



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:53 AM GMT

PDB ID : 2BV8  
Title : THE CRYSTAL STRUCTURE OF PHYCOCYANIN FROM GRACILARIA CHILENSIS.  
Authors : Contreras-Martel, C.; Martinez-Oyanedel, J.; Poo-Caama, G.; Bruna, C.; Bunter, M.  
Deposited on : 2005-06-23  
Resolution : 2.01 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

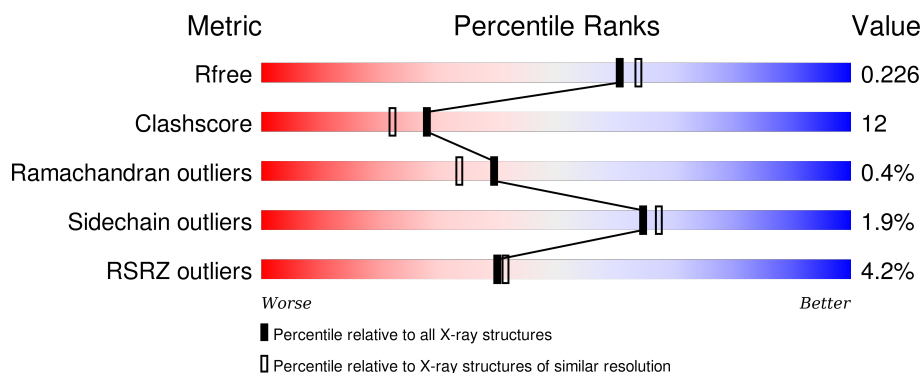
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 6249 (2.00-2.00)                                      |
| Clashscore            | 102246                      | 7340 (2.00-2.00)                                      |
| Ramachandran outliers | 100387                      | 7248 (2.00-2.00)                                      |
| Sidechain outliers    | 100360                      | 7247 (2.00-2.00)                                      |
| RSRZ outliers         | 91569                       | 6262 (2.00-2.00)                                      |

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  $\geq 3$ , 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     | 162    | <div> <div>7%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>  |
| 1   | C     | 162    | <div> <div>7%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>  |
| 1   | E     | 162    | <div> <div>7%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>  |
| 1   | K     | 162    | <div> <div>7%</div> <div>81%</div> <div>17%</div> <div>..</div> </div> |
| 1   | M     | 162    | <div> <div>7%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | O     | 162    |                  |
| 2   | B     | 172    |                  |
| 2   | D     | 172    |                  |
| 2   | F     | 172    |                  |
| 2   | L     | 172    |                  |
| 2   | N     | 172    |                  |
| 2   | P     | 172    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | PEB  | B     | 1175 | X         | -        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16812 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 C-PHYCOCYANIN ALPHA SUBUNIT.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 771 | 209 | 249 | 6 |         |         |       |
| 1   | C     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 771 | 209 | 249 | 6 |         |         |       |
| 1   | E     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 771 | 209 | 249 | 6 |         |         |       |
| 1   | K     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 771 | 209 | 249 | 6 |         |         |       |
| 1   | M     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 771 | 209 | 249 | 6 |         |         |       |
| 1   | O     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 771 | 209 | 249 | 6 |         |         |       |

There are 90 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 35      | THR      | SER    | CONFLICT | UNP Q6B8L6 |
| A     | 49      | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| A     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| A     | 61      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| A     | 65      | TYR      | PHE    | CONFLICT | UNP Q6B8L6 |
| A     | 70      | GLN      | PRO    | CONFLICT | UNP Q6B8L6 |
| A     | 73      | ASN      | THR    | CONFLICT | UNP Q6B8L6 |
| A     | 76      | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| A     | 77      | ASP      | SER    | CONFLICT | UNP Q6B8L6 |
| A     | 79      | THR      | ILE    | CONFLICT | UNP Q6B8L6 |
| A     | 95      | VAL      | THR    | CONFLICT | UNP Q6B8L6 |
| A     | 116     | SER      | GLU    | CONFLICT | UNP Q6B8L6 |
| A     | 134     | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| A     | 138     | ASP      | ASN    | CONFLICT | UNP Q6B8L6 |
| A     | 141     | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| C     | 35      | THR      | SER    | CONFLICT | UNP Q6B8L6 |
| C     | 49      | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| C     | 61      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| C     | 65      | TYR      | PHE    | CONFLICT | UNP Q6B8L6 |
| C     | 70      | GLN      | PRO    | CONFLICT | UNP Q6B8L6 |
| C     | 73      | ASN      | THR    | CONFLICT | UNP Q6B8L6 |
| C     | 76      | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| C     | 77      | ASP      | SER    | CONFLICT | UNP Q6B8L6 |
| C     | 79      | THR      | ILE    | CONFLICT | UNP Q6B8L6 |
| C     | 95      | VAL      | THR    | CONFLICT | UNP Q6B8L6 |
| C     | 116     | SER      | GLU    | CONFLICT | UNP Q6B8L6 |
| C     | 134     | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| C     | 138     | ASP      | ASN    | CONFLICT | UNP Q6B8L6 |
| C     | 141     | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| E     | 35      | THR      | SER    | CONFLICT | UNP Q6B8L6 |
| E     | 49      | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| E     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| E     | 61      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| E     | 65      | TYR      | PHE    | CONFLICT | UNP Q6B8L6 |
| E     | 70      | GLN      | PRO    | CONFLICT | UNP Q6B8L6 |
| E     | 73      | ASN      | THR    | CONFLICT | UNP Q6B8L6 |
| E     | 76      | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| E     | 77      | ASP      | SER    | CONFLICT | UNP Q6B8L6 |
| E     | 79      | THR      | ILE    | CONFLICT | UNP Q6B8L6 |
| E     | 95      | VAL      | THR    | CONFLICT | UNP Q6B8L6 |
| E     | 116     | SER      | GLU    | CONFLICT | UNP Q6B8L6 |
| E     | 134     | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| E     | 138     | ASP      | ASN    | CONFLICT | UNP Q6B8L6 |
| E     | 141     | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| K     | 35      | THR      | SER    | CONFLICT | UNP Q6B8L6 |
| K     | 49      | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| K     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| K     | 61      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| K     | 65      | TYR      | PHE    | CONFLICT | UNP Q6B8L6 |
| K     | 70      | GLN      | PRO    | CONFLICT | UNP Q6B8L6 |
| K     | 73      | ASN      | THR    | CONFLICT | UNP Q6B8L6 |
| K     | 76      | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| K     | 77      | ASP      | SER    | CONFLICT | UNP Q6B8L6 |
| K     | 79      | THR      | ILE    | CONFLICT | UNP Q6B8L6 |
| K     | 95      | VAL      | THR    | CONFLICT | UNP Q6B8L6 |
| K     | 116     | SER      | GLU    | CONFLICT | UNP Q6B8L6 |
| K     | 134     | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| K     | 138     | ASP      | ASN    | CONFLICT | UNP Q6B8L6 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| K     | 141     | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| M     | 35      | THR      | SER    | CONFLICT | UNP Q6B8L6 |
| M     | 49      | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| M     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| M     | 61      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| M     | 65      | TYR      | PHE    | CONFLICT | UNP Q6B8L6 |
| M     | 70      | GLN      | PRO    | CONFLICT | UNP Q6B8L6 |
| M     | 73      | ASN      | THR    | CONFLICT | UNP Q6B8L6 |
| M     | 76      | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| M     | 77      | ASP      | SER    | CONFLICT | UNP Q6B8L6 |
| M     | 79      | THR      | ILE    | CONFLICT | UNP Q6B8L6 |
| M     | 95      | VAL      | THR    | CONFLICT | UNP Q6B8L6 |
| M     | 116     | SER      | GLU    | CONFLICT | UNP Q6B8L6 |
| M     | 134     | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| M     | 138     | ASP      | ASN    | CONFLICT | UNP Q6B8L6 |
| M     | 141     | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| O     | 35      | THR      | SER    | CONFLICT | UNP Q6B8L6 |
| O     | 49      | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| O     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| O     | 61      | SER      | THR    | CONFLICT | UNP Q6B8L6 |
| O     | 65      | TYR      | PHE    | CONFLICT | UNP Q6B8L6 |
| O     | 70      | GLN      | PRO    | CONFLICT | UNP Q6B8L6 |
| O     | 73      | ASN      | THR    | CONFLICT | UNP Q6B8L6 |
| O     | 76      | ALA      | SER    | CONFLICT | UNP Q6B8L6 |
| O     | 77      | ASP      | SER    | CONFLICT | UNP Q6B8L6 |
| O     | 79      | THR      | ILE    | CONFLICT | UNP Q6B8L6 |
| O     | 95      | VAL      | THR    | CONFLICT | UNP Q6B8L6 |
| O     | 116     | SER      | GLU    | CONFLICT | UNP Q6B8L6 |
| O     | 134     | GLU      | GLN    | CONFLICT | UNP Q6B8L6 |
| O     | 138     | ASP      | ASN    | CONFLICT | UNP Q6B8L6 |
| O     | 141     | ALA      | SER    | CONFLICT | UNP Q6B8L6 |

- Molecule 2 is a protein called C-PHYCOCYANIN BETA SUBUNIT.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 773 | 226 | 263 | 8 |         |         |       |
| 2   | D     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 773 | 226 | 263 | 8 |         |         |       |
| 2   | F     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 773 | 226 | 263 | 8 |         |         |       |
| 2   | L     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 773 | 226 | 263 | 8 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | N     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 773 | 226 | 263 | 8 |         |         |       |
| 2   | P     | 172      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 773 | 226 | 263 | 8 |         |         |       |

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 31      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| B     | 43      | ARG      | LYS    | CONFLICT | UNP Q6B8L7 |
| B     | 52      | VAL      | ILE    | CONFLICT | UNP Q6B8L7 |
| B     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| B     | 58      | ALA      | SER    | CONFLICT | UNP Q6B8L7 |
| B     | 67      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| B     | 97      | GLU      | MET    | CONFLICT | UNP Q6B8L7 |
| B     | 125     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| B     | 132     | GLU      | GLN    | CONFLICT | UNP Q6B8L7 |
| B     | 141     | ASP      | LEU    | CONFLICT | UNP Q6B8L7 |
| B     | 146     | SER      | ASN    | CONFLICT | UNP Q6B8L7 |
| B     | 150     | SER      | ILE    | CONFLICT | UNP Q6B8L7 |
| B     | 157     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| B     | 162     | THR      | VAL    | CONFLICT | UNP Q6B8L7 |
| B     | 169     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| B     | 172     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| D     | 31      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| D     | 43      | ARG      | LYS    | CONFLICT | UNP Q6B8L7 |
| D     | 52      | VAL      | ILE    | CONFLICT | UNP Q6B8L7 |
| D     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| D     | 58      | ALA      | SER    | CONFLICT | UNP Q6B8L7 |
| D     | 67      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| D     | 97      | GLU      | MET    | CONFLICT | UNP Q6B8L7 |
| D     | 125     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| D     | 132     | GLU      | GLN    | CONFLICT | UNP Q6B8L7 |
| D     | 141     | ASP      | LEU    | CONFLICT | UNP Q6B8L7 |
| D     | 146     | SER      | ASN    | CONFLICT | UNP Q6B8L7 |
| D     | 150     | SER      | ILE    | CONFLICT | UNP Q6B8L7 |
| D     | 157     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| D     | 162     | THR      | VAL    | CONFLICT | UNP Q6B8L7 |
| D     | 169     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| D     | 172     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| F     | 31      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| F     | 43      | ARG      | LYS    | CONFLICT | UNP Q6B8L7 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 52      | VAL      | ILE    | CONFLICT | UNP Q6B8L7 |
| F     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| F     | 58      | ALA      | SER    | CONFLICT | UNP Q6B8L7 |
| F     | 67      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| F     | 97      | GLU      | MET    | CONFLICT | UNP Q6B8L7 |
| F     | 125     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| F     | 132     | GLU      | GLN    | CONFLICT | UNP Q6B8L7 |
| F     | 141     | ASP      | LEU    | CONFLICT | UNP Q6B8L7 |
| F     | 146     | SER      | ASN    | CONFLICT | UNP Q6B8L7 |
| F     | 150     | SER      | ILE    | CONFLICT | UNP Q6B8L7 |
| F     | 157     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| F     | 162     | THR      | VAL    | CONFLICT | UNP Q6B8L7 |
| F     | 169     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| F     | 172     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| L     | 31      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| L     | 43      | ARG      | LYS    | CONFLICT | UNP Q6B8L7 |
| L     | 52      | VAL      | ILE    | CONFLICT | UNP Q6B8L7 |
| L     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| L     | 58      | ALA      | SER    | CONFLICT | UNP Q6B8L7 |
| L     | 67      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| L     | 97      | GLU      | MET    | CONFLICT | UNP Q6B8L7 |
| L     | 125     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| L     | 132     | GLU      | GLN    | CONFLICT | UNP Q6B8L7 |
| L     | 141     | ASP      | LEU    | CONFLICT | UNP Q6B8L7 |
| L     | 146     | SER      | ASN    | CONFLICT | UNP Q6B8L7 |
| L     | 150     | SER      | ILE    | CONFLICT | UNP Q6B8L7 |
| L     | 157     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| L     | 162     | THR      | VAL    | CONFLICT | UNP Q6B8L7 |
| L     | 169     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| L     | 172     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| N     | 31      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| N     | 43      | ARG      | LYS    | CONFLICT | UNP Q6B8L7 |
| N     | 52      | VAL      | ILE    | CONFLICT | UNP Q6B8L7 |
| N     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| N     | 58      | ALA      | SER    | CONFLICT | UNP Q6B8L7 |
| N     | 67      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| N     | 97      | GLU      | MET    | CONFLICT | UNP Q6B8L7 |
| N     | 125     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| N     | 132     | GLU      | GLN    | CONFLICT | UNP Q6B8L7 |
| N     | 141     | ASP      | LEU    | CONFLICT | UNP Q6B8L7 |
| N     | 146     | SER      | ASN    | CONFLICT | UNP Q6B8L7 |
| N     | 150     | SER      | ILE    | CONFLICT | UNP Q6B8L7 |

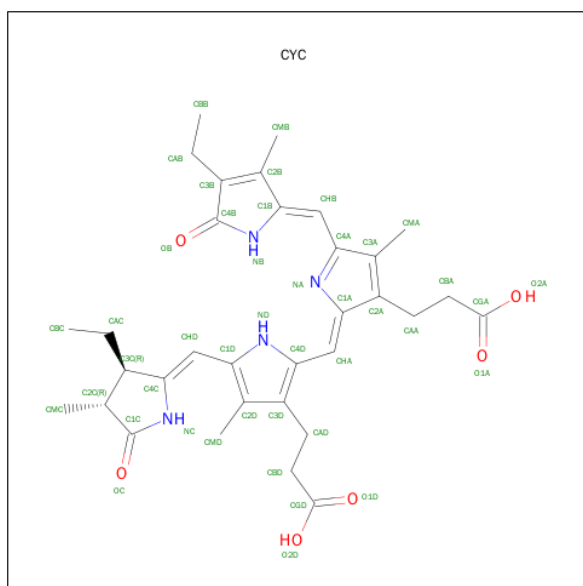
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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| N     | 157     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| N     | 162     | THR      | VAL    | CONFLICT | UNP Q6B8L7 |
| N     | 169     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| N     | 172     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| P     | 31      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| P     | 43      | ARG      | LYS    | CONFLICT | UNP Q6B8L7 |
| P     | 52      | VAL      | ILE    | CONFLICT | UNP Q6B8L7 |
| P     | 53      | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| P     | 58      | ALA      | SER    | CONFLICT | UNP Q6B8L7 |
| P     | 67      | ILE      | VAL    | CONFLICT | UNP Q6B8L7 |
| P     | 97      | GLU      | MET    | CONFLICT | UNP Q6B8L7 |
| P     | 125     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| P     | 132     | GLU      | GLN    | CONFLICT | UNP Q6B8L7 |
| P     | 141     | ASP      | LEU    | CONFLICT | UNP Q6B8L7 |
| P     | 146     | SER      | ASN    | CONFLICT | UNP Q6B8L7 |
| P     | 150     | SER      | ILE    | CONFLICT | UNP Q6B8L7 |
| P     | 157     | SER      | THR    | CONFLICT | UNP Q6B8L7 |
| P     | 162     | THR      | VAL    | CONFLICT | UNP Q6B8L7 |
| P     | 169     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |
| P     | 172     | SER      | VAL    | CONFLICT | UNP Q6B8L7 |

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ).



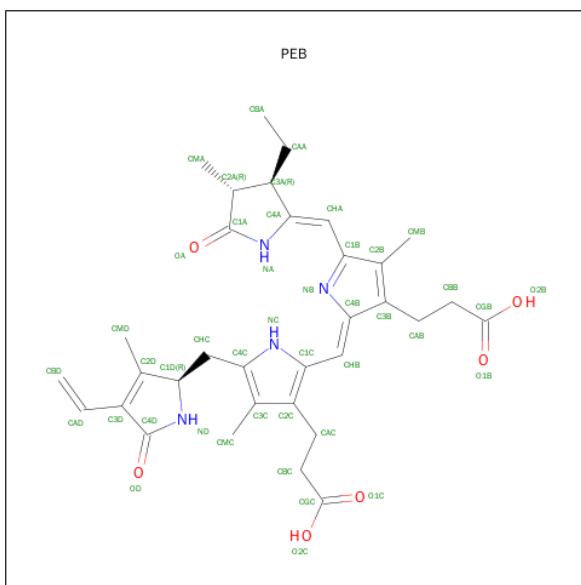
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | O     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 3   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |

- Molecule 4 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula:  $C_{33}H_{40}N_4O_6$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 81       | Total O<br>81 81   | 0       | 0       |
| 5   | B     | 114      | Total O<br>114 114 | 0       | 0       |
| 5   | C     | 83       | Total O<br>83 83   | 0       | 0       |
| 5   | D     | 80       | Total O<br>80 80   | 0       | 0       |
| 5   | E     | 100      | Total O<br>100 100 | 0       | 0       |
| 5   | F     | 66       | Total O<br>66 66   | 0       | 0       |
| 5   | K     | 95       | Total O<br>95 95   | 0       | 0       |
| 5   | L     | 85       | Total O<br>85 85   | 0       | 0       |
| 5   | M     | 91       | Total O<br>91 91   | 0       | 0       |
| 5   | N     | 99       | Total O<br>99 99   | 0       | 0       |
| 5   | O     | 59       | Total O<br>59 59   | 0       | 0       |

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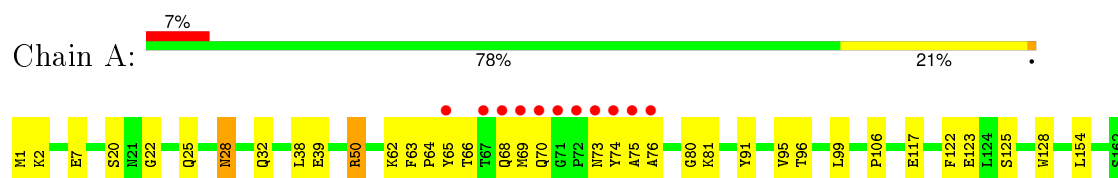
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | P     | 55       | Total | O  | 0       | 0       |
|     |       |          | 55    | 55 |         |         |

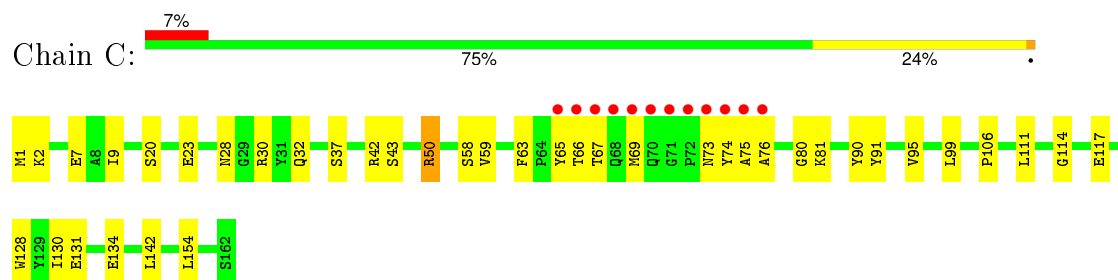
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

