



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:08 am GMT

PDB ID : 4FM4  
Title : Wild Type Fe-type Nitrile Hydratase from *Comamonas testosteroni* N1  
Authors : Kuhn, M.L.; Martinez, S.; Gumataotao, N.; Bornscheuer, U.; Liu, D.; Holz, R.C.  
Deposited on : 2012-06-15  
Resolution : 2.38 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

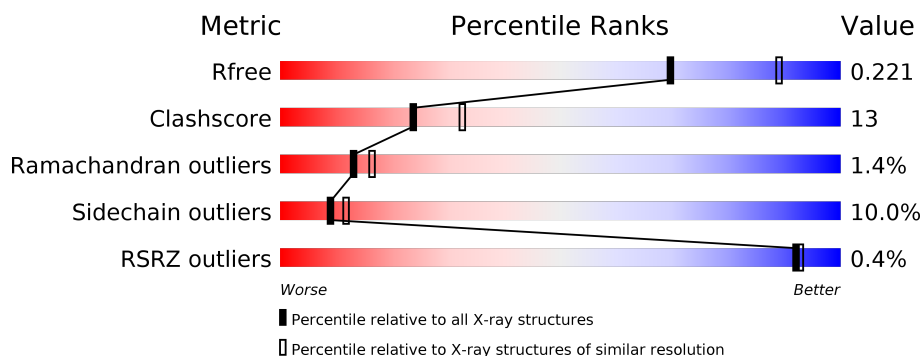
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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.











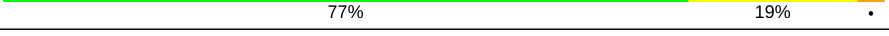

| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 4388 (2.40-2.36)                                      |
| Clashscore            | 112137                      | 4984 (2.40-2.36)                                      |
| Ramachandran outliers | 110173                      | 4907 (2.40-2.36)                                      |
| Sidechain outliers    | 110143                      | 4909 (2.40-2.36)                                      |
| RSRZ outliers         | 101464                      | 4423 (2.40-2.36)                                      |

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     | 209    | <div> <div>71%</div> <div>21%</div> <div>7%</div> <div>.</div> </div> |
| 1   | C     | 209    | <div> <div>69%</div> <div>24%</div> <div>6%</div> <div>.</div> </div> |
| 1   | E     | 209    | <div> <div>72%</div> <div>22%</div> <div>5%</div> <div>.</div> </div> |
| 1   | G     | 209    | <div> <div>72%</div> <div>22%</div> <div>5%</div> <div>.</div> </div> |
| 1   | I     | 209    | <div> <div>71%</div> <div>23%</div> <div>.</div> <div>.</div> </div>  |
| 1   | K     | 209    | <div> <div>73%</div> <div>20%</div> <div>5%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | M     | 209    |  71% 22% 5% • |
| 1   | O     | 209    |  74% 18% 7% • |
| 2   | B     | 206    |  79% 18% •    |
| 2   | D     | 206    |  75% 20% •    |
| 2   | F     | 206    |  76% 19% •    |
| 2   | H     | 206    |  81% 14% •    |
| 2   | J     | 206    |  75% 20% •    |
| 2   | L     | 206    |  76% 20% •    |
| 2   | N     | 206    |  77% 19% •    |
| 2   | P     | 206    |  75% 21% •    |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1   | CSD  | E     | 104 | -         | -        | X       | -                |
| 3   | PO4  | O     | 301 | -         | -        | -       | X                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27326 atoms, of which 8 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 Nitrile hydratase alpha subunit.

| Mol | Chain | Residues | Atoms |      |   |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|---|-----|-----|---|---------|---------|-------|
| 1   | A     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | C     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | E     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | G     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | I     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | K     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | M     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |
| 1   | O     | 206      | Total | C    | H | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1610  | 1026 | 1 | 268 | 306 | 9 |         |         |       |

- Molecule 2 is a protein called Nitrile hydratase beta subunit.

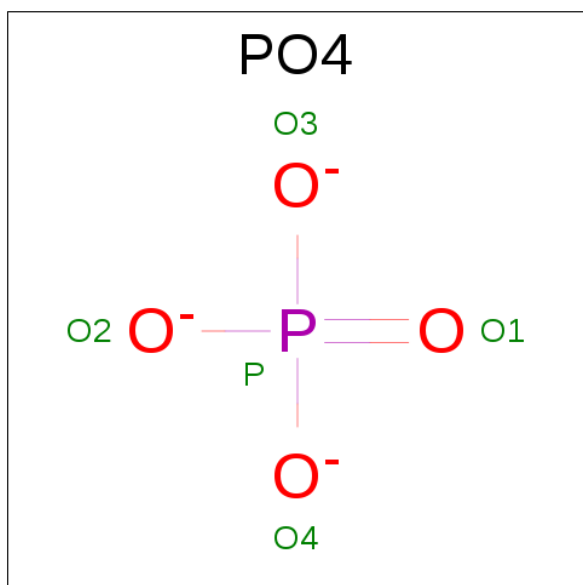
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |
| 2   | D     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |
| 2   | F     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |
| 2   | H     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |
| 2   | J     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |
| 2   | L     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | N     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |
| 2   | P     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1589  | 1017 | 271 | 293 | 8 |         |         |       |

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | I     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | K     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | M     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | O     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | G     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | K     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | E     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | I     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | A     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | O     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 4   | M     | 1        | Total Fe<br>1 1 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 98       | Total O<br>98 98   | 0       | 0       |
| 5   | B     | 113      | Total O<br>113 113 | 0       | 0       |
| 5   | C     | 91       | Total O<br>91 91   | 0       | 0       |
| 5   | D     | 106      | Total O<br>106 106 | 0       | 0       |
| 5   | E     | 107      | Total O<br>107 107 | 0       | 0       |
| 5   | F     | 112      | Total O<br>112 112 | 0       | 0       |
| 5   | G     | 93       | Total O<br>93 93   | 0       | 0       |
| 5   | H     | 110      | Total O<br>110 110 | 0       | 0       |
| 5   | I     | 108      | Total O<br>108 108 | 0       | 0       |
| 5   | J     | 92       | Total O<br>92 92   | 0       | 0       |
| 5   | K     | 113      | Total O<br>113 113 | 0       | 0       |
| 5   | L     | 122      | Total O<br>122 122 | 0       | 0       |

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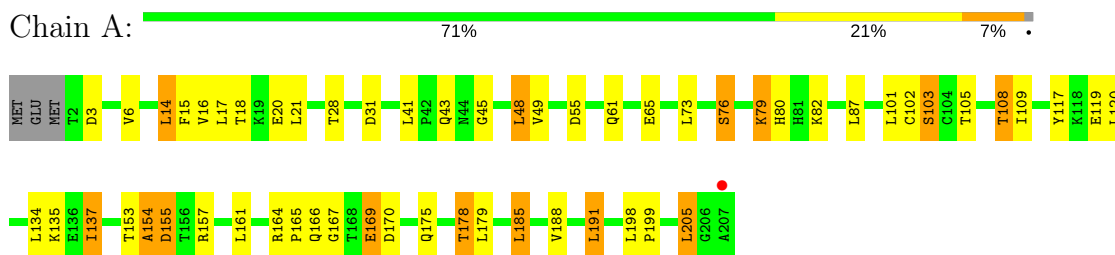
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | M     | 99       | Total<br>99  | O<br>99  | 0       | 0       |
| 5   | N     | 104      | Total<br>104 | O<br>104 | 0       | 0       |
| 5   | O     | 115      | Total<br>115 | O<br>115 | 0       | 0       |
| 5   | P     | 103      | Total<br>103 | O<br>103 | 0       | 0       |

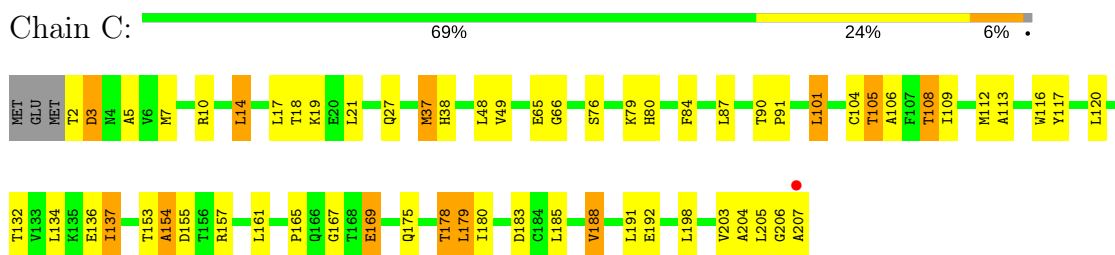
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

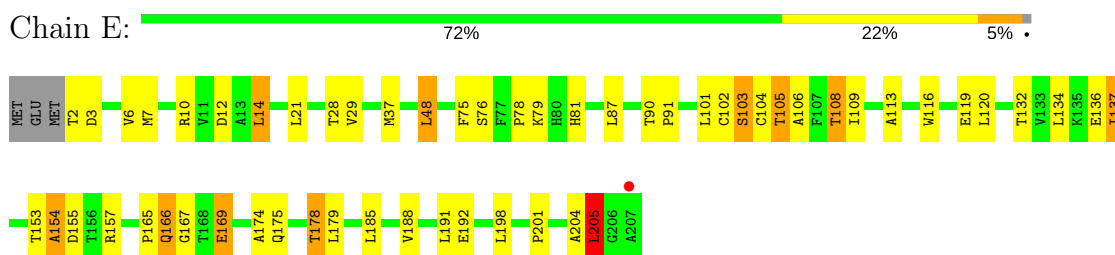
#### • Molecule 1: Nitrile hydratase alpha subunit



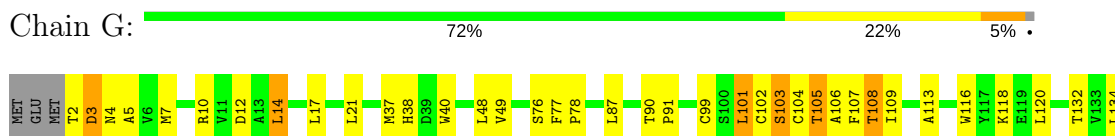
#### • Molecule 1: Nitrile hydratase alpha subunit



#### • Molecule 1: Nitrile hydratase alpha subunit



#### • Molecule 1: Nitrile hydratase alpha subunit

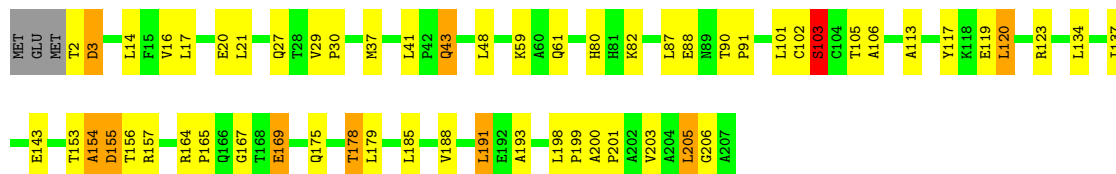






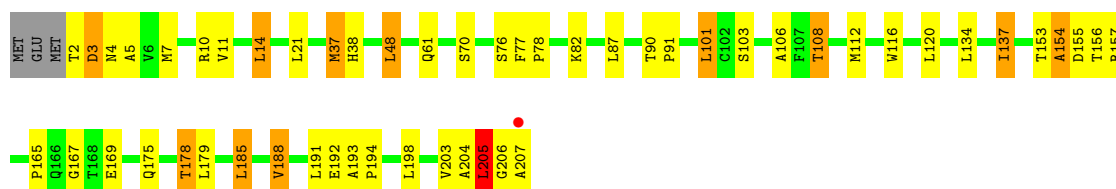
• Molecule 1: Nitrile hydratase alpha subunit

Chain I: 71% 23% . .



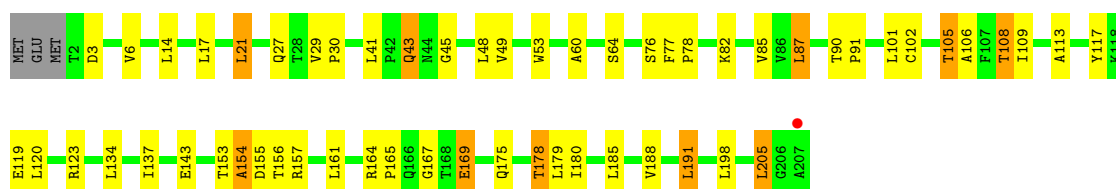
• Molecule 1: Nitrile hydratase alpha subunit

Chain K: 73% 20% 5% .



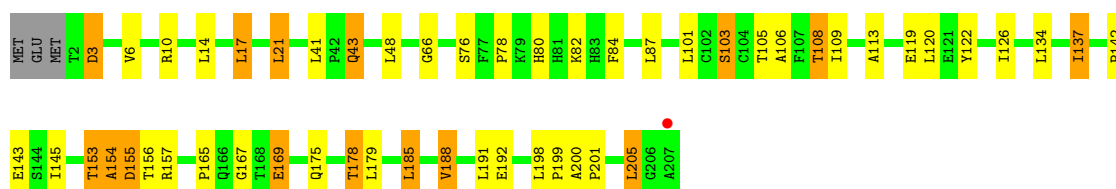
• Molecule 1: Nitrile hydratase alpha subunit

Chain M: 71% 22% 5% .



• Molecule 1: Nitrile hydratase alpha subunit

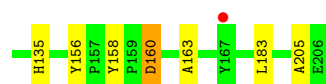
Chain O: 74% 18% 7% .



• Molecule 2: Nitrile hydratase beta subunit

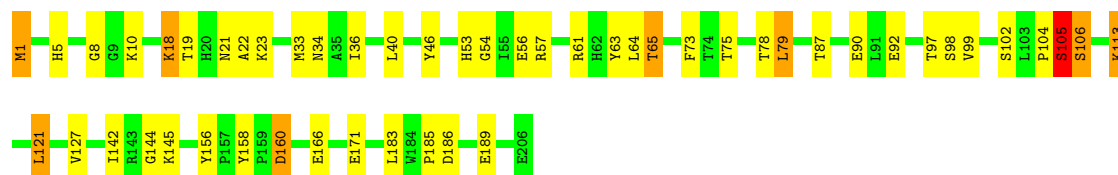
Chain B: 79% 18% .





