



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:57 AM UTC

PDB ID : 1QX5 / pdb\_00001qx5  
Title : Crystal structure of apoCalmodulin  
Authors : Schumacher, M.A.; Crum, M.; Miller, M.C.  
Deposited on : 2003-09-04  
Resolution : 2.54 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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.49

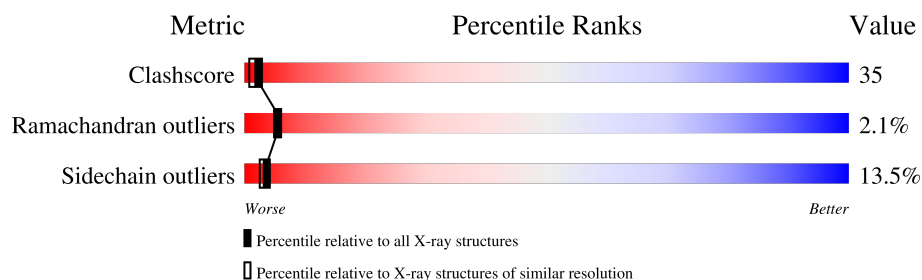
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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                      | 1120 (2.54-2.54)                                      |
| Ramachandran outliers | 187476                      | 1106 (2.54-2.54)                                      |
| Sidechain outliers    | 187428                      | 1106 (2.54-2.54)                                      |

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   | B     | 148    | 42% 45% 8% . .   |
| 1   | D     | 148    | 42% 44% 12% .    |
| 1   | I     | 148    | 45% 41% 11% . .  |
| 1   | J     | 148    | 45% 45% 7% . .   |
| 1   | K     | 148    | 45% 41% 9% . .   |
| 1   | R     | 148    | 46% 41% 10% . .  |
| 1   | T     | 148    | 47% 47% . .      |
| 1   | Y     | 148    | 43% 46% 9% .     |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9333 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 Calmodulin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | D     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 184 | 251 | 9 |         |         |       |
| 1   | I     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 184 | 251 | 9 |         |         |       |
| 1   | B     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 184 | 251 | 9 |         |         |       |
| 1   | J     | 144      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1138  | 698 | 183 | 248 | 9 |         |         |       |
| 1   | K     | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 693 | 181 | 246 | 9 |         |         |       |
| 1   | T     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 184 | 251 | 9 |         |         |       |
| 1   | R     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1161  | 711 | 187 | 254 | 9 |         |         |       |
| 1   | Y     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 184 | 251 | 9 |         |         |       |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | D     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 2   | I     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |
| 2   | B     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 2   | J     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 2   | K     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 2   | T     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |

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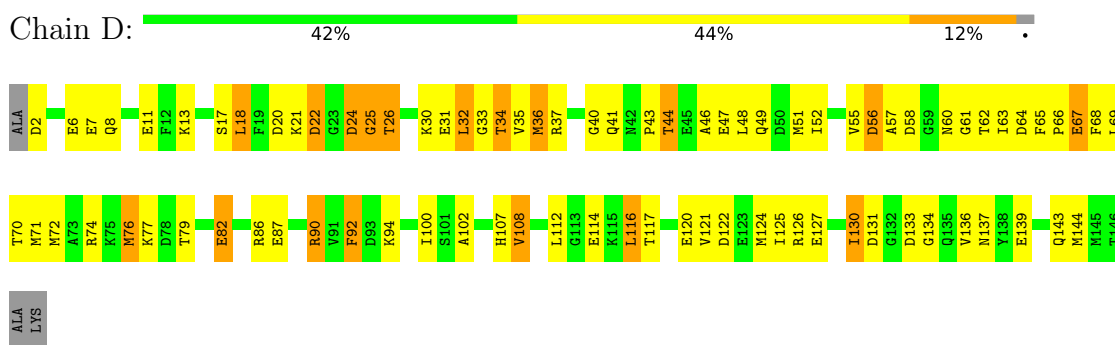
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | R     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |
| 2   | Y     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |

### 3 Residue-property plots

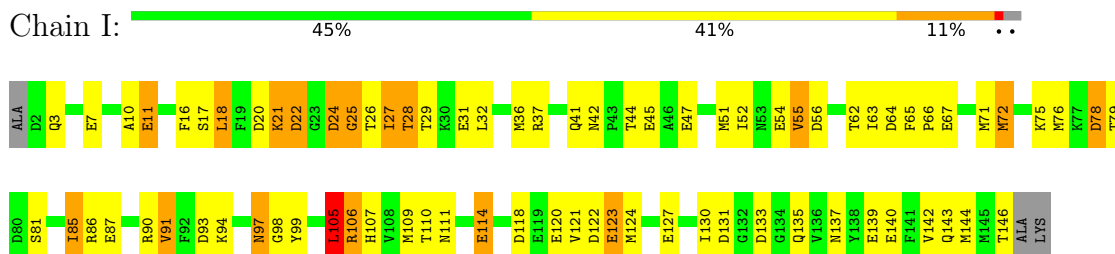
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

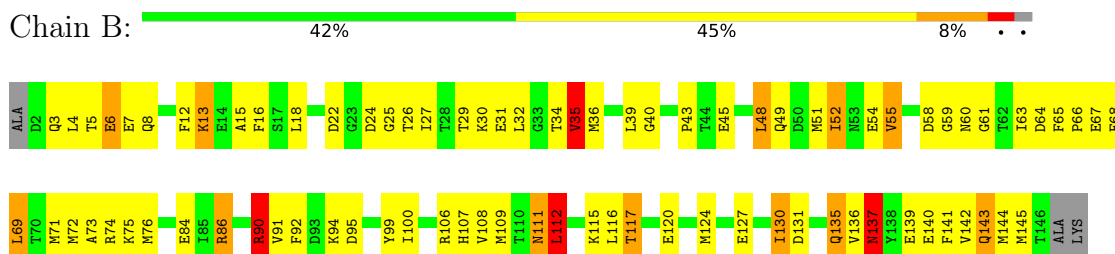
- Molecule 1: Calmodulin



- Molecule 1: Calmodulin

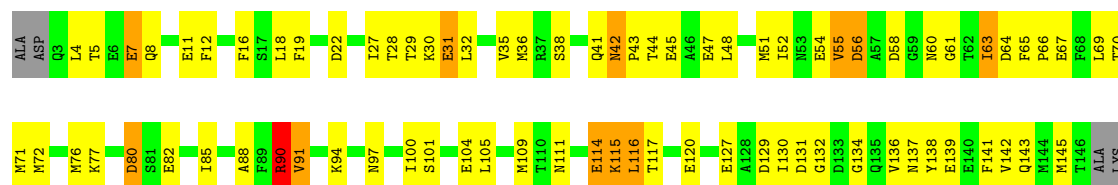


- Molecule 1: Calmodulin



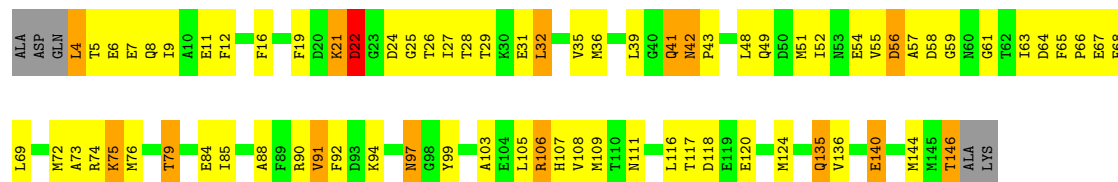
- Molecule 1: Calmodulin





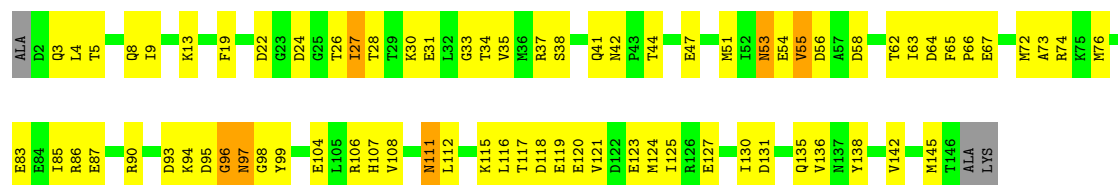
• Molecule 1: Calmodulin

Chain K: 45% 41% 9% . .



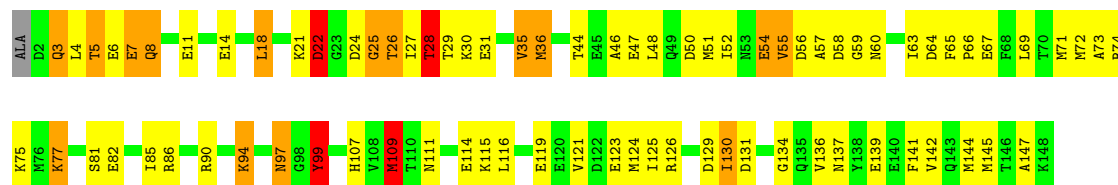
• Molecule 1: Calmodulin

Chain T: 47% 47% . .



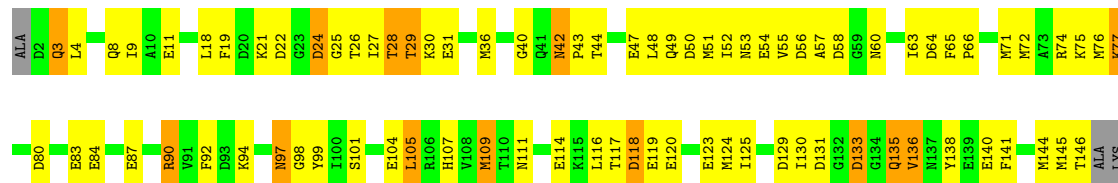
• Molecule 1: Calmodulin

Chain R: 46% 41% 10% . .



• Molecule 1: Calmodulin

Chain Y: 43% 46% 9% .



## 4 Data and refinement statistics

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

| Property                                                 | Value                                                      | Source    |
|----------------------------------------------------------|------------------------------------------------------------|-----------|
| Space group                                              | P 31                                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 146.00 Å   146.00 Å   78.00 Å<br>90.00°   90.00°   120.00° | Depositor |
| Resolution (Å)                                           | 66.39 – 2.54                                               | Depositor |
| % Data completeness<br>(in resolution range)             | 98.5 (66.39-2.54)                                          | Depositor |
| $R_{merge}$                                              | (Not available)                                            | Depositor |
| $R_{sym}$                                                | 0.05                                                       | Depositor |
| Refinement program                                       | CNS 1.0                                                    | Depositor |
| R, $R_{free}$                                            | 0.227 , 0.277                                              | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                     | Xtriage   |
| Total number of atoms                                    | 9333                                                       | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 70.0                                                       | wwPDB-VP  |

## 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   | B     | 1.07         | 3/1158 (0.3%)  | 1.16        | 6/1555 (0.4%)   |
| 1   | D     | 1.05         | 1/1158 (0.1%)  | 1.15        | 3/1555 (0.2%)   |
| 1   | I     | 1.28         | 5/1158 (0.4%)  | 1.36        | 7/1555 (0.5%)   |
| 1   | J     | 0.84         | 0/1150         | 0.96        | 2/1544 (0.1%)   |
| 1   | K     | 1.02         | 1/1141 (0.1%)  | 1.06        | 1/1532 (0.1%)   |
| 1   | R     | 1.21         | 6/1173 (0.5%)  | 1.24        | 5/1573 (0.3%)   |
| 1   | T     | 0.72         | 1/1158 (0.1%)  | 0.95        | 0/1555          |
| 1   | Y     | 1.00         | 1/1158 (0.1%)  | 1.13        | 1/1555 (0.1%)   |
| All | All   | 1.04         | 18/9254 (0.2%) | 1.14        | 25/12424 (0.2%) |

