



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XC1  
Title : Oxo Zirconium(IV) Cluster in the Ferric Binding Protein (FBP)  
Authors : Zhong, W.; Alexeev, D.; Harvey, I.; Guo, M.; Hunter, D.J.B.; Zhu, H.; Campopiano, D.J.; Sadler, P.J.  
Deposited on : 2004-08-31  
Resolution : 1.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

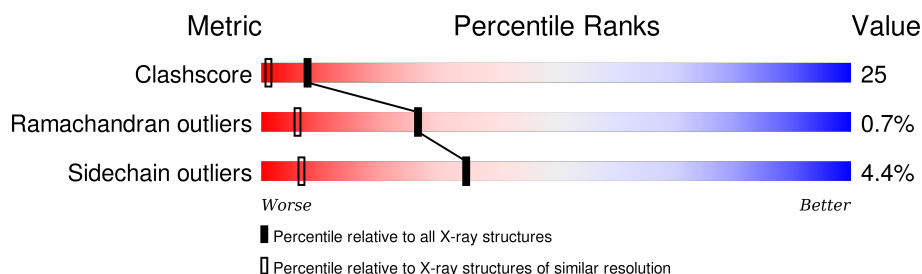
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.51 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            | 102246                      | 2887 (1.54-1.50)                                      |
| Ramachandran outliers | 100387                      | 2818 (1.54-1.50)                                      |
| Sidechain outliers    | 100360                      | 2816 (1.54-1.50)                                      |



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 309    |                  |
| 1   | B     | 309    |                  |
| 1   | C     | 309    |                  |
| 1   | D     | 309    |                  |
| 1   | E     | 309    |                  |
| 1   | F     | 309    |                  |
| 1   | G     | 309    |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | H     | 309    | <br>55% 42% • |
| 1   | I     | 309    | <br>58% 39% • |

## 2 Entry composition

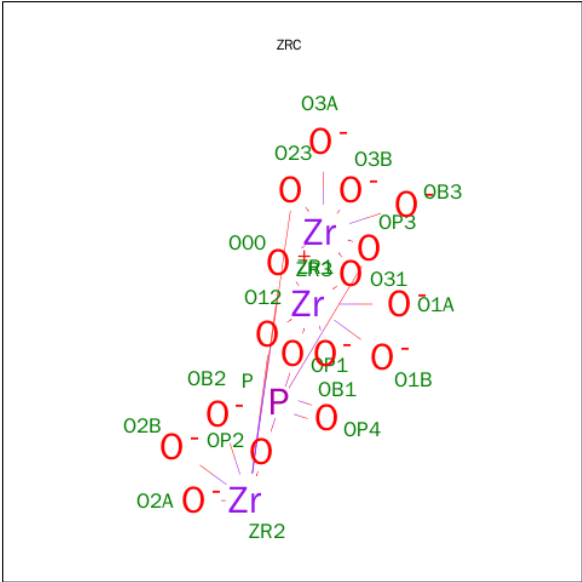
There are 3 unique types of molecules in this entry. The entry contains 22547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 periplasmic iron-binding protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | B     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | C     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | D     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | E     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | F     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | G     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | H     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |
| 1   | I     | 309      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2378  | 1508 | 423 | 446 | 1 |         |         |       |

- Molecule 2 is OXO ZIRCONIUM(IV) CLUSTER (three-letter code: ZRC) (formula: O<sub>17</sub>PZr<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 2   | A     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | B     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | D     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | G     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | H     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | I     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | C     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | E     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |
| 2   | F     | 1        | Total | O  | P | Zr | 0       | 0       |
|     |       |          | 19    | 15 | 1 | 3  |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 142      | Total | O   | 0       | 0       |
|     |       |          | 142   | 142 |         |         |
| 3   | B     | 103      | Total | O   | 0       | 0       |
|     |       |          | 103   | 103 |         |         |
| 3   | C     | 111      | Total | O   | 0       | 0       |
|     |       |          | 111   | 111 |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | D     | 113      | Total<br>113 | O<br>113 | 0       | 0       |
| 3   | E     | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 3   | F     | 124      | Total<br>124 | O<br>124 | 0       | 0       |
| 3   | G     | 79       | Total<br>79  | O<br>79  | 0       | 0       |
| 3   | H     | 81       | Total<br>81  | O<br>81  | 0       | 0       |
| 3   | I     | 85       | Total<br>85  | O<br>85  | 0       | 0       |

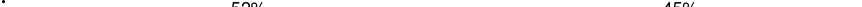


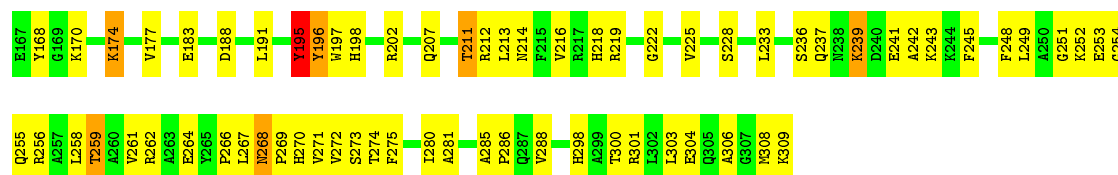
Note EDS was not executed.

- Chain A:
- 
- |    |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D1 | K111 | V216 | S228 | L233 | K234 | S235 | S236 | K239 | K243 | K244 | F245 | F248 | L249 | K252 | K253 | G254 | G255 | K256 | T259 | K262 | P266 | L267 | K268 | P269 | H270 | V271 | E278 | P279 | K282 | L283 | E284 | V288 | E297 | T300 | R301 | L302 | E304 | G305 | A306 | K309 |      |
| V4 | K115 | K130 | K132 | I133 | G134 | I135 | V136 | P137 | F142 | L143 | E144 | Q145 | I146 | K151 | A158 | L159 | L162 | K163 | G164 | V168 | G169 | K170 | K174 | V177 | A181 | V182 | E183 | E186 | I187 | D188 | L191 | I192 | E203 | K204 | G205 | V206 | V209 | H210 | T211 | R212 | L213 |
| Q8 | R9   | E10  | A12  | V16  | T26  | L30  | Q37  | L38  | Q41  | E45  | E46  | S47  | E48  | P49  | A51  | E57  | G58  | I59  | P60  | T64  | L71  | E72  | P73  | L74  | E75  | A76  | E80  | E81  | T82  | V89  | D94  | R101 | S102 | R103 | V106 | I107 | D108 | T109 | E110 |      |      |

- Chain B: 63% ● 35%

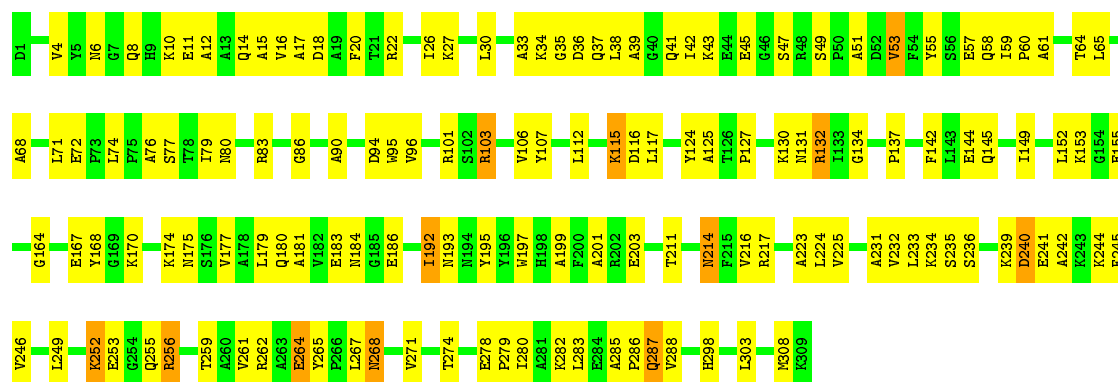
| Amino Acid | Category |
|------------|----------|
| K296       | Green    |
| E297       | Green    |
| R301       | Green    |
| K309       | Green    |
| D1         | Green    |
| I2         | Green    |
| Y5         | Green    |
| N6         | Green    |
| G7         | Green    |
| Q8         | Green    |
| H9         | Green    |
| K10        | Green    |
| E11        | Green    |
| A12        | Green    |
| A13        | Green    |
| Q14        | Green    |
| A15        | Green    |
| V16        | Green    |
| A17        | Green    |
| D18        | Green    |
| A19        | Green    |
| F20        | Green    |
| T21        | Green    |
| R22        | Green    |
| A23        | Green    |
| T24        | Green    |
| G25        | Green    |
| I26        | Green    |
| K27        | Green    |
| V28        | Green    |
| K29        | Green    |
| L30        | Green    |
| N31        | Green    |
| S32        | Green    |
| A33        | Green    |
| D36        | Green    |
| Q37        | Green    |
| L38        | Green    |
| A39        | Green    |
| G40        | Green    |
| Q41        | Green    |
| I42        | Green    |
| K43        | Green    |
| E44        | Green    |
| E45        | Green    |
| S49        | Green    |
| P50        | Green    |
| A51        | Green    |
| D52        | Green    |
| E57        | Green    |
| Q58        | Green    |
| I59        | Green    |
| P60        | Green    |
| T64        | Green    |
| L71        | Green    |
| R83        | Green    |
| V89        | Green    |
| A90        | Green    |
| A91        | Green    |
| K92        | Green    |
| K93        | Red      |
| D94        | Green    |
| W95        | Green    |
| R101       | Green    |
| S102       | Green    |
| R103       | Red      |
| V104       | Green    |
| V105       | Green    |
| V106       | Green    |
| K111       | Green    |
| L117       | Green    |
| E118       | Green    |
| K119       | Green    |
| A125       | Green    |
| N131       | Green    |
| R132       | Green    |
| I133       | Green    |
| V136       | Green    |
| G140       | Green    |
| A141       | Green    |
| E144       | Green    |
| V147       | Green    |
| K151       | Green    |
| L159       | Green    |
| K163       | Green    |
| G164       | Green    |
| K170       | Green    |
| K174       | Green    |
| M175       | Red      |
| E183       | Green    |
| I187       | Green    |
| D188       | Green    |
| L191       | Green    |
| I192       | Green    |
| N193       | Green    |
| N194       | Green    |
| Y195       | Green    |
| Y196       | Green    |
| H202       | Green    |
| G205       | Green    |
| V209       | Green    |
| H210       | Green    |
| T211       | Red      |
| N214       | Green    |
| F215       | Green    |
| V216       | Green    |
| R217       | Green    |
| V225       | Green    |
| T226       | Green    |
| Y227       | Green    |
| L233       | Green    |
| K234       | Green    |
| S235       | Green    |
| S236       | Green    |
| Q237       | Red      |
| N238       | Green    |
| R239       | Green    |
| D240       | Green    |
| E241       | Green    |
| A242       | Green    |
| K243       | Green    |
| K244       | Green    |
| F245       | Green    |
| F248       | Green    |
| L249       | Green    |
| K252       | Green    |
| E253       | Green    |
| G254       | Green    |
| Q255       | Green    |
| R256       | Green    |
| A257       | Green    |
| L258       | Green    |
| T259       | Green    |
| A260       | Green    |
| E264       | Green    |
| H270       | Green    |
| V271       | Green    |
| T274       | Green    |
| E278       | Green    |
| A285       | Green    |
| T291       | Green    |
| T292       | Green    |
| T299       | Green    |
| E305       | Green    |

- Chain C: 
- | Block | Color  |
|-------|--------|
| D1    | Yellow |
| T2    | Green  |
| T3    | Yellow |
| V4    | Yellow |
| V5    | Yellow |
| V6    | Yellow |
| G7    | Yellow |
| Q8    | Yellow |
| H9    | Yellow |
| K10   | Yellow |
| F11   | Yellow |
| A12   | Yellow |
| A13   | Green  |
| V14   | Yellow |
| A15   | Yellow |
| V16   | Green  |
| A17   | Yellow |
| D18   | Yellow |
| A19   | Yellow |
| F20   | Yellow |
| T21   | Yellow |
| R22   | Yellow |
| T26   | Yellow |
| K27   | Yellow |
| V28   | Yellow |
| F29   | Green  |
| L30   | Yellow |
| A33   | Yellow |
| L38   | Yellow |
| A39   | Green  |
| G40   | Yellow |
| Q41   | Yellow |
| A42   | Yellow |
| K43   | Yellow |
| E44   | Yellow |
| E45   | Yellow |
| G46   | Yellow |
| S47   | Yellow |
| R48   | Yellow |
| A51   | Yellow |
| D52   | Yellow |
| V53   | Yellow |
| F54   | Yellow |
| V55   | Yellow |
| S56   | Yellow |
| T59   | Yellow |
| P60   | Yellow |
| T64   | Yellow |
| E72   | Yellow |
| P73   | Yellow |
| I79   | Yellow |
- | Block | Color  |
|-------|--------|
| T82   | Yellow |
| A90   | Green  |
| A91   | Yellow |
| K92   | Yellow |
| K93   | Yellow |
| D94   | Yellow |
| W95   | Yellow |
| K101  | Yellow |
| S102  | Yellow |
| R103  | Yellow |
| V104  | Yellow |
| V105  | Yellow |
| V106  | Yellow |
| V107  | Yellow |
| D108  | Yellow |
| T109  | Yellow |
| R110  | Yellow |
| S113  | Yellow |
| E114  | Yellow |
| K115  | Yellow |
| D116  | Yellow |
| L117  | Yellow |
| E118  | Yellow |
| K119  | Yellow |
| S120  | Yellow |
| V121  | Yellow |
| L122  | Yellow |
| M123  | Yellow |
| Y124  | Yellow |
| A125  | Yellow |
| K130  | Yellow |
| M131  | Yellow |
| R132  | Yellow |
| G140  | Yellow |
| L143  | Yellow |
| E144  | Yellow |
| Q145  | Yellow |
| L146  | Yellow |
| V147  | Yellow |
| A148  | Yellow |
| I149  | Yellow |
| V150  | Yellow |
| K151  | Yellow |
| L152  | Yellow |
| K153  | Yellow |
| G154  | Yellow |
| E155  | Yellow |
| W161  | Yellow |
| L162  | Yellow |
| K163  | Yellow |
| G164  | Yellow |
| L165  | Yellow |