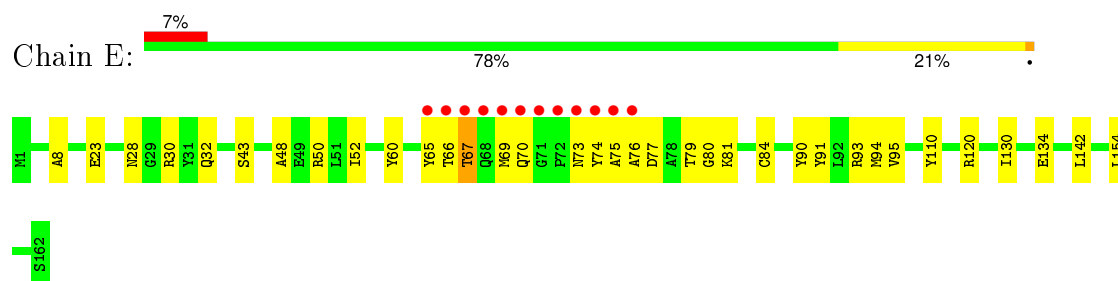
- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



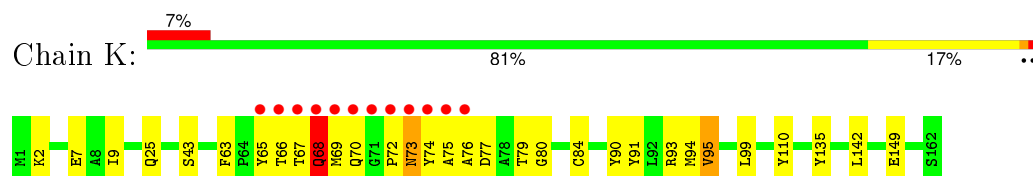
- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



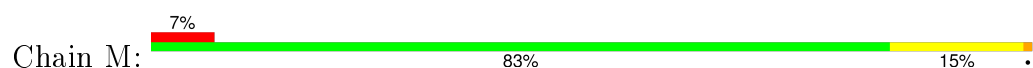
- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

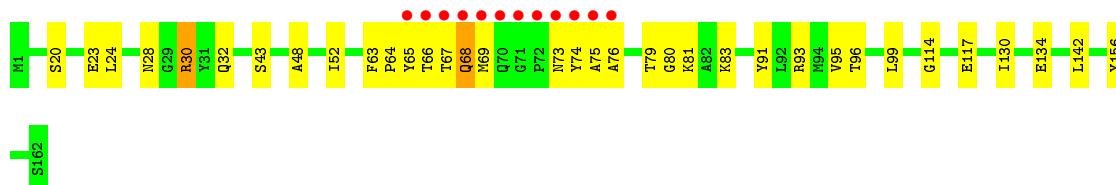
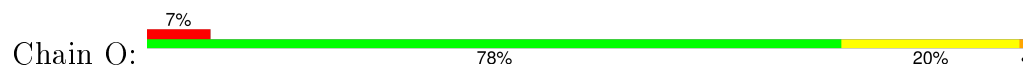


- Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT





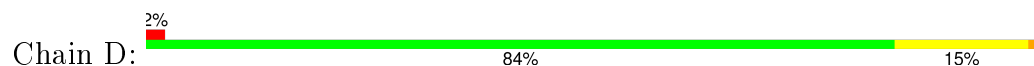
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



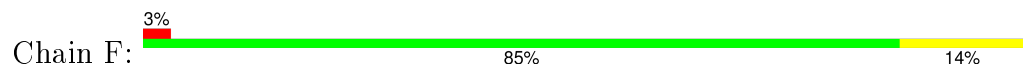
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



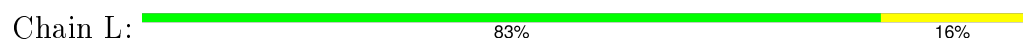
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



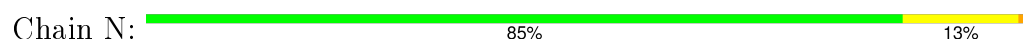
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



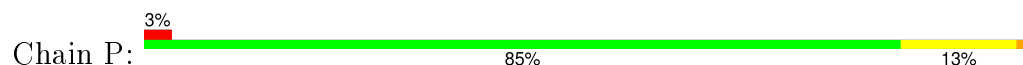
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

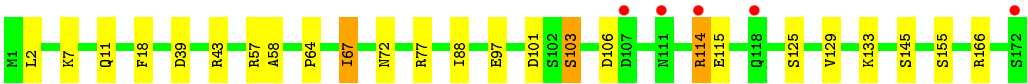


• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 1 21 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 101.98Å 151.80Å 101.55Å<br>90.00° 117.45° 90.00°   | Depositor        |
| Resolution (Å)  | 52.83 – 2.01<br>52.83 – 2.01   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.7 (52.83-2.01)<br>97.9 (52.83-2.01)   | Depositor<br>EDS |
| $R_{merge}$   | 0.06   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.96 (at 2.01Å)  | Xtriage          |
| Refinement program  | CNS 1.1  | Depositor        |
| R, $R_{free}$   | 0.199 , 0.231<br>0.196 , 0.226   | Depositor<br>DCC |
| $R_{free}$ test set   | 7100 reflections (3.98%)   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.3   | Xtriage          |
| Anisotropy  | 0.114  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 56.0  | EDS              |
| Estimated twinning fraction   | 0.008 for l,k,-h-l<br>0.008 for -h-l,k,h<br>0.028 for -h-l,-k,l<br>0.023 for h,-k,-h-l<br>0.021 for l,-k,h | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$  | Xtriage          |
| Outliers  | 0 of 178324 reflections  | Xtriage          |
| $F_o, F_c$ correlation  | 0.95   | EDS              |
| Total number of atoms   | 16812  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: CYC, MEN, PEB

