



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:01 PM GMT

PDB ID : 4EO2  
Title : Structure of the bacteriophage C1 tail knob protein, gp12  
Authors : Aksyuk, A.A.; Rossmann, M.G.  
Deposited on : 2012-04-13  
Resolution : 3.01 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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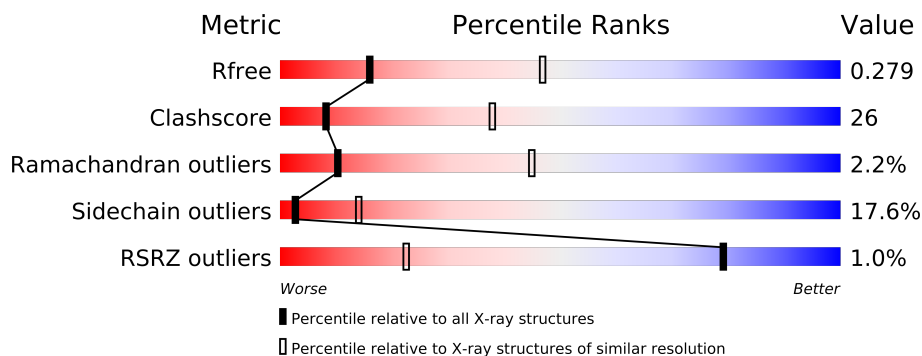
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.01 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 1216 (3.00-3.00)                                      |
| Clashscore            | 79885                       | 1594 (3.00-3.00)                                      |
| Ramachandran outliers | 78287                       | 1537 (3.00-3.00)                                      |
| Sidechain outliers    | 78261                       | 1540 (3.00-3.00)                                      |
| RSRZ outliers         | 66119                       | 1217 (3.00-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 583    |                  |
| 1   | B     | 583    |                  |
| 1   | C     | 583    |                  |
| 1   | D     | 583    |                  |
| 1   | E     | 583    |                  |
| 1   | F     | 583    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23688 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Major tail protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3948  | 2504 | 665 | 761 | 18 |         |         |       |
| 1   | B     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3948  | 2504 | 665 | 761 | 18 |         |         |       |
| 1   | C     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3948  | 2504 | 665 | 761 | 18 |         |         |       |
| 1   | D     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3948  | 2504 | 665 | 761 | 18 |         |         |       |
| 1   | E     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3948  | 2504 | 665 | 761 | 18 |         |         |       |
| 1   | F     | 488      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3948  | 2504 | 665 | 761 | 18 |         |         |       |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 575     | SER      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 576     | LEU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 577     | GLU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 578     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 579     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 580     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 581     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 582     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| A     | 583     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 575     | SER      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 576     | LEU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 577     | GLU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 578     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 579     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 580     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 581     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| B     | 582     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |

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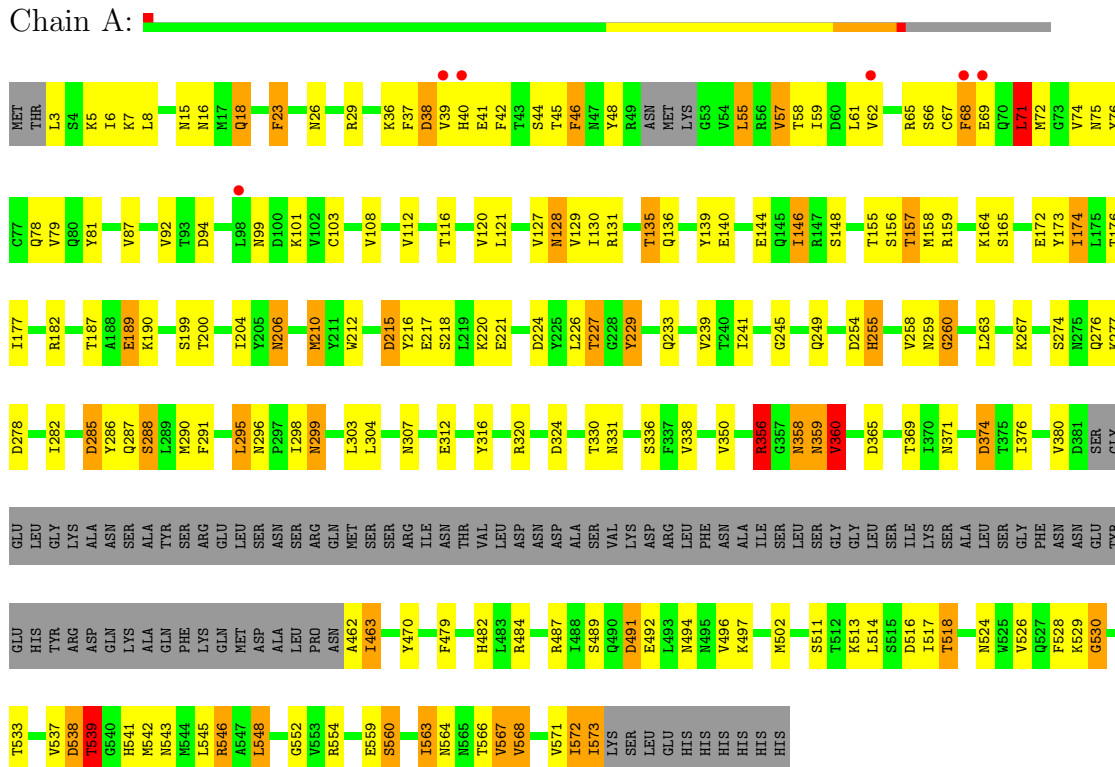
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 583     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 575     | SER      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 576     | LEU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 577     | GLU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 578     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 579     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 580     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 581     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 582     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| C     | 583     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 575     | SER      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 576     | LEU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 577     | GLU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 578     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 579     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 580     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 581     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 582     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| D     | 583     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 575     | SER      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 576     | LEU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 577     | GLU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 578     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 579     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 580     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 581     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 582     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| E     | 583     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 575     | SER      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 576     | LEU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 577     | GLU      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 578     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 579     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 580     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 581     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 582     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |
| F     | 583     | HIS      | -      | EXPRESSION TAG | UNP Q7Y3F0 |

### 3 Residue-property plots

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

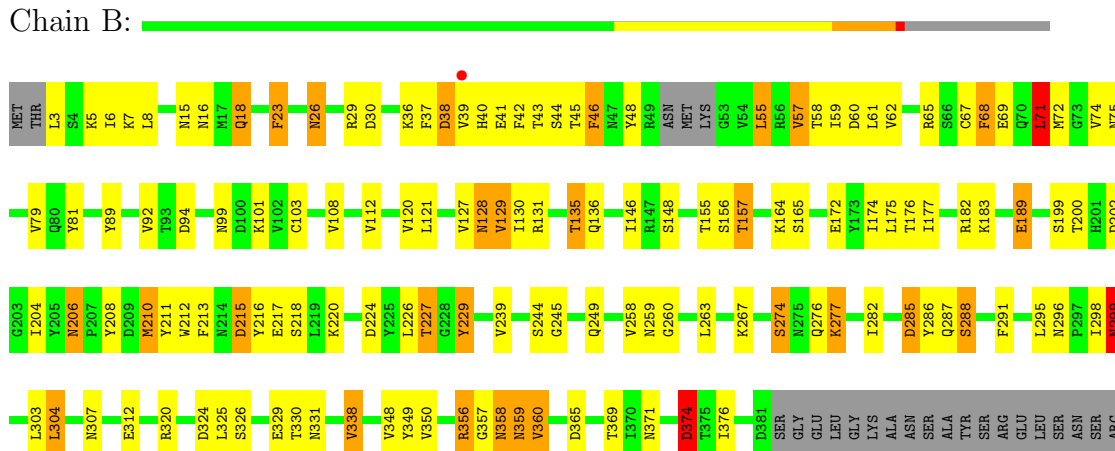
#### • Molecule 1: Major tail protein

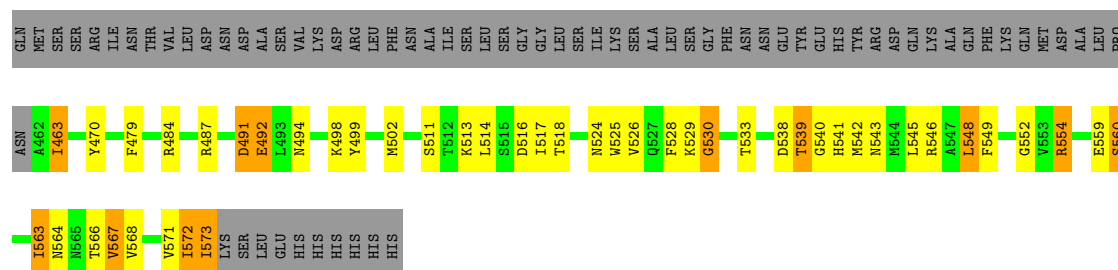
Chain A:



#### • Molecule 1: Major tail protein

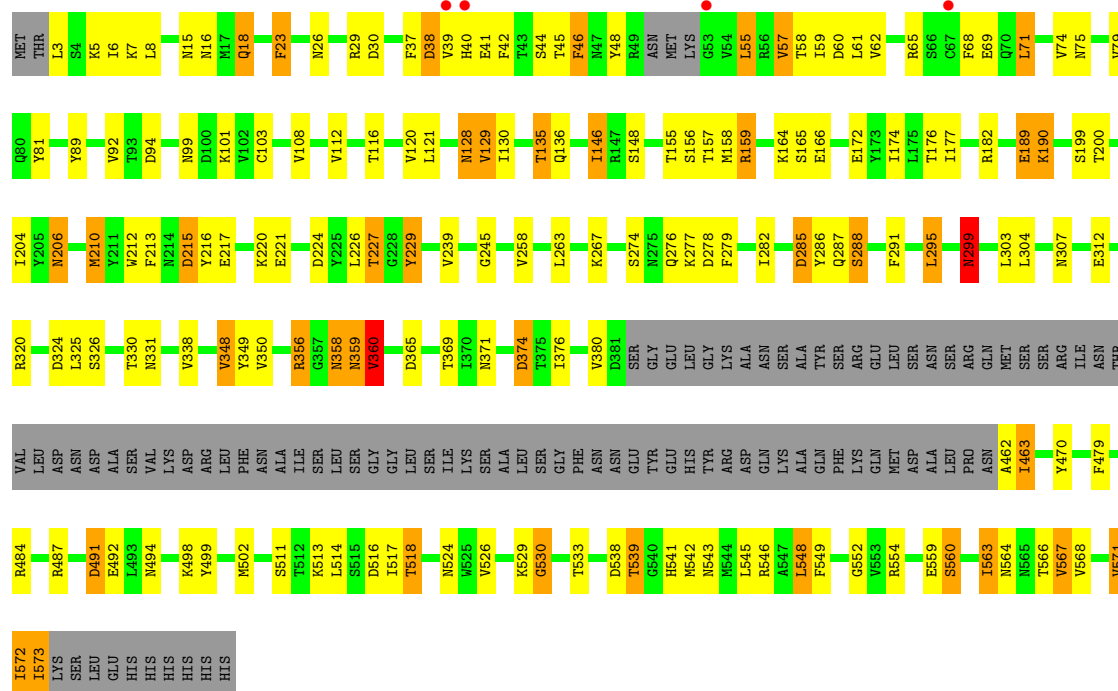
Chain B:





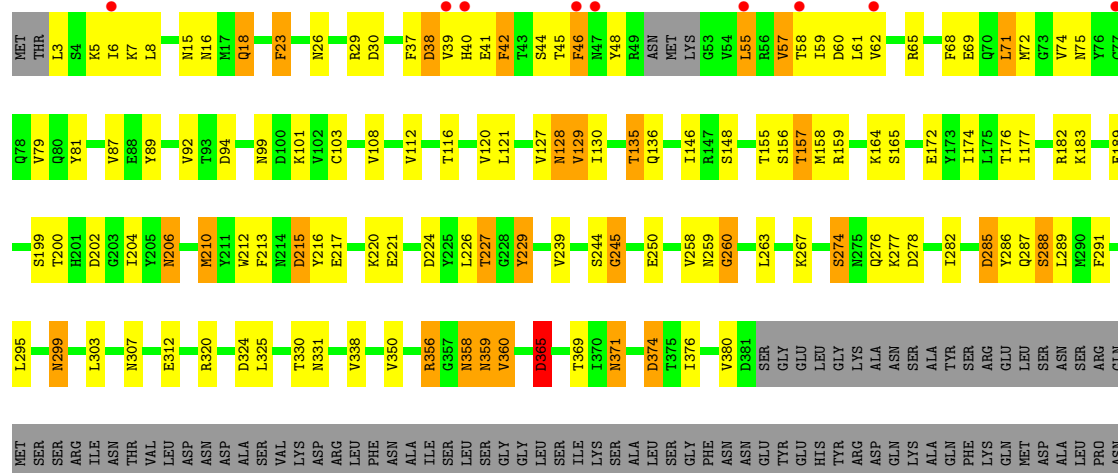
### • Molecule 1: Major tail protein

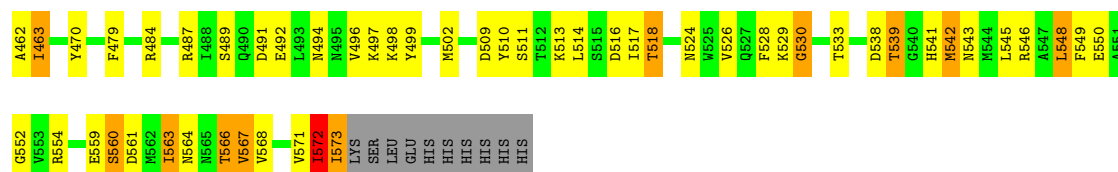
Chain C:



### • Molecule 1: Major tail protein

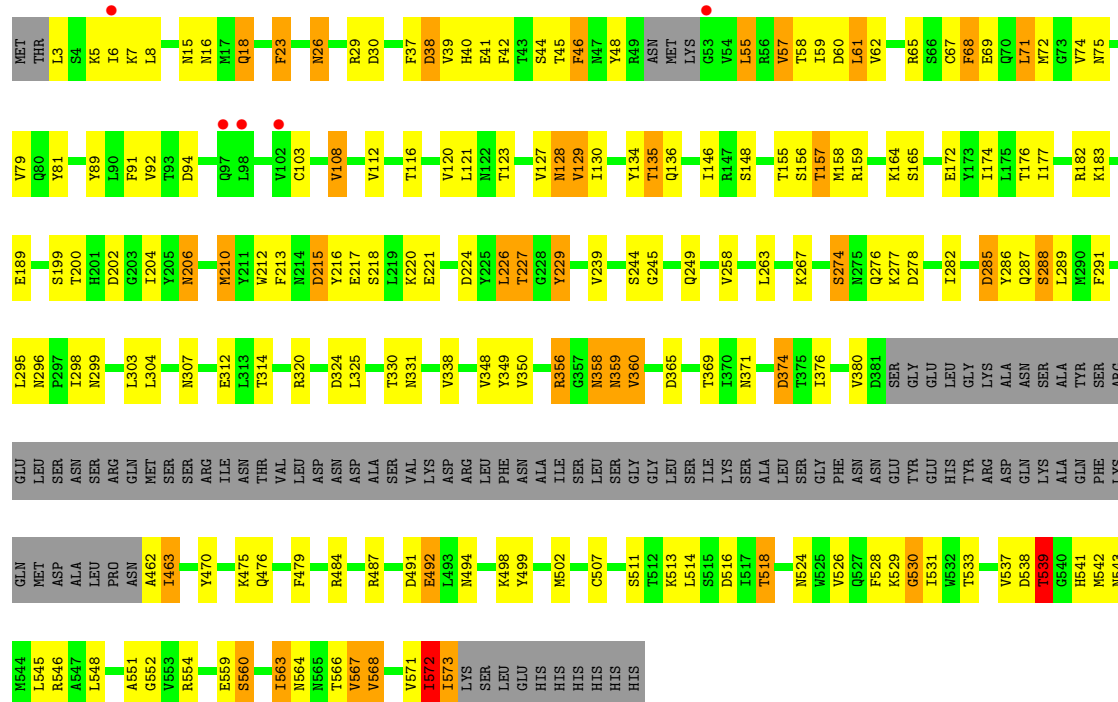
Chain D:





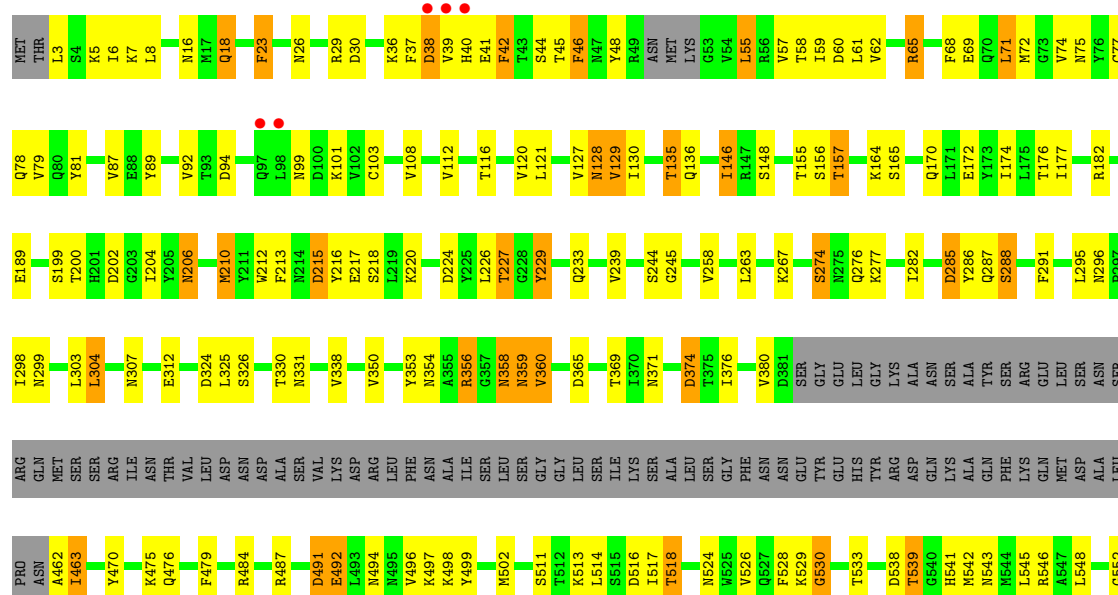
### • Molecule 1: Major tail protein

#### Chain E:



### • Molecule 1: Major tail protein

#### Chain F:



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| V553 | V554 | E559 | S560 | I563 | N564 | N565 | T566 | V567 | V568 | N569 | N570 | V571 | V572 | V573 | LYS | SER | LEU | GLU | HIS | HIS | HIS | HIS | HIS | HIS |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 205.61Å 209.64Å 102.97Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 50.00 – 3.01<br>50.00 – 3.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (50.00-3.01)<br>98.1 (50.00-3.01)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | 0.07  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.21 (at 3.01Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.7.3_928)                           | Depositor        |
| R, $R_{free}$   | 0.238 , 0.282<br>0.235 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4387 reflections (5.02%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 75.3  | Xtriage          |
| Anisotropy  | 0.837   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 71.7   | EDS              |
| Estimated twinning fraction   | 0.000 for k,h,-l  | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Outliers  | 0 of 87455 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 23688   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 108.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.90         | 0/4030         | 0.97        | 4/5464 (0.1%)   |
| 1   | B     | 0.89         | 3/4030 (0.1%)  | 0.94        | 3/5464 (0.1%)   |
| 1   | C     | 0.80         | 1/4030 (0.0%)  | 0.89        | 2/5464 (0.0%)   |
| 1   | D     | 0.77         | 0/4030         | 0.88        | 1/5464 (0.0%)   |
| 1   | E     | 0.81         | 2/4030 (0.0%)  | 0.90        | 1/5464 (0.0%)   |
| 1   | F     | 0.87         | 1/4030 (0.0%)  | 0.94        | 1/5464 (0.0%)   |
| All | All   | 0.84         | 7/24180 (0.0%) | 0.92        | 12/32784 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 3                   |
| 1   | E     | 0                   | 3                   |
| 1   | F     | 0                   | 2                   |
| All | All   | 0                   | 15                  |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 299 | ASN  | CG-ND2 | -9.03 | 1.10        | 1.32     |
| 1   | B     | 299 | ASN  | CG-OD1 | -7.23 | 1.08        | 1.24     |
| 1   | C     | 299 | ASN  | CG-ND2 | -6.63 | 1.16        | 1.32     |
| 1   | F     | 492 | GLU  | CG-CD  | 5.74  | 1.60        | 1.51     |
| 1   | E     | 551 | ALA  | CA-CB  | -5.69 | 1.40        | 1.52     |
| 1   | B     | 492 | GLU  | CB-CG  | 5.43  | 1.62        | 1.52     |
| 1   | E     | 492 | GLU  | CB-CG  | 5.26  | 1.62        | 1.52     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 304 | LEU  | CB-CG-CD1 | -8.30 | 96.89       | 111.00   |
| 1   | B     | 374 | ASP  | CB-CG-OD2 | -6.55 | 112.40      | 118.30   |
| 1   | C     | 304 | LEU  | CB-CG-CD1 | -5.99 | 100.81      | 111.00   |
| 1   | B     | 304 | LEU  | CB-CG-CD1 | -5.98 | 100.83      | 111.00   |
| 1   | D     | 365 | ASP  | CB-CG-OD2 | 5.83  | 123.55      | 118.30   |
| 1   | E     | 304 | LEU  | CB-CG-CD1 | -5.60 | 101.48      | 111.00   |
| 1   | B     | 554 | ARG  | NE-CZ-NH1 | -5.56 | 117.52      | 120.30   |
| 1   | A     | 356 | ARG  | NE-CZ-NH2 | -5.53 | 117.54      | 120.30   |
| 1   | A     | 304 | LEU  | CB-CG-CD1 | -5.38 | 101.85      | 111.00   |
| 1   | A     | 278 | ASP  | CB-CG-OD1 | -5.33 | 113.50      | 118.30   |
| 1   | C     | 159 | ARG  | NE-CZ-NH2 | -5.25 | 117.68      | 120.30   |
| 1   | A     | 241 | ILE  | CB-CA-C   | -5.10 | 101.41      | 111.60   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 356 | ARG  | Peptide |
| 1   | A     | 71  | LEU  | Peptide |
| 1   | B     | 183 | LYS  | Peptide |
| 1   | B     | 356 | ARG  | Peptide |
| 1   | B     | 71  | LEU  | Peptide |
| 1   | C     | 356 | ARG  | Peptide |
| 1   | C     | 71  | LEU  | Peptide |
| 1   | D     | 183 | LYS  | Peptide |
| 1   | D     | 356 | ARG  | Peptide |
| 1   | D     | 71  | LEU  | Peptide |
| 1   | E     | 183 | LYS  | Peptide |
| 1   | E     | 356 | ARG  | Peptide |
| 1   | E     | 71  | LEU  | Peptide |
| 1   | F     | 356 | ARG  | Peptide |
| 1   | F     | 71  | LEU  | Peptide |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3948  | 0        | 0        | 114     | 3            |
| 1   | B     | 3948  | 0        | 0        | 112     | 3            |
| 1   | C     | 3948  | 0        | 0        | 105     | 1            |
| 1   | D     | 3948  | 0        | 0        | 107     | 0            |
| 1   | E     | 3948  | 0        | 0        | 108     | 0            |
| 1   | F     | 3948  | 0        | 0        | 104     | 1            |
| All | All   | 23688 | 0        | 0        | 627     | 4            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

All (627) close contacts within the same asymmetric unit are listed below.

| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:E:285:ASP:OD1 | 1:E:288:SER:OG  | 1.90        | 0.88     |
| 1:C:285:ASP:OD1 | 1:C:288:SER:OG  | 1.93        | 0.86     |
| 1:A:573:ILE:O   | 1:A:573:ILE:CG2 | 2.23        | 0.86     |
| 1:D:285:ASP:OD1 | 1:D:288:SER:OG  | 1.92        | 0.85     |
| 1:F:215:ASP:OD1 | 1:F:216:TYR:N   | 2.10        | 0.85     |
| 1:B:215:ASP:OD1 | 1:B:216:TYR:N   | 2.12        | 0.82     |
| 1:F:285:ASP:OD1 | 1:F:288:SER:OG  | 1.97        | 0.82     |
| 1:F:573:ILE:CG2 | 1:F:573:ILE:O   | 2.27        | 0.81     |
| 1:D:215:ASP:OD1 | 1:D:216:TYR:N   | 2.13        | 0.80     |
| 1:B:26:ASN:OD1  | 1:B:29:ARG:NH2  | 2.15        | 0.80     |
| 1:D:573:ILE:O   | 1:D:573:ILE:CG2 | 2.31        | 0.79     |
| 1:F:26:ASN:OD1  | 1:F:29:ARG:NH2  | 2.16        | 0.79     |
| 1:E:26:ASN:OD1  | 1:E:29:ARG:NH2  | 2.16        | 0.78     |
| 1:A:285:ASP:OD1 | 1:A:288:SER:OG  | 2.02        | 0.78     |
| 1:B:516:ASP:OD2 | 1:B:518:THR:N   | 2.18        | 0.77     |
| 1:C:215:ASP:OD1 | 1:C:216:TYR:N   | 2.16        | 0.77     |
| 1:C:299:ASN:N   | 1:C:299:ASN:ND2 | 2.26        | 0.77     |
| 1:E:215:ASP:OD1 | 1:E:216:TYR:N   | 2.17        | 0.77     |
| 1:A:3:LEU:N     | 1:A:44:SER:O    | 2.18        | 0.77     |
| 1:A:37:PHE:CZ   | 1:A:40:HIS:O    | 2.39        | 0.76     |
| 1:B:573:ILE:CG2 | 1:B:573:ILE:O   | 2.33        | 0.76     |
| 1:C:573:ILE:O   | 1:C:573:ILE:CG2 | 2.34        | 0.76     |
| 1:B:75:ASN:O    | 1:B:92:VAL:N    | 2.18        | 0.76     |
| 1:E:516:ASP:OD2 | 1:E:518:THR:N   | 2.19        | 0.76     |
| 1:E:37:PHE:CZ   | 1:E:40:HIS:O    | 2.39        | 0.75     |
| 1:D:516:ASP:OD2 | 1:D:518:THR:N   | 2.19        | 0.75     |
| 1:C:312:GLU:OE2 | 1:C:484:ARG:NH1 | 2.19        | 0.75     |
| 1:A:516:ASP:OD2 | 1:A:518:THR:N   | 2.20        | 0.75     |
| 1:C:516:ASP:OD2 | 1:C:518:THR:N   | 2.20        | 0.75     |
| 1:B:285:ASP:OD1 | 1:B:288:SER:OG  | 2.06        | 0.74     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:215:ASP:OD1 | 1:A:216:TYR:N   | 2.21        | 0.74     |
| 1:F:516:ASP:OD2 | 1:F:518:THR:N   | 2.20        | 0.73     |
| 1:D:26:ASN:OD1  | 1:D:29:ARG:NH2  | 2.21        | 0.73     |
| 1:A:26:ASN:OD1  | 1:A:29:ARG:NH2  | 2.22        | 0.73     |
| 1:D:542:MET:O   | 1:D:545:LEU:N   | 2.22        | 0.73     |
| 1:A:75:ASN:O    | 1:A:92:VAL:N    | 2.23        | 0.72     |
| 1:F:529:LYS:O   | 1:F:530:GLY:O   | 2.08        | 0.72     |
| 1:E:573:ILE:CG2 | 1:E:573:ILE:O   | 2.38        | 0.72     |
| 1:B:37:PHE:CZ   | 1:B:40:HIS:O    | 2.42        | 0.71     |
| 1:A:542:MET:O   | 1:A:545:LEU:N   | 2.23        | 0.71     |
| 1:D:37:PHE:CZ   | 1:D:40:HIS:O    | 2.43        | 0.71     |
| 1:C:26:ASN:OD1  | 1:C:29:ARG:NH2  | 2.24        | 0.71     |
| 1:C:3:LEU:N     | 1:C:44:SER:O    | 2.24        | 0.70     |
| 1:C:30:ASP:OD2  | 1:C:89:TYR:OH   | 2.11        | 0.69     |
| 1:F:37:PHE:CZ   | 1:F:40:HIS:O    | 2.46        | 0.69     |
| 1:D:224:ASP:O   | 1:D:227:THR:OG1 | 2.10        | 0.68     |
| 1:F:542:MET:O   | 1:F:545:LEU:N   | 2.27        | 0.68     |
| 1:C:374:ASP:OD1 | 1:C:374:ASP:N   | 2.25        | 0.68     |
| 1:A:470:TYR:CG  | 1:A:479:PHE:CE1 | 2.82        | 0.67     |
| 1:D:312:GLU:OE2 | 1:D:484:ARG:NH1 | 2.28        | 0.67     |
| 1:A:286:TYR:N   | 1:A:331:ASN:OD1 | 2.28        | 0.66     |
| 1:E:312:GLU:OE2 | 1:E:484:ARG:NH1 | 2.29        | 0.66     |
| 1:B:164:LYS:C   | 1:B:282:ILE:CD1 | 2.64        | 0.66     |
| 1:C:37:PHE:CZ   | 1:C:40:HIS:O    | 2.49        | 0.66     |
| 1:B:470:TYR:CG  | 1:B:479:PHE:CE1 | 2.83        | 0.66     |
| 1:B:312:GLU:OE2 | 1:B:484:ARG:NH1 | 2.28        | 0.66     |
| 1:A:374:ASP:OD1 | 1:A:374:ASP:N   | 2.29        | 0.66     |
| 1:E:470:TYR:CG  | 1:E:479:PHE:CE1 | 2.83        | 0.65     |
| 1:E:75:ASN:O    | 1:E:92:VAL:N    | 2.30        | 0.65     |
| 1:B:542:MET:O   | 1:B:545:LEU:N   | 2.29        | 0.65     |
| 1:C:463:ILE:O   | 1:C:463:ILE:CD1 | 2.45        | 0.64     |
| 1:B:37:PHE:CD1  | 1:B:38:ASP:N    | 2.65        | 0.64     |
| 1:C:224:ASP:O   | 1:C:227:THR:OG1 | 2.14        | 0.64     |
| 1:D:75:ASN:O    | 1:D:92:VAL:N    | 2.31        | 0.64     |
| 1:A:57:VAL:O    | 1:A:57:VAL:CG1  | 2.45        | 0.64     |
| 1:B:463:ILE:CD1 | 1:B:463:ILE:O   | 2.46        | 0.64     |
| 1:F:206:ASN:OD1 | 1:F:210:MET:CE  | 2.46        | 0.64     |
| 1:C:542:MET:O   | 1:C:545:LEU:N   | 2.31        | 0.64     |
| 1:C:164:LYS:C   | 1:C:282:ILE:CD1 | 2.67        | 0.63     |
| 1:F:312:GLU:OE2 | 1:F:484:ARG:NH1 | 2.32        | 0.63     |
| 1:D:157:THR:CG2 | 1:D:157:THR:O   | 2.47        | 0.63     |
| 1:B:18:GLN:NE2  | 1:B:552:GLY:O   | 2.32        | 0.62     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:A:135:THR:O   | 1:A:136:GLN:C   | 2.38        | 0.62     |
| 1:B:46:PHE:CD2  | 1:B:46:PHE:O    | 2.53        | 0.62     |
| 1:B:224:ASP:O   | 1:B:227:THR:OG1 | 2.17        | 0.62     |
| 1:C:286:TYR:N   | 1:C:331:ASN:OD1 | 2.33        | 0.62     |
| 1:E:356:ARG:NH2 | 1:F:487:ARG:O   | 2.32        | 0.62     |
| 1:C:37:PHE:CD1  | 1:C:38:ASP:N    | 2.68        | 0.62     |
| 1:F:75:ASN:O    | 1:F:92:VAL:N    | 2.33        | 0.62     |
| 1:C:5:LYS:NZ    | 1:C:41:GLU:OE2  | 2.33        | 0.61     |
| 1:A:312:GLU:OE2 | 1:A:484:ARG:NH1 | 2.34        | 0.61     |
| 1:A:224:ASP:O   | 1:A:227:THR:OG1 | 2.18        | 0.61     |
| 1:E:8:LEU:O     | 1:E:37:PHE:CZ   | 2.54        | 0.61     |
| 1:F:3:LEU:N     | 1:F:44:SER:O    | 2.33        | 0.61     |
| 1:E:164:LYS:C   | 1:E:282:ILE:CD1 | 2.69        | 0.61     |
| 1:E:463:ILE:O   | 1:E:463:ILE:CD1 | 2.49        | 0.61     |
| 1:F:217:GLU:O   | 1:F:220:LYS:N   | 2.33        | 0.61     |
| 1:F:224:ASP:O   | 1:F:227:THR:OG1 | 2.19        | 0.61     |
| 1:C:18:GLN:NE2  | 1:C:552:GLY:O   | 2.34        | 0.60     |
| 1:D:566:THR:O   | 1:D:567:VAL:C   | 2.39        | 0.60     |
| 1:A:18:GLN:NE2  | 1:A:552:GLY:O   | 2.34        | 0.60     |
| 1:F:135:THR:O   | 1:F:136:GLN:C   | 2.39        | 0.60     |
| 1:B:75:ASN:N    | 1:B:75:ASN:OD1  | 2.34        | 0.60     |
| 1:A:164:LYS:C   | 1:A:282:ILE:CD1 | 2.70        | 0.60     |
| 1:C:470:TYR:CG  | 1:C:479:PHE:CE1 | 2.89        | 0.60     |
| 1:D:560:SER:O   | 1:D:564:ASN:ND2 | 2.34        | 0.60     |
| 1:E:206:ASN:OD1 | 1:E:210:MET:CE  | 2.48        | 0.60     |
| 1:C:566:THR:O   | 1:C:567:VAL:C   | 2.40        | 0.60     |
| 1:D:374:ASP:OD1 | 1:D:374:ASP:N   | 2.35        | 0.60     |
| 1:A:8:LEU:O     | 1:A:37:PHE:CZ   | 2.54        | 0.60     |
| 1:D:158:MET:O   | 1:D:159:ARG:CD  | 2.50        | 0.60     |
| 1:B:128:ASN:ND2 | 1:B:128:ASN:C   | 2.54        | 0.60     |
| 1:A:15:ASN:CG   | 1:F:546:ARG:NH2 | 2.56        | 0.60     |
| 1:A:463:ILE:O   | 1:A:463:ILE:CD1 | 2.50        | 0.60     |
| 1:E:542:MET:O   | 1:E:545:LEU:N   | 2.35        | 0.59     |
| 1:C:546:ARG:NH2 | 1:D:15:ASN:OD1  | 2.35        | 0.59     |
| 1:F:374:ASP:N   | 1:F:374:ASP:OD1 | 2.32        | 0.59     |
| 1:F:470:TYR:CG  | 1:F:479:PHE:CE1 | 2.91        | 0.59     |
| 1:A:359:ASN:ND2 | 1:A:360:VAL:O   | 2.36        | 0.59     |
| 1:E:5:LYS:NZ    | 1:E:41:GLU:OE2  | 2.35        | 0.59     |
| 1:F:30:ASP:OD2  | 1:F:89:TYR:OH   | 2.20        | 0.59     |
| 1:F:566:THR:O   | 1:F:567:VAL:C   | 2.41        | 0.59     |
| 1:F:463:ILE:O   | 1:F:463:ILE:CD1 | 2.51        | 0.59     |
| 1:B:30:ASP:OD2  | 1:B:89:TYR:OH   | 2.21        | 0.59     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:D:215:ASP:C   | 1:D:215:ASP:OD1 | 2.41        | 0.59     |
| 1:A:128:ASN:ND2 | 1:A:128:ASN:C   | 2.55        | 0.59     |
| 1:C:206:ASN:OD1 | 1:C:210:MET:CE  | 2.50        | 0.59     |
| 1:A:359:ASN:O   | 1:A:360:VAL:C   | 2.41        | 0.59     |
| 1:B:6:ILE:CG2   | 1:B:7:LYS:N     | 2.65        | 0.59     |
| 1:B:566:THR:O   | 1:B:567:VAL:C   | 2.39        | 0.59     |
| 1:C:135:THR:O   | 1:C:136:GLN:C   | 2.38        | 0.59     |
| 1:D:3:LEU:N     | 1:D:44:SER:O    | 2.36        | 0.59     |
| 1:F:164:LYS:C   | 1:F:282:ILE:CD1 | 2.71        | 0.59     |
| 1:D:470:TYR:CG  | 1:D:479:PHE:CE1 | 2.91        | 0.59     |
| 1:B:502:MET:O   | 1:B:554:ARG:NH1 | 2.36        | 0.59     |
| 1:F:563:ILE:O   | 1:F:564:ASN:ND2 | 2.36        | 0.58     |
| 1:B:44:SER:OG   | 1:B:45:THR:N    | 2.36        | 0.58     |
| 1:F:566:THR:O   | 1:F:568:VAL:N   | 2.35        | 0.58     |
| 1:E:374:ASP:OD1 | 1:E:374:ASP:N   | 2.36        | 0.58     |
| 1:D:164:LYS:C   | 1:D:282:ILE:CD1 | 2.72        | 0.58     |
| 1:F:286:TYR:N   | 1:F:331:ASN:OD1 | 2.36        | 0.58     |
| 1:F:215:ASP:C   | 1:F:215:ASP:OD1 | 2.42        | 0.58     |
| 1:D:546:ARG:NH2 | 1:E:15:ASN:CG   | 2.57        | 0.58     |
| 1:D:299:ASN:ND2 | 1:D:299:ASN:N   | 2.51        | 0.58     |
| 1:D:5:LYS:NZ    | 1:D:41:GLU:OE2  | 2.36        | 0.58     |
| 1:B:59:ILE:CG2  | 1:B:59:ILE:O    | 2.51        | 0.58     |
| 1:B:5:LYS:NZ    | 1:B:41:GLU:OE2  | 2.37        | 0.58     |
| 1:E:529:LYS:O   | 1:E:530:GLY:O   | 2.22        | 0.58     |
| 1:B:307:ASN:N   | 1:B:307:ASN:OD1 | 2.36        | 0.58     |
| 1:D:57:VAL:CG1  | 1:D:57:VAL:O    | 2.51        | 0.58     |
| 1:E:229:TYR:N   | 1:E:229:TYR:CD2 | 2.71        | 0.58     |
| 1:B:529:LYS:O   | 1:B:530:GLY:O   | 2.21        | 0.58     |
| 1:E:224:ASP:O   | 1:E:227:THR:OG1 | 2.21        | 0.57     |
| 1:B:563:ILE:O   | 1:B:564:ASN:ND2 | 2.37        | 0.57     |
| 1:D:30:ASP:OD2  | 1:D:89:TYR:OH   | 2.21        | 0.57     |
| 1:E:286:TYR:N   | 1:E:331:ASN:OD1 | 2.37        | 0.57     |
| 1:D:463:ILE:O   | 1:D:463:ILE:CD1 | 2.53        | 0.57     |
| 1:D:8:LEU:O     | 1:D:37:PHE:CZ   | 2.58        | 0.57     |
| 1:A:572:ILE:O   | 1:A:572:ILE:CG2 | 2.50        | 0.57     |
| 1:A:215:ASP:C   | 1:A:215:ASP:OD1 | 2.43        | 0.57     |
| 1:D:37:PHE:CD1  | 1:D:38:ASP:N    | 2.73        | 0.57     |
| 1:B:491:ASP:O   | 1:B:492:GLU:C   | 2.39        | 0.57     |
| 1:C:215:ASP:C   | 1:C:215:ASP:OD1 | 2.44        | 0.57     |
| 1:B:374:ASP:N   | 1:B:374:ASP:OD1 | 2.38        | 0.57     |
| 1:C:356:ARG:NH2 | 1:D:487:ARG:O   | 2.38        | 0.57     |
| 1:D:135:THR:O   | 1:D:136:GLN:C   | 2.42        | 0.56     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:B:356:ARG:NH2 | 1:C:487:ARG:O   | 2.38        | 0.56     |
| 1:F:44:SER:OG   | 1:F:45:THR:N    | 2.37        | 0.56     |
| 1:D:18:GLN:NE2  | 1:D:552:GLY:O   | 2.39        | 0.56     |
| 1:F:18:GLN:NE2  | 1:F:552:GLY:O   | 2.38        | 0.56     |
| 1:B:229:TYR:N   | 1:B:229:TYR:CD2 | 2.73        | 0.56     |
| 1:E:46:PHE:O    | 1:E:46:PHE:CD2  | 2.58        | 0.56     |
| 1:D:286:TYR:N   | 1:D:331:ASN:OD1 | 2.38        | 0.56     |
| 1:C:148:SER:CB  | 1:D:156:SER:O   | 2.54        | 0.56     |
| 1:D:148:SER:CB  | 1:E:156:SER:O   | 2.53        | 0.56     |
| 1:D:572:ILE:CG2 | 1:D:572:ILE:O   | 2.50        | 0.56     |
| 1:B:572:ILE:CG2 | 1:B:572:ILE:O   | 2.49        | 0.56     |
| 1:F:5:LYS:NZ    | 1:F:41:GLU:OE2  | 2.38        | 0.56     |
| 1:C:6:ILE:CG2   | 1:C:7:LYS:N     | 2.69        | 0.56     |
| 1:E:18:GLN:NE2  | 1:E:552:GLY:O   | 2.39        | 0.56     |
| 1:C:8:LEU:O     | 1:C:37:PHE:CZ   | 2.59        | 0.56     |
| 1:E:3:LEU:N     | 1:E:44:SER:O    | 2.39        | 0.56     |
| 1:E:67:CYS:SG   | 1:E:68:PHE:N    | 2.79        | 0.56     |
| 1:C:42:PHE:CE1  | 1:C:59:ILE:CD1  | 2.89        | 0.56     |
| 1:E:572:ILE:CG2 | 1:E:572:ILE:O   | 2.51        | 0.55     |
| 1:C:572:ILE:CG2 | 1:C:572:ILE:O   | 2.52        | 0.55     |
| 1:D:566:THR:O   | 1:D:568:VAL:N   | 2.40        | 0.55     |
| 1:E:566:THR:O   | 1:E:567:VAL:C   | 2.43        | 0.55     |
| 1:B:8:LEU:O     | 1:B:37:PHE:CZ   | 2.60        | 0.55     |
| 1:A:206:ASN:OD1 | 1:A:210:MET:CE  | 2.55        | 0.55     |
| 1:B:57:VAL:CG1  | 1:B:57:VAL:O    | 2.55        | 0.55     |
| 1:A:359:ASN:C   | 1:A:360:VAL:O   | 2.41        | 0.55     |
| 1:F:157:THR:CG2 | 1:F:157:THR:O   | 2.54        | 0.55     |
| 1:E:128:ASN:C   | 1:E:128:ASN:ND2 | 2.58        | 0.55     |
| 1:C:566:THR:O   | 1:C:568:VAL:N   | 2.40        | 0.55     |
| 1:A:156:SER:O   | 1:F:148:SER:CB  | 2.55        | 0.55     |
| 1:A:37:PHE:CD1  | 1:A:38:ASP:N    | 2.75        | 0.55     |
| 1:B:566:THR:O   | 1:B:568:VAL:N   | 2.39        | 0.55     |
| 1:E:563:ILE:O   | 1:E:564:ASN:ND2 | 2.40        | 0.55     |
| 1:C:75:ASN:O    | 1:C:92:VAL:N    | 2.40        | 0.55     |
| 1:F:572:ILE:O   | 1:F:572:ILE:CG2 | 2.54        | 0.54     |
| 1:A:15:ASN:OD1  | 1:F:546:ARG:NH2 | 2.40        | 0.54     |
| 1:C:546:ARG:NH2 | 1:D:15:ASN:CG   | 2.60        | 0.54     |
| 1:B:560:SER:O   | 1:B:564:ASN:ND2 | 2.41        | 0.54     |
| 1:A:566:THR:O   | 1:A:567:VAL:C   | 2.46        | 0.54     |
| 1:B:546:ARG:NH2 | 1:C:15:ASN:OD1  | 2.41        | 0.54     |
| 1:D:229:TYR:CD2 | 1:D:229:TYR:N   | 2.75        | 0.54     |
| 1:D:206:ASN:OD1 | 1:D:210:MET:CE  | 2.56        | 0.54     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:B:538:ASP:O   | 1:B:541:HIS:N   | 2.40        | 0.54     |
| 1:E:135:THR:O   | 1:E:136:GLN:C   | 2.46        | 0.54     |
| 1:E:157:THR:O   | 1:E:157:THR:CG2 | 2.55        | 0.54     |
| 1:F:8:LEU:O     | 1:F:37:PHE:CZ   | 2.61        | 0.54     |
| 1:D:44:SER:OG   | 1:D:45:THR:N    | 2.41        | 0.54     |
| 1:E:44:SER:OG   | 1:E:45:THR:N    | 2.40        | 0.54     |
| 1:F:46:PHE:O    | 1:F:46:PHE:CD2  | 2.61        | 0.54     |