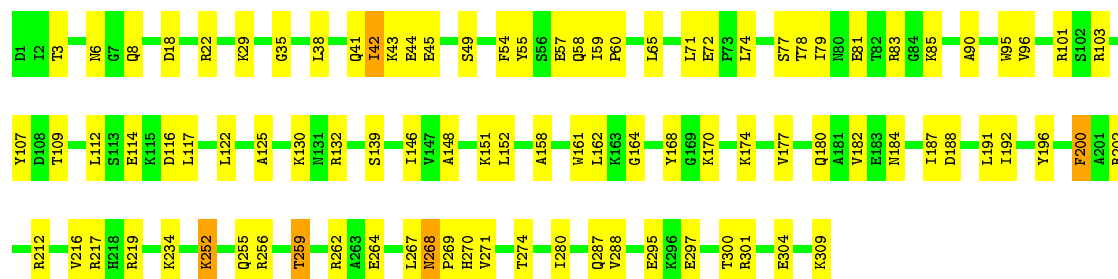
- Molecule 1: periplasmic iron-binding protein

Chain D: 54% 42%



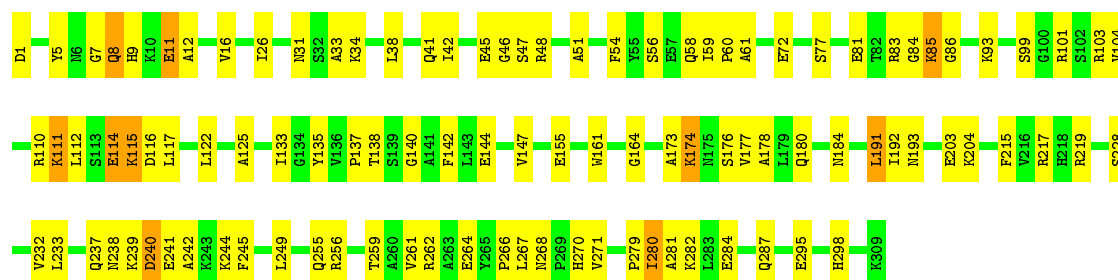
- Molecule 1: periplasmic iron-binding protein

Chain E: 70% 29%



- Molecule 1: periplasmic iron-binding protein

Chain F: 66% 30%

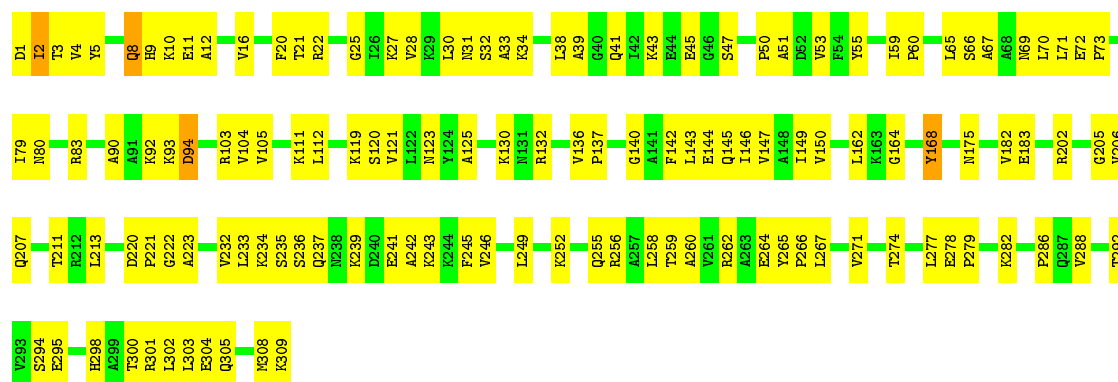


- Molecule 1: periplasmic iron-binding protein

Chain G: 57% 41%

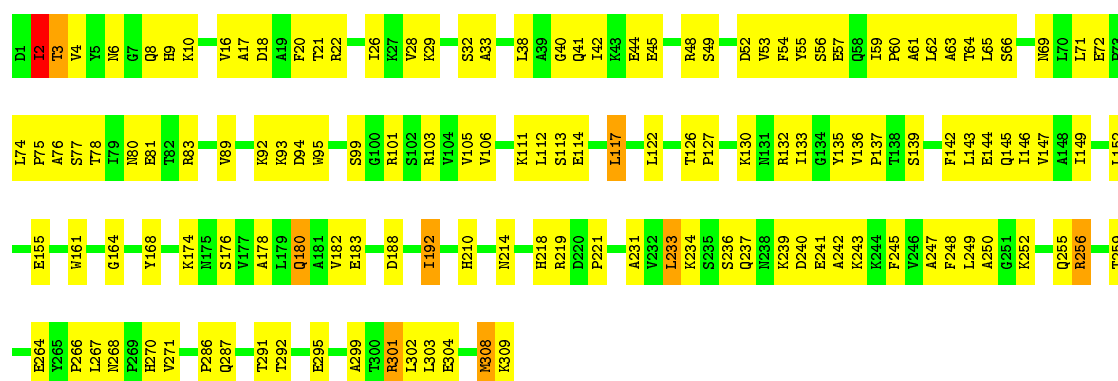






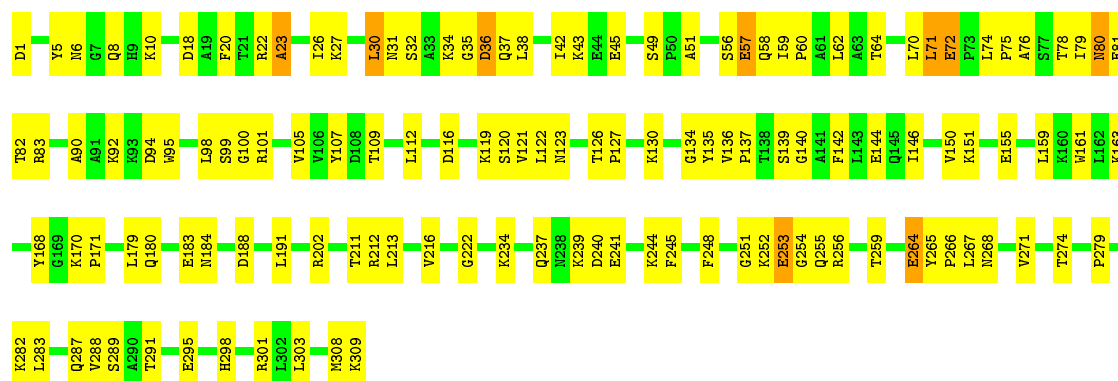
- Molecule 1: periplasmic iron-binding protein

Chain H: 55% 42% .



- Molecule 1: periplasmic iron-binding protein

Chain I: 58% 39% .



## 4 Data and refinement statistics

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

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 32  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 146.20 Å   146.20 Å   113.56 Å<br>90.00°   90.00°   120.00° | Depositor |
| Resolution (Å)   | 20.00 – 1.51  | Depositor |
| % Data completeness<br>(in resolution range)             | 97.3 (20.00-1.51)   | Depositor |
| $R_{merge}$  | 0.10  | Depositor |
| $R_{sym}$  | 0.10  | Depositor |
| Refinement program                                       | CNS 1.0   | Depositor |
| R, $R_{free}$  | 0.191 , 0.275   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 22547   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0  | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZRC

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     | 0.39         | 0/2423      | 0.63        | 0/3280         |
| 1   | B     | 0.36         | 0/2423      | 0.63        | 1/3280 (0.0%)  |
| 1   | C     | 0.41         | 0/2423      | 0.65        | 2/3280 (0.1%)  |
| 1   | D     | 0.37         | 0/2423      | 0.59        | 0/3280         |
| 1   | E     | 0.38         | 0/2423      | 0.63        | 0/3280         |
| 1   | F     | 0.37         | 0/2423      | 0.63        | 0/3280         |
| 1   | G     | 0.34         | 0/2423      | 0.60        | 0/3280         |
| 1   | H     | 0.35         | 0/2423      | 0.60        | 0/3280         |
| 1   | I     | 0.36         | 0/2423      | 0.61        | 0/3280         |
| All | All   | 0.37         | 0/21807     | 0.62        | 3/29520 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 195 | TYR  | CB-CG-CD1 | 5.81  | 124.49      | 121.00   |
| 1   | B     | 205 | GLY  | N-CA-C    | -5.34 | 99.75       | 113.10   |
| 1   | C     | 196 | TYR  | CB-CG-CD2 | 5.22  | 124.13      | 121.00   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2378  | 0        | 2424     | 98      | 0            |
| 1   | B     | 2378  | 0        | 2424     | 102     | 0            |
| 1   | C     | 2378  | 0        | 2424     | 149     | 0            |
| 1   | D     | 2378  | 0        | 2424     | 147     | 0            |
| 1   | E     | 2378  | 0        | 2424     | 93      | 0            |
| 1   | F     | 2378  | 0        | 2424     | 95      | 0            |
| 1   | G     | 2378  | 0        | 2424     | 140     | 0            |
| 1   | H     | 2378  | 0        | 2424     | 139     | 0            |
| 1   | I     | 2378  | 0        | 2424     | 127     | 0            |
| 2   | A     | 19    | 0        | 0        | 0       | 0            |
| 2   | B     | 19    | 0        | 0        | 1       | 0            |
| 2   | C     | 19    | 0        | 0        | 1       | 0            |
| 2   | D     | 19    | 0        | 0        | 2       | 0            |
| 2   | E     | 19    | 0        | 0        | 0       | 0            |
| 2   | F     | 19    | 0        | 0        | 0       | 0            |
| 2   | G     | 19    | 0        | 0        | 0       | 0            |
| 2   | H     | 19    | 0        | 0        | 1       | 0            |
| 2   | I     | 19    | 0        | 0        | 1       | 0            |
| 3   | A     | 142   | 0        | 0        | 3       | 0            |
| 3   | B     | 103   | 0        | 0        | 4       | 0            |
| 3   | C     | 111   | 0        | 0        | 11      | 0            |
| 3   | D     | 113   | 0        | 0        | 10      | 0            |
| 3   | E     | 136   | 0        | 0        | 5       | 0            |
| 3   | F     | 124   | 0        | 0        | 8       | 0            |
| 3   | G     | 79    | 0        | 0        | 5       | 0            |
| 3   | H     | 81    | 0        | 0        | 6       | 0            |
| 3   | I     | 85    | 0        | 0        | 3       | 0            |
| All | All   | 22547 | 0        | 21816    | 1086    | 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 25.

