



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:48 PM EDT

PDB ID : 1OCR / pdb\_00001ocr  
Title : BOVINE HEART CYTOCHROME C OXIDASE IN THE FULLY REDUCED STATE  
Authors : Tsukihara, T.; Yao, M.  
Deposited on : 1998-07-07  
Resolution : 2.35 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

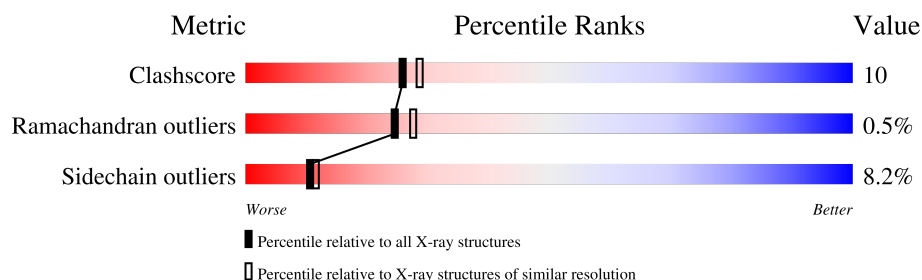
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1663 (2.36-2.36)                                      |
| Ramachandran outliers | 187476                      | 1646 (2.36-2.36)                                      |
| Sidechain outliers    | 187428                      | 1646 (2.36-2.36)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 514    | 73% 24% .        |
| 1   | N     | 514    | 71% 25% .        |
| 2   | B     | 227    | 65% 30% . .      |
| 2   | O     | 227    | 62% 33% . .      |
| 3   | C     | 261    | 75% 20% .        |
| 3   | P     | 261    | 78% 18% .        |
| 4   | D     | 147    | 71% 22% . .      |
| 4   | Q     | 147    | 68% 24% 5% .     |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 109    |    |
| 5   | R     | 109    |    |
| 6   | F     | 98     |    |
| 6   | S     | 98     |    |
| 7   | G     | 84     |    |
| 7   | T     | 84     |    |
| 8   | H     | 85     |    |
| 8   | U     | 85     |    |
| 9   | I     | 73     |    |
| 9   | V     | 73     |    |
| 10  | J     | 59     |    |
| 10  | W     | 59     |   |
| 11  | K     | 56     |  |
| 11  | X     | 56     |  |
| 12  | L     | 47     |  |
| 12  | Y     | 47     |  |
| 13  | M     | 46     |  |
| 13  | Z     | 46     |  |

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 28926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 514      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4025  | 2690 | 623 | 677 | 35 |         |         |       |
| 1   | N     | 514      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4025  | 2690 | 623 | 677 | 35 |         |         |       |

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 227      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 1870  | 1212 | 289 | 351 | 18 |         |         |       |
| 2   | O     | 227      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 1870  | 1212 | 289 | 351 | 18 |         |         |       |

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 261      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2124  | 1420 | 338 | 353 | 13 |         |         |       |
| 3   | P     | 261      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2124  | 1420 | 338 | 353 | 13 |         |         |       |

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1195  | 777 | 196 | 218 | 4 |         |         |       |
| 4   | Q     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1195  | 777 | 196 | 218 | 4 |         |         |       |

- Molecule 5 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 878   | 558 | 150 | 168 | 2 |         |         |       |
| 5   | R     | 109      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 878   | 558 | 150 | 168 | 2 |         |         |       |

- Molecule 6 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 748   | 464 | 134 | 145 | 5 |         |         |       |
| 6   | S     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 748   | 464 | 134 | 145 | 5 |         |         |       |

- Molecule 7 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 672   | 431 | 129 | 111 | 1 |         |         |       |
| 7   | T     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 672   | 431 | 129 | 111 | 1 |         |         |       |

- Molecule 8 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 417 | 121 | 119 | 5 |         |         |       |
| 8   | U     | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 662   | 417 | 121 | 119 | 5 |         |         |       |

- Molecule 9 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 9   | I     | 73       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 598   | 388 | 107 | 99 | 4 |         |         |       |
| 9   | V     | 73       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 598   | 388 | 107 | 99 | 4 |         |         |       |

- Molecule 10 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 460   | 297 | 78 | 82 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | W     | 58       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 460   | 297 | 78 | 82 | 3 |         |         |       |

- Molecule 11 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11  | K     | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 250 | 65 | 67 | 2 |         |         |       |
| 11  | X     | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 384   | 250 | 65 | 67 | 2 |         |         |       |

- Molecule 12 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | L     | 47       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 386   | 257 | 65 | 62 | 2 |         |         |       |
| 12  | Y     | 47       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 386   | 257 | 65 | 62 | 2 |         |         |       |

- Molecule 13 is a protein called CYTOCHROME C OXIDASE.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 13  | M     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 335   | 223 | 53 | 59 |         |         |       |
| 13  | Z     | 43       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 335   | 223 | 53 | 59 |         |         |       |

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | A     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | B     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 14  | N     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 14  | O     | 2        | Total | Cu | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

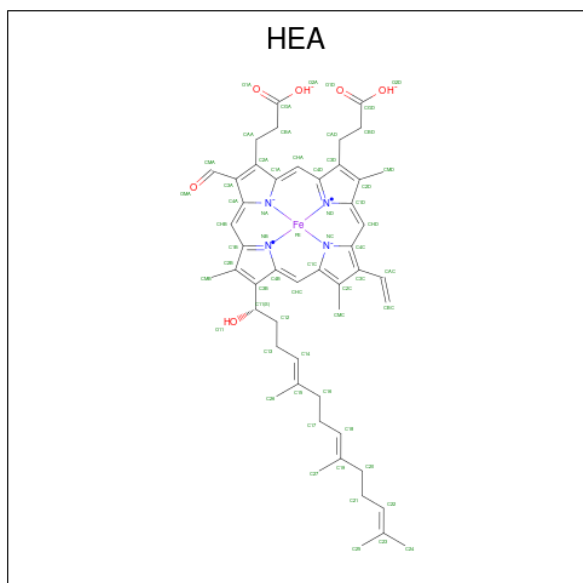
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 15  | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 15  | N     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 16  | A     | 1        | Total Na<br>1 1 | 0       | 0       |
| 16  | N     | 1        | Total Na<br>1 1 | 0       | 0       |

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms                         | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------------|---------|---------|
| 17  | A     | 1        | Total C Fe N O<br>60 49 1 4 6 | 0       | 0       |
| 17  | A     | 1        | Total C Fe N O<br>60 49 1 4 6 | 0       | 0       |
| 17  | N     | 1        | Total C Fe N O<br>60 49 1 4 6 | 0       | 0       |
| 17  | N     | 1        | Total C Fe N O<br>60 49 1 4 6 | 0       | 0       |

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

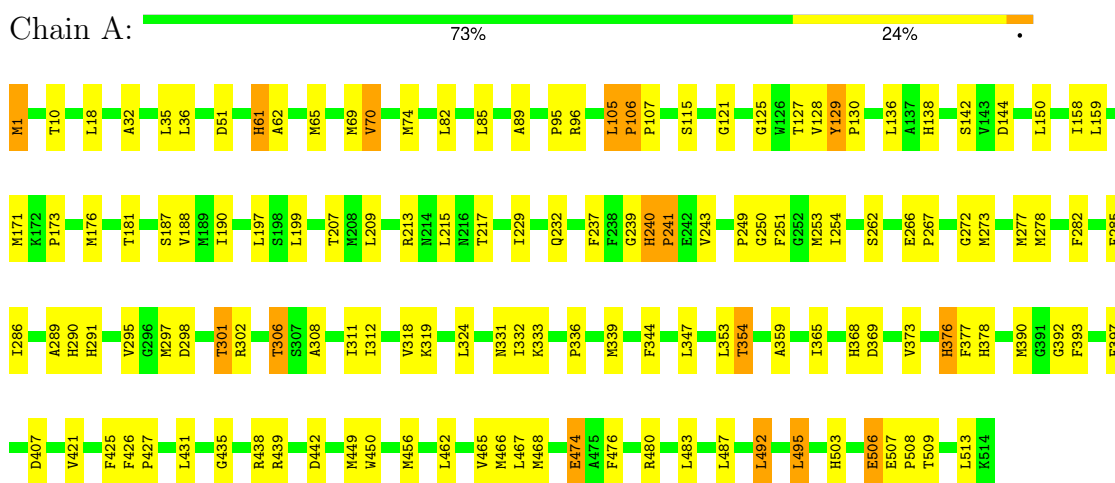
| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 18  | F     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 18  | S     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

### 3 Residue-property plots

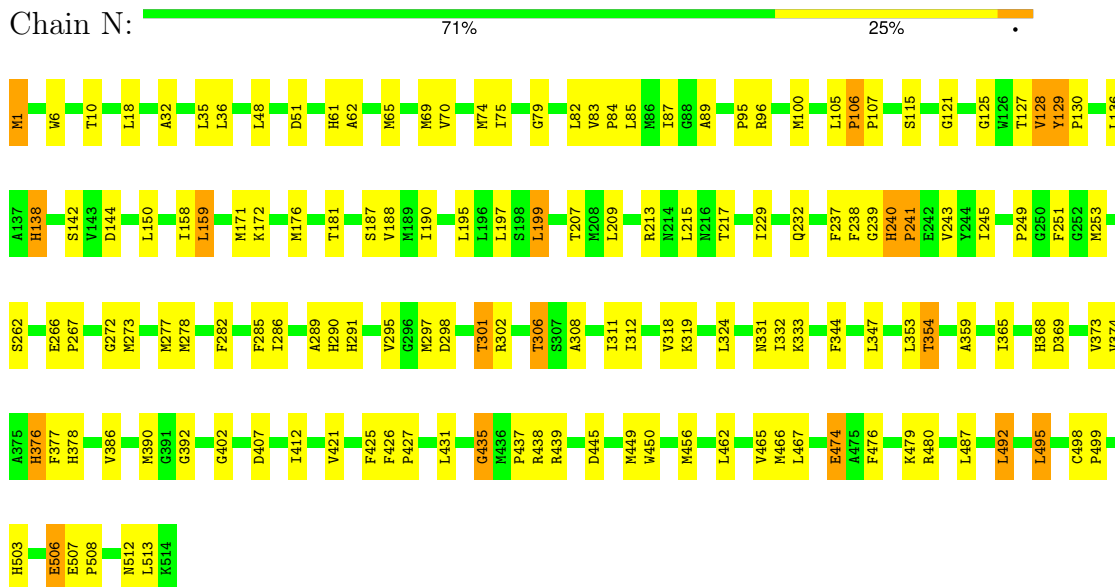
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: CYTOCHROME C OXIDASE

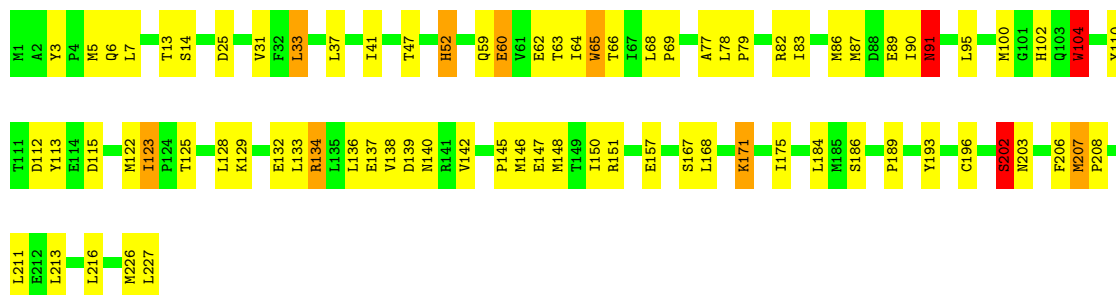


#### • Molecule 1: CYTOCHROME C OXIDASE



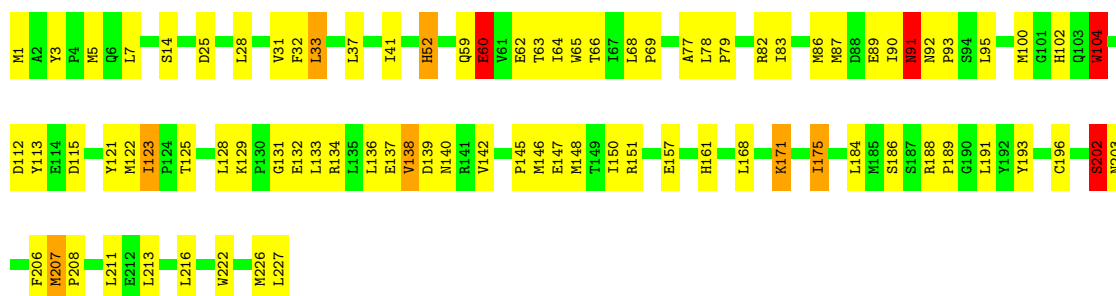
#### • Molecule 2: CYTOCHROME C OXIDASE

Chain B:  65% 30% . .



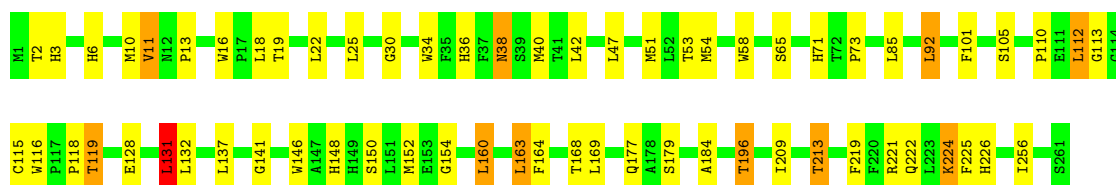
• Molecule 2: CYTOCHROME C OXIDASE

Chain O:  62% 33% . .



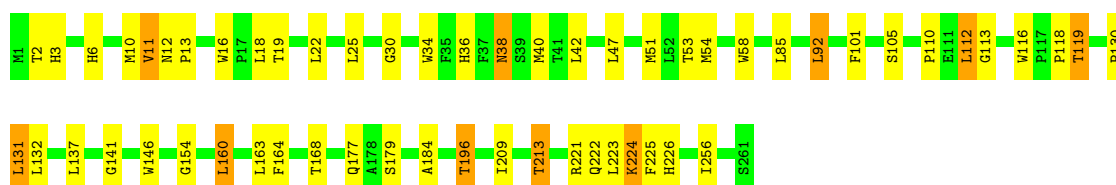
• Molecule 3: CYTOCHROME C OXIDASE

Chain C:  75% 20% .



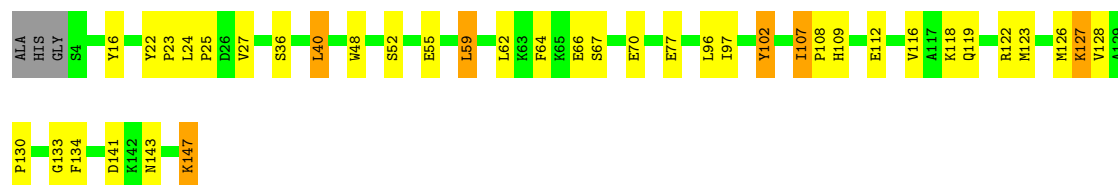
• Molecule 3: CYTOCHROME C OXIDASE

Chain P:  78% 18% .

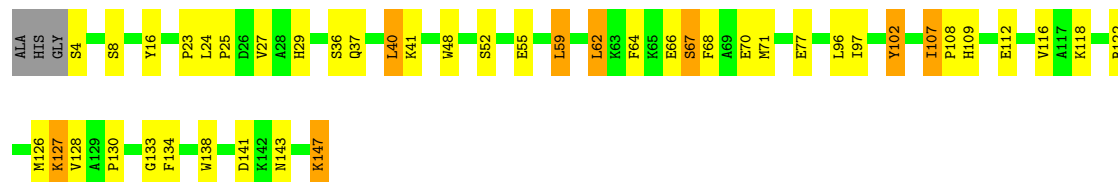


• Molecule 4: CYTOCHROME C OXIDASE

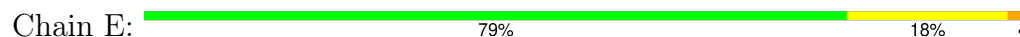
Chain D:  71% 22% . .



• Molecule 4: CYTOCHROME C OXIDASE



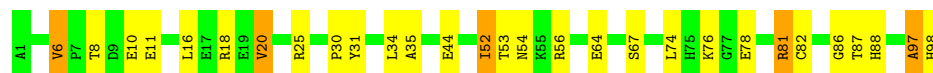
• Molecule 5: CYTOCHROME C OXIDASE



• Molecule 5: CYTOCHROME C OXIDASE



• Molecule 6: CYTOCHROME C OXIDASE



• Molecule 6: CYTOCHROME C OXIDASE



• Molecule 7: CYTOCHROME C OXIDASE



- Molecule 7: CYTOCHROME C OXIDASE

Chain T:  64% 26% 7% .



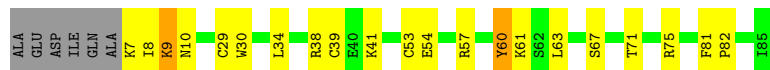
- Molecule 8: CYTOCHROME C OXIDASE

Chain H:  67% 24% 7% .



- Molecule 8: CYTOCHROME C OXIDASE

Chain U:  68% 22% 7% .



- Molecule 9: CYTOCHROME C OXIDASE

Chain I:  79% 19% .



- Molecule 9: CYTOCHROME C OXIDASE

Chain V:  70% 29% .



- Molecule 10: CYTOCHROME C OXIDASE

Chain J:  76% 17% 5% .



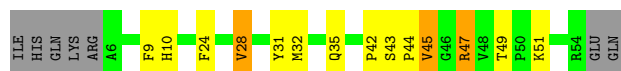
- Molecule 10: CYTOCHROME C OXIDASE

Chain W:  73% 20% 5% .