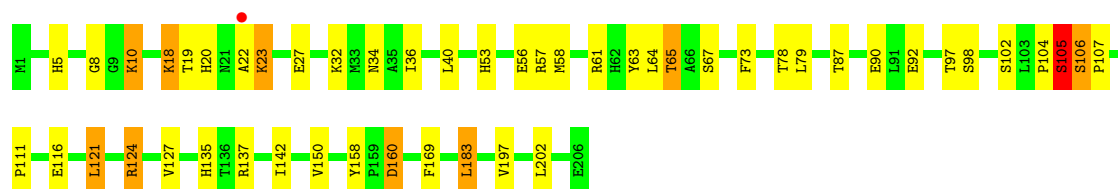
• Molecule 2: Nitrile hydratase beta subunit

Chain D: 75% 20% •



• Molecule 2: Nitrile hydratase beta subunit

Chain F: 76% 19% •



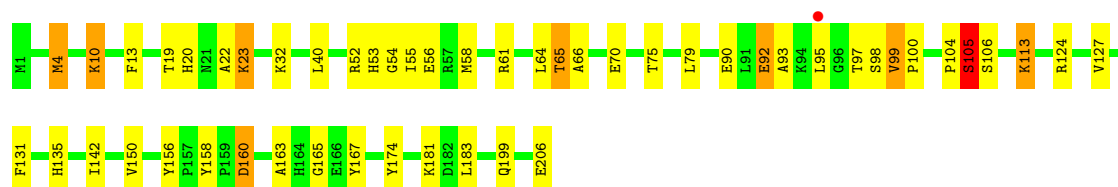
• Molecule 2: Nitrile hydratase beta subunit

Chain H: 81% 14% •



• Molecule 2: Nitrile hydratase beta subunit

Chain J: 75% 20% •



• Molecule 2: Nitrile hydratase beta subunit

Chain L: 76% 20% •





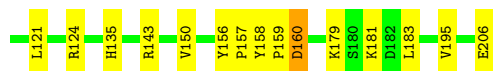
- Molecule 2: Nitrile hydratase beta subunit

Chain N: 77% 19%



- Molecule 2: Nitrile hydratase beta subunit

Chain P: 75% 21%



## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 31   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 111.40Å 111.40Å 475.31Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)  | 36.16 – 2.38<br>36.16 – 2.38                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (36.16-2.38)<br>87.0 (36.16-2.38)                         | Depositor<br>EDS |
| $R_{merge}$   | 0.13   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.14 (at 2.39Å)  | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.7.3_928)                              | Depositor        |
| R, $R_{free}$   | 0.188 , 0.227<br>0.177 , 0.221                                 | Depositor<br>DCC |
| $R_{free}$ test set   | 13123 reflections (5.02%)                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 33.1   | Xtriage          |
| Anisotropy  | 0.642  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | (Not available) , (Not available)                              | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$    | Xtriage          |
| Estimated twinning fraction   | 0.487 for -h,-k,l<br>0.487 for h,-h-k,-l<br>0.487 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.96   | EDS              |
| Total number of atoms   | 27326  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, PO4, FE

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     | 0.54         | 0/1630  | 0.66        | 0/2227         |
| 1   | C     | 0.57         | 0/1630  | 0.71        | 0/2227         |
| 1   | E     | 0.57         | 0/1630  | 0.69        | 0/2227         |
| 1   | G     | 0.57         | 0/1630  | 0.70        | 0/2227         |
| 1   | I     | 0.53         | 0/1630  | 0.67        | 0/2227         |
| 1   | K     | 0.57         | 0/1630  | 0.71        | 0/2227         |
| 1   | M     | 0.55         | 0/1630  | 0.68        | 0/2227         |
| 1   | O     | 0.55         | 0/1630  | 0.67        | 0/2227         |
| 2   | B     | 0.56         | 0/1636  | 0.65        | 0/2216         |
| 2   | D     | 0.58         | 0/1636  | 0.65        | 1/2216 (0.0%)  |
| 2   | F     | 0.59         | 0/1636  | 0.67        | 1/2216 (0.0%)  |
| 2   | H     | 0.59         | 0/1636  | 0.66        | 1/2216 (0.0%)  |
| 2   | J     | 0.56         | 0/1636  | 0.66        | 0/2216         |
| 2   | L     | 0.60         | 0/1636  | 0.67        | 1/2216 (0.0%)  |
| 2   | N     | 0.57         | 0/1636  | 0.65        | 0/2216         |
| 2   | P     | 0.58         | 0/1636  | 0.66        | 0/2216         |
| All | All   | 0.57         | 0/26128 | 0.67        | 4/35544 (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   | A     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | K     | 0                   | 1                   |
| 1   | M     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | O     | 0                   | 1                   |
| All | All   | 0                   | 8                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | H     | 105 | SER  | N-CA-C | -6.11 | 94.51       | 111.00   |
| 2   | F     | 105 | SER  | N-CA-C | -5.75 | 95.47       | 111.00   |
| 2   | L     | 105 | SER  | N-CA-C | -5.52 | 96.10       | 111.00   |
| 2   | D     | 105 | SER  | N-CA-C | -5.26 | 96.79       | 111.00   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 153 | THR  | Peptide |
| 1   | C     | 153 | THR  | Peptide |
| 1   | E     | 153 | THR  | Peptide |
| 1   | G     | 153 | THR  | Peptide |
| 1   | I     | 153 | THR  | Peptide |
| 1   | K     | 153 | THR  | Peptide |
| 1   | M     | 153 | THR  | Peptide |
| 1   | O     | 153 | THR  | Peptide |

## 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     | 1609  | 1        | 1592     | 43      | 0            |
| 1   | C     | 1609  | 1        | 1590     | 49      | 0            |
| 1   | E     | 1609  | 1        | 1591     | 42      | 0            |
| 1   | G     | 1609  | 1        | 1591     | 42      | 0            |
| 1   | I     | 1609  | 1        | 1591     | 48      | 0            |
| 1   | K     | 1609  | 1        | 1590     | 48      | 0            |
| 1   | M     | 1609  | 1        | 1590     | 52      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | O     | 1609  | 1        | 1590     | 44      | 0            |
| 2   | B     | 1589  | 0        | 1538     | 37      | 0            |
| 2   | D     | 1589  | 0        | 1538     | 43      | 0            |
| 2   | F     | 1589  | 0        | 1538     | 41      | 0            |
| 2   | H     | 1589  | 0        | 1538     | 38      | 0            |
| 2   | J     | 1589  | 0        | 1538     | 48      | 0            |
| 2   | L     | 1589  | 0        | 1538     | 46      | 0            |
| 2   | N     | 1589  | 0        | 1538     | 33      | 0            |
| 2   | P     | 1589  | 0        | 1538     | 47      | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 3   | C     | 5     | 0        | 0        | 1       | 0            |
| 3   | E     | 5     | 0        | 0        | 1       | 0            |
| 3   | G     | 5     | 0        | 0        | 0       | 0            |
| 3   | I     | 5     | 0        | 0        | 0       | 0            |
| 3   | K     | 5     | 0        | 0        | 0       | 0            |
| 3   | M     | 5     | 0        | 0        | 0       | 0            |
| 3   | O     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 1     | 0        | 0        | 0       | 0            |
| 4   | O     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 98    | 0        | 0        | 7       | 0            |
| 5   | B     | 113   | 0        | 0        | 4       | 0            |
| 5   | C     | 91    | 0        | 0        | 5       | 1            |
| 5   | D     | 106   | 0        | 0        | 2       | 0            |
| 5   | E     | 107   | 0        | 0        | 6       | 0            |
| 5   | F     | 112   | 0        | 0        | 4       | 1            |
| 5   | G     | 93    | 0        | 0        | 4       | 0            |
| 5   | H     | 110   | 0        | 0        | 8       | 0            |
| 5   | I     | 108   | 0        | 0        | 5       | 0            |
| 5   | J     | 92    | 0        | 0        | 8       | 0            |
| 5   | K     | 113   | 0        | 0        | 8       | 0            |
| 5   | L     | 122   | 0        | 0        | 5       | 0            |
| 5   | M     | 99    | 0        | 0        | 7       | 0            |
| 5   | N     | 104   | 0        | 0        | 1       | 0            |
| 5   | O     | 115   | 0        | 0        | 4       | 1            |
| 5   | P     | 103   | 0        | 0        | 3       | 1            |
| All | All   | 27318 | 8        | 25029    | 640     | 2            |

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 13.