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   | D     | 0                   | 1                   |
| 1   | R     | 0                   | 1                   |
| 1   | Y     | 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   | R     | 109 | MET  | SD-CE | -10.35 | 1.53        | 1.79     |
| 1   | B     | 35  | VAL  | CA-CB | 9.49   | 1.66        | 1.54     |
| 1   | Y     | 109 | MET  | SD-CE | -8.44  | 1.58        | 1.79     |
| 1   | R     | 36  | MET  | SD-CE | 7.56   | 1.98        | 1.79     |
| 1   | I     | 27  | ILE  | CA-CB | 6.61   | 1.62        | 1.55     |
| 1   | B     | 15  | ALA  | CA-CB | 6.45   | 1.63        | 1.53     |
| 1   | I     | 87  | GLU  | C-O   | 6.22   | 1.31        | 1.24     |
| 1   | R     | 142 | VAL  | CA-CB | 6.21   | 1.61        | 1.54     |
| 1   | I     | 72  | MET  | SD-CE | 6.09   | 1.94        | 1.79     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | I     | 10  | ALA  | CA-CB | 6.01  | 1.62        | 1.53     |
| 1   | R     | 28  | THR  | CA-CB | -5.93 | 1.44        | 1.53     |
| 1   | D     | 36  | MET  | SD-CE | -5.91 | 1.64        | 1.79     |
| 1   | R     | 35  | VAL  | CA-CB | 5.63  | 1.60        | 1.54     |
| 1   | B     | 91  | VAL  | CA-C  | 5.58  | 1.60        | 1.52     |
| 1   | I     | 105 | LEU  | CA-C  | 5.55  | 1.59        | 1.52     |
| 1   | K     | 91  | VAL  | CA-C  | 5.33  | 1.59        | 1.52     |
| 1   | R     | 129 | ASP  | CA-C  | 5.06  | 1.59        | 1.53     |
| 1   | T     | 34  | THR  | CA-C  | 5.06  | 1.59        | 1.52     |