All (1086) 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:A:259:THR:HG21 | 1:A:266:PRO:HG3  | 1.24                     | 1.17              |
| 1:F:259:THR:HG21 | 1:F:266:PRO:HG3  | 1.14                     | 1.11              |
| 1:H:80:ASN:HA    | 1:H:83:ARG:HG2   | 1.27                     | 1.10              |
| 1:H:259:THR:HG21 | 1:H:266:PRO:HG3  | 1.35                     | 1.07              |
| 1:G:259:THR:HG21 | 1:G:266:PRO:HG3  | 1.35                     | 1.06              |
| 1:C:202:ARG:HH22 | 1:C:274:THR:HG23 | 1.07                     | 1.06              |
| 1:E:202:ARG:HH22 | 1:E:274:THR:HG22 | 1.19                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:202:ARG:NH2  | 1:E:274:THR:HG22 | 1.72                     | 1.05              |
| 1:C:162:LEU:HB3  | 1:C:308:MET:HE2  | 1.44                     | 0.98              |
| 1:G:119:LYS:HE2  | 1:G:119:LYS:HA   | 1.40                     | 0.98              |
| 1:I:259:THR:HG21 | 1:I:266:PRO:HG3  | 1.42                     | 0.97              |
| 1:I:56:SER:HB3   | 1:I:62:LEU:HD11  | 1.45                     | 0.97              |
| 1:B:93:LYS:HE2   | 1:B:93:LYS:H     | 1.30                     | 0.96              |
| 1:I:80:ASN:HA    | 1:I:83:ARG:HG2   | 1.45                     | 0.94              |
| 1:I:43:LYS:HD2   | 1:I:70:LEU:HD11  | 1.47                     | 0.93              |
| 1:B:170:LYS:HD2  | 1:B:187:ILE:HD12 | 1.51                     | 0.92              |
| 1:C:202:ARG:NH2  | 1:C:274:THR:HG23 | 1.84                     | 0.91              |
| 1:C:202:ARG:HH22 | 1:C:274:THR:CG2  | 1.84                     | 0.91              |
| 1:F:176:SER:O    | 1:F:180:GLN:HG2  | 1.72                     | 0.90              |
| 1:I:71:LEU:HB3   | 1:I:94:ASP:HB2   | 1.55                     | 0.89              |
| 1:D:256:ARG:HH11 | 1:D:256:ARG:HG3  | 1.37                     | 0.88              |
| 1:C:162:LEU:HD22 | 1:C:308:MET:HE1  | 1.56                     | 0.88              |
| 1:C:262:ARG:HG2  | 1:C:264:GLU:HG3  | 1.53                     | 0.88              |
| 1:B:255:GLN:HB2  | 1:B:271:VAL:HG21 | 1.57                     | 0.87              |
| 1:C:256:ARG:NH1  | 1:C:272:VAL:H    | 1.72                     | 0.86              |
| 1:I:202:ARG:NH2  | 1:I:274:THR:HG22 | 1.90                     | 0.86              |
| 1:A:159:LEU:HD13 | 1:A:302:LEU:HD22 | 1.56                     | 0.86              |
| 1:H:259:THR:CG2  | 1:H:266:PRO:HG3  | 2.06                     | 0.86              |
| 1:C:256:ARG:HD3  | 1:C:271:VAL:HG13 | 1.58                     | 0.85              |
| 1:E:72:GLU:HG2   | 1:E:234:LYS:HG2  | 1.59                     | 0.84              |
| 1:H:268:ASN:HD22 | 1:H:271:VAL:HG23 | 1.42                     | 0.84              |
| 1:D:174:LYS:HE3  | 1:D:177:VAL:HG23 | 1.59                     | 0.84              |
| 1:D:101:ARG:CZ   | 1:D:264:GLU:HG2  | 2.08                     | 0.84              |
| 1:A:288:VAL:HB   | 3:A:471:HOH:O    | 1.77                     | 0.83              |
| 1:H:17:ALA:HB1   | 1:H:28:VAL:HG21  | 1.58                     | 0.83              |
| 1:E:85:LYS:N     | 1:E:85:LYS:HD2   | 1.94                     | 0.83              |
| 1:B:93:LYS:HE2   | 1:B:93:LYS:N     | 1.94                     | 0.83              |
| 1:A:304:GLU:HG2  | 1:A:309:LYS:HG2  | 1.58                     | 0.83              |
| 1:B:2:ILE:HG23   | 1:B:241:GLU:OE2  | 1.79                     | 0.82              |
| 1:E:85:LYS:H     | 1:E:85:LYS:HD2   | 1.44                     | 0.82              |
| 1:C:120:SER:HB3  | 1:C:123:ASN:ND2  | 1.95                     | 0.82              |
| 1:I:18:ASP:HB3   | 1:I:22:ARG:HH12  | 1.45                     | 0.81              |
| 1:C:121:VAL:HB   | 3:C:460:HOH:O    | 1.78                     | 0.81              |
| 1:A:278:GLU:HB2  | 1:A:282:LYS:NZ   | 1.96                     | 0.81              |
| 1:E:202:ARG:HH22 | 1:E:274:THR:CG2  | 1.93                     | 0.80              |
| 1:H:2:ILE:HD11   | 1:H:53:VAL:HG23  | 1.65                     | 0.79              |
| 1:D:132:ARG:HH11 | 1:D:132:ARG:HB3  | 1.47                     | 0.79              |
| 1:C:252:LYS:O    | 1:C:256:ARG:HG2  | 1.83                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:239:LYS:O    | 1:G:243:LYS:HG3  | 1.84                     | 0.78              |
| 1:I:202:ARG:HH22 | 1:I:274:THR:HG22 | 1.46                     | 0.78              |
| 1:G:202:ARG:NH2  | 1:G:274:THR:HG22 | 1.99                     | 0.78              |
| 1:C:259:THR:HG23 | 1:C:273:SER:HA   | 1.66                     | 0.78              |
| 1:I:279:PRO:HD2  | 1:I:282:LYS:HD2  | 1.64                     | 0.77              |
| 1:G:72:GLU:HG3   | 1:G:73:PRO:HD2   | 1.66                     | 0.77              |
| 1:H:255:GLN:HB3  | 1:H:271:VAL:HG21 | 1.66                     | 0.77              |
| 1:F:280:ILE:O    | 1:F:280:ILE:HD13 | 1.85                     | 0.77              |
| 1:G:90:ALA:HB3   | 1:G:93:LYS:HA    | 1.66                     | 0.77              |
| 1:H:4:VAL:HG22   | 1:H:53:VAL:HB    | 1.65                     | 0.77              |
| 1:C:52:ASP:HA    | 1:C:236:SER:HB2  | 1.66                     | 0.77              |
| 1:I:240:ASP:O    | 1:I:244:LYS:HG2  | 1.85                     | 0.76              |
| 1:F:11:GLU:HG2   | 1:F:12:ALA:N     | 2.00                     | 0.76              |
| 1:I:309:LYS:NZ   | 1:I:309:LYS:HB3  | 2.00                     | 0.76              |
| 1:G:234:LYS:NZ   | 1:G:234:LYS:HB3  | 2.01                     | 0.76              |
| 1:D:42:ILE:HD13  | 1:D:233:LEU:HD21 | 1.68                     | 0.76              |
| 1:G:292:THR:OG1  | 1:G:295:GLU:HG3  | 1.86                     | 0.76              |
| 1:F:147:VAL:HG13 | 1:F:295:GLU:HG2  | 1.68                     | 0.76              |
| 1:H:255:GLN:CB   | 1:H:271:VAL:HG21 | 2.16                     | 0.75              |
| 1:C:48:ARG:HE    | 1:C:237:GLN:NE2  | 1.84                     | 0.75              |
| 1:C:79:ILE:HD12  | 1:C:93:LYS:HG3   | 1.68                     | 0.75              |
| 1:D:132:ARG:HB3  | 1:D:132:ARG:NH1  | 2.00                     | 0.74              |
| 1:C:195:TYR:CE2  | 1:C:196:TYR:CE1  | 2.74                     | 0.74              |
| 1:A:101:ARG:HH22 | 1:A:228:SER:HB3  | 1.51                     | 0.74              |
| 1:I:130:LYS:HG2  | 1:I:168:TYR:HD2  | 1.52                     | 0.74              |
| 1:E:262:ARG:HG2  | 1:E:264:GLU:HG3  | 1.69                     | 0.74              |
| 1:A:130:LYS:HE3  | 1:A:131:ASN:HD22 | 1.52                     | 0.74              |
| 1:B:60:PRO:O     | 1:B:64:THR:HG23  | 1.88                     | 0.74              |
| 1:A:125:ALA:HB1  | 1:A:164:GLY:HA3  | 1.70                     | 0.73              |
| 1:B:197:TRP:HE1  | 1:B:211:THR:HG22 | 1.53                     | 0.73              |
| 1:I:80:ASN:HB3   | 1:I:83:ARG:NH2   | 2.03                     | 0.73              |
| 1:F:9:HIS:CD2    | 1:F:11:GLU:HB3   | 2.23                     | 0.73              |
| 1:H:99:SER:HA    | 1:H:267:LEU:HG   | 1.69                     | 0.73              |
| 1:F:192:ILE:HG22 | 1:F:193:ASN:N    | 2.03                     | 0.73              |
| 1:D:61:ALA:O     | 1:D:65:LEU:HD23  | 1.88                     | 0.73              |
| 1:B:5:TYR:CE1    | 1:B:51:ALA:HB2   | 2.24                     | 0.73              |
| 1:E:158:ALA:O    | 1:E:162:LEU:HD13 | 1.89                     | 0.73              |
| 1:G:259:THR:CG2  | 1:G:266:PRO:HG3  | 2.15                     | 0.72              |
| 1:F:259:THR:CG2  | 1:F:266:PRO:HG3  | 2.06                     | 0.72              |
| 1:D:256:ARG:NH1  | 1:D:256:ARG:HG3  | 1.99                     | 0.72              |
| 1:C:130:LYS:HD3  | 1:C:131:ASN:N    | 2.05                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:130:LYS:CD   | 1:G:168:TYR:HB3  | 2.19                     | 0.72              |
| 1:A:47:SER:HA    | 1:A:235:SER:HB3  | 1.72                     | 0.72              |
| 1:F:85:LYS:NZ    | 1:F:219:ARG:HH12 | 1.87                     | 0.72              |
| 1:D:39:ALA:HB1   | 1:D:65:LEU:HD21  | 1.72                     | 0.71              |
| 1:A:72:GLU:OE1   | 1:A:73:PRO:HD2   | 1.89                     | 0.71              |
| 1:G:302:LEU:HD23 | 1:G:305:GLN:NE2  | 2.05                     | 0.71              |
| 1:B:209:VAL:HG12 | 1:B:211:THR:H    | 1.53                     | 0.71              |
| 1:F:85:LYS:HZ1   | 1:F:284:GLU:HA   | 1.55                     | 0.71              |
| 1:E:3:THR:HG22   | 1:E:29:LYS:HD3   | 1.71                     | 0.71              |
| 1:B:41:GLN:O     | 1:B:45:GLU:HG2   | 1.88                     | 0.71              |
| 1:D:174:LYS:HE3  | 1:D:177:VAL:CG2  | 2.19                     | 0.71              |
| 1:G:236:SER:HB3  | 1:G:239:LYS:HG2  | 1.73                     | 0.71              |
| 1:B:197:TRP:NE1  | 1:B:211:THR:HG22 | 2.05                     | 0.71              |
| 1:H:268:ASN:ND2  | 1:H:271:VAL:HG23 | 2.04                     | 0.71              |
| 1:H:3:THR:HB     | 1:H:29:LYS:HE2   | 1.73                     | 0.71              |
| 1:H:80:ASN:HA    | 1:H:83:ARG:CG    | 2.15                     | 0.70              |
| 1:B:252:LYS:HE2  | 1:B:256:ARG:NH2  | 2.06                     | 0.70              |
| 1:H:71:LEU:O     | 1:H:234:LYS:HE3  | 1.90                     | 0.70              |
| 1:C:303:LEU:HG   | 1:C:309:LYS:HA   | 1.73                     | 0.70              |
| 1:B:45:GLU:HB3   | 1:B:49:SER:HB3   | 1.73                     | 0.70              |
| 1:C:104:VAL:HG23 | 3:C:511:HOH:O    | 1.90                     | 0.70              |
| 1:C:259:THR:O    | 1:C:274:THR:HG22 | 1.92                     | 0.70              |
| 1:B:45:GLU:CB    | 1:B:49:SER:HB3   | 2.21                     | 0.70              |
| 1:H:8:GLN:HG3    | 1:H:9:HIS:H      | 1.54                     | 0.70              |
| 1:H:259:THR:HG21 | 1:H:266:PRO:CG   | 2.20                     | 0.70              |
| 1:D:265:TYR:HB3  | 1:D:280:ILE:HG23 | 1.74                     | 0.70              |
| 1:D:259:THR:HG23 | 3:D:411:HOH:O    | 1.92                     | 0.69              |
| 1:G:4:VAL:HB     | 1:G:30:LEU:HD23  | 1.73                     | 0.69              |
| 1:A:143:LEU:O    | 1:A:146:ILE:HG23 | 1.93                     | 0.69              |
| 1:C:255:GLN:HE21 | 1:C:268:ASN:H    | 1.39                     | 0.69              |
| 1:A:89:VAL:HG12  | 3:A:465:HOH:O    | 1.92                     | 0.69              |
| 1:I:259:THR:CG2  | 1:I:266:PRO:HG3  | 2.20                     | 0.69              |
| 1:I:81:GLU:OE1   | 1:I:251:GLY:HA2  | 1.93                     | 0.69              |
| 1:I:30:LEU:C     | 1:I:31:ASN:HD22  | 1.96                     | 0.69              |
| 1:E:252:LYS:O    | 1:E:256:ARG:HG3  | 1.93                     | 0.69              |
| 1:H:112:LEU:HD11 | 1:H:188:ASP:HB3  | 1.75                     | 0.69              |
| 1:A:60:PRO:O     | 1:A:64:THR:HG23  | 1.93                     | 0.68              |
| 1:I:126:THR:HB   | 1:I:127:PRO:HD2  | 1.75                     | 0.68              |
| 1:I:43:LYS:HD2   | 1:I:70:LEU:CD1   | 2.22                     | 0.68              |
| 1:A:112:LEU:HD11 | 1:A:188:ASP:HB3  | 1.75                     | 0.68              |
| 1:G:300:THR:O    | 1:G:304:GLU:HG3  | 1.92                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:174:LYS:NZ   | 2:H:400:ZRC:O23  | 2.25                     | 0.68              |
| 1:H:192:ILE:N    | 1:H:192:ILE:HD13 | 2.09                     | 0.68              |