All (640) 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:K:207:ALA:CB   | 2:P:42:SER:HB3   | 1.71                     | 1.20              |
| 2:F:124:ARG:HH11 | 2:F:124:ARG:HG3  | 0.99                     | 1.13              |
| 1:G:154:ALA:O    | 5:G:447:HOH:O    | 1.83                     | 0.96              |
| 2:F:97:THR:HG22  | 2:F:98:SER:H     | 1.30                     | 0.96              |
| 1:K:207:ALA:HB1  | 2:P:42:SER:HB3   | 1.46                     | 0.95              |
| 1:M:43:GLN:H     | 1:M:43:GLN:HE21  | 1.04                     | 0.95              |
| 1:I:43:GLN:N     | 1:I:43:GLN:HE21  | 1.64                     | 0.94              |
| 1:K:204:ALA:O    | 1:K:205:LEU:HB2  | 1.68                     | 0.93              |
| 2:F:104:PRO:CA   | 2:F:105:SER:HB2  | 1.97                     | 0.93              |
| 1:O:43:GLN:HE21  | 1:O:43:GLN:N     | 1.67                     | 0.93              |
| 2:H:10:LYS:HE3   | 5:H:378:HOH:O    | 1.66                     | 0.93              |
| 2:D:104:PRO:CA   | 2:D:105:SER:HB2  | 2.01                     | 0.91              |
| 1:K:154:ALA:O    | 5:K:403:HOH:O    | 1.88                     | 0.91              |
| 2:D:104:PRO:CB   | 2:D:105:SER:HB2  | 2.00                     | 0.91              |
| 1:I:43:GLN:H     | 1:I:43:GLN:NE2   | 1.69                     | 0.90              |
| 1:E:204:ALA:O    | 1:E:205:LEU:HB2  | 1.69                     | 0.90              |
| 2:F:124:ARG:NH1  | 2:F:124:ARG:HG3  | 1.78                     | 0.89              |
| 1:O:43:GLN:NE2   | 1:O:43:GLN:H     | 1.69                     | 0.89              |
| 2:P:104:PRO:CA   | 2:P:105:SER:HB2  | 2.03                     | 0.89              |
| 2:B:163:ALA:O    | 5:B:349:HOH:O    | 1.91                     | 0.88              |
| 1:E:2:THR:N      | 5:E:460:HOH:O    | 2.06                     | 0.88              |
| 1:O:43:GLN:HE21  | 1:O:43:GLN:H     | 0.87                     | 0.86              |
| 1:E:154:ALA:O    | 5:E:473:HOH:O    | 1.93                     | 0.85              |
| 2:P:104:PRO:CB   | 2:P:105:SER:HB2  | 2.06                     | 0.85              |
| 2:D:1:MET:HE3    | 2:D:56:GLU:HB3   | 1.58                     | 0.85              |
| 2:H:104:PRO:CA   | 2:H:105:SER:HB2  | 2.05                     | 0.84              |
| 2:N:104:PRO:CA   | 2:N:105:SER:HB2  | 2.07                     | 0.84              |
| 1:M:167:GLY:N    | 1:M:169:GLU:OE1  | 2.10                     | 0.84              |
| 2:J:163:ALA:O    | 5:J:344:HOH:O    | 1.94                     | 0.84              |
| 2:P:59:GLU:OE1   | 5:P:333:HOH:O    | 1.96                     | 0.83              |
| 2:N:104:PRO:CB   | 2:N:105:SER:HB2  | 2.08                     | 0.83              |
| 2:L:10:LYS:HA    | 2:L:10:LYS:HE3   | 1.59                     | 0.83              |
| 1:M:43:GLN:N     | 1:M:43:GLN:HE21  | 1.77                     | 0.83              |
| 1:A:167:GLY:N    | 1:A:169:GLU:OE1  | 2.12                     | 0.82              |
| 1:K:154:ALA:HB3  | 5:K:507:HOH:O    | 1.78                     | 0.82              |
| 1:O:76:SER:O     | 1:O:108:THR:HG21 | 1.78                     | 0.82              |
| 2:B:104:PRO:CB   | 2:B:105:SER:HB2  | 2.10                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:10:LYS:HA    | 2:J:10:LYS:HE3   | 1.61                     | 0.82              |
| 2:F:104:PRO:HA   | 2:F:105:SER:CB   | 2.09                     | 0.82              |
| 2:J:97:THR:HG22  | 2:J:98:SER:N     | 1.94                     | 0.82              |
| 1:C:175:GLN:O    | 1:C:178:THR:HB   | 1.80                     | 0.81              |
| 1:O:167:GLY:N    | 1:O:169:GLU:OE1  | 2.12                     | 0.81              |
| 1:C:154:ALA:O    | 5:C:402:HOH:O    | 1.98                     | 0.80              |
| 1:G:108:THR:HG22 | 1:G:109:ILE:HG12 | 1.64                     | 0.80              |
| 1:G:2:THR:HG21   | 1:G:7:MET:SD     | 2.21                     | 0.80              |
| 2:F:104:PRO:HA   | 2:F:105:SER:HB2  | 1.63                     | 0.79              |
| 2:F:104:PRO:CB   | 2:F:105:SER:HB2  | 2.12                     | 0.79              |
| 2:N:92:GLU:OE1   | 2:N:98:SER:HA    | 1.83                     | 0.79              |
| 1:C:2:THR:HG21   | 1:C:7:MET:SD     | 2.22                     | 0.79              |
| 1:K:205:LEU:O    | 1:K:207:ALA:N    | 2.16                     | 0.79              |
| 1:A:154:ALA:O    | 5:A:412:HOH:O    | 1.99                     | 0.79              |
| 1:E:175:GLN:O    | 1:E:178:THR:HB   | 1.83                     | 0.79              |
| 1:O:205:LEU:C    | 1:O:205:LEU:HD23 | 2.04                     | 0.78              |
| 1:K:207:ALA:HA   | 2:P:42:SER:CB    | 2.14                     | 0.78              |
| 2:H:104:PRO:CB   | 2:H:105:SER:HB2  | 2.15                     | 0.77              |
| 2:H:78:THR:HG21  | 2:H:102:SER:HB2  | 1.66                     | 0.77              |
| 1:G:175:GLN:O    | 1:G:178:THR:HB   | 1.85                     | 0.77              |
| 1:E:76:SER:O     | 1:E:108:THR:HG21 | 1.84                     | 0.77              |
| 2:L:92:GLU:HG2   | 2:L:98:SER:HA    | 1.66                     | 0.77              |
| 1:K:175:GLN:O    | 1:K:178:THR:HB   | 1.84                     | 0.76              |
| 1:I:43:GLN:H     | 1:I:43:GLN:HE21  | 0.83                     | 0.76              |
| 1:I:154:ALA:O    | 5:I:461:HOH:O    | 2.03                     | 0.76              |
| 2:P:61:ARG:O     | 2:P:65:THR:HB    | 1.86                     | 0.76              |
| 2:H:113:LYS:HA   | 2:H:113:LYS:HE3  | 1.68                     | 0.76              |
| 1:G:102:CSD:O    | 1:G:103:SER:HB3  | 1.86                     | 0.76              |
| 2:N:104:PRO:HA   | 2:N:105:SER:CB   | 2.15                     | 0.76              |
| 1:K:207:ALA:HB2  | 2:P:42:SER:HB3   | 1.67                     | 0.76              |
| 2:J:61:ARG:O     | 2:J:65:THR:HB    | 1.86                     | 0.76              |
| 1:K:207:ALA:CA   | 2:P:42:SER:HB3   | 2.17                     | 0.76              |
| 2:B:104:PRO:CA   | 2:B:105:SER:HB2  | 2.15                     | 0.75              |
| 1:G:105:THR:HG21 | 1:G:113:ALA:HB2  | 1.66                     | 0.75              |
| 1:O:154:ALA:O    | 5:O:412:HOH:O    | 2.02                     | 0.75              |
| 1:C:104:CSD:HA   | 3:C:301:PO4:O4   | 1.87                     | 0.75              |
| 1:M:17:LEU:HD23  | 1:M:21:LEU:CD2   | 2.15                     | 0.75              |
| 2:J:92:GLU:OE1   | 2:J:98:SER:HA    | 1.86                     | 0.75              |
| 1:M:105:THR:HG21 | 1:M:113:ALA:HB2  | 1.68                     | 0.75              |
| 2:F:97:THR:HG22  | 2:F:98:SER:N     | 2.02                     | 0.74              |
| 2:F:58:MET:O     | 5:F:397:HOH:O    | 2.03                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:105:THR:HG21 | 1:E:113:ALA:HB2  | 1.68                     | 0.73              |
| 2:F:10:LYS:NZ    | 5:F:345:HOH:O    | 2.20                     | 0.73              |
| 1:C:167:GLY:N    | 1:C:169:GLU:OE1  | 2.20                     | 0.73              |
| 1:M:43:GLN:H     | 1:M:43:GLN:NE2   | 1.84                     | 0.73              |
| 1:E:2:THR:HG21   | 1:E:7:MET:SD     | 2.29                     | 0.73              |
| 1:I:82:LYS:HE2   | 1:I:155:ASP:OD2  | 1.89                     | 0.73              |
| 2:B:59:GLU:OE1   | 5:B:408:HOH:O    | 2.07                     | 0.73              |
| 2:B:61:ARG:O     | 2:B:65:THR:HB    | 1.89                     | 0.73              |
| 2:F:22:ALA:O     | 2:F:23:LYS:HB2   | 1.87                     | 0.73              |
| 2:N:61:ARG:O     | 2:N:65:THR:HB    | 1.89                     | 0.73              |
| 1:K:207:ALA:HA   | 2:P:42:SER:HB2   | 1.70                     | 0.72              |
| 2:D:104:PRO:HA   | 2:D:105:SER:CB   | 2.18                     | 0.72              |
| 1:I:37:MET:HE2   | 1:I:37:MET:HA    | 1.71                     | 0.72              |
| 2:P:104:PRO:HA   | 2:P:105:SER:CB   | 2.18                     | 0.72              |
| 1:I:167:GLY:N    | 1:I:169:GLU:OE1  | 2.22                     | 0.72              |
| 1:O:82:LYS:HE2   | 1:O:155:ASP:OD2  | 1.88                     | 0.72              |
| 1:M:154:ALA:O    | 5:M:447:HOH:O    | 2.08                     | 0.71              |
| 1:K:154:ALA:N    | 5:K:403:HOH:O    | 2.22                     | 0.71              |
| 2:H:104:PRO:HA   | 2:H:105:SER:HB2  | 1.72                     | 0.71              |
| 1:A:205:LEU:C    | 1:A:205:LEU:HD23 | 2.10                     | 0.71              |
| 1:G:191:LEU:O    | 5:G:420:HOH:O    | 2.09                     | 0.70              |
| 2:D:97:THR:HG22  | 2:D:98:SER:N     | 2.07                     | 0.70              |
| 2:H:104:PRO:HA   | 2:H:105:SER:CB   | 2.22                     | 0.70              |
| 2:P:104:PRO:CA   | 2:P:105:SER:CB   | 2.71                     | 0.69              |
| 2:J:97:THR:CG2   | 2:J:98:SER:N     | 2.56                     | 0.69              |
| 1:G:3:ASP:OD1    | 1:G:5:ALA:N      | 2.26                     | 0.69              |
| 2:D:61:ARG:O     | 2:D:65:THR:HB    | 1.93                     | 0.68              |
| 1:C:154:ALA:N    | 5:C:402:HOH:O    | 2.25                     | 0.68              |
| 2:F:87:THR:OG1   | 2:F:90:GLU:HG3   | 1.94                     | 0.68              |
| 2:P:67:SER:HB3   | 5:P:373:HOH:O    | 1.93                     | 0.68              |
| 1:M:154:ALA:N    | 5:M:447:HOH:O    | 2.27                     | 0.68              |
| 1:K:207:ALA:CB   | 2:P:42:SER:CB    | 2.63                     | 0.68              |
| 1:K:2:THR:HG21   | 1:K:7:MET:SD     | 2.33                     | 0.68              |
| 1:I:137:ILE:CD1  | 1:I:188:VAL:CG2  | 2.72                     | 0.67              |
| 2:J:104:PRO:CA   | 2:J:105:SER:HB2  | 2.25                     | 0.67              |
| 1:E:154:ALA:N    | 5:E:473:HOH:O    | 2.28                     | 0.67              |
| 2:F:61:ARG:O     | 2:F:65:THR:HB    | 1.95                     | 0.67              |
| 2:N:104:PRO:CA   | 2:N:105:SER:CB   | 2.69                     | 0.67              |
| 1:O:76:SER:O     | 1:O:108:THR:CG2  | 2.43                     | 0.67              |
| 2:B:97:THR:HG22  | 2:B:98:SER:O     | 1.95                     | 0.67              |
| 1:E:102:CSD:O    | 1:E:103:SER:HB3  | 1.93                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:124:ARG:HD2  | 2:N:206:GLU:OE1  | 1.95                     | 0.67              |
| 1:G:204:ALA:O    | 1:G:205:LEU:CB   | 2.43                     | 0.67              |
| 2:L:10:LYS:HE3   | 2:L:10:LYS:CA    | 2.24                     | 0.67              |
| 2:H:185:PRO:HD2  | 2:N:131:PHE:CE2  | 2.30                     | 0.67              |
| 1:A:154:ALA:HB3  | 5:B:410:HOH:O    | 1.94                     | 0.67              |
| 1:I:41:LEU:HB3   | 1:I:43:GLN:NE2   | 2.09                     | 0.67              |
| 2:L:177:CYS:O    | 5:L:337:HOH:O    | 2.11                     | 0.67              |
| 1:E:167:GLY:N    | 1:E:169:GLU:OE1  | 2.27                     | 0.66              |
| 2:F:53:HIS:O     | 2:F:57:ARG:HG3   | 1.95                     | 0.66              |
| 2:H:58:MET:O     | 5:H:358:HOH:O    | 2.12                     | 0.66              |
| 1:M:82:LYS:HE2   | 1:M:155:ASP:OD2  | 1.93                     | 0.66              |
| 2:N:52:ARG:O     | 2:N:56:GLU:HG3   | 1.96                     | 0.66              |
| 2:P:19:THR:HG22  | 2:P:20:HIS:N     | 2.11                     | 0.66              |
| 1:K:207:ALA:HB1  | 2:P:42:SER:CB    | 2.24                     | 0.66              |
| 1:A:137:ILE:CD1  | 1:A:188:VAL:CG2  | 2.74                     | 0.66              |
| 2:P:97:THR:HG22  | 2:P:98:SER:O     | 1.96                     | 0.66              |
| 1:A:28:THR:O     | 5:A:428:HOH:O    | 2.15                     | 0.65              |
| 1:A:31:ASP:O     | 5:A:477:HOH:O    | 2.13                     | 0.65              |
| 2:P:104:PRO:HA   | 2:P:105:SER:HB2  | 1.77                     | 0.65              |
| 1:G:76:SER:O     | 1:G:108:THR:HG21 | 1.97                     | 0.65              |
| 2:D:92:GLU:HG2   | 2:D:98:SER:HA    | 1.78                     | 0.65              |
| 1:A:61:GLN:NE2   | 5:A:451:HOH:O    | 2.20                     | 0.65              |
| 1:M:17:LEU:HD23  | 1:M:21:LEU:HD22  | 1.78                     | 0.65              |
| 2:J:52:ARG:O     | 2:J:56:GLU:HG3   | 1.96                     | 0.64              |
| 2:J:104:PRO:CB   | 2:J:105:SER:HB2  | 2.27                     | 0.64              |
| 1:K:198:LEU:HD12 | 1:M:198:LEU:HD12 | 1.79                     | 0.64              |
| 1:M:205:LEU:C    | 1:M:205:LEU:HD23 | 2.16                     | 0.64              |
| 1:E:166:GLN:HG3  | 1:I:193:ALA:CB   | 2.27                     | 0.64              |
| 2:F:124:ARG:CG   | 2:F:124:ARG:HH11 | 1.91                     | 0.64              |
| 1:I:61:GLN:NE2   | 5:I:478:HOH:O    | 1.86                     | 0.64              |
| 1:K:116:TRP:CD1  | 2:L:18:LYS:HG2   | 2.33                     | 0.64              |
| 1:G:14:LEU:HD13  | 2:H:36:ILE:HG21  | 1.81                     | 0.63              |
| 1:K:112:MET:HE3  | 5:K:464:HOH:O    | 1.98                     | 0.63              |
| 1:K:207:ALA:CA   | 2:P:42:SER:CB    | 2.76                     | 0.63              |
| 2:H:10:LYS:CE    | 5:H:378:HOH:O    | 2.36                     | 0.63              |
| 2:J:22:ALA:O     | 2:J:23:LYS:HB2   | 1.97                     | 0.63              |
| 1:I:105:THR:HG21 | 1:I:113:ALA:HB2  | 1.79                     | 0.63              |
| 1:G:4:ASN:OD1    | 2:H:29:TRP:NE1   | 2.23                     | 0.63              |
| 2:D:22:ALA:O     | 2:D:23:LYS:HB2   | 1.96                     | 0.63              |
| 1:M:137:ILE:CD1  | 1:M:188:VAL:CG2  | 2.77                     | 0.62              |
| 1:K:82:LYS:HE2   | 1:K:155:ASP:OD2  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:PRO:HG3  | 1:A:191:LEU:HB3  | 1.80                     | 0.62              |
| 1:E:76:SER:O     | 1:E:108:THR:CG2  | 2.47                     | 0.62              |
| 1:M:137:ILE:HD12 | 1:M:188:VAL:HG21 | 1.81                     | 0.62              |
| 2:L:10:LYS:HA    | 2:L:10:LYS:CE    | 2.30                     | 0.62              |
| 2:P:143:ARG:HD2  | 5:P:360:HOH:O    | 2.00                     | 0.62              |
| 1:A:108:THR:HG22 | 1:A:109:ILE:HG12 | 1.80                     | 0.62              |
| 2:P:92:GLU:OE1   | 2:P:98:SER:HA    | 1.99                     | 0.62              |
| 2:B:19:THR:HG22  | 2:B:20:HIS:O     | 2.00                     | 0.62              |
| 1:M:175:GLN:O    | 1:M:178:THR:HB   | 1.98                     | 0.62              |
| 1:O:175:GLN:O    | 1:O:178:THR:HB   | 2.00                     | 0.62              |
| 2:D:78:THR:HG21  | 2:D:102:SER:HB2  | 1.81                     | 0.61              |
| 1:G:132:THR:O    | 1:G:136:GLU:HG3  | 2.00                     | 0.61              |
| 2:J:10:LYS:NZ    | 5:J:386:HOH:O    | 2.14                     | 0.61              |
| 2:B:87:THR:OG1   | 2:B:90:GLU:HG3   | 2.00                     | 0.61              |
| 2:B:97:THR:HG22  | 2:B:98:SER:N     | 2.14                     | 0.61              |
| 1:C:105:THR:HG21 | 1:C:113:ALA:HB2  | 1.82                     | 0.61              |
| 2:L:22:ALA:O     | 2:L:23:LYS:HB2   | 1.99                     | 0.61              |
| 2:N:22:ALA:O     | 2:N:23:LYS:HB2   | 1.99                     | 0.61              |
| 1:A:76:SER:O     | 1:A:108:THR:HG21 | 2.00                     | 0.61              |
| 2:B:1:MET:HE3    | 2:L:12:GLY:CA    | 2.30                     | 0.61              |
| 2:D:1:MET:CE     | 2:D:56:GLU:HB3   | 2.28                     | 0.61              |
| 2:L:97:THR:HG22  | 2:L:98:SER:N     | 2.16                     | 0.61              |
| 2:F:158:TYR:CE2  | 2:F:160:ASP:HB2  | 2.36                     | 0.61              |
| 1:I:137:ILE:HD12 | 1:I:188:VAL:CG2  | 2.30                     | 0.61              |
| 2:J:97:THR:CG2   | 2:J:98:SER:H     | 2.12                     | 0.61              |
| 2:L:104:PRO:CB   | 2:L:105:SER:HB2  | 2.30                     | 0.61              |
| 2:B:104:PRO:HA   | 2:B:105:SER:CB   | 2.30                     | 0.61              |
| 2:J:92:GLU:HG3   | 2:J:97:THR:O     | 2.01                     | 0.60              |
| 2:P:104:PRO:HB2  | 2:P:105:SER:HB2  | 1.81                     | 0.60              |
| 1:K:76:SER:O     | 1:K:108:THR:OG1  | 2.19                     | 0.60              |
| 2:D:5:HIS:CG     | 2:D:56:GLU:HG2   | 2.36                     | 0.60              |
| 2:P:90:GLU:O     | 2:P:93:ALA:HB3   | 2.01                     | 0.60              |
| 2:P:10:LYS:HE3   | 2:P:10:LYS:HA    | 1.84                     | 0.60              |
| 1:E:3:ASP:HB2    | 1:E:6:VAL:HG23   | 1.82                     | 0.60              |
| 1:A:175:GLN:O    | 1:A:178:THR:HB   | 2.02                     | 0.60              |
| 2:B:104:PRO:HB2  | 2:B:105:SER:HB2  | 1.82                     | 0.60              |
| 1:C:204:ALA:O    | 1:C:205:LEU:CB   | 2.50                     | 0.60              |
| 2:J:104:PRO:HA   | 2:J:105:SER:CB   | 2.32                     | 0.60              |
| 1:K:205:LEU:HD22 | 1:O:78:PRO:HB3   | 1.83                     | 0.60              |
| 2:B:104:PRO:CA   | 2:B:105:SER:CB   | 2.79                     | 0.60              |
| 2:B:131:PHE:CE2  | 2:L:185:PRO:HD2  | 2.37                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:165:PRO:HG3  | 1:M:191:LEU:HB3  | 1.83                     | 0.60              |
| 1:C:137:ILE:CD1  | 1:C:188:VAL:CG2  | 2.80                     | 0.59              |
| 1:G:116:TRP:CD1  | 2:H:18:LYS:HG2   | 2.37                     | 0.59              |
| 1:K:106:ALA:HB2  | 1:K:157:ARG:HB3  | 1.83                     | 0.59              |
| 1:A:119:GLU:HB3  | 5:A:437:HOH:O    | 2.01                     | 0.59              |
| 2:B:97:THR:CG2   | 2:B:98:SER:N     | 2.64                     | 0.59              |
| 1:C:112:MET:HE3  | 5:C:486:HOH:O    | 2.02                     | 0.59              |
| 1:O:108:THR:HG22 | 1:O:109:ILE:HG12 | 1.84                     | 0.59              |
| 1:E:108:THR:HG22 | 1:E:109:ILE:HG12 | 1.85                     | 0.59              |
| 1:M:76:SER:O     | 1:M:108:THR:HG21 | 2.03                     | 0.59              |
| 1:E:28:THR:O     | 5:E:453:HOH:O    | 2.17                     | 0.59              |
| 2:J:10:LYS:HD3   | 5:J:386:HOH:O    | 2.01                     | 0.59              |
| 2:N:163:ALA:O    | 5:N:345:HOH:O    | 2.17                     | 0.59              |
| 1:K:204:ALA:O    | 1:K:205:LEU:CB   | 2.43                     | 0.59              |
| 2:P:10:LYS:HA    | 2:P:10:LYS:CE    | 2.32                     | 0.59              |
| 2:L:10:LYS:NZ    | 5:L:392:HOH:O    | 2.36                     | 0.59              |
| 2:P:52:ARG:O     | 2:P:56:GLU:HG3   | 2.03                     | 0.59              |
| 2:L:158:TYR:CE2  | 2:L:160:ASP:HB2  | 2.38                     | 0.59              |
| 1:E:204:ALA:O    | 1:E:205:LEU:CB   | 2.47                     | 0.58              |
| 2:F:106:SER:HB3  | 5:F:382:HOH:O    | 2.02                     | 0.58              |
| 2:B:92:GLU:OE1   | 2:B:98:SER:HA    | 2.04                     | 0.58              |
| 1:K:137:ILE:CD1  | 1:K:188:VAL:HG22 | 2.33                     | 0.58              |
| 1:A:82:LYS:HE2   | 1:A:155:ASP:OD2  | 2.03                     | 0.58              |
| 2:B:88:ALA:O     | 2:B:92:GLU:HG3   | 2.03                     | 0.58              |
| 1:E:198:LEU:HD12 | 1:I:198:LEU:HD12 | 1.84                     | 0.58              |
| 1:K:37:MET:HG2   | 1:K:38:HIS:CE1   | 2.37                     | 0.58              |
| 1:O:41:LEU:HB3   | 1:O:43:GLN:NE2   | 2.19                     | 0.58              |
| 2:L:78:THR:HG21  | 2:L:102:SER:HB2  | 1.84                     | 0.58              |
| 1:G:137:ILE:CD1  | 1:G:188:VAL:HG22 | 2.34                     | 0.58              |
| 2:J:97:THR:HG22  | 2:J:98:SER:H     | 1.66                     | 0.58              |
| 2:N:97:THR:HG22  | 2:N:98:SER:N     | 2.18                     | 0.58              |
| 1:O:3:ASP:HB3    | 1:O:6:VAL:H      | 1.68                     | 0.57              |
| 2:J:158:TYR:CE2  | 2:J:160:ASP:HB2  | 2.39                     | 0.57              |
| 2:L:97:THR:CG2   | 2:L:98:SER:N     | 2.67                     | 0.57              |
| 1:M:29:VAL:HG21  | 2:N:32:LYS:HD3   | 1.86                     | 0.57              |
| 1:E:14:LEU:HD13  | 2:F:36:ILE:HG21  | 1.86                     | 0.57              |
| 1:G:76:SER:O     | 1:G:108:THR:CG2  | 2.52                     | 0.57              |
| 2:L:104:PRO:HA   | 2:L:105:SER:CB   | 2.34                     | 0.57              |
| 1:M:17:LEU:CD2   | 1:M:21:LEU:CD2   | 2.82                     | 0.57              |
| 1:O:198:LEU:HB3  | 1:O:199:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:137:ILE:HD11 | 1:A:188:VAL:CG2  | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:137:ILE:HD12 | 1:I:188:VAL:HG21 | 1.86                     | 0.57              |
| 2:H:106:SER:HB3  | 5:H:368:HOH:O    | 2.03                     | 0.57              |
| 2:B:75:THR:O     | 2:B:79:LEU:HB2   | 2.05                     | 0.57              |
| 1:C:14:LEU:HD13  | 2:D:36:ILE:HG21  | 1.86                     | 0.56              |
| 1:A:154:ALA:N    | 5:A:412:HOH:O    | 2.38                     | 0.56              |
| 2:D:5:HIS:CD2    | 2:D:56:GLU:HG2   | 2.40                     | 0.56              |
| 1:I:165:PRO:HG3  | 1:I:191:LEU:HB3  | 1.88                     | 0.56              |
| 1:C:137:ILE:HD11 | 1:C:188:VAL:CG2  | 2.35                     | 0.56              |
| 2:D:104:PRO:HB2  | 2:D:105:SER:HB2  | 1.88                     | 0.56              |
| 1:I:119:GLU:HB3  | 5:I:408:HOH:O    | 2.04                     | 0.56              |
| 1:C:76:SER:O     | 1:C:108:THR:OG1  | 2.22                     | 0.56              |
| 2:L:104:PRO:CA   | 2:L:105:SER:HB2  | 2.36                     | 0.56              |
| 2:D:171:GLU:OE1  | 5:D:379:HOH:O    | 2.18                     | 0.56              |
| 1:M:137:ILE:HD12 | 1:M:188:VAL:CG2  | 2.34                     | 0.56              |
| 1:C:106:ALA:HB2  | 1:C:157:ARG:HB3  | 1.88                     | 0.56              |
| 1:E:167:GLY:CA   | 1:E:169:GLU:OE1  | 2.53                     | 0.56              |
| 2:P:19:THR:CG2   | 2:P:20:HIS:N     | 2.69                     | 0.56              |
| 1:A:49:VAL:HG13  | 1:A:161:LEU:HD12 | 1.88                     | 0.55              |
| 2:B:1:MET:CE     | 2:L:12:GLY:CA    | 2.84                     | 0.55              |
| 1:M:119:GLU:HB3  | 5:M:410:HOH:O    | 2.06                     | 0.55              |
| 2:L:10:LYS:NZ    | 5:L:347:HOH:O    | 2.39                     | 0.55              |
| 2:B:52:ARG:O     | 2:B:56:GLU:HG3   | 2.06                     | 0.55              |
| 2:D:106:SER:HB3  | 5:D:391:HOH:O    | 2.05                     | 0.55              |
| 2:L:5:HIS:CG     | 2:L:56:GLU:HG2   | 2.42                     | 0.55              |
| 1:M:108:THR:HG22 | 1:M:109:ILE:HG12 | 1.87                     | 0.55              |
| 2:F:92:GLU:HG2   | 2:F:98:SER:HA    | 1.88                     | 0.55              |
| 2:J:10:LYS:CD    | 5:J:386:HOH:O    | 2.55                     | 0.55              |
| 1:M:3:ASP:HB3    | 1:M:6:VAL:H      | 1.71                     | 0.55              |
| 1:A:137:ILE:HD12 | 1:A:188:VAL:CG2  | 2.37                     | 0.55              |
| 2:H:5:HIS:CG     | 2:H:56:GLU:HG2   | 2.42                     | 0.55              |
| 1:I:175:GLN:O    | 1:I:178:THR:HB   | 2.07                     | 0.55              |
| 1:A:45:GLY:O     | 1:A:49:VAL:HG23  | 2.07                     | 0.55              |
| 2:L:92:GLU:CG    | 2:L:98:SER:HA    | 2.34                     | 0.55              |
| 2:H:23:LYS:N     | 5:H:402:HOH:O    | 2.15                     | 0.55              |
| 2:L:104:PRO:CA   | 2:L:105:SER:CB   | 2.85                     | 0.55              |
| 2:N:158:TYR:CE2  | 2:N:160:ASP:HB2  | 2.42                     | 0.55              |
| 2:N:92:GLU:HG3   | 2:N:97:THR:O     | 2.06                     | 0.55              |
| 2:D:97:THR:HG22  | 2:D:98:SER:H     | 1.71                     | 0.55              |
| 1:C:101:LEU:HB2  | 5:C:406:HOH:O    | 2.06                     | 0.55              |
| 1:I:37:MET:HE2   | 1:I:37:MET:CA    | 2.37                     | 0.54              |
| 1:K:207:ALA:N    | 5:K:428:HOH:O    | 2.39                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:46:TYR:CG    | 2:L:79:LEU:HD23  | 2.42                     | 0.54              |
| 1:E:104:CSD:C    | 1:E:105:THR:CG2  | 2.85                     | 0.54              |
| 1:I:3:ASP:OD2    | 1:I:3:ASP:N      | 2.25                     | 0.54              |
| 2:L:145:LYS:HG3  | 2:L:183:LEU:HD12 | 1.88                     | 0.54              |
| 1:M:41:LEU:HB3   | 1:M:43:GLN:NE2   | 2.23                     | 0.54              |
| 2:N:79:LEU:O     | 2:N:83:LYS:HG3   | 2.08                     | 0.54              |
| 1:O:142:PRO:HD2  | 1:O:145:ILE:HD12 | 1.89                     | 0.54              |
| 1:A:16:VAL:O     | 1:A:20:GLU:HG3   | 2.08                     | 0.54              |
| 1:G:137:ILE:HD11 | 1:G:188:VAL:HG22 | 1.89                     | 0.54              |
| 1:M:102:CSD:O    | 1:M:123:ARG:HD2  | 2.08                     | 0.54              |
| 1:M:105:THR:CG2  | 1:M:113:ALA:HB2  | 2.35                     | 0.54              |
| 1:E:166:GLN:HG3  | 1:I:193:ALA:HB3  | 1.88                     | 0.54              |
| 2:H:113:LYS:CA   | 2:H:113:LYS:HE3  | 2.32                     | 0.54              |
| 1:A:49:VAL:HG13  | 1:A:161:LEU:CD1  | 2.38                     | 0.54              |
| 2:H:158:TYR:CE2  | 2:H:160:ASP:HB2  | 2.43                     | 0.54              |
| 1:M:60:ALA:O     | 5:M:484:HOH:O    | 2.18                     | 0.54              |
| 1:O:153:THR:HG21 | 2:P:195:VAL:HG13 | 1.90                     | 0.54              |
| 1:E:165:PRO:HB3  | 1:E:192:GLU:HA   | 1.90                     | 0.54              |
| 2:J:19:THR:HG22  | 2:J:20:HIS:N     | 2.23                     | 0.54              |
| 2:H:104:PRO:CA   | 2:H:105:SER:CB   | 2.77                     | 0.53              |
| 2:N:19:THR:HG22  | 2:N:20:HIS:N     | 2.23                     | 0.53              |
| 1:O:200:ALA:HB1  | 1:O:201:PRO:HD2  | 1.90                     | 0.53              |
| 2:P:22:ALA:O     | 2:P:23:LYS:HB2   | 2.08                     | 0.53              |
| 1:C:3:ASP:OD1    | 1:C:5:ALA:N      | 2.42                     | 0.53              |
| 1:K:137:ILE:HD11 | 1:K:188:VAL:HG22 | 1.90                     | 0.53              |
| 1:I:103:SER:OG   | 1:I:103:SER:O    | 2.24                     | 0.52              |
| 1:C:37:MET:HB3   | 1:C:38:HIS:CD2   | 2.43                     | 0.52              |
| 2:J:20:HIS:ND1   | 5:J:392:HOH:O    | 2.29                     | 0.52              |
| 1:I:143:GLU:N    | 2:L:116:GLU:OE2  | 2.27                     | 0.52              |
| 2:F:78:THR:HG21  | 2:F:102:SER:HB2  | 1.91                     | 0.52              |
| 1:I:106:ALA:HB2  | 1:I:157:ARG:HB3  | 1.91                     | 0.52              |
| 1:I:156:THR:HB   | 5:I:407:HOH:O    | 2.08                     | 0.52              |
| 2:J:19:THR:CG2   | 2:J:20:HIS:N     | 2.72                     | 0.52              |
| 2:P:53:HIS:CG    | 2:P:135:HIS:HB2  | 2.45                     | 0.52              |
| 2:B:53:HIS:CG    | 2:B:135:HIS:HB2  | 2.45                     | 0.52              |
| 2:J:53:HIS:CG    | 2:J:135:HIS:HB2  | 2.44                     | 0.52              |
| 1:O:137:ILE:CD1  | 1:O:188:VAL:HG22 | 2.39                     | 0.52              |
| 1:A:137:ILE:CD1  | 1:A:188:VAL:HG22 | 2.39                     | 0.52              |
| 1:K:3:ASP:OD1    | 1:K:5:ALA:N      | 2.43                     | 0.52              |
| 2:B:19:THR:HG22  | 2:B:20:HIS:N     | 2.24                     | 0.52              |
| 2:H:53:HIS:CG    | 2:H:135:HIS:HB2  | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:104:PRO:HB2  | 2:N:105:SER:HB2  | 1.89                     | 0.52              |
| 1:C:108:THR:HG23 | 1:C:109:ILE:HG12 | 1.92                     | 0.52              |
| 2:F:124:ARG:CG   | 2:F:124:ARG:NH1  | 2.59                     | 0.52              |
| 2:F:97:THR:CG2   | 2:F:98:SER:H     | 2.10                     | 0.51              |
| 1:C:37:MET:C     | 1:C:38:HIS:HD2   | 2.13                     | 0.51              |
| 2:J:10:LYS:CE    | 5:J:386:HOH:O    | 2.58                     | 0.51              |
| 2:H:22:ALA:N     | 5:H:402:HOH:O    | 2.44                     | 0.51              |
| 1:E:104:CSD:O    | 1:E:105:THR:HG22 | 2.10                     | 0.51              |
| 1:K:103:SER:HB3  | 2:L:68:TYR:HE1   | 1.75                     | 0.51              |
| 2:B:10:LYS:CE    | 2:B:10:LYS:HA    | 2.40                     | 0.51              |
| 2:F:19:THR:CG2   | 2:F:20:HIS:N     | 2.74                     | 0.51              |
| 2:N:19:THR:HG22  | 2:N:20:HIS:O     | 2.10                     | 0.51              |
| 2:F:197:VAL:HG11 | 2:F:202:LEU:HD21 | 1.92                     | 0.51              |
| 1:G:101:LEU:HB2  | 5:G:403:HOH:O    | 2.09                     | 0.51              |
| 1:I:137:ILE:HD11 | 1:I:188:VAL:CG2  | 2.39                     | 0.51              |
| 1:K:155:ASP:HB2  | 2:L:156:TYR:CD2  | 2.46                     | 0.51              |
| 1:E:104:CSD:C    | 1:E:105:THR:HG22 | 2.41                     | 0.51              |
| 1:G:106:ALA:HB2  | 1:G:157:ARG:HB3  | 1.92                     | 0.51              |
| 2:D:64:LEU:HD21  | 2:J:4:MET:CE     | 2.41                     | 0.51              |
| 1:K:2:THR:N      | 5:K:455:HOH:O    | 2.43                     | 0.51              |
| 2:F:19:THR:HG22  | 2:F:20:HIS:O     | 2.10                     | 0.51              |
| 2:B:92:GLU:CD    | 2:B:98:SER:HA    | 2.31                     | 0.51              |
| 1:C:90:THR:HB    | 1:C:91:PRO:CD    | 2.41                     | 0.51              |
| 1:E:174:ALA:HB1  | 1:I:203:VAL:HG11 | 1.92                     | 0.51              |
| 1:M:45:GLY:O     | 1:M:49:VAL:HG23  | 2.11                     | 0.51              |
| 1:E:116:TRP:CD1  | 2:F:18:LYS:HG2   | 2.46                     | 0.50              |
| 1:E:29:VAL:HG21  | 2:F:32:LYS:HG3   | 1.92                     | 0.50              |
| 1:A:3:ASP:HB3    | 1:A:6:VAL:HG23   | 1.92                     | 0.50              |
| 2:L:59:GLU:OE1   | 5:L:408:HOH:O    | 2.20                     | 0.50              |
| 2:N:19:THR:CG2   | 2:N:20:HIS:N     | 2.74                     | 0.50              |
| 2:F:5:HIS:CG     | 2:F:56:GLU:HG2   | 2.46                     | 0.50              |
| 1:I:16:VAL:O     | 1:I:20:GLU:HG3   | 2.11                     | 0.50              |
| 2:J:10:LYS:CA    | 2:J:10:LYS:HE3   | 2.37                     | 0.50              |
| 2:J:90:GLU:O     | 2:J:93:ALA:HB3   | 2.11                     | 0.50              |
| 1:G:155:ASP:H    | 1:G:157:ARG:HH12 | 1.59                     | 0.50              |
| 2:P:97:THR:CG2   | 2:P:98:SER:N     | 2.74                     | 0.50              |
| 1:C:37:MET:C     | 1:C:38:HIS:CD2   | 2.85                     | 0.50              |
| 1:I:105:THR:HG22 | 1:I:117:TYR:CE2  | 2.47                     | 0.50              |
| 1:I:37:MET:CE    | 1:I:37:MET:CA    | 2.89                     | 0.50              |
| 1:G:3:ASP:OD1    | 1:G:3:ASP:C      | 2.50                     | 0.50              |
| 1:M:49:VAL:HG13  | 1:M:161:LEU:CD1  | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:127:VAL:O    | 2:H:144:GLY:HA2  | 2.11                     | 0.50              |
| 1:A:137:ILE:HD12 | 1:A:188:VAL:HG21 | 1.94                     | 0.50              |
| 2:D:97:THR:CG2   | 2:D:98:SER:N     | 2.74                     | 0.50              |
| 2:H:113:LYS:HA   | 2:H:113:LYS:CE   | 2.38                     | 0.50              |
| 2:L:63:TYR:CD2   | 2:L:63:TYR:C     | 2.84                     | 0.50              |
| 2:D:64:LEU:HD21  | 2:J:4:MET:HE2    | 1.93                     | 0.50              |
| 2:L:104:PRO:HB2  | 2:L:105:SER:HB2  | 1.92                     | 0.50              |
| 1:K:167:GLY:N    | 1:K:169:GLU:OE1  | 2.42                     | 0.49              |
| 1:K:167:GLY:CA   | 1:K:169:GLU:OE1  | 2.61                     | 0.49              |
| 2:L:97:THR:HG22  | 2:L:98:SER:O     | 2.11                     | 0.49              |
| 1:A:135:LYS:NZ   | 5:A:494:HOH:O    | 2.29                     | 0.49              |
| 1:A:155:ASP:HB2  | 2:B:156:TYR:CD2  | 2.47                     | 0.49              |
| 1:C:137:ILE:HD12 | 1:C:188:VAL:HG21 | 1.94                     | 0.49              |
| 2:B:1:MET:CE     | 2:L:12:GLY:HA3   | 2.42                     | 0.49              |
| 1:G:99:CYS:HB3   | 1:G:103:SER:HA   | 1.93                     | 0.49              |
| 2:J:104:PRO:CA   | 2:J:105:SER:CB   | 2.86                     | 0.49              |
| 2:N:97:THR:CG2   | 2:N:98:SER:N     | 2.76                     | 0.49              |
| 2:D:63:TYR:CD2   | 2:D:63:TYR:C     | 2.85                     | 0.49              |
| 1:E:201:PRO:HG3  | 1:I:178:THR:HG21 | 1.94                     | 0.49              |
| 2:F:53:HIS:CG    | 2:F:135:HIS:HB2  | 2.47                     | 0.49              |
| 2:D:185:PRO:HD2  | 2:J:131:PHE:CE2  | 2.48                     | 0.49              |
| 1:I:80:HIS:O     | 1:I:155:ASP:HA   | 2.12                     | 0.49              |
| 2:J:19:THR:HG22  | 2:J:20:HIS:O     | 2.13                     | 0.49              |
| 1:O:155:ASP:H    | 1:O:157:ARG:HH12 | 1.60                     | 0.49              |
| 2:P:97:THR:HG22  | 2:P:98:SER:N     | 2.27                     | 0.49              |
| 1:E:104:CSD:HA   | 3:E:301:PO4:O3   | 2.13                     | 0.49              |
| 2:B:19:THR:CG2   | 2:B:20:HIS:N     | 2.75                     | 0.48              |
| 1:C:37:MET:CE    | 1:C:37:MET:HA    | 2.43                     | 0.48              |
| 1:A:167:GLY:CA   | 1:A:169:GLU:OE1  | 2.61                     | 0.48              |
| 2:H:55:ILE:HG23  | 2:H:71:ARG:HB3   | 1.95                     | 0.48              |
| 1:O:106:ALA:HB2  | 1:O:157:ARG:HB3  | 1.93                     | 0.48              |
| 1:A:76:SER:O     | 1:A:108:THR:CG2  | 2.61                     | 0.48              |
| 1:O:137:ILE:CD1  | 1:O:188:VAL:CG2  | 2.91                     | 0.48              |
| 1:C:104:CSD:C    | 1:C:105:THR:CG2  | 2.91                     | 0.48              |
| 2:H:5:HIS:ND1    | 2:H:56:GLU:HG2   | 2.28                     | 0.48              |
| 1:I:205:LEU:C    | 1:I:205:LEU:HD23 | 2.34                     | 0.48              |
| 1:K:10:ARG:HA    | 2:L:95:LEU:HD11  | 1.94                     | 0.48              |
| 2:L:160:ASP:OD2  | 2:L:160:ASP:N    | 2.47                     | 0.48              |
| 1:G:167:GLY:CA   | 1:G:169:GLU:OE1  | 2.62                     | 0.48              |
| 1:I:29:VAL:HB    | 1:I:30:PRO:HD3   | 1.96                     | 0.48              |
| 1:I:59:LYS:NZ    | 1:I:88:GLU:OE2   | 2.39                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:3:ASP:HB3    | 1:M:6:VAL:HG23   | 1.95                     | 0.48              |
| 2:B:10:LYS:HE3   | 2:B:10:LYS:HA    | 1.93                     | 0.48              |
| 1:C:14:LEU:HD22  | 1:C:14:LEU:O     | 2.14                     | 0.48              |
| 1:K:14:LEU:HD13  | 2:L:36:ILE:HG21  | 1.94                     | 0.47              |
| 1:E:137:ILE:CD1  | 1:E:188:VAL:CG2  | 2.92                     | 0.47              |
| 2:N:127:VAL:HG21 | 2:N:142:ILE:HD12 | 1.95                     | 0.47              |
| 1:C:154:ALA:CA   | 5:C:402:HOH:O    | 2.63                     | 0.47              |
| 1:C:206:GLY:HA2  | 1:C:207:ALA:HA   | 1.70                     | 0.47              |
| 1:E:78:PRO:HG2   | 1:E:81:HIS:CG    | 2.49                     | 0.47              |
| 2:H:10:LYS:NZ    | 5:H:385:HOH:O    | 2.20                     | 0.47              |
| 1:M:106:ALA:HB2  | 1:M:157:ARG:HB3  | 1.95                     | 0.47              |
| 1:G:204:ALA:O    | 1:G:205:LEU:HB2  | 2.15                     | 0.47              |
| 2:J:10:LYS:CE    | 2:J:10:LYS:HA    | 2.41                     | 0.47              |
| 2:L:53:HIS:CG    | 2:L:135:HIS:HB2  | 2.50                     | 0.47              |
| 2:P:160:ASP:N    | 2:P:160:ASP:OD2  | 2.48                     | 0.47              |
| 2:N:78:THR:HG21  | 2:N:102:SER:HB2  | 1.95                     | 0.47              |
| 1:G:154:ALA:N    | 5:G:447:HOH:O    | 2.47                     | 0.47              |
| 2:D:92:GLU:CG    | 2:D:98:SER:HA    | 2.42                     | 0.47              |
| 1:M:137:ILE:HD11 | 1:M:188:VAL:CG2  | 2.44                     | 0.47              |
| 2:P:10:LYS:CA    | 2:P:10:LYS:HE3   | 2.44                     | 0.47              |
| 1:C:155:ASP:HB2  | 2:D:156:TYR:CD2  | 2.50                     | 0.47              |
| 1:K:90:THR:HB    | 1:K:91:PRO:CD    | 2.45                     | 0.47              |
| 1:E:106:ALA:HB2  | 1:E:157:ARG:HB3  | 1.96                     | 0.46              |
| 2:H:145:LYS:HG3  | 2:H:183:LEU:HD12 | 1.97                     | 0.46              |
| 2:P:64:LEU:HA    | 2:P:64:LEU:HD12  | 1.58                     | 0.46              |
| 1:C:37:MET:HA    | 1:C:37:MET:HE2   | 1.97                     | 0.46              |
| 1:I:137:ILE:HD11 | 1:I:188:VAL:HG23 | 1.96                     | 0.46              |
| 1:O:155:ASP:N    | 1:O:157:ARG:HH12 | 2.13                     | 0.46              |
| 2:F:116:GLU:OE2  | 1:M:143:GLU:N    | 2.39                     | 0.46              |
| 1:K:156:THR:OG1  | 5:K:422:HOH:O    | 2.19                     | 0.46              |
| 2:D:46:TYR:CG    | 2:D:79:LEU:HD23  | 2.50                     | 0.46              |
| 2:J:113:LYS:HD3  | 2:J:113:LYS:HA   | 1.80                     | 0.46              |
| 2:D:158:TYR:CE2  | 2:D:160:ASP:HB2  | 2.51                     | 0.46              |
| 1:M:53:TRP:CE2   | 1:M:164:ARG:HB2  | 2.51                     | 0.46              |
| 1:C:132:THR:O    | 1:C:136:GLU:HG3  | 2.16                     | 0.46              |
| 2:D:104:PRO:HA   | 2:D:105:SER:HB2  | 1.77                     | 0.46              |
| 1:G:14:LEU:CD1   | 2:H:36:ILE:HG21  | 2.46                     | 0.46              |
| 1:K:3:ASP:C      | 1:K:3:ASP:OD1    | 2.54                     | 0.46              |
| 1:K:3:ASP:OD1    | 1:K:4:ASN:N      | 2.49                     | 0.46              |
| 1:O:154:ALA:O    | 1:O:155:ASP:HB2  | 2.16                     | 0.46              |
| 1:C:204:ALA:O    | 1:C:205:LEU:HB3  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:166:GLN:CG   | 1:I:193:ALA:HB3  | 2.46                     | 0.46              |
| 2:P:54:GLY:HA3   | 2:P:75:THR:OG1   | 2.16                     | 0.46              |
| 1:A:15:PHE:HB2   | 2:B:36:ILE:HD11  | 1.98                     | 0.46              |
| 1:I:198:LEU:HB3  | 1:I:199:PRO:HD2  | 1.97                     | 0.46              |
| 2:J:99:VAL:HA    | 2:J:100:PRO:HD3  | 1.83                     | 0.46              |
| 1:O:156:THR:OG1  | 5:O:467:HOH:O    | 2.21                     | 0.45              |
| 2:H:121:LEU:HD12 | 2:H:121:LEU:HA   | 1.79                     | 0.45              |
| 1:A:164:ARG:HA   | 1:A:165:PRO:HD3  | 1.88                     | 0.45              |
| 1:E:102:CSD:O    | 1:E:103:SER:CB   | 2.64                     | 0.45              |
| 2:D:33:MET:SD    | 2:D:73:PHE:HA    | 2.56                     | 0.45              |
| 2:J:55:ILE:HG13  | 2:J:75:THR:HB    | 1.97                     | 0.45              |
| 2:D:54:GLY:HA3   | 2:D:75:THR:OG1   | 2.17                     | 0.45              |
| 1:G:40:TRP:HB3   | 1:G:107:PHE:O    | 2.17                     | 0.45              |
| 1:G:37:MET:HG2   | 1:G:38:HIS:NE2   | 2.32                     | 0.45              |
| 2:N:90:GLU:O     | 2:N:93:ALA:HB3   | 2.16                     | 0.45              |
| 1:O:167:GLY:CA   | 1:O:169:GLU:OE1  | 2.64                     | 0.45              |
| 1:A:14:LEU:HD22  | 1:A:18:THR:HG23  | 1.99                     | 0.45              |
| 1:A:48:LEU:CD1   | 1:A:73:LEU:HD12  | 2.46                     | 0.45              |
| 1:G:204:ALA:O    | 1:G:205:LEU:HB3  | 2.17                     | 0.45              |
| 2:H:64:LEU:HA    | 2:H:64:LEU:HD12  | 1.58                     | 0.45              |
| 2:L:87:THR:OG1   | 2:L:90:GLU:HG3   | 2.16                     | 0.45              |
| 1:O:105:THR:HG21 | 1:O:113:ALA:HB2  | 1.98                     | 0.45              |
| 1:C:132:THR:OG1  | 2:D:189:GLU:OE1  | 2.25                     | 0.45              |
| 2:D:127:VAL:HG21 | 2:D:142:ILE:HD12 | 1.98                     | 0.45              |
| 2:J:55:ILE:O     | 2:J:58:MET:HG3   | 2.17                     | 0.45              |
| 2:J:97:THR:HG22  | 2:J:98:SER:O     | 2.16                     | 0.45              |
| 2:P:158:TYR:CE2  | 2:P:160:ASP:HB2  | 2.52                     | 0.45              |
| 1:E:90:THR:HB    | 1:E:91:PRO:CD    | 2.46                     | 0.45              |
| 1:C:14:LEU:HD22  | 1:C:18:THR:HG23  | 1.99                     | 0.44              |
| 1:C:66:GLY:HA3   | 1:C:84:PHE:O     | 2.17                     | 0.44              |
| 1:I:37:MET:HB2   | 1:I:37:MET:HE3   | 1.73                     | 0.44              |
| 1:O:137:ILE:HD11 | 1:O:188:VAL:CG2  | 2.47                     | 0.44              |
| 1:G:77:PHE:HB3   | 1:G:78:PRO:HD2   | 1.99                     | 0.44              |
| 1:C:49:VAL:HB    | 1:C:180:ILE:HD13 | 1.99                     | 0.44              |
| 2:F:64:LEU:HD12  | 2:F:64:LEU:HA    | 1.64                     | 0.44              |
| 2:L:19:THR:HB    | 5:L:314:HOH:O    | 2.17                     | 0.44              |
| 1:O:80:HIS:O     | 1:O:155:ASP:HA   | 2.17                     | 0.44              |
| 2:B:126:HIS:HB2  | 2:B:205:ALA:HB2  | 1.99                     | 0.44              |
| 2:B:12:GLY:HA3   | 2:L:1:MET:CE     | 2.48                     | 0.44              |
| 1:M:27:GLN:HB2   | 5:M:462:HOH:O    | 2.18                     | 0.44              |
| 2:D:53:HIS:O     | 2:D:57:ARG:HG2   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:53:HIS:CG    | 2:N:135:HIS:HB2  | 2.52                     | 0.44              |
| 1:M:82:LYS:HD2   | 2:N:156:TYR:CD1  | 2.52                     | 0.44              |
| 2:N:55:ILE:O     | 2:N:58:MET:HG3   | 2.16                     | 0.44              |
| 1:O:3:ASP:HB2    | 1:O:6:VAL:HG23   | 2.00                     | 0.44              |
| 2:P:157:PRO:O    | 2:P:159:PRO:HD3  | 2.18                     | 0.44              |
| 2:B:64:LEU:HA    | 2:B:64:LEU:HD12  | 1.55                     | 0.44              |
| 2:F:111:PRO:HG2  | 2:F:169:PHE:CD1  | 2.53                     | 0.44              |
| 1:I:155:ASP:HB2  | 2:J:156:TYR:CD2  | 2.53                     | 0.44              |
| 1:M:17:LEU:CD2   | 1:M:21:LEU:HD21  | 2.47                     | 0.44              |
| 2:B:40:LEU:HA    | 2:B:40:LEU:HD12  | 1.86                     | 0.44              |
| 2:F:127:VAL:HG21 | 2:F:142:ILE:HD12 | 1.99                     | 0.44              |
| 2:D:87:THR:OG1   | 2:D:90:GLU:HG3   | 2.17                     | 0.43              |
| 1:I:200:ALA:HB1  | 1:I:201:PRO:HD2  | 2.00                     | 0.43              |
| 2:J:20:HIS:HB3   | 5:J:392:HOH:O    | 2.17                     | 0.43              |
| 1:E:132:THR:O    | 1:E:136:GLU:HG3  | 2.18                     | 0.43              |
| 1:O:205:LEU:HD23 | 1:O:205:LEU:O    | 2.17                     | 0.43              |
| 2:J:104:PRO:HB2  | 2:J:105:SER:HB2  | 1.99                     | 0.43              |
| 2:L:111:PRO:HG2  | 2:L:169:PHE:CD1  | 2.53                     | 0.43              |
| 1:M:29:VAL:HB    | 1:M:30:PRO:HD3   | 2.00                     | 0.43              |
| 1:G:104:CSD:C    | 1:G:105:THR:CG2  | 2.96                     | 0.43              |
| 1:I:154:ALA:N    | 5:I:461:HOH:O    | 2.51                     | 0.43              |
| 1:I:37:MET:HA    | 1:I:37:MET:CE    | 2.45                     | 0.43              |
| 2:L:110:GLN:HB3  | 2:L:111:PRO:HD2  | 2.01                     | 0.43              |
| 1:M:49:VAL:HG13  | 1:M:161:LEU:HD12 | 2.00                     | 0.43              |
| 2:N:47:ASN:OD1   | 2:N:50:GLU:HG3   | 2.18                     | 0.43              |
| 1:K:11:VAL:HG12  | 2:L:32:LYS:HG2   | 2.01                     | 0.43              |
| 1:M:105:THR:HG22 | 1:M:117:TYR:CE2  | 2.54                     | 0.43              |
| 1:C:178:THR:HG22 | 1:C:179:LEU:HD13 | 2.01                     | 0.43              |
| 2:F:137:ARG:HD2  | 2:F:137:ARG:HA   | 1.82                     | 0.43              |
| 1:M:77:PHE:HB3   | 1:M:78:PRO:HD2   | 2.00                     | 0.43              |
| 1:A:41:LEU:HB3   | 1:A:43:GLN:OE1   | 2.18                     | 0.43              |
| 1:E:154:ALA:CA   | 5:E:473:HOH:O    | 2.67                     | 0.43              |
| 1:C:198:LEU:HA   | 1:C:198:LEU:HD23 | 1.75                     | 0.43              |
| 1:A:105:THR:CG2  | 1:A:117:TYR:CE2  | 3.01                     | 0.43              |
| 1:C:116:TRP:CD1  | 2:D:18:LYS:HG2   | 2.54                     | 0.43              |
| 2:D:64:LEU:HA    | 2:D:64:LEU:HD12  | 1.80                     | 0.43              |
| 2:F:92:GLU:CG    | 2:F:98:SER:HA    | 2.48                     | 0.43              |
| 2:H:104:PRO:HB2  | 2:H:105:SER:HB2  | 1.99                     | 0.43              |
| 1:A:48:LEU:HD12  | 1:A:73:LEU:HD12  | 2.00                     | 0.43              |
| 1:I:120:LEU:HB3  | 2:J:13:PHE:CE1   | 2.54                     | 0.43              |
| 1:C:49:VAL:HG22  | 1:C:161:LEU:CD1  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:137:ILE:HD12 | 1:E:188:VAL:HG21 | 2.01                     | 0.42              |
| 1:G:103:SER:HB2  | 1:G:118:LYS:HG3  | 2.00                     | 0.42              |
| 2:J:127:VAL:HG21 | 2:J:142:ILE:HD12 | 1.99                     | 0.42              |
| 2:J:160:ASP:OD2  | 2:J:160:ASP:N    | 2.52                     | 0.42              |
| 1:K:101:LEU:HB2  | 5:K:404:HOH:O    | 2.18                     | 0.42              |
| 1:O:137:ILE:HG22 | 2:P:18:LYS:HB2   | 2.01                     | 0.42              |
| 1:M:17:LEU:O     | 1:M:21:LEU:HD22  | 2.18                     | 0.42              |
| 2:P:19:THR:HG22  | 2:P:20:HIS:O     | 2.19                     | 0.42              |
| 2:D:10:LYS:HE3   | 5:J:381:HOH:O    | 2.19                     | 0.42              |
| 1:G:105:THR:CG2  | 1:G:113:ALA:HB2  | 2.44                     | 0.42              |
| 2:L:19:THR:CG2   | 2:L:20:HIS:N     | 2.83                     | 0.42              |
| 1:C:137:ILE:CD1  | 1:C:188:VAL:HG22 | 2.48                     | 0.42              |
| 1:O:154:ALA:N    | 5:O:412:HOH:O    | 2.51                     | 0.42              |
| 1:O:165:PRO:HB3  | 1:O:192:GLU:HA   | 2.01                     | 0.42              |
| 2:P:78:THR:HG21  | 2:P:102:SER:HB2  | 2.01                     | 0.42              |
| 2:N:40:LEU:HD12  | 2:N:40:LEU:HA    | 1.93                     | 0.42              |
| 1:O:185:LEU:HA   | 1:O:185:LEU:HD12 | 1.88                     | 0.42              |
| 1:G:10:ARG:HA    | 2:H:95:LEU:CD1   | 2.50                     | 0.42              |
| 2:J:165:GLY:HA2  | 2:J:167:TYR:CZ   | 2.55                     | 0.42              |
| 1:K:48:LEU:HD11  | 1:K:70:SER:HA    | 2.01                     | 0.42              |
| 1:O:122:TYR:O    | 1:O:126:ILE:HG22 | 2.18                     | 0.42              |
| 1:A:170:ASP:N    | 1:A:170:ASP:OD1  | 2.49                     | 0.42              |
| 1:G:17:LEU:HA    | 1:G:17:LEU:HD23  | 1.83                     | 0.42              |
| 1:K:193:ALA:HB1  | 1:K:194:PRO:HA   | 2.01                     | 0.42              |
| 2:L:110:GLN:HB3  | 2:L:111:PRO:CD   | 2.50                     | 0.42              |
| 1:O:137:ILE:HD11 | 1:O:188:VAL:HG22 | 2.02                     | 0.42              |
| 1:C:183:ASP:OD1  | 2:D:18:LYS:HE2   | 2.19                     | 0.42              |
| 1:G:49:VAL:HG22  | 1:G:161:LEU:HD13 | 2.01                     | 0.42              |
| 2:H:13:PHE:CD1   | 2:N:60:PRO:HG2   | 2.55                     | 0.42              |
| 2:J:64:LEU:HA    | 2:J:64:LEU:HD12  | 1.67                     | 0.42              |
| 1:M:156:THR:HB   | 5:M:404:HOH:O    | 2.20                     | 0.42              |
| 2:N:103:LEU:HD12 | 2:N:103:LEU:N    | 2.35                     | 0.42              |
| 1:O:155:ASP:HB2  | 2:P:156:TYR:CD2  | 2.55                     | 0.42              |
| 1:C:169:GLU:HG2  | 1:C:169:GLU:H    | 1.47                     | 0.42              |
| 1:C:17:LEU:HA    | 1:C:17:LEU:HD23  | 1.88                     | 0.42              |
| 1:C:137:ILE:CD1  | 1:C:188:VAL:HG21 | 2.50                     | 0.42              |
| 2:D:113:LYS:HA   | 2:D:113:LYS:HD3  | 1.81                     | 0.42              |
| 2:D:127:VAL:O    | 2:D:144:GLY:HA2  | 2.19                     | 0.42              |
| 1:E:155:ASP:N    | 1:E:157:ARG:HH12 | 2.18                     | 0.42              |
| 1:E:48:LEU:HD13  | 1:E:75:PHE:HE2   | 1.85                     | 0.42              |
| 2:J:54:GLY:HA3   | 2:J:75:THR:OG1   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:64:LEU:HA    | 2:N:64:LEU:HD12  | 1.80                     | 0.42              |
| 1:A:155:ASP:N    | 1:A:157:ARG:HH12 | 2.17                     | 0.41              |
| 1:E:10:ARG:HB3   | 2:F:73:PHE:CZ    | 2.55                     | 0.41              |
| 1:G:137:ILE:HD12 | 1:G:188:VAL:HG22 | 2.01                     | 0.41              |
| 1:I:102:CSD:O    | 1:I:123:ARG:HD2  | 2.19                     | 0.41              |
| 1:A:102:CSD:O    | 1:A:103:SER:HB3  | 2.19                     | 0.41              |
| 2:D:145:LYS:HD3  | 2:D:145:LYS:HA   | 1.77                     | 0.41              |
| 2:H:19:THR:CG2   | 2:H:20:HIS:N     | 2.82                     | 0.41              |
| 1:O:156:THR:HB   | 5:O:410:HOH:O    | 2.20                     | 0.41              |
| 1:O:205:LEU:C    | 1:O:205:LEU:CD2  | 2.78                     | 0.41              |
| 2:B:99:VAL:HA    | 2:B:100:PRO:HD3  | 1.86                     | 0.41              |
| 2:B:158:TYR:CE2  | 2:B:160:ASP:HB2  | 2.56                     | 0.41              |
| 1:C:80:HIS:O     | 1:C:155:ASP:HA   | 2.20                     | 0.41              |
| 2:H:137:ARG:HD2  | 2:H:137:ARG:HA   | 1.93                     | 0.41              |
| 1:M:76:SER:O     | 1:M:108:THR:CG2  | 2.67                     | 0.41              |
| 1:O:17:LEU:O     | 1:O:21:LEU:HD22  | 2.20                     | 0.41              |
| 2:B:160:ASP:N    | 2:B:160:ASP:OD2  | 2.53                     | 0.41              |
| 1:G:104:CSD:C    | 1:G:105:THR:HG22 | 2.51                     | 0.41              |
| 1:K:137:ILE:CD1  | 1:K:188:VAL:CG2  | 2.98                     | 0.41              |
| 1:K:185:LEU:HA   | 1:K:185:LEU:HD12 | 1.86                     | 0.41              |
| 1:K:77:PHE:HB3   | 1:K:78:PRO:HD2   | 2.02                     | 0.41              |
| 1:M:85:VAL:HG12  | 1:M:87:LEU:HD13  | 2.02                     | 0.41              |
| 1:A:80:HIS:O     | 1:A:155:ASP:HA   | 2.20                     | 0.41              |
| 1:K:165:PRO:HB3  | 1:K:192:GLU:HA   | 2.03                     | 0.41              |
| 2:D:121:LEU:HA   | 2:D:121:LEU:HD12 | 1.82                     | 0.41              |
| 1:C:137:ILE:HD12 | 1:C:188:VAL:CG2  | 2.51                     | 0.41              |
| 1:G:37:MET:C     | 1:G:38:HIS:CD2   | 2.94                     | 0.41              |
| 2:L:5:HIS:ND1    | 2:L:56:GLU:HG2   | 2.36                     | 0.41              |
| 1:M:64:SER:HB3   | 5:M:484:HOH:O    | 2.21                     | 0.41              |
| 1:O:10:ARG:HB3   | 2:P:73:PHE:CZ    | 2.56                     | 0.41              |
| 2:P:179:LYS:HD3  | 2:P:181:LYS:HE3  | 2.03                     | 0.41              |
| 2:P:55:ILE:O     | 2:P:58:MET:HG3   | 2.20                     | 0.41              |
| 1:A:198:LEU:HB3  | 1:A:199:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:165:PRO:HB3  | 1:C:192:GLU:HA   | 2.03                     | 0.41              |
| 2:F:121:LEU:HA   | 2:F:121:LEU:HD12 | 1.91                     | 0.41              |
| 1:M:3:ASP:CB     | 1:M:6:VAL:HG23   | 2.51                     | 0.41              |
| 2:F:106:SER:OG   | 2:F:107:PRO:HD2  | 2.21                     | 0.41              |
| 2:J:92:GLU:O     | 2:J:95:LEU:O     | 2.39                     | 0.41              |
| 1:M:180:ILE:N    | 1:M:180:ILE:HD12 | 2.36                     | 0.41              |
| 1:M:90:THR:HB    | 1:M:91:PRO:CD    | 2.51                     | 0.41              |
| 2:L:137:ARG:HA   | 2:L:137:ARG:HD2  | 1.90                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:45:ILE:O     | 2:N:83:LYS:HD2   | 2.21                     | 0.41              |
| 1:O:66:GLY:HA3   | 1:O:84:PHE:O     | 2.21                     | 0.41              |
| 2:H:19:THR:HB    | 5:H:326:HOH:O    | 2.21                     | 0.41              |
| 2:J:66:ALA:HB1   | 2:J:70:GLU:HB3   | 2.02                     | 0.41              |
| 1:M:198:LEU:HA   | 1:M:198:LEU:HD23 | 1.81                     | 0.41              |
| 2:P:7:LEU:O      | 2:P:10:LYS:HB2   | 2.20                     | 0.41              |
| 2:D:97:THR:CG2   | 2:D:98:SER:H     | 2.33                     | 0.40              |
| 1:C:105:THR:HG22 | 1:C:117:TYR:CE2  | 2.56                     | 0.40              |
| 2:F:27:GLU:HA    | 5:F:400:HOH:O    | 2.21                     | 0.40              |
| 1:G:90:THR:HB    | 1:G:91:PRO:CD    | 2.51                     | 0.40              |
| 1:I:205:LEU:HD23 | 1:I:206:GLY:N    | 2.37                     | 0.40              |
| 1:M:108:THR:CG2  | 1:M:109:ILE:HG12 | 2.50                     | 0.40              |
| 1:A:185:LEU:HA   | 1:A:185:LEU:HD12 | 1.88                     | 0.40              |
| 1:A:55:ASP:OD1   | 1:A:55:ASP:C     | 2.60                     | 0.40              |
| 1:A:79:LYS:HE2   | 5:B:407:HOH:O    | 2.22                     | 0.40              |
| 2:B:55:ILE:HG23  | 2:B:71:ARG:HB3   | 2.04                     | 0.40              |
| 1:E:119:GLU:HB3  | 5:E:407:HOH:O    | 2.21                     | 0.40              |
| 2:H:22:ALA:O     | 2:H:23:LYS:HB2   | 2.22                     | 0.40              |
| 1:M:155:ASP:H    | 1:M:157:ARG:HH12 | 1.68                     | 0.40              |
| 1:C:10:ARG:HB3   | 2:D:73:PHE:CZ    | 2.56                     | 0.40              |
| 2:P:113:LYS:HA   | 2:P:113:LYS:HD3  | 1.84                     | 0.40              |
| 2:F:183:LEU:HA   | 2:F:183:LEU:HD12 | 1.83                     | 0.40              |
| 2:F:63:TYR:CD2   | 2:F:63:TYR:C     | 2.94                     | 0.40              |
| 1:G:155:ASP:HB2  | 2:H:156:TYR:CD2  | 2.56                     | 0.40              |
| 1:G:155:ASP:N    | 1:G:157:ARG:HH12 | 2.18                     | 0.40              |
| 1:I:164:ARG:HA   | 1:I:165:PRO:HD3  | 1.88                     | 0.40              |
| 1:I:90:THR:HB    | 1:I:91:PRO:CD    | 2.52                     | 0.40              |
| 2:J:174:TYR:HE2  | 2:J:199:GLN:HG3  | 1.86                     | 0.40              |
| 1:O:43:GLN:NE2   | 1:O:43:GLN:N     | 2.46                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 5:C:490:HOH:O | 5:O:511:HOH:O[2_555] | 1.77                     | 0.43              |
| 5:F:376:HOH:O | 5:P:374:HOH:O[1_565] | 2.12                     | 0.08              |