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     | 0.82         | 0/1257          | 0.78        | 0/1703         |
| 1   | C     | 0.79         | 0/1257          | 0.78        | 0/1703         |
| 1   | E     | 0.86         | 0/1257          | 0.81        | 0/1703         |
| 1   | K     | 0.85         | 1/1257 (0.1%)   | 0.83        | 0/1703         |
| 1   | M     | 0.86         | 1/1257 (0.1%)   | 0.88        | 1/1703 (0.1%)  |
| 1   | O     | 0.73         | 0/1257          | 0.77        | 0/1703         |
| 2   | B     | 0.95         | 2/1272 (0.2%)   | 0.85        | 1/1717 (0.1%)  |
| 2   | D     | 0.76         | 1/1272 (0.1%)   | 0.81        | 0/1717         |
| 2   | F     | 0.82         | 2/1272 (0.2%)   | 0.81        | 0/1717         |
| 2   | L     | 0.84         | 1/1272 (0.1%)   | 0.80        | 0/1717         |
| 2   | N     | 0.88         | 1/1272 (0.1%)   | 0.87        | 1/1717 (0.1%)  |
| 2   | P     | 0.76         | 1/1272 (0.1%)   | 0.80        | 0/1717         |
| All | All   | 0.83         | 10/15174 (0.1%) | 0.82        | 3/20520 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | K     | 0                   | 1                   |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | L     | 97  | GLU  | CD-OE1 | -9.87 | 1.14        | 1.25     |
| 2   | B     | 97  | GLU  | CD-OE1 | -8.84 | 1.16        | 1.25     |
| 2   | N     | 97  | GLU  | CD-OE1 | -8.32 | 1.16        | 1.25     |
| 2   | B     | 153 | CYS  | CB-SG  | -6.59 | 1.71        | 1.82     |
| 1   | M     | 94  | MET  | SD-CE  | -6.11 | 1.43        | 1.77     |
| 2   | P     | 97  | GLU  | CD-OE1 | -6.00 | 1.19        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 95  | VAL  | CB-CG2 | -5.45 | 1.41        | 1.52     |
| 2   | F     | 97  | GLU  | CD-OE1 | -5.38 | 1.19        | 1.25     |
| 2   | F     | 153 | CYS  | CB-SG  | -5.18 | 1.73        | 1.81     |
| 2   | D     | 97  | GLU  | CD-OE1 | -5.06 | 1.20        | 1.25     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 94  | MET  | CG-SD-CE   | -7.80 | 87.71       | 100.20   |
| 2   | B     | 13  | ASP  | CB-CG-OD2  | 5.19  | 122.97      | 118.30   |
| 2   | N     | 97  | GLU  | OE1-CD-OE2 | -5.01 | 117.28      | 123.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | K     | 135 | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1235  | 0        | 1199     | 33      | 0            |
| 1   | C     | 1235  | 0        | 1199     | 35      | 0            |
| 1   | E     | 1235  | 0        | 1199     | 34      | 0            |
| 1   | K     | 1235  | 0        | 1199     | 37      | 0            |
| 1   | M     | 1235  | 0        | 1199     | 26      | 0            |
| 1   | O     | 1235  | 0        | 1199     | 30      | 0            |
| 2   | B     | 1270  | 0        | 1243     | 13      | 0            |
| 2   | D     | 1270  | 0        | 1243     | 18      | 0            |
| 2   | F     | 1270  | 0        | 1243     | 30      | 0            |
| 2   | L     | 1270  | 0        | 1243     | 25      | 0            |
| 2   | N     | 1270  | 0        | 1243     | 23      | 0            |
| 2   | P     | 1270  | 0        | 1243     | 24      | 0            |
| 3   | A     | 43    | 0        | 37       | 6       | 0            |
| 3   | B     | 43    | 0        | 37       | 4       | 0            |
| 3   | C     | 43    | 0        | 37       | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 86    | 0        | 74       | 11      | 0            |
| 3   | E     | 43    | 0        | 37       | 7       | 0            |
| 3   | F     | 86    | 0        | 74       | 8       | 0            |
| 3   | K     | 43    | 0        | 37       | 7       | 0            |
| 3   | L     | 86    | 0        | 74       | 11      | 0            |
| 3   | M     | 43    | 0        | 37       | 5       | 0            |
| 3   | N     | 86    | 0        | 74       | 7       | 0            |
| 3   | O     | 43    | 0        | 37       | 7       | 0            |
| 3   | P     | 86    | 0        | 74       | 9       | 0            |
| 4   | B     | 43    | 0        | 36       | 2       | 0            |
| 5   | A     | 81    | 0        | 0        | 3       | 0            |
| 5   | B     | 114   | 0        | 0        | 0       | 0            |
| 5   | C     | 83    | 0        | 0        | 1       | 0            |
| 5   | D     | 80    | 0        | 0        | 1       | 0            |
| 5   | E     | 100   | 0        | 0        | 3       | 0            |
| 5   | F     | 66    | 0        | 0        | 1       | 0            |
| 5   | K     | 95    | 0        | 0        | 2       | 0            |
| 5   | L     | 85    | 0        | 0        | 0       | 0            |
| 5   | M     | 91    | 0        | 0        | 0       | 0            |
| 5   | N     | 99    | 0        | 0        | 1       | 0            |
| 5   | O     | 59    | 0        | 0        | 1       | 0            |
| 5   | P     | 55    | 0        | 0        | 0       | 0            |
| All | All   | 16812 | 0        | 15317    | 365     | 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 12.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:75:ALA:HB1    | 1:C:81:LYS:HG3    | 1.28                     | 1.14              |
| 1:C:73:ASN:HA     | 3:C:1163:CYC:HBD2 | 1.24                     | 1.12              |
| 1:E:73:ASN:HB3    | 5:E:2098:HOH:O    | 1.56                     | 1.04              |
| 1:K:94:MET:HE1    | 1:K:110:TYR:HB2   | 1.39                     | 1.04              |
| 1:K:73:ASN:HB3    | 5:K:2095:HOH:O    | 1.65                     | 0.96              |
| 2:N:43:ARG:HG2    | 2:N:43:ARG:HH11   | 1.30                     | 0.94              |
| 2:L:107:ASP:HA    | 2:L:111:ASN:ND2   | 1.85                     | 0.91              |
| 3:C:1163:CYC:HC   | 3:C:1163:CYC:HMD2 | 1.35                     | 0.91              |
| 3:A:1163:CYC:HC   | 3:A:1163:CYC:CMD  | 1.84                     | 0.91              |
| 2:P:101:ASP:OD2   | 2:P:103:SER:HB3   | 1.72                     | 0.89              |
| 3:A:1163:CYC:HMD2 | 3:A:1163:CYC:HC   | 1.36                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:L:107:ASP:HA    | 2:L:111:ASN:HD22  | 1.42                     | 0.83              |
| 2:D:77:ARG:NH1    | 3:D:1174:CYC:O1D  | 2.11                     | 0.83              |
| 1:C:75:ALA:HB1    | 1:C:81:LYS:CG     | 2.08                     | 0.83              |
| 1:C:69:MET:O      | 1:C:76:ALA:HB2    | 1.77                     | 0.83              |
| 2:L:1:MET:HE3     | 2:L:104:VAL:HB    | 1.61                     | 0.83              |
| 1:K:94:MET:CE     | 1:K:110:TYR:HB2   | 2.09                     | 0.83              |
| 1:K:70:GLN:HG2    | 1:K:76:ALA:HB1    | 1.62                     | 0.82              |
| 2:F:108:ARG:O     | 3:F:1174:CYC:HBB1 | 1.78                     | 0.82              |
| 2:L:101:ASP:OD2   | 2:L:103:SER:HB3   | 1.79                     | 0.82              |
| 1:E:94:MET:HE1    | 1:E:110:TYR:HD2   | 1.44                     | 0.81              |
| 2:F:83:LEU:HD23   | 2:F:86:MET:HE1    | 1.63                     | 0.80              |
| 1:O:91:TYR:O      | 1:O:95:VAL:HG23   | 1.81                     | 0.80              |
| 3:O:1163:CYC:HMD2 | 3:O:1163:CYC:HC   | 1.48                     | 0.79              |
| 2:D:15:ARG:NH1    | 2:D:17:GLU:OE1    | 2.17                     | 0.78              |
| 2:F:103:SER:HB3   | 5:F:2005:HOH:O    | 1.83                     | 0.78              |
| 2:D:132:GLU:HG3   | 2:D:136:GLU:OE2   | 1.83                     | 0.78              |
| 1:A:22:GLY:HA2    | 1:A:25:GLN:HE21   | 1.49                     | 0.78              |
| 1:K:77:ASP:OD1    | 1:K:79:THR:HG22   | 1.85                     | 0.77              |
| 1:M:73:ASN:HA     | 3:M:1163:CYC:HBD2 | 1.67                     | 0.76              |
| 1:M:94:MET:HE1    | 1:M:110:TYR:HD2   | 1.48                     | 0.76              |
| 3:O:1163:CYC:HC   | 3:O:1163:CYC:CMD  | 1.99                     | 0.76              |
| 2:P:77:ARG:NH1    | 3:P:1174:CYC:O1D  | 2.19                     | 0.75              |
| 1:A:66:THR:HA     | 1:A:74:TYR:CD2    | 2.21                     | 0.75              |
| 2:F:43:ARG:HH11   | 2:F:43:ARG:HG3    | 1.50                     | 0.75              |
| 1:E:75:ALA:HB2    | 3:E:1163:CYC:OC   | 1.87                     | 0.74              |
| 3:D:1174:CYC:HC   | 3:D:1174:CYC:HMD2 | 1.52                     | 0.74              |
| 1:A:65:TYR:HB2    | 1:A:69:MET:HE3    | 1.70                     | 0.73              |
| 1:A:66:THR:O      | 1:A:74:TYR:HB3    | 1.87                     | 0.73              |
| 1:C:91:TYR:O      | 1:C:95:VAL:HG23   | 1.89                     | 0.73              |
| 2:P:106:ASP:OD1   | 2:P:166:ARG:NE    | 2.18                     | 0.73              |
| 2:N:43:ARG:NH2    | 2:N:144:ASP:O     | 2.21                     | 0.73              |
| 1:K:73:ASN:HB2    | 5:K:2043:HOH:O    | 1.88                     | 0.72              |
| 2:B:43:ARG:HH11   | 2:B:43:ARG:HG2    | 1.55                     | 0.72              |
| 2:P:7:LYS:O       | 2:P:11:GLN:HG3    | 1.90                     | 0.72              |
| 1:A:64:PRO:O      | 1:A:68:GLN:HG3    | 1.92                     | 0.70              |
| 1:K:65:TYR:HA     | 1:K:68:GLN:HB3    | 1.74                     | 0.70              |
| 1:M:70:GLN:HB3    | 1:M:76:ALA:HB1    | 1.73                     | 0.70              |
| 2:L:1:MET:CE      | 2:L:104:VAL:HB    | 2.22                     | 0.69              |
| 1:E:91:TYR:O      | 1:E:95:VAL:HG23   | 1.91                     | 0.69              |
| 1:A:75:ALA:HB1    | 1:A:81:LYS:HG2    | 1.74                     | 0.69              |
| 1:M:63:PHE:HB3    | 1:M:65:TYR:CE1    | 2.28                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:73:ASN:HA     | 3:O:1163:CYC:HBD2 | 1.72                     | 0.69              |
| 1:C:73:ASN:CA     | 3:C:1163:CYC:HBD2 | 2.15                     | 0.69              |
| 2:N:64:PRO:O      | 2:N:67:ILE:HD12   | 1.93                     | 0.69              |
| 1:K:65:TYR:HB2    | 1:K:69:MET:HE2    | 1.75                     | 0.68              |
| 2:B:101:ASP:OD2   | 2:B:103:SER:HB3   | 1.94                     | 0.68              |
| 2:F:101:ASP:OD2   | 2:F:103:SER:HB2   | 1.94                     | 0.68              |
| 2:L:43:ARG:NH2    | 2:L:144:ASP:O     | 2.26                     | 0.68              |
| 1:M:90:TYR:O      | 1:M:94:MET:HG2    | 1.93                     | 0.68              |
| 2:P:67:ILE:HD13   | 2:P:67:ILE:H      | 1.59                     | 0.68              |
| 1:M:77:ASP:OD2    | 1:M:79:THR:HB     | 1.94                     | 0.68              |
| 2:N:43:ARG:NH1    | 2:N:43:ARG:HG2    | 2.02                     | 0.68              |
| 1:O:68:GLN:HE21   | 1:O:68:GLN:HA     | 1.59                     | 0.67              |
| 2:F:72:MEN:HE22   | 3:F:1174:CYC:HBD2 | 1.75                     | 0.67              |
| 1:A:73:ASN:HA     | 3:A:1163:CYC:HBD2 | 1.76                     | 0.67              |
| 2:F:67:ILE:HD12   | 2:F:68:GLN:N      | 2.09                     | 0.67              |
| 3:E:1163:CYC:HMD3 | 3:E:1163:CYC:HC   | 1.58                     | 0.67              |
| 2:P:106:ASP:CG    | 2:P:166:ARG:HE    | 1.99                     | 0.67              |
| 1:K:91:TYR:O      | 1:K:95:VAL:HG23   | 1.94                     | 0.67              |
| 1:A:66:THR:HA     | 1:A:74:TYR:HD2    | 1.58                     | 0.66              |
| 3:L:1174:CYC:HMD2 | 3:L:1174:CYC:HC   | 1.59                     | 0.66              |
| 1:E:90:TYR:O      | 1:E:94:MET:HG2    | 1.95                     | 0.66              |
| 1:M:94:MET:HE1    | 1:M:110:TYR:CD2   | 2.30                     | 0.66              |
| 2:F:43:ARG:HG3    | 2:F:43:ARG:NH1    | 2.11                     | 0.66              |
| 2:B:65:GLN:NE2    | 2:B:65:GLN:H      | 1.93                     | 0.66              |
| 1:E:94:MET:HE1    | 1:E:110:TYR:CD2   | 2.27                     | 0.65              |
| 1:A:69:MET:O      | 1:A:74:TYR:HB2    | 1.96                     | 0.65              |
| 1:O:68:GLN:CA     | 1:O:68:GLN:HE21   | 2.09                     | 0.65              |
| 2:B:114:ARG:O     | 2:B:118:GLN:HG3   | 1.95                     | 0.65              |
| 1:A:1:MET:SD      | 1:A:106:PRO:HG3   | 2.37                     | 0.65              |
| 2:D:7:LYS:O       | 2:D:11:GLN:HG3    | 1.97                     | 0.65              |
| 2:P:64:PRO:O      | 2:P:67:ILE:HD13   | 1.96                     | 0.64              |
| 1:M:140:HIS:O     | 1:M:141:ALA:HB3   | 1.96                     | 0.64              |
| 1:A:91:TYR:O      | 1:A:95:VAL:HG23   | 1.98                     | 0.64              |
| 2:F:114:ARG:HG2   | 2:F:118:GLN:NE2   | 2.12                     | 0.64              |
| 2:F:83:LEU:HA     | 2:F:86:MET:CE     | 2.28                     | 0.64              |
| 1:K:90:TYR:O      | 1:K:94:MET:HG2    | 1.98                     | 0.64              |
| 1:M:65:TYR:O      | 1:M:69:MET:HB2    | 1.98                     | 0.64              |
| 3:O:1163:CYC:HMA1 | 3:O:1163:CYC:NB   | 2.13                     | 0.64              |
| 2:B:43:ARG:HG2    | 2:B:43:ARG:NH1    | 2.11                     | 0.64              |
| 1:M:91:TYR:O      | 1:M:95:VAL:HG23   | 1.97                     | 0.64              |
| 3:P:1174:CYC:HC   | 3:P:1174:CYC:HMD2 | 1.63                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:58:ALA:O      | 2:D:62:GLU:HG2    | 1.97                     | 0.64              |
| 3:M:1163:CYC:HC   | 3:M:1163:CYC:HMD2 | 1.63                     | 0.63              |
| 1:E:77:ASP:OD2    | 1:E:80:GLY:N      | 2.25                     | 0.63              |
| 2:F:113:LEU:HD13  | 3:F:1174:CYC:HMB3 | 1.80                     | 0.63              |
| 1:K:65:TYR:HA     | 1:K:68:GLN:HE21   | 1.63                     | 0.62              |
| 1:K:94:MET:HE1    | 1:K:110:TYR:CB    | 2.24                     | 0.62              |
| 2:D:43:ARG:NH2    | 2:D:144:ASP:O     | 2.32                     | 0.62              |
| 2:F:67:ILE:HD12   | 2:F:67:ILE:C      | 2.20                     | 0.62              |
| 2:N:65:GLN:NE2    | 2:N:65:GLN:H      | 1.98                     | 0.62              |
| 2:L:113:LEU:HD13  | 3:L:1174:CYC:HMB3 | 1.81                     | 0.61              |
| 1:A:20:SER:HA     | 5:A:2010:HOH:O    | 2.00                     | 0.61              |
| 4:B:1175:PEB:NA   | 4:B:1175:PEB:HMB2 | 2.15                     | 0.61              |
| 3:A:1163:CYC:NC   | 3:A:1163:CYC:CMD  | 2.62                     | 0.61              |
| 3:N:1174:CYC:HMD2 | 3:N:1174:CYC:HC   | 1.65                     | 0.61              |
| 2:N:67:ILE:C      | 2:N:67:ILE:CD1    | 2.69                     | 0.61              |
| 1:C:65:TYR:HB2    | 1:C:69:MET:SD     | 2.40                     | 0.61              |
| 3:P:1175:CYC:HMD2 | 3:P:1175:CYC:HC   | 1.65                     | 0.61              |
| 2:N:36:LYS:HD3    | 3:N:1175:CYC:HMD3 | 1.83                     | 0.61              |
| 3:F:1174:CYC:HMD2 | 3:F:1174:CYC:HC   | 1.66                     | 0.61              |
| 2:F:65:GLN:H      | 2:F:65:GLN:CD     | 2.04                     | 0.61              |
| 2:N:113:LEU:HD13  | 3:N:1174:CYC:HMB3 | 1.82                     | 0.61              |
| 3:D:1175:CYC:NC   | 3:D:1175:CYC:HMD2 | 2.16                     | 0.60              |
| 1:K:69:MET:O      | 1:K:76:ALA:HB2    | 2.00                     | 0.60              |
| 2:D:101:ASP:OD2   | 2:D:103:SER:HB3   | 2.01                     | 0.60              |
| 2:F:145:SER:HA    | 3:F:1175:CYC:HMC3 | 1.83                     | 0.59              |
| 1:M:65:TYR:CD2    | 1:M:69:MET:HE3    | 2.36                     | 0.59              |
| 1:M:130:ILE:O     | 1:M:134:GLU:HG2   | 2.02                     | 0.59              |
| 3:B:1174:CYC:HMD2 | 3:B:1174:CYC:HC   | 1.68                     | 0.59              |
| 2:B:67:ILE:HD12   | 3:C:1163:CYC:O1A  | 2.03                     | 0.58              |
| 1:K:94:MET:HE1    | 1:K:110:TYR:CD2   | 2.38                     | 0.58              |
| 1:K:67:THR:HA     | 1:K:75:ALA:C      | 2.24                     | 0.58              |
| 2:N:58:ALA:HB3    | 2:N:133:LYS:HD3   | 1.85                     | 0.58              |
| 1:K:75:ALA:HB2    | 3:K:1163:CYC:OC   | 2.04                     | 0.58              |
| 3:C:1163:CYC:HC   | 3:C:1163:CYC:CMD  | 2.13                     | 0.58              |
| 1:K:66:THR:HA     | 1:K:74:TYR:CD1    | 2.40                     | 0.57              |
| 3:P:1175:CYC:HMD2 | 3:P:1175:CYC:NC   | 2.19                     | 0.57              |
| 1:C:28:ASN:O      | 1:C:32:GLN:HG2    | 2.05                     | 0.57              |
| 2:D:166:ARG:HG3   | 5:D:2069:HOH:O    | 2.04                     | 0.57              |
| 2:P:77:ARG:HG2    | 2:P:77:ARG:HH11   | 1.69                     | 0.57              |
| 3:D:1174:CYC:NB   | 3:D:1174:CYC:HMA1 | 2.20                     | 0.56              |
| 1:E:74:TYR:C      | 1:E:76:ALA:H      | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:N:114:ARG:O     | 2:N:118:GLN:HG3   | 2.04                     | 0.56              |
| 1:O:75:ALA:HB1    | 1:O:81:LYS:HG2    | 1.86                     | 0.56              |
| 1:O:65:TYR:O      | 1:O:69:MET:N      | 2.29                     | 0.56              |
| 1:E:67:THR:O      | 1:E:76:ALA:HA     | 2.06                     | 0.56              |
| 1:C:20:SER:N      | 1:C:23:GLU:OE1    | 2.29                     | 0.56              |
| 1:E:30:ARG:O      | 1:E:30:ARG:HD2    | 2.05                     | 0.56              |
| 1:O:28:ASN:O      | 1:O:32:GLN:HG2    | 2.07                     | 0.55              |
| 3:K:1163:CYC:HC   | 3:K:1163:CYC:HMD3 | 1.71                     | 0.55              |
| 1:O:114:GLY:HA2   | 1:O:117:GLU:OE1   | 2.07                     | 0.55              |
| 1:O:68:GLN:NE2    | 1:O:68:GLN:HA     | 2.22                     | 0.55              |
| 4:B:1175:PEB:HNA  | 4:B:1175:PEB:HMB2 | 1.72                     | 0.54              |
| 2:P:88:ILE:HG21   | 3:P:1174:CYC:HBB3 | 1.88                     | 0.54              |
| 1:O:73:ASN:O      | 1:O:73:ASN:ND2    | 2.41                     | 0.54              |
| 2:F:83:LEU:HA     | 2:F:86:MET:HE2    | 1.89                     | 0.54              |
| 3:L:1174:CYC:NB   | 3:L:1174:CYC:HMA1 | 2.23                     | 0.54              |
| 1:C:130:ILE:O     | 1:C:134:GLU:HG2   | 2.07                     | 0.54              |
| 1:E:77:ASP:OD2    | 1:E:79:THR:N      | 2.41                     | 0.54              |
| 2:F:67:ILE:C      | 2:F:67:ILE:CD1    | 2.77                     | 0.53              |
| 2:P:114:ARG:HD2   | 2:P:115:GLU:OE2   | 2.08                     | 0.53              |
| 2:P:145:SER:HA    | 3:P:1175:CYC:HMC3 | 1.90                     | 0.53              |
| 1:C:30:ARG:O      | 1:C:30:ARG:HD2    | 2.09                     | 0.53              |
| 3:F:1174:CYC:HMA1 | 3:F:1174:CYC:NB   | 2.24                     | 0.53              |
| 2:B:108:ARG:O     | 3:B:1174:CYC:HBB1 | 2.09                     | 0.53              |
| 2:F:113:LEU:HD23  | 2:F:171:VAL:HG12  | 1.90                     | 0.53              |
| 1:K:67:THR:O      | 1:K:76:ALA:HA     | 2.10                     | 0.52              |
| 1:K:94:MET:HE1    | 1:K:110:TYR:HD2   | 1.75                     | 0.52              |
| 1:K:66:THR:HA     | 1:K:74:TYR:CE1    | 2.44                     | 0.52              |
| 1:E:75:ALA:CB     | 3:E:1163:CYC:OC   | 2.55                     | 0.52              |
| 1:M:70:GLN:HA     | 1:M:76:ALA:CB     | 2.39                     | 0.52              |
| 1:O:30:ARG:C      | 1:O:30:ARG:HD3    | 2.29                     | 0.52              |
| 1:M:94:MET:HE3    | 1:M:94:MET:HA     | 1.91                     | 0.52              |
| 3:E:1163:CYC:HC   | 3:E:1163:CYC:CMD  | 2.22                     | 0.52              |
| 2:L:112:GLY:HA2   | 2:L:115:GLU:OE1   | 2.08                     | 0.52              |
| 2:F:43:ARG:NH2    | 2:F:144:ASP:O     | 2.43                     | 0.52              |
| 2:L:145:SER:HA    | 3:L:1175:CYC:HMC3 | 1.92                     | 0.52              |
| 1:O:63:PHE:HB3    | 1:O:65:TYR:CE1    | 2.45                     | 0.52              |
| 3:L:1175:CYC:HMD2 | 3:L:1175:CYC:HC   | 1.74                     | 0.52              |
| 1:E:28:ASN:O      | 1:E:32:GLN:HG2    | 2.11                     | 0.51              |
| 2:P:77:ARG:HG2    | 2:P:77:ARG:NH1    | 2.25                     | 0.51              |
| 1:E:74:TYR:C      | 1:E:76:ALA:N      | 2.64                     | 0.51              |
| 1:O:24:LEU:HB3    | 3:P:1175:CYC:HBB3 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1175:CYC:HC   | 3:D:1175:CYC:HMD2 | 1.75                     | 0.51              |
| 2:P:125:SER:O     | 2:P:129:VAL:HG23  | 2.11                     | 0.51              |
| 2:D:36:LYS:HG2    | 3:D:1175:CYC:C1D  | 2.41                     | 0.51              |
| 3:O:1163:CYC:HMA1 | 3:O:1163:CYC:HB   | 1.73                     | 0.51              |
| 1:A:22:GLY:HA2    | 1:A:25:GLN:NE2    | 2.21                     | 0.51              |
| 1:M:74:TYR:C      | 1:M:76:ALA:H      | 2.13                     | 0.51              |
| 2:N:43:ARG:NH1    | 5:N:2026:HOH:O    | 2.43                     | 0.50              |
| 2:P:2:LEU:HD13    | 2:P:7:LYS:HA      | 1.93                     | 0.50              |
| 1:C:67:THR:HG23   | 1:C:81:LYS:HZ1    | 1.75                     | 0.50              |
| 2:F:83:LEU:HA     | 2:F:86:MET:HE1    | 1.91                     | 0.50              |
| 1:E:66:THR:HA     | 1:E:74:TYR:CD2    | 2.46                     | 0.50              |
| 1:K:63:PHE:HB3    | 1:K:65:TYR:CE2    | 2.46                     | 0.50              |
| 1:O:43:SER:HB3    | 1:O:142:LEU:HD21  | 1.93                     | 0.50              |
| 2:B:115:GLU:HA    | 2:B:118:GLN:HE21  | 1.77                     | 0.50              |
| 2:P:39:ASP:O      | 2:P:43:ARG:HG3    | 2.11                     | 0.50              |
| 2:L:60:PHE:HB3    | 2:L:67:ILE:HD12   | 1.93                     | 0.49              |
| 2:N:35:ASN:ND2    | 3:N:1175:CYC:HAA2 | 2.28                     | 0.49              |
| 3:L:1175:CYC:HMA1 | 3:L:1175:CYC:NB   | 2.27                     | 0.49              |
| 1:K:9:ILE:HG21    | 2:L:1:MET:HE1     | 1.94                     | 0.49              |
| 3:F:1175:CYC:HMD2 | 3:F:1175:CYC:HC   | 1.77                     | 0.49              |
| 3:N:1174:CYC:NB   | 3:N:1174:CYC:HMA1 | 2.28                     | 0.49              |
| 1:C:117:GLU:CD    | 1:C:117:GLU:H     | 2.16                     | 0.49              |
| 1:O:156:TYR:HA    | 5:O:2055:HOH:O    | 2.13                     | 0.49              |
| 1:C:95:VAL:HG21   | 1:C:154:LEU:HD23  | 1.94                     | 0.49              |
| 2:D:1:MET:CE      | 2:D:104:VAL:HB    | 2.43                     | 0.49              |
| 2:L:114:ARG:NE    | 2:L:172:SER:OXT   | 2.39                     | 0.49              |
| 2:N:67:ILE:C      | 2:N:67:ILE:HD13   | 2.33                     | 0.48              |
| 1:C:75:ALA:HA     | 1:C:80:GLY:HA3    | 1.96                     | 0.48              |
| 1:M:62:LYS:HD3    | 1:M:63:PHE:CE2    | 2.47                     | 0.48              |
| 3:M:1163:CYC:NC   | 3:M:1163:CYC:HMD2 | 2.27                     | 0.48              |
| 3:L:1175:CYC:NC   | 3:L:1175:CYC:HMD2 | 2.28                     | 0.48              |
| 2:N:7:LYS:HD3     | 2:N:101:ASP:OD1   | 2.13                     | 0.48              |
| 3:D:1174:CYC:HB   | 3:D:1174:CYC:CMA  | 2.27                     | 0.48              |
| 2:N:98:ILE:O      | 2:N:98:ILE:HD12   | 2.14                     | 0.48              |
| 1:C:2:LYS:HB3     | 5:C:2045:HOH:O    | 2.12                     | 0.48              |
| 1:C:43:SER:HB3    | 1:C:142:LEU:HD21  | 1.96                     | 0.48              |
| 1:C:65:TYR:O      | 1:C:69:MET:N      | 2.47                     | 0.48              |
| 1:K:43:SER:HB3    | 1:K:142:LEU:HD21  | 1.95                     | 0.48              |
| 1:A:39:GLU:HA     | 1:A:39:GLU:OE1    | 2.13                     | 0.48              |
| 1:O:75:ALA:O      | 1:O:81:LYS:HG3    | 2.13                     | 0.48              |
| 1:C:114:GLY:HA2   | 1:C:117:GLU:OE1   | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:N:7:LYS:O       | 2:N:11:GLN:HG3    | 2.13                     | 0.48              |
| 1:O:48:ALA:O      | 1:O:52:ILE:HG13   | 2.14                     | 0.48              |
| 1:A:2:LYS:HE2     | 5:A:2045:HOH:O    | 2.14                     | 0.47              |
| 3:D:1174:CYC:HB   | 3:D:1174:CYC:HMA1 | 1.79                     | 0.47              |
| 1:K:68:GLN:HG2    | 1:K:69:MET:N      | 2.29                     | 0.47              |
| 2:F:83:LEU:HD23   | 2:F:86:MET:CE     | 2.38                     | 0.47              |
| 1:E:95:VAL:HG21   | 1:E:154:LEU:HD23  | 1.96                     | 0.47              |
| 1:A:75:ALA:HA     | 1:A:80:GLY:HA3    | 1.95                     | 0.47              |
| 2:L:43:ARG:HH11   | 2:L:43:ARG:HG2    | 1.78                     | 0.47              |
| 1:C:50:ARG:HH11   | 1:C:50:ARG:HG2    | 1.79                     | 0.47              |
| 1:A:73:ASN:ND2    | 1:A:123:GLU:O     | 2.48                     | 0.47              |
| 2:F:7:LYS:HB3     | 2:F:7:LYS:NZ      | 2.29                     | 0.47              |
| 1:E:66:THR:HB     | 3:E:1163:CYC:HMC2 | 1.95                     | 0.47              |
| 1:A:64:PRO:C      | 1:A:68:GLN:HE21   | 2.18                     | 0.47              |
| 2:L:113:LEU:CD1   | 3:L:1174:CYC:HMB3 | 2.44                     | 0.47              |
| 3:F:1175:CYC:HMD2 | 3:F:1175:CYC:NC   | 2.29                     | 0.47              |
| 2:D:135:LYS:HB2   | 2:D:164:PHE:CG    | 2.50                     | 0.47              |
| 2:P:57:ARG:NH1    | 2:P:57:ARG:CB     | 2.76                     | 0.47              |
| 2:B:57:ARG:HE     | 3:C:1163:CYC:CGD  | 2.28                     | 0.47              |
| 1:M:70:GLN:HA     | 1:M:76:ALA:HB2    | 1.97                     | 0.47              |
| 2:L:43:ARG:HG2    | 2:L:43:ARG:NH1    | 2.30                     | 0.47              |
| 1:C:67:THR:HG23   | 1:C:81:LYS:NZ     | 2.30                     | 0.47              |
| 2:P:88:ILE:CG2    | 3:P:1174:CYC:HBB3 | 2.44                     | 0.47              |
| 1:E:75:ALA:O      | 1:E:81:LYS:HG3    | 2.15                     | 0.47              |
| 1:O:66:THR:O      | 1:O:74:TYR:HB3    | 2.15                     | 0.47              |
| 2:F:123:PRO:HG2   | 2:F:126:SER:HB2   | 1.96                     | 0.47              |
| 2:P:57:ARG:HH11   | 2:P:57:ARG:CB     | 2.28                     | 0.46              |
| 1:A:28:ASN:O      | 1:A:32:GLN:HG2    | 2.15                     | 0.46              |
| 2:P:57:ARG:NH1    | 2:P:57:ARG:HB2    | 2.31                     | 0.46              |
| 2:N:135:LYS:HB2   | 2:N:164:PHE:CG    | 2.49                     | 0.46              |
| 1:O:65:TYR:HD2    | 1:O:69:MET:SD     | 2.39                     | 0.46              |
| 2:P:43:ARG:HG2    | 2:P:43:ARG:NH1    | 2.31                     | 0.46              |
| 2:B:43:ARG:CG     | 2:B:43:ARG:HH11   | 2.27                     | 0.46              |
| 1:C:66:THR:HG22   | 1:C:74:TYR:HD2    | 1.80                     | 0.46              |
| 1:M:100:VAL:HG21  | 2:N:19:LEU:CD1    | 2.46                     | 0.46              |
| 2:N:59:LEU:HD22   | 2:N:130:ALA:HB2   | 1.97                     | 0.46              |
| 1:A:50:ARG:HD3    | 5:A:2060:HOH:O    | 2.15                     | 0.46              |
| 2:L:68:GLN:HB3    | 2:L:68:GLN:HE21   | 1.57                     | 0.46              |
| 1:E:75:ALA:CA     | 3:E:1163:CYC:OC   | 2.64                     | 0.45              |
| 1:E:48:ALA:O      | 1:E:52:ILE:HG13   | 2.17                     | 0.45              |
| 1:O:130:ILE:O     | 1:O:134:GLU:HG2   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:70:GLN:HA     | 1:K:76:ALA:CB     | 2.47                     | 0.45              |
| 2:B:39:ASP:O      | 2:B:43:ARG:HG3    | 2.16                     | 0.45              |
| 2:D:113:LEU:HD13  | 3:D:1174:CYC:HMB3 | 1.98                     | 0.45              |
| 1:C:66:THR:HG22   | 1:C:74:TYR:CD2    | 2.51                     | 0.45              |
| 2:P:57:ARG:HB3    | 2:P:57:ARG:HH11   | 1.81                     | 0.45              |
| 2:L:114:ARG:HB2   | 2:L:170:ALA:O     | 2.17                     | 0.45              |
| 1:K:67:THR:N      | 1:K:75:ALA:HB3    | 2.31                     | 0.45              |
| 1:E:94:MET:CE     | 1:E:110:TYR:HB2   | 2.47                     | 0.45              |
| 1:A:117:GLU:N     | 1:A:117:GLU:OE1   | 2.36                     | 0.45              |
| 1:O:74:TYR:C      | 1:O:76:ALA:H      | 2.20                     | 0.45              |
| 2:L:114:ARG:HB3   | 2:L:114:ARG:HH11  | 1.82                     | 0.44              |
| 1:K:68:GLN:CG     | 1:K:69:MET:N      | 2.79                     | 0.44              |
| 1:A:62:LYS:C      | 1:A:64:PRO:HD3    | 2.38                     | 0.44              |
| 3:M:1163:CYC:NB   | 3:M:1163:CYC:HMA1 | 2.31                     | 0.44              |
| 2:N:43:ARG:CG     | 2:N:43:ARG:NH1    | 2.69                     | 0.44              |
| 2:F:86:MET:HB2    | 2:F:86:MET:HE2    | 1.58                     | 0.44              |
| 1:A:95:VAL:HG21   | 1:A:154:LEU:HD23  | 1.99                     | 0.44              |
| 2:F:7:LYS:HD3     | 2:F:101:ASP:OD1   | 2.17                     | 0.44              |
| 1:O:75:ALA:HA     | 1:O:80:GLY:C      | 2.38                     | 0.44              |
| 1:K:99:LEU:CD2    | 1:K:149:GLU:HB3   | 2.48                     | 0.44              |
| 1:A:96:THR:HA     | 1:A:99:LEU:HD12   | 2.00                     | 0.44              |
| 1:E:8:ALA:HB1     | 1:E:23:GLU:HB3    | 1.99                     | 0.44              |
| 3:B:1174:CYC:HMA1 | 3:B:1174:CYC:NB   | 2.33                     | 0.44              |
| 1:K:2:LYS:HE2     | 1:K:7:GLU:CD      | 2.38                     | 0.44              |
| 1:E:50:ARG:NH2    | 5:E:2043:HOH:O    | 2.50                     | 0.44              |
| 2:L:1:MET:HB2     | 2:L:1:MET:HE3     | 1.92                     | 0.44              |
| 1:M:62:LYS:HD3    | 1:M:63:PHE:CZ     | 2.53                     | 0.44              |
| 1:E:43:SER:HB3    | 1:E:142:LEU:HD21  | 2.00                     | 0.44              |
| 3:D:1174:CYC:NC   | 3:D:1174:CYC:HMD2 | 2.27                     | 0.43              |
| 2:F:114:ARG:HG2   | 2:F:118:GLN:HE22  | 1.83                     | 0.43              |
| 1:O:20:SER:N      | 1:O:23:GLU:OE1    | 2.40                     | 0.43              |
| 1:C:58:SER:OG     | 1:C:131:GLU:OE2   | 2.35                     | 0.43              |
| 1:C:63:PHE:HB3    | 1:C:65:TYR:CE1    | 2.54                     | 0.43              |
| 3:O:1163:CYC:HB   | 3:O:1163:CYC:CMA  | 2.32                     | 0.43              |
| 2:P:72:MEN:HB2    | 3:P:1174:CYC:OC   | 2.19                     | 0.43              |
| 1:O:68:GLN:CA     | 1:O:68:GLN:NE2    | 2.79                     | 0.43              |
| 1:O:67:THR:HA     | 1:O:75:ALA:O      | 2.18                     | 0.43              |
| 2:F:98:ILE:HA     | 2:F:98:ILE:HD12   | 1.85                     | 0.43              |
| 1:E:66:THR:O      | 1:E:75:ALA:N      | 2.52                     | 0.43              |
| 1:E:69:MET:C      | 1:E:76:ALA:HB2    | 2.38                     | 0.43              |
| 3:L:1174:CYC:HMD2 | 3:L:1174:CYC:NC   | 2.31                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:36:LYS:NZ     | 2:B:152:ASP:O     | 2.45                     | 0.43              |
| 3:K:1163:CYC:NB   | 3:K:1163:CYC:HMA1 | 2.33                     | 0.43              |
| 1:M:83:LYS:NZ     | 3:M:1163:CYC:O1A  | 2.47                     | 0.43              |
| 1:C:37:SER:HB3    | 1:C:99:LEU:O      | 2.19                     | 0.43              |
| 1:K:74:TYR:O      | 1:K:80:GLY:HA3    | 2.19                     | 0.42              |
| 2:N:98:ILE:HD13   | 2:N:98:ILE:HA     | 1.73                     | 0.42              |
| 1:O:96:THR:HA     | 1:O:99:LEU:HD12   | 2.01                     | 0.42              |
| 1:O:66:THR:HB     | 3:O:1163:CYC:OC   | 2.20                     | 0.42              |
| 1:M:68:GLN:O      | 1:M:70:GLN:N      | 2.52                     | 0.42              |
| 2:L:39:ASP:OD1    | 3:L:1175:CYC:HHB  | 2.19                     | 0.42              |
| 2:L:15:ARG:NH1    | 2:L:15:ARG:HG2    | 2.33                     | 0.42              |
| 1:C:42:ARG:NH2    | 2:D:25:ASP:OD1    | 2.52                     | 0.42              |
| 1:E:84:CYS:HB2    | 3:E:1163:CYC:C1C  | 2.49                     | 0.42              |
| 1:E:65:TYR:HD2    | 1:E:69:MET:SD     | 2.43                     | 0.42              |
| 1:M:100:VAL:HG21  | 2:N:19:LEU:HD13   | 2.01                     | 0.42              |
| 1:C:111:LEU:C     | 1:C:111:LEU:HD23  | 2.39                     | 0.42              |
| 1:A:38:LEU:HA     | 1:A:38:LEU:HD23   | 1.89                     | 0.42              |
| 1:E:120:ARG:HH11  | 1:E:120:ARG:HG2   | 1.83                     | 0.42              |
| 1:A:73:ASN:ND2    | 1:A:122:PHE:O     | 2.51                     | 0.42              |
| 1:A:64:PRO:CB     | 1:A:68:GLN:HE21   | 2.33                     | 0.42              |
| 2:D:67:ILE:HD13   | 2:D:67:ILE:H      | 1.85                     | 0.42              |
| 1:O:79:THR:O      | 1:O:83:LYS:HG2    | 2.20                     | 0.42              |
| 1:O:93:ARG:HA     | 2:P:18:PHE:CE2    | 2.54                     | 0.42              |
| 1:E:130:ILE:O     | 1:E:134:GLU:HG2   | 2.20                     | 0.42              |
| 1:K:67:THR:HA     | 1:K:75:ALA:O      | 2.19                     | 0.42              |
| 1:K:66:THR:C      | 1:K:75:ALA:HB3    | 2.41                     | 0.42              |
| 1:E:50:ARG:HD3    | 5:E:2039:HOH:O    | 2.20                     | 0.42              |
| 2:B:72:MEN:HE22   | 3:B:1174:CYC:HBD2 | 2.02                     | 0.41              |
| 1:E:93:ARG:HA     | 2:F:18:PHE:CE1    | 2.55                     | 0.41              |
| 1:C:128:TRP:CD2   | 3:C:1163:CYC:HMC3 | 2.55                     | 0.41              |
| 1:K:70:GLN:HA     | 1:K:76:ALA:HB3    | 2.01                     | 0.41              |
| 1:A:74:TYR:C      | 1:A:76:ALA:H      | 2.24                     | 0.41              |
| 1:C:1:MET:SD      | 1:C:106:PRO:HG3   | 2.60                     | 0.41              |
| 2:F:77:ARG:NH1    | 2:F:77:ARG:HG2    | 2.36                     | 0.41              |
| 1:E:77:ASP:OD2    | 1:E:79:THR:HB     | 2.21                     | 0.41              |
| 3:N:1174:CYC:HMA3 | 3:N:1174:CYC:HBA1 | 2.02                     | 0.41              |
| 2:D:112:GLY:HA2   | 2:D:115:GLU:OE1   | 2.20                     | 0.41              |
| 1:C:59:VAL:HG11   | 3:C:1163:CYC:HMC1 | 2.01                     | 0.41              |
| 2:N:36:LYS:NZ     | 2:N:152:ASP:O     | 2.52                     | 0.41              |
| 1:K:84:CYS:HB2    | 3:K:1163:CYC:NC   | 2.35                     | 0.41              |
| 1:M:28:ASN:ND2    | 3:N:1175:CYC:OB   | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:63:PHE:HB3    | 1:A:65:TYR:CE1    | 2.56                     | 0.41              |
| 1:C:90:TYR:CD2    | 3:C:1163:CYC:HBB3 | 2.56                     | 0.41              |
| 1:A:73:ASN:O      | 3:A:1163:CYC:HMD2 | 2.21                     | 0.41              |
| 1:A:63:PHE:HA     | 1:M:69:MET:HE1    | 2.03                     | 0.41              |
| 1:M:66:THR:HG22   | 1:M:74:TYR:CE1    | 2.56                     | 0.41              |
| 2:D:39:ASP:OD1    | 3:D:1175:CYC:HHB  | 2.20                     | 0.41              |
| 1:O:64:PRO:O      | 1:O:67:THR:HG22   | 2.21                     | 0.41              |
| 1:M:108:ASP:HA    | 1:M:112:ILE:HB    | 2.02                     | 0.41              |
| 2:L:123:PRO:HG2   | 2:L:126:SER:HB2   | 2.03                     | 0.41              |
| 2:F:77:ARG:HH11   | 2:F:77:ARG:HG2    | 1.86                     | 0.41              |
| 1:C:2:LYS:HE2     | 1:C:7:GLU:OE1     | 2.22                     | 0.40              |
| 1:A:125:SER:HB3   | 1:A:128:TRP:CE2   | 2.55                     | 0.40              |
| 3:A:1163:CYC:HBB2 | 2:F:75:THR:HA     | 2.02                     | 0.40              |
| 1:E:60:TYR:CE1    | 1:E:75:ALA:HB1    | 2.57                     | 0.40              |
| 1:C:9:ILE:HG21    | 2:D:1:MET:HE1     | 2.04                     | 0.40              |
| 1:K:93:ARG:HA     | 2:L:18:PHE:CE2    | 2.56                     | 0.40              |
| 1:A:64:PRO:CB     | 1:A:68:GLN:NE2    | 2.85                     | 0.40              |
| 1:C:30:ARG:C      | 1:C:30:ARG:HD2    | 2.41                     | 0.40              |
| 3:K:1163:CYC:HBA1 | 3:K:1163:CYC:HMA3 | 2.03                     | 0.40              |
| 3:K:1163:CYC:CMD  | 3:K:1163:CYC:HC   | 2.34                     | 0.40              |
| 2:L:77:ARG:CZ     | 3:L:1174:CYC:O1D  | 2.70                     | 0.40              |
| 1:K:75:ALA:CB     | 3:K:1163:CYC:OC   | 2.68                     | 0.40              |
| 1:K:65:TYR:CD1    | 1:K:69:MET:CE     | 3.04                     | 0.40              |
| 2:D:64:PRO:O      | 2:D:67:ILE:HD13   | 2.22                     | 0.40              |
| 2:L:89:VAL:HG11   | 2:L:131:ILE:HG12  | 2.03                     | 0.40              |
| 2:P:58:ALA:HB3    | 2:P:133:LYS:HD3   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 160/162 (99%)   | 156 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | C     | 160/162 (99%)   | 155 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | E     | 160/162 (99%)   | 156 (98%)  | 3 (2%)  | 1 (1%)   | 30          | 22  |
| 1   | K     | 160/162 (99%)   | 153 (96%)  | 5 (3%)  | 2 (1%)   | 15          | 7   |
| 1   | M     | 160/162 (99%)   | 156 (98%)  | 2 (1%)  | 2 (1%)   | 15          | 7   |
| 1   | O     | 160/162 (99%)   | 156 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 2   | B     | 169/172 (98%)   | 166 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 2   | D     | 169/172 (98%)   | 165 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 2   | F     | 169/172 (98%)   | 166 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 2   | L     | 169/172 (98%)   | 167 (99%)  | 1 (1%)  | 1 (1%)   | 30          | 22  |
| 2   | N     | 169/172 (98%)   | 167 (99%)  | 1 (1%)  | 1 (1%)   | 30          | 22  |
| 2   | P     | 169/172 (98%)   | 166 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| All | All   | 1974/2004 (98%) | 1929 (98%) | 38 (2%) | 7 (0%)   | 39          | 33  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 70  | GLN  |
| 1   | M     | 69  | MET  |
| 1   | K     | 68  | GLN  |
| 2   | L     | 75  | THR  |
| 2   | N     | 75  | THR  |
| 1   | K     | 72  | PRO  |
| 1   | M     | 105 | GLY  |