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | I     | 91  | VAL  | CB-CA-C | -7.81 | 100.05      | 112.16   |
| 1   | I     | 130 | ILE  | CB-CA-C | -7.13 | 101.22      | 110.98   |
| 1   | J     | 90  | ARG  | N-CA-C  | -6.50 | 103.46      | 111.33   |
| 1   | I     | 93  | ASP  | CA-C-N  | 6.30  | 128.73      | 120.28   |
| 1   | I     | 93  | ASP  | C-N-CA  | 6.30  | 128.73      | 120.28   |
| 1   | I     | 85  | ILE  | N-CA-C  | -6.24 | 104.67      | 110.53   |
| 1   | R     | 99  | TYR  | N-CA-C  | 5.91  | 119.03      | 109.40   |
| 1   | J     | 91  | VAL  | CB-CA-C | -5.89 | 104.32      | 112.04   |
| 1   | Y     | 133 | ASP  | N-CA-C  | -5.89 | 104.29      | 112.30   |
| 1   | B     | 90  | ARG  | N-CA-C  | -5.78 | 104.98      | 111.28   |
| 1   | B     | 86  | ARG  | N-CA-C  | -5.70 | 105.59      | 112.54   |
| 1   | R     | 30  | LYS  | N-CA-C  | -5.54 | 105.16      | 111.14   |
| 1   | I     | 121 | VAL  | N-CA-C  | -5.50 | 105.01      | 110.62   |
| 1   | I     | 94  | LYS  | N-CA-C  | 5.45  | 117.22      | 111.28   |
| 1   | R     | 94  | LYS  | N-CA-C  | 5.43  | 117.20      | 111.28   |
| 1   | K     | 140 | GLU  | N-CA-C  | -5.37 | 105.34      | 111.14   |
| 1   | D     | 40  | GLY  | CA-C-N  | -5.32 | 113.62      | 122.92   |
| 1   | D     | 40  | GLY  | C-N-CA  | -5.32 | 113.62      | 122.92   |
| 1   | D     | 32  | LEU  | N-CA-C  | -5.31 | 105.41      | 111.14   |
| 1   | B     | 137 | ASN  | N-CA-C  | -5.20 | 100.03      | 108.41   |
| 1   | B     | 90  | ARG  | N-CA-CB | 5.20  | 117.76      | 110.12   |
| 1   | B     | 6   | GLU  | N-CA-C  | -5.18 | 106.23      | 112.54   |
| 1   | B     | 112 | LEU  | N-CA-C  | -5.18 | 105.32      | 111.69   |
| 1   | R     | 54  | GLU  | N-CA-C  | -5.14 | 106.70      | 113.12   |
| 1   | R     | 6   | GLU  | N-CA-C  | -5.10 | 106.31      | 112.54   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 92  | PHE  | Sidechain |
| 1   | R     | 99  | TYR  | Sidechain |
| 1   | Y     | 138 | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1146  | 0        | 1070     | 97      | 0            |
| 1   | D     | 1146  | 0        | 1070     | 90      | 0            |
| 1   | I     | 1146  | 0        | 1070     | 68      | 0            |
| 1   | J     | 1138  | 0        | 1066     | 83      | 0            |
| 1   | K     | 1129  | 0        | 1058     | 102     | 0            |
| 1   | R     | 1161  | 0        | 1088     | 81      | 0            |
| 1   | T     | 1146  | 0        | 1070     | 81      | 0            |
| 1   | Y     | 1146  | 0        | 1070     | 76      | 0            |
| 2   | B     | 26    | 0        | 0        | 1       | 0            |
| 2   | D     | 24    | 0        | 0        | 2       | 0            |
| 2   | I     | 30    | 0        | 0        | 2       | 0            |
| 2   | J     | 15    | 0        | 0        | 2       | 0            |
| 2   | K     | 20    | 0        | 0        | 2       | 0            |
| 2   | R     | 30    | 0        | 0        | 1       | 0            |
| 2   | T     | 7     | 0        | 0        | 2       | 0            |
| 2   | Y     | 23    | 0        | 0        | 2       | 0            |
| All | All   | 9333  | 0        | 8562     | 628     | 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 35.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:94:LYS:HG3  | 1:K:94:LYS:HG2  | 1.39                     | 1.04              |
| 1:R:124:MET:HA  | 1:R:144:MET:HE1 | 1.40                     | 1.04              |
| 1:K:4:LEU:HD21  | 1:K:73:ALA:HA   | 1.39                     | 1.04              |
| 1:D:44:THR:HG21 | 1:I:131:ASP:OD2 | 1.59                     | 1.03              |
| 1:J:90:ARG:HG2  | 1:J:90:ARG:HH11 | 1.24                     | 1.01              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:Y:55:VAL:HG11  | 1:Y:63:ILE:HG23 | 1.42                     | 1.00              |
| 1:D:55:VAL:HG13  | 1:D:56:ASP:H    | 1.30                     | 0.93              |
| 1:Y:97:ASN:ND2   | 1:Y:99:TYR:H    | 1.67                     | 0.91              |
| 1:R:55:VAL:HG11  | 1:R:63:ILE:HG23 | 1.51                     | 0.90              |
| 1:B:29:THR:HG23  | 1:B:52:ILE:HG13 | 1.55                     | 0.88              |
| 1:I:28:THR:HG23  | 1:I:31:GLU:OE2  | 1.71                     | 0.88              |
| 1:B:5:THR:HG23   | 1:B:8:GLN:H     | 1.37                     | 0.88              |
| 1:B:137:ASN:HD21 | 1:B:139:GLU:HB2 | 1.38                     | 0.85              |
| 1:D:55:VAL:HG21  | 1:D:67:GLU:CD   | 2.01                     | 0.84              |
| 1:K:97:ASN:ND2   | 1:K:99:TYR:H    | 1.75                     | 0.84              |
| 1:K:28:THR:OG1   | 1:K:31:GLU:HG3  | 1.78                     | 0.84              |
| 1:R:5:THR:H      | 1:R:8:GLN:HG3   | 1.42                     | 0.84              |
| 1:K:97:ASN:ND2   | 2:K:164:HOH:O   | 2.11                     | 0.84              |
| 1:K:54:GLU:HG2   | 1:K:74:ARG:HH22 | 1.42                     | 0.84              |
| 1:B:94:LYS:HG3   | 1:K:94:LYS:CG   | 2.08                     | 0.83              |
| 1:B:4:LEU:HD21   | 1:B:73:ALA:HA   | 1.58                     | 0.83              |
| 1:B:31:GLU:O     | 1:B:35:VAL:HG12 | 1.78                     | 0.83              |
| 1:K:124:MET:HA   | 1:K:144:MET:HE1 | 1.61                     | 0.82              |
| 1:R:26:THR:HA    | 1:R:63:ILE:O    | 1.80                     | 0.82              |
| 1:T:55:VAL:HG11  | 1:T:63:ILE:HG13 | 1.59                     | 0.82              |
| 1:J:27:ILE:HB    | 1:J:31:GLU:HG3  | 1.62                     | 0.81              |
| 1:T:27:ILE:HG22  | 1:T:63:ILE:HG22 | 1.63                     | 0.79              |
| 1:D:124:MET:HA   | 1:D:144:MET:HE1 | 1.62                     | 0.79              |
| 1:T:116:LEU:HD21 | 1:T:124:MET:HE1 | 1.65                     | 0.79              |
| 1:B:94:LYS:CG    | 1:K:94:LYS:HG2  | 2.13                     | 0.79              |
| 1:I:97:ASN:ND2   | 2:I:171:HOH:O   | 2.17                     | 0.78              |
| 1:I:20:ASP:HA    | 1:I:21:LYS:NZ   | 1.99                     | 0.78              |
| 1:D:44:THR:CG2   | 1:I:131:ASP:OD2 | 2.32                     | 0.77              |
| 1:I:55:VAL:HG12  | 1:I:56:ASP:N    | 1.99                     | 0.77              |
| 1:J:44:THR:HB    | 1:J:47:GLU:HG3  | 1.67                     | 0.77              |
| 1:Y:48:LEU:HD23  | 1:Y:51:MET:HE3  | 1.66                     | 0.77              |
| 1:J:32:LEU:HD21  | 1:J:51:MET:HE3  | 1.66                     | 0.76              |
| 1:D:108:VAL:HG23 | 1:Y:109:MET:HE1 | 1.68                     | 0.76              |
| 1:I:91:VAL:O     | 1:R:94:LYS:HE2  | 1.85                     | 0.76              |
| 1:B:117:THR:HG23 | 1:B:120:GLU:OE1 | 1.87                     | 0.75              |
| 1:T:22:ASP:HB2   | 1:T:24:ASP:OD1  | 1.86                     | 0.75              |
| 1:B:68:PHE:HA    | 1:B:71:MET:HE3  | 1.68                     | 0.75              |
| 1:R:44:THR:HG22  | 1:R:47:GLU:HG3  | 1.66                     | 0.75              |
| 1:K:55:VAL:HG22  | 1:K:67:GLU:HB3  | 1.66                     | 0.75              |
| 1:D:76:MET:HE3   | 1:D:76:MET:HA   | 1.69                     | 0.74              |
| 1:B:94:LYS:HE2   | 1:K:94:LYS:HG2  | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:119:GLU:O    | 1:Y:123:GLU:HG3  | 1.86                     | 0.74              |
| 1:I:55:VAL:HG23  | 1:I:71:MET:HE1   | 1.70                     | 0.74              |
| 1:B:116:LEU:HD21 | 1:B:145:MET:SD   | 2.27                     | 0.74              |
| 1:D:36:MET:HE1   | 1:D:51:MET:HE1   | 1.69                     | 0.73              |
| 1:J:29:THR:HB    | 1:J:52:ILE:HD13  | 1.68                     | 0.73              |
| 1:K:140:GLU:O    | 1:K:144:MET:HG3  | 1.88                     | 0.73              |
| 1:Y:140:GLU:O    | 1:Y:144:MET:HG2  | 1.89                     | 0.73              |
| 1:I:24:ASP:CG    | 1:I:25:GLY:H     | 1.95                     | 0.73              |
| 1:K:124:MET:CA   | 1:K:144:MET:HE1  | 2.18                     | 0.73              |
| 1:J:7:GLU:HG2    | 1:J:8:GLN:N      | 2.03                     | 0.72              |
| 1:K:29:THR:HG23  | 1:K:52:ILE:HD12  | 1.70                     | 0.72              |
| 1:R:5:THR:OG1    | 1:R:7:GLU:HB3    | 1.89                     | 0.72              |
| 1:I:97:ASN:ND2   | 1:I:99:TYR:H     | 1.85                     | 0.72              |
| 1:J:90:ARG:NE    | 1:T:138:TYR:OH   | 2.23                     | 0.72              |
| 1:R:31:GLU:O     | 1:R:35:VAL:HG23  | 1.87                     | 0.72              |
| 1:Y:36:MET:HE2   | 1:Y:51:MET:HE1   | 1.70                     | 0.72              |
| 1:K:25:GLY:O     | 1:K:64:ASP:HA    | 1.89                     | 0.71              |
| 1:R:44:THR:HG21  | 1:Y:131:ASP:CG   | 2.15                     | 0.71              |
| 1:J:55:VAL:HG23  | 1:J:71:MET:HE1   | 1.72                     | 0.71              |
| 1:J:42:ASN:H     | 1:J:42:ASN:HD22  | 1.38                     | 0.71              |
| 1:I:22:ASP:HB2   | 1:I:24:ASP:OD1   | 1.90                     | 0.71              |
| 1:T:44:THR:HG23  | 1:T:47:GLU:OE1   | 1.91                     | 0.71              |
| 1:D:30:LYS:HE2   | 1:D:133:ASP:OD1  | 1.91                     | 0.70              |
| 1:B:131:ASP:OD2  | 1:J:44:THR:HG21  | 1.91                     | 0.70              |
| 1:B:137:ASN:ND2  | 1:B:139:GLU:HB2  | 2.07                     | 0.70              |
| 1:D:44:THR:HG22  | 1:D:47:GLU:H     | 1.55                     | 0.70              |
| 1:K:42:ASN:HD22  | 1:K:42:ASN:H     | 1.40                     | 0.70              |
| 1:D:24:ASP:O     | 1:D:26:THR:N     | 2.21                     | 0.70              |
| 1:R:44:THR:HG21  | 1:Y:131:ASP:OD1  | 1.92                     | 0.70              |
| 1:J:117:THR:OG1  | 1:J:120:GLU:HG3  | 1.91                     | 0.70              |
| 1:I:55:VAL:HG11  | 1:I:63:ILE:HG12  | 1.73                     | 0.70              |
| 1:B:130:ILE:HD12 | 1:B:136:VAL:CG2  | 2.22                     | 0.69              |
| 1:D:48:LEU:HA    | 1:D:51:MET:HE3   | 1.75                     | 0.69              |
| 1:B:130:ILE:HD12 | 1:B:136:VAL:HG21 | 1.74                     | 0.69              |
| 1:B:107:HIS:O    | 1:B:111:ASN:HB3  | 1.93                     | 0.69              |
| 1:K:64:ASP:HB2   | 1:K:67:GLU:HG3   | 1.73                     | 0.69              |
| 1:K:4:LEU:HA     | 1:K:8:GLN:OE1    | 1.93                     | 0.69              |
| 1:R:29:THR:OG1   | 1:R:52:ILE:HG13  | 1.93                     | 0.68              |
| 1:B:86:ARG:O     | 1:B:90:ARG:HG2   | 1.94                     | 0.68              |
| 1:B:109:MET:HE1  | 1:K:108:VAL:HG12 | 1.76                     | 0.68              |
| 1:R:119:GLU:O    | 1:R:123:GLU:HG3  | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:7:GLU:O      | 1:D:11:GLU:HG3   | 1.93                     | 0.68              |
| 1:D:55:VAL:HG13  | 1:D:56:ASP:N     | 2.07                     | 0.68              |
| 1:Y:72:MET:HE2   | 1:Y:72:MET:HA    | 1.75                     | 0.68              |
| 1:D:63:ILE:HD11  | 1:D:71:MET:HE1   | 1.75                     | 0.67              |
| 1:D:70:THR:O     | 1:D:74:ARG:HD3   | 1.94                     | 0.67              |
| 1:K:55:VAL:HG13  | 1:K:67:GLU:CD    | 2.19                     | 0.67              |
| 1:D:63:ILE:HG13  | 1:D:67:GLU:HG3   | 1.75                     | 0.67              |
| 1:B:5:THR:HG22   | 1:B:8:GLN:CD     | 2.18                     | 0.67              |
| 1:R:55:VAL:HG23  | 1:R:71:MET:HE1   | 1.76                     | 0.67              |
| 1:D:92:PHE:O     | 1:D:94:LYS:HD2   | 1.95                     | 0.67              |
| 1:B:108:VAL:HG12 | 1:B:109:MET:CE   | 2.24                     | 0.66              |
| 1:J:130:ILE:HG22 | 2:J:160:HOH:O    | 1.93                     | 0.66              |