| 1:C:128:ASN:ND2 | 1:C:128:ASN:C   | 2.62        | 0.54     |
| 1:B:291:PHE:C   | 1:B:291:PHE:CD2 | 2.80        | 0.54     |
| 1:A:59:ILE:CG2  | 1:A:59:ILE:O    | 2.56        | 0.54     |
| 1:D:46:PHE:CE1  | 1:D:55:LEU:CD1  | 2.91        | 0.54     |
| 1:A:229:TYR:CD2 | 1:A:229:TYR:N   | 2.75        | 0.53     |
| 1:B:23:PHE:N    | 1:B:23:PHE:CD2  | 2.75        | 0.53     |
| 1:F:229:TYR:N   | 1:F:229:TYR:CD2 | 2.76        | 0.53     |
| 1:A:502:MET:O   | 1:A:554:ARG:NH1 | 2.41        | 0.53     |
| 1:E:30:ASP:OD2  | 1:E:89:TYR:OH   | 2.26        | 0.53     |
| 1:E:37:PHE:CD1  | 1:E:38:ASP:N    | 2.77        | 0.53     |
| 1:F:112:VAL:O   | 1:F:116:THR:OG1 | 2.26        | 0.53     |
| 1:B:286:TYR:N   | 1:B:331:ASN:OD1 | 2.41        | 0.53     |
| 1:A:44:SER:OG   | 1:A:45:THR:N    | 2.40        | 0.53     |
| 1:E:46:PHE:CE1  | 1:E:55:LEU:CD1  | 2.91        | 0.53     |
| 1:E:491:ASP:O   | 1:E:492:GLU:C   | 2.47        | 0.53     |
| 1:F:502:MET:O   | 1:F:554:ARG:NH1 | 2.41        | 0.53     |
| 1:D:46:PHE:O    | 1:D:46:PHE:CD2  | 2.62        | 0.52     |
| 1:B:259:ASN:O   | 1:B:260:GLY:C   | 2.46        | 0.52     |
| 1:B:157:THR:O   | 1:B:157:THR:CG2 | 2.56        | 0.52     |
| 1:A:358:ASN:CG  | 1:A:358:ASN:O   | 2.47        | 0.52     |
| 1:E:285:ASP:OD2 | 1:E:287:GLN:N   | 2.42        | 0.52     |
| 1:E:215:ASP:OD1 | 1:E:215:ASP:C   | 2.46        | 0.52     |
| 1:C:46:PHE:O    | 1:C:46:PHE:CD2  | 2.63        | 0.52     |
| 1:F:359:ASN:O   | 1:F:360:VAL:C   | 2.45        | 0.52     |
| 1:C:516:ASP:OD2 | 1:C:517:ILE:N   | 2.42        | 0.52     |
| 1:A:542:MET:O   | 1:A:543:ASN:C   | 2.48        | 0.52     |
| 1:A:529:LYS:O   | 1:A:530:GLY:O   | 2.28        | 0.52     |
| 1:A:491:ASP:O   | 1:A:494:ASN:N   | 2.41        | 0.52     |
| 1:D:358:ASN:O   | 1:D:358:ASN:CG  | 2.48        | 0.52     |
| 1:A:217:GLU:O   | 1:A:220:LYS:N   | 2.42        | 0.52     |
| 1:F:359:ASN:C   | 1:F:360:VAL:O   | 2.48        | 0.52     |
| 1:A:470:TYR:CB  | 1:A:479:PHE:CE1 | 2.93        | 0.52     |
| 1:B:217:GLU:O   | 1:B:220:LYS:N   | 2.42        | 0.52     |
| 1:D:546:ARG:NH2 | 1:E:15:ASN:OD1  | 2.43        | 0.52     |
| 1:C:172:GLU:CD  | 1:C:212:TRP:CZ2 | 2.83        | 0.52     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:D:356:ARG:NH2 | 1:E:487:ARG:O   | 2.42        | 0.52     |
| 1:B:135:THR:O   | 1:B:136:GLN:C   | 2.44        | 0.52     |
| 1:F:37:PHE:CD1  | 1:F:38:ASP:N    | 2.78        | 0.52     |
| 1:B:3:LEU:N     | 1:B:44:SER:O    | 2.43        | 0.52     |
| 1:B:42:PHE:CE1  | 1:B:59:ILE:CD1  | 2.93        | 0.52     |
| 1:D:120:VAL:CG2 | 1:D:121:LEU:N   | 2.73        | 0.52     |
| 1:A:563:ILE:O   | 1:A:564:ASN:ND2 | 2.42        | 0.52     |
| 1:A:5:LYS:NZ    | 1:A:41:GLU:OE2  | 2.43        | 0.51     |
| 1:B:359:ASN:ND2 | 1:B:360:VAL:O   | 2.43        | 0.51     |
| 1:C:560:SER:O   | 1:C:564:ASN:ND2 | 2.43        | 0.51     |
| 1:D:128:ASN:ND2 | 1:D:128:ASN:C   | 2.64        | 0.51     |
| 1:C:44:SER:OG   | 1:C:45:THR:N    | 2.42        | 0.51     |
| 1:C:172:GLU:OE1 | 1:C:212:TRP:CH2 | 2.63        | 0.51     |
| 1:B:324:ASP:OD1 | 1:B:324:ASP:C   | 2.48        | 0.51     |
| 1:D:511:SER:O   | 1:D:511:SER:OG  | 2.28        | 0.51     |
| 1:B:148:SER:CB  | 1:C:156:SER:O   | 2.58        | 0.51     |
| 1:D:542:MET:O   | 1:D:543:ASN:C   | 2.48        | 0.51     |
| 1:F:6:ILE:CG2   | 1:F:7:LYS:N     | 2.73        | 0.51     |
| 1:A:307:ASN:N   | 1:A:307:ASN:OD1 | 2.44        | 0.51     |
| 1:F:92:VAL:O    | 1:F:92:VAL:CG2  | 2.59        | 0.51     |
| 1:C:46:PHE:CE1  | 1:C:55:LEU:CD1  | 2.94        | 0.51     |
| 1:B:164:LYS:O   | 1:B:282:ILE:CD1 | 2.59        | 0.51     |
| 1:E:566:THR:O   | 1:E:568:VAL:N   | 2.44        | 0.51     |
| 1:E:6:ILE:CG2   | 1:E:7:LYS:N     | 2.74        | 0.51     |
| 1:F:78:GLN:CG   | 1:F:79:VAL:N    | 2.73        | 0.51     |
| 1:D:563:ILE:O   | 1:D:564:ASN:ND2 | 2.44        | 0.51     |
| 1:B:215:ASP:OD1 | 1:B:215:ASP:C   | 2.48        | 0.51     |
| 1:A:537:VAL:O   | 1:A:538:ASP:C   | 2.48        | 0.51     |
| 1:E:79:VAL:CG1  | 1:E:81:TYR:CE2  | 2.93        | 0.51     |
| 1:F:491:ASP:O   | 1:F:492:GLU:C   | 2.47        | 0.51     |
| 1:E:324:ASP:C   | 1:E:324:ASP:OD1 | 2.49        | 0.51     |
| 1:E:560:SER:O   | 1:E:564:ASN:ND2 | 2.44        | 0.50     |
| 1:C:502:MET:O   | 1:C:554:ARG:NH1 | 2.44        | 0.50     |
| 1:E:57:VAL:O    | 1:E:57:VAL:CG1  | 2.58        | 0.50     |
| 1:F:217:GLU:O   | 1:F:218:SER:C   | 2.48        | 0.50     |
| 1:F:358:ASN:O   | 1:F:358:ASN:CG  | 2.50        | 0.50     |
| 1:B:46:PHE:CE1  | 1:B:55:LEU:CD1  | 2.94        | 0.50     |
| 1:F:46:PHE:CE1  | 1:F:55:LEU:CD1  | 2.94        | 0.50     |
| 1:F:491:ASP:O   | 1:F:494:ASN:N   | 2.44        | 0.50     |
| 1:B:172:GLU:OE2 | 1:B:245:GLY:N   | 2.45        | 0.50     |
| 1:A:46:PHE:CD2  | 1:A:46:PHE:O    | 2.64        | 0.50     |
| 1:E:359:ASN:O   | 1:E:360:VAL:C   | 2.50        | 0.50     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:F:172:GLU:CD  | 1:F:212:TRP:CH2 | 2.85        | 0.50     |
| 1:C:212:TRP:O   | 1:C:213:PHE:CD2 | 2.65        | 0.50     |
| 1:A:560:SER:O   | 1:A:564:ASN:ND2 | 2.44        | 0.50     |
| 1:C:559:GLU:O   | 1:C:560:SER:C   | 2.50        | 0.50     |
| 1:F:172:GLU:OE1 | 1:F:212:TRP:CH2 | 2.64        | 0.50     |
| 1:D:491:ASP:O   | 1:D:494:ASN:N   | 2.44        | 0.50     |
| 1:E:172:GLU:OE1 | 1:E:212:TRP:CH2 | 2.64        | 0.50     |
| 1:C:229:TYR:CD2 | 1:C:229:TYR:N   | 2.79        | 0.50     |
| 1:B:79:VAL:CG1  | 1:B:81:TYR:CE2  | 2.94        | 0.50     |
| 1:B:99:ASN:OD1  | 1:B:101:LYS:N   | 2.44        | 0.50     |
| 1:C:545:LEU:O   | 1:C:546:ARG:C   | 2.50        | 0.50     |
| 1:A:46:PHE:CE1  | 1:A:55:LEU:CD1  | 2.94        | 0.50     |
| 1:E:59:ILE:O    | 1:E:59:ILE:CG2  | 2.59        | 0.50     |
| 1:F:99:ASN:OD1  | 1:F:101:LYS:N   | 2.45        | 0.50     |
| 1:D:538:ASP:O   | 1:D:541:HIS:N   | 2.45        | 0.50     |
| 1:D:502:MET:O   | 1:D:554:ARG:NH1 | 2.45        | 0.50     |
| 1:F:172:GLU:CD  | 1:F:212:TRP:CZ2 | 2.85        | 0.50     |
| 1:D:307:ASN:N   | 1:D:307:ASN:OD1 | 2.45        | 0.50     |
| 1:F:285:ASP:OD2 | 1:F:287:GLN:N   | 2.45        | 0.49     |
| 1:F:202:ASP:OD2 | 1:F:274:SER:OG  | 2.30        | 0.49     |
| 1:A:6:ILE:CG2   | 1:A:7:LYS:N     | 2.75        | 0.49     |
| 1:D:172:GLU:OE1 | 1:D:212:TRP:CH2 | 2.65        | 0.49     |
| 1:E:172:GLU:CD  | 1:E:212:TRP:CH2 | 2.85        | 0.49     |
| 1:F:23:PHE:N    | 1:F:23:PHE:CD2  | 2.80        | 0.49     |
| 1:E:172:GLU:CD  | 1:E:212:TRP:CZ2 | 2.85        | 0.49     |
| 1:B:67:CYS:SG   | 1:B:68:PHE:N    | 2.85        | 0.49     |
| 1:D:112:VAL:O   | 1:D:116:THR:OG1 | 2.30        | 0.49     |
| 1:C:164:LYS:O   | 1:C:282:ILE:CD1 | 2.60        | 0.49     |
| 1:B:202:ASP:OD2 | 1:B:274:SER:OG  | 2.30        | 0.49     |
| 1:C:359:ASN:ND2 | 1:C:360:VAL:O   | 2.45        | 0.49     |
| 1:F:75:ASN:N    | 1:F:75:ASN:OD1  | 2.45        | 0.49     |
| 1:A:164:LYS:O   | 1:A:282:ILE:CD1 | 2.60        | 0.49     |
| 1:D:244:SER:O   | 1:D:245:GLY:C   | 2.51        | 0.49     |
| 1:B:286:TYR:CD2 | 1:B:286:TYR:C   | 2.85        | 0.49     |
| 1:C:291:PHE:CD2 | 1:C:291:PHE:C   | 2.86        | 0.49     |
| 1:F:566:THR:C   | 1:F:568:VAL:N   | 2.64        | 0.49     |
| 1:C:23:PHE:N    | 1:C:23:PHE:CD2  | 2.80        | 0.49     |
| 1:A:144:GLU:OE1 | 1:A:356:ARG:NH1 | 2.46        | 0.49     |
| 1:B:285:ASP:OD2 | 1:B:287:GLN:N   | 2.46        | 0.49     |
| 1:C:324:ASP:C   | 1:C:324:ASP:OD1 | 2.51        | 0.49     |
| 1:E:129:VAL:CG2 | 1:E:130:ILE:N   | 2.76        | 0.49     |
| 1:F:307:ASN:N   | 1:F:307:ASN:OD1 | 2.46        | 0.49     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:D:276:GLN:O   | 1:D:277:LYS:C   | 2.50        | 0.48     |
| 1:D:285:ASP:O   | 1:D:286:TYR:C   | 2.50        | 0.48     |
| 1:E:470:TYR:CB  | 1:E:479:PHE:CE1 | 2.95        | 0.48     |
| 1:B:172:GLU:OE1 | 1:B:212:TRP:CH2 | 2.65        | 0.48     |
| 1:B:276:GLN:O   | 1:B:277:LYS:C   | 2.51        | 0.48     |
| 1:A:37:PHE:CE1  | 1:A:40:HIS:O    | 2.66        | 0.48     |
| 1:B:542:MET:O   | 1:B:543:ASN:C   | 2.51        | 0.48     |
| 1:E:559:GLU:O   | 1:E:560:SER:C   | 2.50        | 0.48     |
| 1:D:172:GLU:CD  | 1:D:212:TRP:CH2 | 2.86        | 0.48     |
| 1:F:120:VAL:CG2 | 1:F:121:LEU:N   | 2.76        | 0.48     |
| 1:A:148:SER:CB  | 1:B:156:SER:O   | 2.62        | 0.48     |
| 1:F:359:ASN:ND2 | 1:F:360:VAL:O   | 2.46        | 0.48     |
| 1:C:172:GLU:OE2 | 1:C:245:GLY:N   | 2.47        | 0.48     |
| 1:C:172:GLU:CD  | 1:C:212:TRP:CH2 | 2.87        | 0.48     |
| 1:C:158:MET:O   | 1:C:159:ARG:CD  | 2.61        | 0.48     |
| 1:E:23:PHE:CD2  | 1:E:23:PHE:N    | 2.80        | 0.48     |
| 1:B:129:VAL:CG2 | 1:B:130:ILE:N   | 2.77        | 0.48     |
| 1:D:559:GLU:O   | 1:D:560:SER:C   | 2.51        | 0.48     |
| 1:D:212:TRP:O   | 1:D:213:PHE:CD2 | 2.66        | 0.48     |
| 1:F:496:VAL:O   | 1:F:497:LYS:C   | 2.52        | 0.48     |
| 1:B:511:SER:OG  | 1:B:511:SER:O   | 2.28        | 0.48     |
| 1:E:380:VAL:O   | 1:E:462:ALA:N   | 2.47        | 0.48     |
| 1:E:498:LYS:O   | 1:E:499:TYR:C   | 2.52        | 0.48     |
| 1:C:511:SER:O   | 1:C:511:SER:OG  | 2.30        | 0.48     |
| 1:D:285:ASP:OD2 | 1:D:287:GLN:N   | 2.46        | 0.48     |
| 1:B:559:GLU:O   | 1:B:560:SER:C   | 2.53        | 0.48     |
| 1:E:212:TRP:O   | 1:E:213:PHE:CD2 | 2.67        | 0.47     |
| 1:D:172:GLU:CD  | 1:D:212:TRP:CZ2 | 2.87        | 0.47     |
| 1:A:172:GLU:CD  | 1:A:212:TRP:CZ2 | 2.87        | 0.47     |
| 1:B:563:ILE:C   | 1:B:564:ASN:ND2 | 2.68        | 0.47     |
| 1:D:549:PHE:O   | 1:D:552:GLY:N   | 2.47        | 0.47     |
| 1:B:120:VAL:CG2 | 1:B:121:LEU:N   | 2.77        | 0.47     |
| 1:B:470:TYR:CB  | 1:B:479:PHE:CE1 | 2.98        | 0.47     |
| 1:E:61:LEU:CD2  | 1:E:67:CYS:SG   | 3.02        | 0.47     |
| 1:A:380:VAL:O   | 1:A:462:ALA:N   | 2.47        | 0.47     |
| 1:A:290:MET:CE  | 1:A:295:LEU:CB  | 2.93        | 0.47     |
| 1:A:296:ASN:OD1 | 1:A:298:ILE:N   | 2.48        | 0.47     |
| 1:C:498:LYS:O   | 1:C:499:TYR:C   | 2.52        | 0.47     |
| 1:D:129:VAL:CG2 | 1:D:130:ILE:N   | 2.78        | 0.47     |
| 1:A:217:GLU:O   | 1:A:218:SER:C   | 2.52        | 0.47     |
| 1:F:542:MET:O   | 1:F:543:ASN:C   | 2.52        | 0.47     |
| 1:F:212:TRP:O   | 1:F:213:PHE:CD2 | 2.67        | 0.47     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:E:307:ASN:N   | 1:E:307:ASN:OD1 | 2.48        | 0.47     |
| 1:E:502:MET:O   | 1:E:554:ARG:NH1 | 2.48        | 0.47     |
| 1:A:187:THR:N   | 1:A:190:LYS:O   | 2.48        | 0.47     |
| 1:C:563:ILE:O   | 1:C:564:ASN:ND2 | 2.48        | 0.47     |
| 1:E:212:TRP:O   | 1:E:213:PHE:CG  | 2.68        | 0.47     |
| 1:E:120:VAL:CG2 | 1:E:121:LEU:N   | 2.78        | 0.47     |
| 1:A:173:TYR:N   | 1:A:173:TYR:CD2 | 2.83        | 0.47     |
| 1:F:172:GLU:OE2 | 1:F:245:GLY:N   | 2.48        | 0.47     |
| 1:E:537:VAL:O   | 1:E:539:THR:N   | 2.48        | 0.47     |
| 1:C:285:ASP:O   | 1:C:286:TYR:C   | 2.53        | 0.47     |
| 1:B:212:TRP:O   | 1:B:213:PHE:CD2 | 2.68        | 0.47     |
| 1:C:307:ASN:N   | 1:C:307:ASN:OD1 | 2.46        | 0.47     |
| 1:A:23:PHE:CD2  | 1:A:23:PHE:N    | 2.82        | 0.47     |
| 1:F:128:ASN:ND2 | 1:F:128:ASN:C   | 2.67        | 0.47     |
| 1:E:37:PHE:CE1  | 1:E:40:HIS:O    | 2.68        | 0.46     |
| 1:F:324:ASP:OD1 | 1:F:324:ASP:C   | 2.52        | 0.46     |
| 1:A:276:GLN:O   | 1:A:277:LYS:C   | 2.52        | 0.46     |
| 1:A:286:TYR:C   | 1:A:286:TYR:CD2 | 2.88        | 0.46     |
| 1:A:491:ASP:O   | 1:A:492:GLU:C   | 2.51        | 0.46     |
| 1:A:120:VAL:CG2 | 1:A:121:LEU:N   | 2.77        | 0.46     |
| 1:D:529:LYS:O   | 1:D:530:GLY:O   | 2.33        | 0.46     |
| 1:F:291:PHE:CD2 | 1:F:291:PHE:C   | 2.89        | 0.46     |
| 1:A:285:ASP:O   | 1:A:286:TYR:C   | 2.53        | 0.46     |
| 1:B:516:ASP:OD2 | 1:B:517:ILE:N   | 2.47        | 0.46     |
| 1:A:563:ILE:CD1 | 1:A:563:ILE:N   | 2.78        | 0.46     |
| 1:A:172:GLU:CD  | 1:A:212:TRP:CH2 | 2.88        | 0.46     |
| 1:C:286:TYR:C   | 1:C:286:TYR:CD2 | 2.89        | 0.46     |
| 1:E:542:MET:O   | 1:E:543:ASN:C   | 2.54        | 0.46     |
| 1:E:291:PHE:C   | 1:E:291:PHE:CD2 | 2.89        | 0.46     |
| 1:F:285:ASP:O   | 1:F:286:TYR:C   | 2.54        | 0.46     |
| 1:B:172:GLU:CD  | 1:B:212:TRP:CZ2 | 2.88        | 0.46     |
| 1:E:172:GLU:OE2 | 1:E:245:GLY:N   | 2.48        | 0.46     |
| 1:A:157:THR:CG2 | 1:A:157:THR:O   | 2.64        | 0.46     |
| 1:C:190:LYS:O   | 1:C:190:LYS:CG  | 2.62        | 0.46     |
| 1:C:79:VAL:CG1  | 1:C:81:TYR:CE2  | 2.99        | 0.46     |
| 1:D:217:GLU:O   | 1:D:220:LYS:N   | 2.49        | 0.46     |
| 1:C:348:VAL:CG2 | 1:C:349:TYR:N   | 2.77        | 0.46     |
| 1:C:57:VAL:O    | 1:C:57:VAL:CG1  | 2.63        | 0.46     |
| 1:E:358:ASN:O   | 1:E:358:ASN:CG  | 2.53        | 0.46     |
| 1:A:546:ARG:NH2 | 1:B:15:ASN:CG   | 2.69        | 0.46     |
| 1:B:276:GLN:O   | 1:B:277:LYS:O   | 2.33        | 0.46     |
| 1:C:380:VAL:O   | 1:C:462:ALA:N   | 2.48        | 0.46     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:D:491:ASP:O   | 1:D:492:GLU:C   | 2.54        | 0.46     |
| 1:D:498:LYS:O   | 1:D:499:TYR:C   | 2.54        | 0.46     |
| 1:C:371:ASN:OD1 | 1:C:371:ASN:C   | 2.55        | 0.46     |
