 | 0 |
| 7 | С | 1 | Total 5 | 0 4 | S 1 | 0 | 0 |

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8 | В | 2 | Total Ca 2 2 | 0 | 0 |
| 8 | D | 2 | Total Ca 2 2 | 0 | 0 |

• Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).





| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--|---------|---------|
| 9 | В | 1 | Total C O 13 8 5 | 0 | 0 |
| 9 | С | 1 | Total C O 13 8 5 | 0 | 0 |

• Molecule 10 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 10 | А | 438 | Total O 438 438 | 0 | 0 |
| 10 | В | 28 | TotalO2828 | 0 | 0 |
| 10 | С | 379 | Total O 379 379 | 0 | 0 |
| 10 | D | 32 | Total O 32 32 | 0 | 0 |



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Isoform 2 of Neutral alpha-glucosidase AB

• Molecule 1: Isoform 2 of Neutral alpha-glucosidase AB





| THR LLVS LLVS LLVS LLVS LLVS LLVS LLVS LLVS LLVS P245 P245 P245 P245 P263 P |
|--|
| 1388 1404 1407 1407 1407 1407 1407 1407 1407 1407 1407 1407 1407 1407 1407 1407 1407 1417 1425 1426 1445 1455 1456 1456 1457 |
| W685 W685 L701 L711 L711 L711 L711 P756 P756 P756 P756 P756 P756 P756 P756 |
| • Molecule 2: Glucosidase 2 subunit beta |
| Chain B: 14% • 85% |
| MET LEU LEU PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO |
| D54 661 661 661 710 661 710 710 710 710 7115 7115 7115 7115 7115 7115 7115 7103 7115 7103 7115 |
| GLU LEU LEU LEU LEU LEU LEU LEU CLEU CLEU |
| ALA ALA SALA SALA ALA ALA ALA ALA ALA AL |
| ALA ALA ALA ALA ASP ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG |
| PRO LEU CALU PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO |
| ASP ASP CRU CRU CRU CRU CRU CRU CRU CRU CRU CRU |
| SER ALA ALA ALA ALA ALA ALA CUV GLU GLU GLU ARA ARA ARA ARA ARA CVS ARA ARA ALA ALA ALA ALA ALA ALA ALA ALA |
| SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP |
| • Molecule 2: Glucosidase 2 subunit beta |
| Chain D: 14% • 85% |
| MET ILLE ILLE ILLE PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO |
| CS6 C56 C70 C70 C70 C70 C70 C70 C70 C70 C70 C70 |
| LEU LEU LEU CLU CLU CLU CLU CLU CLU CLU CLU CLU CL |
| |

ALA TTRP SER. HISS PRO GLN CLN GLU LVS GLU LVS GLU LVS HISS HISS HISS HISS HISS



4 Data and refinement statistics (i)

| Property | Value | Source |
|--|--|-----------|
| Space group | P 32 | Depositor |
| Cell constants | 102.91Å 102.91Å 239.83Å | Deperitor |
| a, b, c, α , β , γ | 90.00° 90.00° 120.00° | Depositor |
| $\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$ | 44.56 - 2.20 | Depositor |
| Resolution (A) | 44.56 - 2.20 | EDS |
| % Data completeness | 97.5 (44.56-2.20) | Depositor |
| (in resolution range) | 92.0(44.56-2.20) | EDS |
| R_{merge} | 0.13 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | $1.01 (at 2.20 \text{\AA})$ | Xtriage |
| Refinement program | PHENIX 1.18.2_3874 | Depositor |
| B B c | 0.167 , 0.194 | Depositor |
| It, Itfree | 0.167 , 0.194 | DCC |
| R_{free} test set | 1958 reflections $(1.39%)$ | wwPDB-VP |
| Wilson B-factor $(Å^2)$ | 33.1 | Xtriage |
| Anisotropy | 0.300 | Xtriage |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$ | 0.33 , 45.5 | EDS |
| L-test for $twinning^2$ | $< L > = 0.49, < L^2 > = 0.32$ | Xtriage |
| | 0.009 for -h,-k,l | |
| Estimated twinning fraction | 0.037 for h,-h-k,-l | Xtriage |
| | 0.022 for -k,-h,-l | |
| F_o, F_c correlation | 0.96 | EDS |
| Total number of atoms | 16287 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 43.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, PGE, SO4, CA, XOD, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mal | Chain | Bond | lengths | Bond angles | |
|-----------|-------|------|----------|-------------|----------|
| Moi Chain | | RMSZ | # Z > 5 | RMSZ | # Z > 5 |
| 1 | А | 0.27 | 0/7095 | 0.48 | 0/9663 |
| 1 | С | 0.27 | 0/7069 | 0.47 | 0/9636 |
| 2 | В | 0.25 | 0/585 | 0.53 | 0/803 |
| 2 | D | 0.28 | 0/603 | 0.51 | 0/826 |
| All | All | 0.27 | 0/15352 | 0.48 | 0/20928 |

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 (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | А | 6878 | 0 | 6592 | 52 | 0 |
| 1 | С | 6848 | 0 | 6532 | 62 | 0 |
| 2 | В | 575 | 0 | 457 | 4 | 0 |
| 2 | D | 591 | 0 | 474 | 3 | 0 |
| 3 | А | 50 | 0 | 70 | 3 | 0 |
| 3 | С | 30 | 0 | 42 | 1 | 0 |
| 3 | D | 10 | 0 | 14 | 0 | 0 |
| 4 | А | 96 | 0 | 140 | 12 | 0 |
| 4 | B | 4 | 0 | 6 | 0 | 0 |



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | С | 76 | 0 | 113 | 13 | 0 |
| 4 | D | 4 | 0 | 6 | 0 | 0 |
| 5 | А | 49 | 0 | 70 | 6 | 0 |
| 5 | В | 7 | 0 | 10 | 0 | 0 |
| 5 | С | 42 | 0 | 60 | 6 | 0 |
| 6 | А | 35 | 0 | 0 | 1 | 0 |
| 6 | С | 35 | 0 | 0 | 0 | 0 |
| 7 | А | 20 | 0 | 0 | 0 | 0 |
| 7 | В | 5 | 0 | 0 | 0 | 0 |
| 7 | С | 25 | 0 | 0 | 2 | 0 |
| 8 | В | 2 | 0 | 0 | 0 | 0 |
| 8 | D | 2 | 0 | 0 | 0 | 0 |
| 9 | В | 13 | 0 | 18 | 0 | 0 |
| 9 | С | 13 | 0 | 18 | 2 | 0 |
| 10 | А | 438 | 0 | 0 | 4 | 0 |
| 10 | В | 28 | 0 | 0 | 2 | 0 |
| 10 | С | 379 | 0 | 0 | 18 | 0 |
| 10 | D | 32 | 0 | 0 | 0 | 0 |
| All | All | 16287 | 0 | 14622 | 129 | 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 (129) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic | Clash |
|-----------------|------------------|----------------|-------------|
| | 1100111-2 | distance $(Å)$ | overlap (Å) |
| 1:A:910:TRP:HE1 | 4:A:1222:EDO:H12 | 1.25 | 0.99 |
| 1:C:104:ASP:OD2 | 10:C:1302:HOH:O | 1.92 | 0.88 |
| 1:A:180:HIS:O | 10:A:1301:HOH:O | 1.92 | 0.84 |
| 1:C:407:THR:H | 4:C:1209:EDO:H21 | 1.40 | 0.84 |
| 1:A:97:ASP:OD2 | 10:A:1302:HOH:O | 2.04 | 0.75 |
| 1:C:500:ARG:HB3 | 5:C:1217:PEG:H21 | 1.67 | 0.75 |
| 7:C:1235:SO4:O3 | 10:C:1304:HOH:O | 2.03 | 0.75 |
| 1:A:588:TRP:HE1 | 3:A:1201:PGE:H52 | 1.52 | 0.73 |
| 1:C:385:ASP:OD2 | 10:C:1305:HOH:O | 2.07 | 0.71 |
| 9:C:1230:PG4:O5 | 10:C:1307:HOH:O | 2.09 | 0.71 |
| 1:A:802:GLN:NE2 | 10:A:1307:HOH:O | 2.24 | 0.71 |
| 7:C:1235:SO4:O1 | 10:C:1308:HOH:O | 2.11 | 0.69 |
| 4:C:1215:EDO:O1 | 10:C:1306:HOH:O | 2.07 | 0.67 |
| 1:C:112:ARG:NH2 | 1:C:179:GLU:O | 2.27 | 0.67 |
| 1:C:796:GLU:OE1 | 10:C:1309:HOH:O | 2.13 | 0.67 |