- Molecule 11: CYTOCHROME C OXIDASE

Chain K:  62% 20% 5% 12%



• Molecule 11: CYTOCHROME C OXIDASE

Chain X:  57% 25% 5% 12%



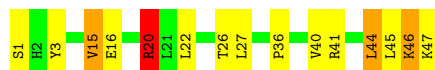
• Molecule 12: CYTOCHROME C OXIDASE

Chain L:  72% 19% 6% •



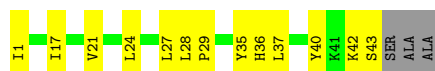
• Molecule 12: CYTOCHROME C OXIDASE

Chain Y:  68% 23% 6% •



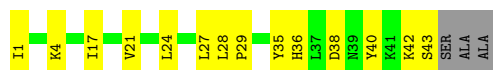
• Molecule 13: CYTOCHROME C OXIDASE

Chain M:  65% 28% 7%



• Molecule 13: CYTOCHROME C OXIDASE

Chain Z:  63% 30% 7%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 189.10Å 210.50Å 178.60Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 15.00 – 2.35                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 89.8 (15.00-2.35)                               | Depositor |
| $R_{merge}$                                              | 0.06                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR 3.84                                     | Depositor |
| R, $R_{free}$                                            | 0.203 , 0.247                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 28926                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 39.0                                            | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEA, MG, NA, ZN

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     | 1.02         | 8/4164 (0.2%)   | 1.20        | 40/5688 (0.7%)   |
| 1   | N     | 0.86         | 8/4164 (0.2%)   | 1.15        | 40/5688 (0.7%)   |
| 2   | B     | 0.90         | 1/1917 (0.1%)   | 1.19        | 17/2612 (0.7%)   |
| 2   | O     | 0.80         | 1/1917 (0.1%)   | 1.17        | 16/2612 (0.6%)   |
| 3   | C     | 0.92         | 0/2211          | 1.02        | 11/3023 (0.4%)   |
| 3   | P     | 0.79         | 0/2211          | 1.01        | 9/3023 (0.3%)    |
| 4   | D     | 0.75         | 0/1229          | 0.99        | 4/1658 (0.2%)    |
| 4   | Q     | 0.67         | 0/1229          | 1.04        | 4/1658 (0.2%)    |
| 5   | E     | 0.79         | 0/898           | 1.08        | 7/1218 (0.6%)    |
| 5   | R     | 0.69         | 0/898           | 1.09        | 8/1218 (0.7%)    |
| 6   | F     | 0.82         | 0/765           | 1.20        | 7/1038 (0.7%)    |
| 6   | S     | 0.75         | 0/765           | 1.16        | 4/1038 (0.4%)    |
| 7   | G     | 0.81         | 0/699           | 1.22        | 12/950 (1.3%)    |
| 7   | T     | 0.75         | 0/699           | 1.22        | 11/950 (1.2%)    |
| 8   | H     | 0.82         | 0/682           | 1.14        | 7/921 (0.8%)     |
| 8   | U     | 0.72         | 0/682           | 1.11        | 6/921 (0.7%)     |
| 9   | I     | 0.85         | 0/611           | 0.97        | 2/810 (0.2%)     |
| 9   | V     | 0.76         | 0/611           | 0.94        | 2/810 (0.2%)     |
| 10  | J     | 0.78         | 0/471           | 0.96        | 0/636            |
| 10  | W     | 0.68         | 0/471           | 0.93        | 0/636            |
| 11  | K     | 0.95         | 0/398           | 1.11        | 0/546            |
| 11  | X     | 0.73         | 0/398           | 1.08        | 0/546            |
| 12  | L     | 0.91         | 0/399           | 1.04        | 2/534 (0.4%)     |
| 12  | Y     | 0.71         | 0/399           | 1.04        | 3/534 (0.6%)     |
| 13  | M     | 0.81         | 0/345           | 0.99        | 1/470 (0.2%)     |
| 13  | Z     | 0.66         | 0/345           | 1.00        | 1/470 (0.2%)     |
| All | All   | 0.84         | 18/29578 (0.1%) | 1.11        | 214/40208 (0.5%) |

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   | N     | 0                   | 1                   |
| 2   | B     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 376 | HIS  | ND1-CE1 | 9.63  | 1.42        | 1.32     |
| 1   | A     | 61  | HIS  | CD2-NE2 | 9.27  | 1.48        | 1.37     |
| 1   | N     | 376 | HIS  | ND1-CE1 | 9.07  | 1.41        | 1.32     |
| 1   | N     | 378 | HIS  | ND1-CE1 | 8.96  | 1.41        | 1.32     |
| 1   | A     | 378 | HIS  | ND1-CE1 | 8.90  | 1.41        | 1.32     |
| 1   | A     | 61  | HIS  | ND1-CE1 | 7.91  | 1.40        | 1.32     |
| 1   | N     | 61  | HIS  | CG-CD2  | 7.30  | 1.43        | 1.35     |
| 1   | N     | 376 | HIS  | CD2-NE2 | 7.03  | 1.45        | 1.37     |
| 1   | A     | 378 | HIS  | CD2-NE2 | 7.02  | 1.45        | 1.37     |
| 1   | A     | 376 | HIS  | CD2-NE2 | 6.84  | 1.45        | 1.37     |
| 1   | N     | 376 | HIS  | CG-CD2  | 6.83  | 1.43        | 1.35     |
| 1   | N     | 378 | HIS  | CG-CD2  | 6.69  | 1.43        | 1.35     |
| 1   | N     | 378 | HIS  | CD2-NE2 | 6.59  | 1.45        | 1.37     |
| 2   | O     | 175 | ILE  | CA-CB   | 6.50  | 1.59        | 1.54     |
| 1   | N     | 61  | HIS  | ND1-CE1 | 6.15  | 1.38        | 1.32     |
| 1   | A     | 130 | PRO  | CA-C    | 6.12  | 1.57        | 1.52     |
| 1   | A     | 61  | HIS  | CG-CD2  | 6.07  | 1.42        | 1.35     |
| 2   | B     | 104 | TRP  | CA-C    | -5.23 | 1.45        | 1.52     |