| 1:A:279:PRO:HD2  | 1:A:282:LYS:NZ   | 2.09                     | 0.68              |
| 1:H:81:GLU:HB2   | 1:H:250:ALA:HB1  | 1.75                     | 0.68              |
| 1:E:170:LYS:HD2  | 1:E:187:ILE:HD12 | 1.76                     | 0.68              |
| 1:G:130:LYS:HD2  | 1:G:168:TYR:HB3  | 1.75                     | 0.67              |
| 1:D:77:SER:HA    | 1:D:80:ASN:HD22  | 1.56                     | 0.67              |
| 1:I:56:SER:HB3   | 1:I:62:LEU:CD1   | 2.21                     | 0.67              |
| 1:B:125:ALA:HB1  | 1:B:164:GLY:HA3  | 1.75                     | 0.67              |
| 1:I:127:PRO:O    | 1:I:130:LYS:HG3  | 1.94                     | 0.67              |
| 1:I:60:PRO:O     | 1:I:64:THR:HG23  | 1.93                     | 0.67              |
| 1:C:151:LYS:HD2  | 1:C:288:VAL:HG23 | 1.77                     | 0.67              |
| 1:D:8:GLN:HE22   | 1:D:101:ARG:HH22 | 1.41                     | 0.67              |
| 1:F:5:TYR:CE1    | 1:F:51:ALA:HB2   | 2.30                     | 0.67              |
| 1:A:278:GLU:HB2  | 1:A:282:LYS:HZ2  | 1.59                     | 0.67              |
| 1:D:255:GLN:O    | 1:D:259:THR:HG22 | 1.95                     | 0.67              |
| 1:G:125:ALA:HB1  | 1:G:164:GLY:HA3  | 1.77                     | 0.67              |
| 1:G:5:TYR:CE1    | 1:G:51:ALA:HB2   | 2.30                     | 0.66              |
| 1:F:125:ALA:HB1  | 1:F:164:GLY:HA3  | 1.76                     | 0.66              |
| 1:B:255:GLN:CB   | 1:B:271:VAL:HG21 | 2.26                     | 0.66              |
| 1:C:197:TRP:HE1  | 1:C:211:THR:HG23 | 1.59                     | 0.66              |
| 1:B:8:GLN:HA     | 1:B:57:GLU:HG3   | 1.77                     | 0.66              |
| 1:C:259:THR:CG2  | 1:C:273:SER:HA   | 2.24                     | 0.66              |
| 1:B:106:VAL:HG22 | 1:B:211:THR:HG23 | 1.77                     | 0.66              |
| 1:D:80:ASN:O     | 1:D:83:ARG:HG2   | 1.95                     | 0.66              |
| 1:I:59:ILE:N     | 1:I:60:PRO:HD2   | 2.11                     | 0.66              |
| 1:A:252:LYS:HE3  | 1:A:256:ARG:NH2  | 2.10                     | 0.66              |
| 1:F:259:THR:HG21 | 1:F:266:PRO:CG   | 2.09                     | 0.66              |
| 1:C:236:SER:H    | 1:C:239:LYS:HE2  | 1.59                     | 0.66              |
| 1:I:266:PRO:HD2  | 3:I:417:HOH:O    | 1.96                     | 0.65              |
| 1:D:236:SER:HB3  | 1:D:239:LYS:HG2  | 1.78                     | 0.65              |
| 1:G:8:GLN:HG3    | 1:G:9:HIS:H      | 1.61                     | 0.65              |
| 1:D:240:ASP:HB2  | 3:D:508:HOH:O    | 1.95                     | 0.65              |
| 1:G:33:ALA:HB3   | 1:G:38:LEU:CD2   | 2.26                     | 0.65              |
| 1:I:119:LYS:O    | 1:I:216:VAL:HG23 | 1.97                     | 0.65              |
| 1:A:279:PRO:HG2  | 1:A:282:LYS:HG3  | 1.79                     | 0.65              |
| 1:F:192:ILE:HG22 | 1:F:193:ASN:H    | 1.61                     | 0.65              |
| 1:C:121:VAL:HG21 | 1:C:222:GLY:HA3  | 1.79                     | 0.65              |
| 1:D:201:ALA:HB3  | 3:D:512:HOH:O    | 1.97                     | 0.65              |
| 1:A:133:ILE:HD11 | 1:A:191:LEU:HD13 | 1.77                     | 0.65              |
| 1:D:15:ALA:CB    | 1:D:261:VAL:HG21 | 2.26                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:255:GLN:NE2  | 1:C:268:ASN:H    | 1.95                     | 0.65              |
| 1:G:202:ARG:HH22 | 1:G:274:THR:HG22 | 1.59                     | 0.64              |
| 1:C:48:ARG:HH21  | 1:C:237:GLN:HG3  | 1.61                     | 0.64              |
| 1:A:110:ARG:HH21 | 1:A:210:HIS:CD2  | 2.15                     | 0.64              |
| 1:A:82:THR:HB    | 1:A:267:LEU:HB3  | 1.79                     | 0.64              |
| 1:H:78:THR:HG23  | 1:H:247:ALA:HA   | 1.77                     | 0.64              |
| 1:D:155:GLU:OE2  | 1:D:298:HIS:HE1  | 1.81                     | 0.64              |
| 1:H:292:THR:OG1  | 1:H:295:GLU:HG3  | 1.97                     | 0.64              |
| 1:A:174:LYS:HB2  | 1:A:177:VAL:HG23 | 1.79                     | 0.64              |
| 1:I:72:GLU:HG3   | 1:I:239:LYS:HD2  | 1.78                     | 0.64              |
| 1:D:267:LEU:HD23 | 1:D:280:ILE:HD13 | 1.78                     | 0.64              |
| 1:B:38:LEU:O     | 1:B:42:ILE:HG13  | 1.97                     | 0.64              |
| 1:D:45:GLU:HB2   | 1:D:49:SER:HB2   | 1.79                     | 0.64              |
| 1:C:119:LYS:O    | 1:C:216:VAL:HG13 | 1.97                     | 0.64              |
| 1:F:245:PHE:O    | 1:F:249:LEU:HG   | 1.98                     | 0.64              |
| 1:H:38:LEU:O     | 1:H:42:ILE:HG13  | 1.97                     | 0.63              |
| 1:G:162:LEU:HD22 | 1:G:308:MET:HE1  | 1.80                     | 0.63              |
| 1:A:9:HIS:HB3    | 1:A:12:ALA:CB    | 2.28                     | 0.63              |
| 1:H:126:THR:HB   | 1:H:127:PRO:HD2  | 1.81                     | 0.63              |
| 1:H:8:GLN:HG3    | 1:H:9:HIS:N      | 2.13                     | 0.63              |
| 1:B:292:THR:OG1  | 1:B:295:GLU:HG3  | 1.98                     | 0.63              |
| 1:B:5:TYR:CD1    | 1:B:51:ALA:HB2   | 2.33                     | 0.63              |
| 1:G:140:GLY:O    | 1:G:144:GLU:HG2  | 1.98                     | 0.63              |
| 1:B:101:ARG:NH2  | 1:B:226:THR:HG22 | 2.13                     | 0.63              |
| 1:C:113:SER:C    | 1:C:115:LYS:H    | 2.02                     | 0.63              |
| 1:H:18:ASP:O     | 1:H:22:ARG:HG3   | 1.98                     | 0.63              |
| 1:H:57:GLU:HB2   | 1:H:101:ARG:NH2  | 2.14                     | 0.63              |
| 1:F:192:ILE:CG2  | 1:F:193:ASN:H    | 2.12                     | 0.63              |
| 1:G:9:HIS:HB3    | 1:G:12:ALA:HB3   | 1.80                     | 0.63              |
| 1:B:252:LYS:HE3  | 1:B:270:HIS:O    | 1.99                     | 0.63              |
| 1:C:2:ILE:HG13   | 1:C:28:VAL:HG13  | 1.81                     | 0.62              |
| 1:I:202:ARG:HH22 | 1:I:274:THR:CG2  | 2.12                     | 0.62              |
| 1:E:287:GLN:HB3  | 3:E:498:HOH:O    | 1.99                     | 0.62              |
| 1:G:130:LYS:HA   | 1:G:168:TYR:HB2  | 1.79                     | 0.62              |
| 1:C:28:VAL:HG11  | 3:C:462:HOH:O    | 1.99                     | 0.62              |
| 1:C:107:TYR:CD1  | 1:C:117:LEU:HD11 | 2.34                     | 0.62              |
| 1:C:162:LEU:HB3  | 1:C:308:MET:CE   | 2.25                     | 0.62              |
| 1:H:33:ALA:HB3   | 1:H:38:LEU:HG    | 1.80                     | 0.62              |
| 1:I:240:ASP:HB3  | 1:I:241:GLU:OE2  | 1.99                     | 0.62              |
| 1:E:268:ASN:HD22 | 1:E:268:ASN:C    | 2.03                     | 0.62              |
| 1:G:34:LYS:O     | 1:G:38:LEU:HD23  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:114:GLU:OE2  | 1:C:214:ASN:HB2  | 1.99                     | 0.62              |
| 1:H:41:GLN:O     | 1:H:45:GLU:HG3   | 2.00                     | 0.62              |
| 1:D:72:GLU:HG2   | 1:D:234:LYS:HA   | 1.82                     | 0.62              |
| 1:I:101:ARG:NH1  | 2:I:400:ZRC:O1A  | 2.33                     | 0.62              |
| 1:G:5:TYR:HB3    | 1:G:38:LEU:HD12  | 1.82                     | 0.61              |
| 1:F:115:LYS:O    | 1:F:116:ASP:CG   | 2.39                     | 0.61              |
| 1:F:85:LYS:HD2   | 1:F:281:ALA:HA   | 1.82                     | 0.61              |
| 1:G:300:THR:O    | 1:G:303:LEU:HB3  | 1.99                     | 0.61              |
| 1:H:54:PHE:CE2   | 1:H:56:SER:HB2   | 2.35                     | 0.61              |
| 1:E:72:GLU:HG2   | 1:E:234:LYS:HA   | 1.83                     | 0.61              |
| 1:F:122:LEU:HA   | 1:F:161:TRP:CD1  | 2.35                     | 0.61              |
| 1:C:105:VAL:HG22 | 1:C:191:LEU:HD23 | 1.82                     | 0.61              |
| 1:C:268:ASN:HD22 | 1:C:268:ASN:C    | 2.04                     | 0.61              |
| 1:G:303:LEU:HD22 | 1:G:308:MET:CE   | 2.30                     | 0.61              |
| 1:E:38:LEU:O     | 1:E:42:ILE:HG13  | 2.01                     | 0.61              |
| 1:H:16:VAL:HG11  | 1:H:249:LEU:CD2  | 2.30                     | 0.61              |
| 1:G:162:LEU:HD22 | 1:G:308:MET:CE   | 2.31                     | 0.61              |
| 1:A:236:SER:HB3  | 1:A:239:LYS:HG2  | 1.83                     | 0.61              |
| 1:C:120:SER:HB3  | 1:C:123:ASN:HD21 | 1.66                     | 0.60              |
| 1:H:136:VAL:O    | 1:H:139:SER:HB3  | 2.01                     | 0.60              |
| 1:G:2:ILE:HD11   | 1:G:28:VAL:HG22  | 1.81                     | 0.60              |
| 1:F:38:LEU:HD13  | 3:F:494:HOH:O    | 2.01                     | 0.60              |
| 1:C:17:ALA:O     | 1:C:20:PHE:HB3   | 2.00                     | 0.60              |
| 1:B:237:GLN:NE2  | 1:B:237:GLN:H    | 1.99                     | 0.60              |
| 1:C:5:TYR:CD1    | 1:C:51:ALA:HB2   | 2.36                     | 0.60              |
| 1:G:202:ARG:HH22 | 1:G:274:THR:CG2  | 2.14                     | 0.60              |
| 1:G:104:VAL:HG12 | 1:G:105:VAL:N    | 2.16                     | 0.60              |
| 1:C:162:LEU:HD22 | 1:C:308:MET:CE   | 2.30                     | 0.60              |
| 1:A:304:GLU:HA   | 1:A:309:LYS:HB3  | 1.84                     | 0.60              |
| 1:H:3:THR:HB     | 1:H:29:LYS:HB3   | 1.82                     | 0.60              |
| 1:I:252:LYS:NZ   | 1:I:256:ARG:HD2  | 2.17                     | 0.60              |
| 1:H:95:TRP:HB3   | 1:H:231:ALA:HB2  | 1.82                     | 0.60              |
| 1:F:280:ILE:C    | 1:F:280:ILE:HD13 | 2.22                     | 0.60              |
| 1:G:2:ILE:HB     | 3:G:443:HOH:O    | 2.01                     | 0.60              |
| 1:G:162:LEU:HB3  | 1:G:308:MET:HE2  | 1.83                     | 0.60              |
| 1:G:1:ASP:OD1    | 1:G:27:LYS:HD3   | 2.01                     | 0.60              |
| 1:E:125:ALA:HB1  | 1:E:164:GLY:HA3  | 1.83                     | 0.60              |
| 1:A:45:GLU:HB3   | 1:A:49:SER:HB3   | 1.82                     | 0.60              |
| 1:H:59:ILE:N     | 1:H:60:PRO:HD2   | 2.16                     | 0.60              |
| 1:F:85:LYS:NZ    | 1:F:284:GLU:HA   | 2.17                     | 0.60              |
| 1:G:279:PRO:HD2  | 1:G:282:LYS:HG3  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:10:LYS:HE2   | 1:I:32:SER:HB2   | 1.84                     | 0.60              |
| 1:A:203:GLU:OE1  | 1:A:204:LYS:HE2  | 2.01                     | 0.60              |
| 1:D:27:LYS:HB3   | 1:D:27:LYS:NZ    | 2.16                     | 0.60              |
| 1:H:75:PRO:HB2   | 1:H:77:SER:OG    | 2.00                     | 0.60              |
| 1:C:121:VAL:CG2  | 1:C:222:GLY:HA3  | 2.32                     | 0.60              |
| 1:G:53:VAL:HG22  | 1:G:232:VAL:HG22 | 1.83                     | 0.60              |
| 1:G:70:LEU:HD22  | 3:G:470:HOH:O    | 2.02                     | 0.59              |
| 1:B:59:ILE:HD11  | 1:B:227:TYR:HB2  | 1.82                     | 0.59              |
| 1:D:279:PRO:HB2  | 1:D:282:LYS:HE2  | 1.84                     | 0.59              |
| 1:A:108:ASP:OD2  | 1:A:110:ARG:HD2  | 2.02                     | 0.59              |
| 1:F:77:SER:O     | 1:F:81:GLU:HG3   | 2.01                     | 0.59              |
| 1:F:101:ARG:NH1  | 1:F:101:ARG:HB2  | 2.18                     | 0.59              |