| | 1 J | Interatomic | Clash |
|--------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:C:399:ARG:NH1 | 10:C:1321:HOH:O | 2.29 | 0.64 |
| 1:A:682:LEU:HD23 | 1:A:711:LEU:HD11 | 1.81 | 0.63 |
| 1:A:960:ASP:HB3 | 5:A:1215:PEG:H12 | 1.81 | 0.63 |
| 1:A:112:ARG:NH2 | 1:A:179:GLU:O | 2.33 | 0.62 |
| 1:C:110:ARG:NH2 | 10:C:1327:HOH:O | 2.33 | 0.60 |
| 1:A:447:VAL:HG11 | 1:A:486:VAL:HG23 | 1.85 | 0.59 |
| 1:C:423:TRP:O | 1:C:701:LEU:HA | 2.03 | 0.59 |
| 1:C:945:THR:O | 10:C:1310:HOH:O | 2.17 | 0.58 |
| 1:C:484:LYS:HZ1 | 4:C:1204:EDO:H12 | 1.69 | 0.57 |
| 1:A:293:THR:HG22 | 4:A:1219:EDO:H12 | 1.86 | 0.57 |
| 1:A:849:PRO:HD3 | 4:A:1222:EDO:H11 | 1.86 | 0.57 |
| 1:C:247:ALA:HB1 | 1:C:263:PRO:HG3 | 1.86 | 0.57 |
| 1:A:423:TRP:O | 1:A:701:LEU:HA | 2.04 | 0.57 |
| 5:C:1206:PEG:H22 | 3:C:1208:PGE:H12 | 1.87 | 0.57 |
| 1:C:682:LEU:HD23 | 1:C:711:LEU:HD11 | 1.86 | 0.56 |
| 1:C:327:HIS:ND1 | 1:C:332:ASP:OD1 | 2.36 | 0.55 |
| 1:A:701:LEU:HD23 | 4:A:1213:EDO:H21 | 1.89 | 0.54 |
| 1:C:91:LEU:HD21 | 1:C:149:ILE:HG21 | 1.89 | 0.53 |
| 1:C:168:LEU:HD11 | 1:C:388:LEU:HD13 | 1.89 | 0.53 |
| 1:C:336:PHE:HB3 | 1:C:387:PHE:HB2 | 1.90 | 0.53 |
| 1:C:442:ASN:OD1 | 5:C:1211:PEG:H12 | 2.09 | 0.53 |
| 1:C:458:LYS:HG2 | 1:C:525:TRP:HB3 | 1.91 | 0.53 |
| 1:C:58:SER:HB2 | 1:C:174:GLY:HA2 | 1.91 | 0.52 |
| 1:A:523:TRP:HE1 | 5:A:1214:PEG:H41 | 1.74 | 0.52 |
| 2:B:35:LYS:N | 10:B:702:HOH:O | 2.42 | 0.52 |
| 1:A:458:LYS:HG2 | 1:A:525:TRP:HB3 | 1.93 | 0.51 |
| 1:A:721:ASP:OD1 | 5:A:1212:PEG:O1 | 2.19 | 0.51 |
| 1:A:370:THR:N | 1:A:371:PRO:HD2 | 2.26 | 0.51 |
| 1:A:67:LEU:HD21 | 1:A:74:LEU:HD11 | 1.93 | 0.51 |
| 1:A:54:ARG:HH22 | 4:A:1218:EDO:H21 | 1.74 | 0.51 |
| 1:C:960:ASP:HB3 | 5:C:1202:PEG:H41 | 1.93 | 0.51 |
| 1:C:460:TYR:CE2 | 1:C:490:ASP:HB2 | 2.46 | 0.51 |
| 1:C:892:SER:N | 10:C:1303:HOH:O | 1.98 | 0.50 |
| 1:A:424:ASN:OD1 | 1:A:451:ASP:HB3 | 2.12 | 0.50 |
| 1:A:168:LEU:HD11 | 1:A:388:LEU:HD13 | 1.94 | 0.49 |
| 1:C:930:LYS:HD3 | 1:C:960:ASP:HB2 | 1.95 | 0.49 |
| 5:C:1211:PEG:H11 | 2:D:90:SER:OG | 2.12 | 0.49 |
| 1:C:114:ARG:HH12 | 4:C:1214:EDO:H12 | 1.77 | 0.49 |
| 1:C:756:PRO:HD2 | 4:C:1227:EDO:H22 | 1.94 | 0.48 |
| 1:A:58:SER:HB2 | 1:A:174:GLY:HA2 | 1.95 | 0.48 |
| 1:C:721[B]:ASP:OD1 | 4:C:1201:EDO:O2 | 2.16 | 0.48 |



| | A de la compage | Interatomic | Clash |
|--------------------|--------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:250:GLU:OE1 | 1:A:259:LYS:NZ | 2.33 | 0.48 |
| 1:A:278:VAL:HG22 | 4:A:1232:EDO:H21 | 1.96 | 0.48 |
| 4:A:1222:EDO:O1 | 2:B:54:ASP:OD2 | 2.29 | 0.48 |
| 1:C:721[A]:ASP:OD1 | 10:C:1311:HOH:O | 2.19 | 0.48 |
| 1:A:171:ASN:HA | 1:A:269:ASP:OD1 | 2.14 | 0.47 |
| 1:C:297:GLU:O | 4:C:1225:EDO:O2 | 2.22 | 0.47 |
| 1:C:426:ARG:NH2 | 10:C:1344:HOH:O | 2.47 | 0.47 |
| 1:C:447:VAL:HG11 | 1:C:486:VAL:HG23 | 1.96 | 0.47 |
| 1:C:74:LEU:HD13 | 1:C:140:LEU:HD21 | 1.96 | 0.47 |
| 1:C:964[A]:HIS:CD2 | 1:C:966:ARG:HG2 | 2.50 | 0.46 |
| 1:C:560:TYR:OH | 4:C:1204:EDO:H11 | 2.14 | 0.46 |
| 1:C:311:LEU:HD22 | 1:C:650:ILE:HD13 | 1.98 | 0.46 |
| 1:A:432:LEU:HD22 | 1:A:477[A]:HIS:ND1 | 2.30 | 0.46 |
| 1:A:910:TRP:NE1 | 4:A:1222:EDO:H12 | 2.09 | 0.46 |
| 1:C:423:TRP:CD2 | 1:C:701:LEU:HB2 | 2.51 | 0.46 |
| 1:C:114:ARG:HH22 | 4:C:1214:EDO:H12 | 1.79 | 0.46 |
| 1:A:523:TRP:NE1 | 5:A:1214:PEG:H41 | 2.30 | 0.46 |
| 1:A:459:ARG:NH1 | 1:A:494:LYS:HE2 | 2.31 | 0.46 |
| 1:C:879:ARG:NH2 | 10:C:1342:HOH:O | 2.46 | 0.46 |
| 1:C:171:ASN:HA | 1:C:269:ASP:OD1 | 2.16 | 0.46 |
| 1:C:484:LYS:NZ | 4:C:1204:EDO:H12 | 2.31 | 0.45 |
| 2:D:61:GLY:HA2 | 2:D:70:CYS:SG | 2.57 | 0.45 |
| 1:A:318:TYR:CE2 | 1:A:639:GLY:HA3 | 2.51 | 0.45 |
| 1:C:814:TYR:CE2 | 10:C:1301:HOH:O | 2.69 | 0.45 |
| 1:C:158:LEU:HB2 | 1:C:170:VAL:HB | 1.99 | 0.45 |
| 1:C:846:LYS:HB2 | 4:C:1203:EDO:H11 | 1.99 | 0.45 |
| 1:A:159:ASP:OD2 | 10:A:1304:HOH:O | 2.21 | 0.45 |
| 1:C:102:ARG:HA | 1:C:384:ILE:O | 2.16 | 0.44 |
| 1:C:847:ASP:HB3 | 1:C:908:PRO:HG2 | 1.99 | 0.44 |
| 1:C:720:ARG:HG2 | 4:C:1201:EDO:H22 | 1.99 | 0.44 |
| 1:C:426:ARG:NH2 | 10:C:1313:HOH:O | 2.29 | 0.44 |
| 1:A:287:SER:HB3 | 4:A:1229:EDO:H21 | 1.99 | 0.44 |
| 1:A:460:TYR:CE2 | 1:A:490:ASP:HB2 | 2.52 | 0.44 |
| 1:A:485:LEU:HD23 | 1:A:486:VAL:N | 2.33 | 0.44 |
| 1:A:520:TYR:HE2 | 1:A:579:LEU:HD12 | 1.82 | 0.44 |
| 1:C:72:ASP:O | 10:C:1312:HOH:O | 2.21 | 0.44 |
| 1:C:632:ARG:HD2 | 4:C:1209:EDO:H22 | 2.00 | 0.43 |
| 1:C:485:LEU:HD23 | 1:C:486:VAL:N | 2.33 | 0.43 |
| 2:B:61:GLY:HA2 | 2:B:70:CYS:SG | 2.59 | 0.43 |
| 1:C:499:TYR:CD1 | 5:C:1217:PEG:H22 | 2.53 | 0.43 |
| 1:A:450:LEU:HG | 1:A:485:LEU:HD21 | 2.00 | 0.43 |



