



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2017 – 07:10 PM EST

PDB ID : 5UQY
Title : Crystal structure of Marburg virus GP in complex with the human survivor antibody MR78
Authors : Hashiguchi, T.; Fusco, M.L.; Hastie, K.M.; Bomholdt, Z.A.; Lee, J.E.; Flyak, A.I.; Matsuoka, R.; Kohda, D.; Yanagi, Y.; Hammel, M.; Crowe, J.E.; Saphire, E.O.
Deposited on : 2017-02-08
Resolution : 3.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20028442 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20028442 |

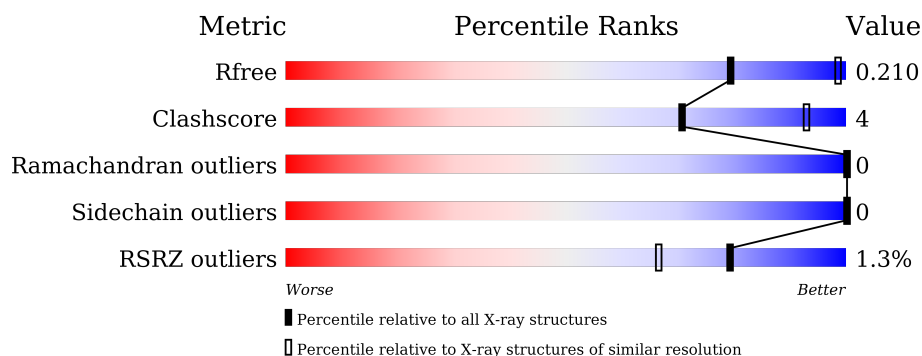
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1408 (3.80-3.40) |
| Clashscore | 102246 | 1010 (3.74-3.46) |
| Ramachandran outliers | 100387 | 1007 (3.76-3.44) |
| Sidechain outliers | 100360 | 1007 (3.76-3.44) |
| RSRZ outliers | 91569 | 1003 (3.78-3.42) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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 | A | 250 | <div> <div>51%</div> <div>7%</div> <div>42%</div> </div> |
| 1 | E | 250 | <div>2%</div> <div>52%</div> <div>6%</div> <div>42%</div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | J | 237 | |
| 2 | N | 237 | |
| 3 | C | 211 | |
| 3 | G | 211 | |
| 3 | K | 211 | |
| 3 | O | 211 | |
| 4 | D | 226 | |
| 4 | H | 226 | |
| 4 | L | 226 | |
| 4 | P | 226 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | NAG | N | 701 | - | - | - | X |

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN GP1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 145 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1131 | 717 | 198 | 209 | 7 | | | |
| 1 | E | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 712 | 197 | 207 | 6 | | | |
| 1 | I | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 706 | 195 | 205 | 6 | | | |
| 1 | M | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1112 | 706 | 195 | 205 | 6 | | | |

- Molecule 2 is a protein called ENVELOPE GLYCOPROTEIN GP2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 962 | 608 | 167 | 182 | 5 | | | |
| 2 | F | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 740 | 470 | 131 | 137 | 2 | | | |
| 2 | J | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 752 | 477 | 133 | 140 | 2 | | | |
| 2 | N | 92 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 722 | 460 | 128 | 132 | 2 | | | |

There are 156 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 438 | LEU | PHE | engineered mutation | UNP Q1PDC7 |
| B | 439 | ALA | TRP | engineered mutation | UNP Q1PDC7 |
| B | 445 | GLY | PHE | engineered mutation | UNP Q1PDC7 |
| B | 447 | ASN | PHE | engineered mutation | UNP Q1PDC7 |
| B | 638 | ASP | - | expression tag | UNP Q1PDC7 |
| B | 639 | ASP | - | expression tag | UNP Q1PDC7 |
| B | 640 | ASP | - | expression tag | UNP Q1PDC7 |
| B | 641 | ASP | - | expression tag | UNP Q1PDC7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | 642 | LYS | - | expression tag | UNP Q1PDC7 |
| B | 643 | ALA | - | expression tag | UNP Q1PDC7 |
| B | 644 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 645 | TRP | - | expression tag | UNP Q1PDC7 |
| B | 646 | SER | - | expression tag | UNP Q1PDC7 |
| B | 647 | HIS | - | expression tag | UNP Q1PDC7 |
| B | 648 | PRO | - | expression tag | UNP Q1PDC7 |
| B | 649 | GLN | - | expression tag | UNP Q1PDC7 |
| B | 650 | PHE | - | expression tag | UNP Q1PDC7 |
| B | 651 | GLU | - | expression tag | UNP Q1PDC7 |
| B | 652 | LYS | - | expression tag | UNP Q1PDC7 |
| B | 653 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 654 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 655 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 656 | SER | - | expression tag | UNP Q1PDC7 |
| B | 657 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 658 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 659 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 660 | SER | - | expression tag | UNP Q1PDC7 |
| B | 661 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 662 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 663 | GLY | - | expression tag | UNP Q1PDC7 |
| B | 664 | SER | - | expression tag | UNP Q1PDC7 |
| B | 665 | TRP | - | expression tag | UNP Q1PDC7 |
| B | 666 | SER | - | expression tag | UNP Q1PDC7 |
| B | 667 | HIS | - | expression tag | UNP Q1PDC7 |
| B | 668 | PRO | - | expression tag | UNP Q1PDC7 |
| B | 669 | GLN | - | expression tag | UNP Q1PDC7 |
| B | 670 | PHE | - | expression tag | UNP Q1PDC7 |
| B | 671 | GLU | - | expression tag | UNP Q1PDC7 |
| B | 672 | LYS | - | expression tag | UNP Q1PDC7 |
| F | 438 | LEU | PHE | engineered mutation | UNP Q1PDC7 |
| F | 439 | ALA | TRP | engineered mutation | UNP Q1PDC7 |
| F | 445 | GLY | PHE | engineered mutation | UNP Q1PDC7 |
| F | 447 | ASN | PHE | engineered mutation | UNP Q1PDC7 |
| F | 638 | ASP | - | expression tag | UNP Q1PDC7 |
| F | 639 | ASP | - | expression tag | UNP Q1PDC7 |
| F | 640 | ASP | - | expression tag | UNP Q1PDC7 |
| F | 641 | ASP | - | expression tag | UNP Q1PDC7 |
| F | 642 | LYS | - | expression tag | UNP Q1PDC7 |
| F | 643 | ALA | - | expression tag | UNP Q1PDC7 |
| F | 644 | GLY | - | expression tag | UNP Q1PDC7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| F | 645 | TRP | - | expression tag | UNP Q1PDC7 |
| F | 646 | SER | - | expression tag | UNP Q1PDC7 |
| F | 647 | HIS | - | expression tag | UNP Q1PDC7 |
| F | 648 | PRO | - | expression tag | UNP Q1PDC7 |
| F | 649 | GLN | - | expression tag | UNP Q1PDC7 |
| F | 650 | PHE | - | expression tag | UNP Q1PDC7 |
| F | 651 | GLU | - | expression tag | UNP Q1PDC7 |
| F | 652 | LYS | - | expression tag | UNP Q1PDC7 |
| F | 653 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 654 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 655 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 656 | SER | - | expression tag | UNP Q1PDC7 |
| F | 657 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 658 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 659 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 660 | SER | - | expression tag | UNP Q1PDC7 |
| F | 661 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 662 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 663 | GLY | - | expression tag | UNP Q1PDC7 |
| F | 664 | SER | - | expression tag | UNP Q1PDC7 |
| F | 665 | TRP | - | expression tag | UNP Q1PDC7 |
| F | 666 | SER | - | expression tag | UNP Q1PDC7 |
| F | 667 | HIS | - | expression tag | UNP Q1PDC7 |
| F | 668 | PRO | - | expression tag | UNP Q1PDC7 |
| F | 669 | GLN | - | expression tag | UNP Q1PDC7 |
| F | 670 | PHE | - | expression tag | UNP Q1PDC7 |
| F | 671 | GLU | - | expression tag | UNP Q1PDC7 |
| F | 672 | LYS | - | expression tag | UNP Q1PDC7 |
| J | 438 | LEU | PHE | engineered mutation | UNP Q1PDC7 |
| J | 439 | ALA | TRP | engineered mutation | UNP Q1PDC7 |
| J | 445 | GLY | PHE | engineered mutation | UNP Q1PDC7 |
| J | 447 | ASN | PHE | engineered mutation | UNP Q1PDC7 |
| J | 638 | ASP | - | expression tag | UNP Q1PDC7 |
| J | 639 | ASP | - | expression tag | UNP Q1PDC7 |
| J | 640 | ASP | - | expression tag | UNP Q1PDC7 |
| J | 641 | ASP | - | expression tag | UNP Q1PDC7 |
| J | 642 | LYS | - | expression tag | UNP Q1PDC7 |
| J | 643 | ALA | - | expression tag | UNP Q1PDC7 |
| J | 644 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 645 | TRP | - | expression tag | UNP Q1PDC7 |
| J | 646 | SER | - | expression tag | UNP Q1PDC7 |
| J | 647 | HIS | - | expression tag | UNP Q1PDC7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| J | 648 | PRO | - | expression tag | UNP Q1PDC7 |
| J | 649 | GLN | - | expression tag | UNP Q1PDC7 |
| J | 650 | PHE | - | expression tag | UNP Q1PDC7 |
| J | 651 | GLU | - | expression tag | UNP Q1PDC7 |
| J | 652 | LYS | - | expression tag | UNP Q1PDC7 |
| J | 653 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 654 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 655 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 656 | SER | - | expression tag | UNP Q1PDC7 |
| J | 657 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 658 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 659 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 660 | SER | - | expression tag | UNP Q1PDC7 |
| J | 661 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 662 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 663 | GLY | - | expression tag | UNP Q1PDC7 |
| J | 664 | SER | - | expression tag | UNP Q1PDC7 |
| J | 665 | TRP | - | expression tag | UNP Q1PDC7 |
| J | 666 | SER | - | expression tag | UNP Q1PDC7 |
| J | 667 | HIS | - | expression tag | UNP Q1PDC7 |
| J | 668 | PRO | - | expression tag | UNP Q1PDC7 |
| J | 669 | GLN | - | expression tag | UNP Q1PDC7 |
| J | 670 | PHE | - | expression tag | UNP Q1PDC7 |
| J | 671 | GLU | - | expression tag | UNP Q1PDC7 |
| J | 672 | LYS | - | expression tag | UNP Q1PDC7 |
| N | 438 | LEU | PHE | engineered mutation | UNP Q1PDC7 |
| N | 439 | ALA | TRP | engineered mutation | UNP Q1PDC7 |
| N | 445 | GLY | PHE | engineered mutation | UNP Q1PDC7 |
| N | 447 | ASN | PHE | engineered mutation | UNP Q1PDC7 |
| N | 638 | ASP | - | expression tag | UNP Q1PDC7 |
| N | 639 | ASP | - | expression tag | UNP Q1PDC7 |
| N | 640 | ASP | - | expression tag | UNP Q1PDC7 |
| N | 641 | ASP | - | expression tag | UNP Q1PDC7 |
| N | 642 | LYS | - | expression tag | UNP Q1PDC7 |
| N | 643 | ALA | - | expression tag | UNP Q1PDC7 |
| N | 644 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 645 | TRP | - | expression tag | UNP Q1PDC7 |
| N | 646 | SER | - | expression tag | UNP Q1PDC7 |
| N | 647 | HIS | - | expression tag | UNP Q1PDC7 |
| N | 648 | PRO | - | expression tag | UNP Q1PDC7 |
| N | 649 | GLN | - | expression tag | UNP Q1PDC7 |
| N | 650 | PHE | - | expression tag | UNP Q1PDC7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| N | 651 | GLU | - | expression tag | UNP Q1PDC7 |
| N | 652 | LYS | - | expression tag | UNP Q1PDC7 |
| N | 653 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 654 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 655 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 656 | SER | - | expression tag | UNP Q1PDC7 |
| N | 657 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 658 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 659 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 660 | SER | - | expression tag | UNP Q1PDC7 |
| N | 661 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 662 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 663 | GLY | - | expression tag | UNP Q1PDC7 |
| N | 664 | SER | - | expression tag | UNP Q1PDC7 |
| N | 665 | TRP | - | expression tag | UNP Q1PDC7 |
| N | 666 | SER | - | expression tag | UNP Q1PDC7 |
| N | 667 | HIS | - | expression tag | UNP Q1PDC7 |
| N | 668 | PRO | - | expression tag | UNP Q1PDC7 |
| N | 669 | GLN | - | expression tag | UNP Q1PDC7 |
| N | 670 | PHE | - | expression tag | UNP Q1PDC7 |
| N | 671 | GLU | - | expression tag | UNP Q1PDC7 |
| N | 672 | LYS | - | expression tag | UNP Q1PDC7 |