### 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     | 127/127 (100%) | 123 (97%) | 4 (3%)   | 47          | 46 |
| 1   | C     | 127/127 (100%) | 126 (99%) | 1 (1%)   | 86          | 89 |
| 1   | E     | 127/127 (100%) | 126 (99%) | 1 (1%)   | 86          | 89 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 1   | K     | 127/127 (100%)   | 124 (98%)  | 3 (2%)   | 57          | 58  |
| 1   | M     | 127/127 (100%)   | 127 (100%) | 0        | 100         | 100 |
| 1   | O     | 127/127 (100%)   | 125 (98%)  | 2 (2%)   | 70          | 73  |
| 2   | B     | 133/133 (100%)   | 132 (99%)  | 1 (1%)   | 86          | 89  |
| 2   | D     | 133/133 (100%)   | 129 (97%)  | 4 (3%)   | 48          | 47  |
| 2   | F     | 133/133 (100%)   | 130 (98%)  | 3 (2%)   | 58          | 60  |
| 2   | L     | 133/133 (100%)   | 130 (98%)  | 3 (2%)   | 58          | 60  |
| 2   | N     | 133/133 (100%)   | 129 (97%)  | 4 (3%)   | 48          | 47  |
| 2   | P     | 133/133 (100%)   | 129 (97%)  | 4 (3%)   | 48          | 47  |
| All | All   | 1560/1560 (100%) | 1530 (98%) | 30 (2%)  | 65          | 67  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | GLU  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 50  | ARG  |
| 1   | A     | 70  | GLN  |
| 2   | B     | 65  | GLN  |
| 1   | C     | 50  | ARG  |
| 2   | D     | 62  | GLU  |
| 2   | D     | 67  | ILE  |
| 2   | D     | 103 | SER  |
| 2   | D     | 120 | LEU  |
| 1   | E     | 67  | THR  |
| 2   | F     | 65  | GLN  |
| 2   | F     | 103 | SER  |
| 2   | F     | 155 | SER  |
| 1   | K     | 25  | GLN  |
| 1   | K     | 68  | GLN  |
| 1   | K     | 73  | ASN  |
| 2   | L     | 22  | THR  |
| 2   | L     | 67  | ILE  |
| 2   | L     | 103 | SER  |
| 2   | N     | 57  | ARG  |
| 2   | N     | 65  | GLN  |
| 2   | N     | 67  | ILE  |
| 2   | N     | 98  | ILE  |
| 1   | O     | 30  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 68  | GLN  |
| 2   | P     | 67  | ILE  |
| 2   | P     | 103 | SER  |
| 2   | P     | 114 | ARG  |
| 2   | P     | 155 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | GLN  |
| 2   | B     | 11  | GLN  |
| 2   | B     | 65  | GLN  |
| 2   | B     | 68  | GLN  |
| 2   | B     | 118 | GLN  |
| 1   | C     | 15  | GLN  |
| 1   | C     | 21  | ASN  |
| 2   | D     | 68  | GLN  |
| 2   | D     | 118 | GLN  |
| 2   | F     | 68  | GLN  |
| 2   | F     | 118 | GLN  |
| 2   | F     | 143 | ASN  |
| 1   | K     | 68  | GLN  |
| 2   | L     | 11  | GLN  |
| 2   | L     | 68  | GLN  |
| 2   | L     | 111 | ASN  |
| 2   | L     | 118 | GLN  |
| 1   | M     | 57  | GLN  |
| 1   | M     | 68  | GLN  |
| 2   | N     | 47  | ASN  |
| 2   | N     | 65  | GLN  |
| 2   | N     | 118 | GLN  |
| 1   | O     | 21  | ASN  |
| 1   | O     | 68  | GLN  |
| 1   | O     | 73  | ASN  |
| 2   | P     | 11  | GLN  |
| 2   | P     | 68  | GLN  |
| 2   | P     | 118 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 2   | MEN  | B     | 72  | 2    | 7,8,9        | 0.60 | 0           | 5,9,11      | 1.13 | 1 (20%)     |
| 2   | MEN  | D     | 72  | 2    | 7,8,9        | 0.75 | 0           | 5,9,11      | 1.26 | 1 (20%)     |
| 2   | MEN  | F     | 72  | 2    | 7,8,9        | 0.68 | 0           | 5,9,11      | 1.00 | 1 (20%)     |
| 2   | MEN  | L     | 72  | 2    | 7,8,9        | 0.79 | 0           | 5,9,11      | 1.26 | 1 (20%)     |
| 2   | MEN  | N     | 72  | 2    | 7,8,9        | 1.07 | 1 (14%)     | 5,9,11      | 0.87 | 0           |
| 2   | MEN  | P     | 72  | 2    | 7,8,9        | 1.20 | 1 (14%)     | 5,9,11      | 1.08 | 1 (20%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 2   | MEN  | B     | 72  | 2    | -       | 0/6/8/10 | 0/0/0/0 |
| 2   | MEN  | D     | 72  | 2    | -       | 0/6/8/10 | 0/0/0/0 |
| 2   | MEN  | F     | 72  | 2    | -       | 0/6/8/10 | 0/0/0/0 |
| 2   | MEN  | L     | 72  | 2    | -       | 0/6/8/10 | 0/0/0/0 |
| 2   | MEN  | N     | 72  | 2    | -       | 0/6/8/10 | 0/0/0/0 |
| 2   | MEN  | P     | 72  | 2    | -       | 0/6/8/10 | 0/0/0/0 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | P     | 72  | MEN  | CE2-ND2 | 2.17 | 1.49        | 1.45     |
| 2   | N     | 72  | MEN  | CE2-ND2 | 2.52 | 1.50        | 1.45     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | L     | 72  | MEN  | O-C-CA | -2.79 | 118.22      | 125.49   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | D     | 72  | MEN  | O-C-CA | -2.64 | 118.62      | 125.49   |
| 2   | B     | 72  | MEN  | O-C-CA | -2.44 | 119.12      | 125.49   |
| 2   | P     | 72  | MEN  | O-C-CA | -2.39 | 119.27      | 125.49   |
| 2   | F     | 72  | MEN  | O-C-CA | -2.23 | 119.69      | 125.49   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 72  | MEN  | 1       | 0            |
| 2   | F     | 72  | MEN  | 1       | 0            |
| 2   | P     | 72  | MEN  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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 |
| 3   | CYC  | A     | 1163 | 1    | 35,46,46     | 3.08 | 12 (34%) | 47,67,67    | 2.87 | 18 (38%) |
| 3   | CYC  | B     | 1174 | 2    | 35,46,46     | 3.07 | 15 (42%) | 47,67,67    | 2.47 | 16 (34%) |
| 4   | PEB  | B     | 1175 | 2    | 36,46,46     | 3.17 | 17 (47%) | 38,67,67    | 2.85 | 18 (47%) |
| 3   | CYC  | C     | 1163 | 1    | 35,46,46     | 3.29 | 12 (34%) | 47,67,67    | 2.93 | 18 (38%) |
| 3   | CYC  | D     | 1174 | 2    | 35,46,46     | 3.18 | 17 (48%) | 47,67,67    | 2.73 | 19 (40%) |
| 3   | CYC  | D     | 1175 | 2    | 35,46,46     | 2.92 | 16 (45%) | 47,67,67    | 3.86 | 17 (36%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | CYC  | E     | 1163 | 1    | 35,46,46     | 3.14 | 17 (48%) | 47,67,67    | 2.79 | 16 (34%) |
| 3   | CYC  | F     | 1174 | 2    | 35,46,46     | 2.61 | 12 (34%) | 47,67,67    | 2.57 | 14 (29%) |
| 3   | CYC  | F     | 1175 | 2    | 35,46,46     | 3.19 | 18 (51%) | 47,67,67    | 2.97 | 25 (53%) |
| 3   | CYC  | K     | 1163 | 1    | 35,46,46     | 2.98 | 17 (48%) | 47,67,67    | 2.75 | 16 (34%) |
| 3   | CYC  | L     | 1174 | 2    | 35,46,46     | 2.65 | 13 (37%) | 47,67,67    | 2.59 | 21 (44%) |
| 3   | CYC  | L     | 1175 | 2    | 35,46,46     | 3.25 | 17 (48%) | 47,67,67    | 2.68 | 17 (36%) |
| 3   | CYC  | M     | 1163 | 1    | 35,46,46     | 3.25 | 14 (40%) | 47,67,67    | 3.02 | 17 (36%) |
| 3   | CYC  | N     | 1174 | 2    | 35,46,46     | 3.74 | 17 (48%) | 47,67,67    | 2.68 | 20 (42%) |
| 3   | CYC  | N     | 1175 | 2    | 35,46,46     | 3.12 | 13 (37%) | 47,67,67    | 2.71 | 14 (29%) |
| 3   | CYC  | O     | 1163 | 1    | 35,46,46     | 3.03 | 19 (54%) | 47,67,67    | 2.60 | 17 (36%) |
| 3   | CYC  | P     | 1174 | 2    | 35,46,46     | 3.27 | 16 (45%) | 47,67,67    | 2.60 | 20 (42%) |
| 3   | CYC  | P     | 1175 | 2    | 35,46,46     | 2.84 | 13 (37%) | 47,67,67    | 2.14 | 17 (36%) |