All (214) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | Q     | 133 | GLY  | N-CA-C      | 14.89 | 130.50      | 112.49   |
| 1   | A     | 61  | HIS  | ND1-CE1-NE2 | 10.43 | 118.83      | 108.40   |
| 1   | A     | 378 | HIS  | ND1-CE1-NE2 | 9.79  | 118.19      | 108.40   |
| 1   | A     | 376 | HIS  | ND1-CE1-NE2 | 8.90  | 117.30      | 108.40   |
| 1   | N     | 332 | ILE  | N-CA-C      | 8.79  | 120.50      | 108.89   |
| 1   | A     | 332 | ILE  | N-CA-C      | 8.71  | 120.38      | 108.89   |
| 5   | E     | 7   | THR  | N-CA-C      | -8.52 | 99.53       | 110.53   |
| 1   | N     | 61  | HIS  | ND1-CE1-NE2 | 8.52  | 116.92      | 108.40   |
| 5   | R     | 42  | VAL  | N-CA-C      | -8.50 | 98.05       | 107.73   |
| 6   | F     | 97  | ALA  | N-CA-C      | 8.48  | 122.84      | 111.30   |
| 6   | S     | 97  | ALA  | N-CA-C      | 8.44  | 122.78      | 111.30   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 435 | GLY  | N-CA-C      | 8.26  | 126.91      | 115.27   |
| 5   | E     | 42  | VAL  | N-CA-C      | -8.22 | 98.36       | 107.73   |
| 1   | N     | 376 | HIS  | ND1-CE1-NE2 | 8.15  | 116.56      | 108.40   |
| 5   | R     | 7   | THR  | N-CA-C      | -8.15 | 100.02      | 110.53   |
| 1   | N     | 130 | PRO  | N-CA-C      | -8.10 | 100.82      | 110.70   |
| 1   | N     | 378 | HIS  | ND1-CE1-NE2 | 7.94  | 116.34      | 108.40   |
| 1   | A     | 376 | HIS  | CE1-NE2-CD2 | -7.92 | 101.08      | 109.00   |
| 1   | N     | 378 | HIS  | CA-CB-CG    | -7.81 | 105.99      | 113.80   |
| 1   | A     | 378 | HIS  | CE1-NE2-CD2 | -7.77 | 101.23      | 109.00   |
| 1   | N     | 125 | GLY  | N-CA-C      | -7.69 | 103.00      | 112.68   |
| 1   | A     | 61  | HIS  | CE1-NE2-CD2 | -7.63 | 101.37      | 109.00   |
| 12  | Y     | 46  | LYS  | N-CA-C      | -7.58 | 104.55      | 113.88   |
| 1   | A     | 125 | GLY  | N-CA-C      | -7.50 | 103.23      | 112.68   |
| 8   | H     | 8   | ILE  | N-CA-C      | 7.50  | 118.60      | 108.11   |
| 1   | N     | 435 | GLY  | N-CA-C      | 7.49  | 125.83      | 115.27   |
| 1   | A     | 130 | PRO  | N-CA-C      | -7.47 | 101.58      | 110.70   |
| 8   | U     | 10  | ASN  | N-CA-C      | -7.45 | 104.16      | 112.57   |
| 3   | C     | 184 | ALA  | CA-C-N      | 7.40  | 128.66      | 120.45   |
| 3   | C     | 184 | ALA  | C-N-CA      | 7.40  | 128.66      | 120.45   |
| 1   | A     | 376 | HIS  | CA-CB-CG    | 7.34  | 121.14      | 113.80   |
| 8   | H     | 10  | ASN  | N-CA-C      | -7.30 | 104.32      | 112.57   |
| 4   | D     | 133 | GLY  | N-CA-C      | 7.29  | 130.46      | 113.18   |
| 7   | G     | 44  | ARG  | CA-C-N      | 7.29  | 127.27      | 119.76   |
| 7   | G     | 44  | ARG  | C-N-CA      | 7.29  | 127.27      | 119.76   |
| 2   | B     | 104 | TRP  | N-CA-C      | 7.20  | 126.13      | 110.80   |
| 1   | N     | 10  | THR  | N-CA-C      | -7.19 | 102.61      | 112.03   |
| 3   | P     | 256 | ILE  | N-CA-C      | 7.17  | 117.77      | 110.82   |
| 7   | T     | 44  | ARG  | CA-C-N      | 7.10  | 127.07      | 119.76   |
| 7   | T     | 44  | ARG  | C-N-CA      | 7.10  | 127.07      | 119.76   |
| 1   | A     | 239 | GLY  | N-CA-C      | 7.03  | 121.41      | 112.83   |
| 2   | O     | 59  | GLN  | N-CA-C      | 7.00  | 122.84      | 111.37   |
| 8   | U     | 8   | ILE  | N-CA-C      | 6.97  | 117.87      | 108.11   |
| 12  | L     | 46  | LYS  | N-CA-C      | -6.96 | 105.32      | 113.88   |
| 1   | A     | 142 | SER  | N-CA-C      | 6.91  | 119.45      | 111.02   |
| 2   | B     | 59  | GLN  | N-CA-C      | 6.88  | 122.65      | 111.37   |
| 2   | O     | 104 | TRP  | N-CA-C      | 6.88  | 125.44      | 110.80   |
| 3   | P     | 184 | ALA  | CA-C-N      | 6.87  | 128.07      | 120.45   |
| 3   | P     | 184 | ALA  | C-N-CA      | 6.87  | 128.07      | 120.45   |
| 1   | A     | 10  | THR  | N-CA-C      | -6.85 | 103.06      | 112.03   |
| 7   | T     | 17  | ARG  | N-CA-C      | -6.84 | 103.28      | 111.69   |
| 5   | R     | 76  | GLY  | CA-C-N      | 6.80  | 126.51      | 119.64   |
| 5   | R     | 76  | GLY  | C-N-CA      | 6.80  | 126.51      | 119.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | T     | 69  | PHE  | N-CA-C      | 6.72  | 119.18      | 111.11   |
| 8   | U     | 81  | PHE  | CA-C-N      | 6.66  | 126.60      | 119.28   |
| 8   | U     | 81  | PHE  | C-N-CA      | 6.66  | 126.60      | 119.28   |
| 1   | N     | 82  | LEU  | N-CA-C      | 6.65  | 121.70      | 112.45   |
| 7   | T     | 72  | ASN  | CA-C-N      | 6.60  | 127.12      | 119.47   |
| 7   | T     | 72  | ASN  | C-N-CA      | 6.60  | 127.12      | 119.47   |
| 5   | E     | 21  | LYS  | CA-C-N      | 6.56  | 126.33      | 119.05   |
| 5   | E     | 21  | LYS  | C-N-CA      | 6.56  | 126.33      | 119.05   |
| 3   | C     | 256 | ILE  | N-CA-C      | 6.55  | 117.18      | 110.82   |
| 7   | G     | 17  | ARG  | N-CA-C      | -6.55 | 103.63      | 111.69   |
| 1   | A     | 82  | LEU  | N-CA-C      | 6.55  | 121.56      | 112.45   |
| 5   | R     | 21  | LYS  | CA-C-N      | 6.54  | 126.31      | 119.05   |
| 5   | R     | 21  | LYS  | C-N-CA      | 6.54  | 126.31      | 119.05   |
| 8   | H     | 81  | PHE  | CA-C-N      | 6.53  | 126.46      | 119.28   |
| 8   | H     | 81  | PHE  | C-N-CA      | 6.53  | 126.46      | 119.28   |
| 2   | B     | 134 | ARG  | N-CA-C      | 6.46  | 124.57      | 110.80   |
| 5   | E     | 76  | GLY  | CA-C-N      | 6.42  | 126.12      | 119.64   |
| 5   | E     | 76  | GLY  | C-N-CA      | 6.42  | 126.12      | 119.64   |
| 3   | C     | 113 | GLY  | N-CA-C      | -6.41 | 105.77      | 115.00   |
| 2   | O     | 134 | ARG  | N-CA-C      | 6.38  | 124.39      | 110.80   |
| 1   | A     | 466 | MET  | N-CA-C      | -6.31 | 104.32      | 111.14   |
| 2   | B     | 202 | SER  | N-CA-C      | 6.30  | 118.96      | 111.33   |
| 7   | T     | 37  | LEU  | N-CA-C      | -6.30 | 105.88      | 112.93   |
| 1   | N     | 262 | SER  | N-CA-C      | -6.29 | 105.65      | 113.38   |
| 1   | N     | 376 | HIS  | CE1-NE2-CD2 | -6.26 | 102.74      | 109.00   |
| 1   | N     | 89  | ALA  | CA-C-N      | 6.25  | 125.82      | 119.19   |
| 1   | N     | 89  | ALA  | C-N-CA      | 6.25  | 125.82      | 119.19   |
| 2   | O     | 77  | ALA  | N-CA-C      | 6.25  | 117.75      | 111.07   |
| 1   | N     | 495 | LEU  | N-CA-C      | 6.19  | 120.39      | 112.34   |
| 2   | B     | 66  | THR  | N-CA-C      | -6.18 | 104.81      | 112.72   |
| 1   | A     | 89  | ALA  | CA-C-N      | 6.18  | 125.74      | 119.19   |
| 1   | A     | 89  | ALA  | C-N-CA      | 6.18  | 125.74      | 119.19   |
| 7   | G     | 69  | PHE  | N-CA-C      | 6.17  | 118.52      | 111.11   |
| 3   | P     | 113 | GLY  | N-CA-C      | -6.16 | 106.12      | 115.00   |
| 7   | G     | 11  | THR  | N-CA-C      | 6.09  | 123.78      | 110.80   |
| 7   | T     | 11  | THR  | N-CA-C      | 6.08  | 123.74      | 110.80   |
| 1   | N     | 239 | GLY  | N-CA-C      | 6.06  | 120.23      | 112.83   |
| 1   | N     | 237 | PHE  | N-CA-C      | -6.06 | 104.79      | 111.82   |
| 1   | A     | 251 | PHE  | N-CA-C      | -6.05 | 104.68      | 111.28   |
| 13  | M     | 27  | LEU  | N-CA-C      | 6.04  | 119.12      | 111.69   |
| 3   | C     | 3   | HIS  | N-CA-C      | -6.02 | 99.89       | 109.76   |
| 13  | Z     | 27  | LEU  | N-CA-C      | 6.02  | 119.82      | 112.23   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 207 | MET  | CA-C-N    | 6.01  | 125.98      | 120.21   |
| 2   | B     | 207 | MET  | C-N-CA    | 6.01  | 125.98      | 120.21   |
| 8   | H     | 63  | LEU  | N-CA-C    | 6.00  | 119.07      | 111.69   |
| 7   | G     | 72  | ASN  | CA-C-N    | 5.99  | 126.15      | 119.32   |
| 7   | G     | 72  | ASN  | C-N-CA    | 5.99  | 126.15      | 119.32   |
| 6   | F     | 35  | ALA  | CA-C-N    | 5.98  | 125.74      | 119.76   |
| 6   | F     | 35  | ALA  | C-N-CA    | 5.98  | 125.74      | 119.76   |
| 7   | G     | 37  | LEU  | N-CA-C    | -5.98 | 106.23      | 112.93   |
| 1   | N     | 507 | GLU  | N-CA-C    | -5.96 | 97.64       | 108.85   |
| 1   | N     | 425 | PHE  | N-CA-C    | 5.95  | 120.82      | 113.50   |
| 1   | N     | 171 | MET  | N-CA-C    | 5.95  | 120.97      | 111.81   |
| 1   | N     | 466 | MET  | N-CA-C    | -5.92 | 104.74      | 111.14   |
| 1   | A     | 105 | LEU  | CA-C-N    | -5.92 | 114.28      | 120.38   |
| 1   | A     | 105 | LEU  | C-N-CA    | -5.92 | 114.28      | 120.38   |
| 2   | B     | 77  | ALA  | N-CA-C    | 5.90  | 117.38      | 111.07   |
| 1   | A     | 129 | TYR  | CB-CA-C   | -5.88 | 100.18      | 109.42   |
| 4   | D     | 102 | TYR  | N-CA-C    | 5.88  | 120.73      | 113.50   |
| 1   | N     | 272 | GLY  | N-CA-C    | -5.87 | 105.50      | 113.37   |
| 1   | N     | 61  | HIS  | CB-CG-CD2 | -5.80 | 123.67      | 131.20   |
| 2   | B     | 129 | LYS  | N-CA-C    | -5.79 | 102.75      | 109.93   |
| 1   | N     | 506 | GLU  | N-CA-C    | -5.76 | 105.08      | 111.71   |
| 9   | V     | 20  | HIS  | N-CA-C    | 5.75  | 118.33      | 111.71   |
| 4   | Q     | 102 | TYR  | N-CA-C    | 5.73  | 120.54      | 113.50   |
| 3   | P     | 141 | GLY  | N-CA-C    | -5.71 | 105.46      | 112.77   |
| 1   | A     | 272 | GLY  | N-CA-C    | -5.71 | 105.72      | 113.37   |
| 8   | U     | 9   | LYS  | N-CA-C    | -5.70 | 104.19      | 113.19   |
| 3   | C     | 141 | GLY  | N-CA-C    | -5.69 | 105.33      | 113.86   |
| 2   | O     | 147 | GLU  | N-CA-C    | 5.64  | 119.34      | 111.90   |
| 3   | C     | 225 | PHE  | N-CA-C    | 5.62  | 119.72      | 112.86   |
| 1   | A     | 237 | PHE  | N-CA-C    | -5.62 | 105.31      | 111.82   |
| 2   | O     | 66  | THR  | N-CA-C    | -5.60 | 105.55      | 112.72   |
| 1   | N     | 412 | ILE  | N-CA-C    | -5.58 | 105.06      | 110.42   |
| 1   | N     | 142 | SER  | N-CA-C    | 5.57  | 117.81      | 111.02   |
| 2   | O     | 123 | ILE  | CA-C-N    | 5.54  | 125.55      | 119.90   |
| 2   | O     | 123 | ILE  | C-N-CA    | 5.54  | 125.55      | 119.90   |
| 9   | I     | 37  | PHE  | N-CA-C    | 5.53  | 117.11      | 111.14   |
| 3   | P     | 225 | PHE  | N-CA-C    | 5.53  | 119.60      | 112.86   |
| 1   | A     | 495 | LEU  | N-CA-C    | 5.52  | 119.52      | 112.34   |
| 12  | Y     | 45  | LEU  | N-CA-C    | 5.50  | 118.99      | 112.72   |
| 3   | P     | 3   | HIS  | N-CA-C    | -5.49 | 100.29      | 109.24   |
| 1   | A     | 158 | ILE  | N-CA-C    | -5.49 | 105.37      | 110.53   |
| 1   | A     | 487 | LEU  | N-CA-C    | 5.48  | 119.00      | 111.54   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 171 | MET  | N-CA-C    | 5.47  | 120.23      | 111.81   |
| 5   | R     | 29  | LEU  | N-CA-C    | -5.47 | 105.24      | 111.14   |
| 1   | N     | 129 | TYR  | CB-CA-C   | -5.46 | 100.84      | 109.42   |
| 4   | Q     | 67  | SER  | N-CA-C    | -5.46 | 103.49      | 110.53   |
| 1   | N     | 331 | ASN  | N-CA-C    | -5.44 | 97.63       | 107.75   |
| 1   | A     | 262 | SER  | N-CA-C    | -5.43 | 106.71      | 113.38   |
| 1   | A     | 331 | ASN  | N-CA-C    | -5.41 | 97.69       | 107.75   |
| 2   | O     | 202 | SER  | N-CA-C    | 5.41  | 117.88      | 111.33   |
| 1   | A     | 506 | GLU  | N-CA-C    | -5.40 | 105.50      | 111.71   |
| 1   | N     | 251 | PHE  | N-CA-C    | -5.39 | 105.30      | 111.07   |
| 12  | L     | 20  | ARG  | N-CA-C    | -5.38 | 105.58      | 111.82   |
| 9   | I     | 20  | HIS  | N-CA-C    | 5.38  | 117.90      | 111.71   |
| 1   | N     | 6   | TRP  | N-CA-C    | 5.38  | 120.12      | 113.50   |
| 3   | C     | 131 | LEU  | N-CA-C    | -5.38 | 105.50      | 111.36   |
| 8   | H     | 9   | LYS  | N-CA-C    | -5.37 | 104.70      | 113.19   |
| 7   | G     | 83  | GLU  | N-CA-C    | 5.36  | 116.98      | 111.03   |
| 8   | H     | 12  | GLN  | N-CA-C    | -5.36 | 104.40      | 111.96   |
| 1   | N     | 407 | ASP  | N-CA-C    | 5.36  | 117.81      | 111.33   |
| 12  | Y     | 20  | ARG  | N-CA-C    | -5.36 | 105.61      | 111.82   |
| 1   | N     | 376 | HIS  | CB-CG-CD2 | -5.34 | 124.26      | 131.20   |
| 2   | O     | 60  | GLU  | N-CA-C    | 5.32  | 122.12      | 110.80   |
| 1   | N     | 421 | VAL  | N-CA-C    | 5.31  | 116.03      | 110.62   |
| 4   | D     | 22  | TYR  | CA-C-N    | 5.31  | 124.94      | 119.05   |
| 4   | D     | 22  | TYR  | C-N-CA    | 5.31  | 124.94      | 119.05   |
| 2   | O     | 129 | LYS  | N-CA-C    | -5.30 | 102.50      | 110.24   |
| 3   | P     | 131 | LEU  | N-CA-C    | -5.30 | 105.58      | 111.36   |
| 1   | A     | 70  | VAL  | N-CA-C    | 5.29  | 115.43      | 110.30   |
| 9   | V     | 37  | PHE  | N-CA-C    | 5.28  | 117.12      | 111.36   |
| 2   | O     | 161 | HIS  | N-CA-C    | -5.28 | 101.10      | 108.96   |
| 1   | A     | 421 | VAL  | N-CA-C    | 5.27  | 115.99      | 110.62   |
| 2   | B     | 52  | HIS  | N-CA-C    | -5.27 | 99.58       | 110.80   |
| 6   | F     | 82  | CYS  | CA-C-N    | 5.27  | 124.93      | 119.56   |
| 6   | F     | 82  | CYS  | C-N-CA    | 5.27  | 124.93      | 119.56   |
| 1   | N     | 386 | VAL  | N-CA-C    | 5.27  | 115.99      | 110.62   |
| 5   | E     | 29  | LEU  | N-CA-C    | -5.26 | 105.63      | 111.36   |
| 7   | G     | 36  | TRP  | CB-CA-C   | 5.25  | 117.32      | 109.13   |
| 2   | O     | 207 | MET  | CA-C-N    | 5.25  | 125.25      | 120.21   |
| 2   | O     | 207 | MET  | C-N-CA    | 5.25  | 125.25      | 120.21   |
| 1   | N     | 479 | LYS  | N-CA-C    | 5.25  | 118.37      | 111.28   |
| 1   | N     | 158 | ILE  | N-CA-C    | -5.25 | 105.60      | 110.53   |
| 2   | B     | 147 | GLU  | N-CA-C    | 5.24  | 118.81      | 111.90   |
| 1   | N     | 217 | THR  | N-CA-C    | -5.24 | 103.00      | 110.59   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 128 | GLU  | CA-C-O  | 5.23  | 120.97      | 117.94   |
| 3   | C     | 150 | SER  | N-CA-C  | -5.22 | 105.58      | 111.28   |
| 3   | C     | 36  | HIS  | N-CA-C  | 5.21  | 120.12      | 113.55   |
| 7   | T     | 36  | TRP  | CB-CA-C | 5.20  | 117.24      | 109.13   |
| 5   | R     | 79  | LYS  | N-CA-C  | 5.19  | 119.10      | 112.87   |
| 2   | B     | 64  | ILE  | CB-CA-C | -5.18 | 105.34      | 111.97   |
| 6   | F     | 52  | ILE  | N-CA-C  | -5.17 | 107.43      | 112.29   |
| 6   | S     | 76  | LYS  | N-CA-C  | -5.16 | 102.41      | 110.10   |
| 1   | A     | 509 | THR  | N-CA-C  | -5.16 | 104.07      | 110.41   |
| 2   | O     | 52  | HIS  | N-CA-C  | -5.16 | 99.82       | 110.80   |
| 2   | B     | 60  | GLU  | N-CA-C  | 5.15  | 121.78      | 110.80   |
| 1   | N     | 445 | ASP  | N-CA-C  | 5.15  | 117.56      | 111.33   |
| 7   | T     | 48  | ILE  | CA-C-N  | 5.15  | 126.27      | 119.84   |
| 7   | T     | 48  | ILE  | C-N-CA  | 5.15  | 126.27      | 119.84   |
| 1   | A     | 507 | GLU  | N-CA-C  | -5.14 | 99.19       | 108.85   |
| 1   | A     | 217 | THR  | N-CA-C  | -5.14 | 103.14      | 110.59   |
| 7   | G     | 48  | ILE  | CA-C-N  | 5.13  | 126.26      | 119.84   |
| 7   | G     | 48  | ILE  | C-N-CA  | 5.13  | 126.26      | 119.84   |
| 6   | S     | 35  | ALA  | CA-C-N  | 5.13  | 124.89      | 119.76   |
| 6   | S     | 35  | ALA  | C-N-CA  | 5.13  | 124.89      | 119.76   |
| 1   | A     | 425 | PHE  | N-CA-C  | 5.12  | 119.80      | 113.50   |
| 1   | A     | 207 | THR  | N-CA-C  | -5.12 | 105.40      | 111.69   |
| 1   | A     | 173 | PRO  | N-CA-C  | -5.10 | 104.48      | 110.70   |
| 2   | B     | 65  | TRP  | N-CA-C  | 5.09  | 119.07      | 113.21   |
| 2   | B     | 123 | ILE  | CA-C-N  | 5.09  | 125.09      | 119.90   |
| 2   | B     | 123 | ILE  | C-N-CA  | 5.09  | 125.09      | 119.90   |
| 3   | P     | 36  | HIS  | N-CA-C  | 5.09  | 119.96      | 113.55   |
| 1   | A     | 407 | ASP  | N-CA-C  | 5.08  | 117.48      | 111.33   |
| 2   | B     | 47  | THR  | N-CA-C  | 5.08  | 118.96      | 112.26   |
| 1   | N     | 207 | THR  | N-CA-C  | -5.07 | 105.46      | 111.69   |
| 8   | U     | 63  | LEU  | N-CA-C  | 5.06  | 119.49      | 112.45   |
| 4   | Q     | 62  | LEU  | N-CA-C  | -5.05 | 105.86      | 112.23   |
| 6   | F     | 76  | LYS  | N-CA-C  | -5.02 | 102.62      | 110.10   |
| 2   | O     | 64  | ILE  | CB-CA-C | -5.01 | 105.55      | 111.97   |
| 1   | N     | 487 | LEU  | N-CA-C  | 5.00  | 118.35      | 111.54   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 240 | HIS  | Sidechain |
| 2   | B     | 110 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | N     | 240 | HIS  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4025  | 0        | 4002     | 75      | 0            |
| 1   | N     | 4025  | 0        | 4002     | 87      | 0            |
| 2   | B     | 1870  | 0        | 1873     | 57      | 0            |
| 2   | O     | 1870  | 0        | 1873     | 58      | 0            |
| 3   | C     | 2124  | 0        | 2044     | 42      | 0            |
| 3   | P     | 2124  | 0        | 2044     | 39      | 0            |
| 4   | D     | 1195  | 0        | 1183     | 30      | 0            |
| 4   | Q     | 1195  | 0        | 1183     | 36      | 0            |
| 5   | E     | 878   | 0        | 868      | 15      | 0            |
| 5   | R     | 878   | 0        | 868      | 18      | 0            |
| 6   | F     | 748   | 0        | 728      | 18      | 0            |
| 6   | S     | 748   | 0        | 728      | 17      | 0            |
| 7   | G     | 672   | 0        | 645      | 21      | 0            |
| 7   | T     | 672   | 0        | 645      | 25      | 0            |
| 8   | H     | 662   | 0        | 623      | 11      | 0            |
| 8   | U     | 662   | 0        | 625      | 11      | 0            |
| 9   | I     | 598   | 0        | 612      | 8       | 0            |
| 9   | V     | 598   | 0        | 612      | 14      | 0            |
| 10  | J     | 460   | 0        | 459      | 9       | 0            |
| 10  | W     | 460   | 0        | 459      | 9       | 0            |
| 11  | K     | 384   | 0        | 366      | 12      | 0            |
| 11  | X     | 384   | 0        | 366      | 14      | 0            |
| 12  | L     | 386   | 0        | 388      | 8       | 0            |
| 12  | Y     | 386   | 0        | 388      | 10      | 0            |
| 13  | M     | 335   | 0        | 352      | 8       | 0            |
| 13  | Z     | 335   | 0        | 352      | 10      | 0            |
| 14  | A     | 1     | 0        | 0        | 0       | 0            |
| 14  | B     | 2     | 0        | 0        | 0       | 0            |
| 14  | N     | 1     | 0        | 0        | 0       | 0            |
| 14  | O     | 2     | 0        | 0        | 0       | 0            |
| 15  | A     | 1     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | A     | 1     | 0        | 0        | 0       | 0            |
| 16  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 120   | 0        | 108      | 9       | 0            |
| 17  | N     | 120   | 0        | 108      | 6       | 0            |
| 18  | F     | 1     | 0        | 0        | 0       | 0            |
| 18  | S     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 28926 | 0        | 28504    | 544     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (544) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 6:S:10:GLU:HG2   | 6:S:25:ARG:HH22   | 1.30                     | 0.94              |
| 6:F:10:GLU:HG2   | 6:F:25:ARG:HH22   | 1.30                     | 0.94              |
| 1:A:176:MET:HE3  | 1:A:181:THR:HG22  | 1.58                     | 0.85              |
| 3:C:101:PHE:HD1  | 3:C:196:THR:HG21  | 1.43                     | 0.84              |
| 1:A:278:MET:HE2  | 7:T:18:PHE:HE2    | 1.42                     | 0.84              |
| 2:B:78:LEU:HB2   | 2:B:79:PRO:HD3    | 1.60                     | 0.83              |
| 1:N:176:MET:HE3  | 1:N:181:THR:HG22  | 1.60                     | 0.82              |
| 2:O:78:LEU:HB2   | 2:O:79:PRO:HD3    | 1.62                     | 0.81              |
| 2:B:33:LEU:HD23  | 9:I:28:SER:HB3    | 1.62                     | 0.81              |
| 6:S:81:ARG:HD3   | 6:S:88:HIS:NE2    | 1.95                     | 0.80              |
| 1:N:508:PRO:HG3  | 3:P:6:HIS:HB3     | 1.62                     | 0.80              |
| 1:N:449:MET:SD   | 2:O:5:MET:HE2     | 2.22                     | 0.79              |
| 1:A:449:MET:SD   | 2:B:5:MET:HE2     | 2.23                     | 0.79              |
| 3:P:101:PHE:HD1  | 3:P:196:THR:HG21  | 1.45                     | 0.79              |
| 1:N:95:PRO:HG2   | 3:P:11:VAL:HG13   | 1.64                     | 0.78              |
| 7:G:18:PHE:HE2   | 1:N:278:MET:HE2   | 1.49                     | 0.77              |
| 1:A:95:PRO:HG2   | 3:C:11:VAL:HG13   | 1.67                     | 0.76              |
| 2:O:33:LEU:HD23  | 9:V:28:SER:HB3    | 1.66                     | 0.76              |
| 1:A:508:PRO:HG3  | 3:C:6:HIS:HB3     | 1.67                     | 0.76              |
| 1:A:197:LEU:HD12 | 7:T:4:ALA:HB2     | 1.68                     | 0.75              |
| 11:K:43:SER:OG   | 11:K:45:VAL:HG13  | 1.87                     | 0.75              |
| 1:N:365:ILE:HG13 | 2:O:87:MET:HE1    | 1.69                     | 0.75              |
| 1:N:306:THR:HB   | 1:N:359:ALA:O     | 1.89                     | 0.73              |
| 11:X:43:SER:OG   | 11:X:45:VAL:HG13  | 1.87                     | 0.73              |
| 6:F:81:ARG:HD3   | 6:F:88:HIS:NE2    | 2.03                     | 0.73              |
| 4:Q:67:SER:OG    | 4:Q:70:GLU:HG3    | 1.88                     | 0.72              |
| 1:N:390:MET:HE1  | 17:N:515:HEA:H242 | 1.72                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:G:4:ALA:HB2     | 1:N:197:LEU:HD12   | 1.71                     | 0.71              |
| 1:A:365:ILE:HG13  | 2:B:87:MET:HE1     | 1.72                     | 0.71              |
| 2:O:193:TYR:HE1   | 4:Q:126:MET:HE1    | 1.56                     | 0.71              |
| 2:O:145:PRO:HG3   | 2:O:148:MET:HE2    | 1.73                     | 0.70              |
| 1:A:1:MET:SD      | 1:A:1:MET:N        | 2.58                     | 0.70              |
| 3:C:19:THR:HG22   | 3:C:53:THR:OG1     | 1.91                     | 0.70              |
| 8:U:71:THR:O      | 8:U:75:ARG:HG2     | 1.93                     | 0.69              |
| 1:A:390:MET:HE1   | 17:A:515:HEA:H242  | 1.75                     | 0.68              |
| 17:N:515:HEA:O11  | 17:N:515:HEA:H262  | 1.92                     | 0.68              |
| 4:Q:52:SER:OG     | 4:Q:55:GLU:HG3     | 1.93                     | 0.68              |
| 6:F:53:THR:HG22   | 6:F:54:ASN:H       | 1.57                     | 0.68              |
| 2:O:196:CYS:HB2   | 2:O:207:MET:HG3    | 1.74                     | 0.68              |
| 2:B:145:PRO:HG3   | 2:B:148:MET:HE2    | 1.75                     | 0.68              |
| 3:P:221:ARG:HE    | 3:P:226:HIS:HD2    | 1.42                     | 0.68              |
| 6:S:10:GLU:HG2    | 6:S:25:ARG:NH2     | 2.07                     | 0.68              |
| 5:E:82:TYR:HB3    | 5:E:83:PRO:HD3     | 1.76                     | 0.68              |
| 2:O:186:SER:HB3   | 2:O:213:LEU:HD22   | 1.75                     | 0.68              |
| 4:D:52:SER:OG     | 4:D:55:GLU:HG3     | 1.94                     | 0.68              |
| 1:N:456:MET:HG2   | 4:Q:96:LEU:HD13    | 1.74                     | 0.68              |
| 6:S:53:THR:HG22   | 6:S:54:ASN:H       | 1.59                     | 0.67              |
| 4:D:67:SER:OG     | 4:D:70:GLU:HG3     | 1.93                     | 0.67              |
| 4:D:40:LEU:HD22   | 4:D:59:LEU:HD13    | 1.76                     | 0.67              |
| 2:B:89[B]:GLU:HB2 | 2:B:91[B]:ASN:HD21 | 1.60                     | 0.67              |
| 2:B:186:SER:HB3   | 2:B:213:LEU:HD22   | 1.77                     | 0.67              |
| 2:B:193:TYR:HE1   | 4:D:126:MET:HE1    | 1.60                     | 0.67              |
| 3:P:209:ILE:O     | 3:P:213:THR:HG23   | 1.94                     | 0.67              |
| 3:P:34:TRP:HE1    | 3:P:40:MET:HE2     | 1.59                     | 0.66              |
| 7:G:6:GLY:HA3     | 1:N:190:ILE:HG12   | 1.77                     | 0.66              |
| 3:C:119:THR:HG21  | 8:H:82:PRO:O       | 1.95                     | 0.66              |
| 8:H:71:THR:O      | 8:H:75:ARG:HG2     | 1.95                     | 0.66              |
| 3:P:19:THR:HG22   | 3:P:53:THR:OG1     | 1.95                     | 0.66              |
| 1:N:1:MET:SD      | 1:N:1:MET:N        | 2.63                     | 0.66              |
| 8:H:39:CYS:CB     | 8:H:53:CYS:SG      | 2.83                     | 0.66              |
| 1:N:209:LEU:O     | 1:N:213:ARG:HG3    | 1.96                     | 0.66              |
| 1:A:306:THR:HB    | 1:A:359:ALA:O      | 1.95                     | 0.66              |
| 3:C:34:TRP:NE1    | 3:C:40:MET:HE2     | 2.11                     | 0.65              |
| 3:C:34:TRP:HE1    | 3:C:40:MET:HE2     | 1.59                     | 0.65              |
| 3:C:209:ILE:O     | 3:C:213:THR:HG23   | 1.96                     | 0.65              |
| 17:A:515:HEA:O11  | 17:A:515:HEA:H262  | 1.97                     | 0.65              |
| 7:G:5:LYS:HE3     | 7:G:23:LEU:HD22    | 1.79                     | 0.65              |
| 1:A:282:PHE:HB2   | 7:T:5:LYS:HB3      | 1.79                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:Q:40:LEU:HD22   | 4:Q:59:LEU:HD13    | 1.79                     | 0.65              |
| 6:F:10:GLU:HG2    | 6:F:25:ARG:NH2     | 2.07                     | 0.65              |
| 3:P:34:TRP:NE1    | 3:P:40:MET:HE2     | 2.12                     | 0.64              |
| 1:A:456:MET:HG2   | 4:D:96:LEU:HD13    | 1.80                     | 0.64              |
| 7:T:5:LYS:HE3     | 7:T:23:LEU:HD22    | 1.78                     | 0.64              |
| 1:N:431:LEU:HD21  | 1:N:450:TRP:HB2    | 1.79                     | 0.64              |
| 2:O:68:LEU:HB3    | 2:O:69:PRO:HD3     | 1.79                     | 0.63              |
| 7:G:5:LYS:HB3     | 1:N:282:PHE:HB2    | 1.79                     | 0.63              |
| 1:N:290:HIS:CD2   | 1:N:291:HIS:CD2    | 2.86                     | 0.63              |
| 1:N:85:LEU:O      | 1:N:492:LEU:HD13   | 1.99                     | 0.63              |
| 1:A:190:ILE:HG12  | 7:T:6:GLY:HA3      | 1.79                     | 0.63              |
| 2:B:196:CYS:HB2   | 2:B:207:MET:HG3    | 1.80                     | 0.63              |
| 2:O:89[B]:GLU:HB2 | 2:O:91[B]:ASN:HD21 | 1.62                     | 0.63              |
| 1:A:431:LEU:HD21  | 1:A:450:TRP:HB2    | 1.80                     | 0.63              |
| 2:O:14:SER:HB3    | 2:O:168:LEU:HD23   | 1.80                     | 0.63              |
| 3:P:119:THR:HG21  | 8:U:82:PRO:O       | 1.98                     | 0.63              |
| 2:B:14:SER:HB3    | 2:B:168:LEU:HD23   | 1.81                     | 0.62              |
| 2:O:89[B]:GLU:HB2 | 2:O:91[B]:ASN:ND2  | 2.15                     | 0.62              |
| 1:N:138:HIS:O     | 1:N:213:ARG:NH2    | 2.33                     | 0.62              |
| 1:A:278:MET:CE    | 7:T:18:PHE:HE2     | 2.13                     | 0.62              |
| 7:T:9:GLY:HA2     | 7:T:19:LEU:HD11    | 1.82                     | 0.62              |
| 2:B:68:LEU:HB3    | 2:B:69:PRO:HD3     | 1.82                     | 0.62              |
| 1:N:32:ALA:HB3    | 12:Y:36:PRO:HG2    | 1.82                     | 0.62              |
| 2:B:89[B]:GLU:HB2 | 2:B:91[B]:ASN:ND2  | 2.14                     | 0.61              |
| 3:C:221:ARG:HE    | 3:C:226:HIS:HD2    | 1.48                     | 0.61              |
| 5:R:82:TYR:HB3    | 5:R:83:PRO:HD3     | 1.81                     | 0.61              |
| 8:U:39:CYS:CB     | 8:U:53:CYS:SG      | 2.88                     | 0.61              |
| 1:N:368:HIS:O     | 2:O:171:LYS:HE3    | 2.01                     | 0.61              |
| 1:A:209:LEU:O     | 1:A:213:ARG:HG3    | 2.00                     | 0.61              |
| 2:B:145:PRO:CG    | 2:B:148:MET:HE2    | 2.30                     | 0.60              |
| 12:Y:20:ARG:HH11  | 12:Y:20:ARG:HB3    | 1.66                     | 0.60              |
| 1:A:176:MET:CE    | 1:A:181:THR:HG22   | 2.32                     | 0.60              |
| 1:N:390:MET:CE    | 17:N:515:HEA:H242  | 2.30                     | 0.60              |
| 1:A:187:SER:HB2   | 1:A:277:MET:HE1    | 1.84                     | 0.60              |
| 7:G:9:GLY:HA2     | 7:G:19:LEU:HD11    | 1.82                     | 0.60              |
| 6:F:16:LEU:O      | 6:F:20:VAL:HG13    | 2.01                     | 0.60              |
| 4:Q:23:PRO:O      | 4:Q:25:PRO:HD3     | 2.02                     | 0.59              |
| 1:A:289:ALA:HB1   | 1:A:297:MET:HE1    | 1.84                     | 0.59              |
| 2:O:226:MET:O     | 2:O:227:LEU:HB2    | 2.02                     | 0.59              |
| 1:A:32:ALA:HB3    | 12:L:36:PRO:HG2    | 1.84                     | 0.59              |
| 1:A:197:LEU:CD1   | 7:T:4:ALA:HB2      | 2.32                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:N:176:MET:CE     | 1:N:181:THR:HG22  | 2.30                     | 0.59              |
| 1:N:289:ALA:HB1    | 1:N:297:MET:HE1   | 1.83                     | 0.59              |
| 2:O:145:PRO:CG     | 2:O:148:MET:HE2   | 2.32                     | 0.59              |
| 1:A:368:HIS:O      | 2:B:171:LYS:HE3   | 2.02                     | 0.59              |
| 1:A:390:MET:CE     | 17:A:515:HEA:H242 | 2.32                     | 0.59              |
| 2:O:146:MET:SD     | 2:O:189:PRO:HB3   | 2.43                     | 0.59              |
| 1:A:278:MET:HE2    | 7:T:18:PHE:CE2    | 2.30                     | 0.58              |
| 4:D:23:PRO:O       | 4:D:25:PRO:HD3    | 2.03                     | 0.58              |
| 1:A:138:HIS:O      | 1:A:213:ARG:NH2   | 2.36                     | 0.58              |
| 4:D:147:LYS:HE3    | 4:D:147:LYS:HA    | 1.86                     | 0.58              |
| 10:J:10:LYS:HE2    | 10:J:10:LYS:HA    | 1.85                     | 0.58              |
| 1:A:290:HIS:CD2    | 1:A:291:HIS:CD2   | 2.92                     | 0.58              |
| 7:G:4:ALA:HB2      | 1:N:197:LEU:CD1   | 2.33                     | 0.58              |
| 4:Q:66:GLU:O       | 5:R:66:ARG:NH2    | 2.37                     | 0.58              |
| 4:Q:102:TYR:CD1    | 13:Z:35:TYR:HE1   | 2.21                     | 0.58              |
| 8:H:60:TYR:CD1     | 8:H:60:TYR:C      | 2.82                     | 0.58              |
| 2:O:90[B]:ILE:HD11 | 2:O:151:ARG:HH21  | 1.69                     | 0.57              |
| 4:D:23:PRO:O       | 5:E:66:ARG:HD3    | 2.04                     | 0.57              |
| 6:F:8:THR:OG1      | 6:F:11:GLU:HG2    | 2.04                     | 0.57              |
| 1:N:302:ARG:O      | 1:N:306:THR:HG23  | 2.04                     | 0.57              |
| 2:O:125:THR:HA     | 2:O:128:LEU:HG    | 1.86                     | 0.57              |
| 1:N:65:MET:HE3     | 17:N:515:HEA:HMC2 | 1.86                     | 0.57              |
| 1:A:302:ARG:O      | 1:A:306:THR:HG23  | 2.05                     | 0.57              |
| 1:A:354:THR:CG2    | 1:A:376:HIS:HB2   | 2.35                     | 0.56              |
| 9:I:19:PHE:CD1     | 9:I:19:PHE:C      | 2.83                     | 0.56              |
| 2:B:5:MET:HE3      | 11:K:42:PRO:HA    | 1.88                     | 0.56              |
| 2:B:226:MET:O      | 2:B:227:LEU:HB2   | 2.04                     | 0.56              |
| 2:O:86:MET:O       | 2:O:89[B]:GLU:HG2 | 2.05                     | 0.56              |
| 6:S:16:LEU:O       | 6:S:20:VAL:HG13   | 2.05                     | 0.56              |
| 10:W:10:LYS:HE2    | 10:W:10:LYS:HA    | 1.87                     | 0.56              |
| 8:U:57:ARG:O       | 8:U:61:LYS:HB2    | 2.05                     | 0.56              |
| 1:N:187:SER:HB2    | 1:N:277:MET:HE1   | 1.87                     | 0.56              |
| 1:A:240:HIS:O      | 1:A:243:VAL:HG22  | 2.05                     | 0.56              |
| 1:A:197:LEU:HD12   | 7:T:4:ALA:CB      | 2.35                     | 0.56              |
| 2:B:100:MET:HE3    | 2:B:157:GLU:HG3   | 1.88                     | 0.55              |
| 12:L:20:ARG:HH11   | 12:L:20:ARG:HB3   | 1.71                     | 0.55              |
| 6:S:8:THR:OG1      | 6:S:11:GLU:HG2    | 2.07                     | 0.55              |
| 3:P:110:PRO:HB3    | 8:U:30:TRP:CE3    | 2.40                     | 0.55              |
| 8:U:39:CYS:C       | 8:U:53:CYS:SG     | 2.89                     | 0.55              |
| 9:V:19:PHE:CD1     | 9:V:19:PHE:C      | 2.84                     | 0.55              |
| 6:F:10:GLU:O       | 6:F:18:ARG:NH2    | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:N:354:THR:CG2   | 1:N:376:HIS:HB2   | 2.36                     | 0.55              |
| 8:H:57:ARG:O      | 8:H:61:LYS:HB2    | 2.07                     | 0.55              |
| 8:H:39:CYS:C      | 8:H:53:CYS:SG     | 2.90                     | 0.55              |
| 1:N:128:VAL:HG22  | 1:N:128:VAL:O     | 2.06                     | 0.55              |
| 4:Q:23:PRO:O      | 5:R:66:ARG:HD3    | 2.07                     | 0.55              |
| 8:U:75:ARG:HG3    | 8:U:75:ARG:HH11   | 1.72                     | 0.55              |
| 17:A:515:HEA:HBC1 | 17:A:515:HEA:HMC1 | 1.88                     | 0.55              |
| 4:D:102:TYR:CD2   | 13:M:35:TYR:HE1   | 2.25                     | 0.54              |
| 3:P:154:GLY:HA2   | 6:S:6:VAL:HG22    | 1.89                     | 0.54              |
| 2:O:150:ILE:HD12  | 2:O:150:ILE:N     | 2.22                     | 0.54              |
| 6:S:10:GLU:O      | 6:S:18:ARG:NH2    | 2.41                     | 0.54              |
| 11:X:24:PHE:O     | 11:X:28:VAL:HG23  | 2.06                     | 0.54              |
| 2:B:150:ILE:N     | 2:B:150:ILE:HD12  | 2.23                     | 0.54              |
| 4:D:127:LYS:O     | 4:D:130:PRO:HD3   | 2.08                     | 0.54              |
| 13:M:35:TYR:HD2   | 13:M:36:HIS:CD2   | 2.26                     | 0.54              |
| 7:G:18:PHE:HE2    | 1:N:278:MET:CE    | 2.20                     | 0.54              |
| 6:F:81:ARG:HD2    | 6:F:86:GLY:O      | 2.08                     | 0.54              |
| 13:Z:28:LEU:HB2   | 13:Z:29:PRO:HD3   | 1.90                     | 0.54              |
| 5:E:79:LYS:H      | 5:E:79:LYS:HD3    | 1.73                     | 0.54              |
| 7:G:4:ALA:CB      | 1:N:197:LEU:HD12  | 2.38                     | 0.54              |
| 2:O:5:MET:HE3     | 11:X:42:PRO:HA    | 1.90                     | 0.54              |
| 1:A:35:LEU:HD11   | 1:A:462:LEU:HD13  | 1.90                     | 0.53              |
| 2:B:125:THR:HA    | 2:B:128:LEU:HG    | 1.90                     | 0.53              |
| 5:R:43:PRO:HB2    | 5:R:48:ILE:HD11   | 1.91                     | 0.53              |
| 1:A:62:ALA:HB2    | 17:A:515:HEA:HBD1 | 1.90                     | 0.53              |
| 9:I:29:LEU:O      | 9:I:33:THR:HG23   | 2.09                     | 0.53              |
| 4:Q:97:ILE:HG13   | 11:X:32:MET:HG3   | 1.91                     | 0.53              |
| 1:A:229:ILE:HD11  | 2:B:175:ILE:HD13  | 1.90                     | 0.53              |
| 13:Z:35:TYR:HD2   | 13:Z:36:HIS:CD2   | 2.27                     | 0.53              |
| 12:L:41:ARG:HD2   | 13:M:40:TYR:CZ    | 2.43                     | 0.53              |
| 12:Y:41:ARG:HD2   | 13:Z:40:TYR:CZ    | 2.44                     | 0.53              |
| 1:N:456:MET:HG2   | 4:Q:96:LEU:CD1    | 2.39                     | 0.53              |
| 2:B:89[A]:GLU:O   | 2:B:91[A]:ASN:ND2 | 2.42                     | 0.53              |
| 12:L:46:LYS:O     | 12:L:47:LYS:HB2   | 2.09                     | 0.53              |
| 2:O:100:MET:HE3   | 2:O:157:GLU:HG3   | 1.91                     | 0.53              |
| 8:U:34:LEU:O      | 8:U:38:ARG:HG3    | 2.08                     | 0.53              |
| 5:E:63:SER:O      | 5:E:67:ILE:HG13   | 2.09                     | 0.53              |
| 1:A:85:LEU:O      | 1:A:492:LEU:HD13  | 2.08                     | 0.52              |
| 1:N:197:LEU:O     | 3:P:92:LEU:HD22   | 2.09                     | 0.52              |
| 1:A:273:MET:HG3   | 1:A:319:LYS:HZ1   | 1.74                     | 0.52              |
| 6:F:52:ILE:O      | 6:F:98:HIS:HA     | 2.08                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:Q:147:LYS:HE3  | 4:Q:147:LYS:HA    | 1.90                     | 0.52              |
| 3:C:154:GLY:HA2  | 6:F:6:VAL:HG22    | 1.90                     | 0.52              |
| 1:A:298:ASP:HB2  | 1:A:301:THR:HG23  | 1.91                     | 0.52              |
| 1:N:115:SER:O    | 1:N:121:GLY:HA2   | 2.09                     | 0.52              |
| 7:G:18:PHE:CE2   | 1:N:278:MET:HE2   | 2.38                     | 0.52              |
| 3:C:101:PHE:HD1  | 3:C:196:THR:CG2   | 2.20                     | 0.52              |
| 1:N:240:HIS:O    | 1:N:243:VAL:HG22  | 2.09                     | 0.52              |
| 2:O:136:LEU:HB3  | 2:O:193:TYR:CD2   | 2.44                     | 0.52              |
| 2:O:186:SER:CB   | 2:O:213:LEU:HD22  | 2.38                     | 0.52              |
| 3:P:30:GLY:HA2   | 3:P:42:LEU:HB3    | 1.92                     | 0.52              |
| 4:D:66:GLU:O     | 5:E:66:ARG:NH2    | 2.42                     | 0.52              |
| 7:G:36:TRP:HD1   | 7:G:36:TRP:O      | 1.93                     | 0.52              |
| 1:N:36:LEU:HD13  | 12:Y:40:VAL:HG21  | 1.91                     | 0.52              |
| 1:A:106:PRO:HB2  | 1:A:107:PRO:HD3   | 1.92                     | 0.51              |
| 5:R:79:LYS:HD3   | 5:R:79:LYS:H      | 1.74                     | 0.51              |
| 2:B:186:SER:CB   | 2:B:213:LEU:HD22  | 2.39                     | 0.51              |
| 1:N:229:ILE:HD11 | 2:O:175:ILE:HD13  | 1.92                     | 0.51              |
| 1:N:290:HIS:HD2  | 1:N:291:HIS:CD2   | 2.26                     | 0.51              |
| 2:O:62:GLU:HA    | 2:O:65:TRP:CD1    | 2.45                     | 0.51              |
| 1:A:128:VAL:HG22 | 1:A:128:VAL:O     | 2.09                     | 0.51              |
| 1:N:144:ASP:OD1  | 1:N:213:ARG:HD3   | 2.10                     | 0.51              |
| 1:N:390:MET:HE2  | 1:N:390:MET:HA    | 1.91                     | 0.51              |
| 3:P:146:TRP:CZ2  | 7:T:17:ARG:HG3    | 2.46                     | 0.51              |
| 3:P:112:LEU:HG   | 3:P:118:PRO:HB3   | 1.93                     | 0.51              |
| 2:B:102:HIS:O    | 2:B:104:TRP:N     | 2.43                     | 0.51              |
| 1:N:62:ALA:HB2   | 17:N:515:HEA:HBD1 | 1.93                     | 0.51              |
| 2:O:100:MET:CE   | 2:O:157:GLU:HG3   | 2.41                     | 0.51              |
| 2:O:146:MET:HA   | 2:O:213:LEU:HD23  | 1.92                     | 0.51              |
| 7:T:36:TRP:O     | 7:T:36:TRP:HD1    | 1.93                     | 0.51              |
| 8:U:60:TYR:CD1   | 8:U:60:TYR:C      | 2.89                     | 0.51              |
| 2:B:33:LEU:CD2   | 9:I:28:SER:HB3    | 2.39                     | 0.51              |
| 2:B:86:MET:O     | 2:B:89[B]:GLU:HG2 | 2.11                     | 0.51              |
| 2:B:146:MET:SD   | 2:B:189:PRO:HB3   | 2.51                     | 0.51              |
| 4:D:97:ILE:HG13  | 11:K:32:MET:HG3   | 1.93                     | 0.51              |
| 2:O:121:TYR:O    | 2:O:138:VAL:HA    | 2.11                     | 0.51              |
| 2:O:132:GLU:HB3  | 2:O:137:GLU:HG3   | 1.92                     | 0.51              |
| 2:B:100:MET:CE   | 2:B:157:GLU:HG3   | 2.40                     | 0.51              |
| 2:O:89[A]:GLU:O  | 2:O:91[A]:ASN:ND2 | 2.44                     | 0.50              |
| 5:R:63:SER:O     | 5:R:67:ILE:HG13   | 2.11                     | 0.50              |
| 1:A:286:ILE:HG22 | 7:T:1:ALA:HB1     | 1.93                     | 0.50              |
| 2:O:52:HIS:CD2   | 5:R:40:ASP:HB2    | 2.47                     | 0.50              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:P:101:PHE:HD1    | 3:P:196:THR:CG2  | 2.19                     | 0.50              |
| 1:A:187:SER:CB     | 1:A:277:MET:HE1  | 2.41                     | 0.50              |
| 3:C:222:GLN:HE21   | 3:C:222:GLN:HA   | 1.76                     | 0.50              |
| 5:E:43:PRO:HB2     | 5:E:48:ILE:HD11  | 1.92                     | 0.50              |
| 3:C:30:GLY:HA2     | 3:C:42:LEU:HB3   | 1.94                     | 0.50              |
| 8:H:75:ARG:HG3     | 8:H:75:ARG:HH11  | 1.76                     | 0.50              |
| 3:P:164:PHE:O      | 3:P:168:THR:HG23 | 2.11                     | 0.50              |
| 4:D:16:TYR:CE1     | 4:D:25:PRO:HG2   | 2.47                     | 0.50              |
| 13:M:28:LEU:HB2    | 13:M:29:PRO:HD3  | 1.93                     | 0.50              |
| 1:N:187:SER:CB     | 1:N:277:MET:HE1  | 2.42                     | 0.50              |
| 12:Y:46:LYS:O      | 12:Y:47:LYS:HB2  | 2.12                     | 0.50              |
| 2:B:62:GLU:HA      | 2:B:65:TRP:CD1   | 2.47                     | 0.49              |
| 8:H:34:LEU:O       | 8:H:38:ARG:HG3   | 2.11                     | 0.49              |
| 1:N:106:PRO:HB2    | 1:N:107:PRO:HD3  | 1.95                     | 0.49              |
| 2:O:132:GLU:HA     | 4:Q:122:ARG:NH1  | 2.27                     | 0.49              |
| 2:B:90[B]:ILE:HD11 | 2:B:151:ARG:HH21 | 1.77                     | 0.49              |
| 4:D:107:ILE:HD13   | 4:D:107:ILE:H    | 1.77                     | 0.49              |
| 1:A:36:LEU:HD13    | 12:L:40:VAL:HG21 | 1.94                     | 0.49              |
| 1:A:69:MET:HE2     | 1:A:70:VAL:N     | 2.28                     | 0.49              |
| 3:P:19:THR:HG23    | 10:W:39:CYS:SG   | 2.53                     | 0.49              |
| 11:K:24:PHE:O      | 11:K:28:VAL:HG23 | 2.12                     | 0.49              |
| 1:N:240:HIS:HB3    | 1:N:241:PRO:HD3  | 1.94                     | 0.49              |
| 6:S:81:ARG:HD2     | 6:S:86:GLY:O     | 2.13                     | 0.49              |
| 2:B:52:HIS:CD2     | 5:E:40:ASP:HB2   | 2.48                     | 0.49              |
| 2:B:83:ILE:O       | 2:B:87:MET:HG3   | 2.13                     | 0.49              |
| 3:C:164:PHE:O      | 3:C:168:THR:HG23 | 2.13                     | 0.49              |
| 1:A:74:MET:HE3     | 1:A:249:PRO:HB2  | 1.95                     | 0.49              |
| 4:D:126:MET:HG3    | 4:D:128:VAL:HG23 | 1.95                     | 0.49              |
| 12:Y:1:SER:HB2     | 12:Y:3:TYR:CE2   | 2.47                     | 0.49              |
| 1:A:476:PHE:CD1    | 12:L:15:VAL:HG21 | 2.48                     | 0.48              |
| 3:C:146:TRP:CZ2    | 7:G:17:ARG:HG3   | 2.48                     | 0.48              |
| 1:A:61:HIS:CD2     | 17:A:515:HEA:ND  | 2.80                     | 0.48              |
| 1:N:35:LEU:HD11    | 1:N:462:LEU:HD13 | 1.95                     | 0.48              |
| 1:N:273:MET:HG3    | 1:N:319:LYS:HZ1  | 1.78                     | 0.48              |
| 1:N:298:ASP:HB2    | 1:N:301:THR:HG23 | 1.94                     | 0.48              |
| 3:C:19:THR:HG23    | 10:J:39:CYS:SG   | 2.54                     | 0.48              |
| 10:W:11:LEU:HD23   | 10:W:11:LEU:O    | 2.14                     | 0.48              |
| 10:W:30:ILE:O      | 10:W:34:VAL:HG23 | 2.12                     | 0.48              |
| 1:A:285:PHE:CE2    | 7:T:4:ALA:HB3    | 2.48                     | 0.48              |
| 3:C:154:GLY:HA2    | 6:F:6:VAL:CG2    | 2.44                     | 0.48              |
| 3:P:154:GLY:HA2    | 6:S:6:VAL:CG2    | 2.43                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:177:GLN:HA    | 3:C:177:GLN:OE1  | 2.13                     | 0.48              |
| 1:N:503:HIS:CD2   | 3:P:10:MET:HE2   | 2.49                     | 0.48              |
| 17:A:516:HEA:H243 | 2:B:69:PRO:HB3   | 1.95                     | 0.48              |
| 2:O:102:HIS:O     | 2:O:104:TRP:N    | 2.46                     | 0.48              |
| 1:A:240:HIS:HB3   | 1:A:241:PRO:HD3  | 1.95                     | 0.47              |
| 1:A:253:MET:HE3   | 1:A:392:GLY:HA3  | 1.95                     | 0.47              |
| 4:Q:127:LYS:O     | 4:Q:130:PRO:HD3  | 2.14                     | 0.47              |
| 9:V:55:ASP:HB3    | 9:V:58:LYS:HB3   | 1.96                     | 0.47              |
| 2:O:184:LEU:HD11  | 2:O:211:LEU:HD21 | 1.96                     | 0.47              |
| 11:X:22:ALA:O     | 11:X:26:VAL:HG23 | 2.15                     | 0.47              |
| 4:Q:16:TYR:CE1    | 4:Q:25:PRO:HG2   | 2.50                     | 0.47              |
| 2:B:132:GLU:HB3   | 2:B:137:GLU:HG3  | 1.95                     | 0.47              |
| 6:S:52:ILE:O      | 6:S:98:HIS:HA    | 2.13                     | 0.47              |
| 3:C:224:LYS:HZ2   | 3:C:224:LYS:HB3  | 1.79                     | 0.47              |
| 4:D:24:LEU:HD12   | 5:E:30:ARG:HA    | 1.95                     | 0.47              |
| 1:N:51:ASP:HB2    | 2:O:202:SER:O    | 2.14                     | 0.47              |
| 2:O:191:LEU:HB2   | 4:Q:126:MET:HE3  | 1.97                     | 0.47              |
| 1:A:51:ASP:HB2    | 2:B:202:SER:O    | 2.14                     | 0.47              |
| 1:A:474:GLU:CD    | 1:A:480:ARG:HH22 | 2.22                     | 0.47              |
| 4:Q:24:LEU:HD12   | 5:R:30:ARG:HA    | 1.96                     | 0.47              |
| 4:Q:107:ILE:HD13  | 4:Q:107:ILE:H    | 1.79                     | 0.47              |
| 4:Q:118:LYS:HA    | 11:X:51:LYS:O    | 2.15                     | 0.47              |
| 1:N:435:GLY:O     | 1:N:437:PRO:HD3  | 2.15                     | 0.47              |
| 1:N:474:GLU:CD    | 1:N:480:ARG:HH22 | 2.21                     | 0.47              |
| 4:Q:77:GLU:HA     | 11:X:10:HIS:CG   | 2.49                     | 0.47              |
| 5:E:52:LEU:O      | 5:E:55:CYS:HB2   | 2.14                     | 0.47              |
| 1:N:266:GLU:HB2   | 1:N:267:PRO:HD2  | 1.96                     | 0.47              |
| 1:A:290:HIS:HD2   | 1:A:291:HIS:CD2  | 2.33                     | 0.47              |
| 9:I:35:TYR:O      | 9:I:39:VAL:HB    | 2.15                     | 0.47              |
| 6:F:97:ALA:O      | 6:F:98:HIS:HB2   | 2.13                     | 0.46              |
| 2:O:203:ASN:HD22  | 2:O:206:PHE:HD2  | 1.63                     | 0.46              |
| 3:P:177:GLN:OE1   | 3:P:177:GLN:HA   | 2.14                     | 0.46              |
| 4:Q:40:LEU:HD21   | 4:Q:55:GLU:HB3   | 1.97                     | 0.46              |
| 12:Y:20:ARG:HB3   | 12:Y:20:ARG:NH1  | 2.30                     | 0.46              |
| 1:A:144:ASP:OD1   | 1:A:213:ARG:HD3  | 2.15                     | 0.46              |
| 1:A:115:SER:O     | 1:A:121:GLY:HA2  | 2.16                     | 0.46              |
| 2:B:37:LEU:O      | 2:B:41:ILE:HG12  | 2.16                     | 0.46              |
| 2:B:132:GLU:HA    | 4:D:122:ARG:NH1  | 2.31                     | 0.46              |
| 10:J:30:ILE:O     | 10:J:34:VAL:HG23 | 2.15                     | 0.46              |
| 13:M:17:ILE:O     | 13:M:21:VAL:HG23 | 2.15                     | 0.46              |
| 1:N:426:PHE:N     | 1:N:427:PRO:CD   | 2.79                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:37:LEU:O     | 2:O:41:ILE:HG12  | 2.16                     | 0.46              |
| 3:C:110:PRO:HB3  | 8:H:30:TRP:CE3   | 2.51                     | 0.46              |
| 6:F:81:ARG:HD3   | 6:F:88:HIS:CE1   | 2.51                     | 0.46              |
| 1:N:95:PRO:CG    | 3:P:11:VAL:HG13  | 2.41                     | 0.46              |
| 1:N:107:PRO:HB3  | 3:P:25:LEU:HB2   | 1.97                     | 0.46              |
| 2:O:122:MET:HB2  | 2:O:208:PRO:HD2  | 1.96                     | 0.46              |
| 4:D:109:HIS:O    | 4:D:112:GLU:HG2  | 2.15                     | 0.46              |
| 1:N:492:LEU:HD22 | 1:N:492:LEU:O    | 2.15                     | 0.46              |
| 4:Q:68:PHE:HA    | 4:Q:71:MET:HG2   | 1.97                     | 0.46              |
| 5:R:52:LEU:O     | 5:R:55:CYS:HB2   | 2.15                     | 0.46              |
| 7:T:67:HIS:NE2   | 7:T:78:LEU:HD21  | 2.31                     | 0.46              |
| 9:V:29:LEU:O     | 9:V:33:THR:HG23  | 2.15                     | 0.46              |
| 9:V:60:PHE:CE1   | 9:V:69:PHE:CE2   | 3.04                     | 0.46              |
| 3:P:16:TRP:HA    | 3:P:16:TRP:CE3   | 2.51                     | 0.46              |
| 2:B:148:MET:O    | 2:B:150:ILE:HD12 | 2.15                     | 0.46              |
| 2:B:139:ASP:OD1  | 2:B:140:ASN:N    | 2.49                     | 0.46              |
| 3:P:222:GLN:HE21 | 3:P:222:GLN:HA   | 1.80                     | 0.46              |
| 2:B:136:LEU:HB3  | 2:B:193:TYR:CD2  | 2.51                     | 0.46              |
| 1:N:390:MET:HE1  | 17:N:515:HEA:C24 | 2.44                     | 0.46              |
| 2:O:95:LEU:HD12  | 2:O:112:ASP:OD2  | 2.15                     | 0.46              |
| 13:Z:17:ILE:O    | 13:Z:21:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:107:PRO:HB3  | 3:C:25:LEU:HB2   | 1.97                     | 0.45              |
| 13:M:42:LYS:O    | 13:M:43:SER:HB2  | 2.16                     | 0.45              |
| 7:T:36:TRP:CD1   | 7:T:36:TRP:C     | 2.95                     | 0.45              |
| 7:G:15:THR:O     | 7:G:18:PHE:HB3   | 2.16                     | 0.45              |
| 3:P:160:LEU:HD13 | 3:P:222:GLN:HG2  | 1.98                     | 0.45              |
| 1:A:503:HIS:CD2  | 3:C:10:MET:HE2   | 2.51                     | 0.45              |
| 1:N:253:MET:HE3  | 1:N:392:GLY:HA3  | 1.99                     | 0.45              |
| 2:O:62:GLU:HA    | 2:O:65:TRP:NE1   | 2.30                     | 0.45              |
| 2:O:139:ASP:OD1  | 2:O:140:ASN:N    | 2.48                     | 0.45              |
| 9:V:63:MET:HB3   | 9:V:68:ILE:HD11  | 1.97                     | 0.45              |
| 11:K:9:PHE:CD1   | 11:K:9:PHE:C     | 2.94                     | 0.45              |
| 5:R:41:LEU:C     | 5:R:41:LEU:HD12  | 2.41                     | 0.45              |
| 2:B:62:GLU:HA    | 2:B:65:TRP:NE1   | 2.31                     | 0.45              |
| 2:B:25:ASP:OD2   | 9:I:43:ARG:HD2   | 2.16                     | 0.45              |
| 6:S:97:ALA:O     | 6:S:98:HIS:HB2   | 2.16                     | 0.45              |
| 7:G:36:TRP:CD1   | 7:G:36:TRP:C     | 2.94                     | 0.45              |
| 4:Q:126:MET:HG3  | 4:Q:128:VAL:HG23 | 1.98                     | 0.45              |
| 6:S:81:ARG:HA    | 6:S:87:THR:O     | 2.16                     | 0.45              |
| 1:N:172:LYS:HD2  | 1:N:176:MET:HE2  | 1.98                     | 0.45              |
| 2:O:123:ILE:HD12 | 2:O:137:GLU:HB3  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:Z:38:ASP:O    | 13:Z:42:LYS:HG2   | 2.17                     | 0.45              |
| 1:A:65:MET:HE3   | 17:A:515:HEA:HMC3 | 1.99                     | 0.45              |
| 1:A:197:LEU:O    | 3:C:92:LEU:HD22   | 2.17                     | 0.45              |
| 8:H:39:CYS:HB3   | 8:H:53:CYS:SG     | 2.57                     | 0.45              |
| 7:T:53:LEU:O     | 7:T:54:ARG:C      | 2.60                     | 0.45              |
| 8:U:54:GLU:OE1   | 8:U:57:ARG:NH1    | 2.50                     | 0.45              |
| 12:L:1:SER:HB2   | 12:L:3:TYR:CE2    | 2.53                     | 0.44              |
| 4:Q:138:TRP:CH2  | 11:X:50:PRO:HG2   | 2.52                     | 0.44              |
| 2:B:203:ASN:HD22 | 2:B:206:PHE:HD2   | 1.64                     | 0.44              |
| 1:A:456:MET:HG2  | 4:D:96:LEU:CD1    | 2.45                     | 0.44              |
| 2:B:82:ARG:HH21  | 2:B:86:MET:HE1    | 1.82                     | 0.44              |
| 2:O:33:LEU:CD2   | 9:V:28:SER:HB3    | 2.42                     | 0.44              |
| 6:S:81:ARG:HD3   | 6:S:88:HIS:CE1    | 2.52                     | 0.44              |
| 1:A:250:GLY:O    | 1:A:254:ILE:HG12  | 2.17                     | 0.44              |
| 7:G:1:ALA:HB1    | 1:N:286:ILE:HG22  | 1.99                     | 0.44              |
| 10:J:50:LEU:HD22 | 10:J:50:LEU:O     | 2.18                     | 0.44              |
| 2:O:82:ARG:HH21  | 2:O:86:MET:HE1    | 1.82                     | 0.44              |
| 2:B:133:LEU:HA   | 2:B:133:LEU:HD23  | 1.69                     | 0.44              |
| 2:B:184:LEU:HD11 | 2:B:211:LEU:HD21  | 1.99                     | 0.44              |
| 1:N:69:MET:HE2   | 1:N:70:VAL:N      | 2.32                     | 0.44              |
| 1:N:100:MET:HE3  | 1:N:159:LEU:HD21  | 1.99                     | 0.44              |
| 11:X:43:SER:HG   | 11:X:45:VAL:HG13  | 1.78                     | 0.44              |
| 3:C:42:LEU:HD12  | 3:C:42:LEU:HA     | 1.81                     | 0.44              |
| 2:O:83:ILE:O     | 2:O:87:MET:HG3    | 2.17                     | 0.44              |
| 4:Q:102:TYR:HD1  | 13:Z:35:TYR:HE1   | 1.66                     | 0.44              |
| 2:B:122:MET:HB2  | 2:B:208:PRO:HD2   | 1.99                     | 0.44              |
| 2:B:123:ILE:HD12 | 2:B:137:GLU:HB3   | 2.00                     | 0.44              |
| 7:G:4:ALA:HB3    | 1:N:285:PHE:CE2   | 2.53                     | 0.44              |
| 7:T:44:ARG:HA    | 7:T:45:PRO:HD3    | 1.71                     | 0.44              |
| 1:A:129:TYR:CE1  | 1:A:232:GLN:HG2   | 2.53                     | 0.43              |
| 3:P:42:LEU:HD12  | 3:P:42:LEU:HA     | 1.76                     | 0.43              |
| 1:A:426:PHE:N    | 1:A:427:PRO:CD    | 2.81                     | 0.43              |
| 1:N:344:PHE:CD1  | 1:N:344:PHE:C     | 2.96                     | 0.43              |
| 3:P:54:MET:HB3   | 3:P:58:TRP:CZ3    | 2.53                     | 0.43              |
| 12:Y:44:LEU:HD12 | 12:Y:44:LEU:HA    | 1.73                     | 0.43              |
| 1:A:492:LEU:O    | 1:A:492:LEU:HD22  | 2.18                     | 0.43              |
| 7:G:34:ASN:C     | 7:G:36:TRP:H      | 2.26                     | 0.43              |
| 10:W:11:LEU:HD23 | 10:W:11:LEU:C     | 2.44                     | 0.43              |
| 2:B:95:LEU:HD12  | 2:B:112:ASP:OD2   | 2.19                     | 0.43              |
| 3:C:16:TRP:CE3   | 3:C:16:TRP:HA     | 2.53                     | 0.43              |
| 11:X:9:PHE:CD1   | 11:X:9:PHE:C      | 2.96                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:402:GLY:HA3  | 1:N:499:PRO:HD3  | 2.01                     | 0.43              |
| 2:O:131:GLY:O    | 4:Q:122:ARG:HD3  | 2.18                     | 0.43              |
| 3:P:146:TRP:CE2  | 7:T:17:ARG:HG3   | 2.54                     | 0.43              |
| 3:P:224:LYS:HB3  | 3:P:224:LYS:HZ2  | 1.83                     | 0.43              |
| 1:N:100:MET:HE3  | 1:N:159:LEU:CD2  | 2.49                     | 0.43              |
| 6:F:53:THR:HG22  | 6:F:54:ASN:N     | 2.30                     | 0.43              |
| 1:N:495:LEU:HD23 | 1:N:495:LEU:HA   | 1.79                     | 0.43              |
| 3:P:47:LEU:O     | 3:P:51:MET:HG2   | 2.19                     | 0.43              |
| 1:A:468:MET:HE2  | 1:A:468:MET:HB3  | 1.85                     | 0.43              |
| 1:A:483:LEU:HD23 | 1:A:483:LEU:HA   | 1.85                     | 0.43              |
| 2:B:68:LEU:HD12  | 2:B:68:LEU:HA    | 1.87                     | 0.43              |
| 3:C:163:LEU:HD13 | 3:C:219:PHE:HD1  | 1.84                     | 0.43              |
| 10:J:47:LEU:HD12 | 10:J:47:LEU:HA   | 1.73                     | 0.43              |
| 1:N:87:ILE:HG22  | 1:N:176:MET:HE1  | 2.00                     | 0.43              |
| 2:O:3:TYR:CD1    | 2:O:3:TYR:N      | 2.87                     | 0.43              |
| 4:Q:48:TRP:HB2   | 5:R:96:LEU:O     | 2.19                     | 0.43              |
| 7:T:34:ASN:C     | 7:T:36:TRP:H     | 2.27                     | 0.43              |
| 1:A:495:LEU:HD23 | 1:A:495:LEU:HA   | 1.77                     | 0.43              |
| 1:A:513:LEU:HD12 | 1:A:513:LEU:HA   | 1.78                     | 0.43              |
| 8:H:54:GLU:OE1   | 8:H:57:ARG:NH1   | 2.52                     | 0.43              |
| 1:N:508:PRO:O    | 6:S:56:ARG:HD3   | 2.19                     | 0.42              |
| 2:O:188:ARG:HG2  | 9:V:54:TYR:CZ    | 2.53                     | 0.42              |
| 4:Q:37:GLN:O     | 4:Q:41:LYS:HG2   | 2.19                     | 0.42              |
| 11:X:44:PRO:HA   | 11:X:47:ARG:NH1  | 2.33                     | 0.42              |
| 3:C:154:GLY:O    | 6:F:6:VAL:HG13   | 2.20                     | 0.42              |
| 11:K:32:MET:HB3  | 11:K:32:MET:HE2  | 1.70                     | 0.42              |
| 1:N:144:ASP:CG   | 1:N:213:ARG:HH11 | 2.26                     | 0.42              |
| 12:L:44:LEU:HD12 | 12:L:44:LEU:HA   | 1.73                     | 0.42              |
| 1:N:476:PHE:CD1  | 12:Y:15:VAL:HG21 | 2.54                     | 0.42              |
| 5:R:106:LEU:HA   | 5:R:106:LEU:HD23 | 1.84                     | 0.42              |
| 9:V:35:TYR:O     | 9:V:39:VAL:HB    | 2.20                     | 0.42              |
| 13:Z:42:LYS:O    | 13:Z:43:SER:HB2  | 2.20                     | 0.42              |
| 1:A:308:ALA:O    | 1:A:311:ILE:HG12 | 2.19                     | 0.42              |
| 3:C:146:TRP:CE2  | 7:G:17:ARG:HG3   | 2.54                     | 0.42              |
| 1:N:176:MET:HE3  | 1:N:181:THR:CG2  | 2.41                     | 0.42              |
| 1:A:344:PHE:CD1  | 1:A:344:PHE:C    | 2.97                     | 0.42              |
| 5:E:41:LEU:C     | 5:E:41:LEU:HD12  | 2.44                     | 0.42              |
| 6:F:81:ARG:HA    | 6:F:87:THR:O     | 2.20                     | 0.42              |
| 4:Q:102:TYR:CD1  | 13:Z:35:TYR:CE1  | 3.06                     | 0.42              |
| 2:B:3:TYR:CD1    | 2:B:3:TYR:N      | 2.86                     | 0.42              |
| 3:C:54:MET:HB3   | 3:C:58:TRP:CZ3   | 2.54                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D:119:GLN:O      | 4:D:123:MET:HG3   | 2.20                     | 0.42              |
| 5:E:86:ILE:HD13    | 5:E:86:ILE:HA     | 1.83                     | 0.42              |
| 2:O:1:MET:HE1      | 2:O:133:LEU:HD13  | 2.00                     | 0.42              |
| 4:Q:4:SER:N        | 4:Q:29:HIS:O      | 2.52                     | 0.42              |
| 12:Y:15:VAL:O      | 12:Y:15:VAL:HG13  | 2.20                     | 0.42              |
| 11:K:44:PRO:HA     | 11:K:47:ARG:NH1   | 2.34                     | 0.42              |
| 5:R:9:GLU:CD       | 5:R:9:GLU:H       | 2.28                     | 0.42              |
| 3:C:169:LEU:HD23   | 3:C:169:LEU:HA    | 1.85                     | 0.42              |
| 4:D:118:LYS:HA     | 11:K:51:LYS:O     | 2.20                     | 0.42              |
| 1:N:129:TYR:CE1    | 1:N:232:GLN:HG2   | 2.55                     | 0.42              |
| 2:B:146:MET:HA     | 2:B:213:LEU:HD23  | 2.01                     | 0.42              |
| 3:C:154:GLY:C      | 6:F:6:VAL:HG13    | 2.45                     | 0.42              |
| 6:F:30:PRO:HG2     | 6:F:31:TYR:CD2    | 2.55                     | 0.42              |
| 1:N:498:CYS:HA     | 1:N:499:PRO:HA    | 1.87                     | 0.42              |
| 2:O:25:ASP:OD2     | 9:V:43:ARG:HD2    | 2.20                     | 0.42              |
| 4:D:40:LEU:HD22    | 4:D:59:LEU:CD1    | 2.49                     | 0.41              |
| 5:R:80:GLU:H       | 5:R:80:GLU:CD     | 2.28                     | 0.41              |
| 13:M:37:LEU:HA     | 13:M:37:LEU:HD23  | 1.81                     | 0.41              |
| 1:N:48:LEU:HD23    | 1:N:48:LEU:HA     | 1.80                     | 0.41              |
| 1:N:75:ILE:O       | 1:N:79:GLY:HA3    | 2.20                     | 0.41              |
| 4:Q:8:SER:OG       | 13:Z:4:LYS:HE2    | 2.20                     | 0.41              |
| 1:A:266:GLU:HB2    | 1:A:267:PRO:HD2   | 2.01                     | 0.41              |
| 1:A:377:PHE:CD2    | 17:A:516:HEA:HAD1 | 2.55                     | 0.41              |
| 3:C:19:THR:CG2     | 3:C:53:THR:OG1    | 2.65                     | 0.41              |
| 3:C:42:LEU:HD13    | 10:J:45:TYR:CD2   | 2.56                     | 0.41              |
| 4:D:134:PHE:CZ     | 11:K:44:PRO:HG2   | 2.55                     | 0.41              |
| 10:J:11:LEU:HD23   | 10:J:11:LEU:O     | 2.21                     | 0.41              |
| 5:R:25:ASP:OD1     | 5:R:28:GLU:HG3    | 2.20                     | 0.41              |
| 3:C:160:LEU:HD13   | 3:C:222:GLN:HG2   | 2.00                     | 0.41              |
| 3:C:224:LYS:HZ2    | 3:C:224:LYS:CB    | 2.32                     | 0.41              |
| 2:O:60:GLU:H       | 2:O:60:GLU:HG3    | 1.71                     | 0.41              |
| 10:W:8:LYS:O       | 10:W:12:PHE:HD2   | 2.04                     | 0.41              |
| 2:B:90[B]:ILE:HG12 | 2:B:91[B]:ASN:N   | 2.34                     | 0.41              |
| 5:E:80:GLU:CD      | 5:E:80:GLU:H      | 2.29                     | 0.41              |
| 1:N:74:MET:HE3     | 1:N:249:PRO:HB2   | 2.01                     | 0.41              |
| 1:N:513:LEU:HA     | 1:N:513:LEU:HD12  | 1.77                     | 0.41              |
| 2:O:28:LEU:HG      | 2:O:32:PHE:CE2    | 2.55                     | 0.41              |
| 4:Q:64:PHE:CE1     | 5:R:66:ARG:HD2    | 2.55                     | 0.41              |
| 4:Q:134:PHE:CZ     | 11:X:44:PRO:HG2   | 2.55                     | 0.41              |
| 7:T:15:THR:O       | 7:T:18:PHE:HB3    | 2.20                     | 0.41              |
| 9:V:42:LYS:HE2     | 9:V:42:LYS:HB3    | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:442:ASP:OD2  | 2:B:134:ARG:NH2  | 2.54                     | 0.41              |
| 3:C:105:SER:HA   | 3:C:116:TRP:CE3  | 2.56                     | 0.41              |
| 3:C:148:HIS:O    | 3:C:152:MET:HG3  | 2.21                     | 0.41              |
| 4:D:77:GLU:HA    | 11:K:10:HIS:CG   | 2.55                     | 0.41              |
| 4:D:96:LEU:HA    | 4:D:96:LEU:HD23  | 1.87                     | 0.41              |
| 1:N:438:ARG:O    | 1:N:439:ARG:HB2  | 2.20                     | 0.41              |
| 3:P:12:ASN:O     | 3:P:13:PRO:C     | 2.63                     | 0.41              |
| 3:P:105:SER:HA   | 3:P:116:TRP:CE3  | 2.55                     | 0.41              |
| 1:A:390:MET:HE2  | 1:A:390:MET:HA   | 2.02                     | 0.41              |
| 4:D:66:GLU:HA    | 4:D:70:GLU:OE1   | 2.21                     | 0.41              |
| 10:J:11:LEU:HD23 | 10:J:11:LEU:C    | 2.46                     | 0.41              |
| 1:N:308:ALA:O    | 1:N:311:ILE:HG12 | 2.21                     | 0.41              |
| 10:W:4:ARG:HG2   | 10:W:8:LYS:HZ3   | 1.84                     | 0.41              |
| 11:X:31:TYR:CD1  | 11:X:35:GLN:HG3  | 2.55                     | 0.41              |
| 3:C:47:LEU:O     | 3:C:51:MET:HG2   | 2.21                     | 0.41              |
| 1:N:311:ILE:HD13 | 1:N:311:ILE:HG21 | 1.75                     | 0.41              |
| 2:O:222:TRP:HB2  | 9:V:71:SER:HB2   | 2.02                     | 0.41              |
| 10:J:8:LYS:O     | 10:J:12:PHE:HD2  | 2.04                     | 0.41              |
| 11:K:31:TYR:CD1  | 11:K:35:GLN:HG3  | 2.56                     | 0.41              |
| 1:N:508:PRO:CG   | 3:P:6:HIS:HB3    | 2.43                     | 0.41              |
| 3:P:42:LEU:HD13  | 10:W:45:TYR:CD2  | 2.55                     | 0.41              |
| 3:P:221:ARG:HE   | 3:P:226:HIS:CD2  | 2.30                     | 0.41              |
| 3:P:223:LEU:HD23 | 3:P:223:LEU:HA   | 1.91                     | 0.41              |
| 6:S:30:PRO:HG2   | 6:S:31:TYR:CD2   | 2.56                     | 0.41              |
| 7:T:3:ALA:O      | 7:T:4:ALA:HB2    | 2.21                     | 0.41              |
| 7:T:67:HIS:CD2   | 7:T:78:LEU:HD11  | 2.55                     | 0.41              |
| 2:B:13:THR:OG1   | 2:B:167:SER:HB3  | 2.21                     | 0.41              |
| 3:C:131:LEU:HD23 | 3:C:131:LEU:HA   | 1.91                     | 0.41              |
| 7:G:44:ARG:HA    | 7:G:45:PRO:HD3   | 1.71                     | 0.41              |
| 1:N:83:VAL:HB    | 1:N:84:PRO:HD3   | 2.03                     | 0.41              |
| 8:U:57:ARG:HA    | 8:U:60:TYR:CD2   | 2.55                     | 0.41              |
| 1:A:336:PRO:O    | 1:A:339:MET:HB2  | 2.21                     | 0.40              |
| 1:A:393:PHE:O    | 1:A:397:PHE:HB2  | 2.21                     | 0.40              |
| 2:B:78:LEU:HB2   | 2:B:79:PRO:CD    | 2.42                     | 0.40              |
| 3:C:115:CYS:SG   | 3:C:119:THR:HG22 | 2.61                     | 0.40              |
| 4:D:102:TYR:CD2  | 13:M:35:TYR:CE1  | 3.09                     | 0.40              |
| 7:G:53:LEU:O     | 7:G:54:ARG:C     | 2.65                     | 0.40              |
| 9:I:55:ASP:HB3   | 9:I:58:LYS:HB3   | 2.01                     | 0.40              |
| 1:N:374:VAL:HA   | 1:N:377:PHE:CE2  | 2.56                     | 0.40              |
| 4:Q:134:PHE:CE1  | 11:X:44:PRO:HG2  | 2.57                     | 0.40              |
| 5:R:99:SER:HB2   | 5:R:104:LEU:HD21 | 2.02                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:S:55:LYS:HA      | 6:S:74:LEU:O      | 2.21                     | 0.40              |
| 10:W:50:LEU:O      | 10:W:50:LEU:HD22  | 2.21                     | 0.40              |
| 3:C:112:LEU:HG     | 3:C:118:PRO:HB3   | 2.03                     | 0.40              |
| 5:E:90:ARG:HD3     | 5:E:90:ARG:HA     | 1.87                     | 0.40              |
| 2:O:193:TYR:CE1    | 4:Q:126:MET:HE1   | 2.45                     | 0.40              |
| 4:Q:109:HIS:O      | 4:Q:112:GLU:HG2   | 2.21                     | 0.40              |
| 9:V:68:ILE:HG13    | 9:V:69:PHE:N      | 2.36                     | 0.40              |
| 7:G:72:ASN:HA      | 7:G:73:PRO:HD3    | 1.87                     | 0.40              |
| 1:N:195:LEU:HD23   | 1:N:245:ILE:HD13  | 2.02                     | 0.40              |
| 1:N:199:LEU:HD13   | 1:N:238:PHE:CE1   | 2.56                     | 0.40              |
| 9:V:21:ILE:HA      | 9:V:21:ILE:HD12   | 1.83                     | 0.40              |
| 3:C:65:SER:HB3     | 3:C:71:HIS:CE1    | 2.55                     | 0.40              |
| 4:D:48:TRP:CH2     | 5:E:56:ARG:HA     | 2.56                     | 0.40              |
| 2:O:133:LEU:HA     | 2:O:133:LEU:HD23  | 1.71                     | 0.40              |
| 5:R:21:LYS:HA      | 5:R:22:PRO:HD2    | 1.90                     | 0.40              |
| 1:A:438:ARG:O      | 1:A:439:ARG:HB2   | 2.20                     | 0.40              |
| 2:B:3:TYR:CZ       | 2:B:6:GLN:HG3     | 2.56                     | 0.40              |
| 2:B:90[B]:ILE:HG23 | 2:B:91[B]:ASN:H   | 1.87                     | 0.40              |
| 4:D:64:PHE:CE1     | 5:E:66:ARG:HD2    | 2.56                     | 0.40              |
| 4:D:134:PHE:CE1    | 11:K:44:PRO:HG2   | 2.56                     | 0.40              |
| 9:I:68:ILE:HG13    | 9:I:69:PHE:N      | 2.35                     | 0.40              |
| 2:O:92[A]:ASN:HA   | 2:O:93[A]:PRO:HD2 | 1.86                     | 0.40              |
| 3:P:146:TRP:CZ2    | 7:T:17:ARG:CG     | 3.05                     | 0.40              |
| 3:P:224:LYS:HZ2    | 3:P:224:LYS:CB    | 2.34                     | 0.40              |
| 7:T:25:LEU:HD23    | 7:T:25:LEU:HA     | 1.84                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 512/514 (100%) | 491 (96%) | 21 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | N     | 512/514 (100%)  | 492 (96%)  | 20 (4%)  | 0        | 100         | 100 |
| 2   | B     | 231/227 (102%)  | 208 (90%)  | 20 (9%)  | 3 (1%)   | 9           | 8   |
| 2   | O     | 231/227 (102%)  | 207 (90%)  | 21 (9%)  | 3 (1%)   | 9           | 8   |
| 3   | C     | 259/261 (99%)   | 252 (97%)  | 6 (2%)   | 1 (0%)   | 30          | 34  |
| 3   | P     | 259/261 (99%)   | 252 (97%)  | 6 (2%)   | 1 (0%)   | 30          | 34  |
| 4   | D     | 142/147 (97%)   | 137 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 4   | Q     | 142/147 (97%)   | 135 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 5   | E     | 107/109 (98%)   | 105 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 5   | R     | 107/109 (98%)   | 105 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 6   | F     | 96/98 (98%)     | 90 (94%)   | 5 (5%)   | 1 (1%)   | 12          | 12  |
| 6   | S     | 96/98 (98%)     | 91 (95%)   | 4 (4%)   | 1 (1%)   | 12          | 12  |
| 7   | G     | 82/84 (98%)     | 67 (82%)   | 11 (13%) | 4 (5%)   | 1           | 0   |
| 7   | T     | 82/84 (98%)     | 67 (82%)   | 11 (13%) | 4 (5%)   | 1           | 0   |
| 8   | H     | 77/85 (91%)     | 73 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 8   | U     | 77/85 (91%)     | 74 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 9   | I     | 71/73 (97%)     | 65 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 9   | V     | 71/73 (97%)     | 65 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 10  | J     | 56/59 (95%)     | 53 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 10  | W     | 56/59 (95%)     | 52 (93%)   | 3 (5%)   | 1 (2%)   | 6           | 5   |
| 11  | K     | 47/56 (84%)     | 45 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 11  | X     | 47/56 (84%)     | 45 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 12  | L     | 45/47 (96%)     | 42 (93%)   | 3 (7%)   | 0        | 100         | 100 |
| 12  | Y     | 45/47 (96%)     | 43 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 13  | M     | 41/46 (89%)     | 41 (100%)  | 0        | 0        | 100         | 100 |
| 13  | Z     | 41/46 (89%)     | 41 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 3532/3612 (98%) | 3338 (94%) | 175 (5%) | 19 (0%)  | 24          | 27  |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 2   | B     | 91[A] | ASN  |
| 2   | B     | 91[B] | ASN  |
| 7   | G     | 4     | ALA  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 2   | O     | 91[A] | ASN  |
| 2   | O     | 91[B] | ASN  |
| 7   | T     | 4     | ALA  |
| 2   | B     | 104   | TRP  |
| 2   | O     | 104   | TRP  |
| 7   | G     | 11    | THR  |
| 7   | T     | 11    | THR  |
| 3   | C     | 38    | ASN  |
| 6   | F     | 64    | GLU  |
| 7   | G     | 8     | HIS  |
| 7   | G     | 35    | SER  |
| 3   | P     | 38    | ASN  |
| 7   | T     | 35    | SER  |
| 6   | S     | 64    | GLU  |
| 7   | T     | 8     | HIS  |
| 10  | W     | 15    | ASP  |