- Molecule 3 is a protein called MR78 Fab light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 210 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1632 | 1024 | 273 | 330 | 5 | | | |
| 3 | G | 210 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1632 | 1024 | 273 | 330 | 5 | | | |
| 3 | K | 210 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1632 | 1024 | 273 | 330 | 5 | | | |
| 3 | O | 210 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1626 | 1021 | 270 | 330 | 5 | | | |

- Molecule 4 is a protein called MR78 Fab heavy chain.

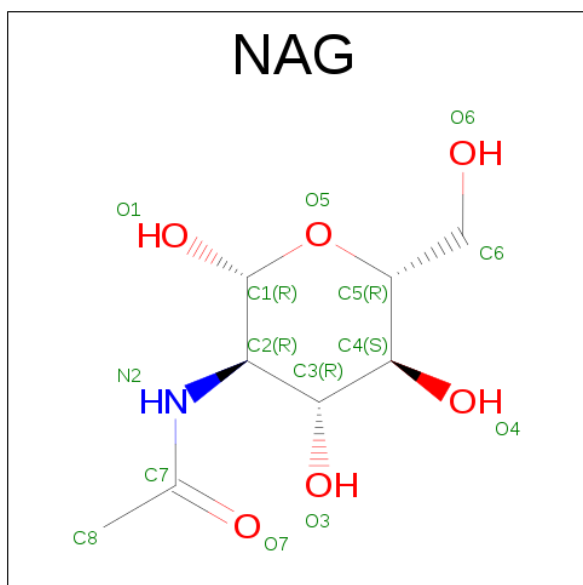
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1635 | 1045 | 259 | 326 | 5 | | | |
| 4 | H | 220 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1640 | 1047 | 260 | 328 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | L | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1655 | 1055 | 263 | 332 | 5 | | | |
| 4 | P | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1594 | 1019 | 252 | 318 | 5 | | | |

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



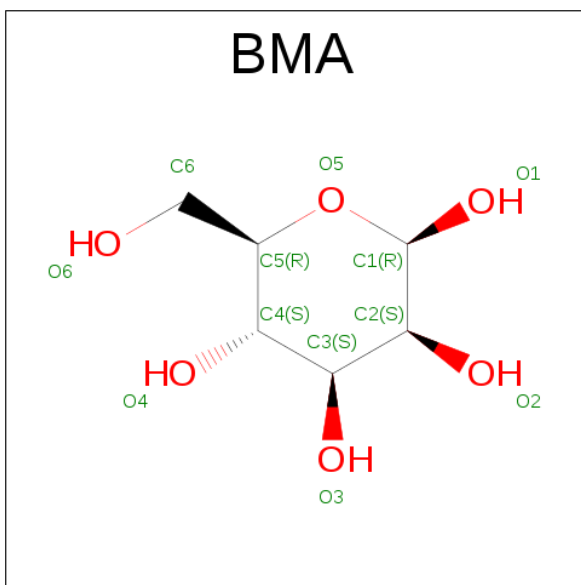
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

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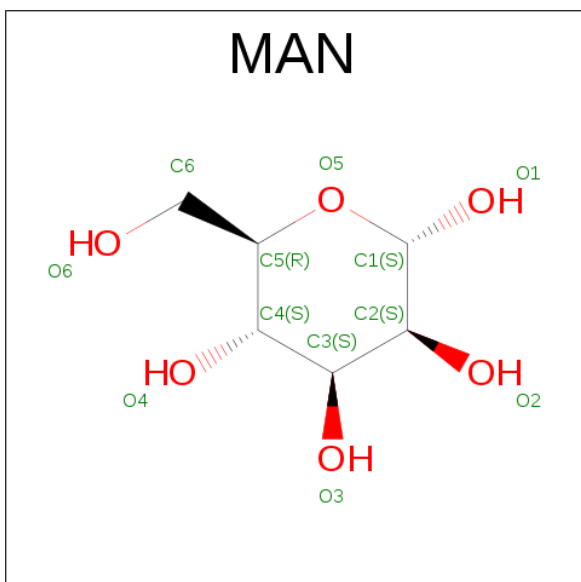
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5 | F | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | F | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | I | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | I | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | I | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | I | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | J | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | J | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | N | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | N | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).

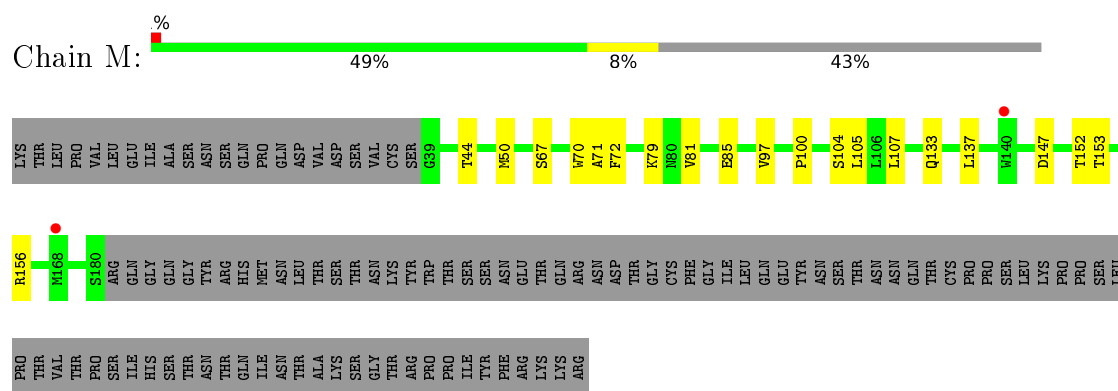


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6 | B | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 6 | F | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 6 | I | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 6 | J | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 6 | N | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |

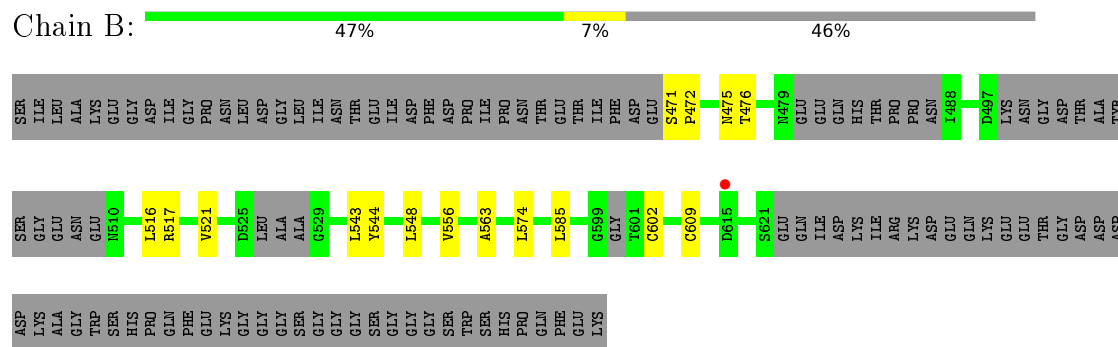
- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



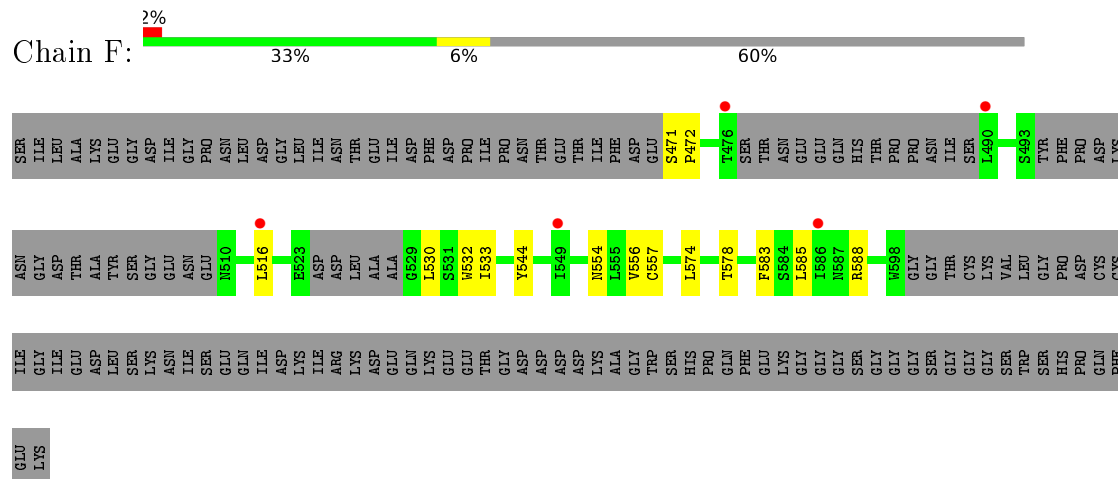
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7 | B | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | B | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | B | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | F | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | F | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | F | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | I | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | I | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | J | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | M | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | N | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |
| 7 | N | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 6 | 5 | | |



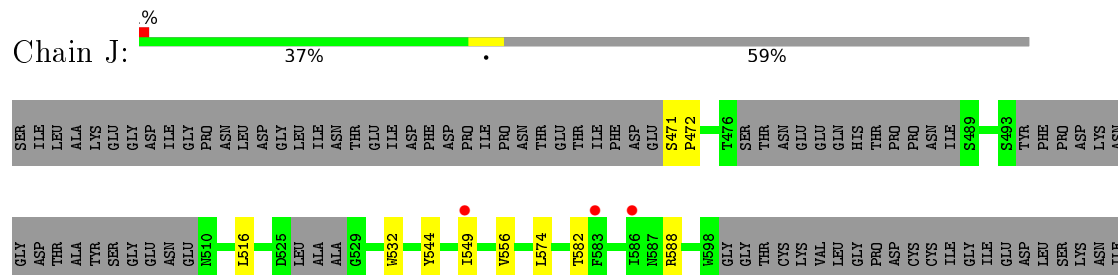
- Molecule 2: ENVELOPE GLYCOPROTEIN GP2



- Molecule 2: ENVELOPE GLYCOPROTEIN GP2



- Molecule 2: ENVELOPE GLYCOPROTEIN GP2



SER GLU GLN ILE ASP LYS ASP ILE ARG LYS LYS ASP GLU GLN LYS GLU GLU THR GLY ASP ASP ASP LYS ASP ALA GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY SER GLY GLY GLY TRP HIS PRO GLN PHE LYS

• Molecule 2: ENVELOPE GLYCOPROTEIN GP2


Chain N:  34% 5% 61%

SER ILE ALA LYS GLY ASP ILE GLY PRO ASN LEU ASP GLY ILE ASN THR GLU ILE THR PRO ASN THR GLU THR ILE PHE ASP GLY S471 H475 F476 SER THR ASN GLU GLN HIS THR PRO ASN ILE SER L490 T491 F492 S493 TTR PHE PRO ASP

LYS ASN GLY ASP THR ALA TYR SER GLY ASN GLY ASP GLN LYS L516 V521 GLN GLU ASP ASP ASP LYS ALA ALA G529 T102 W532 Y544 I549 Q552 V556 L574 R575 G599 GLY THR CYS VAL LEU GLY PRO ASP CYS ILE GLY ILE ASP LEU SER LYS


ASN ILE GLU GLN ILE LYS ARG LYS GLU ASN GLN LYS LYS GLU THR GLY ASP ASP ASP LYS ALA GLY TRP SER HIS PRO GLN PHE GLY SER GLY GLY SER GLY GLY GLY TRP HIS PRO GLN PHE GLU LYS

• Molecule 3: MR78 Fab light chain

Chain C:  2% 87% 13%

ASP I2 Q6 I21 R31 Y36 Q37 Q38 K39 K42 L46 L47 Q79 P80 T85 P100 G101 T102 K103 V104 D105 P113 S114 V115 F116 I117 V132 L136 N137 F139 K149 L154 S159 T164 L175 L179 L201 R211

• Molecule 3: MR78 Fab light chain

Chain G:  0% 85% 15%

ASP I2 Q6 S7 P8 I21 I29 S30 Y36 Q37 Q38 K39 K42 L46 L47 L54 V58 P59 S60 R61 F73 I83 A84 T85 P100 G101 T102 K103 P113 S114 P120 V132 V137 N138 F139 W148 N158 Q166 L181 A193

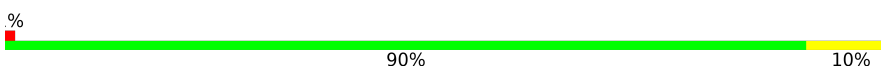
L201 S208 R211

• Molecule 3: MR78 Fab light chain

Chain K:  90% 10%


ASP I2 Q6 I21 Y36 Q37 L46 L47 F73 T85 L94 P100 G101 T102 K103 P113 P120 V132 F139 S159 L179 A193 Q199 S200 L201 S208 R211

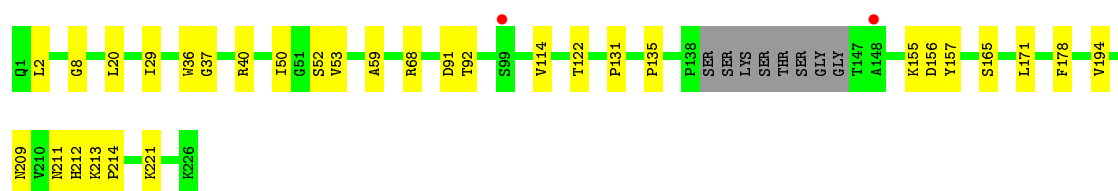
• Molecule 3: MR78 Fab light chain

Chain O:  90% 10%

ASP I2 Q6 I21 Y36 K39 K42 L46 L47 F73 P100 P113 S114 I117 V132 N137 N138 F139 N158 S159 L179 T180 L181 A193 T197 H198 L201 S208 R211

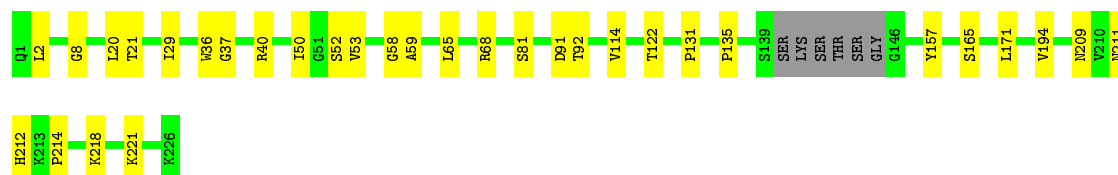
• Molecule 4: MR78 Fab heavy chain

Chain D:  83% 14% 3%



- Molecule 4: MR78 Fab heavy chain

Chain H: 83% 14% .



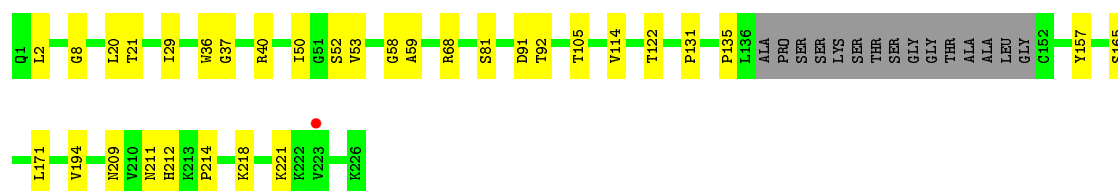
- Molecule 4: MR78 Fab heavy chain

Chain L: 87% 12% .