| A 4 amo 1 | A4 ama 2 | Interatomic | Clash |
|--------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:A:336:PHE:HB3 | 1:A:387:PHE:HB2 | 1.99 | 0.43 |
| 1:C:534:PHE:HB3 | 1:C:600:TYR:HB3 | 2.01 | 0.43 |
| 1:C:892:SER:HB3 | 1:C:965:LEU:HB2 | 1.99 | 0.43 |
| 1:A:50:GLN:O | 1:A:376:ARG:NH2 | 2.52 | 0.42 |
| 1:A:846:LYS:HB2 | 4:A:1225:EDO:H11 | 2.01 | 0.42 |
| 5:A:1212:PEG:H42 | 5:A:1212:PEG:H21 | 1.64 | 0.42 |
| 9:C:1230:PG4:H32 | 2:D:56:CYS:SG | 2.60 | 0.42 |
| 1:C:891:GLY:HA3 | 10:C:1303:HOH:O | 2.20 | 0.42 |
| 1:A:567:GLU:N | 1:A:568:PRO:HA | 2.35 | 0.42 |
| 1:A:294:GLU:HA | 4:A:1218:EDO:O1 | 2.20 | 0.41 |
| 1:A:320:SER:O | 1:A:627:PHE:HA | 2.20 | 0.41 |
| 1:C:152:THR:HB | 1:C:157:ARG:HB3 | 2.00 | 0.41 |
| 1:A:278:VAL:HG23 | 1:A:290:LEU:HB2 | 2.02 | 0.41 |
| 1:A:154:GLN:HA | 1:A:155:PRO:HA | 1.95 | 0.41 |
| 1:A:755:TYR:HH | 1:A:798:TRP:HZ2 | 1.65 | 0.41 |
| 5:A:1214:PEG:H22 | 6:A:1237:XOD:C19 | 2.51 | 0.41 |
| 1:A:453:GLU:OE1 | 1:A:458:LYS:NZ | 2.49 | 0.41 |
| 1:C:450:LEU:HG | 1:C:485:LEU:HD21 | 2.01 | 0.41 |
| 1:A:648:LEU:HD13 | 1:A:685:TRP:CG | 2.56 | 0.41 |
| 1:C:424:ASN:OD1 | 1:C:451:ASP:HB3 | 2.20 | 0.41 |
| 1:C:635:ALA:HB2 | 1:C:665:PHE:CD2 | 2.56 | 0.41 |
| 1:A:276:GLU:O | 4:A:1232:EDO:H22 | 2.21 | 0.41 |
| 1:A:547:PHE:CE1 | 1:A:561:VAL:HG21 | 2.56 | 0.41 |
| 1:A:910:TRP:CE3 | 1:A:954:GLY:HA2 | 2.56 | 0.41 |
| 1:A:952:LYS:NZ | 3:A:1223:PGE:H22 | 2.36 | 0.41 |
| 1:C:105:GLU:HB2 | 1:C:108:PRO:HB3 | 2.03 | 0.41 |
| 1:C:964[A]:HIS:HD2 | 1:C:966:ARG:HG2 | 1.84 | 0.41 |
| 1:A:678:GLU:HG3 | 1:A:681:LEU:H | 1.85 | 0.41 |
| 3:A:1201:PGE:H5 | 3:A:1201:PGE:H3 | 1.89 | 0.40 |
| 2:B:103:THR:OG1 | 10:B:701:HOH:O | 2.21 | 0.40 |
| 1:C:120:VAL:HG22 | 1:C:404:LEU:O | 2.22 | 0.40 |
| 1:C:320:SER:O | 1:C:627:PHE:HA | 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 X-ray entries followed by that with respect to entries



All

of similar resolution.

All

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | | | |
|-----|-------|---------------|-----------|---------|----------|-------------|--|--|--|
| 1 | А | 852/977~(87%) | 821 (96%) | 30 (4%) | 1 (0%) | 51 60 | | | |
| 1 | С | 856/977~(88%) | 820 (96%) | 36 (4%) | 0 | 100 100 | | | |
| 2 | В | 81/554~(15%) | 77 (95%) | 4 (5%) | 0 | 100 100 | | | |
| 2 | D | 81/554 (15%) | 76 (94%) | 3 (4%) | 2(2%) | 5 3 | | | |

1794 (96%)

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

73(4%)

3(0%)

47

55

All (3) Ramachandran outliers are listed below:

1870/3062 (61%)

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 36 | PRO |
| 2 | D | 83 | LYS |
| 1 | А | 643 | ALA |

5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Perce | ntiles |
|-----|-------|-----------------|------------|----------|-------|--------|
| 1 | А | 741/846~(88%) | 728~(98%) | 13 (2%) | 59 | 72 |
| 1 | С | 730/846~(86%) | 712 (98%) | 18 (2%) | 47 | 60 |
| 2 | В | 63/485~(13%) | 62~(98%) | 1 (2%) | 62 | 76 |
| 2 | D | 65/485~(13%) | 64 (98%) | 1 (2%) | 65 | 78 |
| All | All | 1599/2662~(60%) | 1566 (98%) | 33~(2%) | 53 | 67 |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 35 | ARG |
| 1 | А | 36 | SER |
| 1 | А | 37 | ASN |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 61 | ARG |
| 1 | А | 67 | LEU |
| 1 | А | 137 | SER |
| 1 | А | 251 | THR |
| 1 | А | 424 | ASN |
| 1 | А | 446 | ASP |
| 1 | А | 552 | TYR |
| 1 | А | 637 | TRP |
| 1 | А | 665 | PHE |
| 1 | А | 706 | ARG |
| 2 | В | 78 | THR |
| 1 | С | 74 | LEU |
| 1 | С | 110 | ARG |
| 1 | С | 144 | GLU |
| 1 | С | 163 | ASP |
| 1 | С | 173 | ARG |
| 1 | С | 312 | ASN |
| 1 | С | 324 | LEU |
| 1 | С | 424 | ASN |
| 1 | С | 446 | ASP |
| 1 | С | 500 | ARG |
| 1 | С | 538 | ARG |
| 1 | С | 637 | TRP |
| 1 | С | 665 | PHE |
| 1 | С | 685 | TRP |
| 1 | С | 706 | ARG |
| 1 | С | 714 | GLN |
| 1 | С | 797 | VAL |
| 1 | С | 808 | HIS |
| 2 | D | 48 | PHE |

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 964 | HIS |

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 86 ligands modelled in this entry, 4 are monoatomic - leaving 82 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).

| Mal | Turne | Chain | Dec | Tiple | Bo | Bond lengths | | | Bond angles | | |
|-------|-------|-------|------|-------|-------------|--------------|--------|-------------|-------------|--------|--|
| INIOI | туре | Unain | nes | LIIIK | Counts | RMSZ | # Z >2 | Counts | RMSZ | # Z >2 | |
| 4 | EDO | А | 1225 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.44 | 0 | |
| 4 | EDO | А | 1235 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.36 | 0 | |
| 4 | EDO | А | 1216 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.42 | 0 | |
| 4 | EDO | А | 1233 | - | 3,3,3 | 0.49 | 0 | 2,2,2 | 0.33 | 0 | |
| 4 | EDO | С | 1224 | - | 3,3,3 | 0.45 | 0 | 2,2,2 | 0.39 | 0 | |
| 4 | EDO | А | 1204 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.31 | 0 | |
| 4 | EDO | А | 1226 | - | 3,3,3 | 0.51 | 0 | 2,2,2 | 0.21 | 0 | |
| 5 | PEG | С | 1202 | - | $6,\!6,\!6$ | 0.49 | 0 | $5,\!5,\!5$ | 0.27 | 0 | |
| 3 | PGE | А | 1221 | - | $9,\!9,\!9$ | 0.29 | 0 | 8,8,8 | 0.38 | 0 | |
| 4 | EDO | С | 1203 | - | 3,3,3 | 0.41 | 0 | 2,2,2 | 0.55 | 0 | |
| 3 | PGE | А | 1223 | - | $9,\!9,\!9$ | 0.31 | 0 | 8,8,8 | 0.27 | 0 | |
| 7 | SO4 | С | 1232 | - | 4,4,4 | 0.16 | 0 | $6,\!6,\!6$ | 0.13 | 0 | |
| 3 | PGE | А | 1201 | - | $9,\!9,\!9$ | 0.30 | 0 | 8,8,8 | 0.32 | 0 | |
| 9 | PG4 | В | 603 | - | 12,12,12 | 0.52 | 0 | 11,11,11 | 0.22 | 0 | |
| 7 | SO4 | В | 606 | - | 4,4,4 | 0.12 | 0 | $6,\!6,\!6$ | 0.15 | 0 | |
| 5 | PEG | А | 1214 | - | 6,6,6 | 0.49 | 0 | $5,\!5,\!5$ | 0.35 | 0 | |
| 5 | PEG | С | 1219 | - | $6,\!6,\!6$ | 0.48 | 0 | $5,\!5,\!5$ | 0.27 | 0 | |
| 3 | PGE | А | 1207 | - | $9,\!9,\!9$ | 0.33 | 0 | 8,8,8 | 0.23 | 0 | |
| 4 | EDO | А | 1219 | - | 3,3,3 | 0.44 | 0 | 2,2,2 | 0.42 | 0 | |
| 4 | EDO | А | 1202 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.39 | 0 | |
| 3 | PGE | D | 603 | - | $9,\!9,\!9$ | 0.31 | 0 | 8,8,8 | 0.30 | 0 | |
| 3 | PGE | С | 1205 | - | $9,\!9,\!9$ | 0.31 | 0 | 8,8,8 | 0.35 | 0 | |