## 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     | 202/209 (97%)   | 192 (95%)  | 8 (4%)   | 2 (1%)   | 18          | 24 |
| 1   | C     | 202/209 (97%)   | 195 (96%)  | 6 (3%)   | 1 (0%)   | 32          | 44 |
| 1   | E     | 202/209 (97%)   | 195 (96%)  | 4 (2%)   | 3 (2%)   | 12          | 15 |
| 1   | G     | 202/209 (97%)   | 193 (96%)  | 6 (3%)   | 3 (2%)   | 12          | 15 |
| 1   | I     | 202/209 (97%)   | 196 (97%)  | 4 (2%)   | 2 (1%)   | 18          | 24 |
| 1   | K     | 202/209 (97%)   | 194 (96%)  | 5 (2%)   | 3 (2%)   | 12          | 15 |
| 1   | M     | 202/209 (97%)   | 194 (96%)  | 7 (4%)   | 1 (0%)   | 32          | 44 |
| 1   | O     | 202/209 (97%)   | 194 (96%)  | 6 (3%)   | 2 (1%)   | 18          | 24 |
| 2   | B     | 204/206 (99%)   | 196 (96%)  | 6 (3%)   | 2 (1%)   | 18          | 24 |
| 2   | D     | 204/206 (99%)   | 196 (96%)  | 4 (2%)   | 4 (2%)   | 9           | 9  |
| 2   | F     | 204/206 (99%)   | 194 (95%)  | 6 (3%)   | 4 (2%)   | 9           | 9  |
| 2   | H     | 204/206 (99%)   | 194 (95%)  | 6 (3%)   | 4 (2%)   | 9           | 9  |
| 2   | J     | 204/206 (99%)   | 190 (93%)  | 11 (5%)  | 3 (2%)   | 12          | 15 |
| 2   | L     | 204/206 (99%)   | 195 (96%)  | 6 (3%)   | 3 (2%)   | 12          | 15 |
| 2   | N     | 204/206 (99%)   | 192 (94%)  | 7 (3%)   | 5 (2%)   | 6           | 6  |
| 2   | P     | 204/206 (99%)   | 191 (94%)  | 11 (5%)  | 2 (1%)   | 18          | 24 |
| All | All   | 3248/3320 (98%) | 3101 (96%) | 103 (3%) | 44 (1%)  | 13          | 16 |