- Molecule 4: MR78 Fab heavy chain

Chain P: 79% 14% 7%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 63 | Depositor |
| Cell constants a, b, c, α , β , γ | 204.65Å 204.65Å 192.96Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 84.74 – 3.60 130.53 – 3.60 | Depositor EDS |
| % Data completeness (in resolution range) | 99.4 (84.74-3.60) 99.4 (130.53-3.60) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.14 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.23 (at 3.58Å) | Xtriage |
| Refinement program | PHENIX (1.10.1_2155: ???) | Depositor |
| R, R_{free} | 0.221 , 0.262 0.184 , 0.210 | Depositor DCC |
| R_{free} test set | 2676 reflections (5.07%) | DCC |
| Wilson B-factor (Å ²) | 105.0 | Xtriage |
| Anisotropy | 0.180 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 75.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$ | Xtriage |
| Estimated twinning fraction | 0.178 for h,-h-k,-l | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 21208 | wwPDB-VP |
| Average B, all atoms (Å ²) | 106.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: BMA, NAG, MAN

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 | 0.25 | 0/1159 | 0.43 | 0/1571 |
| 1 | E | 0.25 | 0/1150 | 0.43 | 0/1559 |
| 1 | I | 0.25 | 0/1140 | 0.43 | 0/1545 |
| 1 | M | 0.24 | 0/1140 | 0.43 | 0/1545 |
| 2 | B | 0.24 | 0/976 | 0.42 | 0/1324 |
| 2 | F | 0.24 | 0/751 | 0.39 | 0/1017 |
| 2 | J | 0.24 | 0/763 | 0.40 | 0/1034 |
| 2 | N | 0.23 | 0/733 | 0.40 | 0/992 |
| 3 | C | 0.25 | 0/1667 | 0.45 | 0/2263 |
| 3 | G | 0.24 | 0/1667 | 0.45 | 0/2263 |
| 3 | K | 0.24 | 0/1667 | 0.45 | 0/2263 |
| 3 | O | 0.24 | 0/1661 | 0.45 | 0/2256 |
| 4 | D | 0.25 | 0/1680 | 0.45 | 0/2294 |
| 4 | H | 0.25 | 0/1685 | 0.45 | 0/2303 |
| 4 | L | 0.25 | 0/1700 | 0.45 | 0/2320 |
| 4 | P | 0.24 | 0/1638 | 0.44 | 0/2235 |
| All | All | 0.24 | 0/21177 | 0.44 | 0/28784 |