| | T | | D | T | Bo | ond leng | \mathbf{ths} | B | ond ang | gles |
|------|----------|-------|-------------------|------|-------------|----------|----------------|-------------|---------|----------|
| NIOI | Type | Chain | Res | Link | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | EDO | С | 1225 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.51 | 0 |
| 7 | SO4 | С | 1233 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.08 | 0 |
| 4 | EDO | С | 1215 | - | 3,3,3 | 0.47 | 0 | $2,\!2,\!2$ | 0.30 | 0 |
| 4 | EDO | С | 1222 | _ | 3,3,3 | 0.49 | 0 | 2,2,2 | 0.28 | 0 |
| 4 | EDO | D | 604 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.41 | 0 |
| 4 | EDO | С | 1204 | - | 3,3,3 | 0.46 | 0 | $2,\!2,\!2$ | 0.34 | 0 |
| 4 | EDO | С | 1213 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.34 | 0 |
| 4 | EDO | С | 1223 | - | 3,3,3 | 0.48 | 0 | $2,\!2,\!2$ | 0.31 | 0 |
| 4 | EDO | А | 1205 | - | 3,3,3 | 0.42 | 0 | $2,\!2,\!2$ | 0.42 | 0 |
| 4 | EDO | С | 1228 | - | 3,3,3 | 0.47 | 0 | $2,\!2,\!2$ | 0.36 | 0 |
| 4 | EDO | С | 1227 | - | 3,3,3 | 0.57 | 0 | $2,\!2,\!2$ | 0.19 | 0 |
| 4 | EDO | С | 1221 | - | 3,3,3 | 0.44 | 0 | 2,2,2 | 0.41 | 0 |
| 5 | PEG | С | 1217 | - | $6,\!6,\!6$ | 0.50 | 0 | $5,\!5,\!5$ | 0.25 | 0 |
| 5 | PEG | С | 1212 | - | 6,6,6 | 0.47 | 0 | $5,\!5,\!5$ | 0.24 | 0 |
| 7 | SO4 | С | 1234 | - | 4,4,4 | 0.14 | 0 | $6,\!6,\!6$ | 0.05 | 0 |
| 5 | PEG | А | 1212 | _ | 6,6,6 | 0.50 | 0 | $5,\!5,\!5$ | 0.28 | 0 |
| 4 | EDO | А | 1203 | - | 3,3,3 | 0.42 | 0 | 2,2,2 | 0.43 | 0 |
| 4 | EDO | А | 1230 | _ | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.31 | 0 |
| 4 | EDO | А | 1227 | - | 3,3,3 | 0.52 | 0 | 2,2,2 | 0.65 | 0 |
| 7 | SO4 | С | 1235 | - | 4,4,4 | 0.14 | 0 | $6,\!6,\!6$ | 0.07 | 0 |
| 7 | SO4 | А | 1241 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 3 | PGE | А | 1210 | - | $9,\!9,\!9$ | 0.31 | 0 | 8,8,8 | 0.29 | 0 |
| 4 | EDO | С | 1209 | - | 3,3,3 | 0.47 | 0 | $2,\!2,\!2$ | 0.31 | 0 |
| 5 | PEG | В | 604 | - | $6,\!6,\!6$ | 0.48 | 0 | $5,\!5,\!5$ | 0.24 | 0 |
| 4 | EDO | С | 1214 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.38 | 0 |
| 5 | PEG | А | 1208 | - | 6,6,6 | 0.49 | 0 | $5,\!5,\!5$ | 0.30 | 0 |
| 4 | EDO | А | 1229 | - | 3,3,3 | 0.46 | 0 | $2,\!2,\!2$ | 0.34 | 0 |
| 4 | EDO | А | 1224 | - | 3,3,3 | 0.46 | 0 | $2,\!2,\!2$ | 0.36 | 0 |
| 5 | PEG | А | 1217 | - | 6,6,6 | 0.49 | 0 | $5,\!5,\!5$ | 0.26 | 0 |
| 5 | PEG | А | 1220 | - | 6,6,6 | 0.49 | 0 | $5,\!5,\!5$ | 0.23 | 0 |
| 9 | PG4 | С | 1230 | - | 12,12,12 | 0.52 | 0 | 11,11,11 | 0.23 | 0 |
| 4 | EDO | С | 1216 | - | 3, 3, 3 | 0.48 | 0 | $2,\!2,\!2$ | 0.33 | 0 |
| 4 | EDO | С | 1226 | - | 3,3,3 | 0.45 | 0 | $2,\!2,\!2$ | 0.38 | 0 |
| 7 | SO4 | А | 1240 | - | 4,4,4 | 0.14 | 0 | $6,\!6,\!6$ | 0.06 | 0 |
| 4 | EDO | А | 1234 | - | 3, 3, 3 | 0.44 | 0 | $2,\!2,\!2$ | 0.41 | 0 |
| 4 | EDO | А | 1236 | - | 3,3,3 | 0.44 | 0 | $2,\!2,\!2$ | 0.49 | 0 |
| 4 | EDO | A | 1209 | - | 3,3,3 | 0.47 | 0 | 2,2,2 | 0.23 | 0 |
| 3 | PGE | С | 1208 | - | $9,\!9,\!9$ | 0.35 | 0 | 8,8,8 | 0.25 | 0 |
| 4 | EDO | A | 1211 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.42 | 0 |
| 5 | PEG | A | $1\overline{215}$ | - | $6,\!6,\!6$ | 0.48 | 0 | 5, 5, 5 | 0.29 | 0 |
| 4 | EDO | C | 1201 | - | 3,3,3 | 0.39 | 0 | 2,2,2 | 0.59 | 0 |
| 4 | EDO | A | 1232 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.40 | 0 |
| 4 | EDO | A | 1206 | - | 3,3,3 | 0.47 | 0 | 2,2,2 | 0.32 | 0 |



| Mal | Type | Chain | ain Res | Link | Bo | ond leng | ths | E | ond ang | gles |
|------|------|---------|---------|-------|-------------|----------|----------------------|-------------|---------|----------|
| WIOI | Type | Ullalli | nes | LIIIK | Counts | RMSZ | # Z >2 | Counts | RMSZ | # Z >2 |
| 5 | PEG | С | 1206 | - | $6,\!6,\!6$ | 0.49 | 0 | $5,\!5,\!5$ | 0.27 | 0 |
| 3 | PGE | С | 1220 | - | $9,\!9,\!9$ | 0.32 | 0 | 8,8,8 | 0.29 | 0 |
| 7 | SO4 | А | 1239 | - | $4,\!4,\!4$ | 0.15 | 0 | $6,\!6,\!6$ | 0.06 | 0 |
| 4 | EDO | С | 1218 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.30 | 0 |
| 7 | SO4 | С | 1231 | - | 4,4,4 | 0.13 | 0 | $6,\!6,\!6$ | 0.11 | 0 |
| 4 | EDO | В | 605 | - | 3,3,3 | 0.47 | 0 | 2,2,2 | 0.32 | 0 |
| 4 | EDO | А | 1222 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.41 | 0 |
| 6 | XOD | А | 1237 | - | 36,37,37 | 2.04 | 4 (11%) | 44,51,51 | 1.64 | 7 (15%) |
| 4 | EDO | А | 1218 | - | 3,3,3 | 0.47 | 0 | 2,2,2 | 0.33 | 0 |
| 5 | PEG | А | 1228 | - | $6,\!6,\!6$ | 0.49 | 0 | $5,\!5,\!5$ | 0.20 | 0 |
| 4 | EDO | А | 1231 | - | 3,3,3 | 0.43 | 0 | 2,2,2 | 0.47 | 0 |
| 4 | EDO | А | 1213 | - | 3,3,3 | 0.48 | 0 | 2,2,2 | 0.28 | 0 |
| 4 | EDO | С | 1207 | - | 3,3,3 | 0.46 | 0 | 2,2,2 | 0.27 | 0 |
| 7 | SO4 | А | 1238 | - | 4,4,4 | 0.14 | 0 | $6,\!6,\!6$ | 0.05 | 0 |
| 4 | EDO | С | 1210 | - | 3,3,3 | 0.42 | 0 | 2,2,2 | 0.39 | 0 |
| 5 | PEG | С | 1211 | - | $6,\!6,\!6$ | 0.50 | 0 | $5,\!5,\!5$ | 0.26 | 0 |
| 6 | XOD | С | 1229 | - | 36,37,37 | 2.01 | 3 (8%) | 44,51,51 | 1.70 | 10 (22%) |