| 1:H:69:ASN:HB3   | 1:H:92:LYS:NZ    | 2.16                     | 0.59              |
| 1:G:260:ALA:HA   | 1:G:274:THR:OG1  | 2.02                     | 0.59              |
| 1:G:302:LEU:HD23 | 1:G:305:GLN:HE22 | 1.68                     | 0.59              |
| 1:I:82:THR:HB    | 1:I:267:LEU:HB3  | 1.83                     | 0.59              |
| 1:I:109:THR:O    | 1:I:109:THR:HG22 | 2.03                     | 0.59              |
| 1:A:146:ILE:CD1  | 1:A:158:ALA:HB1  | 2.32                     | 0.59              |
| 1:F:192:ILE:CG2  | 1:F:193:ASN:N    | 2.64                     | 0.59              |
| 1:G:130:LYS:HD3  | 1:G:168:TYR:HB3  | 1.84                     | 0.59              |
| 1:E:78:THR:HG22  | 1:E:96:VAL:HG21  | 1.84                     | 0.59              |
| 1:I:80:ASN:HD22  | 1:I:80:ASN:N     | 2.01                     | 0.59              |
| 1:I:130:LYS:HG2  | 1:I:168:TYR:CD2  | 2.37                     | 0.59              |
| 1:G:3:THR:CG2    | 1:G:31:ASN:HD21  | 2.15                     | 0.59              |
| 1:E:148:ALA:O    | 1:E:152:LEU:HD23 | 2.03                     | 0.59              |
| 1:G:5:TYR:CD1    | 1:G:51:ALA:HB2   | 2.38                     | 0.59              |
| 1:D:4:VAL:HB     | 1:D:30:LEU:HD23  | 1.85                     | 0.59              |
| 1:F:99:SER:HA    | 1:F:267:LEU:HG   | 1.84                     | 0.59              |
| 1:I:309:LYS:HB3  | 1:I:309:LYS:HZ3  | 1.68                     | 0.59              |
| 1:I:5:TYR:CE1    | 1:I:51:ALA:HB2   | 2.38                     | 0.59              |
| 1:C:266:PRO:HD2  | 3:C:457:HOH:O    | 2.03                     | 0.58              |
| 1:B:245:PHE:O    | 1:B:248:PHE:HB3  | 2.02                     | 0.58              |
| 1:D:79:ILE:HG12  | 1:D:96:VAL:HG22  | 1.85                     | 0.58              |
| 1:C:106:VAL:HB   | 3:C:511:HOH:O    | 2.02                     | 0.58              |
| 1:D:16:VAL:HG11  | 1:D:249:LEU:HD22 | 1.83                     | 0.58              |
| 1:E:255:GLN:HE22 | 1:E:267:LEU:H    | 1.51                     | 0.58              |
| 1:B:133:ILE:HD11 | 1:B:191:LEU:CD1  | 2.32                     | 0.58              |
| 1:C:130:LYS:HD2  | 1:C:131:ASN:ND2  | 2.19                     | 0.58              |
| 1:E:252:LYS:HE2  | 1:E:252:LYS:H    | 1.69                     | 0.58              |
| 1:H:146:ILE:HD11 | 1:H:303:LEU:HD21 | 1.86                     | 0.58              |
| 1:F:233:LEU:HD12 | 1:F:233:LEU:N    | 2.18                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:135:TYR:CD2  | 1:F:137:PRO:HD3  | 2.39                     | 0.58              |
| 1:C:252:LYS:HG2  | 1:C:268:ASN:OD1  | 2.03                     | 0.58              |
| 1:I:22:ARG:HG3   | 3:I:426:HOH:O    | 2.02                     | 0.58              |
| 1:D:96:VAL:HG13  | 3:D:513:HOH:O    | 2.03                     | 0.58              |
| 1:E:180:GLN:NE2  | 1:E:184:ASN:HD21 | 2.01                     | 0.58              |
| 1:D:34:LYS:HB3   | 1:D:37:GLN:CD    | 2.24                     | 0.58              |
| 1:H:17:ALA:HB1   | 1:H:28:VAL:CG2   | 2.33                     | 0.58              |
| 1:D:4:VAL:HG13   | 1:D:53:VAL:HG22  | 1.85                     | 0.58              |
| 1:G:234:LYS:HB3  | 1:G:234:LYS:HZ2  | 1.68                     | 0.58              |
| 1:C:106:VAL:CG2  | 1:C:211:THR:OG1  | 2.52                     | 0.58              |
| 1:B:8:GLN:HA     | 1:B:57:GLU:CG    | 2.34                     | 0.58              |
| 1:H:80:ASN:CA    | 1:H:83:ARG:HG2   | 2.18                     | 0.57              |
| 1:B:59:ILE:N     | 1:B:60:PRO:HD2   | 2.18                     | 0.57              |
| 1:C:104:VAL:HG21 | 1:C:213:LEU:HD22 | 1.84                     | 0.57              |
| 1:E:268:ASN:HD22 | 1:E:270:HIS:H    | 1.52                     | 0.57              |
| 1:B:197:TRP:CD1  | 1:B:211:THR:HG22 | 2.39                     | 0.57              |
| 1:I:31:ASN:HD22  | 1:I:31:ASN:N     | 2.00                     | 0.57              |
| 1:G:255:GLN:O    | 1:G:259:THR:HG23 | 2.04                     | 0.57              |
| 1:F:178:ALA:HB3  | 1:F:192:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:106:VAL:HG13 | 1:A:213:LEU:HD23 | 1.85                     | 0.57              |
| 1:D:184:ASN:HB2  | 1:D:186:GLU:HG3  | 1.87                     | 0.57              |
| 1:D:51:ALA:HB3   | 1:D:233:LEU:HD22 | 1.86                     | 0.57              |
| 1:F:85:LYS:HB2   | 3:F:514:HOH:O    | 2.05                     | 0.57              |
| 1:I:34:LYS:HE3   | 1:I:36:ASP:OD2   | 2.05                     | 0.57              |
| 1:H:152:LEU:HD12 | 3:H:481:HOH:O    | 2.05                     | 0.57              |
| 1:E:255:GLN:NE2  | 1:E:268:ASN:H    | 2.02                     | 0.57              |
| 1:E:268:ASN:ND2  | 1:E:270:HIS:H    | 2.02                     | 0.57              |
| 1:G:43:LYS:HZ3   | 1:G:65:LEU:HD23  | 1.69                     | 0.57              |
| 1:H:83:ARG:HA    | 1:H:83:ARG:NE    | 2.19                     | 0.57              |
| 1:G:90:ALA:CB    | 1:G:93:LYS:HA    | 2.34                     | 0.57              |
| 1:I:179:LEU:O    | 1:I:183:GLU:HB2  | 2.05                     | 0.57              |
| 1:C:268:ASN:HD22 | 1:C:269:PRO:N    | 2.03                     | 0.56              |
| 1:D:101:ARG:HH21 | 1:D:262:ARG:HE   | 1.53                     | 0.56              |
| 1:F:147:VAL:HG22 | 1:F:295:GLU:HG3  | 1.86                     | 0.56              |
| 1:D:47:SER:HA    | 1:D:235:SER:HB3  | 1.86                     | 0.56              |
| 2:D:400:ZRC:O1B  | 3:D:407:HOH:O    | 2.18                     | 0.56              |
| 1:B:83:ARG:HB3   | 1:B:83:ARG:HH11  | 1.71                     | 0.56              |
| 1:D:255:GLN:CB   | 1:D:271:VAL:HG21 | 2.35                     | 0.56              |
| 1:F:85:LYS:NZ    | 1:F:219:ARG:NH1  | 2.53                     | 0.56              |
| 1:C:197:TRP:HB3  | 1:C:213:LEU:HD11 | 1.87                     | 0.56              |
| 1:D:77:SER:HA    | 1:D:80:ASN:ND2   | 2.20                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:9:HIS:CE1    | 1:G:11:GLU:HB3   | 2.40                     | 0.56              |
| 1:C:22:ARG:HD3   | 1:D:184:ASN:HB3  | 1.87                     | 0.56              |
| 1:B:136:VAL:HG21 | 1:B:175:ASN:HD22 | 1.71                     | 0.56              |
| 1:B:141:ALA:CB   | 1:B:193:ASN:HD21 | 2.18                     | 0.56              |
| 1:G:20:PHE:C     | 1:G:22:ARG:H     | 2.09                     | 0.56              |
| 1:G:47:SER:HA    | 1:G:235:SER:HB3  | 1.86                     | 0.56              |
| 1:B:8:GLN:NE2    | 1:B:57:GLU:HG2   | 2.21                     | 0.56              |
| 1:D:41:GLN:O     | 1:D:45:GLU:HG3   | 2.04                     | 0.56              |
| 1:H:92:LYS:HB2   | 1:H:94:ASP:OD1   | 2.06                     | 0.56              |
| 1:D:252:LYS:HG3  | 1:D:253:GLU:H    | 1.70                     | 0.56              |
| 1:F:256:ARG:HG2  | 1:F:271:VAL:HG13 | 1.86                     | 0.56              |
| 1:D:57:GLU:N     | 1:D:57:GLU:OE2   | 2.36                     | 0.56              |
| 1:B:43:LYS:NZ    | 1:B:64:THR:HB    | 2.19                     | 0.56              |
| 1:A:16:VAL:HG11  | 1:A:249:LEU:CD2  | 2.36                     | 0.56              |
| 1:D:11:GLU:CD    | 1:D:11:GLU:H     | 2.09                     | 0.56              |
| 1:H:117:LEU:HD23 | 1:H:214:ASN:ND2  | 2.20                     | 0.56              |
| 1:B:18:ASP:O     | 1:B:22:ARG:HB2   | 2.06                     | 0.56              |
| 1:I:155:GLU:OE1  | 1:I:298:HIS:HE1  | 1.89                     | 0.56              |
| 1:G:303:LEU:HD12 | 1:G:309:LYS:HB2  | 1.88                     | 0.56              |
| 1:D:107:TYR:HB2  | 1:D:112:LEU:HD12 | 1.88                     | 0.56              |
| 1:F:177:VAL:HA   | 1:F:180:GLN:CG   | 2.36                     | 0.56              |
| 1:G:79:ILE:HD11  | 1:G:93:LYS:HB2   | 1.87                     | 0.56              |
| 1:I:288:VAL:HG12 | 1:I:289:SER:O    | 2.05                     | 0.56              |
| 1:D:137:PRO:HB3  | 1:D:308:MET:HE3  | 1.87                     | 0.56              |
| 1:I:253:GLU:OE1  | 1:I:254:GLY:N    | 2.38                     | 0.56              |
| 1:B:159:LEU:O    | 1:B:163:LYS:HG3  | 2.06                     | 0.55              |
| 1:H:164:GLY:O    | 1:H:168:TYR:HD1  | 1.89                     | 0.55              |
| 1:G:41:GLN:O     | 1:G:45:GLU:HG3   | 2.05                     | 0.55              |
| 1:H:236:SER:HB2  | 1:H:239:LYS:HG2  | 1.86                     | 0.55              |
| 1:F:203:GLU:HG3  | 1:F:204:LYS:N    | 2.20                     | 0.55              |
| 1:E:182:VAL:HG22 | 1:E:187:ILE:HG23 | 1.88                     | 0.55              |
| 1:B:239:LYS:O    | 1:B:243:LYS:HG3  | 2.06                     | 0.55              |
| 1:A:47:SER:HA    | 1:A:235:SER:CB   | 2.34                     | 0.55              |
| 1:H:57:GLU:N     | 1:H:57:GLU:OE2   | 2.25                     | 0.55              |
| 1:H:26:ILE:HD13  | 1:H:241:GLU:HG3  | 1.89                     | 0.55              |
| 1:D:144:GLU:HG3  | 1:D:224:LEU:HD21 | 1.89                     | 0.55              |
| 1:D:255:GLN:HB3  | 1:D:271:VAL:HG21 | 1.88                     | 0.55              |
| 1:G:233:LEU:HD12 | 1:G:233:LEU:N    | 2.22                     | 0.55              |
| 1:A:1:ASP:HB2    | 1:A:26:ILE:HG23  | 1.87                     | 0.55              |
| 1:G:71:LEU:O     | 1:G:234:LYS:HD3  | 2.07                     | 0.55              |
| 1:B:233:LEU:CD1  | 1:B:233:LEU:N    | 2.70                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:HIS:HB3    | 1:A:12:ALA:HB2   | 1.87                     | 0.55              |
| 1:A:170:LYS:HG3  | 3:A:450:HOH:O    | 2.06                     | 0.55              |
| 1:C:7:GLY:HA2    | 1:C:33:ALA:O     | 2.07                     | 0.55              |
| 1:I:58:GLN:O     | 1:I:62:LEU:HD13  | 2.07                     | 0.55              |
| 1:G:33:ALA:HB3   | 1:G:38:LEU:HD21  | 1.88                     | 0.55              |
| 1:H:89:VAL:HG12  | 3:H:456:HOH:O    | 2.07                     | 0.55              |
| 1:I:255:GLN:CB   | 1:I:271:VAL:HG21 | 2.36                     | 0.55              |
| 1:D:10:LYS:O     | 1:D:14:GLN:HG3   | 2.07                     | 0.55              |
| 1:H:61:ALA:O     | 1:H:64:THR:HG22  | 2.07                     | 0.55              |
| 1:I:98:LEU:O     | 1:I:267:LEU:HB2  | 2.07                     | 0.55              |
| 1:H:72:GLU:OE2   | 1:H:239:LYS:HD3  | 2.07                     | 0.55              |
| 1:H:21:THR:HA    | 1:H:26:ILE:O     | 2.07                     | 0.55              |
| 1:F:85:LYS:HZ3   | 1:F:219:ARG:HH12 | 1.54                     | 0.54              |
| 1:B:141:ALA:HB1  | 1:B:193:ASN:HD21 | 1.72                     | 0.54              |
| 1:E:130:LYS:HD3  | 1:E:168:TYR:HD2  | 1.72                     | 0.54              |
| 1:A:9:HIS:ND1    | 1:A:262:ARG:HD3  | 2.22                     | 0.54              |
| 1:I:27:LYS:C     | 1:I:27:LYS:HD3   | 2.27                     | 0.54              |
| 1:H:40:GLY:O     | 1:H:44:GLU:HG3   | 2.06                     | 0.54              |
| 1:B:91:ALA:O     | 1:B:93:LYS:HE3   | 2.07                     | 0.54              |
| 1:G:71:LEU:CB    | 1:G:94:ASP:HB2   | 2.37                     | 0.54              |
| 1:G:256:ARG:HG2  | 1:G:271:VAL:HG13 | 1.88                     | 0.54              |
| 1:G:72:GLU:OE1   | 1:G:239:LYS:HD3  | 2.07                     | 0.54              |