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 | A | 1131 | 0 | 1115 | 11 | 0 |
| 1 | E | 1122 | 0 | 1101 | 10 | 0 |
| 1 | I | 1112 | 0 | 1097 | 14 | 0 |
| 1 | M | 1112 | 0 | 1097 | 13 | 0 |
| 2 | B | 962 | 0 | 918 | 10 | 0 |
| 2 | F | 740 | 0 | 726 | 12 | 0 |
| 2 | J | 752 | 0 | 729 | 9 | 0 |
| 2 | N | 722 | 0 | 715 | 9 | 0 |
| 3 | C | 1632 | 0 | 1590 | 15 | 0 |
| 3 | G | 1632 | 0 | 1590 | 17 | 0 |
| 3 | K | 1632 | 0 | 1590 | 12 | 0 |
| 3 | O | 1626 | 0 | 1579 | 12 | 0 |
| 4 | D | 1635 | 0 | 1591 | 16 | 0 |
| 4 | H | 1640 | 0 | 1588 | 17 | 0 |
| 4 | L | 1655 | 0 | 1607 | 14 | 0 |
| 4 | P | 1594 | 0 | 1548 | 18 | 0 |
| 5 | A | 56 | 0 | 50 | 0 | 0 |
| 5 | B | 28 | 0 | 24 | 0 | 0 |
| 5 | E | 42 | 0 | 38 | 0 | 0 |
| 5 | F | 28 | 0 | 24 | 1 | 0 |
| 5 | I | 56 | 0 | 49 | 0 | 0 |
| 5 | J | 28 | 0 | 24 | 1 | 0 |
| 5 | M | 56 | 0 | 50 | 0 | 0 |
| 5 | N | 28 | 0 | 24 | 1 | 0 |
| 6 | B | 11 | 0 | 8 | 0 | 0 |
| 6 | F | 11 | 0 | 8 | 0 | 0 |
| 6 | I | 11 | 0 | 9 | 0 | 0 |
| 6 | J | 11 | 0 | 9 | 0 | 0 |
| 6 | N | 11 | 0 | 9 | 0 | 0 |
| 7 | B | 33 | 0 | 29 | 1 | 0 |
| 7 | F | 33 | 0 | 29 | 0 | 0 |
| 7 | I | 22 | 0 | 20 | 0 | 0 |
| 7 | J | 11 | 0 | 10 | 0 | 0 |
| 7 | M | 11 | 0 | 10 | 0 | 0 |
| 7 | N | 22 | 0 | 19 | 0 | 0 |
| All | All | 21208 | 0 | 20624 | 185 | 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 (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:L:68:ARG:NH2 | 4:L:91:ASP:OD2 | 2.19 | 0.75 |
| 1:I:147:ASP:OD2 | 2:J:544:TYR:OH | 2.07 | 0.71 |
| 1:A:147:ASP:OD2 | 2:B:544:TYR:OH | 2.06 | 0.71 |
| 4:H:68:ARG:NH2 | 4:H:91:ASP:OD2 | 2.23 | 0.69 |
| 4:D:68:ARG:NH2 | 4:D:91:ASP:OD2 | 2.25 | 0.69 |
| 3:O:158:ASN:HD22 | 3:O:181:LEU:HD21 | 1.60 | 0.67 |
| 1:M:147:ASP:OD2 | 2:N:544:TYR:OH | 2.11 | 0.67 |
| 4:P:8:GLY:HA3 | 4:P:20:LEU:HD23 | 1.78 | 0.65 |
| 4:D:135:PRO:HD3 | 4:D:221:LYS:HE2 | 1.79 | 0.65 |
| 4:H:8:GLY:HA3 | 4:H:20:LEU:HD23 | 1.79 | 0.64 |
| 1:M:100:PRO:HB2 | 4:P:58:GLY:HA3 | 1.80 | 0.64 |
| 4:D:8:GLY:HA3 | 4:D:20:LEU:HD23 | 1.79 | 0.63 |
| 4:L:8:GLY:HA3 | 4:L:20:LEU:HD23 | 1.81 | 0.62 |
| 2:B:517:ARG:HD3 | 2:B:548:LEU:HD13 | 1.82 | 0.61 |
| 3:O:113:PRO:HD2 | 3:O:201:LEU:HD13 | 1.83 | 0.61 |
| 2:J:588:ARG:HG3 | 1:M:44:THR:HG21 | 1.82 | 0.60 |
| 4:D:171:LEU:HD21 | 4:D:194:VAL:HG21 | 1.84 | 0.59 |
| 4:P:68:ARG:NH2 | 4:P:91:ASP:OD2 | 2.33 | 0.59 |
| 4:D:92:THR:HG23 | 4:D:122:THR:HA | 1.85 | 0.58 |
| 3:G:120:PRO:HD3 | 3:G:132:VAL:HG22 | 1.83 | 0.58 |
| 4:H:92:THR:HG23 | 4:H:122:THR:HA | 1.85 | 0.58 |
| 1:M:81:VAL:HG23 | 2:N:574:LEU:HD21 | 1.85 | 0.58 |
| 2:B:475:ASN:OD1 | 2:B:476:THR:N | 2.37 | 0.57 |
| 3:O:132:VAL:HG23 | 3:O:179:LEU:HB3 | 1.87 | 0.57 |
| 3:C:113:PRO:HB3 | 3:C:139:PHE:HB3 | 1.87 | 0.57 |
| 3:G:6:GLN:HB2 | 3:G:100:PRO:HD2 | 1.87 | 0.56 |
| 1:E:81:VAL:HG23 | 2:F:574:LEU:HD21 | 1.86 | 0.56 |
| 4:P:171:LEU:HD21 | 4:P:194:VAL:HG21 | 1.88 | 0.56 |
| 4:P:135:PRO:HD3 | 4:P:221:LYS:HE2 | 1.87 | 0.56 |
| 4:P:53:VAL:HG12 | 4:P:59:ALA:HA | 1.88 | 0.56 |
| 3:G:8:PRO:HD2 | 3:G:21:ILE:HG22 | 1.88 | 0.55 |
| 1:E:50:MET:HG2 | 1:E:85:GLU:HB2 | 1.87 | 0.55 |
| 3:K:120:PRO:HD3 | 3:K:132:VAL:HG22 | 1.88 | 0.55 |
| 3:C:113:PRO:HD2 | 3:C:201:LEU:HD13 | 1.88 | 0.55 |
| 3:K:113:PRO:HD2 | 3:K:201:LEU:HD13 | 1.87 | 0.55 |
| 3:G:113:PRO:HB3 | 3:G:139:PHE:HB3 | 1.88 | 0.55 |
| 3:G:21:ILE:HG21 | 3:G:102:THR:HG21 | 1.88 | 0.55 |
| 4:P:211:ASN:HD22 | 4:P:218:LYS:HG2 | 1.71 | 0.55 |
| 3:G:21:ILE:HG13 | 3:G:73:PHE:HB3 | 1.89 | 0.55 |
| 4:L:211:ASN:HD22 | 4:L:218:LYS:HG2 | 1.71 | 0.55 |
| 4:H:171:LEU:HD21 | 4:H:194:VAL:HG21 | 1.88 | 0.55 |
| 3:G:158:ASN:HD22 | 3:G:181:LEU:HD21 | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:516:LEU:HD22 | 2:B:556:VAL:HG13 | 1.90 | 0.54 |
| 1:I:81:VAL:HG23 | 2:J:574:LEU:HD21 | 1.89 | 0.54 |
| 4:H:131:PRO:HB3 | 4:H:157:TYR:HB3 | 1.90 | 0.54 |
| 1:A:81:VAL:HG23 | 2:B:574:LEU:HD21 | 1.90 | 0.53 |
| 3:K:113:PRO:HB3 | 3:K:139:PHE:HB3 | 1.89 | 0.53 |
| 3:K:21:ILE:HG13 | 3:K:73:PHE:HB3 | 1.90 | 0.53 |
| 3:C:21:ILE:HD12 | 3:C:102:THR:HG21 | 1.90 | 0.53 |
| 4:D:211:ASN:HD21 | 4:D:213:LYS:HG2 | 1.74 | 0.53 |
| 3:O:39:LYS:HB2 | 3:O:42:LYS:HG2 | 1.90 | 0.53 |
| 4:H:165:SER:HB3 | 4:H:209:ASN:HB2 | 1.91 | 0.53 |
| 3:G:36:TYR:CE1 | 3:G:46:LEU:HB3 | 2.44 | 0.53 |
| 4:P:92:THR:HG23 | 4:P:122:THR:HA | 1.91 | 0.52 |
| 4:P:165:SER:HB3 | 4:P:209:ASN:HB2 | 1.90 | 0.52 |
| 4:D:29:ILE:HG13 | 4:D:36:TRP:CE2 | 2.45 | 0.52 |
| 4:H:211:ASN:HB2 | 4:H:218:LYS:HD2 | 1.91 | 0.51 |
| 4:L:92:THR:HG23 | 4:L:122:THR:HA | 1.92 | 0.51 |
| 3:O:113:PRO:HB3 | 3:O:139:PHE:HB3 | 1.92 | 0.51 |
| 4:D:2:LEU:HB2 | 4:D:114:VAL:HG21 | 1.93 | 0.51 |
| 3:C:85:THR:HG22 | 3:C:103:LYS:HG2 | 1.92 | 0.51 |
| 3:C:39:LYS:HB2 | 3:C:42:LYS:HG2 | 1.92 | 0.51 |
| 3:G:54:LEU:HB2 | 3:G:58:VAL:HG21 | 1.93 | 0.51 |
| 1:I:128:GLN:HE21 | 3:K:94:LEU:HD23 | 1.76 | 0.51 |
| 4:L:165:SER:HB3 | 4:L:209:ASN:HB2 | 1.92 | 0.51 |
| 5:J:701:NAG:H83 | 2:N:532:TRP:HH2 | 1.76 | 0.51 |
| 4:L:135:PRO:HD3 | 4:L:221:LYS:HE2 | 1.93 | 0.51 |
| 4:D:131:PRO:HB3 | 4:D:157:TYR:HB3 | 1.94 | 0.50 |
| 3:K:21:ILE:HG21 | 3:K:102:THR:HG21 | 1.93 | 0.50 |
| 4:P:21:THR:HG22 | 4:P:81:SER:HB3 | 1.92 | 0.50 |
| 1:E:148:ARG:NH1 | 2:N:575:ARG:O | 2.45 | 0.50 |
| 3:G:114:SER:HB2 | 3:G:137:ASN:HB3 | 1.94 | 0.50 |
| 3:O:21:ILE:HG13 | 3:O:73:PHE:HB3 | 1.94 | 0.50 |
| 2:F:516:LEU:HD22 | 2:F:556:VAL:HG13 | 1.93 | 0.50 |
| 4:L:29:ILE:HG13 | 4:L:36:TRP:CE2 | 2.46 | 0.50 |
| 4:L:171:LEU:HD21 | 4:L:194:VAL:HG21 | 1.93 | 0.49 |
| 1:I:100:PRO:HB2 | 4:L:58:GLY:HA3 | 1.94 | 0.49 |
| 3:K:6:GLN:HB2 | 3:K:100:PRO:HD2 | 1.94 | 0.49 |
| 4:L:131:PRO:HB3 | 4:L:157:TYR:HB3 | 1.94 | 0.49 |
| 1:I:79:LYS:HB3 | 2:J:574:LEU:HD22 | 1.93 | 0.49 |
| 3:C:6:GLN:HB2 | 3:C:100:PRO:HD2 | 1.94 | 0.49 |
| 1:E:147:ASP:OD2 | 2:F:544:TYR:OH | 2.12 | 0.49 |
| 4:P:131:PRO:HB3 | 4:P:157:TYR:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:578:THR:HG22 | 1:I:114:ARG:HH22 | 1.78 | 0.49 |
| 2:B:521:VAL:HG13 | 2:B:543:LEU:HG | 1.95 | 0.49 |
| 2:F:588:ARG:HG3 | 1:I:44:THR:HG21 | 1.95 | 0.49 |
| 4:D:212:HIS:CD2 | 4:D:214:PRO:HD2 | 2.48 | 0.48 |
| 1:I:50:MET:HG2 | 1:I:85:GLU:HB2 | 1.95 | 0.48 |
| 1:A:50:MET:HG2 | 1:A:85:GLU:HB2 | 1.95 | 0.48 |
| 4:H:21:THR:HG22 | 4:H:81:SER:HB3 | 1.94 | 0.48 |
| 2:N:490:LEU:N | 2:N:552:GLN:HE22 | 2.10 | 0.48 |
| 2:F:532:TRP:HH2 | 5:N:701:NAG:H83 | 1.78 | 0.48 |
| 3:C:114:SER:HB2 | 3:C:137:ASN:HB3 | 1.94 | 0.48 |
| 1:M:50:MET:HG2 | 1:M:85:GLU:HB2 | 1.94 | 0.48 |
| 2:F:583:PHE:HZ | 2:F:588:ARG:HE | 1.61 | 0.48 |
| 3:G:113:PRO:HD2 | 3:G:201:LEU:HD13 | 1.94 | 0.47 |
| 4:P:29:ILE:HG13 | 4:P:36:TRP:CE2 | 2.49 | 0.47 |
| 4:D:40:ARG:HB3 | 4:D:50:ILE:HD11 | 1.97 | 0.47 |
| 4:H:50:ILE:HG23 | 4:H:65:LEU:HD13 | 1.97 | 0.47 |
| 1:A:138:HIS:CE1 | 1:A:140:TRP:HB2 | 2.49 | 0.47 |
| 4:D:165:SER:HB3 | 4:D:209:ASN:HB2 | 1.96 | 0.47 |