| 1:D:34:THR:HB    | 2:D:155:HOH:O    | 1.94                     | 0.66              |
| 1:J:12:PHE:CE1   | 1:J:72:MET:HE3   | 2.31                     | 0.66              |
| 2:J:156:HOH:O    | 1:T:37:ARG:HD3   | 1.94                     | 0.66              |
| 1:T:97:ASN:H     | 1:T:97:ASN:HD22  | 1.44                     | 0.66              |
| 1:R:55:VAL:CG1   | 1:R:63:ILE:HG23  | 2.25                     | 0.66              |
| 1:K:124:MET:CB   | 1:K:144:MET:HE1  | 2.25                     | 0.65              |
| 1:J:90:ARG:HH11  | 1:J:90:ARG:CG    | 2.01                     | 0.65              |
| 1:T:26:THR:HA    | 1:T:63:ILE:O     | 1.97                     | 0.65              |
| 1:R:77:LYS:HA    | 1:R:77:LYS:NZ    | 2.11                     | 0.65              |
| 1:R:55:VAL:HG12  | 1:R:56:ASP:N     | 2.11                     | 0.65              |
| 1:T:33:GLY:O     | 1:T:37:ARG:HG2   | 1.97                     | 0.65              |
| 1:Y:71:MET:HE3   | 1:Y:72:MET:HE3   | 1.78                     | 0.65              |
| 1:T:93:ASP:OD1   | 1:T:93:ASP:C     | 2.39                     | 0.64              |
| 1:B:74:ARG:HB3   | 1:B:74:ARG:NH1   | 2.13                     | 0.64              |
| 1:K:4:LEU:HD11   | 1:K:73:ALA:HB2   | 1.80                     | 0.64              |
| 1:Y:131:ASP:HB2  | 1:Y:135:GLN:O    | 1.96                     | 0.64              |
| 1:I:20:ASP:HA    | 1:I:21:LYS:HZ1   | 1.61                     | 0.64              |
| 1:T:94:LYS:H     | 1:T:94:LYS:HD2   | 1.63                     | 0.64              |
| 1:D:48:LEU:HD23  | 1:D:51:MET:CE    | 2.28                     | 0.64              |
| 1:I:140:GLU:O    | 1:I:144:MET:HG3  | 1.98                     | 0.63              |
| 1:D:44:THR:HG22  | 1:D:46:ALA:H     | 1.63                     | 0.63              |
| 1:T:95:ASP:O     | 1:T:97:ASN:N     | 2.31                     | 0.63              |
| 1:R:48:LEU:HD23  | 1:R:51:MET:HE3   | 1.81                     | 0.63              |
| 1:T:130:ILE:HG12 | 1:T:136:VAL:HG22 | 1.81                     | 0.63              |
| 1:Y:120:GLU:O    | 1:Y:124:MET:HG3  | 1.97                     | 0.63              |
| 1:J:55:VAL:HG22  | 1:J:67:GLU:HB3   | 1.80                     | 0.63              |
| 1:J:54:GLU:CD    | 1:J:71:MET:HE2   | 2.24                     | 0.63              |
| 1:I:86:ARG:O     | 1:I:90:ARG:HG3   | 1.98                     | 0.63              |
| 1:I:91:VAL:O     | 1:I:91:VAL:HG12  | 1.97                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:130:ILE:N    | 1:R:130:ILE:HD12 | 2.14                     | 0.63              |
| 1:D:56:ASP:HB2   | 1:D:62:THR:O     | 1.99                     | 0.63              |
| 1:Y:97:ASN:C     | 1:Y:97:ASN:HD22  | 2.07                     | 0.63              |
| 1:R:18:LEU:HD11  | 1:R:125:ILE:HG21 | 1.81                     | 0.62              |
| 1:I:51:MET:O     | 1:I:54:GLU:HB3   | 1.99                     | 0.62              |
| 1:J:64:ASP:HB3   | 1:J:66:PRO:HD2   | 1.79                     | 0.62              |
| 1:K:65:PHE:HB3   | 1:K:66:PRO:HD3   | 1.82                     | 0.62              |
| 1:R:44:THR:HG23  | 1:R:46:ALA:H     | 1.65                     | 0.62              |
| 1:B:92:PHE:HB2   | 1:B:100:ILE:HG21 | 1.82                     | 0.62              |
| 1:B:139:GLU:OE1  | 1:B:142:VAL:HG11 | 2.00                     | 0.62              |
| 1:I:110:THR:O    | 1:I:114:GLU:HB3  | 2.00                     | 0.61              |
| 1:R:27:ILE:O     | 1:R:63:ILE:HD12  | 2.00                     | 0.61              |
| 1:B:22:ASP:HB2   | 1:B:24:ASP:OD1   | 2.00                     | 0.61              |
| 1:Y:72:MET:O     | 1:Y:76:MET:HB2   | 2.00                     | 0.61              |
| 1:D:21:LYS:HD3   | 1:D:22:ASP:H     | 1.64                     | 0.61              |
| 1:T:86:ARG:HD2   | 1:T:90:ARG:NH2   | 2.15                     | 0.61              |
| 1:T:104:GLU:O    | 1:T:108:VAL:HG23 | 2.01                     | 0.61              |
| 1:J:54:GLU:OE2   | 1:J:71:MET:HE2   | 2.00                     | 0.60              |
| 1:K:54:GLU:HG2   | 1:K:74:ARG:NH2   | 2.14                     | 0.60              |
| 1:K:107:HIS:O    | 1:K:111:ASN:HB3  | 2.01                     | 0.60              |
| 1:R:97:ASN:ND2   | 1:R:99:TYR:H     | 1.98                     | 0.60              |
| 1:I:97:ASN:C     | 1:I:97:ASN:HD22  | 2.08                     | 0.60              |
| 1:R:28:THR:HG23  | 1:R:31:GLU:OE1   | 2.02                     | 0.60              |
| 1:R:130:ILE:HG22 | 1:R:131:ASP:N    | 2.15                     | 0.60              |
| 1:Y:64:ASP:HB3   | 1:Y:66:PRO:HD2   | 1.83                     | 0.60              |
| 1:D:120:GLU:O    | 1:D:124:MET:HG3  | 2.00                     | 0.60              |
| 1:B:139:GLU:HA   | 1:B:142:VAL:HG12 | 1.83                     | 0.60              |
| 1:T:28:THR:HG22  | 1:T:30:LYS:H     | 1.66                     | 0.60              |
| 1:I:41:GLN:OE1   | 1:I:79:THR:HG21  | 2.02                     | 0.60              |
| 1:I:97:ASN:HD22  | 1:I:98:GLY:N     | 1.99                     | 0.60              |
| 1:R:5:THR:N      | 1:R:8:GLN:HG3    | 2.14                     | 0.59              |
| 1:Y:48:LEU:O     | 1:Y:52:ILE:HG13  | 2.02                     | 0.59              |
| 1:J:94:LYS:HG3   | 1:T:94:LYS:HG3   | 1.85                     | 0.59              |
| 1:Y:56:ASP:OD1   | 1:Y:60:ASN:HB2   | 2.01                     | 0.59              |
| 1:R:77:LYS:HA    | 1:R:77:LYS:HZ3   | 1.68                     | 0.59              |
| 1:I:64:ASP:HB3   | 1:I:66:PRO:HD2   | 1.84                     | 0.59              |
| 1:Y:87:GLU:OE2   | 1:Y:90:ARG:NH1   | 2.35                     | 0.59              |
| 1:D:55:VAL:HG21  | 1:D:67:GLU:OE1   | 2.02                     | 0.59              |
| 1:K:29:THR:HG23  | 1:K:52:ILE:CD1   | 2.32                     | 0.59              |
| 1:B:65:PHE:HB3   | 1:B:66:PRO:HD3   | 1.85                     | 0.59              |
| 1:K:116:LEU:HD22 | 1:K:124:MET:HE2  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:27:ILE:HG22  | 1:T:63:ILE:CG2   | 2.32                     | 0.59              |
| 1:K:90:ARG:HG2   | 1:K:90:ARG:HH11  | 1.67                     | 0.59              |
| 1:I:97:ASN:ND2   | 1:I:97:ASN:C     | 2.60                     | 0.58              |
| 1:I:106:ARG:HD2  | 1:I:106:ARG:C    | 2.28                     | 0.58              |
| 1:K:12:PHE:CZ    | 1:K:76:MET:HG3   | 2.38                     | 0.58              |
| 1:T:64:ASP:HB3   | 1:T:66:PRO:HD2   | 1.86                     | 0.58              |
| 1:R:77:LYS:N     | 1:R:77:LYS:HD2   | 2.19                     | 0.58              |
| 1:T:28:THR:HB    | 1:T:31:GLU:HG3   | 1.86                     | 0.58              |
| 1:T:107:HIS:O    | 1:T:111:ASN:HB3  | 2.04                     | 0.58              |
| 1:I:55:VAL:HG12  | 1:I:56:ASP:H     | 1.65                     | 0.58              |
| 1:B:109:MET:HE2  | 1:B:109:MET:HA   | 1.83                     | 0.58              |
| 1:B:115:LYS:HD2  | 1:K:85:ILE:HD11  | 1.86                     | 0.58              |
| 1:D:63:ILE:CD1   | 1:D:71:MET:HE1   | 2.34                     | 0.58              |
| 1:B:5:THR:HG22   | 1:B:8:GLN:NE2    | 2.18                     | 0.58              |
| 1:T:27:ILE:HG23  | 1:T:28:THR:N     | 2.19                     | 0.58              |
| 1:D:21:LYS:HD2   | 1:D:31:GLU:OE1   | 2.03                     | 0.58              |
| 1:K:117:THR:OG1  | 1:K:120:GLU:HG3  | 2.04                     | 0.57              |
| 1:Y:56:ASP:C     | 1:Y:58:ASP:H     | 2.12                     | 0.57              |
| 1:Y:97:ASN:HD22  | 1:Y:98:GLY:N     | 2.01                     | 0.57              |
| 1:B:43:PRO:HB2   | 1:B:48:LEU:HD13  | 1.84                     | 0.57              |
| 1:B:115:LYS:CD   | 1:K:85:ILE:HD11  | 2.35                     | 0.57              |
| 1:T:64:ASP:HB2   | 1:T:67:GLU:HG3   | 1.85                     | 0.57              |
| 1:Y:26:THR:HG22  | 1:Y:64:ASP:OD1   | 2.04                     | 0.57              |
| 1:D:32:LEU:HG    | 1:D:36:MET:HE2   | 1.86                     | 0.57              |
| 1:D:130:ILE:HB   | 1:D:136:VAL:HG22 | 1.87                     | 0.57              |
| 1:I:146:THR:HG21 | 1:R:82:GLU:HG3   | 1.87                     | 0.57              |
| 1:J:137:ASN:ND2  | 1:J:139:GLU:HB2  | 2.19                     | 0.57              |
| 1:B:24:ASP:OD2   | 1:B:26:THR:HB    | 2.04                     | 0.57              |
| 1:B:40:GLY:HA2   | 1:K:107:HIS:CD2  | 2.39                     | 0.57              |
| 1:Y:28:THR:HG23  | 1:Y:31:GLU:OE1   | 2.03                     | 0.57              |
| 1:J:55:VAL:HG13  | 1:J:67:GLU:CD    | 2.29                     | 0.57              |
| 1:I:32:LEU:HD22  | 1:I:52:ILE:CD1   | 2.35                     | 0.56              |
| 1:D:44:THR:CG2   | 1:D:46:ALA:H     | 2.19                     | 0.56              |
| 1:D:63:ILE:HD11  | 1:D:71:MET:CE    | 2.35                     | 0.56              |
| 1:B:108:VAL:HG12 | 1:B:109:MET:HE2  | 1.87                     | 0.56              |
| 1:B:112:LEU:HD13 | 1:K:109:MET:HE2  | 1.86                     | 0.56              |
| 1:K:49:GLN:C     | 1:K:51:MET:H     | 2.12                     | 0.56              |
| 1:R:29:THR:HA    | 1:R:52:ILE:HD11  | 1.86                     | 0.56              |
| 1:I:85:ILE:HD11  | 1:R:115:LYS:HD2  | 1.88                     | 0.56              |
| 1:T:28:THR:HB    | 1:T:31:GLU:CG    | 2.35                     | 0.56              |
| 1:R:44:THR:HG21  | 1:Y:131:ASP:OD2  | 2.04                     | 0.56              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:124:MET:HG2  | 1:K:144:MET:CE  | 2.36                     | 0.56              |
| 1:D:48:LEU:HD23  | 1:D:51:MET:HE3  | 1.87                     | 0.56              |
| 1:J:27:ILE:HG13  | 1:J:63:ILE:HG23 | 1.87                     | 0.56              |
| 1:I:131:ASP:OD1  | 1:I:133:ASP:N   | 2.38                     | 0.56              |
| 1:K:55:VAL:C     | 1:K:57:ALA:H    | 2.13                     | 0.56              |
| 1:K:56:ASP:C     | 1:K:58:ASP:H    | 2.14                     | 0.55              |
| 1:Y:43:PRO:HB2   | 1:Y:48:LEU:HG   | 1.88                     | 0.55              |
| 1:D:87:GLU:OE1   | 2:D:164:HOH:O   | 2.18                     | 0.55              |
| 1:I:24:ASP:CG    | 1:I:25:GLY:N    | 2.64                     | 0.55              |
| 1:J:111:ASN:ND2  | 1:J:115:LYS:HE3 | 2.21                     | 0.55              |
| 1:K:4:LEU:N      | 1:K:4:LEU:HD23  | 2.21                     | 0.55              |
| 1:T:117:THR:O    | 1:T:120:GLU:N   | 2.39                     | 0.55              |
| 1:Y:44:THR:OG1   | 1:Y:47:GLU:HG3  | 2.06                     | 0.55              |
| 1:J:28:THR:O     | 1:J:31:GLU:HG2  | 2.07                     | 0.55              |
| 1:J:29:THR:O     | 1:J:52:ILE:HD11 | 2.07                     | 0.55              |
| 1:D:56:ASP:OD1   | 1:D:60:ASN:HB3  | 2.06                     | 0.55              |
| 1:K:55:VAL:HG21  | 1:K:63:ILE:HD12 | 1.88                     | 0.55              |
| 1:Y:26:THR:HA    | 1:Y:63:ILE:O    | 2.07                     | 0.55              |
| 1:B:112:LEU:CD1  | 1:K:109:MET:HE2 | 2.36                     | 0.55              |
| 1:D:56:ASP:CG    | 1:D:61:GLY:H    | 2.15                     | 0.55              |
| 1:B:36:MET:HE1   | 1:B:51:MET:SD   | 2.47                     | 0.55              |
| 1:K:117:THR:O    | 1:K:118:ASP:C   | 2.50                     | 0.55              |
| 1:I:55:VAL:HG13  | 1:I:67:GLU:CD   | 2.32                     | 0.55              |
| 1:B:13:LYS:HA    | 1:B:65:PHE:CE1  | 2.42                     | 0.55              |
| 1:J:55:VAL:HG23  | 1:J:71:MET:CE   | 2.35                     | 0.55              |
| 1:K:19:PHE:HD2   | 1:K:35:VAL:HG22 | 1.72                     | 0.55              |