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 | EDO | А | 1202 | - | - | 0/1/1/1 | - |
| 3 | PGE | D | 603 | - | - | 1/7/7/7 | - |
| 3 | PGE | С | 1205 | - | - | 5/7/7/7 | - |
| 3 | PGE | А | 1210 | - | - | 0/7/7/7 | - |
| 4 | EDO | А | 1225 | - | - | 1/1/1/1 | - |
| 4 | EDO | А | 1235 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1209 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1225 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1215 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1214 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1222 | - | - | 0/1/1/1 | - |
| 5 | PEG | А | 1208 | - | - | 0/4/4/4 | - |
| 5 | PEG | В | 604 | - | - | 1/4/4/4 | - |
| 4 | EDO | D | 604 | - | - | 0/1/1/1 | - |
| 4 | EDO | А | 1229 | - | - | 0/1/1/1 | - |
| 4 | EDO | A | 1232 | - | - | 1/1/1/1 | - |
| 4 | EDO | А | 1206 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1204 | - | - | 0/1/1/1 | - |



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|--------|----------|-------|----------|------|---------|------------|---------|
| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
| 4 | EDO | А | 1216 | - | - | 0/1/1/1 | - |
| 3 | PGE | С | 1220 | - | - | 3/7/7/7 | - |
| 5 | PEG | С | 1206 | - | - | 2/4/4/4 | - |
| 4 | EDO | А | 1224 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1213 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1218 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1223 | - | - | 1/1/1/1 | - |
| 4 | EDO | А | 1233 | - | - | 1/1/1/1 | - |
| 4 | EDO | A | 1205 | - | - | 1/1/1/1 | - |
| 4 | EDO | C | 1224 | - | - | 0/1/1/1 | - |
| 4 | EDO | A | 1204 | - | - | 0/1/1/1 | - |
| 4 | EDO | A | 1226 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1228 | - | - | 0/1/1/1 | - |
| 5 | PEG | А | 1217 | - | - | 2/4/4/4 | - |
| 5 | PEG | С | 1202 | - | - | 1/4/4/4 | - |
| 5 | PEG | А | 1220 | - | - | 2/4/4/4 | - |
| 9 | PG4 | С | 1230 | - | - | 4/10/10/10 | - |
| 4 | EDO | С | 1227 | - | - | 1/1/1/1 | - |
| 3 | PGE | А | 1221 | - | - | 4/7/7/7 | - |
| 4 | EDO | С | 1203 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1216 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1221 | - | - | 0/1/1/1 | - |
| 4 | EDO | В | 605 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1226 | - | - | 0/1/1/1 | - |
| 5 | PEG | С | 1212 | - | - | 0/4/4/4 | - |
| 3 | PGE | А | 1223 | - | - | 5/7/7/7 | - |
| 5 | PEG | С | 1217 | - | - | 2/4/4/4 | - |
| 4 | EDO | А | 1222 | - | - | 0/1/1/1 | - |
| 6 | XOD | А | 1237 | - | - | 9/20/45/45 | 0/3/3/3 |
| 3 | PGE | А | 1201 | - | - | 3/7/7/7 | - |
| 9 | PG4 | В | 603 | - | - | 7/10/10/10 | - |
| 4 | EDO | А | 1234 | - | - | 0/1/1/1 | - |
| 4 | EDO | А | 1218 | - | - | 0/1/1/1 | - |
| 5 | PEG | А | 1214 | - | - | 2/4/4/4 | - |
| 4 | EDO | С | 1201 | - | - | 0/1/1/1 | - |
| 5 | PEG | А | 1228 | - | - | 1/4/4/4 | - |
| 3 | PGE | А | 1207 | - | - | 1/7/7/7 | - |
| 4 | EDO | А | 1231 | _ | - | 1/1/1/1 | - |
| 5 | PEG | A | 1212 | _ | - | 3/4/4/4 | - |



| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 5 | PEG | С | 1219 | - | - | 1/4/4/4 | - |
| 4 | EDO | А | 1203 | - | - | 0/1/1/1 | - |
| 4 | EDO | А | 1213 | - | - | 0/1/1/1 | - |
| 4 | EDO | А | 1236 | - | - | 0/1/1/1 | - |
| 4 | EDO | С | 1207 | - | - | 1/1/1/1 | - |
| 4 | EDO | А | 1230 | - | - | 1/1/1/1 | - |
| 4 | EDO | С | 1210 | - | - | 0/1/1/1 | - |
| 4 | EDO | А | 1209 | - | - | 0/1/1/1 | - |
| 4 | EDO | А | 1219 | - | - | 0/1/1/1 | - |
| 3 | PGE | С | 1208 | - | - | 1/7/7/7 | - |
| 4 | EDO | А | 1211 | - | - | 0/1/1/1 | - |
| 5 | PEG | С | 1211 | - | - | 2/4/4/4 | - |
| 5 | PEG | А | 1215 | - | - | 0/4/4/4 | - |
| 6 | XOD | С | 1229 | - | - | 12/20/45/45 | 0/3/3/3 |
| 4 | EDO | А | 1227 | - | - | 1/1/1/1 | - |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | | Observed(Å) | $\operatorname{Ideal}(\operatorname{\AA})$ |
|-----|-------|------|------|---------|-------|-------------|--|
| 6 | А | 1237 | XOD | O6-N5 | 10.65 | 1.40 | 1.22 |
| 6 | С | 1229 | XOD | O6-N5 | 10.42 | 1.40 | 1.22 |
| 6 | А | 1237 | XOD | C14-N2 | 3.29 | 1.46 | 1.37 |
| 6 | С | 1229 | XOD | C14-N2 | 3.08 | 1.46 | 1.37 |
| 6 | А | 1237 | XOD | O1-C1 | -2.19 | 1.40 | 1.44 |
| 6 | А | 1237 | XOD | C17-C20 | 2.17 | 1.54 | 1.48 |
| 6 | С | 1229 | XOD | O1-C1 | -2.10 | 1.40 | 1.44 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 6 | А | 1237 | XOD | C21-N3-C20 | 4.86 | 121.16 | 116.08 |
| 6 | С | 1229 | XOD | C21-N3-C20 | 4.82 | 121.12 | 116.08 |
| 6 | А | 1237 | XOD | C8-N1-C5 | -3.96 | 108.60 | 114.20 |
| 6 | А | 1237 | XOD | C23-N4-C20 | 3.63 | 119.87 | 116.08 |
| 6 | С | 1229 | XOD | C4-C3-C2 | -3.34 | 106.70 | 111.30 |
| 6 | С | 1229 | XOD | C8-N1-C5 | -3.18 | 109.70 | 114.20 |
| 6 | А | 1237 | XOD | C17-C20-N3 | 3.16 | 120.81 | 117.41 |
| 6 | С | 1229 | XOD | C23-N4-C20 | 3.09 | 119.31 | 116.08 |
| 6 | С | 1229 | XOD | C4-C5-N1 | -3.02 | 104.14 | 109.66 |
| 6 | С | 1229 | XOD | C22-C21-N3 | -2.79 | 118.87 | 123.43 |
| 6 | А | 1237 | XOD | C4-C5-N1 | -2.75 | 104.64 | 109.66 |
| 6 | C | 1229 | XOD | C15-C14-N2 | -2.73 | 118.53 | 123.33 |

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|------|------|------------|-------|------------------|---------------|
| 6 | А | 1237 | XOD | C22-C21-N3 | -2.69 | 119.03 | 123.43 |
| 6 | А | 1237 | XOD | C13-N2-C14 | -2.66 | 117.00 | 123.39 |
| 6 | С | 1229 | XOD | O5-C2-C3 | -2.45 | 104.60 | 110.03 |
| 6 | С | 1229 | XOD | C17-C20-N4 | 2.20 | 119.78 | 117.41 |
| 6 | С | 1229 | XOD | C12-C13-N2 | -2.02 | 106.06 | 111.49 |

There are no chirality outliers.