| 4:L:212:HIS:CD2 | 4:L:214:PRO:HD2 | 2.49 | 0.47 |
| 3:K:85:THR:HG22 | 3:K:103:LYS:HG2 | 1.96 | 0.47 |
| 4:P:2:LEU:HB2 | 4:P:114:VAL:HG21 | 1.97 | 0.47 |
| 3:K:37:GLN:HB2 | 3:K:47:LEU:HD11 | 1.97 | 0.46 |
| 4:H:40:ARG:HB3 | 4:H:50:ILE:HD11 | 1.98 | 0.46 |
| 1:M:137:LEU:HD22 | 1:M:152:THR:HG22 | 1.97 | 0.46 |
| 3:K:36:TYR:CE1 | 3:K:46:LEU:HB3 | 2.50 | 0.46 |
| 3:C:159:SER:HB3 | 3:C:179:LEU:HD12 | 1.98 | 0.46 |
| 4:D:53:VAL:HG12 | 4:D:59:ALA:HA | 1.97 | 0.46 |
| 3:G:37:GLN:HB2 | 3:G:47:LEU:HD11 | 1.98 | 0.46 |
| 2:J:516:LEU:HD22 | 2:J:556:VAL:HG13 | 1.97 | 0.46 |
| 5:F:701:NAG:H83 | 2:J:532:TRP:HH2 | 1.81 | 0.46 |
| 3:O:193:ALA:HB2 | 3:O:208:SER:HB3 | 1.98 | 0.46 |
| 4:L:53:VAL:HG12 | 4:L:59:ALA:HA | 1.97 | 0.46 |
| 3:C:36:TYR:CE2 | 3:C:46:LEU:HB3 | 2.51 | 0.45 |
| 4:H:212:HIS:CD2 | 4:H:214:PRO:HD2 | 2.52 | 0.45 |
| 1:E:107:LEU:HD12 | 1:E:153:THR:HG21 | 1.99 | 0.45 |
| 4:H:53:VAL:HG12 | 4:H:59:ALA:HA | 1.97 | 0.45 |
| 4:H:29:ILE:HG13 | 4:H:36:TRP:CE2 | 2.51 | 0.45 |
| 3:C:132:VAL:HG13 | 3:C:179:LEU:HB3 | 1.99 | 0.44 |
| 1:A:104:SER:HB3 | 1:A:156:ARG:HE | 1.82 | 0.44 |
| 1:E:100:PRO:HB2 | 4:H:58:GLY:HA3 | 1.99 | 0.44 |
| 4:H:135:PRO:HD3 | 4:H:221:LYS:HE2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:159:SER:HB3 | 3:O:179:LEU:HD12 | 1.98 | 0.44 |
| 1:E:73:ARG:HG2 | 1:E:74:THR:N | 2.32 | 0.44 |
| 3:O:36:TYR:CE2 | 3:O:46:LEU:HB3 | 2.52 | 0.44 |
| 4:P:40:ARG:HB3 | 4:P:50:ILE:HD11 | 1.99 | 0.44 |
| 1:E:138:HIS:CE1 | 1:E:140:TRP:HB2 | 2.53 | 0.43 |
| 2:F:578:THR:HG22 | 1:I:114:ARG:NH2 | 2.32 | 0.43 |
| 3:C:164:THR:HG23 | 4:D:178:PHE:CD2 | 2.53 | 0.43 |
| 4:L:40:ARG:HB3 | 4:L:50:ILE:HD11 | 1.99 | 0.43 |
| 3:O:6:GLN:HB2 | 3:O:100:PRO:HD2 | 2.00 | 0.43 |
| 2:F:471:SER:HA | 2:F:472:PRO:HD3 | 1.88 | 0.43 |
| 3:G:39:LYS:HB2 | 3:G:42:LYS:HG2 | 2.00 | 0.43 |
| 1:M:104:SER:HB3 | 1:M:156:ARG:HE | 1.83 | 0.43 |
| 3:O:114:SER:HB2 | 3:O:137:ASN:HB3 | 2.00 | 0.43 |
| 2:F:530:LEU:HG | 2:F:533:ILE:HD12 | 2.00 | 0.43 |
| 1:I:116:TYR:H | 1:I:159:VAL:HG23 | 1.82 | 0.43 |
| 4:P:37:GLY:HA2 | 4:P:52:SER:HA | 2.00 | 0.43 |
| 2:B:602:CYS:HB2 | 2:B:609:CYS:HB2 | 1.89 | 0.43 |
| 1:I:73:ARG:HG2 | 1:I:74:THR:N | 2.32 | 0.43 |
| 4:D:37:GLY:HA2 | 4:D:52:SER:HA | 2.01 | 0.43 |
| 3:G:193:ALA:HB2 | 3:G:208:SER:HB3 | 2.00 | 0.43 |
| 1:M:71:ALA:HB2 | 4:P:105:THR:HB | 2.00 | 0.43 |
| 3:C:37:GLN:HB2 | 3:C:47:LEU:HD11 | 2.01 | 0.42 |
| 1:I:146:TYR:CE1 | 1:I:160:PHE:HB3 | 2.54 | 0.42 |
| 4:P:40:ARG:HH12 | 4:P:91:ASP:CG | 2.22 | 0.42 |
| 2:J:471:SER:HA | 2:J:472:PRO:HD3 | 1.86 | 0.42 |
| 3:O:198:HIS:HB3 | 3:O:201:LEU:HB2 | 2.00 | 0.42 |
| 3:C:79:GLN:HB3 | 3:C:80:PRO:HD2 | 2.00 | 0.42 |
| 1:A:67:SER:HA | 1:A:70:TRP:CE3 | 2.54 | 0.42 |
| 1:A:166:ALA:HB2 | 2:B:563:ALA:HB2 | 2.00 | 0.42 |
| 2:J:516:LEU:HD23 | 2:J:549:ILE:HB | 2.01 | 0.42 |
| 4:L:167:ASN:HD22 | 4:L:171:LEU:HB2 | 1.84 | 0.42 |
| 2:N:475:ASN:OD1 | 2:N:491:THR:OG1 | 2.37 | 0.42 |
| 1:E:49:LEU:HD11 | 2:F:585:LEU:HB3 | 2.01 | 0.42 |
| 1:M:107:LEU:HD12 | 1:M:153:THR:HG21 | 2.00 | 0.42 |
| 1:A:49:LEU:HD11 | 2:B:585:LEU:HB3 | 2.01 | 0.41 |
| 4:P:212:HIS:CD2 | 4:P:214:PRO:HD2 | 2.55 | 0.41 |
| 1:A:107:LEU:HD12 | 1:A:153:THR:HG21 | 2.01 | 0.41 |
| 3:C:149:LYS:HG2 | 3:C:154:LEU:HD22 | 2.02 | 0.41 |
| 1:E:104:SER:HB3 | 1:E:156:ARG:HE | 1.85 | 0.41 |
| 3:G:59:PRO:HB2 | 3:G:61:ARG:HG2 | 2.02 | 0.41 |
| 3:K:159:SER:HB3 | 3:K:179:LEU:HD12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:2:LEU:HB2 | 4:H:114:VAL:HG21 | 2.01 | 0.41 |
| 4:D:155:LYS:HG2 | 4:D:156:ASP:OD1 | 2.20 | 0.41 |
| 1:M:72:PHE:HB3 | 1:M:133:GLN:O | 2.21 | 0.41 |
| 7:B:704:MAN:H2 | 7:B:705:MAN:H2 | 1.81 | 0.41 |
| 1:M:67:SER:HA | 1:M:70:TRP:CE3 | 2.56 | 0.41 |
| 4:H:37:GLY:HA2 | 4:H:52:SER:HA | 2.02 | 0.41 |
| 1:I:61:ASP:HB3 | 1:I:91:THR:HG21 | 2.03 | 0.41 |
| 1:M:79:LYS:HB3 | 2:N:574:LEU:HD22 | 2.03 | 0.41 |
| 1:A:137:LEU:HD22 | 1:A:152:THR:HG22 | 2.03 | 0.41 |
| 2:F:554:ASN:HB2 | 2:F:557:CYS:HB2 | 2.03 | 0.41 |
| 1:I:112:ASN:ND2 | 2:J:582:THR:HG23 | 2.36 | 0.41 |
| 3:K:193:ALA:HB2 | 3:K:208:SER:HB3 | 2.02 | 0.41 |
| 3:G:85:THR:HG22 | 3:G:103:LYS:HG2 | 2.02 | 0.41 |
| 1:M:97:VAL:HG12 | 1:M:105:LEU:HD12 | 2.02 | 0.41 |
| 1:A:90:LYS:O | 1:A:120:LYS:HB3 | 2.21 | 0.41 |
| 3:C:136:LEU:HB2 | 3:C:175:LEU:HB3 | 2.03 | 0.41 |
| 2:N:516:LEU:HD22 | 2:N:556:VAL:HG13 | 2.02 | 0.40 |
| 2:B:471:SER:HA | 2:B:472:PRO:HD3 | 1.91 | 0.40 |
| 3:G:83:ILE:HD13 | 3:G:166:GLN:HB3 | 2.02 | 0.40 |
| 2:N:516:LEU:HD23 | 2:N:549:ILE:HB | 2.04 | 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 of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | A | 143/250 (57%) | 139 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | E | 142/250 (57%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | I | 140/250 (56%) | 137 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | M | 140/250 (56%) | 136 (97%) | 4 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2 | B | 117/237 (49%) | 110 (94%) | 7 (6%) | 0 | 100 | 100 |
| 2 | F | 86/237 (36%) | 81 (94%) | 5 (6%) | 0 | 100 | 100 |
| 2 | J | 89/237 (38%) | 84 (94%) | 5 (6%) | 0 | 100 | 100 |
| 2 | N | 84/237 (35%) | 80 (95%) | 4 (5%) | 0 | 100 | 100 |
| 3 | C | 208/211 (99%) | 203 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | G | 208/211 (99%) | 202 (97%) | 6 (3%) | 0 | 100 | 100 |
| 3 | K | 208/211 (99%) | 204 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | O | 208/211 (99%) | 202 (97%) | 6 (3%) | 0 | 100 | 100 |
| 4 | D | 214/226 (95%) | 202 (94%) | 12 (6%) | 0 | 100 | 100 |
| 4 | H | 216/226 (96%) | 204 (94%) | 12 (6%) | 0 | 100 | 100 |
| 4 | L | 218/226 (96%) | 205 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | P | 207/226 (92%) | 196 (95%) | 11 (5%) | 0 | 100 | 100 |
| All | All | 2628/3696 (71%) | 2523 (96%) | 105 (4%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 124/222 (56%) | 124 (100%) | 0 | 100 | 100 |
| 1 | E | 121/222 (54%) | 121 (100%) | 0 | 100 | 100 |
| 1 | I | 121/222 (54%) | 121 (100%) | 0 | 100 | 100 |
| 1 | M | 121/222 (54%) | 121 (100%) | 0 | 100 | 100 |
| 2 | B | 103/202 (51%) | 103 (100%) | 0 | 100 | 100 |
| 2 | F | 80/202 (40%) | 80 (100%) | 0 | 100 | 100 |
| 2 | J | 80/202 (40%) | 80 (100%) | 0 | 100 | 100 |
| 2 | N | 78/202 (39%) | 78 (100%) | 0 | 100 | 100 |
| 3 | C | 188/189 (100%) | 188 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 3 | G | 188/189 (100%) | 188 (100%) | 0 | 100 | 100 |
| 3 | K | 188/189 (100%) | 188 (100%) | 0 | 100 | 100 |
| 3 | O | 187/189 (99%) | 187 (100%) | 0 | 100 | 100 |
| 4 | D | 186/192 (97%) | 186 (100%) | 0 | 100 | 100 |
| 4 | H | 186/192 (97%) | 186 (100%) | 0 | 100 | 100 |
| 4 | L | 188/192 (98%) | 188 (100%) | 0 | 100 | 100 |
| 4 | P | 183/192 (95%) | 183 (100%) | 0 | 100 | 100 |
| All | All | 2322/3220 (72%) | 2322 (100%) | 0 | 100 | 100 |