| 1:B:13:LYS:HA    | 1:B:65:PHE:HE1  | 1.72                     | 0.54              |
| 1:J:137:ASN:HD21 | 1:J:139:GLU:HB2 | 1.71                     | 0.54              |
| 1:T:119:GLU:O    | 1:T:123:GLU:HB2 | 2.07                     | 0.54              |
| 1:Y:42:ASN:H     | 1:Y:42:ASN:HD22 | 1.55                     | 0.54              |
| 1:D:32:LEU:HG    | 1:D:36:MET:CE   | 2.38                     | 0.54              |
| 1:T:116:LEU:HD11 | 1:T:145:MET:SD  | 2.47                     | 0.54              |
| 1:D:76:MET:HA    | 1:D:76:MET:CE   | 2.37                     | 0.54              |
| 1:J:36:MET:HE2   | 1:J:51:MET:SD   | 2.47                     | 0.54              |
| 1:T:97:ASN:ND2   | 1:T:99:TYR:H    | 2.04                     | 0.54              |
| 1:R:97:ASN:ND2   | 2:R:158:HOH:O   | 2.39                     | 0.54              |
| 1:J:64:ASP:CB    | 1:J:66:PRO:HD2  | 2.37                     | 0.54              |
| 1:Y:97:ASN:HD22  | 1:Y:99:TYR:H    | 1.52                     | 0.54              |
| 1:D:41:GLN:O     | 1:D:43:PRO:HD3  | 2.08                     | 0.54              |
| 1:I:20:ASP:HA    | 1:I:21:LYS:HZ3  | 1.73                     | 0.54              |
| 1:K:55:VAL:HG11  | 1:K:63:ILE:CB   | 2.38                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:97:ASN:ND2   | 2:T:154:HOH:O    | 2.32                     | 0.54              |
| 1:J:55:VAL:HG12  | 1:J:56:ASP:N     | 2.22                     | 0.53              |
| 1:T:115:LYS:O    | 1:T:116:LEU:HD12 | 2.08                     | 0.53              |
| 1:Y:97:ASN:ND2   | 1:Y:97:ASN:C     | 2.65                     | 0.53              |
| 1:Y:97:ASN:ND2   | 2:Y:163:HOH:O    | 2.40                     | 0.53              |
| 1:K:91:VAL:HG12  | 1:K:91:VAL:O     | 2.08                     | 0.53              |
| 1:R:109:MET:HA   | 1:R:109:MET:CE   | 2.39                     | 0.53              |
| 1:Y:117:THR:OG1  | 1:Y:120:GLU:HG3  | 2.07                     | 0.53              |
| 1:D:44:THR:HG22  | 1:D:46:ALA:N     | 2.23                     | 0.53              |
| 1:I:105:LEU:HD22 | 1:I:109:MET:HG2  | 1.91                     | 0.53              |
| 1:K:7:GLU:O      | 1:K:11:GLU:HG3   | 2.08                     | 0.53              |
| 1:I:120:GLU:O    | 1:I:124:MET:HG3  | 2.09                     | 0.53              |
| 1:B:32:LEU:HG    | 1:B:36:MET:HE2   | 1.90                     | 0.53              |
| 1:B:140:GLU:O    | 1:B:144:MET:HG3  | 2.08                     | 0.53              |
| 1:J:138:TYR:CE2  | 1:T:98:GLY:HA2   | 2.44                     | 0.53              |
| 1:T:115:LYS:C    | 1:T:116:LEU:HD12 | 2.34                     | 0.53              |
| 1:I:72:MET:HE2   | 1:I:72:MET:HA    | 1.90                     | 0.53              |
| 1:K:72:MET:HE2   | 1:K:72:MET:HA    | 1.91                     | 0.53              |
| 1:T:97:ASN:H     | 1:T:97:ASN:ND2   | 2.07                     | 0.53              |
| 1:D:41:GLN:O     | 1:D:41:GLN:HG3   | 2.08                     | 0.52              |
| 1:I:51:MET:HE2   | 1:I:75:LYS:HE3   | 1.91                     | 0.52              |
| 1:I:51:MET:HE2   | 1:I:75:LYS:CE    | 2.40                     | 0.52              |
| 1:J:114:GLU:C    | 1:J:116:LEU:H    | 2.16                     | 0.52              |
| 1:Y:28:THR:HG23  | 1:Y:31:GLU:CD    | 2.34                     | 0.52              |
| 1:Y:77:LYS:HA    | 1:Y:77:LYS:NZ    | 2.23                     | 0.52              |
| 1:I:26:THR:HA    | 1:I:63:ILE:O     | 2.09                     | 0.52              |
| 1:B:117:THR:OG1  | 1:B:120:GLU:HB2  | 2.09                     | 0.52              |
| 1:D:122:ASP:O    | 1:D:126:ARG:HG3  | 2.10                     | 0.52              |
| 1:K:36:MET:O     | 1:K:39:LEU:HB2   | 2.09                     | 0.52              |
| 1:D:48:LEU:HA    | 1:D:51:MET:CE    | 2.39                     | 0.52              |
| 1:T:93:ASP:OD1   | 1:T:93:ASP:O     | 2.28                     | 0.52              |
| 1:D:44:THR:HG23  | 2:I:156:HOH:O    | 2.08                     | 0.52              |
| 1:D:76:MET:HE2   | 1:D:79:THR:HB    | 1.91                     | 0.52              |
| 1:D:108:VAL:CG2  | 1:Y:109:MET:HE1  | 2.38                     | 0.52              |
| 1:B:94:LYS:HE2   | 1:K:94:LYS:CG    | 2.39                     | 0.52              |
| 1:J:136:VAL:HG21 | 1:J:141:PHE:HE1  | 1.75                     | 0.52              |
| 1:R:44:THR:HG23  | 1:R:46:ALA:N     | 2.24                     | 0.52              |
| 1:R:124:MET:HA   | 1:R:144:MET:CE   | 2.28                     | 0.52              |
| 1:Y:49:GLN:HA    | 1:Y:52:ILE:HD12  | 1.92                     | 0.52              |
| 1:D:47:GLU:O     | 1:D:51:MET:HG3   | 2.09                     | 0.52              |
| 1:R:44:THR:HG22  | 1:R:47:GLU:H     | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:18:LEU:HD12  | 1:Y:19:PHE:CE2   | 2.44                     | 0.52              |
| 1:Y:47:GLU:O     | 1:Y:51:MET:HG3   | 2.10                     | 0.52              |
| 1:Y:71:MET:O     | 1:Y:74:ARG:HG2   | 2.10                     | 0.52              |
| 1:D:82:GLU:HB2   | 1:Y:146:THR:HG21 | 1.92                     | 0.51              |
| 1:T:72:MET:HA    | 1:T:72:MET:HE2   | 1.91                     | 0.51              |
| 1:D:116:LEU:O    | 1:D:116:LEU:HD23 | 2.10                     | 0.51              |
| 1:J:48:LEU:HD23  | 1:J:51:MET:HE2   | 1.92                     | 0.51              |
| 1:J:117:THR:HG23 | 1:J:120:GLU:OE1  | 2.10                     | 0.51              |
| 1:Y:53:ASN:HA    | 1:Y:57:ALA:HB2   | 1.93                     | 0.51              |
| 1:J:65:PHE:N     | 1:J:66:PRO:CD    | 2.74                     | 0.51              |
| 1:J:90:ARG:CG    | 1:J:90:ARG:NH1   | 2.67                     | 0.51              |
| 1:J:100:ILE:O    | 1:T:135:GLN:HA   | 2.11                     | 0.51              |
| 1:Y:94:LYS:N     | 1:Y:94:LYS:HD2   | 2.26                     | 0.51              |
| 1:J:80:ASP:OD2   | 1:J:82:GLU:HB3   | 2.10                     | 0.51              |
| 1:K:74:ARG:HB2   | 1:K:75:LYS:NZ    | 2.25                     | 0.51              |
| 1:J:90:ARG:HG2   | 1:J:90:ARG:NH1   | 2.04                     | 0.51              |
| 1:R:29:THR:HG23  | 1:R:52:ILE:HG13  | 1.91                     | 0.51              |
| 1:K:16:PHE:HD1   | 1:K:68:PHE:CD1   | 2.29                     | 0.51              |
| 1:K:55:VAL:HG11  | 1:K:63:ILE:CG1   | 2.40                     | 0.51              |
| 1:T:19:PHE:HD2   | 1:T:35:VAL:HG22  | 1.76                     | 0.51              |
| 1:R:48:LEU:HA    | 1:R:51:MET:HE3   | 1.93                     | 0.51              |
| 1:Y:18:LEU:HD11  | 1:Y:125:ILE:HG21 | 1.93                     | 0.51              |
| 1:J:29:THR:HG23  | 1:J:61:GLY:C     | 2.35                     | 0.51              |
| 1:D:64:ASP:OD1   | 1:D:66:PRO:HD2   | 2.11                     | 0.50              |
| 1:B:95:ASP:OD2   | 1:B:95:ASP:N     | 2.44                     | 0.50              |
| 1:K:28:THR:HG23  | 1:K:31:GLU:OE1   | 2.10                     | 0.50              |
| 1:Y:44:THR:HG23  | 1:Y:47:GLU:OE2   | 2.11                     | 0.50              |
| 1:B:5:THR:HG22   | 1:B:8:GLN:CG     | 2.42                     | 0.50              |
| 1:J:76:MET:HE2   | 1:J:76:MET:HA    | 1.93                     | 0.50              |
| 1:I:97:ASN:HD21  | 1:I:99:TYR:HB2   | 1.76                     | 0.50              |
| 1:K:146:THR:CG2  | 1:K:146:THR:O    | 2.59                     | 0.50              |
| 1:T:51:MET:O     | 1:T:55:VAL:HG23  | 2.11                     | 0.50              |
| 1:Y:42:ASN:O     | 1:Y:42:ASN:ND2   | 2.44                     | 0.50              |
| 1:T:97:ASN:HD22  | 1:T:97:ASN:N     | 2.06                     | 0.50              |
| 1:T:121:VAL:O    | 1:T:125:ILE:HG13 | 2.12                     | 0.50              |
| 1:D:24:ASP:OD2   | 1:D:26:THR:HG23  | 2.10                     | 0.50              |
| 1:D:112:LEU:O    | 1:D:116:LEU:HD22 | 2.11                     | 0.50              |
| 1:I:105:LEU:CD2  | 1:I:109:MET:HG2  | 2.42                     | 0.50              |
| 1:R:58:ASP:OD1   | 1:R:60:ASN:HB2   | 2.10                     | 0.50              |
| 1:Y:48:LEU:HA    | 1:Y:51:MET:HE3   | 1.93                     | 0.50              |
| 1:R:97:ASN:HD22  | 1:R:97:ASN:H     | 1.60                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:29:THR:CG2   | 1:R:52:ILE:HG13  | 2.42                     | 0.49              |
| 1:B:135:GLN:HG2  | 2:K:159:HOH:O    | 2.12                     | 0.49              |
| 1:J:36:MET:HE2   | 1:J:51:MET:HE1   | 1.94                     | 0.49              |
| 1:T:5:THR:O      | 1:T:9:ILE:HG13   | 2.12                     | 0.49              |
| 1:R:25:GLY:O     | 1:R:64:ASP:HA    | 2.12                     | 0.49              |
| 1:Y:116:LEU:HD21 | 1:Y:145:MET:SD   | 2.52                     | 0.49              |
| 1:J:116:LEU:HD13 | 1:J:120:GLU:HB2  | 1.94                     | 0.49              |
| 1:J:130:ILE:HG23 | 1:J:130:ILE:O    | 2.12                     | 0.49              |
| 1:R:130:ILE:HD12 | 1:R:130:ILE:H    | 1.75                     | 0.49              |
| 1:Y:18:LEU:HD12  | 1:Y:19:PHE:CZ    | 2.47                     | 0.49              |
| 1:B:135:GLN:HG3  | 1:K:99:TYR:HB3   | 1.94                     | 0.49              |
| 1:K:55:VAL:HG13  | 1:K:67:GLU:OE1   | 2.13                     | 0.49              |
| 1:Y:8:GLN:O      | 1:Y:9:ILE:C      | 2.52                     | 0.49              |
| 1:J:142:VAL:HG13 | 1:J:143:GLN:N    | 2.27                     | 0.49              |
| 1:T:125:ILE:HG23 | 1:T:130:ILE:HD11 | 1.93                     | 0.49              |
| 1:R:44:THR:HG22  | 1:R:47:GLU:CG    | 2.38                     | 0.49              |
| 1:B:5:THR:CG2    | 1:B:8:GLN:H      | 2.19                     | 0.49              |
| 1:K:12:PHE:HZ    | 1:K:76:MET:HG3   | 1.78                     | 0.49              |
| 1:R:107:HIS:ND1  | 1:R:111:ASN:ND2  | 2.41                     | 0.49              |
| 1:B:58:ASP:C     | 1:B:60:ASN:H     | 2.20                     | 0.49              |
| 1:B:141:PHE:O    | 1:B:145:MET:HG3  | 2.13                     | 0.49              |
| 1:J:109:MET:HE2  | 1:T:112:LEU:HG   | 1.94                     | 0.49              |
| 1:K:55:VAL:HG11  | 1:K:63:ILE:HB    | 1.94                     | 0.49              |
| 1:R:130:ILE:HG13 | 1:R:136:VAL:CG2  | 2.43                     | 0.49              |
| 1:Y:107:HIS:O    | 1:Y:111:ASN:HB2  | 2.12                     | 0.49              |
| 1:B:65:PHE:CZ    | 1:B:69:LEU:HG    | 2.48                     | 0.49              |
| 1:B:108:VAL:HG12 | 1:B:109:MET:HE3  | 1.94                     | 0.49              |
| 1:T:117:THR:H    | 1:T:120:GLU:HB2  | 1.78                     | 0.49              |
| 1:B:99:TYR:HB3   | 1:K:135:GLN:HG3  | 1.95                     | 0.48              |
| 1:J:139:GLU:O    | 1:J:142:VAL:HG12 | 2.13                     | 0.48              |
| 1:K:74:ARG:HB2   | 1:K:75:LYS:HZ2   | 1.77                     | 0.48              |
| 1:K:91:VAL:O     | 1:K:91:VAL:CG1   | 2.61                     | 0.48              |
| 1:Y:125:ILE:HG23 | 1:Y:130:ILE:HD11 | 1.94                     | 0.48              |
| 1:J:16:PHE:C     | 1:J:16:PHE:CD2   | 2.92                     | 0.48              |
| 1:K:48:LEU:O     | 1:K:52:ILE:HG12  | 2.13                     | 0.48              |
| 1:B:51:MET:HE1   | 1:B:75:LYS:HE3   | 1.94                     | 0.48              |
| 1:B:3:GLN:HE21   | 1:B:4:LEU:H      | 1.62                     | 0.48              |
| 1:Y:53:ASN:CA    | 1:Y:57:ALA:HB2   | 2.43                     | 0.48              |
| 1:R:64:ASP:HB3   | 1:R:66:PRO:HD2   | 1.94                     | 0.48              |