All (44) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 103 | SER  |
| 1   | A     | 154 | ALA  |
| 2   | B     | 106 | SER  |
| 1   | C     | 154 | ALA  |
| 2   | D     | 105 | SER  |
| 1   | E     | 103 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 154 | ALA  |
| 1   | E     | 205 | LEU  |
| 2   | F     | 105 | SER  |
| 2   | F     | 106 | SER  |
| 1   | G     | 103 | SER  |
| 1   | G     | 154 | ALA  |
| 2   | H     | 105 | SER  |
| 2   | H     | 106 | SER  |
| 1   | I     | 154 | ALA  |
| 1   | K     | 154 | ALA  |
| 1   | K     | 205 | LEU  |
| 2   | L     | 105 | SER  |
| 2   | L     | 106 | SER  |
| 1   | M     | 154 | ALA  |
| 2   | N     | 105 | SER  |
| 1   | O     | 154 | ALA  |
| 2   | P     | 105 | SER  |
| 2   | B     | 105 | SER  |
| 2   | J     | 105 | SER  |
| 1   | K     | 206 | GLY  |
| 1   | O     | 103 | SER  |
| 2   | D     | 8   | GLY  |
| 2   | D     | 106 | SER  |
| 1   | G     | 205 | LEU  |
| 2   | H     | 96  | GLY  |
| 2   | D     | 21  | ASN  |
| 2   | J     | 106 | SER  |
| 2   | N     | 8   | GLY  |
| 2   | F     | 23  | LYS  |
| 2   | H     | 23  | LYS  |
| 1   | I     | 103 | SER  |
| 2   | J     | 23  | LYS  |
| 2   | N     | 23  | LYS  |
| 2   | P     | 106 | SER  |
| 2   | L     | 8   | GLY  |
| 2   | F     | 8   | GLY  |
| 2   | N     | 106 | SER  |
| 2   | N     | 185 | PRO  |