### 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     | 427/427 (100%) | 397 (93%) | 30 (7%)  | 14          | 15 |
| 1   | N     | 427/427 (100%) | 394 (92%) | 33 (8%)  | 12          | 13 |
| 2   | B     | 217/211 (103%) | 203 (94%) | 14 (6%)  | 15          | 18 |
| 2   | O     | 217/211 (103%) | 203 (94%) | 14 (6%)  | 15          | 18 |
| 3   | C     | 226/226 (100%) | 206 (91%) | 20 (9%)  | 9           | 10 |
| 3   | P     | 226/226 (100%) | 207 (92%) | 19 (8%)  | 10          | 11 |
| 4   | D     | 128/129 (99%)  | 116 (91%) | 12 (9%)  | 8           | 8  |
| 4   | Q     | 128/129 (99%)  | 116 (91%) | 12 (9%)  | 8           | 8  |
| 5   | E     | 95/95 (100%)   | 91 (96%)  | 4 (4%)   | 26          | 35 |
| 5   | R     | 95/95 (100%)   | 91 (96%)  | 4 (4%)   | 26          | 35 |
| 6   | F     | 81/81 (100%)   | 72 (89%)  | 9 (11%)  | 6           | 5  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 6   | S     | 81/81 (100%)     | 72 (89%)   | 9 (11%)  | 6           | 5  |
| 7   | G     | 68/68 (100%)     | 59 (87%)   | 9 (13%)  | 4           | 3  |
| 7   | T     | 68/68 (100%)     | 60 (88%)   | 8 (12%)  | 5           | 5  |
| 8   | H     | 71/75 (95%)      | 65 (92%)   | 6 (8%)   | 10          | 11 |
| 8   | U     | 71/75 (95%)      | 65 (92%)   | 6 (8%)   | 10          | 11 |
| 9   | I     | 58/58 (100%)     | 55 (95%)   | 3 (5%)   | 21          | 25 |
| 9   | V     | 58/58 (100%)     | 54 (93%)   | 4 (7%)   | 14          | 16 |
| 10  | J     | 49/50 (98%)      | 43 (88%)   | 6 (12%)  | 5           | 4  |
| 10  | W     | 49/50 (98%)      | 42 (86%)   | 7 (14%)  | 3           | 3  |
| 11  | K     | 39/46 (85%)      | 35 (90%)   | 4 (10%)  | 7           | 6  |
| 11  | X     | 39/46 (85%)      | 35 (90%)   | 4 (10%)  | 7           | 6  |
| 12  | L     | 40/40 (100%)     | 34 (85%)   | 6 (15%)  | 3           | 2  |
| 12  | Y     | 40/40 (100%)     | 33 (82%)   | 7 (18%)  | 2           | 1  |
| 13  | M     | 37/38 (97%)      | 35 (95%)   | 2 (5%)   | 20          | 24 |
| 13  | Z     | 37/38 (97%)      | 35 (95%)   | 2 (5%)   | 20          | 24 |
| All | All   | 3072/3088 (100%) | 2818 (92%) | 254 (8%) | 10          | 11 |