| All (84) torsion outliers are listed below | w: |
|--|----|
|--|----|

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 6 | А | 1237 | XOD | C14-C15-N5-O6 |
| 6 | А | 1237 | XOD | C16-C15-N5-O6 |
| 6 | С | 1229 | XOD | C15-C14-N2-C13 |
| 5 | С | 1211 | PEG | O1-C1-C2-O2 |
| 5 | А | 1212 | PEG | C4-C3-O2-C2 |
| 6 | С | 1229 | XOD | C19-C14-N2-C13 |
| 6 | А | 1237 | XOD | N1-C8-C9-C10 |
| 6 | А | 1237 | XOD | C11-C12-C13-N2 |
| 9 | В | 603 | PG4 | C6-C5-O3-C4 |
| 3 | А | 1201 | PGE | O2-C3-C4-O3 |
| 3 | D | 603 | PGE | O2-C3-C4-O3 |
| 3 | С | 1208 | PGE | O2-C3-C4-O3 |
| 5 | А | 1212 | PEG | O2-C3-C4-O4 |
| 6 | С | 1229 | XOD | C11-C12-C13-N2 |
| 9 | С | 1230 | PG4 | O3-C5-C6-O4 |
| 6 | А | 1237 | XOD | C15-C14-N2-C13 |
| 3 | С | 1205 | PGE | O2-C3-C4-O3 |
| 9 | В | 603 | PG4 | O3-C5-C6-O4 |
| 3 | А | 1223 | PGE | O1-C1-C2-O2 |
| 6 | С | 1229 | XOD | C16-C17-C20-N4 |
| 6 | С | 1229 | XOD | C16-C17-C20-N3 |
| 6 | С | 1229 | XOD | C18-C17-C20-N3 |
| 6 | А | 1237 | XOD | С11-С10-С9-С8 |
| 6 | С | 1229 | XOD | C18-C17-C20-N4 |
| 6 | А | 1237 | XOD | C9-C10-C11-C12 |
| 9 | В | 603 | PG4 | C8-C7-O4-C6 |
| 6 | А | 1237 | XOD | C10-C11-C12-C13 |
| 5 | A | 1212 | PEG | 01-C1-C2-O2 |
| 4 | А | 1225 | EDO | O1-C1-C2-O2 |
| 4 | А | 1227 | EDO | O1-C1-C2-O2 |
| 4 | А | 1231 | EDO | O1-C1-C2-O2 |
| 4 | С | 1227 | EDO | O1-C1-C2-O2 |



| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 6 | С | 1229 | XOD | C11-C10-C9-C8 |
| 5 | А | 1220 | PEG | O2-C3-C4-O4 |
| 5 | С | 1219 | PEG | O2-C3-C4-O4 |
| 6 | А | 1237 | XOD | C19-C14-N2-C13 |
| 6 | С | 1229 | XOD | C6-C5-N1-C8 |
| 3 | А | 1221 | PGE | O1-C1-C2-O2 |
| 5 | С | 1217 | PEG | O1-C1-C2-O2 |
| 9 | В | 603 | PG4 | O2-C3-C4-O3 |
| 5 | С | 1206 | PEG | O1-C1-C2-O2 |
| 4 | А | 1230 | EDO | O1-C1-C2-O2 |
| 6 | С | 1229 | XOD | C16-C15-N5-O6 |
| 3 | А | 1201 | PGE | C3-C4-O3-C5 |
| 3 | С | 1220 | PGE | C3-C4-O3-C5 |
| 5 | А | 1214 | PEG | O1-C1-C2-O2 |
| 5 | А | 1217 | PEG | O1-C1-C2-O2 |
| 4 | С | 1207 | EDO | O1-C1-C2-O2 |
| 9 | С | 1230 | PG4 | C5-C6-O4-C7 |
| 5 | А | 1228 | PEG | C1-C2-O2-C3 |
| 3 | С | 1205 | PGE | C1-C2-O2-C3 |
| 3 | С | 1205 | PGE | C3-C4-O3-C5 |
| 5 | С | 1211 | PEG | C1-C2-O2-C3 |
| 5 | А | 1214 | PEG | O2-C3-C4-O4 |
| 3 | А | 1221 | PGE | C3-C4-O3-C5 |
| 3 | А | 1201 | PGE | C1-C2-O2-C3 |
| 5 | С | 1206 | PEG | C1-C2-O2-C3 |
| 3 | А | 1207 | PGE | O2-C3-C4-O3 |
| 6 | С | 1229 | XOD | N1-C8-C9-C10 |
| 3 | А | 1221 | PGE | C6-C5-O3-C4 |
| 3 | А | 1223 | PGE | O2-C3-C4-O3 |
| 3 | А | 1221 | PGE | C1-C2-O2-C3 |
| 3 | С | 1205 | PGE | C6-C5-O3-C4 |
| 5 | В | 604 | PEG | C1-C2-O2-C3 |
| 3 | А | 1223 | PGE | O3-C5-C6-O4 |
| 5 | С | 1202 | PEG | O1-C1-C2-O2 |
| 4 | С | 1223 | EDO | O1-C1-C2-O2 |
| 3 | С | 1220 | PGE | O2-C3-C4-O3 |
| 3 | С | 1220 | PGE | C4-C3-O2-C2 |
| 9 | В | 603 | PG4 | C3-C4-O3-C5 |
| 3 | С | 1205 | PGE | O1-C1-C2-O2 |
| 9 | С | 1230 | PG4 | C6-C5-O3-C4 |
| 9 | С | 1230 | PG4 | O2-C3-C4-O3 |
| 3 | А | 1223 | PGE | C4-C3-O2-C2 |

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| | 9 | 1 | 1 5 | |
|-----|-------|---------------------------|------|----------------|
| Mol | Chain | $\overline{\mathrm{Res}}$ | Type | Atoms |
| 9 | В | 603 | PG4 | C5-C6-O4-C7 |
| 6 | С | 1229 | XOD | C9-C10-C11-C12 |
| 5 | А | 1220 | PEG | C4-C3-O2-C2 |
| 4 | А | 1205 | EDO | O1-C1-C2-O2 |
| 4 | А | 1232 | EDO | O1-C1-C2-O2 |
| 4 | А | 1233 | EDO | O1-C1-C2-O2 |
| 5 | А | 1217 | PEG | C1-C2-O2-C3 |
| 9 | В | 603 | PG4 | C4-C3-O2-C2 |
| 3 | А | 1223 | PGE | C6-C5-O3-C4 |
| 5 | С | 1217 | PEG | C1-C2-O2-C3 |

Continued from previous page...

There are no ring outliers.

28 monomers are involved in 44 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | А | 1225 | EDO | 1 | 0 |
| 5 | С | 1202 | PEG | 1 | 0 |
| 4 | С | 1203 | EDO | 1 | 0 |
| 3 | А | 1223 | PGE | 1 | 0 |
| 3 | А | 1201 | PGE | 2 | 0 |
| 5 | А | 1214 | PEG | 3 | 0 |
| 4 | А | 1219 | EDO | 1 | 0 |
| 4 | С | 1225 | EDO | 1 | 0 |
| 4 | С | 1215 | EDO | 1 | 0 |
| 4 | С | 1204 | EDO | 3 | 0 |
| 4 | С | 1227 | EDO | 1 | 0 |
| 5 | С | 1217 | PEG | 2 | 0 |
| 5 | А | 1212 | PEG | 2 | 0 |
| 7 | С | 1235 | SO4 | 2 | 0 |
| 4 | С | 1209 | EDO | 2 | 0 |
| 4 | С | 1214 | EDO | 2 | 0 |
| 4 | А | 1229 | EDO | 1 | 0 |
| 9 | С | 1230 | PG4 | 2 | 0 |
| 3 | С | 1208 | PGE | 1 | 0 |
| 5 | А | 1215 | PEG | 1 | 0 |
| 4 | С | 1201 | EDO | 2 | 0 |
| 4 | А | 1232 | EDO | 2 | 0 |
| 5 | С | 1206 | PEG | 1 | 0 |
| 4 | А | 1222 | EDO | 4 | 0 |
| 6 | A | 1237 | XOD | 1 | 0 |
| 4 | А | 1218 | EDO | 2 | 0 |
| 4 | А | 1213 | EDO | 1 | 0 |



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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5 | С | 1211 | PEG | 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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ $>$ | #RSRZ>2 | $\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$ | $Q{<}0.9$ |
|-----|-------|-----------------|-----------|----------------|--|-----------|
| 1 | А | 850/977~(87%) | -0.26 | 24 (2%) 53 51 | 23, 35, 62, 106 | 0 |
| 1 | С | 856/977~(87%) | -0.09 | 57 (6%) 17 16 | 24, 40, 81, 110 | 0 |
| 2 | В | 83/554~(14%) | 0.50 | 18 (21%) 0 0 | 30, 51, 85, 100 | 0 |
| 2 | D | 83/554~(14%) | 0.43 | 14 (16%) 1 1 | 32, 50, 89, 108 | 0 |
| All | All | 1872/3062~(61%) | -0.12 | 113 (6%) 21 20 | 23, 38, 79, 110 | 0 |