### 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     | 172/175 (98%)   | 151 (88%)  | 21 (12%)  | 6           | 6  |
| 1   | C     | 172/175 (98%)   | 149 (87%)  | 23 (13%)  | 4           | 5  |
| 1   | E     | 172/175 (98%)   | 152 (88%)  | 20 (12%)  | 6           | 7  |
| 1   | G     | 172/175 (98%)   | 155 (90%)  | 17 (10%)  | 9           | 12 |
| 1   | I     | 172/175 (98%)   | 152 (88%)  | 20 (12%)  | 6           | 7  |
| 1   | K     | 172/175 (98%)   | 153 (89%)  | 19 (11%)  | 7           | 9  |
| 1   | M     | 172/175 (98%)   | 156 (91%)  | 16 (9%)   | 10          | 14 |
| 1   | O     | 172/175 (98%)   | 149 (87%)  | 23 (13%)  | 4           | 5  |
| 2   | B     | 164/164 (100%)  | 152 (93%)  | 12 (7%)   | 16          | 23 |
| 2   | D     | 164/164 (100%)  | 149 (91%)  | 15 (9%)   | 11          | 15 |
| 2   | F     | 164/164 (100%)  | 151 (92%)  | 13 (8%)   | 14          | 20 |
| 2   | H     | 164/164 (100%)  | 152 (93%)  | 12 (7%)   | 16          | 23 |
| 2   | J     | 164/164 (100%)  | 148 (90%)  | 16 (10%)  | 9           | 12 |
| 2   | L     | 164/164 (100%)  | 149 (91%)  | 15 (9%)   | 11          | 15 |
| 2   | N     | 164/164 (100%)  | 153 (93%)  | 11 (7%)   | 19          | 27 |
| 2   | P     | 164/164 (100%)  | 147 (90%)  | 17 (10%)  | 8           | 10 |
| All | All   | 2688/2712 (99%) | 2418 (90%) | 270 (10%) | 9           | 12 |