All (254) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 18  | LEU  |
| 1   | A     | 96  | ARG  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 106 | PRO  |
| 1   | A     | 127 | THR  |
| 1   | A     | 136 | LEU  |
| 1   | A     | 150 | LEU  |
| 1   | A     | 159 | LEU  |
| 1   | A     | 188 | VAL  |
| 1   | A     | 199 | LEU  |
| 1   | A     | 215 | LEU  |
| 1   | A     | 241 | PRO  |
| 1   | A     | 295 | VAL  |
| 1   | A     | 301 | THR  |
| 1   | A     | 306 | THR  |
| 1   | A     | 312 | ILE  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 318   | VAL  |
| 1   | A     | 324   | LEU  |
| 1   | A     | 333   | LYS  |
| 1   | A     | 347   | LEU  |
| 1   | A     | 353   | LEU  |
| 1   | A     | 354   | THR  |
| 1   | A     | 369   | ASP  |
| 1   | A     | 373   | VAL  |
| 1   | A     | 465   | VAL  |
| 1   | A     | 467   | LEU  |
| 1   | A     | 474   | GLU  |
| 1   | A     | 492   | LEU  |
| 1   | A     | 506   | GLU  |
| 2   | B     | 7     | LEU  |
| 2   | B     | 31    | VAL  |
| 2   | B     | 33    | LEU  |
| 2   | B     | 60    | GLU  |
| 2   | B     | 63    | THR  |
| 2   | B     | 91[A] | ASN  |
| 2   | B     | 91[B] | ASN  |
| 2   | B     | 113   | TYR  |
| 2   | B     | 115   | ASP  |
| 2   | B     | 138   | VAL  |
| 2   | B     | 142   | VAL  |
| 2   | B     | 171   | LYS  |
| 2   | B     | 202   | SER  |
| 2   | B     | 216   | LEU  |
| 3   | C     | 2     | THR  |
| 3   | C     | 11    | VAL  |
| 3   | C     | 13    | PRO  |
| 3   | C     | 18    | LEU  |
| 3   | C     | 22    | LEU  |
| 3   | C     | 38    | ASN  |
| 3   | C     | 73    | PRO  |
| 3   | C     | 85    | LEU  |
| 3   | C     | 92    | LEU  |
| 3   | C     | 112   | LEU  |
| 3   | C     | 119   | THR  |
| 3   | C     | 131   | LEU  |
| 3   | C     | 132   | LEU  |
| 3   | C     | 137   | LEU  |
| 3   | C     | 160   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 163 | LEU  |
| 3   | C     | 179 | SER  |
| 3   | C     | 196 | THR  |
| 3   | C     | 213 | THR  |
| 3   | C     | 224 | LYS  |
| 4   | D     | 27  | VAL  |
| 4   | D     | 36  | SER  |
| 4   | D     | 40  | LEU  |
| 4   | D     | 59  | LEU  |
| 4   | D     | 62  | LEU  |
| 4   | D     | 107 | ILE  |
| 4   | D     | 108 | PRO  |
| 4   | D     | 116 | VAL  |
| 4   | D     | 127 | LYS  |
| 4   | D     | 141 | ASP  |
| 4   | D     | 143 | ASN  |
| 4   | D     | 147 | LYS  |
| 5   | E     | 29  | LEU  |
| 5   | E     | 79  | LYS  |
| 5   | E     | 80  | GLU  |
| 5   | E     | 109 | VAL  |
| 6   | F     | 6   | VAL  |
| 6   | F     | 20  | VAL  |
| 6   | F     | 34  | LEU  |
| 6   | F     | 44  | GLU  |
| 6   | F     | 56  | ARG  |
| 6   | F     | 67  | SER  |
| 6   | F     | 74  | LEU  |
| 6   | F     | 78  | GLU  |
| 6   | F     | 81  | ARG  |
| 7   | G     | 5   | LYS  |
| 7   | G     | 7   | ASP  |
| 7   | G     | 14  | ARG  |
| 7   | G     | 17  | ARG  |
| 7   | G     | 33  | LEU  |
| 7   | G     | 36  | TRP  |
| 7   | G     | 37  | LEU  |
| 7   | G     | 41  | HIS  |
| 7   | G     | 48  | ILE  |
| 8   | H     | 7   | LYS  |
| 8   | H     | 9   | LYS  |
| 8   | H     | 29  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 41  | LYS  |
| 8   | H     | 60  | TYR  |
| 8   | H     | 67  | SER  |
| 9   | I     | 44  | LYS  |
| 9   | I     | 52  | ARG  |
| 9   | I     | 58  | LYS  |
| 10  | J     | 4   | ARG  |
| 10  | J     | 27  | THR  |
| 10  | J     | 30  | ILE  |
| 10  | J     | 47  | LEU  |
| 10  | J     | 50  | LEU  |
| 10  | J     | 58  | LYS  |
| 11  | K     | 28  | VAL  |
| 11  | K     | 45  | VAL  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 49  | THR  |
| 12  | L     | 15  | VAL  |
| 12  | L     | 16  | GLU  |
| 12  | L     | 20  | ARG  |
| 12  | L     | 22  | LEU  |
| 12  | L     | 26  | THR  |
| 12  | L     | 44  | LEU  |
| 13  | M     | 1   | ILE  |
| 13  | M     | 24  | LEU  |
| 1   | N     | 1   | MET  |
| 1   | N     | 18  | LEU  |
| 1   | N     | 96  | ARG  |
| 1   | N     | 105 | LEU  |
| 1   | N     | 106 | PRO  |
| 1   | N     | 127 | THR  |
| 1   | N     | 128 | VAL  |
| 1   | N     | 136 | LEU  |
| 1   | N     | 138 | HIS  |
| 1   | N     | 150 | LEU  |
| 1   | N     | 159 | LEU  |
| 1   | N     | 188 | VAL  |
| 1   | N     | 199 | LEU  |
| 1   | N     | 215 | LEU  |
| 1   | N     | 241 | PRO  |
| 1   | N     | 295 | VAL  |
| 1   | N     | 301 | THR  |
| 1   | N     | 306 | THR  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | N     | 312   | ILE  |
| 1   | N     | 318   | VAL  |
| 1   | N     | 324   | LEU  |
| 1   | N     | 333   | LYS  |
| 1   | N     | 347   | LEU  |
| 1   | N     | 353   | LEU  |
| 1   | N     | 354   | THR  |
| 1   | N     | 369   | ASP  |
| 1   | N     | 373   | VAL  |
| 1   | N     | 465   | VAL  |
| 1   | N     | 467   | LEU  |
| 1   | N     | 474   | GLU  |
| 1   | N     | 492   | LEU  |
| 1   | N     | 506   | GLU  |
| 1   | N     | 512   | ASN  |
| 2   | O     | 7     | LEU  |
| 2   | O     | 31    | VAL  |
| 2   | O     | 33    | LEU  |
| 2   | O     | 60    | GLU  |
| 2   | O     | 63    | THR  |
| 2   | O     | 91[A] | ASN  |
| 2   | O     | 91[B] | ASN  |
| 2   | O     | 113   | TYR  |
| 2   | O     | 115   | ASP  |
| 2   | O     | 138   | VAL  |
| 2   | O     | 142   | VAL  |
| 2   | O     | 171   | LYS  |
| 2   | O     | 202   | SER  |
| 2   | O     | 216   | LEU  |
| 3   | P     | 2     | THR  |
| 3   | P     | 11    | VAL  |
| 3   | P     | 18    | LEU  |
| 3   | P     | 22    | LEU  |
| 3   | P     | 38    | ASN  |
| 3   | P     | 85    | LEU  |
| 3   | P     | 92    | LEU  |
| 3   | P     | 112   | LEU  |
| 3   | P     | 119   | THR  |
| 3   | P     | 130   | PRO  |
| 3   | P     | 131   | LEU  |
| 3   | P     | 132   | LEU  |
| 3   | P     | 137   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | P     | 160 | LEU  |
| 3   | P     | 163 | LEU  |
| 3   | P     | 179 | SER  |
| 3   | P     | 196 | THR  |
| 3   | P     | 213 | THR  |
| 3   | P     | 224 | LYS  |
| 4   | Q     | 27  | VAL  |
| 4   | Q     | 36  | SER  |
| 4   | Q     | 40  | LEU  |
| 4   | Q     | 59  | LEU  |
| 4   | Q     | 62  | LEU  |
| 4   | Q     | 107 | ILE  |
| 4   | Q     | 108 | PRO  |
| 4   | Q     | 116 | VAL  |
| 4   | Q     | 127 | LYS  |
| 4   | Q     | 141 | ASP  |
| 4   | Q     | 143 | ASN  |
| 4   | Q     | 147 | LYS  |
| 5   | R     | 29  | LEU  |
| 5   | R     | 79  | LYS  |
| 5   | R     | 80  | GLU  |
| 5   | R     | 109 | VAL  |
| 6   | S     | 6   | VAL  |
| 6   | S     | 20  | VAL  |
| 6   | S     | 34  | LEU  |
| 6   | S     | 44  | GLU  |
| 6   | S     | 56  | ARG  |
| 6   | S     | 67  | SER  |
| 6   | S     | 74  | LEU  |
| 6   | S     | 78  | GLU  |
| 6   | S     | 81  | ARG  |
| 7   | T     | 5   | LYS  |
| 7   | T     | 14  | ARG  |
| 7   | T     | 17  | ARG  |
| 7   | T     | 33  | LEU  |
| 7   | T     | 36  | TRP  |
| 7   | T     | 37  | LEU  |
| 7   | T     | 41  | HIS  |
| 7   | T     | 48  | ILE  |
| 8   | U     | 7   | LYS  |
| 8   | U     | 9   | LYS  |
| 8   | U     | 29  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | U     | 41  | LYS  |
| 8   | U     | 60  | TYR  |
| 8   | U     | 67  | SER  |
| 9   | V     | 4   | LEU  |
| 9   | V     | 44  | LYS  |
| 9   | V     | 52  | ARG  |
| 9   | V     | 58  | LYS  |
| 10  | W     | 4   | ARG  |
| 10  | W     | 27  | THR  |
| 10  | W     | 30  | ILE  |
| 10  | W     | 36  | MET  |
| 10  | W     | 47  | LEU  |
| 10  | W     | 50  | LEU  |
| 10  | W     | 58  | LYS  |
| 11  | X     | 28  | VAL  |
| 11  | X     | 45  | VAL  |
| 11  | X     | 47  | ARG  |
| 11  | X     | 49  | THR  |
| 12  | Y     | 15  | VAL  |
| 12  | Y     | 16  | GLU  |
| 12  | Y     | 20  | ARG  |
| 12  | Y     | 22  | LEU  |
| 12  | Y     | 26  | THR  |
| 12  | Y     | 27  | LEU  |
| 12  | Y     | 44  | LEU  |
| 13  | Z     | 1   | ILE  |
| 13  | Z     | 24  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASN  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 503 | HIS  |
| 2   | B     | 52  | HIS  |
| 2   | B     | 203 | ASN  |
| 3   | C     | 148 | HIS  |
| 3   | C     | 222 | GLN  |
| 3   | C     | 226 | HIS  |
| 3   | C     | 230 | ASN  |
| 4   | D     | 72  | ASN  |
| 4   | D     | 109 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 132 | GLN  |
| 7   | G     | 51  | HIS  |
| 7   | G     | 71  | HIS  |
| 8   | H     | 10  | ASN  |
| 8   | H     | 32  | ASN  |
| 9   | I     | 53  | ASN  |
| 11  | K     | 15  | ASN  |
| 12  | L     | 42  | HIS  |
| 13  | M     | 36  | HIS  |
| 1   | N     | 4   | ASN  |
| 1   | N     | 422 | ASN  |
| 1   | N     | 503 | HIS  |
| 2   | O     | 52  | HIS  |
| 2   | O     | 203 | ASN  |
| 3   | P     | 222 | GLN  |
| 3   | P     | 226 | HIS  |
| 3   | P     | 230 | ASN  |
| 4   | Q     | 109 | HIS  |
| 4   | Q     | 119 | GLN  |
| 7   | T     | 51  | HIS  |
| 7   | T     | 71  | HIS  |
| 8   | U     | 10  | ASN  |
| 8   | U     | 32  | ASN  |
| 9   | V     | 53  | ASN  |
| 10  | W     | 29  | ASN  |
| 12  | Y     | 42  | HIS  |
| 13  | Z     | 36  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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 |
| 17  | HEA  | A     | 516 | 1    | 67,67,67     | 1.50 | 9 (13%)  | 81,103,103  | 1.54 | 18 (22%) |
| 17  | HEA  | N     | 516 | 1    | 67,67,67     | 1.15 | 6 (8%)   | 81,103,103  | 1.37 | 12 (14%) |
| 17  | HEA  | N     | 515 | 1    | 67,67,67     | 1.14 | 4 (5%)   | 81,103,103  | 1.57 | 13 (16%) |
| 17  | HEA  | A     | 515 | 1    | 67,67,67     | 1.34 | 8 (11%)  | 81,103,103  | 1.61 | 16 (19%) |