All (113) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | D | 81 | GLY | 8.1 |
| 2 | D | 82 | TYR | 6.3 |
| 1 | С | 370 | THR | 6.0 |
| 1 | А | 183 | ALA | 5.7 |
| 1 | А | 248 | TRP | 5.2 |
| 2 | D | 80 | THR | 5.0 |
| 1 | С | 128 | LEU | 4.5 |
| 1 | С | 129 | SER | 4.4 |
| 2 | D | 43 | THR | 4.3 |
| 1 | А | 251 | THR | 4.3 |
| 1 | С | 136 | ASN | 4.2 |
| 1 | С | 67 | LEU | 4.0 |
| 2 | В | 44 | ALA | 3.9 |
| 1 | С | 85 | VAL | 3.9 |
| 1 | С | 135 | ASP | 3.9 |
| 1 | А | 370 | THR | 3.8 |
| 1 | С | 82 | VAL | 3.8 |
| 2 | В | 42 | GLY | 3.8 |
| 1 | С | 141 | THR | 3.7 |
| 2 | В | B 43 | | 3.7 |
| 2 | D | 84 | PRO | 3.7 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | С | 245 | PRO | 3.7 |
| 1 | С | 137 | SER | 3.6 |
| 2 | В | 84 | PRO | 3.6 |
| 1 | С | 64 | LEU | 3.5 |
| 1 | С | 132 | GLY | 3.5 |
| 1 | А | 658 | LEU | 3.5 |
| 1 | С | 63 | LEU | 3.4 |
| 1 | А | 635 | ALA | 3.4 |
| 1 | А | 249 | GLU | 3.4 |
| 2 | В | 41 | ASP | 3.4 |
| 2 | D | 116 | CYS | 3.4 |
| 1 | С | 69 | LEU | 3.4 |
| 2 | В | 116 | CYS | 3.4 |
| 1 | С | 244 | GLU | 3.4 |
| 1 | С | 33 | VAL | 3.3 |
| 1 | С | 142 | VAL | 3.2 |
| 1 | А | 663 | LEU | 3.2 |
| 2 | В | 78 | THR | 3.2 |
| 1 | С | 164 | ARG | 3.2 |
| 1 | А | 622 | LEU | 3.2 |
| 2 | В | 82 | TYR | 3.1 |
| 1 | А | 636 | VAL | 3.1 |
| 1 | С | 156 | PHE | 3.1 |
| 1 | С | 140 | LEU | 3.1 |
| 1 | С | 153 | ALA | 3.1 |
| 1 | С | 66 | THR | 3.0 |
| 1 | С | 163 | ASP | 3.0 |
| 1 | С | 130 | VAL | 3.0 |
| 1 | С | 138 | VAL | 3.0 |
| 2 | В | 80 | THR | 3.0 |
| 1 | С | 143 | ALA | 3.0 |
| 1 | С | 34 | ASP | 3.0 |
| 1 | С | 60 | TYR | 2.9 |
| 1 | С | 81 | GLU | 2.8 |
| 2 | D | 48 | PHE | 2.8 |
| 1 | A | 254 | THR | 2.8 |
| 1 | С | 83 | THR | 2.8 |
| 1 | A | 665 | PHE | 2.8 |
| 1 | С | 131 | SER | 2.8 |
| 1 | С | 165 | SER | 2.7 |
| 1 | С | 133 | ARG | 2.7 |
| 1 | С | 65 | ASP | 2.7 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | А | 164 | ARG | 2.7 |
| 1 | С | 126 | ALA | 2.7 |
| 2 | В | 86 | TYR | 2.7 |
| 1 | С | 56 | GLY | 2.7 |
| 1 | А | 637 | TRP | 2.6 |
| 1 | А | 667 | GLY | 2.6 |
| 2 | D | 78 | THR | 2.6 |
| 2 | В | 40 | LEU | 2.6 |
| 2 | D | 117 | ARG | 2.6 |
| 2 | В | 45 | THR | 2.5 |
| 2 | В | 117 | ARG | 2.5 |
| 1 | С | 70 | GLY | 2.5 |
| 2 | В | 79 | ASN | 2.5 |
| 2 | D | 44 | ALA | 2.5 |
| 1 | С | 149 | ILE | 2.5 |
| 2 | В | 85 | LEU | 2.5 |
| 1 | А | 182 | ARG | 2.4 |
| 1 | А | 253 | LYS | 2.4 |
| 2 | D | 79 | ASN | 2.4 |
| 1 | С | 134 | ASP | 2.4 |
| 1 | С | 58 | SER | 2.4 |
| 1 | С | 151 | LEU | 2.4 |
| 1 | А | 621 | VAL | 2.4 |
| 1 | С | 155 | PRO | 2.4 |
| 1 | С | 78 | LEU | 2.3 |
| 2 | D | 83 | LYS | 2.3 |
| 2 | В | 100 | CYS | 2.3 |
| 1 | С | 76 | VAL | 2.2 |
| 1 | С | 282 | PRO | 2.2 |
| 2 | D | 85 | LEU | 2.2 |
| 2 | В | 114 | ASN | 2.2 |
| 1 | С | 84 | LYS | 2.2 |
| 1 | А | 252 | PHE | 2.2 |
| 1 | С | 79 | ILE | 2.2 |
| 1 | А | 891 | GLY | 2.2 |
| 1 | С | 57 | LEU | 2.1 |
| 1 | С | 80 | HIS | 2.1 |
| 1 | С | 144 | GLU | 2.1 |
| 1 | А | 694 | PHE | 2.1 |
| 1 | С | 635 | ALA | 2.1 |
| 1 | А | 656 | LEU | 2.1 |
| 1 | С | 74 | LEU | 2.1 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | А | 562 | TRP | 2.0 |
| 1 | С | 658 | LEU | 2.0 |
| 1 | С | 52 | SER | 2.0 |
| 1 | С | 626 | PHE | 2.0 |
| 1 | С | 637 | TRP | 2.0 |
| 1 | А | 623 | SER | 2.0 |
| 2 | В | 115 | THR | 2.0 |
| 2 | D | 45 | THR | 2.0 |

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | $B-factors(A^2)$ | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------------------------|-------|
| 4 | EDO | С | 1215 | 4/4 | 0.65 | 0.30 | 72,74,75,84 | 0 |
| 4 | EDO | С | 1209 | 4/4 | 0.66 | 0.27 | 50,55,69,76 | 0 |
| 3 | PGE | С | 1220 | 10/10 | 0.71 | 0.30 | 58,79,85,95 | 0 |
| 7 | SO4 | A | 1240 | 5/5 | 0.72 | 0.55 | $109,\!135,\!152,\!170$ | 0 |
| 4 | EDO | А | 1233 | 4/4 | 0.74 | 0.27 | 61,71,73,85 | 0 |
| 7 | SO4 | С | 1234 | 5/5 | 0.76 | 0.60 | 135,143,159,180 | 0 |
| 5 | PEG | А | 1217 | 7/7 | 0.77 | 0.20 | 53,59,64,70 | 0 |
| 5 | PEG | А | 1212 | 7/7 | 0.78 | 0.19 | 59,64,77,80 | 0 |
| 5 | PEG | А | 1220 | 7/7 | 0.79 | 0.15 | 49,60,67,73 | 0 |
| 4 | EDO | А | 1235 | 4/4 | 0.80 | 0.21 | 67,71,74,76 | 0 |
| 4 | EDO | А | 1226 | 4/4 | 0.81 | 0.27 | 41,64,66,76 | 0 |
| 4 | EDO | С | 1218 | 4/4 | 0.82 | 0.12 | 59,65,69,70 | 0 |
| 7 | SO4 | A | 1241 | 5/5 | 0.82 | 0.29 | 82,92,110,127 | 0 |
| 4 | EDO | А | 1206 | 4/4 | 0.82 | 0.17 | 55,68,71,76 | 0 |
| 4 | EDO | C | 1216 | 4/4 | 0.83 | 0.15 | 52,62,62,64 | 0 |