All (270) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | LEU  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 21  | LEU  |
| 1   | A     | 48  | LEU  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 76  | SER  |
| 1   | A     | 79  | LYS  |
| 1   | A     | 87  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 101 | LEU  |
| 1   | A     | 108 | THR  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 137 | ILE  |
| 1   | A     | 155 | ASP  |
| 1   | A     | 166 | GLN  |
| 1   | A     | 169 | GLU  |
| 1   | A     | 178 | THR  |
| 1   | A     | 179 | LEU  |
| 1   | A     | 185 | LEU  |
| 1   | A     | 191 | LEU  |
| 1   | A     | 205 | LEU  |
| 2   | B     | 10  | LYS  |
| 2   | B     | 18  | LYS  |
| 2   | B     | 34  | ASN  |
| 2   | B     | 40  | LEU  |
| 2   | B     | 42  | SER  |
| 2   | B     | 65  | THR  |
| 2   | B     | 67  | SER  |
| 2   | B     | 79  | LEU  |
| 2   | B     | 105 | SER  |
| 2   | B     | 121 | LEU  |
| 2   | B     | 160 | ASP  |
| 2   | B     | 183 | LEU  |
| 1   | C     | 3   | ASP  |
| 1   | C     | 14  | LEU  |
| 1   | C     | 19  | LYS  |
| 1   | C     | 21  | LEU  |
| 1   | C     | 27  | GLN  |
| 1   | C     | 37  | MET  |
| 1   | C     | 48  | LEU  |
| 1   | C     | 65  | GLU  |
| 1   | C     | 79  | LYS  |
| 1   | C     | 87  | LEU  |
| 1   | C     | 101 | LEU  |
| 1   | C     | 105 | THR  |
| 1   | C     | 108 | THR  |
| 1   | C     | 120 | LEU  |
| 1   | C     | 134 | LEU  |
| 1   | C     | 137 | ILE  |
| 1   | C     | 169 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 178 | THR  |
| 1   | C     | 179 | LEU  |
| 1   | C     | 185 | LEU  |
| 1   | C     | 188 | VAL  |
| 1   | C     | 191 | LEU  |
| 1   | C     | 203 | VAL  |
| 2   | D     | 1   | MET  |
| 2   | D     | 18  | LYS  |
| 2   | D     | 19  | THR  |
| 2   | D     | 34  | ASN  |
| 2   | D     | 40  | LEU  |
| 2   | D     | 65  | THR  |
| 2   | D     | 79  | LEU  |
| 2   | D     | 99  | VAL  |
| 2   | D     | 105 | SER  |
| 2   | D     | 113 | LYS  |
| 2   | D     | 121 | LEU  |
| 2   | D     | 160 | ASP  |
| 2   | D     | 166 | GLU  |
| 2   | D     | 183 | LEU  |
| 2   | D     | 186 | ASP  |
| 1   | E     | 12  | ASP  |
| 1   | E     | 14  | LEU  |
| 1   | E     | 21  | LEU  |
| 1   | E     | 37  | MET  |
| 1   | E     | 48  | LEU  |
| 1   | E     | 79  | LYS  |
| 1   | E     | 87  | LEU  |
| 1   | E     | 101 | LEU  |
| 1   | E     | 105 | THR  |
| 1   | E     | 108 | THR  |
| 1   | E     | 120 | LEU  |
| 1   | E     | 134 | LEU  |
| 1   | E     | 137 | ILE  |
| 1   | E     | 166 | GLN  |
| 1   | E     | 169 | GLU  |
| 1   | E     | 178 | THR  |
| 1   | E     | 179 | LEU  |
| 1   | E     | 185 | LEU  |
| 1   | E     | 191 | LEU  |
| 1   | E     | 205 | LEU  |
| 2   | F     | 10  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 18  | LYS  |
| 2   | F     | 34  | ASN  |
| 2   | F     | 40  | LEU  |
| 2   | F     | 65  | THR  |
| 2   | F     | 67  | SER  |
| 2   | F     | 79  | LEU  |
| 2   | F     | 105 | SER  |
| 2   | F     | 121 | LEU  |
| 2   | F     | 124 | ARG  |
| 2   | F     | 150 | VAL  |
| 2   | F     | 160 | ASP  |
| 2   | F     | 183 | LEU  |
| 1   | G     | 3   | ASP  |
| 1   | G     | 12  | ASP  |
| 1   | G     | 14  | LEU  |
| 1   | G     | 21  | LEU  |
| 1   | G     | 48  | LEU  |
| 1   | G     | 87  | LEU  |
| 1   | G     | 101 | LEU  |
| 1   | G     | 105 | THR  |
| 1   | G     | 108 | THR  |
| 1   | G     | 120 | LEU  |
| 1   | G     | 134 | LEU  |
| 1   | G     | 166 | GLN  |
| 1   | G     | 179 | LEU  |
| 1   | G     | 185 | LEU  |
| 1   | G     | 188 | VAL  |
| 1   | G     | 191 | LEU  |
| 1   | G     | 203 | VAL  |
| 2   | H     | 10  | LYS  |
| 2   | H     | 18  | LYS  |
| 2   | H     | 19  | THR  |
| 2   | H     | 32  | LYS  |
| 2   | H     | 34  | ASN  |
| 2   | H     | 40  | LEU  |
| 2   | H     | 79  | LEU  |
| 2   | H     | 95  | LEU  |
| 2   | H     | 105 | SER  |
| 2   | H     | 113 | LYS  |
| 2   | H     | 160 | ASP  |
| 2   | H     | 183 | LEU  |
| 1   | I     | 2   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 3   | ASP  |
| 1   | I     | 14  | LEU  |
| 1   | I     | 17  | LEU  |
| 1   | I     | 21  | LEU  |
| 1   | I     | 27  | GLN  |
| 1   | I     | 43  | GLN  |
| 1   | I     | 48  | LEU  |
| 1   | I     | 87  | LEU  |
| 1   | I     | 101 | LEU  |
| 1   | I     | 103 | SER  |
| 1   | I     | 120 | LEU  |
| 1   | I     | 134 | LEU  |
| 1   | I     | 155 | ASP  |
| 1   | I     | 169 | GLU  |
| 1   | I     | 178 | THR  |
| 1   | I     | 179 | LEU  |
| 1   | I     | 185 | LEU  |
| 1   | I     | 191 | LEU  |
| 1   | I     | 205 | LEU  |
| 2   | J     | 4   | MET  |
| 2   | J     | 10  | LYS  |
| 2   | J     | 32  | LYS  |
| 2   | J     | 40  | LEU  |
| 2   | J     | 65  | THR  |
| 2   | J     | 79  | LEU  |
| 2   | J     | 92  | GLU  |
| 2   | J     | 99  | VAL  |
| 2   | J     | 105 | SER  |
| 2   | J     | 113 | LYS  |
| 2   | J     | 124 | ARG  |
| 2   | J     | 150 | VAL  |
| 2   | J     | 160 | ASP  |
| 2   | J     | 181 | LYS  |
| 2   | J     | 183 | LEU  |
| 2   | J     | 206 | GLU  |
| 1   | K     | 3   | ASP  |
| 1   | K     | 14  | LEU  |
| 1   | K     | 21  | LEU  |
| 1   | K     | 37  | MET  |
| 1   | K     | 48  | LEU  |
| 1   | K     | 61  | GLN  |
| 1   | K     | 87  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 101 | LEU  |
| 1   | K     | 108 | THR  |
| 1   | K     | 120 | LEU  |
| 1   | K     | 134 | LEU  |
| 1   | K     | 137 | ILE  |
| 1   | K     | 178 | THR  |
| 1   | K     | 179 | LEU  |
| 1   | K     | 185 | LEU  |
| 1   | K     | 188 | VAL  |
| 1   | K     | 191 | LEU  |
| 1   | K     | 203 | VAL  |
| 1   | K     | 205 | LEU  |
| 2   | L     | 10  | LYS  |
| 2   | L     | 18  | LYS  |
| 2   | L     | 19  | THR  |
| 2   | L     | 32  | LYS  |
| 2   | L     | 34  | ASN  |
| 2   | L     | 40  | LEU  |
| 2   | L     | 67  | SER  |
| 2   | L     | 79  | LEU  |
| 2   | L     | 99  | VAL  |
| 2   | L     | 105 | SER  |
| 2   | L     | 113 | LYS  |
| 2   | L     | 121 | LEU  |
| 2   | L     | 160 | ASP  |
| 2   | L     | 166 | GLU  |
| 2   | L     | 183 | LEU  |
| 1   | M     | 14  | LEU  |
| 1   | M     | 21  | LEU  |
| 1   | M     | 43  | GLN  |
| 1   | M     | 48  | LEU  |
| 1   | M     | 87  | LEU  |
| 1   | M     | 101 | LEU  |
| 1   | M     | 105 | THR  |
| 1   | M     | 108 | THR  |
| 1   | M     | 120 | LEU  |
| 1   | M     | 134 | LEU  |
| 1   | M     | 169 | GLU  |
| 1   | M     | 178 | THR  |
| 1   | M     | 179 | LEU  |
| 1   | M     | 185 | LEU  |
| 1   | M     | 191 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 205 | LEU  |
| 2   | N     | 10  | LYS  |
| 2   | N     | 40  | LEU  |
| 2   | N     | 65  | THR  |
| 2   | N     | 67  | SER  |
| 2   | N     | 79  | LEU  |
| 2   | N     | 92  | GLU  |
| 2   | N     | 98  | SER  |
| 2   | N     | 105 | SER  |
| 2   | N     | 160 | ASP  |
| 2   | N     | 181 | LYS  |
| 2   | N     | 183 | LEU  |
| 1   | O     | 3   | ASP  |
| 1   | O     | 14  | LEU  |
| 1   | O     | 17  | LEU  |
| 1   | O     | 21  | LEU  |
| 1   | O     | 43  | GLN  |
| 1   | O     | 48  | LEU  |
| 1   | O     | 87  | LEU  |
| 1   | O     | 101 | LEU  |
| 1   | O     | 103 | SER  |
| 1   | O     | 108 | THR  |
| 1   | O     | 119 | GLU  |
| 1   | O     | 120 | LEU  |
| 1   | O     | 134 | LEU  |
| 1   | O     | 137 | ILE  |
| 1   | O     | 143 | GLU  |
| 1   | O     | 155 | ASP  |
| 1   | O     | 169 | GLU  |
| 1   | O     | 178 | THR  |
| 1   | O     | 179 | LEU  |
| 1   | O     | 185 | LEU  |
| 1   | O     | 188 | VAL  |
| 1   | O     | 191 | LEU  |
| 1   | O     | 205 | LEU  |
| 2   | P     | 10  | LYS  |
| 2   | P     | 18  | LYS  |
| 2   | P     | 34  | ASN  |
| 2   | P     | 40  | LEU  |
| 2   | P     | 65  | THR  |
| 2   | P     | 67  | SER  |
| 2   | P     | 79  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 92  | GLU  |
| 2   | P     | 99  | VAL  |
| 2   | P     | 105 | SER  |
| 2   | P     | 113 | LYS  |
| 2   | P     | 121 | LEU  |
| 2   | P     | 124 | ARG  |
| 2   | P     | 150 | VAL  |
| 2   | P     | 160 | ASP  |
| 2   | P     | 183 | LEU  |
| 2   | P     | 206 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 38  | HIS  |
| 2   | D     | 5   | HIS  |
| 1   | G     | 38  | HIS  |
| 1   | I     | 43  | GLN  |
| 1   | M     | 38  | HIS  |
| 1   | M     | 43  | GLN  |
| 1   | O     | 38  | HIS  |
| 1   | O     | 43  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | CSD  | A     | 102 | 1,4  | 4,7,8        | 1.45 | 0        | 2,8,10      | 3.23 | 2 (100%) |
| 1   | CSD  | A     | 104 | 1,4  | 4,7,8        | 1.29 | 1 (25%)  | 2,8,10      | 1.97 | 1 (50%)  |
| 1   | CSD  | C     | 102 | 1,4  | 4,7,8        | 1.52 | 0        | 2,8,10      | 3.86 | 2 (100%) |
| 1   | CSD  | C     | 104 | 1,4  | 4,7,8        | 1.51 | 1 (25%)  | 2,8,10      | 1.76 | 1 (50%)  |
| 1   | CSD  | E     | 102 | 1,4  | 4,7,8        | 1.52 | 1 (25%)  | 2,8,10      | 3.95 | 2 (100%) |
| 1   | CSD  | E     | 104 | 1,4  | 4,7,8        | 1.44 | 1 (25%)  | 2,8,10      | 1.93 | 1 (50%)  |
| 1   | CSD  | G     | 102 | 1,4  | 4,7,8        | 1.30 | 1 (25%)  | 2,8,10      | 3.56 | 2 (100%) |
| 1   | CSD  | G     | 104 | 1,4  | 4,7,8        | 1.31 | 0        | 2,8,10      | 1.54 | 0        |
| 1   | CSD  | I     | 102 | 1,4  | 4,7,8        | 1.32 | 0        | 2,8,10      | 3.43 | 2 (100%) |
| 1   | CSD  | I     | 104 | 1,4  | 4,7,8        | 1.31 | 0        | 2,8,10      | 1.72 | 0        |
| 1   | CSD  | K     | 102 | 1,4  | 4,7,8        | 1.21 | 1 (25%)  | 2,8,10      | 3.67 | 2 (100%) |
| 1   | CSD  | K     | 104 | 1,4  | 4,7,8        | 1.46 | 1 (25%)  | 2,8,10      | 1.55 | 0        |
| 1   | CSD  | M     | 102 | 1,4  | 4,7,8        | 1.36 | 0        | 2,8,10      | 3.75 | 2 (100%) |
| 1   | CSD  | M     | 104 | 1,4  | 4,7,8        | 1.45 | 1 (25%)  | 2,8,10      | 1.73 | 1 (50%)  |
| 1   | CSD  | O     | 102 | 1,4  | 4,7,8        | 1.20 | 0        | 2,8,10      | 3.88 | 2 (100%) |
| 1   | CSD  | O     | 104 | 1,4  | 4,7,8        | 1.36 | 1 (25%)  | 2,8,10      | 1.76 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | CSD  | A     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | A     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | C     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | C     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | E     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | E     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | G     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | G     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | I     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | I     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | K     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | K     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | M     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | M     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | O     | 102 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |
| 1   | CSD  | O     | 104 | 1,4  | -       | 0/2/6/8  | 0/0/0/0 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | K     | 104 | CSD  | CB-SG | -2.21 | 1.66        | 1.79     |
| 1   | C     | 104 | CSD  | CB-SG | -2.19 | 1.66        | 1.79     |
| 1   | E     | 104 | CSD  | CB-SG | -2.06 | 1.67        | 1.79     |
| 1   | G     | 102 | CSD  | CB-SG | -2.05 | 1.67        | 1.79     |
| 1   | M     | 104 | CSD  | CB-SG | -2.03 | 1.67        | 1.79     |
| 1   | K     | 102 | CSD  | CB-SG | -2.02 | 1.67        | 1.79     |
| 1   | O     | 104 | CSD  | CB-SG | -2.01 | 1.67        | 1.79     |
| 1   | A     | 104 | CSD  | CB-SG | -2.01 | 1.67        | 1.79     |
| 1   | E     | 102 | CSD  | CB-SG | -2.00 | 1.67        | 1.79     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 102 | CSD  | O-C-CA    | -2.91 | 116.98      | 125.02   |
| 1   | A     | 102 | CSD  | O-C-CA    | -2.79 | 117.32      | 125.02   |
| 1   | G     | 102 | CSD  | O-C-CA    | -2.64 | 117.74      | 125.02   |
| 1   | I     | 102 | CSD  | O-C-CA    | -2.64 | 117.74      | 125.02   |
| 1   | E     | 102 | CSD  | O-C-CA    | -2.56 | 117.94      | 125.02   |
| 1   | M     | 102 | CSD  | O-C-CA    | -2.48 | 118.17      | 125.02   |
| 1   | E     | 104 | CSD  | O-C-CA    | -2.46 | 118.22      | 125.02   |
| 1   | K     | 102 | CSD  | O-C-CA    | -2.27 | 118.75      | 125.02   |
| 1   | C     | 104 | CSD  | O-C-CA    | -2.26 | 118.79      | 125.02   |
| 1   | C     | 102 | CSD  | O-C-CA    | -2.09 | 119.23      | 125.02   |
| 1   | M     | 104 | CSD  | O-C-CA    | -2.08 | 119.27      | 125.02   |
| 1   | A     | 104 | CSD  | O-C-CA    | -2.02 | 119.44      | 125.02   |
| 1   | A     | 102 | CSD  | OD1-SG-CB | 3.63  | 112.41      | 105.61   |
| 1   | I     | 102 | CSD  | OD1-SG-CB | 4.07  | 113.24      | 105.61   |
| 1   | G     | 102 | CSD  | OD1-SG-CB | 4.29  | 113.65      | 105.61   |
| 1   | O     | 102 | CSD  | OD1-SG-CB | 4.65  | 114.32      | 105.61   |
| 1   | K     | 102 | CSD  | OD1-SG-CB | 4.67  | 114.36      | 105.61   |
| 1   | M     | 102 | CSD  | OD1-SG-CB | 4.69  | 114.39      | 105.61   |
| 1   | E     | 102 | CSD  | OD1-SG-CB | 4.97  | 114.93      | 105.61   |
| 1   | C     | 102 | CSD  | OD1-SG-CB | 5.04  | 115.05      | 105.61   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | A     | 102 | CSD  | 1       | 0            |
| 1   | C     | 104 | CSD  | 2       | 0            |
| 1   | E     | 102 | CSD  | 2       | 0            |
| 1   | E     | 104 | CSD  | 4       | 0            |
| 1   | G     | 102 | CSD  | 1       | 0            |
| 1   | G     | 104 | CSD  | 2       | 0            |
| 1   | I     | 102 | CSD  | 1       | 0            |
| 1   | M     | 102 | CSD  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | PO4  | A     | 301 | -    | 4,4,4        | 0.75 | 0           | 6,6,6       | 0.41 | 0           |
| 3   | PO4  | C     | 301 | -    | 4,4,4        | 0.69 | 0           | 6,6,6       | 0.43 | 0           |
| 3   | PO4  | E     | 301 | -    | 4,4,4        | 0.62 | 0           | 6,6,6       | 0.82 | 0           |
| 3   | PO4  | G     | 301 | -    | 4,4,4        | 0.67 | 0           | 6,6,6       | 0.93 | 0           |
| 3   | PO4  | I     | 301 | -    | 4,4,4        | 0.73 | 0           | 6,6,6       | 0.47 | 0           |
| 3   | PO4  | K     | 301 | -    | 4,4,4        | 0.70 | 0           | 6,6,6       | 0.41 | 0           |
| 3   | PO4  | M     | 301 | -    | 4,4,4        | 0.75 | 0           | 6,6,6       | 0.40 | 0           |
| 3   | PO4  | O     | 301 | -    | 4,4,4        | 0.68 | 0           | 6,6,6       | 0.48 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | PO4  | A     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | PO4  | C     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | PO4  | E     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | PO4  | G     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | PO4  | I     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | PO4  | K     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | PO4  | M     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 3   | PO4  | O     | 301 | -    | -       | 0/0/0/0  | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 301 | PO4  | 1       | 0            |
| 3   | E     | 301 | PO4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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     | 204/209 (97%)   | 0.07   | 1 (0%) 90 91  | 32, 45, 70, 131       | 0       |
| 1   | C     | 204/209 (97%)   | 0.06   | 1 (0%) 90 91  | 31, 45, 66, 87        | 1 (0%)  |
| 1   | E     | 204/209 (97%)   | 0.10   | 1 (0%) 90 91  | 32, 45, 69, 90        | 1 (0%)  |
| 1   | G     | 204/209 (97%)   | 0.06   | 0 100 100     | 33, 45, 69, 91        | 1 (0%)  |
| 1   | I     | 204/209 (97%)   | 0.06   | 0 100 100     | 33, 44, 68, 102       | 0       |
| 1   | K     | 204/209 (97%)   | 0.07   | 1 (0%) 90 91  | 33, 45, 68, 110       | 1 (0%)  |
| 1   | M     | 204/209 (97%)   | 0.07   | 1 (0%) 90 91  | 33, 45, 69, 125       | 1 (0%)  |
| 1   | O     | 204/209 (97%)   | 0.09   | 1 (0%) 90 91  | 32, 45, 70, 120       | 0       |
| 2   | B     | 206/206 (100%)  | 0.10   | 1 (0%) 90 91  | 31, 44, 77, 100       | 0       |
| 2   | D     | 206/206 (100%)  | 0.12   | 0 100 100     | 30, 43, 75, 98        | 0       |
| 2   | F     | 206/206 (100%)  | 0.11   | 1 (0%) 90 91  | 30, 43, 74, 96        | 0       |
| 2   | H     | 206/206 (100%)  | 0.07   | 0 100 100     | 33, 43, 77, 96        | 0       |
| 2   | J     | 206/206 (100%)  | 0.08   | 1 (0%) 90 91  | 31, 44, 76, 100       | 0       |
| 2   | L     | 206/206 (100%)  | 0.04   | 1 (0%) 90 91  | 31, 44, 75, 96        | 0       |
| 2   | N     | 206/206 (100%)  | 0.09   | 1 (0%) 90 91  | 30, 45, 79, 102       | 0       |
| 2   | P     | 206/206 (100%)  | 0.10   | 1 (0%) 90 91  | 31, 44, 76, 102       | 0       |
| All | All   | 3280/3320 (98%) | 0.08   | 12 (0%) 92 93 | 30, 44, 75, 131       | 5 (0%)  |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 207 | ALA  | 5.9  |
| 1   | M     | 207 | ALA  | 5.9  |
| 1   | O     | 207 | ALA  | 4.4  |
| 1   | E     | 207 | ALA  | 3.0  |
| 1   | K     | 207 | ALA  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | P     | 116 | GLU  | 2.7  |
| 2   | B     | 167 | TYR  | 2.4  |
| 2   | F     | 22  | ALA  | 2.4  |
| 2   | N     | 95  | LEU  | 2.3  |
| 2   | J     | 95  | LEU  | 2.2  |
| 2   | L     | 22  | ALA  | 2.2  |
| 1   | C     | 207 | ALA  | 2.1  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 1   | CSD  | I     | 104 | 8/9   | 0.96 | 0.13 | -    | 57,60,75,77                | 8     |
| 1   | CSD  | O     | 104 | 8/9   | 0.97 | 0.14 | -    | 52,55,76,78                | 8     |
| 1   | CSD  | M     | 104 | 8/9   | 0.97 | 0.12 | -    | 46,49,73,77                | 8     |
| 1   | CSD  | E     | 102 | 8/9   | 0.93 | 0.19 | -    | 34,49,57,60                | 8     |
| 1   | CSD  | G     | 102 | 8/9   | 0.95 | 0.20 | -    | 37,52,61,66                | 8     |
| 1   | CSD  | A     | 102 | 8/9   | 0.94 | 0.13 | -    | 39,54,61,64                | 8     |
| 1   | CSD  | C     | 102 | 8/9   | 0.92 | 0.19 | -    | 40,55,64,66                | 8     |
| 1   | CSD  | M     | 102 | 8/9   | 0.95 | 0.14 | -    | 41,49,63,63                | 8     |
| 1   | CSD  | O     | 102 | 8/9   | 0.94 | 0.14 | -    | 47,51,61,70                | 8     |
| 1   | CSD  | I     | 102 | 8/9   | 0.96 | 0.14 | -    | 50,62,69,69                | 0     |
| 1   | CSD  | K     | 102 | 8/9   | 0.96 | 0.19 | -    | 34,47,59,60                | 8     |
| 1   | CSD  | C     | 104 | 8/9   | 0.98 | 0.13 | -    | 51,53,66,69                | 8     |
| 1   | CSD  | A     | 104 | 8/9   | 0.96 | 0.13 | -    | 42,50,72,76                | 8     |
| 1   | CSD  | G     | 104 | 8/9   | 0.98 | 0.13 | -    | 56,58,64,64                | 8     |
| 1   | CSD  | E     | 104 | 8/9   | 0.99 | 0.13 | -    | 42,56,66,67                | 8     |
| 1   | CSD  | K     | 104 | 8/9   | 0.98 | 0.13 | -    | 52,59,71,71                | 8     |