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 |
|-----|------|-------|-----|------|---------|-------------|-------|
| 17  | HEA  | A     | 516 | 1    | -       | 6/36/76/76  | -     |
| 17  | HEA  | N     | 516 | 1    | -       | 6/36/76/76  | -     |
| 17  | HEA  | N     | 515 | 1    | -       | 10/36/76/76 | -     |
| 17  | HEA  | A     | 515 | 1    | -       | 10/36/76/76 | -     |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 17  | A     | 516 | HEA  | C4C-NC  | -4.64 | 1.30        | 1.39     |
| 17  | A     | 516 | HEA  | C1D-C2D | 4.25  | 1.53        | 1.44     |
| 17  | A     | 516 | HEA  | FE-NA   | 4.12  | 2.08        | 1.95     |
| 17  | A     | 516 | HEA  | CMA-C3A | -3.88 | 1.36        | 1.45     |
| 17  | N     | 515 | HEA  | C11-C3B | -3.76 | 1.46        | 1.51     |
| 17  | N     | 516 | HEA  | CMA-C3A | -3.71 | 1.37        | 1.45     |
| 17  | A     | 515 | HEA  | C11-C3B | -3.47 | 1.47        | 1.51     |
| 17  | A     | 515 | HEA  | C4B-C3B | 3.17  | 1.50        | 1.44     |
| 17  | A     | 515 | HEA  | C1A-C2A | -3.04 | 1.39        | 1.45     |
| 17  | A     | 515 | HEA  | C1B-C2B | 2.93  | 1.50        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 17  | A     | 516 | HEA  | C1D-ND  | -2.91 | 1.35        | 1.40     |
| 17  | A     | 515 | HEA  | CMA-C3A | -2.84 | 1.39        | 1.45     |
| 17  | A     | 516 | HEA  | FE-NC   | 2.62  | 2.03        | 1.95     |
| 17  | A     | 515 | HEA  | C13-C14 | 2.56  | 1.58        | 1.50     |
| 17  | N     | 515 | HEA  | C4B-C3B | 2.51  | 1.49        | 1.44     |
| 17  | N     | 516 | HEA  | FE-NC   | 2.50  | 2.03        | 1.95     |
| 17  | A     | 515 | HEA  | C1D-ND  | -2.45 | 1.36        | 1.40     |
| 17  | N     | 516 | HEA  | C1D-C2D | 2.37  | 1.49        | 1.44     |
| 17  | N     | 515 | HEA  | C3D-C2D | -2.33 | 1.31        | 1.36     |
| 17  | N     | 516 | HEA  | C4C-NC  | -2.31 | 1.35        | 1.39     |
| 17  | N     | 515 | HEA  | CMA-C3A | -2.29 | 1.40        | 1.45     |
| 17  | A     | 516 | HEA  | C11-C3B | 2.27  | 1.54        | 1.51     |
| 17  | A     | 515 | HEA  | C27-C19 | -2.25 | 1.45        | 1.50     |
| 17  | N     | 516 | HEA  | CMD-C2D | 2.23  | 1.55        | 1.50     |
| 17  | N     | 516 | HEA  | CHC-C1C | -2.14 | 1.34        | 1.39     |
| 17  | A     | 516 | HEA  | C3C-C2C | -2.11 | 1.34        | 1.41     |
| 17  | A     | 516 | HEA  | C4A-NA  | -2.03 | 1.35        | 1.39     |