| 1:D:259:ASN:O   | 1:D:260:GLY:C   | 2.55        | 0.46     |
| 1:B:549:PHE:O   | 1:B:552:GLY:N   | 2.49        | 0.45     |
| 1:F:380:VAL:O   | 1:F:462:ALA:N   | 2.49        | 0.45     |
| 1:A:285:ASP:OD2 | 1:A:287:GLN:N   | 2.50        | 0.45     |
| 1:D:172:GLU:OE2 | 1:D:245:GLY:N   | 2.49        | 0.45     |
| 1:C:120:VAL:CG2 | 1:C:121:LEU:N   | 2.79        | 0.45     |
| 1:A:259:ASN:O   | 1:A:260:GLY:C   | 2.51        | 0.45     |
| 1:C:285:ASP:OD2 | 1:C:285:ASP:C   | 2.55        | 0.45     |
| 1:E:217:GLU:O   | 1:E:220:LYS:N   | 2.49        | 0.45     |
| 1:A:42:PHE:CE1  | 1:A:59:ILE:CD1  | 2.99        | 0.45     |
| 1:C:60:ASP:N    | 1:C:60:ASP:OD2  | 2.49        | 0.45     |
| 1:F:516:ASP:OD2 | 1:F:517:ILE:N   | 2.49        | 0.45     |
| 1:F:559:GLU:O   | 1:F:560:SER:C   | 2.55        | 0.45     |
| 1:C:563:ILE:N   | 1:C:563:ILE:CD1 | 2.80        | 0.45     |
| 1:E:244:SER:O   | 1:E:245:GLY:C   | 2.55        | 0.45     |
| 1:F:59:ILE:O    | 1:F:59:ILE:CG2  | 2.64        | 0.45     |
| 1:A:79:VAL:CG1  | 1:A:81:TYR:CE2  | 3.00        | 0.45     |
| 1:C:75:ASN:OD1  | 1:C:75:ASN:N    | 2.50        | 0.45     |
| 1:A:559:GLU:O   | 1:A:560:SER:C   | 2.55        | 0.45     |
| 1:B:525:TRP:CZ3 | 1:B:554:ARG:NH1 | 2.84        | 0.45     |
| 1:E:286:TYR:C   | 1:E:286:TYR:CD2 | 2.89        | 0.45     |
| 1:C:129:VAL:CG2 | 1:C:130:ILE:N   | 2.79        | 0.45     |
| 1:B:329:GLU:OE2 | 1:B:357:GLY:N   | 2.50        | 0.45     |
| 1:A:324:ASP:OD1 | 1:A:324:ASP:C   | 2.54        | 0.45     |
| 1:C:358:ASN:O   | 1:C:358:ASN:CG  | 2.54        | 0.45     |
| 1:B:498:LYS:O   | 1:B:499:TYR:C   | 2.54        | 0.45     |
| 1:D:99:ASN:OD1  | 1:D:101:LYS:N   | 2.50        | 0.45     |
| 1:C:276:GLN:O   | 1:C:277:LYS:C   | 2.53        | 0.45     |
| 1:D:371:ASN:C   | 1:D:371:ASN:OD1 | 2.55        | 0.45     |
| 1:D:157:THR:CG2 | 1:D:489:SER:N   | 2.80        | 0.45     |
| 1:E:359:ASN:ND2 | 1:E:360:VAL:O   | 2.50        | 0.45     |
| 1:B:206:ASN:OD1 | 1:B:210:MET:CE  | 2.65        | 0.45     |
| 1:E:371:ASN:OD1 | 1:E:371:ASN:C   | 2.55        | 0.45     |
| 1:F:60:ASP:N    | 1:F:60:ASP:OD2  | 2.49        | 0.45     |
| 1:B:546:ARG:NH2 | 1:C:15:ASN:CG   | 2.70        | 0.45     |
| 1:E:359:ASN:C   | 1:E:360:VAL:O   | 2.52        | 0.45     |
| 1:D:212:TRP:O   | 1:D:213:PHE:CG  | 2.70        | 0.45     |
| 1:B:358:ASN:O   | 1:B:358:ASN:CG  | 2.55        | 0.45     |
| 1:B:566:THR:C   | 1:B:568:VAL:N   | 2.67        | 0.44     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:D:202:ASP:OD2 | 1:D:274:SER:OG  | 2.35        | 0.44     |
| 1:D:286:TYR:C   | 1:D:286:TYR:CD2 | 2.90        | 0.44     |
| 1:C:542:MET:O   | 1:C:543:ASN:C   | 2.56        | 0.44     |
| 1:C:566:THR:C   | 1:C:568:VAL:N   | 2.68        | 0.44     |
| 1:B:525:TRP:CE3 | 1:B:554:ARG:NH1 | 2.85        | 0.44     |
| 1:E:276:GLN:O   | 1:E:277:LYS:C   | 2.56        | 0.44     |
| 1:E:220:LYS:O   | 1:E:221:GLU:C   | 2.54        | 0.44     |
| 1:F:529:LYS:O   | 1:F:530:GLY:C   | 2.55        | 0.44     |
| 1:A:566:THR:O   | 1:A:568:VAL:N   | 2.49        | 0.44     |
| 1:B:172:GLU:CD  | 1:B:212:TRP:CH2 | 2.90        | 0.44     |
| 1:C:529:LYS:O   | 1:C:530:GLY:O   | 2.35        | 0.44     |
| 1:F:127:VAL:CG2 | 1:F:528:PHE:CD1 | 2.99        | 0.44     |
| 1:E:75:ASN:N    | 1:E:75:ASN:OD1  | 2.48        | 0.44     |
| 1:D:127:VAL:CG2 | 1:D:528:PHE:CD1 | 3.00        | 0.44     |
| 1:D:79:VAL:CG1  | 1:D:81:TYR:CE2  | 3.00        | 0.44     |
| 1:A:299:ASN:N   | 1:A:299:ASN:ND2 | 2.65        | 0.44     |
| 1:A:516:ASP:OD2 | 1:A:517:ILE:N   | 2.50        | 0.44     |
| 1:A:75:ASN:N    | 1:A:75:ASN:OD1  | 2.50        | 0.44     |
| 1:A:75:ASN:OD1  | 1:A:76:TYR:N    | 2.51        | 0.44     |
| 1:D:509:ASP:O   | 1:D:510:TYR:C   | 2.56        | 0.44     |
| 1:D:359:ASN:O   | 1:D:360:VAL:C   | 2.56        | 0.44     |
| 1:E:158:MET:O   | 1:E:159:ARG:CD  | 2.66        | 0.44     |
| 1:C:491:ASP:O   | 1:C:494:ASN:N   | 2.51        | 0.44     |
| 1:D:37:PHE:CE1  | 1:D:40:HIS:O    | 2.71        | 0.43     |
| 1:D:566:THR:C   | 1:D:568:VAL:N   | 2.70        | 0.43     |
| 1:D:215:ASP:OD1 | 1:D:217:GLU:N   | 2.52        | 0.43     |
| 1:B:285:ASP:C   | 1:B:285:ASP:OD2 | 2.56        | 0.43     |
| 1:E:537:VAL:O   | 1:E:538:ASP:C   | 2.55        | 0.43     |
| 1:D:291:PHE:CD2 | 1:D:291:PHE:C   | 2.91        | 0.43     |
| 1:D:6:ILE:CG2   | 1:D:7:LYS:N     | 2.80        | 0.43     |
| 1:E:217:GLU:O   | 1:E:218:SER:C   | 2.54        | 0.43     |
| 1:C:359:ASN:O   | 1:C:360:VAL:C   | 2.55        | 0.43     |
| 1:A:487:ARG:O   | 1:F:356:ARG:NH2 | 2.51        | 0.43     |
| 1:F:511:SER:O   | 1:F:511:SER:OG  | 2.34        | 0.43     |
| 1:E:215:ASP:OD1 | 1:E:217:GLU:N   | 2.52        | 0.43     |
| 1:D:164:LYS:O   | 1:D:282:ILE:CD1 | 2.66        | 0.43     |
| 1:C:99:ASN:OD1  | 1:C:101:LYS:N   | 2.51        | 0.43     |
| 1:B:299:ASN:OD1 | 1:B:299:ASN:N   | 2.48        | 0.43     |
| 1:B:127:VAL:CG2 | 1:B:528:PHE:CD1 | 3.02        | 0.43     |
| 1:A:215:ASP:OD1 | 1:A:217:GLU:N   | 2.51        | 0.43     |
| 1:C:212:TRP:O   | 1:C:213:PHE:CG  | 2.71        | 0.43     |
| 1:E:538:ASP:O   | 1:E:541:HIS:N   | 2.52        | 0.43     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:F:42:PHE:CE1  | 1:F:59:ILE:CD1  | 3.02        | 0.43     |
| 1:F:498:LYS:O   | 1:F:499:TYR:C   | 2.55        | 0.43     |
| 1:D:23:PHE:CD2  | 1:D:23:PHE:N    | 2.86        | 0.43     |
| 1:D:59:ILE:CG2  | 1:D:59:ILE:O    | 2.66        | 0.43     |
| 1:D:220:LYS:O   | 1:D:221:GLU:C   | 2.57        | 0.43     |
| 1:E:491:ASP:O   | 1:E:494:ASN:N   | 2.51        | 0.43     |
| 1:A:127:VAL:CG2 | 1:A:528:PHE:CD1 | 3.01        | 0.43     |
| 1:A:496:VAL:O   | 1:A:497:LYS:C   | 2.56        | 0.43     |
| 1:E:60:ASP:N    | 1:E:60:ASP:OD2  | 2.52        | 0.43     |
| 1:B:175:LEU:O   | 1:B:211:TYR:N   | 2.52        | 0.43     |
| 1:A:371:ASN:OD1 | 1:A:371:ASN:C   | 2.54        | 0.43     |
| 1:F:286:TYR:CD2 | 1:F:286:TYR:C   | 2.92        | 0.42     |
| 1:F:560:SER:O   | 1:F:564:ASN:ND2 | 2.52        | 0.42     |
| 1:E:120:VAL:O   | 1:E:123:THR:OG1 | 2.37        | 0.42     |
| 1:E:296:ASN:OD1 | 1:E:298:ILE:N   | 2.52        | 0.42     |
| 1:D:365:ASP:OD1 | 1:E:314:THR:OG1 | 2.37        | 0.42     |
| 1:B:189:GLU:N   | 1:B:189:GLU:CD  | 2.73        | 0.42     |
| 1:A:291:PHE:C   | 1:A:291:PHE:CD2 | 2.92        | 0.42     |
| 1:A:112:VAL:CG2 | 1:A:548:LEU:CD1 | 2.97        | 0.42     |
| 1:E:511:SER:OG  | 1:E:511:SER:O   | 2.37        | 0.42     |
| 1:A:542:MET:O   | 1:A:546:ARG:N   | 2.53        | 0.42     |
| 1:C:538:ASP:O   | 1:C:541:HIS:N   | 2.52        | 0.42     |
| 1:C:470:TYR:CB  | 1:C:479:PHE:CE1 | 3.02        | 0.42     |
| 1:B:491:ASP:O   | 1:B:494:ASN:N   | 2.52        | 0.42     |
| 1:E:563:ILE:CD1 | 1:E:563:ILE:N   | 2.83        | 0.42     |
| 1:A:537:VAL:O   | 1:A:539:THR:N   | 2.52        | 0.42     |
| 1:A:538:ASP:O   | 1:A:541:HIS:N   | 2.53        | 0.42     |
| 1:A:277:LYS:O   | 1:A:336:SER:OG  | 2.37        | 0.42     |
| 1:A:112:VAL:O   | 1:A:116:THR:OG1 | 2.37        | 0.42     |
| 1:B:112:VAL:CG2 | 1:B:548:LEU:CD1 | 2.97        | 0.42     |
| 1:F:563:ILE:CD1 | 1:F:563:ILE:N   | 2.82        | 0.42     |
| 1:D:112:VAL:CG2 | 1:D:548:LEU:CD1 | 2.97        | 0.42     |
| 1:A:172:GLU:OE2 | 1:A:245:GLY:N   | 2.52        | 0.42     |
| 1:C:146:ILE:O   | 1:C:146:ILE:CD1 | 2.67        | 0.42     |
| 1:D:285:ASP:O   | 1:D:289:LEU:N   | 2.52        | 0.42     |
| 1:E:164:LYS:O   | 1:E:282:ILE:CD1 | 2.68        | 0.42     |
| 1:E:542:MET:O   | 1:E:546:ARG:N   | 2.52        | 0.42     |
| 1:C:491:ASP:O   | 1:C:492:GLU:C   | 2.58        | 0.42     |
| 1:E:127:VAL:CG2 | 1:E:528:PHE:CD1 | 3.03        | 0.42     |
| 1:B:296:ASN:OD1 | 1:B:298:ILE:N   | 2.52        | 0.42     |
| 1:D:60:ASP:OD2  | 1:D:60:ASP:N    | 2.52        | 0.42     |
| 1:A:99:ASN:OD1  | 1:A:101:LYS:N   | 2.52        | 0.42     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:F:538:ASP:O   | 1:F:541:HIS:N   | 2.52        | 0.42     |
| 1:F:571:VAL:CG1 | 1:F:572:ILE:N   | 2.79        | 0.42     |
| 1:F:224:ASP:O   | 1:F:227:THR:N   | 2.52        | 0.42     |
| 1:D:470:TYR:CB  | 1:D:479:PHE:CE1 | 3.02        | 0.42     |
| 1:B:42:PHE:CG   | 1:B:43:THR:N    | 2.85        | 0.42     |
| 1:B:539:THR:CG2 | 1:B:540:GLY:N   | 2.82        | 0.42     |
| 1:B:244:SER:O   | 1:B:245:GLY:C   | 2.58        | 0.42     |
| 1:A:356:ARG:NH2 | 1:B:487:ARG:O   | 2.52        | 0.42     |
| 1:A:254:ASP:O   | 1:A:255:HIS:C   | 2.57        | 0.42     |
| 1:C:215:ASP:OD1 | 1:C:217:GLU:N   | 2.53        | 0.42     |
| 1:F:542:MET:O   | 1:F:545:LEU:CB  | 2.68        | 0.42     |
| 1:B:359:ASN:O   | 1:B:360:VAL:C   | 2.58        | 0.42     |
| 1:A:157:THR:CG2 | 1:A:489:SER:N   | 2.82        | 0.42     |
| 1:D:359:ASN:C   | 1:D:360:VAL:O   | 2.58        | 0.42     |
| 1:C:112:VAL:O   | 1:C:116:THR:OG1 | 2.37        | 0.42     |
| 1:C:285:ASP:OD2 | 1:C:287:GLN:N   | 2.53        | 0.42     |
| 1:C:549:PHE:O   | 1:C:552:GLY:N   | 2.53        | 0.42     |
| 1:D:563:ILE:CD1 | 1:D:563:ILE:N   | 2.83        | 0.42     |
| 1:D:89:TYR:N    | 1:D:89:TYR:CD2  | 2.88        | 0.42     |
| 1:B:60:ASP:N    | 1:B:60:ASP:OD2  | 2.53        | 0.42     |
| 1:F:296:ASN:OD1 | 1:F:298:ILE:N   | 2.53        | 0.42     |
| 1:A:174:ILE:O   | 1:A:174:ILE:CD1 | 2.68        | 0.42     |
| 1:D:380:VAL:O   | 1:D:462:ALA:N   | 2.53        | 0.42     |
| 1:D:42:PHE:CE1  | 1:D:59:ILE:CD1  | 3.03        | 0.41     |
| 1:B:348:VAL:CG2 | 1:B:349:TYR:N   | 2.81        | 0.41     |
| 1:D:561:ASP:O   | 1:D:563:ILE:N   | 2.53        | 0.41     |
| 1:E:91:PHE:N    | 1:E:108:VAL:O   | 2.53        | 0.41     |
| 1:E:566:THR:C   | 1:E:568:VAL:N   | 2.70        | 0.41     |
| 1:A:563:ILE:C   | 1:A:564:ASN:ND2 | 2.74        | 0.41     |
| 1:A:172:GLU:OE1 | 1:A:212:TRP:CH2 | 2.73        | 0.41     |
| 1:E:531:ILE:CG2 | 1:E:531:ILE:O   | 2.68        | 0.41     |
| 1:A:130:ILE:O   | 1:A:131:ARG:CG  | 2.69        | 0.41     |
| 1:B:37:PHE:C    | 1:B:38:ASP:CG   | 2.79        | 0.41     |
| 1:C:542:MET:O   | 1:C:545:LEU:CB  | 2.69        | 0.41     |
| 1:F:470:TYR:CB  | 1:F:479:PHE:CE1 | 3.03        | 0.41     |
| 1:C:166:GLU:OE1 | 1:C:279:PHE:CA  | 2.68        | 0.41     |
| 1:F:146:ILE:CD1 | 1:F:146:ILE:O   | 2.69        | 0.41     |
| 1:F:371:ASN:OD1 | 1:F:371:ASN:C   | 2.57        | 0.41     |
| 1:C:224:ASP:O   | 1:C:227:THR:N   | 2.54        | 0.41     |
| 1:C:112:VAL:CG2 | 1:C:548:LEU:CD1 | 2.99        | 0.41     |
| 1:F:129:VAL:CG2 | 1:F:130:ILE:N   | 2.83        | 0.41     |
| 1:A:158:MET:O   | 1:A:159:ARG:CD  | 2.69        | 0.41     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 1:F:79:VAL:CG1  | 1:F:81:TYR:CE2  | 3.03        | 0.41     |
| 1:E:42:PHE:CE1  | 1:E:59:ILE:CD1  | 3.03        | 0.41     |
| 1:F:276:GLN:O   | 1:F:277:LYS:C   | 2.59        | 0.41     |
| 1:E:112:VAL:O   | 1:E:116:THR:OG1 | 2.38        | 0.41     |
| 1:A:511:SER:O   | 1:A:511:SER:OG  | 2.39        | 0.41     |
| 1:A:78:GLN:CG   | 1:A:79:VAL:N    | 2.83        | 0.41     |
| 1:E:134:TYR:OH  | 1:E:507:CYS:SG  | 2.79        | 0.41     |
| 1:D:324:ASP:C   | 1:D:324:ASP:OD1 | 2.59        | 0.41     |
| 1:E:285:ASP:O   | 1:E:289:LEU:N   | 2.54        | 0.41     |
| 1:A:572:ILE:O   | 1:A:573:ILE:CB  | 2.67        | 0.41     |
| 1:F:572:ILE:O   | 1:F:573:ILE:C   | 2.59        | 0.41     |
| 1:D:516:ASP:OD2 | 1:D:517:ILE:N   | 2.54        | 0.41     |
| 1:C:542:MET:O   | 1:C:546:ARG:N   | 2.54        | 0.41     |
| 1:E:224:ASP:C   | 1:E:226:LEU:N   | 2.73        | 0.41     |
| 1:A:146:ILE:CD1 | 1:A:146:ILE:O   | 2.69        | 0.41     |
| 1:C:189:GLU:N   | 1:C:189:GLU:CD  | 2.74        | 0.41     |
| 1:C:220:LYS:O   | 1:C:221:GLU:C   | 2.59        | 0.41     |
| 1:B:338:VAL:O   | 1:B:338:VAL:CG2 | 2.67        | 0.41     |
| 1:B:371:ASN:OD1 | 1:B:371:ASN:C   | 2.59        | 0.41     |
| 1:C:571:VAL:CG1 | 1:C:572:ILE:N   | 2.81        | 0.41     |
| 1:B:545:LEU:O   | 1:B:546:ARG:C   | 2.57        | 0.41     |
| 1:B:563:ILE:CD1 | 1:B:563:ILE:N   | 2.84        | 0.41     |
| 1:A:316:TYR:CE2 | 1:A:482:HIS:CD2 | 3.09        | 0.41     |
| 1:F:353:TYR:O   | 1:F:354:ASN:CB  | 2.67        | 0.41     |
| 1:A:220:LYS:O   | 1:A:221:GLU:C   | 2.57        | 0.40     |
| 1:C:89:TYR:N    | 1:C:89:TYR:CD2  | 2.89        | 0.40     |
| 1:D:75:ASN:N    | 1:D:75:ASN:OD1  | 2.53        | 0.40     |
| 1:E:348:VAL:CG2 | 1:E:349:TYR:N   | 2.82        | 0.40     |
| 1:E:148:SER:CB  | 1:F:156:SER:O   | 2.69        | 0.40     |
| 1:A:139:TYR:O   | 1:A:140:GLU:C   | 2.59        | 0.40     |
| 1:F:37:PHE:CE1  | 1:F:40:HIS:O    | 2.74        | 0.40     |
| 1:A:67:CYS:SG   | 1:A:68:PHE:N    | 2.94        | 0.40     |
| 1:A:189:GLU:CD  | 1:A:189:GLU:N   | 2.75        | 0.40     |
| 1:F:170:GLN:O   | 1:F:244:SER:CB  | 2.70        | 0.40     |
| 1:F:215:ASP:OD1 | 1:F:217:GLU:N   | 2.54        | 0.40     |
| 1:B:224:ASP:O   | 1:B:227:THR:N   | 2.54        | 0.40     |
| 1:F:212:TRP:O   | 1:F:213:PHE:CG  | 2.74        | 0.40     |
| 1:E:202:ASP:OD2 | 1:E:274:SER:OG  | 2.40        | 0.40     |
| 1:B:217:GLU:O   | 1:B:218:SER:C   | 2.60        | 0.40     |
| 1:B:130:ILE:O   | 1:B:131:ARG:CG  | 2.69        | 0.40     |
| 1:E:276:GLN:OE1 | 1:F:476:GLN:NE2 | 2.55        | 0.40     |
| 1:D:496:VAL:O   | 1:D:497:LYS:C   | 2.59        | 0.40     |