| 1:G:92:LYS:C     | 1:G:93:LYS:HG2   | 2.28                     | 0.54              |
| 1:H:192:ILE:HD13 | 1:H:192:ILE:H    | 1.70                     | 0.54              |
| 1:D:39:ALA:O     | 1:D:43:LYS:HG2   | 2.08                     | 0.54              |
| 1:H:245:PHE:O    | 1:H:248:PHE:HB3  | 2.07                     | 0.54              |
| 1:C:143:LEU:HA   | 1:C:146:ILE:HD12 | 1.89                     | 0.54              |
| 1:C:262:ARG:CG   | 1:C:264:GLU:HG3  | 2.30                     | 0.54              |
| 1:G:146:ILE:HD13 | 1:G:162:LEU:HD11 | 1.89                     | 0.54              |
| 1:G:303:LEU:HD22 | 1:G:308:MET:HE1  | 1.89                     | 0.54              |
| 1:I:151:LYS:HD2  | 1:I:288:VAL:HG13 | 1.88                     | 0.54              |
| 1:C:51:ALA:HB3   | 1:C:233:LEU:CD2  | 2.38                     | 0.54              |
| 1:I:34:LYS:HE2   | 1:I:37:GLN:HG3   | 1.89                     | 0.54              |
| 1:I:183:GLU:OE1  | 1:I:211:THR:HG23 | 2.08                     | 0.54              |
| 1:C:236:SER:O    | 1:C:237:GLN:HB2  | 2.08                     | 0.54              |
| 1:F:147:VAL:HG13 | 1:F:295:GLU:CG   | 2.37                     | 0.54              |
| 1:A:252:LYS:NZ   | 1:H:237:GLN:HB3  | 2.23                     | 0.54              |
| 1:D:34:LYS:HE3   | 1:D:36:ASP:H     | 1.73                     | 0.54              |
| 1:G:183:GLU:HA   | 1:G:211:THR:HG23 | 1.90                     | 0.54              |
| 1:I:146:ILE:O    | 1:I:150:VAL:HG23 | 2.08                     | 0.54              |
| 1:E:202:ARG:NH2  | 1:E:274:THR:CG2  | 2.57                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:255:GLN:HB2  | 1:H:271:VAL:HG21 | 1.88                     | 0.54              |
| 1:C:303:LEU:CG   | 1:C:309:LYS:HA   | 2.38                     | 0.54              |
| 1:I:57:GLU:HG2   | 1:I:58:GLN:HG3   | 1.89                     | 0.53              |
| 1:C:130:LYS:HD3  | 1:C:130:LYS:C    | 2.29                     | 0.53              |
| 1:I:137:PRO:HA   | 1:I:142:PHE:CD2  | 2.43                     | 0.53              |
| 1:F:173:ALA:HB3  | 1:F:174:LYS:CE   | 2.38                     | 0.53              |
| 1:C:51:ALA:HB3   | 1:C:233:LEU:HD21 | 1.90                     | 0.53              |
| 1:E:216:VAL:HG13 | 3:E:436:HOH:O    | 2.08                     | 0.53              |
| 1:G:303:LEU:CD1  | 1:G:309:LYS:HB2  | 2.38                     | 0.53              |
| 1:C:166:LYS:HD2  | 3:C:417:HOH:O    | 2.07                     | 0.53              |
| 1:G:255:GLN:HB2  | 1:G:271:VAL:HG21 | 1.89                     | 0.53              |
| 1:G:242:ALA:O    | 1:G:246:VAL:HG23 | 2.09                     | 0.53              |
| 1:A:75:PRO:HD3   | 1:A:243:LYS:HZ2  | 1.73                     | 0.53              |
| 1:C:125:ALA:HB1  | 1:C:164:GLY:HA3  | 1.90                     | 0.53              |
| 1:D:262:ARG:HG2  | 1:D:264:GLU:HG3  | 1.90                     | 0.53              |
| 1:G:104:VAL:HG12 | 1:G:105:VAL:H    | 1.72                     | 0.53              |
| 1:E:268:ASN:HD22 | 1:E:269:PRO:N    | 2.06                     | 0.53              |
| 1:F:41:GLN:O     | 1:F:45:GLU:HG3   | 2.09                     | 0.53              |
| 1:E:196:TYR:O    | 1:E:200:PHE:CD1  | 2.62                     | 0.53              |
| 1:F:8:GLN:OE1    | 1:F:12:ALA:HB3   | 2.08                     | 0.53              |
| 1:I:252:LYS:CD   | 1:I:256:ARG:HD2  | 2.39                     | 0.53              |
| 1:B:9:HIS:NE2    | 1:B:11:GLU:HG2   | 2.23                     | 0.53              |
| 1:C:51:ALA:O     | 1:C:233:LEU:HD22 | 2.09                     | 0.53              |
| 1:E:43:LYS:HA    | 3:E:527:HOH:O    | 2.08                     | 0.53              |
| 1:G:255:GLN:CB   | 1:G:271:VAL:HG21 | 2.39                     | 0.53              |
| 1:B:22:ARG:O     | 1:F:110:ARG:NH1  | 2.39                     | 0.53              |
| 1:G:67:ALA:HA    | 1:G:92:LYS:NZ    | 2.24                     | 0.53              |
| 1:B:233:LEU:HD12 | 1:B:233:LEU:N    | 2.24                     | 0.53              |
| 1:H:114:GLU:HA   | 1:H:117:LEU:HD22 | 1.90                     | 0.53              |
| 1:G:256:ARG:NH1  | 1:G:256:ARG:HB3  | 2.23                     | 0.53              |
| 1:E:252:LYS:CD   | 1:E:252:LYS:H    | 2.22                     | 0.53              |
| 1:G:33:ALA:HB3   | 1:G:38:LEU:HD22  | 1.89                     | 0.53              |
| 1:F:255:GLN:HB2  | 1:F:271:VAL:HG21 | 1.90                     | 0.53              |
| 1:G:21:THR:HG22  | 1:G:21:THR:O     | 2.09                     | 0.52              |
| 1:A:297:GLU:OE2  | 1:A:297:GLU:HA   | 2.09                     | 0.52              |
| 1:E:79:ILE:HG12  | 1:E:96:VAL:HG22  | 1.90                     | 0.52              |
| 1:D:233:LEU:N    | 1:D:233:LEU:HD12 | 2.24                     | 0.52              |
| 1:B:291:THR:CG2  | 1:B:296:LYS:HE2  | 2.39                     | 0.52              |
| 1:B:22:ARG:HG2   | 1:F:184:ASN:O    | 2.09                     | 0.52              |
| 1:D:145:GLN:O    | 1:D:149:ILE:HG13 | 2.10                     | 0.52              |
| 1:G:121:VAL:CG1  | 1:G:222:GLY:HA3  | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:THR:OG1  | 1:C:266:PRO:HG3  | 2.09                     | 0.52              |
| 1:I:253:GLU:CD   | 1:I:254:GLY:H    | 2.12                     | 0.52              |
| 1:C:48:ARG:HE    | 1:C:237:GLN:HE21 | 1.54                     | 0.52              |
| 1:E:252:LYS:CE   | 1:E:252:LYS:H    | 2.23                     | 0.52              |
| 1:I:122:LEU:HA   | 1:I:161:TRP:CD1  | 2.44                     | 0.52              |
| 1:B:36:ASP:HB2   | 3:B:489:HOH:O    | 2.09                     | 0.52              |
| 1:E:161:TRP:CE3  | 1:E:162:LEU:HD12 | 2.45                     | 0.52              |
| 1:H:16:VAL:HG11  | 1:H:249:LEU:HD23 | 1.91                     | 0.52              |
| 1:H:105:VAL:HG23 | 3:H:480:HOH:O    | 2.09                     | 0.52              |
| 1:H:268:ASN:HD22 | 1:H:271:VAL:CG2  | 2.18                     | 0.52              |
| 1:D:6:ASN:OD1    | 1:D:55:TYR:HD2   | 1.93                     | 0.52              |
| 1:C:33:ALA:HB3   | 1:C:38:LEU:HD21  | 1.92                     | 0.52              |
| 1:H:66:SER:O     | 1:H:92:LYS:HE2   | 2.10                     | 0.52              |
| 1:I:34:LYS:HE2   | 1:I:37:GLN:CG    | 2.40                     | 0.52              |
| 1:H:240:ASP:HA   | 1:H:243:LYS:HD2  | 1.91                     | 0.52              |
| 1:G:59:ILE:N     | 1:G:60:PRO:CD    | 2.73                     | 0.52              |
| 1:B:216:VAL:HG23 | 3:B:437:HOH:O    | 2.10                     | 0.52              |
| 1:H:304:GLU:HA   | 1:H:309:LYS:O    | 2.09                     | 0.52              |
| 1:I:59:ILE:N     | 1:I:60:PRO:CD    | 2.73                     | 0.52              |
| 1:I:34:LYS:HG2   | 1:I:37:GLN:CD    | 2.30                     | 0.52              |
| 1:D:33:ALA:HB1   | 1:D:37:GLN:OE1   | 2.10                     | 0.52              |
| 1:G:80:ASN:OD1   | 1:G:83:ARG:NH2   | 2.41                     | 0.52              |
| 1:C:121:VAL:HG23 | 1:C:216:VAL:HG21 | 1.92                     | 0.51              |
| 1:C:4:VAL:HG22   | 1:C:53:VAL:HB    | 1.92                     | 0.51              |
| 1:C:300:THR:O    | 1:C:304:GLU:HG3  | 2.10                     | 0.51              |
| 1:C:304:GLU:HG2  | 1:C:309:LYS:HG3  | 1.91                     | 0.51              |
| 1:F:5:TYR:CD1    | 1:F:51:ALA:HB2   | 2.44                     | 0.51              |
| 1:A:8:GLN:CG     | 1:A:9:HIS:H      | 2.23                     | 0.51              |
| 1:H:152:LEU:HD11 | 1:H:286:PRO:HB2  | 1.92                     | 0.51              |
| 1:I:245:PHE:O    | 1:I:248:PHE:HB3  | 2.09                     | 0.51              |
| 1:D:103:ARG:HD2  | 1:D:145:GLN:HB2  | 1.92                     | 0.51              |
| 1:G:2:ILE:O      | 1:G:2:ILE:HG13   | 2.09                     | 0.51              |
| 1:F:262:ARG:HH11 | 1:F:264:GLU:HG3  | 1.74                     | 0.51              |
| 1:I:140:GLY:O    | 1:I:144:GLU:HG2  | 2.10                     | 0.51              |
| 1:I:259:THR:HG21 | 1:I:266:PRO:CG   | 2.29                     | 0.51              |
| 1:H:6:ASN:OD1    | 1:H:8:GLN:HB3    | 2.11                     | 0.51              |
| 1:G:104:VAL:HG11 | 1:G:213:LEU:HB3  | 1.93                     | 0.51              |
| 1:I:34:LYS:HG2   | 1:I:37:GLN:OE1   | 2.09                     | 0.51              |
| 1:D:26:ILE:HD13  | 1:D:241:GLU:HB3  | 1.91                     | 0.51              |
| 1:G:252:LYS:O    | 1:G:256:ARG:HG3  | 2.10                     | 0.51              |
| 1:B:202:ARG:NH2  | 1:B:274:THR:O    | 2.43                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:ARG:NH2  | 1:A:183:GLU:O    | 2.32                     | 0.51              |
| 1:I:20:PHE:CZ    | 1:I:26:ILE:HD12  | 2.45                     | 0.51              |
| 1:I:18:ASP:HB3   | 1:I:22:ARG:NH1   | 2.21                     | 0.51              |
| 1:A:9:HIS:HB3    | 1:A:12:ALA:HB3   | 1.92                     | 0.51              |
| 1:D:10:LYS:HD2   | 1:D:14:GLN:NE2   | 2.25                     | 0.51              |
| 1:F:114:GLU:O    | 1:F:117:LEU:HB2  | 2.10                     | 0.51              |
| 1:C:1:ASP:OD1    | 1:C:27:LYS:HG2   | 2.11                     | 0.51              |
| 1:E:45:GLU:HG3   | 1:E:49:SER:HB2   | 1.91                     | 0.51              |
| 1:F:137:PRO:HA   | 1:F:142:PHE:CD2  | 2.46                     | 0.51              |
| 1:I:121:VAL:HB   | 1:I:222:GLY:HA3  | 1.92                     | 0.51              |
| 1:E:146:ILE:HG12 | 1:E:162:LEU:HD11 | 1.93                     | 0.51              |
| 1:I:252:LYS:HZ3  | 1:I:256:ARG:HD2  | 1.76                     | 0.51              |
| 1:I:234:LYS:O    | 1:I:239:LYS:NZ   | 2.44                     | 0.51              |
| 1:A:245:PHE:O    | 1:A:249:LEU:HG   | 2.10                     | 0.51              |
| 1:D:106:VAL:HG22 | 1:D:211:THR:OG1  | 2.11                     | 0.51              |
| 1:C:174:LYS:HG3  | 1:C:177:VAL:HG23 | 1.93                     | 0.51              |
| 1:G:136:VAL:HG21 | 1:G:175:ASN:HD22 | 1.76                     | 0.51              |
| 1:F:191:LEU:O    | 1:F:192:ILE:HG13 | 2.11                     | 0.51              |
| 1:I:34:LYS:CE    | 1:I:37:GLN:HG3   | 2.40                     | 0.51              |
| 1:H:239:LYS:O    | 1:H:243:LYS:HG3  | 2.11                     | 0.51              |
| 1:C:43:LYS:HE3   | 1:C:64:THR:HG22  | 1.93                     | 0.51              |
| 1:C:109:THR:HG21 | 1:C:212:ARG:NE   | 2.26                     | 0.51              |
| 1:C:255:GLN:CB   | 1:C:271:VAL:HG21 | 2.41                     | 0.51              |
| 1:E:255:GLN:O    | 1:E:259:THR:HB   | 2.11                     | 0.51              |
| 1:F:51:ALA:O     | 1:F:233:LEU:HD22 | 2.11                     | 0.51              |
| 1:I:1:ASP:OD1    | 1:I:27:LYS:HB3   | 2.12                     | 0.51              |
| 1:G:137:PRO:HA   | 1:G:142:PHE:CD2  | 2.46                     | 0.51              |
| 1:I:79:ILE:HG22  | 1:I:83:ARG:NH1   | 2.26                     | 0.50              |
| 1:E:256:ARG:HD3  | 3:E:504:HOH:O    | 2.11                     | 0.50              |
| 1:D:236:SER:O    | 1:D:239:LYS:HG3  | 2.11                     | 0.50              |
| 1:F:54:PHE:CE2   | 1:F:56:SER:HB2   | 2.46                     | 0.50              |
| 1:H:234:LYS:HE2  | 3:H:450:HOH:O    | 2.11                     | 0.50              |