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

40 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 |
| 5 | NAG | A | 301 | 1,5 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.30 | 0 |
| 5 | NAG | A | 302 | 5 | 14,14,15 | 0.23 | 0 | 15,19,21 | 0.39 | 0 |
| 5 | NAG | A | 303 | 1,5 | 14,14,15 | 0.46 | 0 | 15,19,21 | 0.38 | 0 |
| 5 | NAG | A | 304 | 5 | 14,14,15 | 0.34 | 0 | 15,19,21 | 0.32 | 0 |
| 5 | NAG | B | 701 | 2,5 | 14,14,15 | 0.20 | 0 | 15,19,21 | 0.40 | 0 |
| 5 | NAG | B | 702 | 5,6 | 14,14,15 | 0.26 | 0 | 15,19,21 | 0.47 | 0 |
| 6 | BMA | B | 703 | 5,7 | 11,11,12 | 0.64 | 0 | 15,15,17 | 0.82 | 0 |
| 7 | MAN | B | 704 | 7,6 | 11,11,12 | 0.72 | 0 | 15,15,17 | 0.94 | 0 |
| 7 | MAN | B | 705 | 7 | 11,11,12 | 0.78 | 0 | 15,15,17 | 0.91 | 1 (6%) |
| 7 | MAN | B | 706 | 6 | 11,11,12 | 0.87 | 1 (9%) | 15,15,17 | 1.16 | 3 (20%) |
| 5 | NAG | E | 301 | 1,5 | 14,14,15 | 0.32 | 0 | 15,19,21 | 0.25 | 0 |
| 5 | NAG | E | 302 | 5 | 14,14,15 | 0.23 | 0 | 15,19,21 | 0.41 | 0 |
| 5 | NAG | E | 303 | 1 | 14,14,15 | 0.35 | 0 | 15,19,21 | 0.32 | 0 |
| 5 | NAG | F | 701 | 2,5 | 14,14,15 | 0.22 | 0 | 15,19,21 | 0.40 | 0 |
| 5 | NAG | F | 702 | 5,6 | 14,14,15 | 0.26 | 0 | 15,19,21 | 0.38 | 0 |
| 6 | BMA | F | 703 | 5,7 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.75 | 0 |
| 7 | MAN | F | 704 | 7,6 | 11,11,12 | 1.09 | 1 (9%) | 15,15,17 | 0.95 | 0 |
| 7 | MAN | F | 705 | 7 | 11,11,12 | 0.95 | 0 | 15,15,17 | 1.19 | 2 (13%) |
| 7 | MAN | F | 706 | 6 | 11,11,12 | 0.68 | 0 | 15,15,17 | 1.09 | 2 (13%) |
| 5 | NAG | I | 301 | 1,5 | 14,14,15 | 0.42 | 0 | 15,19,21 | 0.30 | 0 |
| 5 | NAG | I | 302 | 5,6 | 14,14,15 | 0.26 | 0 | 15,19,21 | 0.35 | 0 |
| 6 | BMA | I | 303 | 5,7 | 11,11,12 | 0.50 | 0 | 15,15,17 | 0.67 | 0 |
| 7 | MAN | I | 304 | 6 | 11,11,12 | 0.66 | 0 | 15,15,17 | 1.05 | 2 (13%) |
| 7 | MAN | I | 305 | - | 11,11,12 | 0.63 | 0 | 15,15,17 | 1.16 | 2 (13%) |
| 5 | NAG | I | 306 | 1,5 | 14,14,15 | 0.32 | 0 | 15,19,21 | 0.21 | 0 |
| 5 | NAG | I | 307 | 5 | 14,14,15 | 0.30 | 0 | 15,19,21 | 0.41 | 0 |
| 5 | NAG | J | 701 | 2,5 | 14,14,15 | 0.18 | 0 | 15,19,21 | 0.40 | 0 |
| 5 | NAG | J | 702 | 5,6 | 14,14,15 | 0.22 | 0 | 15,19,21 | 0.38 | 0 |
| 6 | BMA | J | 703 | 5,7 | 11,11,12 | 0.71 | 0 | 15,15,17 | 0.79 | 0 |
| 7 | MAN | J | 704 | 6 | 11,11,12 | 0.75 | 0 | 15,15,17 | 0.94 | 1 (6%) |
| 5 | NAG | M | 301 | 1,5 | 14,14,15 | 0.29 | 0 | 15,19,21 | 0.30 | 0 |
| 5 | NAG | M | 302 | 5 | 14,14,15 | 0.24 | 0 | 15,19,21 | 0.40 | 0 |
| 5 | NAG | M | 303 | 1,5 | 14,14,15 | 0.33 | 0 | 15,19,21 | 0.38 | 0 |
| 5 | NAG | M | 304 | 5 | 14,14,15 | 0.37 | 0 | 15,19,21 | 0.51 | 0 |
| 7 | MAN | M | 305 | - | 11,11,12 | 0.94 | 1 (9%) | 15,15,17 | 1.24 | 2 (13%) |
| 5 | NAG | N | 701 | 2,5 | 14,14,15 | 0.24 | 0 | 15,19,21 | 0.43 | 0 |
| 5 | NAG | N | 702 | 5,6 | 14,14,15 | 0.25 | 0 | 15,19,21 | 0.36 | 0 |
| 6 | BMA | N | 703 | 5,7 | 11,11,12 | 0.86 | 0 | 15,15,17 | 1.16 | 1 (6%) |
| 7 | MAN | N | 704 | 7,6 | 11,11,12 | 0.73 | 0 | 15,15,17 | 1.00 | 1 (6%) |
| 7 | MAN | N | 705 | 7 | 11,11,12 | 0.64 | 0 | 15,15,17 | 0.96 | 2 (13%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5 | NAG | A | 301 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 302 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 303 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 304 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 701 | 2,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 702 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | B | 703 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | B | 704 | 7,6 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | B | 705 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | B | 706 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | E | 301 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | E | 302 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | E | 303 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | F | 701 | 2,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | F | 702 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | F | 703 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | F | 704 | 7,6 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | F | 705 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | F | 706 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | I | 301 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 302 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | I | 303 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | I | 304 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | I | 305 | - | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | I | 306 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 307 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | J | 701 | 2,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | J | 702 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | J | 703 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | J | 704 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | M | 301 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 302 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 303 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 304 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | MAN | M | 305 | - | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | N | 701 | 2,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | N | 702 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | N | 703 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | N | 704 | 7,6 | - | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7 | MAN | N | 705 | 7 | - | 0/2/19/22 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7 | M | 305 | MAN | O5-C1 | -2.06 | 1.40 | 1.43 |
| 7 | F | 704 | MAN | C2-C3 | 2.17 | 1.55 | 1.52 |
| 7 | B | 706 | MAN | C1-C2 | 2.36 | 1.58 | 1.52 |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6 | N | 703 | BMA | O6-C6-C5 | -2.50 | 102.97 | 111.30 |
| 7 | B | 706 | MAN | O2-C2-C3 | -2.29 | 105.56 | 110.19 |
| 7 | J | 704 | MAN | O2-C2-C3 | -2.27 | 105.60 | 110.19 |
| 7 | F | 706 | MAN | O2-C2-C3 | -2.27 | 105.61 | 110.19 |
| 7 | B | 705 | MAN | O2-C2-C3 | -2.23 | 105.70 | 110.19 |
| 7 | I | 305 | MAN | O2-C2-C3 | -2.21 | 105.73 | 110.19 |
| 7 | F | 705 | MAN | O2-C2-C3 | -2.20 | 105.76 | 110.19 |
| 7 | M | 305 | MAN | O2-C2-C3 | -2.17 | 105.82 | 110.19 |
| 7 | I | 304 | MAN | O2-C2-C3 | -2.17 | 105.82 | 110.19 |
| 7 | N | 705 | MAN | O2-C2-C3 | -2.04 | 106.08 | 110.19 |
| 7 | I | 305 | MAN | C1-O5-C5 | 2.11 | 115.24 | 112.14 |
| 7 | N | 704 | MAN | O3-C3-C2 | 2.13 | 113.92 | 110.01 |
| 7 | B | 706 | MAN | C1-O5-C5 | 2.22 | 115.40 | 112.14 |
| 7 | M | 305 | MAN | O5-C1-C2 | 2.31 | 114.59 | 110.89 |
| 7 | F | 705 | MAN | C1-O5-C5 | 2.40 | 115.66 | 112.14 |
| 7 | N | 705 | MAN | C1-O5-C5 | 2.42 | 115.70 | 112.14 |
| 7 | B | 706 | MAN | C1-C2-C3 | 2.42 | 112.49 | 109.55 |
| 7 | I | 304 | MAN | C1-O5-C5 | 2.44 | 115.72 | 112.14 |
| 7 | F | 706 | MAN | C1-O5-C5 | 2.87 | 116.35 | 112.14 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 7 | B | 704 | MAN | 1 | 0 |
| 7 | B | 705 | MAN | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | F | 701 | NAG | 1 | 0 |
| 5 | J | 701 | NAG | 1 | 0 |
| 5 | N | 701 | NAG | 1 | 0 |