All (59) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | A     | 515 | HEA  | C13-C14-C15 | -5.24 | 115.63      | 127.62   |
| 17  | N     | 515 | HEA  | C13-C14-C15 | -5.08 | 115.99      | 127.62   |
| 17  | A     | 516 | HEA  | CMD-C2D-C1D | 4.30  | 131.76      | 125.03   |
| 17  | N     | 515 | HEA  | CMB-C2B-C3B | -3.93 | 122.67      | 130.28   |
| 17  | N     | 516 | HEA  | CHB-C4A-NA  | -3.86 | 120.25      | 124.45   |
| 17  | A     | 515 | HEA  | CMB-C2B-C3B | -3.79 | 122.94      | 130.28   |
| 17  | A     | 516 | HEA  | CHB-C4A-NA  | -3.63 | 120.50      | 124.45   |
| 17  | N     | 516 | HEA  | CMD-C2D-C1D | 3.44  | 130.41      | 125.03   |
| 17  | A     | 515 | HEA  | C20-C19-C18 | 3.35  | 128.69      | 121.17   |
| 17  | A     | 516 | HEA  | C3D-C4D-ND  | 3.35  | 113.58      | 110.35   |
| 17  | N     | 515 | HEA  | C26-C15-C14 | -3.33 | 115.09      | 123.63   |
| 17  | N     | 515 | HEA  | O11-C11-C3B | 3.27  | 117.26      | 111.26   |
| 17  | A     | 516 | HEA  | C13-C14-C15 | -3.10 | 120.52      | 127.62   |
| 17  | A     | 515 | HEA  | O11-C11-C3B | 3.07  | 116.90      | 111.26   |
| 17  | N     | 515 | HEA  | C26-C15-C16 | 3.06  | 120.55      | 115.23   |
| 17  | A     | 515 | HEA  | C27-C19-C18 | -3.02 | 115.86      | 123.63   |
| 17  | A     | 515 | HEA  | C26-C15-C14 | -3.02 | 115.87      | 123.63   |
| 17  | N     | 515 | HEA  | C20-C19-C18 | 2.92  | 127.73      | 121.17   |
| 17  | A     | 516 | HEA  | CHA-C1A-NA  | -2.89 | 121.31      | 124.45   |
| 17  | A     | 515 | HEA  | C26-C15-C16 | 2.86  | 120.19      | 115.23   |
| 17  | N     | 516 | HEA  | C3C-C4C-NC  | 2.86  | 112.20      | 109.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | N     | 515 | HEA  | CHC-C4B-NB  | -2.84 | 120.85      | 124.37   |
| 17  | A     | 516 | HEA  | CHD-C1D-ND  | -2.82 | 120.88      | 124.37   |
| 17  | A     | 516 | HEA  | C2D-C1D-ND  | 2.75  | 113.00      | 109.84   |
| 17  | A     | 515 | HEA  | C3B-C4B-NB  | 2.60  | 112.83      | 109.84   |
| 17  | N     | 516 | HEA  | OMA-CMA-C3A | -2.59 | 119.78      | 125.62   |
| 17  | N     | 515 | HEA  | C2A-C1A-NA  | 2.56  | 112.79      | 110.32   |
| 17  | A     | 515 | HEA  | C12-C11-C3B | 2.53  | 116.08      | 112.12   |
| 17  | N     | 515 | HEA  | C3B-C4B-NB  | 2.49  | 112.70      | 109.84   |
| 17  | A     | 515 | HEA  | C4B-NB-C1B  | -2.42 | 102.34      | 105.21   |
| 17  | A     | 516 | HEA  | C1D-ND-C4D  | -2.42 | 102.34      | 105.21   |
| 17  | A     | 515 | HEA  | C17-C18-C19 | -2.40 | 122.13      | 127.62   |
| 17  | N     | 516 | HEA  | C1D-C2D-C3D | -2.40 | 104.46      | 106.98   |
| 17  | A     | 516 | HEA  | C27-C19-C20 | 2.39  | 119.37      | 115.23   |
| 17  | N     | 515 | HEA  | C27-C19-C18 | -2.38 | 117.52      | 123.63   |
| 17  | A     | 516 | HEA  | C20-C19-C18 | -2.36 | 115.86      | 121.17   |
| 17  | N     | 516 | HEA  | C2A-C1A-NA  | 2.35  | 112.59      | 110.32   |
| 17  | A     | 515 | HEA  | CMD-C2D-C1D | 2.31  | 128.65      | 125.03   |
| 17  | A     | 516 | HEA  | C3C-C4C-NC  | 2.30  | 111.73      | 109.80   |
| 17  | N     | 516 | HEA  | CHA-C1A-NA  | -2.29 | 121.96      | 124.45   |
| 17  | A     | 516 | HEA  | C1D-C2D-C3D | -2.27 | 104.59      | 106.98   |
| 17  | N     | 516 | HEA  | C13-C14-C15 | -2.26 | 122.45      | 127.62   |
| 17  | A     | 516 | HEA  | OMA-CMA-C3A | -2.22 | 120.61      | 125.62   |
| 17  | N     | 515 | HEA  | C1B-C2B-C3B | 2.21  | 109.35      | 106.80   |
| 17  | N     | 516 | HEA  | C3D-C4D-ND  | 2.20  | 112.48      | 110.35   |
| 17  | A     | 516 | HEA  | CMB-C2B-C3B | -2.16 | 126.10      | 130.28   |
| 17  | A     | 515 | HEA  | CMB-C2B-C1B | 2.14  | 128.37      | 125.03   |
| 17  | A     | 516 | HEA  | C2A-C1A-NA  | 2.13  | 112.38      | 110.32   |
| 17  | A     | 516 | HEA  | CHB-C4A-C3A | 2.13  | 128.80      | 125.21   |
| 17  | A     | 516 | HEA  | CHA-C4D-C3D | -2.11 | 121.69      | 124.77   |
| 17  | A     | 515 | HEA  | C3C-C2C-C1C | -2.10 | 104.70      | 107.17   |
| 17  | N     | 515 | HEA  | C4B-NB-C1B  | -2.10 | 102.73      | 105.21   |
| 17  | N     | 516 | HEA  | C20-C19-C18 | -2.08 | 116.50      | 121.17   |
| 17  | A     | 515 | HEA  | O11-C11-C12 | -2.06 | 103.68      | 109.14   |
| 17  | A     | 516 | HEA  | O1A-CGA-CBA | -2.05 | 116.58      | 123.09   |
| 17  | N     | 516 | HEA  | C26-C15-C14 | -2.05 | 118.37      | 123.63   |
| 17  | N     | 515 | HEA  | C3C-C2C-C1C | -2.04 | 104.77      | 107.17   |
| 17  | A     | 515 | HEA  | C1D-ND-C4D  | -2.02 | 102.81      | 105.21   |
| 17  | N     | 516 | HEA  | O1D-CGD-CBD | -2.00 | 116.74      | 123.09   |