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   |
|-----|------|-------|------|------|-----------|------------|---------|
| 3   | CYC  | A     | 1163 | 1    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | B     | 1174 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 4   | PEB  | B     | 1175 | 2    | 1/1/14/19 | 2/19/74/74 | 0/4/4/4 |
| 3   | CYC  | C     | 1163 | 1    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | D     | 1174 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | D     | 1175 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | E     | 1163 | 1    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | F     | 1174 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | F     | 1175 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | K     | 1163 | 1    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | L     | 1174 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | L     | 1175 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | M     | 1163 | 1    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | N     | 1174 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | N     | 1175 | 2    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | O     | 1163 | 1    | -         | 2/21/74/74 | 0/4/4/4 |
| 3   | CYC  | P     | 1174 | 2    | -         | 2/21/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | CYC  | P     | 1175 | 2    | -       | 2/21/74/74 | 0/4/4/4 |

All (275) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | B     | 1174 | CYC  | C2C-C1C | -9.45 | 1.43        | 1.52     |
| 3   | N     | 1175 | CYC  | C1C-NC  | -8.56 | 1.26        | 1.37     |
| 3   | A     | 1163 | CYC  | C1A-C2A | -7.66 | 1.32        | 1.45     |
| 3   | L     | 1175 | CYC  | C1A-C2A | -7.14 | 1.33        | 1.45     |
| 3   | F     | 1175 | CYC  | C1A-C2A | -7.10 | 1.33        | 1.45     |
| 3   | K     | 1163 | CYC  | C1B-NB  | -6.25 | 1.27        | 1.37     |
| 4   | B     | 1175 | PEB  | C1D-ND  | -5.84 | 1.36        | 1.46     |
| 3   | E     | 1163 | CYC  | C4B-NB  | -5.80 | 1.24        | 1.37     |
| 3   | P     | 1174 | CYC  | C1C-NC  | -5.75 | 1.30        | 1.37     |
| 3   | M     | 1163 | CYC  | C4C-NC  | -5.70 | 1.24        | 1.37     |
| 3   | F     | 1174 | CYC  | C1A-NA  | -5.52 | 1.26        | 1.38     |
| 3   | P     | 1175 | CYC  | C1A-C2A | -5.44 | 1.36        | 1.45     |
| 3   | N     | 1174 | CYC  | C1A-C2A | -5.42 | 1.36        | 1.45     |
| 4   | B     | 1175 | PEB  | C1A-NA  | -5.40 | 1.30        | 1.37     |
| 3   | E     | 1163 | CYC  | C1B-NB  | -5.27 | 1.28        | 1.37     |
| 3   | L     | 1175 | CYC  | C1C-NC  | -5.06 | 1.31        | 1.37     |
| 3   | O     | 1163 | CYC  | C1A-C2A | -4.96 | 1.37        | 1.45     |
| 3   | O     | 1163 | CYC  | C4B-C3B | -4.86 | 1.37        | 1.48     |
| 3   | D     | 1174 | CYC  | C1A-C2A | -4.69 | 1.37        | 1.45     |
| 4   | B     | 1175 | PEB  | C4B-C3B | -4.62 | 1.37        | 1.45     |
| 3   | K     | 1163 | CYC  | C1C-NC  | -4.54 | 1.31        | 1.37     |
| 3   | C     | 1163 | CYC  | C4C-NC  | -4.51 | 1.27        | 1.37     |
| 3   | P     | 1175 | CYC  | C1A-NA  | -4.44 | 1.28        | 1.38     |
| 3   | E     | 1163 | CYC  | C1C-NC  | -4.42 | 1.32        | 1.37     |
| 3   | B     | 1174 | CYC  | C1A-NA  | -4.32 | 1.29        | 1.38     |
| 3   | D     | 1175 | CYC  | C1B-NB  | -4.26 | 1.30        | 1.37     |
| 3   | N     | 1174 | CYC  | C4C-NC  | -4.10 | 1.28        | 1.37     |
| 3   | N     | 1174 | CYC  | C1B-C2B | -4.06 | 1.37        | 1.45     |
| 4   | B     | 1175 | PEB  | CHC-C1D | -4.00 | 1.44        | 1.54     |
| 3   | O     | 1163 | CYC  | CMC-C2C | -3.76 | 1.44        | 1.53     |
| 3   | A     | 1163 | CYC  | C1C-NC  | -3.75 | 1.32        | 1.37     |
| 3   | P     | 1174 | CYC  | C1A-NA  | -3.75 | 1.30        | 1.38     |
| 3   | L     | 1175 | CYC  | C4A-C3A | -3.75 | 1.37        | 1.45     |
| 3   | N     | 1174 | CYC  | C1A-NA  | -3.74 | 1.30        | 1.38     |
| 3   | B     | 1174 | CYC  | C1B-NB  | -3.61 | 1.31        | 1.37     |
| 3   | F     | 1175 | CYC  | C4A-C3A | -3.60 | 1.37        | 1.45     |
| 3   | F     | 1175 | CYC  | C4B-NB  | -3.59 | 1.29        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | E     | 1163 | CYC  | C4B-C3B | -3.57 | 1.40        | 1.48     |
| 3   | O     | 1163 | CYC  | C2C-C1C | -3.56 | 1.48        | 1.52     |
| 3   | B     | 1174 | CYC  | C4B-C3B | -3.51 | 1.40        | 1.48     |
| 3   | F     | 1175 | CYC  | CAC-C3C | -3.51 | 1.46        | 1.54     |
| 3   | L     | 1174 | CYC  | C1C-NC  | -3.38 | 1.33        | 1.37     |
| 3   | L     | 1175 | CYC  | C1B-C2B | -3.35 | 1.38        | 1.45     |
| 3   | P     | 1174 | CYC  | C2A-C3A | -3.34 | 1.29        | 1.36     |
| 3   | F     | 1174 | CYC  | C1C-NC  | -3.31 | 1.33        | 1.37     |
| 3   | K     | 1163 | CYC  | C4B-NB  | -3.27 | 1.30        | 1.37     |
| 3   | D     | 1174 | CYC  | C4A-NA  | -3.25 | 1.29        | 1.37     |
| 3   | N     | 1175 | CYC  | C4B-NB  | -3.11 | 1.30        | 1.37     |
| 3   | P     | 1174 | CYC  | C1A-C2A | -3.04 | 1.40        | 1.45     |
| 3   | O     | 1163 | CYC  | C1A-NA  | -3.04 | 1.31        | 1.38     |
| 3   | C     | 1163 | CYC  | C4B-NB  | -3.02 | 1.31        | 1.37     |
| 3   | D     | 1175 | CYC  | OB-C4B  | -3.01 | 1.17        | 1.23     |
| 3   | L     | 1174 | CYC  | C1A-C2A | -3.01 | 1.40        | 1.45     |
| 3   | L     | 1174 | CYC  | C1B-NB  | -2.96 | 1.32        | 1.37     |
| 3   | A     | 1163 | CYC  | C1B-NB  | -2.94 | 1.32        | 1.37     |
| 3   | P     | 1175 | CYC  | C4A-C3A | -2.93 | 1.39        | 1.45     |
| 3   | N     | 1174 | CYC  | C4B-C3B | -2.93 | 1.42        | 1.48     |
| 4   | B     | 1175 | PEB  | C1B-C2B | -2.89 | 1.39        | 1.45     |
| 3   | L     | 1175 | CYC  | C4B-NB  | -2.77 | 1.31        | 1.37     |
| 3   | M     | 1163 | CYC  | C1B-NB  | -2.75 | 1.33        | 1.37     |
| 3   | L     | 1174 | CYC  | C4B-C3B | -2.72 | 1.42        | 1.48     |
| 3   | D     | 1175 | CYC  | C1A-C2A | -2.71 | 1.40        | 1.45     |
| 3   | D     | 1174 | CYC  | CMD-C2D | -2.57 | 1.46        | 1.51     |
| 3   | D     | 1174 | CYC  | C4B-C3B | -2.47 | 1.43        | 1.48     |
| 3   | D     | 1174 | CYC  | C1B-NB  | -2.47 | 1.33        | 1.37     |
| 3   | N     | 1175 | CYC  | C3B-C2B | -2.47 | 1.31        | 1.36     |
| 3   | O     | 1163 | CYC  | C4B-NB  | -2.44 | 1.32        | 1.37     |
| 3   | L     | 1175 | CYC  | CBB-CAB | -2.43 | 1.39        | 1.51     |
| 3   | L     | 1174 | CYC  | CHD-C4C | -2.43 | 1.32        | 1.38     |
| 3   | D     | 1174 | CYC  | C1A-NA  | -2.41 | 1.33        | 1.38     |
| 3   | D     | 1175 | CYC  | C1A-NA  | -2.40 | 1.33        | 1.38     |
| 3   | P     | 1175 | CYC  | C3D-C2D | -2.35 | 1.30        | 1.37     |
| 3   | D     | 1175 | CYC  | CBB-CAB | -2.33 | 1.40        | 1.51     |
| 3   | N     | 1175 | CYC  | C4C-NC  | -2.31 | 1.32        | 1.37     |
| 4   | B     | 1175 | PEB  | C4B-NB  | -2.29 | 1.33        | 1.38     |
| 3   | D     | 1175 | CYC  | C4B-C3B | -2.23 | 1.43        | 1.48     |
| 3   | O     | 1163 | CYC  | C1B-NB  | -2.19 | 1.34        | 1.37     |
| 3   | N     | 1175 | CYC  | CAC-C3C | -2.19 | 1.49        | 1.54     |
| 3   | O     | 1163 | CYC  | C4A-C3A | -2.16 | 1.41        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | M     | 1163 | CYC  | C2C-C1C | -2.13 | 1.50        | 1.52     |
| 3   | L     | 1175 | CYC  | C1A-NA  | -2.05 | 1.34        | 1.38     |
| 4   | B     | 1175 | PEB  | C2C-C3C | -2.03 | 1.31        | 1.37     |
| 3   | K     | 1163 | CYC  | CHA-C1A | 2.00  | 1.36        | 1.35     |
| 3   | E     | 1163 | CYC  | CMC-C2C | 2.02  | 1.57        | 1.53     |
| 3   | F     | 1174 | CYC  | CHB-C4A | 2.02  | 1.45        | 1.40     |
| 3   | E     | 1163 | CYC  | CAB-C3B | 2.05  | 1.56        | 1.51     |
| 3   | N     | 1175 | CYC  | CMD-C2D | 2.05  | 1.55        | 1.51     |
| 3   | K     | 1163 | CYC  | CMC-C2C | 2.06  | 1.57        | 1.53     |
| 3   | O     | 1163 | CYC  | CHB-C4A | 2.06  | 1.45        | 1.40     |
| 3   | L     | 1174 | CYC  | C2C-C3C | 2.11  | 1.61        | 1.54     |
| 3   | K     | 1163 | CYC  | CAC-C3C | 2.13  | 1.58        | 1.54     |
| 3   | D     | 1174 | CYC  | CHB-C4A | 2.14  | 1.45        | 1.40     |
| 3   | C     | 1163 | CYC  | CBB-CAB | 2.15  | 1.61        | 1.51     |
| 3   | P     | 1175 | CYC  | C2C-C3C | 2.16  | 1.61        | 1.54     |
| 3   | N     | 1175 | CYC  | C1B-NB  | 2.19  | 1.41        | 1.37     |
| 3   | B     | 1174 | CYC  | CHB-C1B | 2.20  | 1.43        | 1.37     |
| 3   | O     | 1163 | CYC  | CHA-C1A | 2.20  | 1.37        | 1.35     |
| 3   | F     | 1175 | CYC  | CHD-C4C | 2.23  | 1.43        | 1.38     |
| 3   | E     | 1163 | CYC  | C2A-C3A | 2.23  | 1.41        | 1.36     |
| 3   | D     | 1175 | CYC  | C4A-C3A | 2.23  | 1.50        | 1.45     |
| 3   | E     | 1163 | CYC  | C4A-NA  | 2.26  | 1.42        | 1.37     |
| 3   | L     | 1175 | CYC  | CHB-C4A | 2.33  | 1.46        | 1.40     |
| 3   | F     | 1174 | CYC  | CBC-CAC | 2.34  | 1.65        | 1.50     |
| 3   | D     | 1175 | CYC  | C4C-NC  | 2.39  | 1.42        | 1.37     |
| 3   | N     | 1175 | CYC  | CMB-C2B | 2.40  | 1.55        | 1.50     |
| 3   | A     | 1163 | CYC  | CBB-CAB | 2.41  | 1.62        | 1.51     |
| 3   | M     | 1163 | CYC  | C4A-C3A | 2.42  | 1.51        | 1.45     |
| 3   | F     | 1175 | CYC  | CHB-C4A | 2.44  | 1.46        | 1.40     |
| 4   | B     | 1175 | PEB  | CHA-C1B | 2.46  | 1.46        | 1.40     |
| 3   | F     | 1174 | CYC  | C3B-C2B | 2.47  | 1.42        | 1.36     |
| 3   | K     | 1163 | CYC  | CMA-C3A | 2.48  | 1.56        | 1.50     |
| 3   | B     | 1174 | CYC  | C3D-C2D | 2.48  | 1.45        | 1.37     |
| 3   | D     | 1174 | CYC  | CBB-CAB | 2.48  | 1.63        | 1.51     |
| 3   | K     | 1163 | CYC  | CHD-C4C | 2.52  | 1.44        | 1.38     |
| 3   | A     | 1163 | CYC  | OC-C1C  | 2.54  | 1.28        | 1.23     |
| 3   | N     | 1174 | CYC  | CHD-C4C | 2.55  | 1.44        | 1.38     |
| 3   | F     | 1175 | CYC  | CAB-C3B | 2.58  | 1.58        | 1.51     |
| 3   | O     | 1163 | CYC  | C2C-C3C | 2.58  | 1.62        | 1.54     |
| 3   | L     | 1175 | CYC  | C4C-NC  | 2.59  | 1.43        | 1.37     |
| 3   | M     | 1163 | CYC  | CBB-CAB | 2.61  | 1.63        | 1.51     |
| 3   | D     | 1175 | CYC  | CAA-C2A | 2.64  | 1.58        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | P     | 1175 | CYC  | CMD-C2D | 2.66 | 1.57        | 1.51     |
| 3   | E     | 1163 | CYC  | C2C-C3C | 2.67 | 1.62        | 1.54     |
| 3   | K     | 1163 | CYC  | OB-C4B  | 2.70 | 1.28        | 1.23     |
| 3   | P     | 1174 | CYC  | CMD-C2D | 2.71 | 1.57        | 1.51     |
| 3   | F     | 1175 | CYC  | CAD-C3D | 2.71 | 1.56        | 1.52     |
| 3   | M     | 1163 | CYC  | CAA-C2A | 2.73 | 1.58        | 1.51     |
| 3   | K     | 1163 | CYC  | C1B-C2B | 2.74 | 1.50        | 1.45     |
| 3   | O     | 1163 | CYC  | C1D-CHD | 2.75 | 1.50        | 1.40     |
| 3   | B     | 1174 | CYC  | C2A-C3A | 2.77 | 1.42        | 1.36     |
| 3   | L     | 1175 | CYC  | C2A-C3A | 2.77 | 1.42        | 1.36     |
| 3   | B     | 1174 | CYC  | OB-C4B  | 2.78 | 1.28        | 1.23     |
| 3   | B     | 1174 | CYC  | CAA-C2A | 2.78 | 1.59        | 1.51     |
| 3   | P     | 1174 | CYC  | C3B-C2B | 2.79 | 1.42        | 1.36     |
| 3   | F     | 1174 | CYC  | CAC-C3C | 2.82 | 1.59        | 1.54     |
| 3   | F     | 1175 | CYC  | CMD-C2D | 2.86 | 1.57        | 1.51     |
| 3   | B     | 1174 | CYC  | CAB-C3B | 2.90 | 1.59        | 1.51     |
| 3   | F     | 1174 | CYC  | CHB-C1B | 2.95 | 1.44        | 1.37     |
| 3   | M     | 1163 | CYC  | CMC-C2C | 2.96 | 1.60        | 1.53     |
| 3   | N     | 1174 | CYC  | OB-C4B  | 2.98 | 1.29        | 1.23     |
| 4   | B     | 1175 | PEB  | CAC-C2C | 3.00 | 1.57        | 1.52     |
| 3   | K     | 1163 | CYC  | CAA-C2A | 3.08 | 1.59        | 1.51     |
| 3   | L     | 1174 | CYC  | OB-C4B  | 3.09 | 1.29        | 1.23     |
| 4   | B     | 1175 | PEB  | CBD-CAD | 3.11 | 1.45        | 1.30     |
| 3   | F     | 1175 | CYC  | C2A-C3A | 3.11 | 1.43        | 1.36     |
| 3   | E     | 1163 | CYC  | CAC-C3C | 3.15 | 1.60        | 1.54     |
| 4   | B     | 1175 | PEB  | CMB-C2B | 3.19 | 1.57        | 1.50     |
| 3   | F     | 1175 | CYC  | CBC-CAC | 3.20 | 1.71        | 1.50     |
| 3   | P     | 1175 | CYC  | CBC-CAC | 3.22 | 1.71        | 1.50     |
| 3   | D     | 1174 | CYC  | OB-C4B  | 3.25 | 1.29        | 1.23     |
| 3   | N     | 1174 | CYC  | OC-C1C  | 3.25 | 1.29        | 1.23     |
| 3   | D     | 1174 | CYC  | CAC-C3C | 3.27 | 1.60        | 1.54     |
| 3   | N     | 1175 | CYC  | OC-C1C  | 3.28 | 1.29        | 1.23     |
| 3   | F     | 1175 | CYC  | CAA-C2A | 3.29 | 1.60        | 1.51     |
| 3   | K     | 1163 | CYC  | CAB-C3B | 3.42 | 1.60        | 1.51     |
| 3   | D     | 1175 | CYC  | CMA-C3A | 3.44 | 1.58        | 1.50     |
| 3   | P     | 1174 | CYC  | C4A-C3A | 3.44 | 1.53        | 1.45     |
| 3   | L     | 1174 | CYC  | CAB-C3B | 3.49 | 1.60        | 1.51     |
| 3   | C     | 1163 | CYC  | CAB-C3B | 3.55 | 1.61        | 1.51     |
| 3   | L     | 1175 | CYC  | C1B-NB  | 3.59 | 1.44        | 1.37     |
| 3   | F     | 1175 | CYC  | C2C-C3C | 3.60 | 1.65        | 1.54     |
| 3   | B     | 1174 | CYC  | CMC-C2C | 3.60 | 1.61        | 1.53     |
| 3   | B     | 1174 | CYC  | C4A-NA  | 3.61 | 1.45        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | B     | 1175 | PEB  | CHB-C4B | 3.66 | 1.38        | 1.35     |
| 3   | P     | 1174 | CYC  | C1B-NB  | 3.70 | 1.44        | 1.37     |
| 3   | D     | 1174 | CYC  | CMC-C2C | 3.71 | 1.61        | 1.53     |
| 3   | P     | 1174 | CYC  | CAB-C3B | 3.72 | 1.61        | 1.51     |
| 3   | P     | 1175 | CYC  | C2A-C3A | 3.74 | 1.44        | 1.36     |
| 3   | F     | 1174 | CYC  | OB-C4B  | 3.76 | 1.30        | 1.23     |
| 3   | L     | 1174 | CYC  | CAA-C2A | 3.76 | 1.61        | 1.51     |
| 3   | C     | 1163 | CYC  | CMD-C2D | 3.77 | 1.59        | 1.51     |
| 3   | N     | 1175 | CYC  | C2C-C1C | 3.80 | 1.55        | 1.52     |
| 3   | P     | 1174 | CYC  | OB-C4B  | 3.81 | 1.30        | 1.23     |
| 3   | F     | 1174 | CYC  | CAA-C2A | 3.82 | 1.61        | 1.51     |
| 3   | O     | 1163 | CYC  | CMD-C2D | 3.89 | 1.59        | 1.51     |
| 3   | P     | 1175 | CYC  | CAD-C3D | 3.94 | 1.58        | 1.52     |
| 3   | N     | 1175 | CYC  | CAA-C2A | 3.95 | 1.62        | 1.51     |
| 3   | M     | 1163 | CYC  | CHB-C1B | 3.95 | 1.47        | 1.37     |
| 3   | L     | 1175 | CYC  | CAD-C3D | 3.96 | 1.58        | 1.52     |
| 4   | B     | 1175 | PEB  | OD-C4D  | 3.96 | 1.31        | 1.23     |
| 3   | F     | 1175 | CYC  | C1B-NB  | 4.01 | 1.44        | 1.37     |
| 3   | F     | 1175 | CYC  | C4B-C3B | 4.03 | 1.56        | 1.48     |
| 3   | D     | 1175 | CYC  | OC-C1C  | 4.04 | 1.31        | 1.23     |
| 3   | E     | 1163 | CYC  | CMD-C2D | 4.05 | 1.60        | 1.51     |
| 3   | B     | 1174 | CYC  | CHD-C4C | 4.08 | 1.48        | 1.38     |
| 3   | K     | 1163 | CYC  | CHB-C4A | 4.11 | 1.50        | 1.40     |
| 3   | C     | 1163 | CYC  | CMA-C3A | 4.13 | 1.59        | 1.50     |
| 3   | P     | 1174 | CYC  | CMC-C2C | 4.28 | 1.63        | 1.53     |
| 3   | E     | 1163 | CYC  | CAA-C2A | 4.35 | 1.63        | 1.51     |
| 3   | A     | 1163 | CYC  | CAA-C2A | 4.36 | 1.63        | 1.51     |
| 3   | N     | 1174 | CYC  | CAB-C3B | 4.38 | 1.63        | 1.51     |
| 3   | F     | 1174 | CYC  | CMA-C3A | 4.39 | 1.60        | 1.50     |
| 3   | D     | 1174 | CYC  | CAB-C3B | 4.40 | 1.63        | 1.51     |
| 3   | A     | 1163 | CYC  | CAD-C3D | 4.41 | 1.59        | 1.52     |
| 3   | D     | 1175 | CYC  | CAD-C3D | 4.43 | 1.59        | 1.52     |
| 3   | O     | 1163 | CYC  | CMA-C3A | 4.47 | 1.60        | 1.50     |
| 3   | O     | 1163 | CYC  | C1C-NC  | 4.52 | 1.43        | 1.37     |
| 3   | N     | 1175 | CYC  | CMA-C3A | 4.53 | 1.60        | 1.50     |
| 3   | N     | 1174 | CYC  | C1C-NC  | 4.55 | 1.43        | 1.37     |
| 3   | E     | 1163 | CYC  | CAD-C3D | 4.58 | 1.59        | 1.52     |
| 3   | L     | 1175 | CYC  | CAA-C2A | 4.58 | 1.63        | 1.51     |
| 3   | P     | 1175 | CYC  | CHA-C1A | 4.58 | 1.39        | 1.35     |
| 3   | E     | 1163 | CYC  | OC-C1C  | 4.61 | 1.32        | 1.23     |
| 3   | C     | 1163 | CYC  | CAC-C3C | 4.66 | 1.63        | 1.54     |
| 3   | N     | 1174 | CYC  | C3B-C2B | 4.67 | 1.46        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 4   | B     | 1175 | PEB  | CAD-C3D | 4.68 | 1.62        | 1.47     |
| 3   | F     | 1174 | CYC  | CAD-C3D | 4.70 | 1.60        | 1.52     |
| 3   | M     | 1163 | CYC  | OC-C1C  | 4.71 | 1.32        | 1.23     |
| 3   | A     | 1163 | CYC  | CAB-C3B | 4.76 | 1.64        | 1.51     |
| 3   | C     | 1163 | CYC  | OC-C1C  | 4.77 | 1.32        | 1.23     |
| 3   | P     | 1174 | CYC  | C2C-C1C | 4.81 | 1.56        | 1.52     |
| 3   | B     | 1174 | CYC  | CMD-C2D | 4.89 | 1.61        | 1.51     |
| 3   | L     | 1174 | CYC  | CAD-C3D | 4.93 | 1.60        | 1.52     |
| 3   | D     | 1174 | CYC  | CMA-C3A | 4.95 | 1.61        | 1.50     |
| 3   | L     | 1175 | CYC  | OB-C4B  | 4.96 | 1.33        | 1.23     |
| 3   | K     | 1163 | CYC  | CMB-C2B | 4.97 | 1.61        | 1.50     |
| 3   | L     | 1174 | CYC  | CHA-C1A | 5.03 | 1.39        | 1.35     |
| 3   | M     | 1163 | CYC  | CAC-C3C | 5.03 | 1.64        | 1.54     |
| 3   | D     | 1175 | CYC  | CMD-C2D | 5.12 | 1.62        | 1.51     |
| 3   | D     | 1174 | CYC  | CAA-C2A | 5.13 | 1.65        | 1.51     |
| 3   | O     | 1163 | CYC  | OC-C1C  | 5.14 | 1.33        | 1.23     |
| 3   | E     | 1163 | CYC  | CHA-C1A | 5.15 | 1.39        | 1.35     |
| 3   | E     | 1163 | CYC  | CMA-C3A | 5.26 | 1.61        | 1.50     |
| 3   | M     | 1163 | CYC  | CAB-C3B | 5.30 | 1.65        | 1.51     |
| 3   | D     | 1175 | CYC  | CAB-C3B | 5.34 | 1.65        | 1.51     |
| 3   | N     | 1174 | CYC  | CHB-C4A | 5.34 | 1.53        | 1.40     |
| 3   | P     | 1175 | CYC  | CAB-C3B | 5.38 | 1.66        | 1.51     |
| 3   | K     | 1163 | CYC  | CMD-C2D | 5.45 | 1.62        | 1.51     |
| 3   | O     | 1163 | CYC  | CAA-C2A | 5.45 | 1.66        | 1.51     |
| 3   | N     | 1174 | CYC  | C1B-NB  | 5.50 | 1.47        | 1.37     |
| 3   | O     | 1163 | CYC  | CAD-C3D | 5.52 | 1.61        | 1.52     |
| 3   | A     | 1163 | CYC  | CHA-C1A | 5.52 | 1.40        | 1.35     |
| 4   | B     | 1175 | PEB  | CAB-C3B | 5.61 | 1.66        | 1.51     |
| 3   | F     | 1175 | CYC  | CMB-C2B | 5.62 | 1.62        | 1.50     |
| 3   | P     | 1174 | CYC  | CHB-C1B | 5.70 | 1.51        | 1.37     |
| 3   | D     | 1174 | CYC  | CAD-C3D | 5.80 | 1.62        | 1.52     |
| 3   | N     | 1174 | CYC  | CMA-C3A | 5.86 | 1.63        | 1.50     |
| 3   | A     | 1163 | CYC  | C2C-C1C | 5.93 | 1.57        | 1.52     |
| 3   | A     | 1163 | CYC  | CMB-C2B | 6.04 | 1.63        | 1.50     |
| 3   | P     | 1175 | CYC  | CMB-C2B | 6.05 | 1.63        | 1.50     |
| 3   | L     | 1175 | CYC  | CMB-C2B | 6.10 | 1.63        | 1.50     |
| 3   | C     | 1163 | CYC  | C4A-C3A | 6.10 | 1.59        | 1.45     |
| 3   | L     | 1175 | CYC  | CMD-C2D | 6.12 | 1.64        | 1.51     |
| 3   | N     | 1174 | CYC  | CMC-C2C | 6.14 | 1.67        | 1.53     |
| 3   | C     | 1163 | CYC  | CHA-C1A | 6.15 | 1.40        | 1.35     |
| 3   | L     | 1174 | CYC  | CMC-C2C | 6.21 | 1.67        | 1.53     |
| 3   | K     | 1163 | CYC  | OC-C1C  | 6.38 | 1.35        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | F     | 1175 | CYC  | CHA-C1A | 6.41  | 1.40        | 1.35     |
| 3   | D     | 1174 | CYC  | CHA-C1A | 6.43  | 1.40        | 1.35     |
| 3   | D     | 1175 | CYC  | CMB-C2B | 6.43  | 1.64        | 1.50     |
| 3   | P     | 1174 | CYC  | CAA-C2A | 6.45  | 1.69        | 1.51     |
| 3   | P     | 1174 | CYC  | CMA-C3A | 6.57  | 1.64        | 1.50     |
| 4   | B     | 1175 | PEB  | C4D-ND  | 6.63  | 1.44        | 1.34     |
| 3   | O     | 1163 | CYC  | CMB-C2B | 6.64  | 1.64        | 1.50     |
| 3   | L     | 1174 | CYC  | CMA-C3A | 6.70  | 1.64        | 1.50     |
| 3   | A     | 1163 | CYC  | CAC-C3C | 6.78  | 1.67        | 1.54     |
| 3   | K     | 1163 | CYC  | C2C-C1C | 6.92  | 1.58        | 1.52     |
| 3   | C     | 1163 | CYC  | CAD-C3D | 7.27  | 1.64        | 1.52     |
| 3   | P     | 1175 | CYC  | CMA-C3A | 7.28  | 1.66        | 1.50     |
| 4   | B     | 1175 | PEB  | CMC-C3C | 7.29  | 1.66        | 1.51     |
| 3   | M     | 1163 | CYC  | OB-C4B  | 7.44  | 1.37        | 1.23     |
| 3   | M     | 1163 | CYC  | CAD-C3D | 7.44  | 1.64        | 1.52     |
| 3   | E     | 1163 | CYC  | CMB-C2B | 7.61  | 1.66        | 1.50     |
| 3   | F     | 1175 | CYC  | CMA-C3A | 7.63  | 1.66        | 1.50     |
| 3   | D     | 1175 | CYC  | CHA-C1A | 7.68  | 1.41        | 1.35     |
| 3   | L     | 1175 | CYC  | CHA-C1A | 7.85  | 1.42        | 1.35     |
| 3   | P     | 1174 | CYC  | CHA-C1A | 8.05  | 1.42        | 1.35     |
| 3   | N     | 1174 | CYC  | CAC-C3C | 8.13  | 1.70        | 1.54     |
| 3   | B     | 1174 | CYC  | CHA-C1A | 8.27  | 1.42        | 1.35     |
| 3   | F     | 1174 | CYC  | CHA-C1A | 8.29  | 1.42        | 1.35     |
| 3   | M     | 1163 | CYC  | CMD-C2D | 8.40  | 1.68        | 1.51     |
| 3   | D     | 1174 | CYC  | C2C-C1C | 9.45  | 1.60        | 1.52     |
| 3   | N     | 1174 | CYC  | CHA-C1A | 10.06 | 1.44        | 1.35     |
| 3   | C     | 1163 | CYC  | CMB-C2B | 10.15 | 1.72        | 1.50     |
| 3   | N     | 1175 | CYC  | CHA-C1A | 11.80 | 1.45        | 1.35     |