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 | OWAB(Å ²) | Q < 0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1 | A | 145/250 (58%) | 0.14 | 0 100 100 | 55, 86, 119, 147 | 0 |
| 1 | E | 144/250 (57%) | 0.48 | 4 (2%) 56 42 | 70, 94, 132, 148 | 0 |
| 1 | I | 142/250 (56%) | 0.60 | 5 (3%) 48 34 | 70, 99, 133, 149 | 0 |
| 1 | M | 142/250 (56%) | 0.49 | 2 (1%) 78 65 | 94, 116, 139, 155 | 0 |
| 2 | B | 127/237 (53%) | 0.11 | 1 (0%) 87 78 | 73, 110, 158, 174 | 0 |
| 2 | F | 94/237 (39%) | 0.49 | 5 (5%) 30 21 | 79, 120, 149, 158 | 0 |
| 2 | J | 97/237 (40%) | 0.51 | 3 (3%) 52 38 | 80, 120, 149, 176 | 0 |
| 2 | N | 92/237 (38%) | 0.35 | 1 (1%) 82 70 | 93, 124, 150, 173 | 0 |
| 3 | C | 210/211 (99%) | 0.36 | 5 (2%) 62 47 | 72, 116, 136, 149 | 0 |
| 3 | G | 210/211 (99%) | 0.43 | 3 (1%) 78 65 | 68, 99, 128, 161 | 0 |
| 3 | K | 210/211 (99%) | 0.35 | 1 (0%) 91 86 | 61, 95, 124, 141 | 0 |
| 3 | O | 210/211 (99%) | 0.17 | 3 (1%) 78 65 | 110, 138, 158, 168 | 0 |
| 4 | D | 218/226 (96%) | 0.30 | 2 (0%) 85 75 | 59, 86, 127, 155 | 0 |
| 4 | H | 220/226 (97%) | 0.35 | 0 100 100 | 59, 82, 111, 128 | 0 |
| 4 | L | 222/226 (98%) | 0.26 | 0 100 100 | 57, 80, 124, 151 | 0 |
| 4 | P | 211/226 (93%) | 0.12 | 1 (0%) 91 86 | 99, 126, 148, 174 | 0 |
| All | All | 2694/3696 (72%) | 0.33 | 36 (1%) 79 66 | 55, 105, 145, 176 | 0 |

All (36) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | F | 476 | THR | 4.0 |
| 2 | J | 583 | PHE | 3.6 |
| 3 | G | 30 | SER | 3.3 |
| 3 | C | 105 | ASP | 3.0 |
| 1 | E | 50 | MET | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | C | 117 | ILE | 2.9 |
| 3 | K | 199 | GLN | 2.7 |
| 3 | O | 197 | THR | 2.6 |
| 1 | E | 139 | LEU | 2.6 |
| 1 | I | 50 | MET | 2.6 |
| 4 | D | 148 | ALA | 2.5 |
| 2 | J | 549 | ILE | 2.5 |
| 3 | C | 31 | ASN | 2.4 |
| 1 | M | 168 | MET | 2.4 |
| 1 | I | 39 | GLY | 2.4 |
| 3 | O | 47 | LEU | 2.3 |
| 3 | O | 117 | ILE | 2.3 |
| 2 | N | 490 | LEU | 2.3 |
| 3 | C | 115 | VAL | 2.2 |
| 2 | B | 615 | ASP | 2.2 |
| 2 | J | 586 | ILE | 2.2 |
| 2 | F | 586 | ILE | 2.2 |
| 2 | F | 516 | LEU | 2.2 |
| 3 | G | 148 | TRP | 2.2 |
| 1 | I | 167 | ALA | 2.2 |
| 4 | D | 99 | SER | 2.2 |
| 3 | C | 39 | LYS | 2.2 |
| 3 | G | 29 | ILE | 2.1 |
| 1 | I | 168 | MET | 2.1 |
| 1 | I | 52 | PHE | 2.1 |
| 2 | F | 490 | LEU | 2.1 |
| 2 | F | 549 | ILE | 2.1 |
| 1 | M | 140 | TRP | 2.1 |
| 1 | E | 165 | ILE | 2.0 |
| 4 | P | 223 | VAL | 2.0 |
| 1 | E | 167 | ALA | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 5 | NAG | N | 701 | 14/15 | 0.92 | 0.46 | 1.07 | 108,126,155,155 | 0 |
| 5 | NAG | B | 701 | 14/15 | 0.95 | 0.32 | 0.28 | 75,87,93,99 | 0 |
| 5 | NAG | J | 701 | 14/15 | 0.95 | 0.32 | -0.03 | 88,107,118,123 | 0 |
| 5 | NAG | A | 301 | 14/15 | 0.95 | 0.25 | -0.13 | 82,103,124,127 | 0 |
| 5 | NAG | E | 301 | 14/15 | 0.94 | 0.24 | -0.19 | 97,105,130,157 | 0 |
| 5 | NAG | M | 301 | 14/15 | 0.85 | 0.25 | -0.28 | 122,137,150,152 | 0 |
| 5 | NAG | I | 301 | 14/15 | 0.92 | 0.25 | -0.63 | 104,113,126,141 | 0 |
| 5 | NAG | E | 303 | 14/15 | 0.76 | 0.25 | -0.70 | 119,150,167,170 | 0 |
| 5 | NAG | F | 701 | 14/15 | 0.95 | 0.29 | -0.77 | 96,106,115,119 | 0 |
| 5 | NAG | M | 303 | 14/15 | 0.86 | 0.15 | -0.93 | 131,149,167,169 | 0 |
| 5 | NAG | A | 303 | 14/15 | 0.88 | 0.16 | -1.08 | 109,132,148,159 | 0 |
| 5 | NAG | I | 306 | 14/15 | 0.91 | 0.16 | -1.57 | 146,161,166,172 | 0 |
| 7 | MAN | B | 706 | 11/12 | 0.77 | 0.25 | - | 98,121,144,159 | 0 |
| 6 | BMA | J | 703 | 11/12 | 0.86 | 0.17 | - | 89,135,147,164 | 0 |
| 7 | MAN | I | 304 | 11/12 | 0.78 | 0.29 | - | 116,160,172,172 | 0 |
| 5 | NAG | A | 304 | 14/15 | 0.83 | 0.17 | - | 119,161,166,173 | 0 |
| 7 | MAN | I | 305 | 11/12 | 0.72 | 0.21 | - | 115,144,163,168 | 0 |
| 5 | NAG | A | 302 | 14/15 | 0.85 | 0.25 | - | 94,123,152,155 | 0 |
| 7 | MAN | F | 704 | 11/12 | 0.84 | 0.31 | - | 139,150,160,161 | 0 |
| 6 | BMA | B | 703 | 11/12 | 0.87 | 0.21 | - | 129,143,167,173 | 0 |
| 5 | NAG | N | 702 | 14/15 | 0.91 | 0.34 | - | 110,122,148,152 | 0 |
| 7 | MAN | B | 705 | 11/12 | 0.88 | 0.22 | - | 116,129,139,141 | 0 |
| 7 | MAN | F | 705 | 11/12 | 0.89 | 0.20 | - | 129,138,146,157 | 0 |
| 6 | BMA | I | 303 | 11/12 | 0.74 | 0.20 | - | 143,162,184,184 | 0 |
| 5 | NAG | I | 302 | 14/15 | 0.87 | 0.24 | - | 115,138,152,156 | 0 |
| 7 | MAN | F | 706 | 11/12 | 0.75 | 0.21 | - | 107,150,161,168 | 0 |
| 5 | NAG | M | 302 | 14/15 | 0.82 | 0.24 | - | 125,157,178,198 | 0 |
| 7 | MAN | N | 704 | 11/12 | 0.82 | 0.25 | - | 167,178,185,195 | 0 |
| 5 | NAG | B | 702 | 14/15 | 0.91 | 0.35 | - | 90,104,122,125 | 0 |
| 7 | MAN | M | 305 | 11/12 | 0.69 | 0.41 | - | 152,184,193,196 | 0 |
| 6 | BMA | F | 703 | 11/12 | 0.88 | 0.16 | - | 111,118,133,145 | 0 |
| 6 | BMA | N | 703 | 11/12 | 0.85 | 0.22 | - | 143,167,178,180 | 0 |
| 5 | NAG | F | 702 | 14/15 | 0.92 | 0.26 | - | 82,102,128,131 | 0 |
| 7 | MAN | N | 705 | 11/12 | 0.86 | 0.14 | - | 111,156,169,170 | 0 |
| 5 | NAG | J | 702 | 14/15 | 0.90 | 0.24 | - | 88,101,119,124 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 7 | MAN | B | 704 | 11/12 | 0.90 | 0.27 | - | 119,131,156,166 | 0 |
| 5 | NAG | M | 304 | 14/15 | 0.59 | 0.30 | - | 148,168,184,187 | 0 |
| 5 | NAG | I | 307 | 14/15 | 0.67 | 0.23 | - | 101,164,178,181 | 0 |
| 7 | MAN | J | 704 | 11/12 | 0.78 | 0.23 | - | 141,152,161,171 | 0 |
| 5 | NAG | E | 302 | 14/15 | 0.90 | 0.19 | - | 118,143,154,159 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.