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3   | PO4  | O     | 301 | 5/5   | 0.99 | 0.17 | 2.67  | 54,63,67,71                | 0     |
| 3   | PO4  | I     | 301 | 5/5   | 0.99 | 0.15 | 0.60  | 55,64,67,71                | 0     |
| 3   | PO4  | A     | 301 | 5/5   | 0.98 | 0.14 | 0.36  | 54,67,74,76                | 0     |
| 3   | PO4  | M     | 301 | 5/5   | 0.99 | 0.15 | 0.36  | 55,68,72,76                | 0     |
| 3   | PO4  | G     | 301 | 5/5   | 0.99 | 0.14 | 0.13  | 64,70,76,81                | 0     |
| 3   | PO4  | E     | 301 | 5/5   | 0.99 | 0.12 | -0.59 | 69,76,79,85                | 0     |
| 3   | PO4  | C     | 301 | 5/5   | 0.98 | 0.13 | -0.81 | 68,69,81,82                | 0     |
| 3   | PO4  | K     | 301 | 5/5   | 0.98 | 0.12 | -2.78 | 70,78,85,86                | 0     |
| 4   | FE   | K     | 302 | 1/1   | 0.98 | 0.11 | -     | 59,59,59,59                | 1     |
| 4   | FE   | A     | 302 | 1/1   | 0.98 | 0.12 | -     | 65,65,65,65                | 1     |
| 4   | FE   | I     | 302 | 1/1   | 0.94 | 0.11 | -     | 74,74,74,74                | 1     |
| 4   | FE   | M     | 302 | 1/1   | 0.90 | 0.10 | -     | 66,66,66,66                | 1     |
| 4   | FE   | G     | 302 | 1/1   | 0.96 | 0.10 | -     | 60,60,60,60                | 1     |
| 4   | FE   | C     | 302 | 1/1   | 0.97 | 0.09 | -     | 65,65,65,65                | 1     |
| 4   | FE   | E     | 302 | 1/1   | 0.95 | 0.09 | -     | 70,70,70,70                | 1     |
| 4   | FE   | O     | 302 | 1/1   | 0.96 | 0.12 | -     | 68,68,68,68                | 1     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.