All (320) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 3   | D     | 1175 | CYC  | C4B-C3B-C2B | -10.47 | 102.08      | 108.05   |
| 3   | C     | 1163 | CYC  | C3C-C2C-C1C | -9.55  | 95.41       | 103.41   |
| 3   | M     | 1163 | CYC  | C3C-C2C-C1C | -9.10  | 95.78       | 103.41   |
| 3   | O     | 1163 | CYC  | OC-C1C-C2C  | -9.00  | 118.98      | 126.25   |
| 3   | D     | 1174 | CYC  | CBD-CAD-C3D | -8.10  | 98.01       | 112.53   |
| 3   | B     | 1174 | CYC  | CBD-CAD-C3D | -7.74  | 98.66       | 112.53   |
| 3   | M     | 1163 | CYC  | C4B-C3B-C2B | -7.54  | 103.74      | 108.05   |
| 3   | C     | 1163 | CYC  | CBD-CAD-C3D | -7.51  | 99.07       | 112.53   |
| 4   | B     | 1175 | PEB  | CBC-CAC-C2C | -7.04  | 99.91       | 112.53   |
| 3   | E     | 1163 | CYC  | C4B-C3B-C2B | -6.93  | 104.09      | 108.05   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | N     | 1175 | CYC  | CHB-C4A-NA  | -6.79 | 111.99      | 124.91   |
| 3   | F     | 1174 | CYC  | OC-C1C-C2C  | -6.70 | 120.84      | 126.25   |
| 3   | A     | 1163 | CYC  | C3C-C2C-C1C | -6.58 | 97.90       | 103.41   |
| 3   | A     | 1163 | CYC  | C4B-C3B-C2B | -6.45 | 104.37      | 108.05   |
| 3   | L     | 1174 | CYC  | CBD-CAD-C3D | -6.27 | 101.30      | 112.53   |
| 3   | K     | 1163 | CYC  | C4B-C3B-C2B | -6.23 | 104.49      | 108.05   |
| 3   | N     | 1174 | CYC  | C3C-C2C-C1C | -6.21 | 98.21       | 103.41   |
| 3   | E     | 1163 | CYC  | OC-C1C-C2C  | -6.19 | 121.25      | 126.25   |
| 3   | N     | 1175 | CYC  | OC-C1C-NC   | -6.18 | 117.35      | 124.83   |
| 3   | C     | 1163 | CYC  | OC-C1C-NC   | -6.12 | 117.43      | 124.83   |
| 3   | O     | 1163 | CYC  | C2D-C1D-ND  | -6.07 | 100.35      | 110.29   |
| 3   | C     | 1163 | CYC  | OC-C1C-C2C  | -6.07 | 121.35      | 126.25   |
| 4   | B     | 1175 | PEB  | CAA-C3A-C2A | -6.02 | 98.99       | 114.13   |
| 3   | L     | 1174 | CYC  | OC-C1C-C2C  | -5.98 | 121.42      | 126.25   |
| 3   | N     | 1174 | CYC  | C1B-CHB-C4A | -5.97 | 112.61      | 128.06   |
| 3   | D     | 1175 | CYC  | CAA-CBA-CGA | -5.84 | 102.04      | 112.75   |
| 3   | P     | 1174 | CYC  | C2D-C1D-ND  | -5.58 | 101.15      | 110.29   |
| 3   | F     | 1175 | CYC  | C2D-C1D-ND  | -5.53 | 101.24      | 110.29   |
| 3   | F     | 1175 | CYC  | CHB-C4A-NA  | -5.42 | 114.60      | 124.91   |
| 3   | E     | 1163 | CYC  | C2D-C1D-ND  | -5.39 | 101.46      | 110.29   |
| 3   | N     | 1175 | CYC  | C3C-C2C-C1C | -5.37 | 98.91       | 103.41   |
| 3   | B     | 1174 | CYC  | C1B-CHB-C4A | -5.35 | 114.21      | 128.06   |
| 3   | P     | 1174 | CYC  | C1B-CHB-C4A | -5.35 | 114.23      | 128.06   |
| 3   | B     | 1174 | CYC  | C2D-C1D-ND  | -5.33 | 101.57      | 110.29   |
| 3   | P     | 1174 | CYC  | CAD-CBD-CGD | -5.27 | 103.08      | 112.75   |
| 3   | D     | 1175 | CYC  | OC-C1C-C2C  | -5.27 | 121.99      | 126.25   |
| 3   | P     | 1175 | CYC  | CAC-C3C-C2C | -5.23 | 100.99      | 114.13   |
| 3   | D     | 1174 | CYC  | C2D-C1D-ND  | -5.22 | 101.75      | 110.29   |
| 3   | F     | 1175 | CYC  | CAC-C3C-C2C | -5.21 | 101.04      | 114.13   |
| 3   | E     | 1163 | CYC  | CMC-C2C-C1C | -5.12 | 101.67      | 112.43   |
| 3   | K     | 1163 | CYC  | OC-C1C-NC   | -5.09 | 118.67      | 124.83   |
| 3   | F     | 1174 | CYC  | CBD-CAD-C3D | -5.03 | 103.52      | 112.53   |
| 3   | D     | 1174 | CYC  | CAD-C3D-C4D | -4.98 | 121.61      | 127.01   |
| 3   | N     | 1174 | CYC  | C3A-C4A-NA  | -4.97 | 99.21       | 110.55   |
| 3   | D     | 1175 | CYC  | CAC-C3C-C2C | -4.86 | 101.92      | 114.13   |
| 3   | D     | 1174 | CYC  | C1B-CHB-C4A | -4.81 | 115.63      | 128.06   |
| 3   | L     | 1174 | CYC  | C2D-C1D-ND  | -4.80 | 102.42      | 110.29   |
| 3   | L     | 1175 | CYC  | CHB-C4A-NA  | -4.80 | 115.77      | 124.91   |
| 3   | D     | 1175 | CYC  | CHB-C4A-NA  | -4.74 | 115.89      | 124.91   |
| 3   | F     | 1175 | CYC  | CAD-C3D-C4D | -4.65 | 121.96      | 127.01   |
| 3   | P     | 1174 | CYC  | C3A-C4A-NA  | -4.62 | 100.01      | 110.55   |
| 3   | M     | 1163 | CYC  | OC-C1C-NC   | -4.54 | 119.34      | 124.83   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | B     | 1175 | PEB  | C3A-C2A-C1A | -4.54 | 99.61       | 103.41   |
| 3   | M     | 1163 | CYC  | C2D-C1D-ND  | -4.52 | 102.89      | 110.29   |
| 3   | O     | 1163 | CYC  | C3C-C2C-C1C | -4.45 | 99.68       | 103.41   |
| 3   | A     | 1163 | CYC  | C2D-C1D-ND  | -4.43 | 103.04      | 110.29   |
| 3   | D     | 1174 | CYC  | C3A-C4A-NA  | -4.42 | 100.46      | 110.55   |
| 3   | F     | 1174 | CYC  | C3A-C4A-NA  | -4.41 | 100.51      | 110.55   |
| 3   | K     | 1163 | CYC  | CAA-CBA-CGA | -4.40 | 104.68      | 112.75   |
| 3   | C     | 1163 | CYC  | C4B-C3B-C2B | -4.35 | 105.56      | 108.05   |
| 3   | N     | 1175 | CYC  | CAC-C3C-C2C | -4.35 | 103.20      | 114.13   |
| 3   | L     | 1175 | CYC  | CAB-C3B-C2B | -4.34 | 119.90      | 127.51   |
| 3   | L     | 1175 | CYC  | C2D-C1D-ND  | -4.30 | 103.25      | 110.29   |
| 4   | B     | 1175 | PEB  | CMB-C2B-C1B | -4.26 | 118.12      | 125.06   |
| 3   | F     | 1175 | CYC  | C3C-C2C-C1C | -4.25 | 99.85       | 103.41   |
| 3   | P     | 1175 | CYC  | CAA-CBA-CGA | -4.23 | 104.99      | 112.75   |
| 3   | L     | 1175 | CYC  | OC-C1C-C2C  | -4.21 | 122.85      | 126.25   |
| 4   | B     | 1175 | PEB  | OA-C1A-C2A  | -4.21 | 122.85      | 126.25   |
| 3   | P     | 1174 | CYC  | OC-C1C-C2C  | -4.19 | 122.87      | 126.25   |
| 3   | F     | 1174 | CYC  | C1B-CHB-C4A | -4.18 | 117.26      | 128.06   |
| 3   | D     | 1175 | CYC  | C2D-C1D-ND  | -4.14 | 103.50      | 110.29   |
| 3   | N     | 1174 | CYC  | C2D-C1D-ND  | -4.14 | 103.51      | 110.29   |
| 3   | K     | 1163 | CYC  | CAD-C3D-C4D | -4.13 | 122.52      | 127.01   |
| 3   | B     | 1174 | CYC  | C3A-C4A-NA  | -4.12 | 101.16      | 110.55   |
| 3   | A     | 1163 | CYC  | OC-C1C-NC   | -4.09 | 119.88      | 124.83   |
| 4   | B     | 1175 | PEB  | C2B-C1B-NB  | -4.06 | 101.28      | 110.55   |
| 3   | M     | 1163 | CYC  | CBD-CAD-C3D | -4.06 | 105.24      | 112.53   |
| 3   | L     | 1174 | CYC  | CAD-CBD-CGD | -3.97 | 105.47      | 112.75   |
| 3   | K     | 1163 | CYC  | CHB-C4A-NA  | -3.94 | 117.41      | 124.91   |
| 3   | B     | 1174 | CYC  | OC-C1C-C2C  | -3.94 | 123.07      | 126.25   |
| 3   | L     | 1174 | CYC  | CAC-C3C-C2C | -3.92 | 104.28      | 114.13   |
| 3   | P     | 1175 | CYC  | CHB-C4A-NA  | -3.90 | 117.49      | 124.91   |
| 3   | D     | 1174 | CYC  | OC-C1C-C2C  | -3.87 | 123.13      | 126.25   |
| 3   | D     | 1175 | CYC  | CAB-C3B-C2B | -3.87 | 120.73      | 127.51   |
| 3   | L     | 1175 | CYC  | CAC-C3C-C2C | -3.83 | 104.50      | 114.13   |
| 3   | N     | 1174 | CYC  | OB-C4B-C3B  | -3.72 | 123.63      | 128.09   |
| 3   | N     | 1175 | CYC  | C2D-C1D-ND  | -3.68 | 104.27      | 110.29   |
| 3   | C     | 1163 | CYC  | C2D-C1D-ND  | -3.67 | 104.28      | 110.29   |
| 3   | E     | 1163 | CYC  | CHB-C4A-NA  | -3.59 | 118.07      | 124.91   |
| 3   | F     | 1174 | CYC  | C2D-C1D-ND  | -3.56 | 104.46      | 110.29   |
| 3   | M     | 1163 | CYC  | CAD-C3D-C4D | -3.49 | 123.22      | 127.01   |
| 3   | L     | 1174 | CYC  | C3A-C4A-NA  | -3.41 | 102.77      | 110.55   |
| 3   | A     | 1163 | CYC  | C3A-C4A-NA  | -3.41 | 102.78      | 110.55   |
| 3   | O     | 1163 | CYC  | C3A-C4A-NA  | -3.40 | 102.81      | 110.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | F     | 1175 | CYC  | CAC-C3C-C4C | -3.33 | 104.11      | 112.67   |
| 3   | F     | 1174 | CYC  | C3B-C4B-NB  | -3.30 | 103.74      | 106.74   |
| 3   | P     | 1175 | CYC  | OB-C4B-C3B  | -3.28 | 124.17      | 128.09   |
| 3   | F     | 1174 | CYC  | C2A-C1A-NA  | -3.26 | 104.80      | 109.86   |
| 3   | D     | 1174 | CYC  | C4B-C3B-C2B | -3.26 | 106.19      | 108.05   |
| 3   | E     | 1163 | CYC  | CBD-CAD-C3D | -3.20 | 106.78      | 112.53   |
| 3   | D     | 1175 | CYC  | C3C-C2C-C1C | -3.20 | 100.73      | 103.41   |
| 3   | F     | 1175 | CYC  | CAB-C3B-C2B | -3.19 | 121.91      | 127.51   |
| 3   | P     | 1175 | CYC  | C2D-C1D-ND  | -3.19 | 105.07      | 110.29   |
| 3   | P     | 1175 | CYC  | C4B-C3B-C2B | -3.18 | 106.23      | 108.05   |
| 3   | F     | 1175 | CYC  | C3A-C4A-NA  | -3.15 | 103.37      | 110.55   |
| 3   | N     | 1174 | CYC  | C2A-C1A-NA  | -3.14 | 104.98      | 109.86   |
| 3   | K     | 1163 | CYC  | C1B-CHB-C4A | -3.14 | 119.93      | 128.06   |
| 3   | K     | 1163 | CYC  | CBC-CAC-C3C | -3.13 | 105.92      | 113.57   |
| 3   | M     | 1163 | CYC  | C2B-C1B-NB  | -3.10 | 102.50      | 107.00   |
| 3   | D     | 1174 | CYC  | CHA-C1A-NA  | -3.08 | 123.17      | 128.67   |
| 3   | B     | 1174 | CYC  | C4B-C3B-C2B | -3.06 | 106.30      | 108.05   |
| 3   | O     | 1163 | CYC  | C4B-C3B-C2B | -2.97 | 106.35      | 108.05   |
| 4   | B     | 1175 | PEB  | CAD-C3D-C2D | -2.96 | 118.48      | 128.41   |
| 4   | B     | 1175 | PEB  | C3B-C4B-NB  | -2.95 | 105.28      | 109.86   |
| 3   | O     | 1163 | CYC  | CBD-CAD-C3D | -2.94 | 107.26      | 112.53   |
| 3   | A     | 1163 | CYC  | OB-C4B-NB   | -2.88 | 117.50      | 125.14   |
| 4   | B     | 1175 | PEB  | CAB-C3B-C4B | -2.80 | 120.06      | 125.06   |
| 3   | O     | 1163 | CYC  | C1B-CHB-C4A | -2.80 | 120.82      | 128.06   |
| 3   | P     | 1174 | CYC  | C2B-C1B-NB  | -2.80 | 102.95      | 107.00   |
| 3   | L     | 1174 | CYC  | C1B-CHB-C4A | -2.78 | 120.86      | 128.06   |
| 3   | K     | 1163 | CYC  | C2D-C1D-ND  | -2.77 | 105.75      | 110.29   |
| 3   | O     | 1163 | CYC  | CMC-C2C-C1C | -2.76 | 106.64      | 112.43   |
| 3   | M     | 1163 | CYC  | C3A-C4A-NA  | -2.71 | 104.38      | 110.55   |
| 3   | N     | 1174 | CYC  | OC-C1C-C2C  | -2.68 | 124.09      | 126.25   |
| 3   | N     | 1174 | CYC  | OC-C1C-NC   | -2.67 | 121.60      | 124.83   |
| 3   | A     | 1163 | CYC  | C1B-CHB-C4A | -2.65 | 121.20      | 128.06   |
| 3   | D     | 1175 | CYC  | C3A-C4A-NA  | -2.64 | 104.54      | 110.55   |
| 3   | F     | 1175 | CYC  | C2A-C1A-NA  | -2.59 | 105.84      | 109.86   |
| 3   | B     | 1174 | CYC  | CMA-C3A-C2A | -2.59 | 118.43      | 125.94   |
| 3   | A     | 1163 | CYC  | CAD-C3D-C4D | -2.57 | 124.21      | 127.01   |
| 3   | L     | 1175 | CYC  | C3A-C4A-NA  | -2.56 | 104.71      | 110.55   |
| 3   | C     | 1163 | CYC  | CAD-C3D-C4D | -2.55 | 124.24      | 127.01   |
| 3   | A     | 1163 | CYC  | CMC-C2C-C1C | -2.53 | 107.10      | 112.43   |
| 3   | F     | 1174 | CYC  | CBB-CAB-C3B | -2.53 | 104.66      | 112.39   |
| 3   | F     | 1175 | CYC  | OC-C1C-NC   | -2.53 | 121.77      | 124.83   |
| 3   | O     | 1163 | CYC  | C2B-C1B-NB  | -2.53 | 103.33      | 107.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | P     | 1175 | CYC  | C3A-C4A-NA  | -2.52 | 104.81      | 110.55   |
| 3   | F     | 1175 | CYC  | C4B-C3B-C2B | -2.52 | 106.61      | 108.05   |
| 3   | L     | 1175 | CYC  | C3B-C4B-NB  | -2.52 | 104.45      | 106.74   |
| 3   | P     | 1175 | CYC  | C3C-C2C-C1C | -2.51 | 101.31      | 103.41   |
| 3   | L     | 1175 | CYC  | CAC-C3C-C4C | -2.49 | 106.28      | 112.67   |
| 3   | P     | 1174 | CYC  | C4B-C3B-C2B | -2.47 | 106.64      | 108.05   |
| 3   | F     | 1175 | CYC  | C1B-CHB-C4A | -2.46 | 121.69      | 128.06   |
| 3   | F     | 1174 | CYC  | CAD-CBD-CGD | -2.45 | 108.26      | 112.75   |
| 3   | L     | 1174 | CYC  | C3C-C2C-C1C | -2.44 | 101.37      | 103.41   |
| 3   | P     | 1174 | CYC  | CAD-C3D-C2D | -2.43 | 122.06      | 129.00   |
| 3   | N     | 1174 | CYC  | CAC-C3C-C2C | -2.43 | 108.03      | 114.13   |
| 3   | C     | 1163 | CYC  | C3A-C4A-NA  | -2.42 | 105.03      | 110.55   |
| 3   | P     | 1175 | CYC  | OC-C1C-NC   | -2.41 | 121.91      | 124.83   |
| 3   | P     | 1174 | CYC  | CAD-C3D-C4D | -2.41 | 124.39      | 127.01   |
| 4   | B     | 1175 | PEB  | CBD-CAD-C3D | -2.39 | 114.91      | 127.01   |
| 3   | L     | 1175 | CYC  | C3C-C2C-C1C | -2.36 | 101.43      | 103.41   |
| 3   | L     | 1174 | CYC  | C3B-C4B-NB  | -2.35 | 104.60      | 106.74   |
| 3   | P     | 1175 | CYC  | CAC-C3C-C4C | -2.32 | 106.72      | 112.67   |
| 3   | D     | 1174 | CYC  | C3C-C2C-C1C | -2.32 | 101.47      | 103.41   |
| 3   | F     | 1175 | CYC  | OB-C4B-C3B  | -2.31 | 125.33      | 128.09   |
| 3   | N     | 1175 | CYC  | CMC-C2C-C3C | -2.30 | 104.17      | 114.35   |
| 3   | P     | 1174 | CYC  | OC-C1C-NC   | -2.30 | 122.04      | 124.83   |
| 3   | K     | 1163 | CYC  | CMB-C2B-C1B | -2.29 | 121.16      | 124.20   |
| 3   | L     | 1175 | CYC  | C1B-CHB-C4A | -2.27 | 122.19      | 128.06   |
| 3   | C     | 1163 | CYC  | C1B-CHB-C4A | -2.26 | 122.21      | 128.06   |
| 3   | M     | 1163 | CYC  | C1B-CHB-C4A | -2.26 | 122.21      | 128.06   |
| 3   | O     | 1163 | CYC  | OC-C1C-NC   | -2.25 | 122.10      | 124.83   |
| 3   | B     | 1174 | CYC  | CBB-CAB-C3B | -2.25 | 105.53      | 112.39   |
| 3   | F     | 1175 | CYC  | C1B-NB-C4B  | -2.23 | 107.47      | 110.73   |
| 3   | D     | 1175 | CYC  | C1B-CHB-C4A | -2.23 | 122.29      | 128.06   |
| 3   | P     | 1175 | CYC  | CBB-CAB-C3B | -2.23 | 105.60      | 112.39   |
| 3   | L     | 1174 | CYC  | CBB-CAB-C3B | -2.22 | 105.62      | 112.39   |
| 3   | N     | 1175 | CYC  | CAA-CBA-CGA | -2.22 | 108.68      | 112.75   |
| 3   | N     | 1174 | CYC  | CAD-CBD-CGD | -2.20 | 108.70      | 112.75   |
| 3   | P     | 1174 | CYC  | CMC-C2C-C1C | -2.20 | 107.80      | 112.43   |
| 3   | B     | 1174 | CYC  | C2B-C1B-NB  | -2.18 | 103.84      | 107.00   |
| 3   | F     | 1175 | CYC  | CHB-C1B-C2B | -2.17 | 122.38      | 126.89   |
| 3   | N     | 1175 | CYC  | CAB-C3B-C2B | -2.17 | 123.71      | 127.51   |
| 3   | F     | 1174 | CYC  | C3C-C2C-C1C | -2.15 | 101.61      | 103.41   |
| 3   | E     | 1163 | CYC  | OC-C1C-NC   | -2.13 | 122.25      | 124.83   |
| 3   | L     | 1174 | CYC  | C2B-C1B-NB  | -2.12 | 103.94      | 107.00   |
| 3   | L     | 1174 | CYC  | CAB-C3B-C2B | -2.11 | 123.80      | 127.51   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 1163 | CYC  | C2B-C1B-NB  | -2.11 | 103.94      | 107.00   |
| 3   | A     | 1163 | CYC  | CHB-C4A-NA  | -2.09 | 120.92      | 124.91   |
| 3   | F     | 1175 | CYC  | CAA-C2A-C3A | -2.09 | 124.37      | 128.01   |
| 3   | O     | 1163 | CYC  | C3C-C4C-NC  | -2.09 | 105.84      | 107.93   |
| 3   | P     | 1175 | CYC  | C1B-CHB-C4A | -2.08 | 122.67      | 128.06   |
| 3   | C     | 1163 | CYC  | CHB-C4A-NA  | -2.08 | 120.96      | 124.91   |
| 3   | P     | 1175 | CYC  | CHA-C1A-NA  | -2.06 | 124.98      | 128.67   |
| 3   | E     | 1163 | CYC  | C3C-C2C-C1C | -2.06 | 101.69      | 103.41   |
| 3   | M     | 1163 | CYC  | CMD-C2D-C3D | -2.04 | 120.97      | 125.24   |
| 3   | P     | 1174 | CYC  | CHA-C1A-NA  | -2.02 | 125.05      | 128.67   |
| 3   | B     | 1174 | CYC  | OB-C4B-C3B  | -2.01 | 125.68      | 128.09   |
| 3   | D     | 1174 | CYC  | C2B-C1B-NB  | -2.01 | 104.09      | 107.00   |
| 3   | N     | 1174 | CYC  | CMC-C2C-C3C | -2.01 | 105.47      | 114.35   |
| 3   | N     | 1174 | CYC  | OB-C4B-NB   | 2.02  | 130.50      | 125.14   |
| 3   | C     | 1163 | CYC  | C2C-C3C-C4C | 2.04  | 104.95      | 101.50   |
| 3   | N     | 1174 | CYC  | CHB-C4A-C3A | 2.04  | 129.86      | 124.88   |
| 3   | C     | 1163 | CYC  | C3B-C4B-NB  | 2.04  | 108.59      | 106.74   |
| 3   | P     | 1174 | CYC  | C1B-NB-C4B  | 2.06  | 113.75      | 110.73   |
| 3   | N     | 1175 | CYC  | C1A-NA-C4A  | 2.09  | 110.66      | 106.51   |
| 4   | B     | 1175 | PEB  | CAD-C3D-C4D | 2.11  | 130.56      | 123.49   |
| 3   | D     | 1174 | CYC  | CAD-CBD-CGD | 2.11  | 116.62      | 112.75   |
| 4   | B     | 1175 | PEB  | C3A-C4A-NA  | 2.12  | 110.05      | 107.93   |
| 3   | D     | 1175 | CYC  | C1A-C2A-C3A | 2.14  | 109.21      | 106.81   |
| 3   | L     | 1174 | CYC  | CMB-C2B-C1B | 2.17  | 127.08      | 124.20   |
| 4   | B     | 1175 | PEB  | CAB-C3B-C2B | 2.21  | 131.87      | 128.01   |
| 3   | K     | 1163 | CYC  | CHB-C1B-NB  | 2.22  | 130.97      | 126.16   |
| 3   | K     | 1163 | CYC  | C1A-NA-C4A  | 2.26  | 110.97      | 106.51   |
| 3   | O     | 1163 | CYC  | C1B-NB-C4B  | 2.26  | 114.04      | 110.73   |
| 3   | A     | 1163 | CYC  | CAC-C3C-C2C | 2.27  | 119.84      | 114.13   |
| 3   | D     | 1174 | CYC  | CMA-C3A-C4A | 2.32  | 128.83      | 125.06   |
| 3   | C     | 1163 | CYC  | CHB-C4A-C3A | 2.32  | 130.55      | 124.88   |
| 3   | F     | 1175 | CYC  | C1A-NA-C4A  | 2.37  | 111.21      | 106.51   |
| 3   | F     | 1174 | CYC  | C1B-NB-C4B  | 2.39  | 114.24      | 110.73   |
| 3   | L     | 1175 | CYC  | CBC-CAC-C3C | 2.42  | 119.48      | 113.57   |
| 3   | P     | 1175 | CYC  | CBC-CAC-C3C | 2.42  | 119.49      | 113.57   |
| 3   | P     | 1174 | CYC  | CBC-CAC-C3C | 2.45  | 119.56      | 113.57   |
| 3   | P     | 1175 | CYC  | C2C-C1C-NC  | 2.50  | 110.68      | 108.30   |
| 3   | L     | 1174 | CYC  | C1A-NA-C4A  | 2.51  | 111.48      | 106.51   |
| 3   | E     | 1163 | CYC  | C3C-C4C-NC  | 2.52  | 110.45      | 107.93   |
| 3   | F     | 1175 | CYC  | C4A-C3A-C2A | 2.55  | 109.56      | 106.50   |
| 3   | C     | 1163 | CYC  | CMB-C2B-C1B | 2.55  | 127.60      | 124.20   |
| 3   | D     | 1174 | CYC  | C4A-C3A-C2A | 2.59  | 109.61      | 106.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3   | C     | 1163 | CYC  | CMA-C3A-C4A | 2.60 | 129.29      | 125.06   |
| 3   | E     | 1163 | CYC  | CAC-C3C-C4C | 2.60 | 119.36      | 112.67   |
| 3   | N     | 1174 | CYC  | C4A-C3A-C2A | 2.61 | 109.63      | 106.50   |
| 3   | D     | 1175 | CYC  | C2C-C1C-NC  | 2.62 | 110.81      | 108.30   |
| 3   | L     | 1175 | CYC  | CAD-C3D-C4D | 2.62 | 129.86      | 127.01   |
| 3   | N     | 1174 | CYC  | CMA-C3A-C4A | 2.64 | 129.35      | 125.06   |
| 3   | O     | 1163 | CYC  | CHB-C4A-C3A | 2.65 | 131.35      | 124.88   |
| 3   | B     | 1174 | CYC  | C3C-C2C-C1C | 2.68 | 105.66      | 103.41   |
| 3   | N     | 1174 | CYC  | C2C-C3C-C4C | 2.68 | 106.04      | 101.50   |
| 3   | P     | 1174 | CYC  | C4A-C3A-C2A | 2.70 | 109.74      | 106.50   |
| 3   | B     | 1174 | CYC  | C1B-NB-C4B  | 2.71 | 114.70      | 110.73   |
| 3   | D     | 1174 | CYC  | CHB-C1B-C2B | 2.73 | 132.58      | 126.89   |
| 3   | L     | 1174 | CYC  | CHB-C4A-C3A | 2.80 | 131.72      | 124.88   |
| 3   | L     | 1175 | CYC  | C4B-C3B-C2B | 2.84 | 109.67      | 108.05   |
| 3   | F     | 1174 | CYC  | CAB-C3B-C4B | 2.86 | 124.01      | 121.51   |
| 3   | L     | 1174 | CYC  | CAC-C3C-C4C | 2.87 | 120.05      | 112.67   |
| 3   | M     | 1163 | CYC  | OB-C4B-C3B  | 2.92 | 131.60      | 128.09   |
| 3   | M     | 1163 | CYC  | CHB-C4A-C3A | 2.94 | 132.04      | 124.88   |
| 3   | D     | 1175 | CYC  | C3B-C4B-NB  | 2.94 | 109.41      | 106.74   |
| 3   | N     | 1175 | CYC  | OB-C4B-C3B  | 2.96 | 131.65      | 128.09   |
| 3   | M     | 1163 | CYC  | CAC-C3C-C4C | 3.00 | 120.38      | 112.67   |
| 3   | P     | 1174 | CYC  | C1B-C2B-C3B | 3.00 | 111.02      | 107.81   |
| 3   | A     | 1163 | CYC  | C1A-NA-C4A  | 3.01 | 112.47      | 106.51   |
| 3   | B     | 1174 | CYC  | CHB-C4A-C3A | 3.03 | 132.26      | 124.88   |
| 3   | A     | 1163 | CYC  | CMA-C3A-C4A | 3.11 | 130.12      | 125.06   |
| 3   | L     | 1174 | CYC  | C1B-NB-C4B  | 3.12 | 115.30      | 110.73   |
| 3   | D     | 1174 | CYC  | C2C-C1C-NC  | 3.18 | 111.33      | 108.30   |
| 3   | D     | 1175 | CYC  | C1B-C2B-C3B | 3.20 | 111.23      | 107.81   |
| 3   | O     | 1163 | CYC  | CAC-C3C-C4C | 3.20 | 120.90      | 112.67   |
| 3   | L     | 1175 | CYC  | C1A-NA-C4A  | 3.23 | 112.90      | 106.51   |
| 3   | D     | 1175 | CYC  | C1A-NA-C4A  | 3.24 | 112.93      | 106.51   |
| 3   | F     | 1175 | CYC  | CBC-CAC-C3C | 3.28 | 121.59      | 113.57   |
| 3   | B     | 1174 | CYC  | C2C-C1C-NC  | 3.31 | 111.46      | 108.30   |
| 4   | B     | 1175 | PEB  | C2A-C1A-NA  | 3.33 | 111.48      | 108.30   |
| 3   | F     | 1175 | CYC  | CAA-CBA-CGA | 3.37 | 118.92      | 112.75   |
| 3   | M     | 1163 | CYC  | C1B-NB-C4B  | 3.42 | 115.74      | 110.73   |
| 3   | F     | 1175 | CYC  | C2C-C1C-NC  | 3.44 | 111.58      | 108.30   |
| 3   | N     | 1174 | CYC  | CAB-C3B-C4B | 3.46 | 124.53      | 121.51   |
| 3   | P     | 1174 | CYC  | C1A-NA-C4A  | 3.49 | 113.42      | 106.51   |
| 3   | F     | 1175 | CYC  | CAD-CBD-CGD | 3.50 | 119.15      | 112.75   |
| 3   | P     | 1175 | CYC  | C1A-NA-C4A  | 3.52 | 113.47      | 106.51   |
| 4   | B     | 1175 | PEB  | CHA-C1B-C2B | 3.56 | 133.56      | 124.88   |