| 1:I:118:ASP:OD1  | 1:I:118:ASP:C    | 2.56                     | 0.48              |
| 1:K:28:THR:HG1   | 1:K:31:GLU:HG3   | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:123:GLU:O    | 1:I:127:GLU:HG2  | 2.14                     | 0.48              |
| 1:Y:71:MET:CE    | 1:Y:72:MET:HE3   | 2.43                     | 0.48              |
| 1:B:40:GLY:HA2   | 1:K:107:HIS:NE2  | 2.29                     | 0.47              |
| 1:B:145:MET:CE   | 1:K:85:ILE:HD12  | 2.44                     | 0.47              |
| 1:K:5:THR:O      | 1:K:6:GLU:C      | 2.57                     | 0.47              |
| 1:R:65:PHE:HB3   | 1:R:66:PRO:HD3   | 1.96                     | 0.47              |
| 1:J:36:MET:HE3   | 1:J:43:PRO:HG3   | 1.96                     | 0.47              |
| 1:T:111:ASN:C    | 1:T:111:ASN:HD22 | 2.22                     | 0.47              |
| 1:I:76:MET:C     | 1:I:78:ASP:H     | 2.22                     | 0.47              |
| 1:D:22:ASP:HB3   | 1:D:24:ASP:OD1   | 2.14                     | 0.47              |
| 1:D:64:ASP:O     | 1:D:67:GLU:HG2   | 2.15                     | 0.47              |
| 1:D:86:ARG:HD3   | 1:D:90:ARG:NH1   | 2.29                     | 0.47              |
| 1:R:74:ARG:HG3   | 1:R:75:LYS:N     | 2.29                     | 0.47              |
| 1:R:130:ILE:CG2  | 1:R:134:GLY:HA2  | 2.45                     | 0.47              |
| 1:Y:3:GLN:CD     | 1:Y:3:GLN:N      | 2.72                     | 0.47              |
| 1:D:30:LYS:HE2   | 1:D:133:ASP:CG   | 2.39                     | 0.47              |
| 1:D:116:LEU:HD23 | 1:D:116:LEU:C    | 2.37                     | 0.47              |
| 1:R:3:GLN:HE21   | 1:R:3:GLN:HB2    | 1.51                     | 0.47              |
| 1:D:64:ASP:CG    | 1:D:66:PRO:HD2   | 2.39                     | 0.47              |
| 1:B:111:ASN:O    | 1:B:115:LYS:HG3  | 2.15                     | 0.47              |
| 1:T:31:GLU:O     | 1:T:35:VAL:HG23  | 2.15                     | 0.47              |
| 1:R:126:ARG:HG2  | 1:R:126:ARG:HH11 | 1.80                     | 0.47              |
| 1:D:36:MET:HE1   | 1:D:48:LEU:CD2   | 2.44                     | 0.47              |
| 1:I:91:VAL:O     | 1:I:91:VAL:CG1   | 2.63                     | 0.47              |
| 1:B:137:ASN:ND2  | 1:B:139:GLU:H    | 2.12                     | 0.47              |
| 1:R:72:MET:HE2   | 1:R:72:MET:HA    | 1.96                     | 0.47              |
| 1:D:130:ILE:HD11 | 1:D:134:GLY:HA2  | 1.96                     | 0.47              |
| 1:B:111:ASN:C    | 1:B:111:ASN:HD22 | 2.22                     | 0.47              |
| 1:D:137:ASN:OD1  | 1:D:139:GLU:HB2  | 2.14                     | 0.46              |
| 1:I:44:THR:OG1   | 1:I:47:GLU:HG3   | 2.14                     | 0.46              |
| 1:I:131:ASP:OD2  | 1:I:135:GLN:HB2  | 2.15                     | 0.46              |
| 1:I:142:VAL:O    | 1:I:146:THR:HG23 | 2.15                     | 0.46              |
| 1:B:58:ASP:C     | 1:B:60:ASN:N     | 2.71                     | 0.46              |
| 1:J:116:LEU:CD1  | 1:J:120:GLU:HB2  | 2.45                     | 0.46              |
| 1:D:36:MET:HE1   | 1:D:48:LEU:HD23  | 1.96                     | 0.46              |
| 1:B:76:MET:HE2   | 1:B:76:MET:N     | 2.31                     | 0.46              |
| 1:T:130:ILE:HG22 | 1:T:131:ASP:N    | 2.31                     | 0.46              |
| 1:R:71:MET:HE3   | 1:R:71:MET:HB2   | 1.69                     | 0.46              |
| 1:D:102:ALA:HB2  | 1:Y:136:VAL:CG2  | 2.45                     | 0.46              |
| 1:K:52:ILE:CG2   | 1:K:56:ASP:HB3   | 2.45                     | 0.46              |
| 1:K:117:THR:HG23 | 1:K:120:GLU:OE2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:22:ASP:HB2   | 1:Y:24:ASP:OD2   | 2.15                     | 0.46              |
| 1:B:74:ARG:HH11  | 1:B:74:ARG:CB    | 2.28                     | 0.46              |
| 1:K:49:GLN:C     | 1:K:51:MET:N     | 2.72                     | 0.46              |
| 1:R:18:LEU:HD11  | 1:R:125:ILE:CG2  | 2.44                     | 0.46              |
| 1:R:55:VAL:HG13  | 1:R:67:GLU:CD    | 2.40                     | 0.46              |
| 1:Y:117:THR:HG23 | 1:Y:120:GLU:OE2  | 2.15                     | 0.46              |
| 1:D:8:GLN:NE2    | 1:D:76:MET:HG2   | 2.30                     | 0.46              |
| 1:I:107:HIS:O    | 1:I:111:ASN:HB3  | 2.14                     | 0.46              |
| 1:I:131:ASP:OD1  | 1:I:131:ASP:C    | 2.59                     | 0.46              |
| 1:B:115:LYS:HD2  | 1:K:85:ILE:CD1   | 2.46                     | 0.46              |
| 1:J:22:ASP:OD1   | 1:J:22:ASP:N     | 2.49                     | 0.46              |
| 1:J:88:ALA:HB1   | 1:T:112:LEU:HD22 | 1.96                     | 0.46              |
| 1:K:97:ASN:OD1   | 1:K:99:TYR:HB2   | 2.16                     | 0.46              |
| 1:D:127:GLU:CD   | 1:D:144:MET:HE3  | 2.40                     | 0.46              |
| 1:Y:27:ILE:O     | 1:Y:27:ILE:HG13  | 2.16                     | 0.46              |
| 1:J:42:ASN:ND2   | 1:J:42:ASN:O     | 2.49                     | 0.46              |
| 1:R:14:GLU:O     | 1:R:18:LEU:HB2   | 2.16                     | 0.46              |
| 1:R:86:ARG:HD2   | 1:R:90:ARG:NH2   | 2.30                     | 0.46              |
| 1:Y:129:ASP:N    | 1:Y:129:ASP:OD2  | 2.46                     | 0.46              |
| 1:D:13:LYS:HA    | 1:D:65:PHE:CE1   | 2.51                     | 0.46              |
| 1:D:117:THR:OG1  | 1:D:120:GLU:HG3  | 2.16                     | 0.46              |
| 1:D:130:ILE:HD13 | 1:D:130:ILE:O    | 2.16                     | 0.46              |
| 1:J:91:VAL:O     | 1:J:91:VAL:HG12  | 2.16                     | 0.46              |
| 1:R:130:ILE:CG2  | 1:R:131:ASP:N    | 2.79                     | 0.46              |
| 1:D:116:LEU:N    | 1:D:116:LEU:CD2  | 2.78                     | 0.46              |
| 1:J:32:LEU:CD2   | 1:J:51:MET:HE3   | 2.41                     | 0.46              |
| 1:K:52:ILE:O     | 1:K:52:ILE:HG22  | 2.16                     | 0.46              |
| 1:R:4:LEU:HD11   | 1:R:73:ALA:HA    | 1.99                     | 0.45              |
| 1:R:121:VAL:O    | 1:R:125:ILE:HG13 | 2.16                     | 0.45              |
| 1:R:137:ASN:OD1  | 1:R:139:GLU:HB2  | 2.16                     | 0.45              |
| 1:Y:24:ASP:CG    | 1:Y:25:GLY:H     | 2.25                     | 0.45              |
| 1:D:64:ASP:OD1   | 1:D:67:GLU:HG2   | 2.17                     | 0.45              |
| 1:K:21:LYS:HG3   | 1:K:22:ASP:H     | 1.81                     | 0.45              |
| 1:J:101:SER:HB3  | 1:J:104:GLU:HB2  | 1.99                     | 0.45              |
| 1:K:124:MET:CG   | 1:K:144:MET:CE   | 2.93                     | 0.45              |
| 1:T:54:GLU:HG2   | 1:T:74:ARG:HH22  | 1.82                     | 0.45              |
| 1:B:36:MET:HE3   | 1:B:48:LEU:HD11  | 1.97                     | 0.45              |
| 1:Y:92:PHE:O     | 1:Y:94:LYS:HD2   | 2.16                     | 0.45              |
| 1:B:59:GLY:C     | 1:B:61:GLY:H     | 2.24                     | 0.45              |
| 1:R:145:MET:HE2  | 1:R:145:MET:HB3  | 1.77                     | 0.45              |
| 1:B:12:PHE:CE2   | 1:B:72:MET:HB3   | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:141:PHE:HD2  | 1:Y:144:MET:HE3  | 1.81                     | 0.45              |
| 1:R:27:ILE:HG13  | 1:R:63:ILE:HD13  | 1.99                     | 0.45              |
| 1:D:2:ASP:HB3    | 1:D:77:LYS:NZ    | 2.32                     | 0.45              |
| 1:I:27:ILE:HB    | 1:I:31:GLU:HB2   | 1.99                     | 0.45              |
| 1:I:142:VAL:HG11 | 1:R:86:ARG:NH1   | 2.32                     | 0.45              |
| 1:B:64:ASP:OD1   | 1:B:67:GLU:HG3   | 2.17                     | 0.45              |
| 1:J:105:LEU:HD12 | 1:J:109:MET:HG2  | 1.99                     | 0.45              |
| 1:K:64:ASP:HB3   | 1:K:66:PRO:HD2   | 1.98                     | 0.45              |
| 1:K:88:ALA:O     | 1:K:91:VAL:HB    | 2.17                     | 0.45              |
| 1:Y:42:ASN:HD22  | 1:Y:42:ASN:N     | 2.11                     | 0.45              |
| 1:I:37:ARG:HA    | 1:I:41:GLN:O     | 2.17                     | 0.45              |
| 1:I:55:VAL:HG21  | 1:I:63:ILE:CD1   | 2.46                     | 0.45              |
| 1:J:137:ASN:HA   | 1:T:98:GLY:O     | 2.17                     | 0.45              |
| 1:R:109:MET:HA   | 1:R:109:MET:HE2  | 1.97                     | 0.45              |
| 1:R:81:SER:O     | 1:R:85:ILE:HG13  | 2.18                     | 0.44              |
| 1:Y:56:ASP:C     | 1:Y:58:ASP:N     | 2.73                     | 0.44              |
| 1:I:11:GLU:OE2   | 1:I:11:GLU:HA    | 2.17                     | 0.44              |
| 1:I:29:THR:OG1   | 1:I:52:ILE:HG12  | 2.16                     | 0.44              |
| 1:J:28:THR:C     | 1:J:30:LYS:N     | 2.73                     | 0.44              |
| 1:T:28:THR:H     | 1:T:31:GLU:HB2   | 1.82                     | 0.44              |
| 1:K:55:VAL:HG11  | 1:K:63:ILE:HG13  | 1.98                     | 0.44              |
| 1:T:93:ASP:OD2   | 1:T:97:ASN:ND2   | 2.50                     | 0.44              |
| 1:D:13:LYS:HD2   | 1:D:65:PHE:CE1   | 2.53                     | 0.44              |
| 1:B:30:LYS:HA    | 1:B:30:LYS:HD3   | 1.84                     | 0.44              |
| 1:J:31:GLU:HG2   | 1:J:31:GLU:H     | 1.50                     | 0.44              |
| 1:J:85:ILE:HG22  | 1:T:142:VAL:HG22 | 2.00                     | 0.44              |
| 1:B:63:ILE:HD12  | 1:B:71:MET:CE    | 2.48                     | 0.44              |
| 1:K:42:ASN:HD22  | 1:K:42:ASN:N     | 2.10                     | 0.44              |
| 1:D:18:LEU:HD23  | 1:D:18:LEU:HA    | 1.83                     | 0.44              |
| 1:K:120:GLU:O    | 1:K:124:MET:HG3  | 2.18                     | 0.44              |
| 1:I:65:PHE:O     | 1:I:66:PRO:C     | 2.58                     | 0.44              |
| 1:B:137:ASN:C    | 1:B:137:ASN:HD22 | 2.25                     | 0.44              |
| 1:J:97:ASN:OD1   | 1:J:97:ASN:C     | 2.59                     | 0.44              |
| 1:R:56:ASP:OD1   | 1:R:60:ASN:HB3   | 2.17                     | 0.44              |
| 1:D:24:ASP:HB2   | 1:D:26:THR:HG22  | 1.99                     | 0.44              |
| 1:J:90:ARG:CD    | 1:T:138:TYR:OH   | 2.66                     | 0.44              |
| 1:K:42:ASN:CG    | 1:K:42:ASN:O     | 2.61                     | 0.44              |
| 1:T:19:PHE:HE2   | 1:T:38:SER:CB    | 2.30                     | 0.44              |
| 1:K:5:THR:O      | 1:K:8:GLN:N      | 2.51                     | 0.44              |
| 1:T:116:LEU:CD2  | 1:T:124:MET:HE1  | 2.41                     | 0.44              |
| 1:D:52:ILE:N     | 1:D:52:ILE:HD12  | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:137:ASN:OD1  | 1:I:139:GLU:HB2  | 2.18                     | 0.43              |
| 1:B:25:GLY:O     | 1:B:64:ASP:HA    | 2.17                     | 0.43              |
| 1:B:107:HIS:HE1  | 1:K:84:GLU:O     | 2.00                     | 0.43              |
| 1:Y:117:THR:C    | 1:Y:119:GLU:H    | 2.27                     | 0.43              |
| 1:D:33:GLY:O     | 1:D:37:ARG:HG3   | 2.17                     | 0.43              |
| 1:J:28:THR:C     | 1:J:30:LYS:H     | 2.25                     | 0.43              |
| 1:J:47:GLU:O     | 1:J:51:MET:HG3   | 2.17                     | 0.43              |
| 1:J:141:PHE:O    | 1:J:145:MET:HG2  | 2.18                     | 0.43              |
| 1:T:117:THR:OG1  | 1:T:120:GLU:HG3  | 2.18                     | 0.43              |
| 1:K:41:GLN:O     | 1:K:43:PRO:HD3   | 2.18                     | 0.43              |
| 1:T:47:GLU:O     | 1:T:51:MET:HG3   | 2.18                     | 0.43              |
| 1:R:36:MET:HE2   | 1:R:51:MET:HE1   | 2.01                     | 0.43              |