| 1:D:76:ALA:O     | 1:D:80:ASN:ND2   | 2.44                     | 0.50              |
| 1:I:248:PHE:CD1  | 1:I:253:GLU:OE1  | 2.63                     | 0.50              |
| 1:C:109:THR:HG21 | 1:C:212:ARG:CD   | 2.41                     | 0.50              |
| 1:H:252:LYS:HE2  | 1:H:270:HIS:CB   | 2.41                     | 0.50              |
| 1:B:174:LYS:NZ   | 2:B:400:ZRC:O23  | 2.45                     | 0.50              |
| 1:E:77:SER:O     | 1:E:81:GLU:HG3   | 2.11                     | 0.50              |
| 1:C:15:ALA:HB2   | 1:C:261:VAL:HG11 | 1.93                     | 0.50              |
| 1:I:80:ASN:HA    | 1:I:83:ARG:CG    | 2.30                     | 0.50              |
| 1:H:38:LEU:HB3   | 1:H:54:PHE:HE1   | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:58:GLN:HG3   | 1:F:61:ALA:H     | 1.76                     | 0.50              |
| 1:E:255:GLN:CB   | 1:E:271:VAL:HG21 | 2.41                     | 0.50              |
| 1:G:51:ALA:O     | 1:G:233:LEU:HD22 | 2.11                     | 0.50              |
| 1:D:34:LYS:HD2   | 1:D:35:GLY:N     | 2.26                     | 0.50              |
| 1:G:258:LEU:HD11 | 1:G:264:GLU:OE1  | 2.11                     | 0.50              |
| 1:C:130:LYS:HE2  | 1:C:168:TYR:HA   | 1.94                     | 0.50              |
| 1:E:74:LEU:CD1   | 1:E:96:VAL:HG23  | 2.42                     | 0.50              |
| 1:C:252:LYS:HE2  | 1:C:270:HIS:CD2  | 2.46                     | 0.50              |
| 1:C:52:ASP:HA    | 1:C:236:SER:CB   | 2.37                     | 0.50              |
| 1:F:133:ILE:HD11 | 1:F:191:LEU:HD13 | 1.93                     | 0.50              |
| 1:D:34:LYS:O     | 1:D:37:GLN:HG2   | 2.11                     | 0.50              |
| 1:B:111:LYS:HA   | 1:B:111:LYS:HE2  | 1.94                     | 0.50              |
| 1:D:217:ARG:NH1  | 1:D:278:GLU:OE2  | 2.45                     | 0.50              |
| 1:G:3:THR:HG23   | 1:G:31:ASN:HD21  | 1.77                     | 0.50              |
| 1:C:195:TYR:HE2  | 1:C:196:TYR:CE1  | 2.29                     | 0.50              |
| 1:H:236:SER:HB2  | 1:H:239:LYS:CG   | 2.42                     | 0.50              |
| 1:E:6:ASN:HD21   | 1:E:8:GLN:HB2    | 1.75                     | 0.50              |
| 1:E:252:LYS:HE2  | 1:E:252:LYS:N    | 2.27                     | 0.49              |
| 1:G:12:ALA:O     | 1:G:16:VAL:HG22  | 2.12                     | 0.49              |
| 1:H:53:VAL:CG2   | 1:H:242:ALA:HB1  | 2.42                     | 0.49              |
| 1:E:8:GLN:NE2    | 1:E:55:TYR:CE1   | 2.79                     | 0.49              |
| 1:A:269:PRO:HG3  | 1:H:48:ARG:CZ    | 2.41                     | 0.49              |
| 1:E:304:GLU:HG3  | 1:E:309:LYS:HD3  | 1.92                     | 0.49              |
| 1:I:80:ASN:HB3   | 1:I:83:ARG:CZ    | 2.42                     | 0.49              |
| 1:D:42:ILE:CD1   | 1:D:233:LEU:HD21 | 2.39                     | 0.49              |
| 1:A:37:GLN:O     | 1:A:41:GLN:HB2   | 2.12                     | 0.49              |
| 1:D:287:GLN:OE1  | 1:D:288:VAL:N    | 2.46                     | 0.49              |
| 1:A:146:ILE:HD11 | 1:A:302:LEU:CD1  | 2.42                     | 0.49              |
| 1:B:89:VAL:HG22  | 3:B:408:HOH:O    | 2.11                     | 0.49              |
| 1:E:297:GLU:O    | 1:E:301:ARG:HG2  | 2.12                     | 0.49              |
| 1:D:71:LEU:HD13  | 1:D:231:ALA:CB   | 2.43                     | 0.49              |
| 1:A:51:ALA:O     | 1:A:233:LEU:HD22 | 2.13                     | 0.49              |
| 1:H:122:LEU:HD21 | 1:H:149:ILE:HD13 | 1.94                     | 0.49              |
| 1:D:217:ARG:HA   | 1:D:283:LEU:O    | 2.12                     | 0.49              |
| 1:D:4:VAL:HG13   | 1:D:53:VAL:CG2   | 2.42                     | 0.49              |
| 1:G:121:VAL:HG11 | 1:G:222:GLY:HA3  | 1.93                     | 0.49              |
| 1:A:142:PHE:O    | 1:A:146:ILE:HG22 | 2.13                     | 0.49              |
| 1:G:66:SER:OG    | 1:G:92:LYS:HE3   | 2.13                     | 0.49              |
| 1:E:148:ALA:O    | 1:E:152:LEU:CD2  | 2.61                     | 0.49              |
| 1:D:117:LEU:HD12 | 1:D:117:LEU:N    | 2.27                     | 0.49              |
| 1:I:38:LEU:O     | 1:I:42:ILE:HG13  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:90:ALA:HB2   | 1:C:95:TRP:CE2   | 2.46                     | 0.49              |
| 1:A:4:VAL:HB     | 1:A:30:LEU:HD23  | 1.93                     | 0.49              |
| 1:D:268:ASN:HD22 | 1:D:268:ASN:C    | 2.15                     | 0.49              |
| 1:C:301:ARG:HA   | 1:C:304:GLU:OE1  | 2.13                     | 0.49              |
| 1:H:106:VAL:HB   | 1:H:192:ILE:HD11 | 1.94                     | 0.49              |
| 1:H:54:PHE:HD2   | 1:H:62:LEU:HD23  | 1.78                     | 0.49              |
| 1:E:41:GLN:O     | 1:E:45:GLU:HG2   | 2.11                     | 0.49              |
| 1:G:234:LYS:HB3  | 1:G:234:LYS:HZ3  | 1.78                     | 0.49              |
| 1:A:248:PHE:O    | 1:A:254:GLY:HA3  | 2.13                     | 0.49              |
| 1:C:40:GLY:O     | 1:C:44:GLU:HG3   | 2.12                     | 0.49              |
| 1:E:191:LEU:HD22 | 1:E:191:LEU:N    | 2.27                     | 0.49              |
| 1:D:101:ARG:NH2  | 1:D:262:ARG:HE   | 2.11                     | 0.49              |
| 1:H:2:ILE:HG23   | 1:H:2:ILE:O      | 2.13                     | 0.49              |
| 1:C:48:ARG:NH2   | 1:C:237:GLN:HG3  | 2.26                     | 0.49              |
| 1:I:268:ASN:HB3  | 1:I:271:VAL:HG23 | 1.95                     | 0.49              |
| 1:A:110:ARG:HE   | 1:A:210:HIS:CG   | 2.31                     | 0.49              |
| 1:F:155:GLU:OE2  | 1:F:298:HIS:HE1  | 1.96                     | 0.49              |
| 1:D:256:ARG:NH2  | 1:D:274:THR:HG22 | 2.27                     | 0.49              |
| 1:H:81:GLU:HB3   | 1:H:250:ALA:O    | 2.13                     | 0.49              |
| 1:D:37:GLN:HG3   | 3:D:494:HOH:O    | 2.13                     | 0.49              |
| 1:C:122:LEU:HA   | 1:C:161:TRP:CD1  | 2.48                     | 0.49              |
| 1:F:140:GLY:O    | 1:F:144:GLU:HG2  | 2.13                     | 0.49              |
| 1:D:8:GLN:NE2    | 1:D:101:ARG:HH22 | 2.11                     | 0.48              |
| 1:I:105:VAL:HG22 | 1:I:191:LEU:HD23 | 1.94                     | 0.48              |
| 1:D:232:VAL:HG23 | 1:D:246:VAL:HG21 | 1.95                     | 0.48              |
| 1:D:101:ARG:NH1  | 1:D:264:GLU:HG2  | 2.28                     | 0.48              |
| 1:E:255:GLN:HB2  | 1:E:271:VAL:HG21 | 1.95                     | 0.48              |
| 1:I:76:ALA:O     | 1:I:80:ASN:ND2   | 2.46                     | 0.48              |
| 1:H:2:ILE:C      | 1:H:2:ILE:HD13   | 2.34                     | 0.48              |
| 1:A:304:GLU:HG2  | 1:A:309:LYS:CG   | 2.39                     | 0.48              |
| 1:H:99:SER:OG    | 1:H:264:GLU:HG2  | 2.13                     | 0.48              |
| 1:D:17:ALA:O     | 1:D:20:PHE:HB3   | 2.13                     | 0.48              |
| 1:F:237:GLN:O    | 1:F:238:ASN:ND2  | 2.46                     | 0.48              |
| 1:F:111:LYS:HD2  | 1:F:111:LYS:N    | 2.28                     | 0.48              |
| 1:C:255:GLN:HB2  | 1:C:271:VAL:HG21 | 1.95                     | 0.48              |
| 1:B:256:ARG:HA   | 1:B:259:THR:HG22 | 1.94                     | 0.48              |
| 1:C:53:VAL:HG23  | 1:C:242:ALA:HB1  | 1.96                     | 0.48              |
| 1:E:256:ARG:O    | 1:E:259:THR:HG22 | 2.13                     | 0.48              |
| 1:I:309:LYS:HZ2  | 1:I:309:LYS:HB3  | 1.78                     | 0.48              |
| 1:F:191:LEU:C    | 1:F:192:ILE:HG13 | 2.34                     | 0.48              |
| 1:I:100:GLY:O    | 1:I:264:GLU:HG3  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:107:TYR:O    | 1:I:211:THR:HA   | 2.14                     | 0.48              |
| 1:G:245:PHE:O    | 1:G:249:LEU:HG   | 2.13                     | 0.48              |
| 1:G:303:LEU:O    | 1:G:303:LEU:HD13 | 2.13                     | 0.48              |
| 1:B:8:GLN:HG3    | 1:B:9:HIS:N      | 2.28                     | 0.48              |
| 1:D:74:LEU:HD12  | 1:D:96:VAL:HG23  | 1.95                     | 0.48              |
| 1:E:200:PHE:CD1  | 1:E:200:PHE:N    | 2.81                     | 0.48              |
| 1:E:200:PHE:HD1  | 1:E:200:PHE:N    | 2.11                     | 0.48              |
| 1:D:197:TRP:CD1  | 1:D:211:THR:HG23 | 2.47                     | 0.48              |
| 1:C:72:GLU:OE1   | 1:C:73:PRO:HD2   | 2.13                     | 0.48              |
| 1:C:46:GLY:O     | 1:C:47:SER:C     | 2.51                     | 0.48              |
| 1:D:90:ALA:HB2   | 1:D:95:TRP:CD2   | 2.49                     | 0.48              |
| 1:F:72:GLU:OE2   | 1:F:239:LYS:HD3  | 2.14                     | 0.48              |
| 1:I:119:LYS:O    | 1:I:216:VAL:CG2  | 2.60                     | 0.48              |
| 1:C:22:ARG:HG2   | 3:C:433:HOH:O    | 2.13                     | 0.48              |
| 1:G:47:SER:HA    | 1:G:235:SER:CB   | 2.43                     | 0.48              |
| 1:A:111:LYS:HB3  | 1:A:111:LYS:HE2  | 1.74                     | 0.48              |
| 1:G:220:ASP:OD1  | 1:G:221:PRO:HD2  | 2.14                     | 0.48              |
| 1:B:255:GLN:O    | 1:B:259:THR:HG22 | 2.14                     | 0.48              |
| 1:G:71:LEU:HB3   | 1:G:94:ASP:HB2   | 1.96                     | 0.48              |
| 1:D:43:LYS:HZ3   | 1:D:68:ALA:CB    | 2.26                     | 0.48              |
| 1:H:256:ARG:HH11 | 1:H:256:ARG:CB   | 2.26                     | 0.48              |
| 1:F:58:GLN:HB2   | 3:F:508:HOH:O    | 2.13                     | 0.48              |
| 1:C:59:ILE:N     | 1:C:60:PRO:HD2   | 2.29                     | 0.48              |
| 1:H:76:ALA:O     | 1:H:80:ASN:ND2   | 2.46                     | 0.47              |
| 1:G:256:ARG:HH11 | 1:G:256:ARG:CB   | 2.27                     | 0.47              |
| 1:C:183:GLU:HG2  | 1:C:211:THR:CG2  | 2.44                     | 0.47              |
| 1:G:282:LYS:HA   | 1:G:282:LYS:HE2  | 1.95                     | 0.47              |
| 1:H:143:LEU:O    | 1:H:147:VAL:HG23 | 2.13                     | 0.47              |
| 1:F:240:ASP:OD1  | 1:F:241:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:117:LEU:HD22 | 1:B:214:ASN:HB2  | 1.95                     | 0.47              |
| 1:B:9:HIS:CE1    | 1:B:11:GLU:HG2   | 2.49                     | 0.47              |
| 1:I:80:ASN:ND2   | 1:I:80:ASN:N     | 2.61                     | 0.47              |
| 1:G:2:ILE:HG21   | 1:G:241:GLU:O    | 2.14                     | 0.47              |
| 1:G:5:TYR:CB     | 1:G:38:LEU:HD12  | 2.44                     | 0.47              |
| 1:E:41:GLN:O     | 1:E:42:ILE:C     | 2.51                     | 0.47              |
| 1:D:180:GLN:NE2  | 1:D:184:ASN:OD1  | 2.46                     | 0.47              |
| 1:C:113:SER:C    | 1:C:115:LYS:N    | 2.67                     | 0.47              |
| 1:D:34:LYS:HD2   | 1:D:35:GLY:H     | 1.79                     | 0.47              |
| 1:D:197:TRP:NE1  | 1:D:211:THR:HG23 | 2.30                     | 0.47              |
| 1:G:237:GLN:NE2  | 1:G:237:GLN:HA   | 2.29                     | 0.47              |
| 1:I:252:LYS:HD2  | 1:I:256:ARG:HD2  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:233:LEU:HD12 | 1:G:233:LEU:H    | 1.80                     | 0.47              |