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| Atom-1        | Atom-2          | Distance(Å) | Clash(Å) |
|---------------|-----------------|-------------|----------|
| 1:B:71:LEU:O  | 1:B:71:LEU:CG   | 2.69        | 0.40     |
| 1:C:572:ILE:O | 1:C:573:ILE:C   | 2.58        | 0.40     |
| 1:C:541:HIS:O | 1:C:545:LEU:N   | 2.54        | 0.40     |
| 1:D:561:ASP:C | 1:D:563:ILE:N   | 2.74        | 0.40     |
| 1:F:566:THR:O | 1:F:569:ASN:N   | 2.55        | 0.40     |
| 1:E:563:ILE:C | 1:E:564:ASN:ND2 | 2.74        | 0.40     |
| 1:B:538:ASP:O | 1:B:540:GLY:N   | 2.54        | 0.40     |
| 1:B:359:ASN:C | 1:B:360:VAL:O   | 2.59        | 0.40     |
| 1:A:71:LEU:CG | 1:A:71:LEU:O    | 2.68        | 0.40     |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                 | Distance(Å) | Clash(Å) |
|---------------|------------------------|-------------|----------|
| 1:A:255:HIS:O | 1:B:291:PHE:CZ[2_665]  | 1.96        | 0.24     |
| 1:C:295:LEU:O | 1:F:65:ARG:NH2[1_556]  | 2.07        | 0.13     |
| 1:A:255:HIS:O | 1:B:291:PHE:CE2[2_665] | 2.09        | 0.11     |
| 1:A:255:HIS:C | 1:B:291:PHE:CZ[2_665]  | 2.19        | 0.01     |