| 1:Y:4:LEU:HA     | 1:Y:8:GLN:OE1    | 2.18                     | 0.43              |
| 1:D:25:GLY:O     | 1:D:64:ASP:HA    | 2.19                     | 0.43              |
| 1:J:58:ASP:OD2   | 1:J:60:ASN:HB2   | 2.18                     | 0.43              |
| 1:T:56:ASP:C     | 1:T:58:ASP:H     | 2.26                     | 0.43              |
| 1:D:107:HIS:CE1  | 1:Y:40:GLY:CA    | 3.02                     | 0.43              |
| 1:K:27:ILE:HG13  | 1:K:63:ILE:HG23  | 1.99                     | 0.43              |
| 1:D:124:MET:HA   | 1:D:144:MET:CE   | 2.38                     | 0.43              |
| 1:K:26:THR:HA    | 1:K:63:ILE:O     | 2.18                     | 0.43              |
| 1:I:135:GLN:HE21 | 1:R:99:TYR:HB3   | 1.84                     | 0.43              |
| 1:J:139:GLU:O    | 1:J:143:GLN:HG2  | 2.19                     | 0.43              |
| 1:K:51:MET:HE2   | 1:K:75:LYS:HD3   | 2.00                     | 0.43              |
| 1:K:106:ARG:HD2  | 1:K:106:ARG:C    | 2.44                     | 0.43              |
| 1:T:76:MET:O     | 1:T:76:MET:HE3   | 2.19                     | 0.43              |
| 1:T:87:GLU:OE2   | 1:T:90:ARG:NH1   | 2.52                     | 0.43              |
| 1:R:48:LEU:O     | 1:R:51:MET:HB2   | 2.18                     | 0.43              |
| 1:D:55:VAL:CG1   | 1:D:56:ASP:H     | 2.14                     | 0.43              |
| 1:K:8:GLN:O      | 1:K:9:ILE:C      | 2.61                     | 0.43              |
| 1:K:55:VAL:HG21  | 1:K:63:ILE:CD1   | 2.48                     | 0.43              |
| 1:T:95:ASP:O     | 1:T:96:GLY:C     | 2.60                     | 0.43              |
| 1:Y:53:ASN:O     | 1:Y:57:ALA:HB2   | 2.19                     | 0.43              |
| 1:I:97:ASN:HD22  | 1:I:99:TYR:H     | 1.63                     | 0.42              |
| 1:B:69:LEU:HD23  | 1:B:69:LEU:HA    | 1.83                     | 0.42              |
| 1:J:19:PHE:HD1   | 1:J:35:VAL:HG22  | 1.84                     | 0.42              |
| 1:K:69:LEU:HD12  | 1:K:69:LEU:HA    | 1.83                     | 0.42              |
| 1:R:26:THR:HG22  | 1:R:63:ILE:O     | 2.19                     | 0.42              |
| 1:R:50:ASP:O     | 1:R:54:GLU:HB2   | 2.18                     | 0.42              |
| 1:D:55:VAL:O     | 1:D:57:ALA:N     | 2.50                     | 0.42              |
| 1:D:121:VAL:O    | 1:D:125:ILE:HG13 | 2.19                     | 0.42              |
| 1:B:140:GLU:O    | 1:B:144:MET:HE3  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:4:LEU:HD21   | 1:T:73:ALA:HA    | 2.02                     | 0.42              |
| 1:T:117:THR:O    | 1:T:118:ASP:C    | 2.61                     | 0.42              |
| 1:J:27:ILE:CG1   | 1:J:63:ILE:HG23  | 2.48                     | 0.42              |
| 1:K:51:MET:HE2   | 1:K:75:LYS:CD    | 2.49                     | 0.42              |
| 1:B:55:VAL:HG12  | 1:B:67:GLU:HG2   | 2.01                     | 0.42              |
| 1:J:132:GLY:C    | 1:J:134:GLY:H    | 2.28                     | 0.42              |
| 1:R:44:THR:CG2   | 1:R:47:GLU:H     | 2.32                     | 0.42              |
| 1:D:117:THR:N    | 1:D:120:GLU:OE2  | 2.53                     | 0.42              |
| 1:B:115:LYS:HD3  | 1:K:85:ILE:HD11  | 2.02                     | 0.42              |
| 1:T:116:LEU:HD23 | 1:T:121:VAL:HG22 | 2.00                     | 0.42              |
| 1:R:130:ILE:N    | 1:R:130:ILE:CD1  | 2.82                     | 0.42              |
| 1:T:65:PHE:N     | 1:T:66:PRO:CD    | 2.83                     | 0.42              |
| 1:R:51:MET:O     | 1:R:54:GLU:HB3   | 2.20                     | 0.42              |
| 1:B:74:ARG:NH1   | 1:B:74:ARG:CB    | 2.82                     | 0.42              |
| 1:B:131:ASP:OD2  | 1:J:44:THR:CG2   | 2.66                     | 0.42              |
| 1:R:141:PHE:O    | 1:R:145:MET:HG3  | 2.19                     | 0.42              |
| 1:I:56:ASP:HB2   | 1:I:62:THR:O     | 2.19                     | 0.42              |
| 1:B:51:MET:HA    | 1:B:54:GLU:HB3   | 2.01                     | 0.42              |
| 1:B:92:PHE:HB2   | 1:B:100:ILE:CG2  | 2.49                     | 0.42              |
| 1:J:28:THR:H     | 1:J:31:GLU:CD    | 2.28                     | 0.42              |
| 1:K:56:ASP:CG    | 1:K:61:GLY:H     | 2.27                     | 0.42              |
| 1:R:29:THR:OG1   | 1:R:52:ILE:CG1   | 2.65                     | 0.42              |
| 1:B:59:GLY:C     | 1:B:61:GLY:N     | 2.78                     | 0.42              |
| 1:K:55:VAL:HG12  | 1:K:56:ASP:N     | 2.35                     | 0.42              |
| 1:T:145:MET:HE2  | 1:T:145:MET:HB3  | 1.83                     | 0.42              |
| 1:Y:3:GLN:CD     | 1:Y:3:GLN:H      | 2.28                     | 0.42              |
| 1:Y:80:ASP:OD1   | 1:Y:83:GLU:HG2   | 2.19                     | 0.42              |
| 1:D:68:PHE:O     | 1:D:72:MET:HG2   | 2.19                     | 0.42              |
| 1:I:20:ASP:CA    | 1:I:21:LYS:HZ3   | 2.33                     | 0.42              |
| 1:K:92:PHE:CE2   | 1:K:105:LEU:HA   | 2.54                     | 0.42              |
| 1:T:37:ARG:HA    | 1:T:41:GLN:O     | 2.20                     | 0.42              |
| 1:T:56:ASP:OD1   | 1:T:62:THR:O     | 2.37                     | 0.42              |
| 1:T:131:ASP:C    | 1:T:131:ASP:OD2  | 2.63                     | 0.42              |
| 1:Y:29:THR:OG1   | 1:Y:52:ILE:HD13  | 2.20                     | 0.42              |
| 1:B:90:ARG:HB2   | 2:B:156:HOH:O    | 2.20                     | 0.41              |
| 1:R:21:LYS:HG3   | 1:R:22:ASP:N     | 2.35                     | 0.41              |
| 1:J:45:GLU:HA    | 1:J:45:GLU:OE1   | 2.20                     | 0.41              |
| 1:T:86:ARG:HD2   | 1:T:90:ARG:HH22  | 1.84                     | 0.41              |
| 1:R:57:ALA:C     | 1:R:59:GLY:H     | 2.29                     | 0.41              |
| 1:R:131:ASP:OD1  | 1:R:131:ASP:C    | 2.61                     | 0.41              |
| 1:I:55:VAL:CG1   | 1:I:63:ILE:HG12  | 2.48                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:94:LYS:HD3   | 2:T:155:HOH:O    | 2.19                     | 0.41              |
| 1:Y:65:PHE:N     | 1:Y:66:PRO:CD    | 2.83                     | 0.41              |
| 1:D:108:VAL:HG23 | 1:D:108:VAL:O    | 2.20                     | 0.41              |
| 1:D:130:ILE:HD13 | 1:D:131:ASP:O    | 2.21                     | 0.41              |
| 1:B:34:THR:HG23  | 1:K:103:ALA:HB2  | 2.02                     | 0.41              |
| 1:B:130:ILE:HG23 | 1:B:136:VAL:CG2  | 2.50                     | 0.41              |
| 1:J:111:ASN:O    | 1:J:114:GLU:HB3  | 2.20                     | 0.41              |
| 1:T:8:GLN:O      | 1:T:9:ILE:C      | 2.63                     | 0.41              |
| 1:B:12:PHE:HZ    | 1:B:76:MET:SD    | 2.43                     | 0.41              |
| 1:B:142:VAL:HG13 | 1:B:143:GLN:N    | 2.35                     | 0.41              |
| 1:K:90:ARG:HG2   | 1:K:90:ARG:NH1   | 2.34                     | 0.41              |
| 1:D:71:MET:HE3   | 1:D:71:MET:HB2   | 1.97                     | 0.41              |
| 1:B:109:MET:CE   | 1:K:108:VAL:HG12 | 2.48                     | 0.41              |
| 1:I:16:PHE:CD2   | 1:I:16:PHE:C     | 2.99                     | 0.41              |
| 1:I:17:SER:O     | 1:I:18:LEU:C     | 2.64                     | 0.41              |
| 1:Y:117:THR:C    | 1:Y:119:GLU:N    | 2.78                     | 0.41              |
| 1:I:32:LEU:HD22  | 1:I:52:ILE:HD11  | 2.02                     | 0.41              |
| 1:B:130:ILE:CD1  | 1:B:136:VAL:CG2  | 2.97                     | 0.41              |
| 1:J:142:VAL:CG1  | 1:J:143:GLN:N    | 2.84                     | 0.41              |
| 1:K:124:MET:HB3  | 1:K:144:MET:HE1  | 2.02                     | 0.41              |
| 1:B:107:HIS:CE1  | 1:K:84:GLU:O     | 2.74                     | 0.41              |
| 1:J:36:MET:HE2   | 1:J:51:MET:CE    | 2.50                     | 0.41              |
| 1:J:90:ARG:HD2   | 1:T:138:TYR:CZ   | 2.56                     | 0.41              |
| 1:J:131:ASP:OD1  | 1:J:131:ASP:C    | 2.64                     | 0.41              |
| 1:K:12:PHE:CE2   | 1:K:76:MET:HG3   | 2.56                     | 0.41              |
| 1:Y:118:ASP:HB2  | 2:Y:153:HOH:O    | 2.21                     | 0.41              |
| 1:B:16:PHE:CE1   | 1:B:27:ILE:HD13  | 2.56                     | 0.41              |
| 1:B:74:ARG:HB3   | 1:B:74:ARG:HH11  | 1.82                     | 0.41              |
| 1:B:116:LEU:HD11 | 1:B:124:MET:SD   | 2.61                     | 0.41              |
| 1:J:38:SER:HB2   | 1:T:106:ARG:HD3  | 2.02                     | 0.41              |
| 1:T:94:LYS:HD2   | 1:T:94:LYS:N     | 2.35                     | 0.41              |
| 1:D:24:ASP:OD1   | 1:D:24:ASP:N     | 2.53                     | 0.40              |
| 1:D:47:GLU:HG2   | 1:D:51:MET:HE2   | 2.03                     | 0.40              |
| 1:D:55:VAL:HG22  | 1:D:56:ASP:N     | 2.35                     | 0.40              |
| 1:K:32:LEU:HD12  | 1:K:52:ILE:HD11  | 2.04                     | 0.40              |
| 1:B:49:GLN:HA    | 1:B:52:ILE:HB    | 2.02                     | 0.40              |
| 1:I:97:ASN:HD21  | 1:I:99:TYR:H     | 1.66                     | 0.40              |
| 1:T:19:PHE:CE2   | 1:T:38:SER:HB3   | 2.56                     | 0.40              |
| 1:T:108:VAL:O    | 1:T:112:LEU:HB3  | 2.20                     | 0.40              |
| 1:B:51:MET:HE2   | 1:B:51:MET:HB3   | 1.81                     | 0.40              |
| 1:B:130:ILE:N    | 1:B:130:ILE:HD13 | 2.36                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:J:42:ASN:O    | 1:J:42:ASN:CG   | 2.64                     | 0.40              |
| 1:T:53:ASN:HD22 | 1:T:53:ASN:HA   | 1.60                     | 0.40              |
| 1:D:20:ASP:O    | 1:D:21:LYS:C    | 2.64                     | 0.40              |
| 1:I:32:LEU:O    | 1:I:36:MET:HG2  | 2.22                     | 0.40              |
| 1:I:47:GLU:O    | 1:I:51:MET:HG3  | 2.22                     | 0.40              |
| 1:J:115:LYS:HD2 | 1:T:85:ILE:HD11 | 2.04                     | 0.40              |
| 1:Y:104:GLU:O   | 1:Y:105:LEU:C   | 2.63                     | 0.40              |
| 1:Y:131:ASP:HB3 | 1:Y:133:ASP:H   | 1.85                     | 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   | B     | 143/148 (97%)   | 131 (92%)  | 11 (8%)  | 1 (1%)   | 18          | 25 |
| 1   | D     | 143/148 (97%)   | 131 (92%)  | 9 (6%)   | 3 (2%)   | 5           | 5  |
| 1   | I     | 143/148 (97%)   | 130 (91%)  | 10 (7%)  | 3 (2%)   | 5           | 5  |
| 1   | J     | 142/148 (96%)   | 125 (88%)  | 14 (10%) | 3 (2%)   | 5           | 5  |
| 1   | K     | 141/148 (95%)   | 123 (87%)  | 12 (8%)  | 6 (4%)   | 2           | 1  |
| 1   | R     | 145/148 (98%)   | 135 (93%)  | 5 (3%)   | 5 (3%)   | 3           | 1  |
| 1   | T     | 143/148 (97%)   | 128 (90%)  | 13 (9%)  | 2 (1%)   | 9           | 11 |
| 1   | Y     | 143/148 (97%)   | 129 (90%)  | 13 (9%)  | 1 (1%)   | 18          | 25 |
| All | All   | 1143/1184 (96%) | 1032 (90%) | 87 (8%)  | 24 (2%)  | 5           | 5  |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 22  | ASP  |
| 1   | I     | 55  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 96  | GLY  |
| 1   | R     | 55  | VAL  |
| 1   | R     | 147 | ALA  |
| 1   | D     | 25  | GLY  |
| 1   | K     | 75  | LYS  |
| 1   | Y     | 24  | ASP  |
| 1   | D     | 56  | ASP  |
| 1   | I     | 25  | GLY  |
| 1   | J     | 115 | LYS  |
| 1   | K     | 21  | LYS  |
| 1   | K     | 22  | ASP  |
| 1   | K     | 59  | GLY  |
| 1   | K     | 79  | THR  |
| 1   | R     | 24  | ASP  |
| 1   | J     | 56  | ASP  |
| 1   | K     | 56  | ASP  |
| 1   | I     | 24  | ASP  |
| 1   | J     | 55  | VAL  |
| 1   | T     | 55  | VAL  |
| 1   | R     | 22  | ASP  |
| 1   | R     | 25  | GLY  |
| 1   | B     | 55  | VAL  |