There are no chirality outliers.

All (32) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | N     | 516 | HEA  | C4D-C3D-CAD-CBD |
| 17  | A     | 516 | HEA  | C21-C22-C23-C25 |
| 17  | N     | 516 | HEA  | C21-C22-C23-C25 |
| 17  | A     | 516 | HEA  | C4D-C3D-CAD-CBD |
| 17  | A     | 515 | HEA  | C2A-C3A-CMA-OMA |
| 17  | N     | 515 | HEA  | C2A-C3A-CMA-OMA |
| 17  | A     | 515 | HEA  | C26-C15-C16-C17 |
| 17  | N     | 515 | HEA  | C26-C15-C16-C17 |
| 17  | A     | 515 | HEA  | C14-C15-C16-C17 |
| 17  | N     | 515 | HEA  | C14-C15-C16-C17 |
| 17  | A     | 515 | HEA  | O11-C11-C12-C13 |
| 17  | A     | 515 | HEA  | C4A-C3A-CMA-OMA |
| 17  | N     | 515 | HEA  | C4A-C3A-CMA-OMA |
| 17  | A     | 515 | HEA  | C21-C22-C23-C25 |
| 17  | N     | 515 | HEA  | O11-C11-C12-C13 |
| 17  | A     | 516 | HEA  | C21-C22-C23-C24 |
| 17  | N     | 516 | HEA  | C21-C22-C23-C24 |
| 17  | A     | 516 | HEA  | CAD-CBD-CGD-O1D |
| 17  | N     | 516 | HEA  | CAD-CBD-CGD-O1D |
| 17  | A     | 515 | HEA  | CAD-CBD-CGD-O1D |
| 17  | A     | 516 | HEA  | CAD-CBD-CGD-O2D |
| 17  | N     | 516 | HEA  | CAD-CBD-CGD-O2D |
| 17  | N     | 515 | HEA  | CAD-CBD-CGD-O1D |
| 17  | A     | 515 | HEA  | CAD-CBD-CGD-O2D |
| 17  | N     | 515 | HEA  | CAD-CBD-CGD-O2D |
| 17  | A     | 515 | HEA  | C21-C22-C23-C24 |
| 17  | N     | 515 | HEA  | C21-C22-C23-C25 |
| 17  | N     | 515 | HEA  | CAA-CBA-CGA-O2A |
| 17  | A     | 515 | HEA  | CAA-CBA-CGA-O2A |
| 17  | A     | 516 | HEA  | CAA-CBA-CGA-O1A |
| 17  | N     | 515 | HEA  | CAA-CBA-CGA-O1A |
| 17  | N     | 516 | HEA  | CAA-CBA-CGA-O1A |

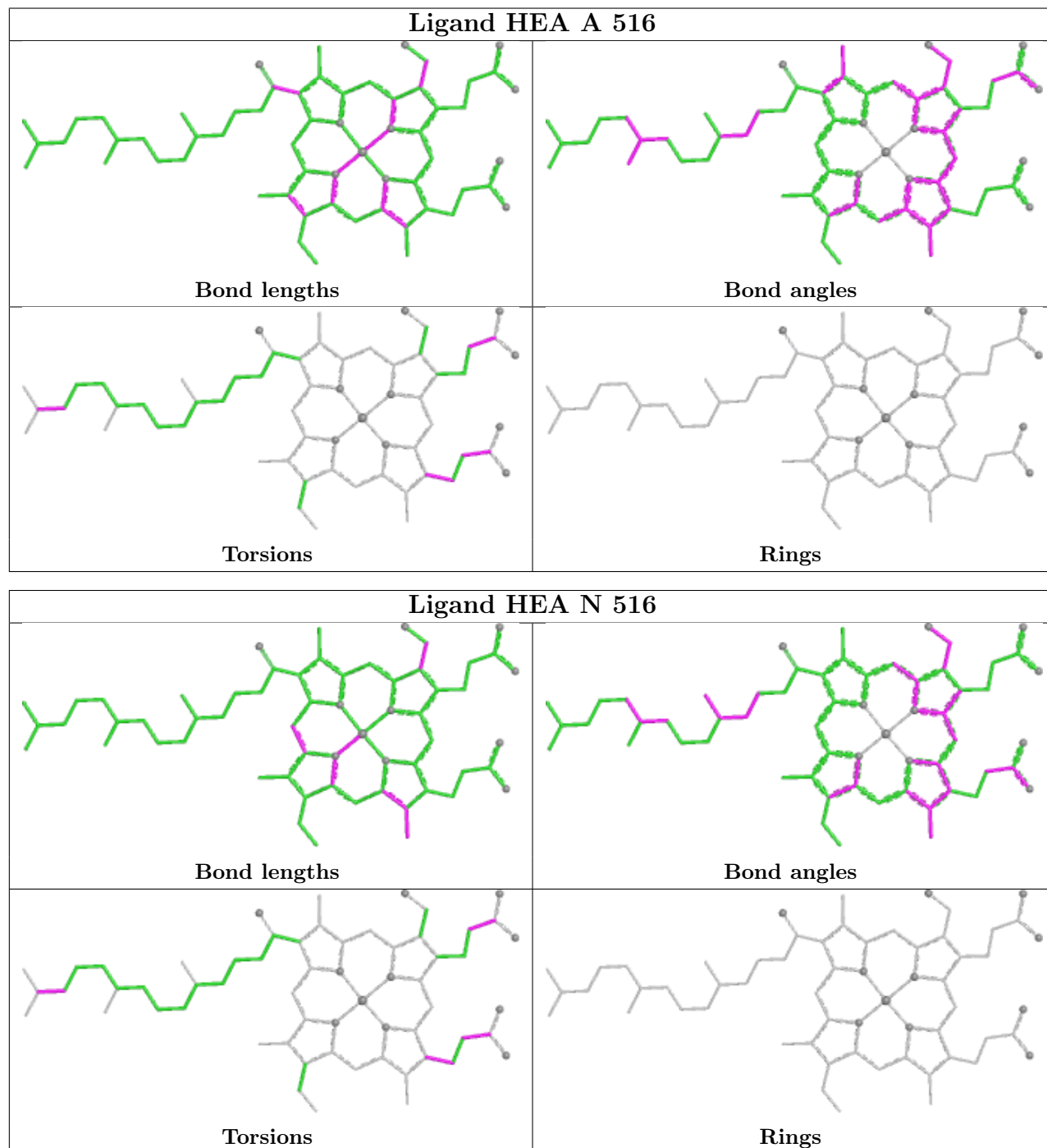
There are no ring outliers.

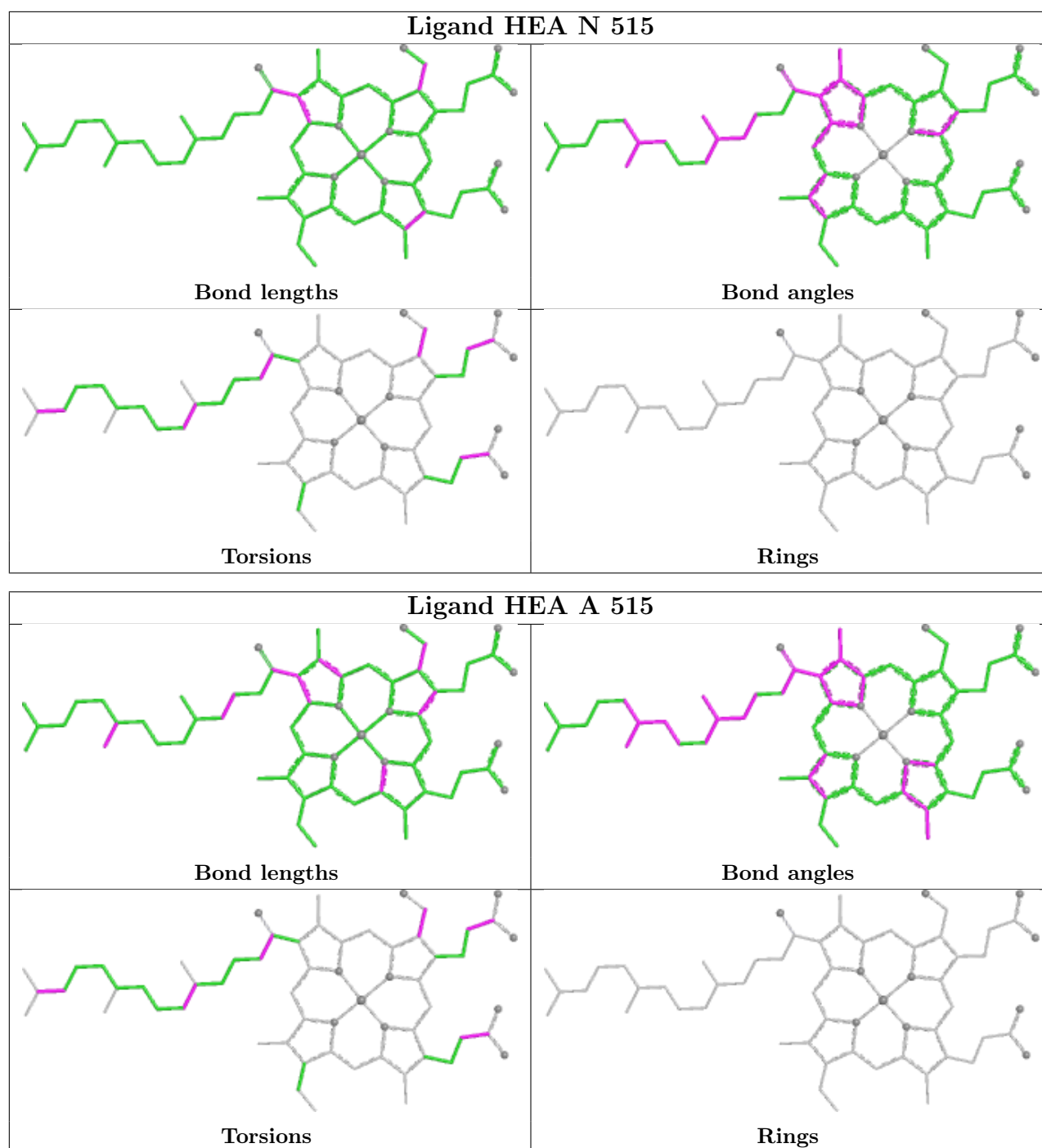
3 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | A     | 516 | HEA  | 2       | 0            |
| 17  | N     | 515 | HEA  | 6       | 0            |
| 17  | A     | 515 | HEA  | 7       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | O     | 1                |
| 2   | B     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | O     | 87:MET    | C      | 88[A]:ASP | N      | 1.17         |
| 1     | B     | 87:MET    | C      | 88[A]:ASP | N      | 1.16         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.