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| Mol | Tvne | Chain | Bes | Atoms | BSCC | BSB | B -factors($Å^2$) | Q<0.9 |
|------------|------------|---------------------|--------------|---------------------------|------|---|-----------------------------------|---------|
| 3 | PCE | С | 1208 | 10/10 | 0.83 | 0.27 | <u>16 77 85 86</u> | Q < 0.5 |
| 0 0 | PG4 | B | 603 | $\frac{10/10}{13/13}$ | 0.83 | 0.21 0.22 | 58 67 76 77 | 0 |
| 4 | EDO | C D | 1227 | $\frac{10/10}{4/4}$ | 0.84 | 0.22 0.47 | 52 56 72 84 | 0 |
| 4 | EDO | C | 1221 | | 0.01 | 0.11 | 49 56 68 77 | 0 |
| 3 | PGE | C | 1210 1205 | 10/10 | 0.85 | 0.20 | 35 61 71 77 | 0 |
| 9 | PG4 | <u>С</u> | 1200 1230 | $\frac{10/10}{13/13}$ | 0.85 | 0.17 | 53 72 78 93 | 0 |
| 4 | EDO | | 1200 1213 | $\frac{10/10}{4/4}$ | 0.86 | 0.11 | 43 49 56 66 | 0 |
| 3 | PGE | | 1210 1207 | 10/10 | 0.86 | $\begin{array}{c} 0.21 \\ 0.28 \end{array}$ | 50 65 73 74 | 0 |
| 5 | PEG | A | 1201 | 7/7 | 0.86 | 0.20 0.24 | 45 50 67 67 | 0 |
| 4 | EDO | A | 1220 1227 | 4/4 | 0.86 | 0.21 0.22 | 49 52 61 68 | 0 |
| 5 | PEG | | 1206 | 7/7 | 0.87 | 0.22 | 62 69 80 99 | 0 |
| 7 | SO4 | A | 1238 | 5/5 | 0.87 | 0.10 | 80 97 131 154 | 0 |
| 4 | EDO | | 1200 1213 | | 0.87 | 0.21 0.12 | 48 56 56 56 | 0 |
| 3 | PGE | | 1210 1221 | 10/10 | 0.87 | 0.12 0.26 | <u>40,30,30,30</u> 56 72 78 78 | 0 |
| 7 | SO4 | $\frac{\Lambda}{C}$ | 1221 1233 | $\frac{10/10}{5/5}$ | 0.87 | 0.20 | 66 89 92 129 | 0 |
| 4 | EDO | <u>А</u> | 1200 1204 | | 0.87 | 0.20 | 57 57 60 66 | 0 |
| 4 | EDO | Δ | 1204 | 4/4 | 0.87 | 0.11 | 18 / 9 59 6/ | 0 |
| 4 | EDO | $\frac{\Lambda}{C}$ | 1224 1223 | 4/4 | 0.87 | 0.14 | 62 63 66 77 | 0 |
| 4 | EDO | | 1220 1218 | 4/4 | 0.88 | 0.30 0.17 | 55 60 71 75 | 0 |
| 5 | PEG | Δ | 1210 1208 | 7/7 | 0.88 | 0.17 | 51 62 65 78 | 0 |
| | FDO | $\frac{\Lambda}{C}$ | 1200 1214 | 1/1 1/1 | 0.00 | 0.10 | 55 65 67 68 | 0 |
| 5 | DEC | B | 604 | 7/7 | 0.88 | 0.10 | 50 60 75 78 | 0 |
| 7 | <u>SO4</u> | Δ | 1230 | 5/5 | 0.80 | 0.31 | 70 81 121 131 | 0 |
| 1 | FDO | Λ | 1209 | | 0.89 | 0.39 | 41 50 58 61 | 0 |
| 4 | PCE | Δ | 1209 1223 | $\frac{4/4}{10/10}$ | 0.89 | 0.19 | 56 64 70 88 | 0 |
| 7 | <u>101</u> | R R | 606 | 5/5 | 0.89 | 0.10 | 65 68 101 107 | 0 |
| 1 | EDO | | 1207 | | 0.89 | 0.00 | 54 55 64 75 | 0 |
| 4 | EDO | | 1207 | 4/4 | 0.89 | 0.21 | 48 61 68 80 | 0 |
| - 4 - 5 | DEC | $\frac{A}{C}$ | 1229 1917 | 4/4 | 0.89 | 0.18 | 45,01,08,80 | 0 |
| | FDO | | 1217 1220 | 1/1 | 0.89 | 0.18 | 45,50,09,78 | 0 |
| 5 | PEC | | 1230 1210 | 7/7 | 0.09 | 0.20 | 50 56 68 71 | 0 |
| 7 | <u> </u> | | 1219 1232 | 5/5 | 0.90 | 0.21 | 76 86 97 131 | 0 |
| 2 | PCE | | 603 | $\frac{0}{5}$ | 0.50 | 0.10 | 54 74 78 70 | 0 |
| 5 | PEC | | 1202 | $\frac{10/10}{7/7}$ | 0.90 | $\begin{array}{c} 0.22 \\ 0.17 \end{array}$ | 51 50 72 75 | 0 |
| 5 | PEG | | 1202 1214 | 7/7 | 0.90 | 0.17 | 47 54 68 74 | 0 |
| 5 | PEC | Δ | 1214 1915 | 7/7 | 0.50 | 0.10 0.14 | 47,54,00,14 | 0 |
| 4 | EDO | R | 605 | $\frac{1}{\Delta}/\Delta$ | 0.90 | 0.14 | 51 57 60 63 | 0 |
| 7 | SO4 | C | 1225 | 5/5 | 0.01 | 0.22 | 75 83 117 110 | 0 |
| 6 | XOD | | 1200 | 35/35 | 0.91 | 0.50 | 27 58 11/ 110 | 0 |
| 1 | EDO | | 1229 | 1/1 | 0.91 | 0.10 | 10 50 60 71 | 0 |
| 4 5 | DEC | | 1204 1911 | ++/++ 7/7 | 0.91 | 0.00 | 38 51 71 74 | 0 |
| 2 2 | PCF | | 1211 | 10/10 | 0.92 | 0.00 | 48 60 72 81 | 0 |
| ა | IGE | Λ | 1210 | 10/10 | 0.92 | 0.20 | 40,00,73,01 | U |



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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------------------------------|-------|
| 4 | EDO | А | 1216 | 4/4 | 0.92 | 0.22 | 45,62,62,63 | 0 |
| 6 | XOD | А | 1237 | 35/35 | 0.92 | 0.19 | 23,53,104,113 | 0 |
| 4 | EDO | С | 1226 | 4/4 | 0.93 | 0.26 | 46,52,61,62 | 0 |
| 3 | PGE | А | 1201 | 10/10 | 0.93 | 0.24 | 51,63,70,70 | 0 |
| 7 | SO4 | С | 1231 | 5/5 | 0.94 | 0.11 | $62,\!67,\!70,\!105$ | 0 |
| 4 | EDO | D | 604 | 4/4 | 0.94 | 0.16 | 48,53,58,62 | 0 |
| 4 | EDO | С | 1204 | 4/4 | 0.94 | 0.10 | 39,49,51,55 | 0 |
| 5 | PEG | С | 1212 | 7/7 | 0.94 | 0.29 | 45,68,73,77 | 0 |
| 4 | EDO | А | 1222 | 4/4 | 0.94 | 0.15 | 42,49,58,60 | 0 |
| 4 | EDO | А | 1232 | 4/4 | 0.94 | 0.16 | $36,\!38,\!56,\!57$ | 0 |
| 4 | EDO | С | 1203 | 4/4 | 0.94 | 0.14 | 35,42,52,57 | 0 |
| 4 | EDO | А | 1231 | 4/4 | 0.95 | 0.11 | 40,45,50,53 | 0 |
| 4 | EDO | С | 1221 | 4/4 | 0.95 | 0.18 | $40,\!48,\!59,\!65$ | 0 |
| 4 | EDO | А | 1202 | 4/4 | 0.95 | 0.14 | 42,44,45,52 | 0 |
| 4 | EDO | С | 1224 | 4/4 | 0.95 | 0.28 | $56,\!57,\!59,\!81$ | 0 |
| 4 | EDO | А | 1225 | 4/4 | 0.95 | 0.17 | 39,42,61,66 | 0 |
| 4 | EDO | С | 1228 | 4/4 | 0.96 | 0.16 | 46,50,50,53 | 0 |
| 4 | EDO | А | 1203 | 4/4 | 0.96 | 0.18 | 53,58,60,61 | 0 |
| 4 | EDO | С | 1225 | 4/4 | 0.96 | 0.14 | 54,60,70,74 | 0 |
| 4 | EDO | С | 1222 | 4/4 | 0.96 | 0.13 | $40,\!44,\!52,\!57$ | 0 |
| 4 | EDO | А | 1205 | 4/4 | 0.96 | 0.09 | $43,\!49,\!55,\!57$ | 0 |
| 4 | EDO | С | 1201 | 4/4 | 0.97 | 0.10 | 45,46,54,66 | 0 |
| 4 | EDO | А | 1236 | 4/4 | 0.97 | 0.25 | $56,\!59,\!64,\!70$ | 0 |
| 4 | EDO | А | 1211 | 4/4 | 0.97 | 0.10 | 35,48,66,69 | 0 |
| 4 | EDO | А | 1219 | 4/4 | 0.98 | 0.09 | $3\overline{5},\!39,\!48,\!52$ | 0 |
| 8 | CA | D | 601 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 8 | CA | В | 602 | 1/1 | 0.99 | 0.05 | 33,33,33,33 | 0 |
| 8 | CA | В | 601 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |
| 8 | CA | D | 602 | 1/1 | 1.00 | 0.04 | $3\overline{2},\!32,\!32,\!32$ | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







6.5 Other polymers (i)

There are no such residues in this entry.