### 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   | B     | 125/126 (99%)  | 104 (83%) | 21 (17%) | 2           | 2  |
| 1   | D     | 125/126 (99%)  | 104 (83%) | 21 (17%) | 2           | 2  |
| 1   | I     | 125/126 (99%)  | 107 (86%) | 18 (14%) | 3           | 2  |
| 1   | J     | 124/126 (98%)  | 106 (86%) | 18 (14%) | 3           | 2  |
| 1   | K     | 123/126 (98%)  | 111 (90%) | 12 (10%) | 7           | 9  |
| 1   | R     | 126/126 (100%) | 110 (87%) | 16 (13%) | 4           | 4  |
| 1   | T     | 125/126 (99%)  | 116 (93%) | 9 (7%)   | 13          | 18 |

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| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | Y     | 125/126 (99%)  | 105 (84%) | 20 (16%)  | 2           | 2 |
| All | All   | 998/1008 (99%) | 863 (86%) | 135 (14%) | 4           | 3 |

All (135) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 6   | GLU  |
| 1   | D     | 17  | SER  |
| 1   | D     | 18  | LEU  |
| 1   | D     | 24  | ASP  |
| 1   | D     | 26  | THR  |
| 1   | D     | 34  | THR  |
| 1   | D     | 35  | VAL  |
| 1   | D     | 44  | THR  |
| 1   | D     | 49  | GLN  |
| 1   | D     | 58  | ASP  |
| 1   | D     | 67  | GLU  |
| 1   | D     | 69  | LEU  |
| 1   | D     | 76  | MET  |
| 1   | D     | 82  | GLU  |
| 1   | D     | 90  | ARG  |
| 1   | D     | 100 | ILE  |
| 1   | D     | 108 | VAL  |
| 1   | D     | 114 | GLU  |
| 1   | D     | 116 | LEU  |
| 1   | D     | 130 | ILE  |
| 1   | D     | 143 | GLN  |
| 1   | I     | 3   | GLN  |
| 1   | I     | 7   | GLU  |
| 1   | I     | 11  | GLU  |
| 1   | I     | 18  | LEU  |
| 1   | I     | 21  | LYS  |
| 1   | I     | 22  | ASP  |
| 1   | I     | 28  | THR  |
| 1   | I     | 42  | ASN  |
| 1   | I     | 45  | GLU  |
| 1   | I     | 78  | ASP  |
| 1   | I     | 81  | SER  |
| 1   | I     | 97  | ASN  |
| 1   | I     | 105 | LEU  |
| 1   | I     | 106 | ARG  |
| 1   | I     | 114 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 122 | ASP  |
| 1   | I     | 123 | GLU  |
| 1   | I     | 143 | GLN  |
| 1   | B     | 6   | GLU  |
| 1   | B     | 7   | GLU  |
| 1   | B     | 13  | LYS  |
| 1   | B     | 18  | LEU  |
| 1   | B     | 35  | VAL  |
| 1   | B     | 39  | LEU  |
| 1   | B     | 45  | GLU  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 52  | ILE  |
| 1   | B     | 69  | LEU  |
| 1   | B     | 84  | GLU  |
| 1   | B     | 90  | ARG  |
| 1   | B     | 106 | ARG  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 112 | LEU  |
| 1   | B     | 117 | THR  |
| 1   | B     | 127 | GLU  |
| 1   | B     | 130 | ILE  |
| 1   | B     | 135 | GLN  |
| 1   | B     | 137 | ASN  |
| 1   | B     | 143 | GLN  |
| 1   | J     | 4   | LEU  |
| 1   | J     | 5   | THR  |
| 1   | J     | 7   | GLU  |
| 1   | J     | 11  | GLU  |
| 1   | J     | 18  | LEU  |
| 1   | J     | 31  | GLU  |
| 1   | J     | 41  | GLN  |
| 1   | J     | 42  | ASN  |
| 1   | J     | 63  | ILE  |
| 1   | J     | 69  | LEU  |
| 1   | J     | 70  | THR  |
| 1   | J     | 77  | LYS  |
| 1   | J     | 80  | ASP  |
| 1   | J     | 90  | ARG  |
| 1   | J     | 114 | GLU  |
| 1   | J     | 116 | LEU  |
| 1   | J     | 127 | GLU  |
| 1   | J     | 129 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 4   | LEU  |
| 1   | K     | 22  | ASP  |
| 1   | K     | 24  | ASP  |
| 1   | K     | 32  | LEU  |
| 1   | K     | 41  | GLN  |
| 1   | K     | 42  | ASN  |
| 1   | K     | 79  | THR  |
| 1   | K     | 97  | ASN  |
| 1   | K     | 106 | ARG  |
| 1   | K     | 135 | GLN  |
| 1   | K     | 136 | VAL  |
| 1   | K     | 146 | THR  |
| 1   | T     | 3   | GLN  |
| 1   | T     | 13  | LYS  |
| 1   | T     | 27  | ILE  |
| 1   | T     | 42  | ASN  |
| 1   | T     | 53  | ASN  |
| 1   | T     | 83  | GLU  |
| 1   | T     | 97  | ASN  |
| 1   | T     | 111 | ASN  |
| 1   | T     | 127 | GLU  |
| 1   | R     | 3   | GLN  |
| 1   | R     | 5   | THR  |
| 1   | R     | 7   | GLU  |
| 1   | R     | 8   | GLN  |
| 1   | R     | 11  | GLU  |
| 1   | R     | 18  | LEU  |
| 1   | R     | 22  | ASP  |
| 1   | R     | 26  | THR  |
| 1   | R     | 28  | THR  |
| 1   | R     | 69  | LEU  |
| 1   | R     | 77  | LYS  |
| 1   | R     | 97  | ASN  |
| 1   | R     | 109 | MET  |
| 1   | R     | 114 | GLU  |
| 1   | R     | 116 | LEU  |
| 1   | R     | 130 | ILE  |
| 1   | Y     | 3   | GLN  |
| 1   | Y     | 11  | GLU  |
| 1   | Y     | 21  | LYS  |
| 1   | Y     | 28  | THR  |
| 1   | Y     | 29  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Y     | 30  | LYS  |
| 1   | Y     | 42  | ASN  |
| 1   | Y     | 50  | ASP  |
| 1   | Y     | 54  | GLU  |
| 1   | Y     | 75  | LYS  |
| 1   | Y     | 77  | LYS  |
| 1   | Y     | 84  | GLU  |
| 1   | Y     | 90  | ARG  |
| 1   | Y     | 97  | ASN  |
| 1   | Y     | 101 | SER  |
| 1   | Y     | 105 | LEU  |
| 1   | Y     | 114 | GLU  |
| 1   | Y     | 118 | ASP  |
| 1   | Y     | 135 | GLN  |
| 1   | Y     | 136 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 3   | GLN  |
| 1   | D     | 49  | GLN  |
| 1   | D     | 60  | ASN  |
| 1   | D     | 111 | ASN  |
| 1   | I     | 3   | GLN  |
| 1   | I     | 8   | GLN  |
| 1   | I     | 53  | ASN  |
| 1   | I     | 60  | ASN  |
| 1   | I     | 97  | ASN  |
| 1   | I     | 135 | GLN  |
| 1   | I     | 143 | GLN  |
| 1   | B     | 3   | GLN  |
| 1   | B     | 8   | GLN  |
| 1   | B     | 41  | GLN  |
| 1   | B     | 53  | ASN  |
| 1   | B     | 107 | HIS  |
| 1   | B     | 111 | ASN  |
| 1   | B     | 137 | ASN  |
| 1   | J     | 41  | GLN  |
| 1   | J     | 42  | ASN  |
| 1   | J     | 60  | ASN  |
| 1   | J     | 107 | HIS  |
| 1   | J     | 137 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 42  | ASN  |
| 1   | K     | 49  | GLN  |
| 1   | K     | 53  | ASN  |
| 1   | K     | 60  | ASN  |
| 1   | K     | 97  | ASN  |
| 1   | K     | 135 | GLN  |
| 1   | T     | 3   | GLN  |
| 1   | T     | 42  | ASN  |
| 1   | T     | 53  | ASN  |
| 1   | T     | 60  | ASN  |
| 1   | T     | 97  | ASN  |
| 1   | T     | 111 | ASN  |
| 1   | T     | 135 | GLN  |
| 1   | R     | 3   | GLN  |
| 1   | R     | 8   | GLN  |
| 1   | R     | 49  | GLN  |
| 1   | R     | 53  | ASN  |
| 1   | R     | 60  | ASN  |
| 1   | R     | 97  | ASN  |
| 1   | R     | 111 | ASN  |
| 1   | Y     | 3   | GLN  |
| 1   | Y     | 42  | ASN  |
| 1   | Y     | 53  | ASN  |
| 1   | Y     | 97  | ASN  |
| 1   | Y     | 111 | ASN  |
| 1   | Y     | 135 | GLN  |

### 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

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

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.