## 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     | 482/583 (83%)   | 386 (80%)  | 82 (17%)  | 14 (3%)  | 7           | 35 |
| 1   | B     | 482/583 (83%)   | 390 (81%)  | 82 (17%)  | 10 (2%)  | 11          | 47 |
| 1   | C     | 482/583 (83%)   | 387 (80%)  | 86 (18%)  | 9 (2%)   | 12          | 51 |
| 1   | D     | 482/583 (83%)   | 388 (80%)  | 81 (17%)  | 13 (3%)  | 8           | 38 |
| 1   | E     | 482/583 (83%)   | 390 (81%)  | 85 (18%)  | 7 (2%)   | 15          | 58 |
| 1   | F     | 482/583 (83%)   | 387 (80%)  | 85 (18%)  | 10 (2%)  | 11          | 47 |
| All | All   | 2892/3498 (83%) | 2328 (80%) | 501 (17%) | 63 (2%)  | 10          | 45 |

All (63) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 258 | VAL  |
| 1   | A     | 530 | GLY  |
| 1   | A     | 539 | THR  |
| 1   | B     | 258 | VAL  |
| 1   | B     | 530 | GLY  |
| 1   | C     | 258 | VAL  |
| 1   | C     | 530 | GLY  |
| 1   | D     | 258 | VAL  |
| 1   | D     | 530 | GLY  |
| 1   | D     | 539 | THR  |
| 1   | E     | 258 | VAL  |
| 1   | E     | 530 | GLY  |
| 1   | E     | 539 | THR  |
| 1   | F     | 258 | VAL  |
| 1   | F     | 530 | GLY  |
| 1   | F     | 539 | THR  |
| 1   | A     | 68  | PHE  |
| 1   | A     | 233 | GLN  |
| 1   | A     | 255 | HIS  |
| 1   | B     | 68  | PHE  |
| 1   | B     | 539 | THR  |
| 1   | C     | 68  | PHE  |
| 1   | C     | 539 | THR  |
| 1   | D     | 68  | PHE  |
| 1   | E     | 68  | PHE  |
| 1   | F     | 68  | PHE  |
| 1   | A     | 36  | LYS  |
| 1   | D     | 550 | GLU  |
| 1   | F     | 567 | VAL  |
| 1   | A     | 546 | ARG  |
| 1   | A     | 567 | VAL  |
| 1   | B     | 304 | LEU  |
| 1   | A     | 39  | VAL  |
| 1   | A     | 360 | VAL  |
| 1   | A     | 538 | ASP  |
| 1   | B     | 39  | VAL  |
| 1   | B     | 277 | LYS  |
| 1   | B     | 567 | VAL  |
| 1   | C     | 567 | VAL  |
| 1   | D     | 250 | GLU  |
| 1   | D     | 567 | VAL  |
| 1   | F     | 233 | GLN  |
| 1   | F     | 304 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 260 | GLY  |
| 1   | B     | 36  | LYS  |
| 1   | C     | 39  | VAL  |
| 1   | D     | 39  | VAL  |
| 1   | D     | 371 | ASN  |
| 1   | D     | 542 | MET  |
| 1   | E     | 39  | VAL  |
| 1   | F     | 36  | LYS  |
| 1   | F     | 39  | VAL  |
| 1   | B     | 572 | ILE  |
| 1   | D     | 245 | GLY  |
| 1   | E     | 567 | VAL  |
| 1   | C     | 190 | LYS  |
| 1   | D     | 260 | GLY  |
| 1   | A     | 572 | ILE  |
| 1   | C     | 360 | VAL  |
| 1   | C     | 572 | ILE  |
| 1   | D     | 572 | ILE  |
| 1   | E     | 572 | ILE  |
| 1   | F     | 572 | ILE  |