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| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3   | C     | 1163 | CYC  | CAC-C3C-C4C | 3.58 | 121.87      | 112.67   |
| 3   | K     | 1163 | CYC  | C1B-NB-C4B  | 3.59 | 115.98      | 110.73   |
| 3   | P     | 1174 | CYC  | C3C-C4C-NC  | 3.63 | 111.56      | 107.93   |
| 3   | A     | 1163 | CYC  | C2C-C1C-NC  | 3.65 | 111.79      | 108.30   |
| 3   | M     | 1163 | CYC  | C1B-C2B-C3B | 3.67 | 111.73      | 107.81   |
| 3   | N     | 1175 | CYC  | OC-C1C-C2C  | 3.68 | 129.23      | 126.25   |
| 3   | E     | 1163 | CYC  | CMB-C2B-C1B | 3.70 | 129.12      | 124.20   |
| 3   | F     | 1175 | CYC  | C3C-C4C-NC  | 3.73 | 111.67      | 107.93   |
| 3   | O     | 1163 | CYC  | C1A-NA-C4A  | 3.78 | 113.98      | 106.51   |
| 3   | D     | 1174 | CYC  | C3C-C4C-NC  | 3.81 | 111.75      | 107.93   |
| 3   | L     | 1174 | CYC  | CAB-C3B-C4B | 3.84 | 124.86      | 121.51   |
| 3   | A     | 1163 | CYC  | CHB-C4A-C3A | 3.86 | 134.31      | 124.88   |
| 4   | B     | 1175 | PEB  | C4B-NB-C1B  | 3.89 | 114.21      | 106.51   |
| 4   | B     | 1175 | PEB  | C1B-C2B-C3B | 3.90 | 111.18      | 106.50   |
| 3   | D     | 1174 | CYC  | CAB-C3B-C4B | 3.99 | 125.00      | 121.51   |
| 3   | L     | 1174 | CYC  | C4A-C3A-C2A | 4.03 | 111.33      | 106.50   |
| 3   | K     | 1163 | CYC  | CMC-C2C-C1C | 4.19 | 121.22      | 112.43   |
| 3   | N     | 1174 | CYC  | CMB-C2B-C1B | 4.25 | 129.86      | 124.20   |
| 3   | K     | 1163 | CYC  | CHB-C4A-C3A | 4.27 | 135.31      | 124.88   |
| 3   | N     | 1175 | CYC  | C2C-C1C-NC  | 4.30 | 112.41      | 108.30   |
| 3   | E     | 1163 | CYC  | C1B-NB-C4B  | 4.33 | 117.08      | 110.73   |
| 3   | E     | 1163 | CYC  | CHB-C4A-C3A | 4.35 | 135.49      | 124.88   |
| 3   | B     | 1174 | CYC  | C1A-NA-C4A  | 4.37 | 115.15      | 106.51   |
| 3   | D     | 1174 | CYC  | CHB-C4A-C3A | 4.42 | 135.67      | 124.88   |
| 3   | L     | 1174 | CYC  | C3C-C4C-NC  | 4.49 | 112.42      | 107.93   |
| 3   | B     | 1174 | CYC  | CMA-C3A-C4A | 4.52 | 132.41      | 125.06   |
| 3   | A     | 1163 | CYC  | CAC-C3C-C4C | 4.66 | 124.64      | 112.67   |
| 3   | L     | 1174 | CYC  | C2C-C1C-NC  | 4.75 | 112.83      | 108.30   |
| 3   | D     | 1174 | CYC  | C1A-NA-C4A  | 4.79 | 115.98      | 106.51   |
| 3   | A     | 1163 | CYC  | OB-C4B-C3B  | 4.90 | 133.97      | 128.09   |
| 3   | P     | 1174 | CYC  | CAB-C3B-C4B | 5.11 | 125.98      | 121.51   |
| 3   | M     | 1163 | CYC  | C2C-C1C-NC  | 5.12 | 113.19      | 108.30   |
| 3   | P     | 1175 | CYC  | CHB-C4A-C3A | 5.16 | 137.48      | 124.88   |
| 4   | B     | 1175 | PEB  | CHC-C4C-C3C | 5.17 | 139.13      | 130.41   |
| 3   | C     | 1163 | CYC  | C2C-C1C-NC  | 5.19 | 113.26      | 108.30   |
| 3   | L     | 1175 | CYC  | C2C-C1C-NC  | 5.26 | 113.32      | 108.30   |
| 3   | E     | 1163 | CYC  | C2C-C1C-NC  | 5.33 | 113.39      | 108.30   |
| 3   | C     | 1163 | CYC  | CAB-C3B-C4B | 5.33 | 126.17      | 121.51   |
| 3   | O     | 1163 | CYC  | CAB-C3B-C4B | 5.45 | 126.27      | 121.51   |
| 3   | O     | 1163 | CYC  | C2C-C1C-NC  | 5.70 | 113.75      | 108.30   |
| 3   | D     | 1175 | CYC  | CHB-C4A-C3A | 5.72 | 138.83      | 124.88   |
| 3   | L     | 1175 | CYC  | CHB-C4A-C3A | 5.93 | 139.36      | 124.88   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | F     | 1174 | CYC  | C1A-NA-C4A  | 5.95  | 118.28      | 106.51   |
| 3   | N     | 1175 | CYC  | CHB-C4A-C3A | 6.09  | 139.74      | 124.88   |
| 3   | N     | 1174 | CYC  | C1A-NA-C4A  | 6.22  | 118.81      | 106.51   |
| 3   | N     | 1174 | CYC  | C2C-C1C-NC  | 6.29  | 114.31      | 108.30   |
| 3   | K     | 1163 | CYC  | OC-C1C-C2C  | 6.75  | 131.71      | 126.25   |
| 3   | F     | 1175 | CYC  | CHB-C4A-C3A | 6.98  | 141.91      | 124.88   |
| 3   | P     | 1174 | CYC  | C2C-C1C-NC  | 7.09  | 115.07      | 108.30   |
| 3   | F     | 1174 | CYC  | C2C-C1C-NC  | 7.89  | 115.83      | 108.30   |
| 3   | F     | 1175 | CYC  | CAB-C3B-C4B | 8.08  | 128.57      | 121.51   |
| 3   | N     | 1175 | CYC  | CAB-C3B-C4B | 8.08  | 128.57      | 121.51   |
| 3   | E     | 1163 | CYC  | CAB-C3B-C4B | 8.08  | 128.57      | 121.51   |
| 3   | K     | 1163 | CYC  | CAB-C3B-C4B | 8.22  | 128.69      | 121.51   |
| 3   | M     | 1163 | CYC  | CAB-C3B-C4B | 9.12  | 129.48      | 121.51   |
| 3   | A     | 1163 | CYC  | CAB-C3B-C4B | 9.60  | 129.89      | 121.51   |
| 3   | L     | 1175 | CYC  | CAB-C3B-C4B | 9.69  | 129.97      | 121.51   |
| 3   | D     | 1175 | CYC  | CAB-C3B-C4B | 17.95 | 137.18      | 121.51   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 4   | B     | 1175 | PEB  | C1D  |