### 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     | 446/529 (84%)   | 368 (82%)  | 78 (18%)  | 3           | 14 |
| 1   | B     | 446/529 (84%)   | 369 (83%)  | 77 (17%)  | 3           | 14 |
| 1   | C     | 446/529 (84%)   | 369 (83%)  | 77 (17%)  | 3           | 14 |
| 1   | D     | 446/529 (84%)   | 367 (82%)  | 79 (18%)  | 3           | 14 |
| 1   | E     | 446/529 (84%)   | 365 (82%)  | 81 (18%)  | 2           | 13 |
| 1   | F     | 446/529 (84%)   | 367 (82%)  | 79 (18%)  | 3           | 14 |
| All | All   | 2676/3174 (84%) | 2205 (82%) | 471 (18%) | 3           | 14 |

All (471) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | ASN  |
| 1   | A     | 18  | GLN  |
| 1   | A     | 23  | PHE  |
| 1   | A     | 38  | ASP  |
| 1   | A     | 46  | PHE  |
| 1   | A     | 48  | TYR  |
| 1   | A     | 55  | LEU  |
| 1   | A     | 57  | VAL  |
| 1   | A     | 58  | THR  |
| 1   | A     | 61  | LEU  |
| 1   | A     | 62  | VAL  |
| 1   | A     | 65  | ARG  |
| 1   | A     | 66  | SER  |
| 1   | A     | 69  | GLU  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 72  | MET  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 87  | VAL  |
| 1   | A     | 94  | ASP  |
| 1   | A     | 103 | CYS  |
| 1   | A     | 108 | VAL  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 129 | VAL  |
| 1   | A     | 135 | THR  |
| 1   | A     | 146 | ILE  |
| 1   | A     | 155 | THR  |
| 1   | A     | 157 | THR  |
| 1   | A     | 165 | SER  |
| 1   | A     | 174 | ILE  |
| 1   | A     | 176 | THR  |
| 1   | A     | 177 | ILE  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 189 | GLU  |
| 1   | A     | 199 | SER  |
| 1   | A     | 200 | THR  |
| 1   | A     | 204 | ILE  |
| 1   | A     | 206 | ASN  |
| 1   | A     | 210 | MET  |
| 1   | A     | 215 | ASP  |
| 1   | A     | 226 | LEU  |
| 1   | A     | 227 | THR  |
| 1   | A     | 229 | TYR  |
| 1   | A     | 239 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 249 | GLN  |
| 1   | A     | 263 | LEU  |
| 1   | A     | 267 | LYS  |
| 1   | A     | 274 | SER  |
| 1   | A     | 285 | ASP  |
| 1   | A     | 288 | SER  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 299 | ASN  |
| 1   | A     | 303 | LEU  |
| 1   | A     | 320 | ARG  |
| 1   | A     | 330 | THR  |
| 1   | A     | 338 | VAL  |
| 1   | A     | 350 | VAL  |
| 1   | A     | 358 | ASN  |
| 1   | A     | 359 | ASN  |
| 1   | A     | 360 | VAL  |
| 1   | A     | 365 | ASP  |
| 1   | A     | 369 | THR  |
| 1   | A     | 374 | ASP  |
| 1   | A     | 376 | ILE  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 491 | ASP  |
| 1   | A     | 513 | LYS  |
| 1   | A     | 514 | LEU  |
| 1   | A     | 518 | THR  |
| 1   | A     | 524 | ASN  |
| 1   | A     | 526 | VAL  |
| 1   | A     | 533 | THR  |
| 1   | A     | 539 | THR  |
| 1   | A     | 548 | LEU  |
| 1   | A     | 560 | SER  |
| 1   | A     | 563 | ILE  |
| 1   | A     | 568 | VAL  |
| 1   | A     | 571 | VAL  |
| 1   | A     | 573 | ILE  |
| 1   | B     | 16  | ASN  |
| 1   | B     | 18  | GLN  |
| 1   | B     | 23  | PHE  |
| 1   | B     | 26  | ASN  |
| 1   | B     | 38  | ASP  |
| 1   | B     | 46  | PHE  |
| 1   | B     | 48  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 55  | LEU  |
| 1   | B     | 57  | VAL  |
| 1   | B     | 58  | THR  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 62  | VAL  |
| 1   | B     | 65  | ARG  |
| 1   | B     | 69  | GLU  |
| 1   | B     | 71  | LEU  |
| 1   | B     | 72  | MET  |
| 1   | B     | 74  | VAL  |
| 1   | B     | 94  | ASP  |
| 1   | B     | 103 | CYS  |
| 1   | B     | 108 | VAL  |
| 1   | B     | 128 | ASN  |
| 1   | B     | 129 | VAL  |
| 1   | B     | 135 | THR  |
| 1   | B     | 146 | ILE  |
| 1   | B     | 155 | THR  |
| 1   | B     | 157 | THR  |
| 1   | B     | 165 | SER  |
| 1   | B     | 174 | ILE  |
| 1   | B     | 176 | THR  |
| 1   | B     | 177 | ILE  |
| 1   | B     | 182 | ARG  |
| 1   | B     | 189 | GLU  |
| 1   | B     | 199 | SER  |
| 1   | B     | 200 | THR  |
| 1   | B     | 204 | ILE  |
| 1   | B     | 206 | ASN  |
| 1   | B     | 208 | TYR  |
| 1   | B     | 210 | MET  |
| 1   | B     | 215 | ASP  |
| 1   | B     | 226 | LEU  |
| 1   | B     | 227 | THR  |
| 1   | B     | 229 | TYR  |
| 1   | B     | 239 | VAL  |
| 1   | B     | 249 | GLN  |
| 1   | B     | 263 | LEU  |
| 1   | B     | 267 | LYS  |
| 1   | B     | 274 | SER  |
| 1   | B     | 285 | ASP  |
| 1   | B     | 288 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 295 | LEU  |
| 1   | B     | 299 | ASN  |
| 1   | B     | 303 | LEU  |
| 1   | B     | 320 | ARG  |
| 1   | B     | 325 | LEU  |
| 1   | B     | 326 | SER  |
| 1   | B     | 330 | THR  |
| 1   | B     | 338 | VAL  |
| 1   | B     | 350 | VAL  |
| 1   | B     | 358 | ASN  |
| 1   | B     | 359 | ASN  |
| 1   | B     | 360 | VAL  |
| 1   | B     | 365 | ASP  |
| 1   | B     | 369 | THR  |
| 1   | B     | 374 | ASP  |
| 1   | B     | 376 | ILE  |
| 1   | B     | 463 | ILE  |
| 1   | B     | 491 | ASP  |
| 1   | B     | 513 | LYS  |
| 1   | B     | 514 | LEU  |
| 1   | B     | 524 | ASN  |
| 1   | B     | 526 | VAL  |
| 1   | B     | 533 | THR  |
| 1   | B     | 548 | LEU  |
| 1   | B     | 560 | SER  |
| 1   | B     | 563 | ILE  |
| 1   | B     | 571 | VAL  |
| 1   | B     | 573 | ILE  |
| 1   | C     | 16  | ASN  |
| 1   | C     | 18  | GLN  |
| 1   | C     | 23  | PHE  |
| 1   | C     | 38  | ASP  |
| 1   | C     | 46  | PHE  |
| 1   | C     | 48  | TYR  |
| 1   | C     | 55  | LEU  |
| 1   | C     | 57  | VAL  |
| 1   | C     | 58  | THR  |
| 1   | C     | 61  | LEU  |
| 1   | C     | 62  | VAL  |
| 1   | C     | 65  | ARG  |
| 1   | C     | 69  | GLU  |
| 1   | C     | 71  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 74  | VAL  |
| 1   | C     | 94  | ASP  |
| 1   | C     | 103 | CYS  |
| 1   | C     | 108 | VAL  |
| 1   | C     | 128 | ASN  |
| 1   | C     | 129 | VAL  |
| 1   | C     | 135 | THR  |
| 1   | C     | 146 | ILE  |
| 1   | C     | 155 | THR  |
| 1   | C     | 157 | THR  |
| 1   | C     | 165 | SER  |
| 1   | C     | 174 | ILE  |
| 1   | C     | 176 | THR  |
| 1   | C     | 177 | ILE  |
| 1   | C     | 182 | ARG  |
| 1   | C     | 189 | GLU  |
| 1   | C     | 199 | SER  |
| 1   | C     | 200 | THR  |
| 1   | C     | 204 | ILE  |
| 1   | C     | 206 | ASN  |
| 1   | C     | 210 | MET  |
| 1   | C     | 215 | ASP  |
| 1   | C     | 226 | LEU  |
| 1   | C     | 227 | THR  |
| 1   | C     | 229 | TYR  |
| 1   | C     | 239 | VAL  |
| 1   | C     | 263 | LEU  |
| 1   | C     | 267 | LYS  |
| 1   | C     | 274 | SER  |
| 1   | C     | 278 | ASP  |
| 1   | C     | 285 | ASP  |
| 1   | C     | 288 | SER  |
| 1   | C     | 295 | LEU  |
| 1   | C     | 299 | ASN  |
| 1   | C     | 303 | LEU  |
| 1   | C     | 320 | ARG  |
| 1   | C     | 325 | LEU  |
| 1   | C     | 326 | SER  |
| 1   | C     | 330 | THR  |
| 1   | C     | 338 | VAL  |
| 1   | C     | 348 | VAL  |
| 1   | C     | 350 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 358 | ASN  |
| 1   | C     | 359 | ASN  |
| 1   | C     | 360 | VAL  |
| 1   | C     | 365 | ASP  |
| 1   | C     | 369 | THR  |
| 1   | C     | 374 | ASP  |
| 1   | C     | 376 | ILE  |
| 1   | C     | 463 | ILE  |
| 1   | C     | 491 | ASP  |
| 1   | C     | 513 | LYS  |
| 1   | C     | 514 | LEU  |
| 1   | C     | 518 | THR  |
| 1   | C     | 524 | ASN  |
| 1   | C     | 526 | VAL  |
| 1   | C     | 533 | THR  |
| 1   | C     | 539 | THR  |
| 1   | C     | 548 | LEU  |
| 1   | C     | 560 | SER  |
| 1   | C     | 563 | ILE  |
| 1   | C     | 571 | VAL  |
| 1   | C     | 573 | ILE  |
| 1   | D     | 16  | ASN  |
| 1   | D     | 18  | GLN  |
| 1   | D     | 23  | PHE  |
| 1   | D     | 38  | ASP  |
| 1   | D     | 42  | PHE  |
| 1   | D     | 46  | PHE  |
| 1   | D     | 48  | TYR  |
| 1   | D     | 55  | LEU  |
| 1   | D     | 57  | VAL  |
| 1   | D     | 58  | THR  |
| 1   | D     | 61  | LEU  |
| 1   | D     | 62  | VAL  |
| 1   | D     | 65  | ARG  |
| 1   | D     | 69  | GLU  |
| 1   | D     | 71  | LEU  |
| 1   | D     | 72  | MET  |
| 1   | D     | 74  | VAL  |
| 1   | D     | 87  | VAL  |
| 1   | D     | 94  | ASP  |
| 1   | D     | 103 | CYS  |
| 1   | D     | 108 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 128 | ASN  |
| 1   | D     | 129 | VAL  |
| 1   | D     | 135 | THR  |
| 1   | D     | 146 | ILE  |
| 1   | D     | 155 | THR  |
| 1   | D     | 157 | THR  |
| 1   | D     | 165 | SER  |
| 1   | D     | 174 | ILE  |
| 1   | D     | 176 | THR  |
| 1   | D     | 177 | ILE  |
| 1   | D     | 182 | ARG  |
| 1   | D     | 189 | GLU  |
| 1   | D     | 199 | SER  |
| 1   | D     | 200 | THR  |
| 1   | D     | 204 | ILE  |
| 1   | D     | 206 | ASN  |
| 1   | D     | 210 | MET  |
| 1   | D     | 215 | ASP  |
| 1   | D     | 226 | LEU  |
| 1   | D     | 227 | THR  |
| 1   | D     | 229 | TYR  |
| 1   | D     | 239 | VAL  |
| 1   | D     | 263 | LEU  |
| 1   | D     | 267 | LYS  |
| 1   | D     | 274 | SER  |
| 1   | D     | 278 | ASP  |
| 1   | D     | 285 | ASP  |
| 1   | D     | 288 | SER  |
| 1   | D     | 295 | LEU  |
| 1   | D     | 299 | ASN  |
| 1   | D     | 303 | LEU  |
| 1   | D     | 320 | ARG  |
| 1   | D     | 325 | LEU  |
| 1   | D     | 330 | THR  |
| 1   | D     | 338 | VAL  |
| 1   | D     | 350 | VAL  |
| 1   | D     | 358 | ASN  |
| 1   | D     | 359 | ASN  |
| 1   | D     | 360 | VAL  |
| 1   | D     | 365 | ASP  |
| 1   | D     | 369 | THR  |
| 1   | D     | 374 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 376 | ILE  |
| 1   | D     | 463 | ILE  |
| 1   | D     | 513 | LYS  |
| 1   | D     | 514 | LEU  |
| 1   | D     | 518 | THR  |
| 1   | D     | 524 | ASN  |
| 1   | D     | 526 | VAL  |
| 1   | D     | 533 | THR  |
| 1   | D     | 539 | THR  |
| 1   | D     | 548 | LEU  |
| 1   | D     | 560 | SER  |
| 1   | D     | 563 | ILE  |
| 1   | D     | 566 | THR  |
| 1   | D     | 571 | VAL  |
| 1   | D     | 572 | ILE  |
| 1   | D     | 573 | ILE  |
| 1   | E     | 16  | ASN  |
| 1   | E     | 18  | GLN  |
| 1   | E     | 23  | PHE  |
| 1   | E     | 26  | ASN  |
| 1   | E     | 38  | ASP  |
| 1   | E     | 46  | PHE  |
| 1   | E     | 48  | TYR  |
| 1   | E     | 55  | LEU  |
| 1   | E     | 57  | VAL  |
| 1   | E     | 58  | THR  |
| 1   | E     | 61  | LEU  |
| 1   | E     | 62  | VAL  |
| 1   | E     | 65  | ARG  |
| 1   | E     | 69  | GLU  |
| 1   | E     | 71  | LEU  |
| 1   | E     | 72  | MET  |
| 1   | E     | 74  | VAL  |
| 1   | E     | 94  | ASP  |
| 1   | E     | 103 | CYS  |
| 1   | E     | 108 | VAL  |
| 1   | E     | 128 | ASN  |
| 1   | E     | 129 | VAL  |
| 1   | E     | 135 | THR  |
| 1   | E     | 146 | ILE  |
| 1   | E     | 155 | THR  |
| 1   | E     | 157 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 165 | SER  |
| 1   | E     | 174 | ILE  |
| 1   | E     | 176 | THR  |
| 1   | E     | 177 | ILE  |
| 1   | E     | 182 | ARG  |
| 1   | E     | 189 | GLU  |
| 1   | E     | 199 | SER  |
| 1   | E     | 200 | THR  |
| 1   | E     | 204 | ILE  |
| 1   | E     | 206 | ASN  |
| 1   | E     | 210 | MET  |
| 1   | E     | 215 | ASP  |
| 1   | E     | 226 | LEU  |
| 1   | E     | 227 | THR  |
| 1   | E     | 229 | TYR  |
| 1   | E     | 239 | VAL  |
| 1   | E     | 249 | GLN  |
| 1   | E     | 263 | LEU  |
| 1   | E     | 267 | LYS  |
| 1   | E     | 274 | SER  |
| 1   | E     | 278 | ASP  |
| 1   | E     | 285 | ASP  |
| 1   | E     | 288 | SER  |
| 1   | E     | 295 | LEU  |
| 1   | E     | 299 | ASN  |
| 1   | E     | 303 | LEU  |
| 1   | E     | 320 | ARG  |
| 1   | E     | 325 | LEU  |
| 1   | E     | 330 | THR  |
| 1   | E     | 338 | VAL  |
| 1   | E     | 350 | VAL  |
| 1   | E     | 358 | ASN  |
| 1   | E     | 359 | ASN  |
| 1   | E     | 360 | VAL  |
| 1   | E     | 365 | ASP  |
| 1   | E     | 369 | THR  |
| 1   | E     | 374 | ASP  |
| 1   | E     | 376 | ILE  |
| 1   | E     | 463 | ILE  |
| 1   | E     | 475 | LYS  |
| 1   | E     | 476 | GLN  |
| 1   | E     | 513 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 514 | LEU  |
| 1   | E     | 518 | THR  |
| 1   | E     | 524 | ASN  |
| 1   | E     | 526 | VAL  |
| 1   | E     | 533 | THR  |
| 1   | E     | 539 | THR  |
| 1   | E     | 548 | LEU  |
| 1   | E     | 560 | SER  |
| 1   | E     | 563 | ILE  |
| 1   | E     | 568 | VAL  |
| 1   | E     | 571 | VAL  |
| 1   | E     | 572 | ILE  |
| 1   | E     | 573 | ILE  |
| 1   | F     | 16  | ASN  |
| 1   | F     | 18  | GLN  |
| 1   | F     | 23  | PHE  |
| 1   | F     | 38  | ASP  |
| 1   | F     | 42  | PHE  |
| 1   | F     | 46  | PHE  |
| 1   | F     | 48  | TYR  |
| 1   | F     | 55  | LEU  |
| 1   | F     | 57  | VAL  |
| 1   | F     | 58  | THR  |
| 1   | F     | 61  | LEU  |
| 1   | F     | 62  | VAL  |
| 1   | F     | 65  | ARG  |
| 1   | F     | 69  | GLU  |
| 1   | F     | 71  | LEU  |
| 1   | F     | 72  | MET  |
| 1   | F     | 74  | VAL  |
| 1   | F     | 77  | CYS  |
| 1   | F     | 87  | VAL  |
| 1   | F     | 94  | ASP  |
| 1   | F     | 103 | CYS  |
| 1   | F     | 108 | VAL  |
| 1   | F     | 128 | ASN  |
| 1   | F     | 129 | VAL  |
| 1   | F     | 135 | THR  |
| 1   | F     | 146 | ILE  |
| 1   | F     | 155 | THR  |
| 1   | F     | 157 | THR  |
| 1   | F     | 165 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 174 | ILE  |
| 1   | F     | 176 | THR  |
| 1   | F     | 177 | ILE  |
| 1   | F     | 182 | ARG  |
| 1   | F     | 189 | GLU  |
| 1   | F     | 199 | SER  |
| 1   | F     | 200 | THR  |
| 1   | F     | 204 | ILE  |
| 1   | F     | 206 | ASN  |
| 1   | F     | 210 | MET  |
| 1   | F     | 215 | ASP  |
| 1   | F     | 226 | LEU  |
| 1   | F     | 227 | THR  |
| 1   | F     | 229 | TYR  |
| 1   | F     | 239 | VAL  |
| 1   | F     | 263 | LEU  |
| 1   | F     | 267 | LYS  |
| 1   | F     | 274 | SER  |
| 1   | F     | 285 | ASP  |
| 1   | F     | 288 | SER  |
| 1   | F     | 295 | LEU  |
| 1   | F     | 299 | ASN  |
| 1   | F     | 303 | LEU  |
| 1   | F     | 325 | LEU  |
| 1   | F     | 326 | SER  |
| 1   | F     | 330 | THR  |
| 1   | F     | 338 | VAL  |
| 1   | F     | 350 | VAL  |
| 1   | F     | 358 | ASN  |
| 1   | F     | 359 | ASN  |
| 1   | F     | 360 | VAL  |
| 1   | F     | 365 | ASP  |
| 1   | F     | 369 | THR  |
| 1   | F     | 374 | ASP  |
| 1   | F     | 376 | ILE  |
| 1   | F     | 463 | ILE  |
| 1   | F     | 475 | LYS  |
| 1   | F     | 491 | ASP  |
| 1   | F     | 513 | LYS  |
| 1   | F     | 514 | LEU  |
| 1   | F     | 518 | THR  |
| 1   | F     | 524 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 526 | VAL  |
| 1   | F     | 533 | THR  |
| 1   | F     | 539 | THR  |
| 1   | F     | 548 | LEU  |
| 1   | F     | 560 | SER  |
| 1   | F     | 563 | ILE  |
| 1   | F     | 571 | VAL  |
| 1   | F     | 573 | ILE  |

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------|-------|-----------------------|-------|
| 1   | A     | 488/583 (83%)   | -0.15  | 6 (1%)  | 75 20 | 48, 91, 189, 275      | 0     |
| 1   | B     | 488/583 (83%)   | -0.24  | 1 (0%)  | 93 54 | 50, 92, 180, 276      | 0     |
| 1   | C     | 488/583 (83%)   | -0.19  | 4 (0%)  | 83 26 | 58, 102, 192, 278     | 0     |
| 1   | D     | 488/583 (83%)   | -0.14  | 9 (1%)  | 65 14 | 65, 104, 205, 279     | 0     |
| 1   | E     | 488/583 (83%)   | -0.18  | 5 (1%)  | 79 22 | 58, 103, 198, 275     | 0     |
| 1   | F     | 488/583 (83%)   | -0.21  | 5 (1%)  | 79 22 | 52, 94, 194, 281      | 0     |
| All | All   | 2928/3498 (83%) | -0.18  | 30 (1%) | 79 22 | 48, 99, 194, 281      | 0     |

All (30) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 39  | VAL  | 6.0  |
| 1   | B     | 39  | VAL  | 5.3  |
| 1   | F     | 39  | VAL  | 4.8  |
| 1   | D     | 40  | HIS  | 4.3  |
| 1   | D     | 62  | VAL  | 4.0  |
| 1   | E     | 98  | LEU  | 4.0  |
| 1   | C     | 40  | HIS  | 3.9  |
| 1   | A     | 68  | PHE  | 3.9  |
| 1   | A     | 40  | HIS  | 3.5  |
| 1   | F     | 98  | LEU  | 3.4  |
| 1   | A     | 39  | VAL  | 3.4  |
| 1   | A     | 69  | GLU  | 3.0  |
| 1   | D     | 46  | PHE  | 2.9  |
| 1   | A     | 98  | LEU  | 2.8  |
| 1   | A     | 62  | VAL  | 2.7  |
| 1   | D     | 47  | ASN  | 2.6  |
| 1   | F     | 97  | GLN  | 2.5  |
| 1   | F     | 38  | ASP  | 2.4  |
| 1   | F     | 40  | HIS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 53  | GLY  | 2.3  |
| 1   | D     | 55  | LEU  | 2.3  |
| 1   | E     | 102 | VAL  | 2.3  |
| 1   | E     | 6   | ILE  | 2.3  |
| 1   | D     | 77  | CYS  | 2.2  |
| 1   | D     | 58  | THR  | 2.2  |
| 1   | D     | 6   | ILE  | 2.2  |
| 1   | C     | 53  | GLY  | 2.2  |
| 1   | C     | 67  | CYS  | 2.2  |
| 1   | D     | 39  | VAL  | 2.2  |
| 1   | E     | 97  | GLN  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.