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | P     | 1174 | CYC  | C1B-CHB-C4A-C3A |
| 3   | N     | 1174 | CYC  | C1B-CHB-C4A-C3A |
| 3   | B     | 1174 | CYC  | C1B-CHB-C4A-C3A |
| 3   | F     | 1174 | CYC  | C1B-CHB-C4A-C3A |
| 3   | F     | 1175 | CYC  | C1B-CHB-C4A-C3A |
| 3   | D     | 1175 | CYC  | C1B-CHB-C4A-C3A |
| 3   | C     | 1163 | CYC  | C1B-CHB-C4A-C3A |
| 3   | O     | 1163 | CYC  | C1B-CHB-C4A-C3A |
| 3   | D     | 1174 | CYC  | C1B-CHB-C4A-C3A |
| 3   | A     | 1163 | CYC  | C1B-CHB-C4A-C3A |
| 3   | K     | 1163 | CYC  | C1B-CHB-C4A-C3A |
| 3   | L     | 1174 | CYC  | C1B-CHB-C4A-C3A |
| 3   | M     | 1163 | CYC  | C1B-CHB-C4A-C3A |
| 3   | L     | 1175 | CYC  | C1B-CHB-C4A-C3A |
| 3   | P     | 1175 | CYC  | C1B-CHB-C4A-C3A |
| 3   | F     | 1175 | CYC  | C1B-CHB-C4A-NA  |
| 3   | N     | 1175 | CYC  | C1B-CHB-C4A-NA  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | E     | 1163 | CYC  | C1B-CHB-C4A-C3A |
| 3   | D     | 1175 | CYC  | C1B-CHB-C4A-NA  |
| 3   | N     | 1175 | CYC  | C1B-CHB-C4A-C3A |
| 4   | B     | 1175 | PEB  | C4A-CHA-C1B-NB  |
| 3   | L     | 1175 | CYC  | C1B-CHB-C4A-NA  |
| 3   | P     | 1175 | CYC  | C1B-CHB-C4A-NA  |
| 3   | E     | 1163 | CYC  | C1B-CHB-C4A-NA  |
| 3   | K     | 1163 | CYC  | C1B-CHB-C4A-NA  |
| 3   | P     | 1174 | CYC  | C1B-CHB-C4A-NA  |
| 3   | N     | 1174 | CYC  | C1B-CHB-C4A-NA  |
| 3   | M     | 1163 | CYC  | C1B-CHB-C4A-NA  |
| 3   | B     | 1174 | CYC  | C1B-CHB-C4A-NA  |
| 4   | B     | 1175 | PEB  | C4A-CHA-C1B-C2B |
| 3   | A     | 1163 | CYC  | C1B-CHB-C4A-NA  |
| 3   | F     | 1174 | CYC  | C1B-CHB-C4A-NA  |
| 3   | L     | 1174 | CYC  | C1B-CHB-C4A-NA  |
| 3   | O     | 1163 | CYC  | C1B-CHB-C4A-NA  |
| 3   | C     | 1163 | CYC  | C1B-CHB-C4A-NA  |
| 3   | D     | 1174 | CYC  | C1B-CHB-C4A-NA  |

There are no ring outliers.

18 monomers are involved in 93 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 1163 | CYC  | 6       | 0            |
| 3   | B     | 1174 | CYC  | 4       | 0            |
| 4   | B     | 1175 | PEB  | 2       | 0            |
| 3   | C     | 1163 | CYC  | 9       | 0            |
| 3   | D     | 1174 | CYC  | 7       | 0            |
| 3   | D     | 1175 | CYC  | 4       | 0            |
| 3   | E     | 1163 | CYC  | 7       | 0            |
| 3   | F     | 1174 | CYC  | 5       | 0            |
| 3   | F     | 1175 | CYC  | 3       | 0            |
| 3   | K     | 1163 | CYC  | 7       | 0            |
| 3   | L     | 1174 | CYC  | 6       | 0            |
| 3   | L     | 1175 | CYC  | 5       | 0            |
| 3   | M     | 1163 | CYC  | 5       | 0            |
| 3   | N     | 1174 | CYC  | 4       | 0            |
| 3   | N     | 1175 | CYC  | 3       | 0            |
| 3   | O     | 1163 | CYC  | 7       | 0            |
| 3   | P     | 1174 | CYC  | 5       | 0            |
| 3   | P     | 1175 | CYC  | 4       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 162/162 (100%)  | -0.10  | 11 (6%) 20 22 | 16, 23, 76, 94        | 0     |
| 1   | C     | 162/162 (100%)  | 0.10   | 12 (7%) 17 18 | 17, 26, 80, 98        | 0     |
| 1   | E     | 162/162 (100%)  | 0.10   | 12 (7%) 17 18 | 15, 21, 75, 102       | 0     |
| 1   | K     | 162/162 (100%)  | 0.20   | 12 (7%) 17 18 | 14, 21, 74, 98        | 0     |
| 1   | M     | 162/162 (100%)  | -0.22  | 12 (7%) 17 18 | 14, 22, 71, 96        | 0     |
| 1   | O     | 162/162 (100%)  | 0.09   | 12 (7%) 17 18 | 17, 26, 79, 96        | 0     |
| 2   | B     | 171/172 (99%)   | -0.48  | 0 100 100     | 14, 22, 36, 46        | 0     |
| 2   | D     | 171/172 (99%)   | -0.41  | 3 (1%) 71 72  | 15, 25, 39, 52        | 0     |
| 2   | F     | 171/172 (99%)   | -0.38  | 5 (2%) 55 56  | 17, 28, 41, 58        | 0     |
| 2   | L     | 171/172 (99%)   | -0.52  | 0 100 100     | 16, 24, 40, 49        | 0     |
| 2   | N     | 171/172 (99%)   | -0.44  | 0 100 100     | 14, 21, 34, 40        | 0     |
| 2   | P     | 171/172 (99%)   | -0.29  | 5 (2%) 55 56  | 17, 28, 46, 57        | 0     |
| All | All   | 1998/2004 (99%) | -0.20  | 84 (4%) 40 41 | 14, 24, 49, 102       | 0     |

All (84) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 75  | ALA  | 11.3 |
| 1   | K     | 72  | PRO  | 10.6 |
| 1   | C     | 67  | THR  | 10.2 |
| 1   | A     | 74  | TYR  | 10.0 |
| 1   | E     | 71  | GLY  | 9.8  |
| 1   | C     | 73  | ASN  | 9.7  |
| 1   | A     | 69  | MET  | 9.3  |
| 1   | A     | 70  | GLN  | 9.3  |
| 1   | C     | 70  | GLN  | 9.1  |
| 1   | O     | 66  | THR  | 9.0  |
| 1   | C     | 74  | TYR  | 9.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 69  | MET  | 8.9  |
| 1   | O     | 68  | GLN  | 8.9  |
| 1   | O     | 69  | MET  | 8.7  |
| 1   | K     | 67  | THR  | 8.7  |
| 1   | M     | 68  | GLN  | 8.5  |
| 1   | C     | 75  | ALA  | 8.4  |
| 1   | O     | 71  | GLY  | 8.4  |
| 1   | K     | 73  | ASN  | 8.2  |
| 1   | E     | 74  | TYR  | 7.8  |
| 1   | C     | 76  | ALA  | 7.7  |
| 1   | C     | 68  | GLN  | 7.7  |
| 1   | A     | 71  | GLY  | 7.7  |
| 1   | K     | 68  | GLN  | 7.7  |
| 1   | C     | 71  | GLY  | 7.6  |
| 1   | O     | 67  | THR  | 7.4  |
| 1   | O     | 75  | ALA  | 7.4  |
| 1   | K     | 74  | TYR  | 7.1  |
| 1   | A     | 68  | GLN  | 7.1  |
| 1   | O     | 72  | PRO  | 7.1  |
| 1   | M     | 69  | MET  | 7.0  |
| 1   | A     | 73  | ASN  | 6.9  |
| 1   | K     | 69  | MET  | 6.9  |
| 1   | O     | 70  | GLN  | 6.8  |
| 1   | E     | 70  | GLN  | 6.7  |
| 1   | A     | 75  | ALA  | 6.7  |
| 1   | O     | 73  | ASN  | 6.7  |
| 1   | O     | 76  | ALA  | 6.6  |
| 1   | M     | 72  | PRO  | 6.5  |
| 1   | E     | 75  | ALA  | 6.5  |
| 1   | M     | 70  | GLN  | 6.5  |
| 1   | E     | 68  | GLN  | 6.5  |
| 1   | O     | 65  | TYR  | 6.4  |
| 1   | E     | 73  | ASN  | 6.3  |
| 1   | C     | 69  | MET  | 6.2  |
| 1   | O     | 74  | TYR  | 6.1  |
| 1   | A     | 65  | TYR  | 6.0  |
| 1   | M     | 65  | TYR  | 5.9  |
| 1   | K     | 65  | TYR  | 5.9  |
| 1   | E     | 67  | THR  | 5.9  |
| 1   | E     | 65  | TYR  | 5.7  |
| 1   | C     | 65  | TYR  | 5.6  |
| 1   | K     | 71  | GLY  | 5.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 76  | ALA  | 5.4  |
| 1   | M     | 71  | GLY  | 5.2  |
| 1   | K     | 76  | ALA  | 5.1  |
| 1   | E     | 66  | THR  | 5.1  |
| 1   | M     | 75  | ALA  | 4.9  |
| 1   | A     | 72  | PRO  | 4.7  |
| 1   | E     | 72  | PRO  | 4.7  |
| 1   | A     | 67  | THR  | 4.6  |
| 1   | C     | 66  | THR  | 4.6  |
| 1   | K     | 70  | GLN  | 4.4  |
| 1   | C     | 72  | PRO  | 4.0  |
| 1   | M     | 67  | THR  | 4.0  |
| 1   | M     | 74  | TYR  | 3.9  |
| 1   | M     | 76  | ALA  | 3.9  |
| 1   | M     | 66  | THR  | 3.8  |
| 1   | M     | 73  | ASN  | 3.7  |
| 1   | K     | 66  | THR  | 3.5  |
| 2   | P     | 111 | ASN  | 3.4  |
| 1   | E     | 76  | ALA  | 3.2  |
| 2   | P     | 118 | GLN  | 2.9  |
| 2   | F     | 111 | ASN  | 2.8  |
| 2   | F     | 115 | GLU  | 2.8  |
| 2   | P     | 172 | SER  | 2.6  |
| 2   | D     | 118 | GLN  | 2.5  |
| 2   | F     | 109 | CYS  | 2.3  |
| 2   | D     | 172 | SER  | 2.3  |
| 2   | F     | 172 | SER  | 2.2  |
| 2   | P     | 107 | ASP  | 2.2  |
| 2   | P     | 114 | ARG  | 2.1  |
| 2   | D     | 109 | CYS  | 2.1  |
| 2   | F     | 120 | LEU  | 2.0  |

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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2   | MEN  | L     | 72  | 9/10  | 0.98 | 0.08 | -    | 16,20,24,25                 | 0     |
| 2   | MEN  | F     | 72  | 9/10  | 0.99 | 0.09 | -    | 21,26,27,34                 | 0     |
| 2   | MEN  | B     | 72  | 9/10  | 0.98 | 0.06 | -    | 14,18,22,23                 | 0     |
| 2   | MEN  | D     | 72  | 9/10  | 0.97 | 0.10 | -    | 19,23,25,27                 | 0     |
| 2   | MEN  | P     | 72  | 9/10  | 0.98 | 0.08 | -    | 21,22,25,26                 | 0     |
| 2   | MEN  | N     | 72  | 9/10  | 0.97 | 0.08 | -    | 16,19,23,27                 | 0     |

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3   | CYC  | F     | 1174 | 43/43 | 0.95 | 0.13 | 0.45  | 16,29,45,49                 | 0     |
| 3   | CYC  | P     | 1174 | 43/43 | 0.94 | 0.13 | 0.40  | 19,29,44,47                 | 0     |
| 3   | CYC  | N     | 1174 | 43/43 | 0.96 | 0.10 | 0.32  | 9,24,38,44                  | 0     |
| 3   | CYC  | P     | 1175 | 43/43 | 0.94 | 0.10 | 0.32  | 20,31,49,52                 | 0     |
| 3   | CYC  | F     | 1175 | 43/43 | 0.96 | 0.10 | 0.25  | 14,24,41,63                 | 0     |
| 3   | CYC  | D     | 1174 | 43/43 | 0.96 | 0.11 | 0.21  | 13,34,47,53                 | 0     |
| 3   | CYC  | L     | 1174 | 43/43 | 0.95 | 0.10 | 0.19  | 15,31,40,49                 | 0     |
| 3   | CYC  | B     | 1174 | 43/43 | 0.95 | 0.10 | 0.15  | 9,21,35,39                  | 0     |
| 3   | CYC  | L     | 1175 | 43/43 | 0.95 | 0.10 | -0.02 | 17,24,40,52                 | 0     |
| 3   | CYC  | N     | 1175 | 43/43 | 0.96 | 0.09 | -0.07 | 14,24,51,59                 | 0     |
| 3   | CYC  | E     | 1163 | 43/43 | 0.96 | 0.12 | -0.34 | 12,18,28,38                 | 0     |
| 3   | CYC  | K     | 1163 | 43/43 | 0.97 | 0.12 | -0.35 | 13,20,29,36                 | 0     |
| 3   | CYC  | M     | 1163 | 43/43 | 0.97 | 0.08 | -0.42 | 15,23,32,40                 | 0     |
| 3   | CYC  | A     | 1163 | 43/43 | 0.96 | 0.08 | -0.43 | 14,25,39,46                 | 0     |
| 3   | CYC  | C     | 1163 | 43/43 | 0.97 | 0.08 | -0.45 | 13,22,35,37                 | 0     |
| 3   | CYC  | D     | 1175 | 43/43 | 0.96 | 0.08 | -0.46 | 14,23,38,56                 | 0     |
| 3   | CYC  | O     | 1163 | 43/43 | 0.96 | 0.08 | -0.47 | 14,23,37,45                 | 0     |
| 4   | PEB  | B     | 1175 | 43/43 | 0.97 | 0.08 | -0.72 | 11,22,44,52                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.