| 1:B:117:LEU:HD12 | 1:B:117:LEU:N    | 2.29                     | 0.47              |
| 1:I:134:GLY:HA2  | 1:I:170:LYS:O    | 2.15                     | 0.47              |
| 1:E:59:ILE:N     | 1:E:60:PRO:CD    | 2.78                     | 0.47              |
| 1:D:267:LEU:CD2  | 1:D:280:ILE:HD13 | 2.44                     | 0.47              |
| 1:I:252:LYS:O    | 1:I:256:ARG:HG3  | 2.15                     | 0.47              |
| 1:I:72:GLU:HG2   | 1:I:234:LYS:HA   | 1.97                     | 0.47              |
| 1:D:279:PRO:HD2  | 1:D:282:LYS:HG3  | 1.96                     | 0.47              |
| 1:E:151:LYS:HE3  | 1:E:295:GLU:OE1  | 2.13                     | 0.47              |
| 1:C:170:LYS:HB2  | 1:C:170:LYS:HE3  | 1.67                     | 0.47              |
| 1:A:279:PRO:CG   | 1:A:282:LYS:HE3  | 2.44                     | 0.47              |
| 1:C:239:LYS:O    | 1:C:243:LYS:HG3  | 2.15                     | 0.47              |
| 1:D:43:LYS:HZ1   | 1:D:64:THR:C     | 2.18                     | 0.47              |
| 1:F:101:ARG:HB2  | 1:F:101:ARG:HH11 | 1.79                     | 0.47              |
| 1:I:98:LEU:C     | 1:I:267:LEU:HD22 | 2.34                     | 0.47              |
| 1:I:135:TYR:O    | 1:I:171:PRO:HA   | 2.15                     | 0.47              |
| 1:H:133:ILE:HG23 | 1:H:133:ILE:O    | 2.14                     | 0.47              |
| 1:I:127:PRO:HA   | 1:I:168:TYR:CD2  | 2.50                     | 0.47              |
| 1:E:74:LEU:HD13  | 1:E:96:VAL:HG23  | 1.97                     | 0.47              |
| 1:D:142:PHE:HE2  | 1:D:308:MET:HE1  | 1.80                     | 0.47              |
| 1:G:21:THR:O     | 1:G:25:GLY:HA2   | 2.15                     | 0.47              |
| 1:F:138:THR:HG23 | 3:F:441:HOH:O    | 2.13                     | 0.47              |
| 1:H:59:ILE:N     | 1:H:60:PRO:CD    | 2.77                     | 0.47              |
| 1:F:59:ILE:N     | 1:F:60:PRO:CD    | 2.77                     | 0.47              |
| 1:A:217:ARG:HG2  | 1:A:217:ARG:HH11 | 1.80                     | 0.47              |
| 1:A:57:GLU:HG2   | 1:A:101:ARG:NH1  | 2.29                     | 0.47              |
| 1:G:303:LEU:HD22 | 1:G:308:MET:HE3  | 1.97                     | 0.47              |
| 1:C:147:VAL:O    | 1:C:151:LYS:HG3  | 2.14                     | 0.47              |
| 1:D:240:ASP:O    | 1:D:244:LYS:HG3  | 2.15                     | 0.47              |
| 1:F:262:ARG:HH11 | 1:F:262:ARG:HG2  | 1.79                     | 0.47              |
| 1:D:197:TRP:HE1  | 1:D:211:THR:HG23 | 1.80                     | 0.47              |
| 1:A:135:TYR:CD2  | 1:A:137:PRO:HD3  | 2.50                     | 0.46              |
| 1:G:71:LEU:HB2   | 1:G:94:ASP:HB2   | 1.96                     | 0.46              |
| 1:E:122:LEU:HA   | 1:E:161:TRP:CD1  | 2.49                     | 0.46              |
| 1:H:71:LEU:HD23  | 1:H:233:LEU:HD12 | 1.97                     | 0.46              |
| 1:A:10:LYS:HE2   | 1:I:81:GLU:OE2   | 2.15                     | 0.46              |
| 1:H:55:TYR:CE1   | 1:H:249:LEU:HD13 | 2.51                     | 0.46              |
| 1:B:6:ASN:HD22   | 1:B:32:SER:HB3   | 1.79                     | 0.46              |
| 1:D:256:ARG:NH2  | 1:D:274:THR:CG2  | 2.78                     | 0.46              |
| 1:F:103:ARG:NH1  | 3:F:411:HOH:O    | 2.48                     | 0.46              |
| 1:H:99:SER:HB2   | 1:H:264:GLU:HG2  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:146:ILE:CD1  | 1:H:303:LEU:HD21 | 2.44                     | 0.46              |
| 1:H:252:LYS:HE2  | 1:H:270:HIS:HB3  | 1.97                     | 0.46              |
| 1:H:183:GLU:OE2  | 1:H:210:HIS:HB2  | 2.14                     | 0.46              |
| 1:D:65:LEU:N     | 1:D:65:LEU:HD22  | 2.30                     | 0.46              |
| 1:D:33:ALA:HB3   | 1:D:38:LEU:HG    | 1.97                     | 0.46              |
| 1:A:106:VAL:HG13 | 1:A:213:LEU:CD2  | 2.45                     | 0.46              |
| 1:F:228:SER:HB3  | 3:F:500:HOH:O    | 2.15                     | 0.46              |
| 1:I:18:ASP:O     | 1:I:22:ARG:NH1   | 2.49                     | 0.46              |
| 1:D:43:LYS:NZ    | 1:D:68:ALA:HB2   | 2.30                     | 0.46              |
| 1:G:301:ARG:O    | 1:G:305:GLN:HG3  | 2.15                     | 0.46              |
| 1:H:69:ASN:HB3   | 1:H:92:LYS:HZ2   | 1.80                     | 0.46              |
| 1:G:3:THR:CG2    | 1:G:31:ASN:ND2   | 2.79                     | 0.46              |
| 1:H:122:LEU:HA   | 1:H:161:TRP:CD1  | 2.51                     | 0.46              |
| 1:E:109:THR:HG21 | 1:E:212:ARG:HG2  | 1.96                     | 0.46              |
| 1:E:112:LEU:N    | 1:E:112:LEU:HD22 | 2.31                     | 0.46              |
| 1:G:112:LEU:HD21 | 1:G:132:ARG:HH12 | 1.79                     | 0.46              |
| 1:H:99:SER:CB    | 1:H:264:GLU:HG2  | 2.46                     | 0.46              |
| 1:I:101:ARG:HG2  | 1:I:264:GLU:CD   | 2.36                     | 0.46              |
| 1:B:258:LEU:C    | 1:B:260:ALA:H    | 2.19                     | 0.46              |
| 1:H:135:TYR:CE2  | 1:H:308:MET:HE3  | 2.50                     | 0.46              |
| 1:A:146:ILE:HD11 | 1:A:302:LEU:HD12 | 1.97                     | 0.46              |
| 1:A:279:PRO:HD2  | 1:A:282:LYS:HZ2  | 1.79                     | 0.46              |
| 1:B:41:GLN:O     | 1:B:45:GLU:CG    | 2.61                     | 0.46              |
| 1:B:117:LEU:HD12 | 1:B:117:LEU:H    | 1.79                     | 0.46              |
| 1:B:117:LEU:HD22 | 1:B:214:ASN:CB   | 2.45                     | 0.46              |
| 1:B:7:GLY:HA2    | 1:B:33:ALA:O     | 2.16                     | 0.46              |
| 1:A:159:LEU:HD12 | 1:A:159:LEU:HA   | 1.81                     | 0.46              |
| 1:G:2:ILE:O      | 1:G:4:VAL:HG23   | 2.15                     | 0.46              |
| 1:D:15:ALA:HB3   | 1:D:261:VAL:HG21 | 1.97                     | 0.46              |
| 1:B:245:PHE:CE2  | 1:B:249:LEU:HD11 | 2.51                     | 0.46              |
| 1:B:83:ARG:NH1   | 1:B:83:ARG:HB3   | 2.31                     | 0.46              |
| 1:D:125:ALA:HB1  | 1:D:164:GLY:HA3  | 1.98                     | 0.46              |
| 1:B:28:VAL:HG12  | 1:B:30:LEU:CD1   | 2.46                     | 0.46              |
| 1:H:192:ILE:N    | 1:H:192:ILE:CD1  | 2.78                     | 0.46              |
| 1:F:112:LEU:HD13 | 1:F:117:LEU:HD11 | 1.97                     | 0.46              |
| 1:C:82:THR:HB    | 1:C:267:LEU:HB3  | 1.97                     | 0.46              |
| 1:A:151:LYS:HD2  | 1:A:288:VAL:CG2  | 2.46                     | 0.46              |
| 1:F:11:GLU:HG3   | 1:F:261:VAL:HG12 | 1.96                     | 0.46              |
| 1:F:34:LYS:O     | 1:F:38:LEU:HD22  | 2.16                     | 0.46              |
| 1:D:242:ALA:O    | 1:D:246:VAL:HG23 | 2.16                     | 0.46              |
| 1:I:120:SER:HB3  | 1:I:123:ASN:ND2  | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:280:ILE:HG23 | 1:C:281:ALA:N    | 2.31                     | 0.46              |
| 1:C:245:PHE:O    | 1:C:248:PHE:HB3  | 2.15                     | 0.46              |
| 1:B:71:LEU:O     | 1:B:234:LYS:HE3  | 2.15                     | 0.46              |
| 1:A:137:PRO:HA   | 1:A:142:PHE:CD2  | 2.50                     | 0.45              |
| 1:C:92:LYS:O     | 1:C:93:LYS:HB3   | 2.15                     | 0.45              |
| 1:D:279:PRO:O    | 1:D:282:LYS:HG2  | 2.16                     | 0.45              |
| 1:H:219:ARG:O    | 1:H:286:PRO:HB3  | 2.17                     | 0.45              |
| 1:I:112:LEU:HB2  | 1:I:116:ASP:HB2  | 1.98                     | 0.45              |
| 1:I:159:LEU:O    | 1:I:163:LYS:HG3  | 2.16                     | 0.45              |
| 1:C:26:ILE:HD13  | 1:C:26:ILE:HA    | 1.85                     | 0.45              |
| 1:C:255:GLN:O    | 1:C:259:THR:HB   | 2.16                     | 0.45              |
| 1:F:174:LYS:HG3  | 1:F:176:SER:OG   | 2.16                     | 0.45              |
| 1:B:106:VAL:HG22 | 1:B:211:THR:CG2  | 2.45                     | 0.45              |
| 1:C:113:SER:O    | 1:C:115:LYS:N    | 2.44                     | 0.45              |
| 1:C:268:ASN:ND2  | 1:C:268:ASN:C    | 2.68                     | 0.45              |
| 1:A:300:THR:O    | 1:A:304:GLU:HG3  | 2.16                     | 0.45              |
| 1:A:130:LYS:HA   | 1:A:168:TYR:HB3  | 1.97                     | 0.45              |
| 1:I:31:ASN:N     | 1:I:31:ASN:ND2   | 2.65                     | 0.45              |
| 1:B:119:LYS:O    | 1:B:216:VAL:HG13 | 2.17                     | 0.45              |
| 1:E:72:GLU:CG    | 1:E:234:LYS:HA   | 2.45                     | 0.45              |
| 1:G:243:LYS:HG2  | 3:G:471:HOH:O    | 2.15                     | 0.45              |
| 1:D:74:LEU:CD1   | 1:D:96:VAL:HG23  | 2.47                     | 0.45              |
| 1:G:10:LYS:HE2   | 1:G:32:SER:HB3   | 1.99                     | 0.45              |
| 1:H:155:GLU:HG3  | 1:H:302:LEU:HD11 | 1.98                     | 0.45              |
| 1:C:219:ARG:O    | 1:C:286:PRO:HB3  | 2.16                     | 0.45              |
| 1:F:85:LYS:CE    | 1:F:219:ARG:HH22 | 2.29                     | 0.45              |
| 1:B:245:PHE:O    | 1:B:249:LEU:HG   | 2.16                     | 0.45              |
| 1:H:52:ASP:HA    | 1:H:236:SER:OG   | 2.17                     | 0.45              |
| 1:F:270:HIS:CG   | 1:I:237:GLN:HG3  | 2.51                     | 0.45              |
| 1:C:106:VAL:HG23 | 1:C:211:THR:OG1  | 2.16                     | 0.45              |
| 1:A:256:ARG:HG3  | 1:A:271:VAL:HG13 | 1.98                     | 0.45              |
| 1:B:291:THR:HG21 | 1:B:296:LYS:HE2  | 1.99                     | 0.45              |
| 1:E:54:PHE:CD2   | 1:E:65:LEU:HD12  | 2.52                     | 0.45              |
| 1:D:4:VAL:HG22   | 1:D:53:VAL:HG22  | 1.98                     | 0.45              |
| 1:G:20:PHE:C     | 1:G:22:ARG:N     | 2.70                     | 0.45              |
| 1:B:106:VAL:HB   | 1:B:192:ILE:HD11 | 1.97                     | 0.45              |
| 1:D:117:LEU:HD22 | 1:D:214:ASN:HB2  | 1.99                     | 0.45              |
| 1:D:137:PRO:HB3  | 1:D:308:MET:CE   | 2.47                     | 0.45              |
| 1:A:212:ARG:HG2  | 1:A:212:ARG:HH11 | 1.81                     | 0.45              |
| 1:I:22:ARG:O     | 1:I:23:ALA:HB2   | 2.17                     | 0.45              |
| 1:A:57:GLU:CG    | 1:A:101:ARG:NH1  | 2.79                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:233:LEU:CD1  | 1:F:233:LEU:N    | 2.80                     | 0.45              |
| 1:D:245:PHE:CE1  | 1:D:249:LEU:HD21 | 2.52                     | 0.45              |
| 1:B:105:VAL:HB   | 1:B:214:ASN:HB3  | 1.98                     | 0.45              |
| 1:E:192:ILE:HB   | 3:E:536:HOH:O    | 2.17                     | 0.45              |
| 1:A:181:ALA:O    | 1:A:186:GLU:HG2  | 2.17                     | 0.45              |
| 1:G:239:LYS:HB3  | 1:G:243:LYS:HE3  | 1.99                     | 0.45              |
| 1:A:252:LYS:HE3  | 1:A:256:ARG:HH22 | 1.78                     | 0.45              |
| 1:G:279:PRO:HB2  | 1:G:282:LYS:HG2  | 1.98                     | 0.45              |
| 1:B:193:ASN:HB3  | 1:B:195:TYR:CE1  | 2.52                     | 0.45              |
| 1:E:90:ALA:HB2   | 1:E:95:TRP:CE2   | 2.52                     | 0.45              |
| 1:H:76:ALA:HB1   | 1:H:80:ASN:HD21  | 1.81                     | 0.45              |
| 1:D:27:LYS:HZ3   | 1:D:27:LYS:HB3   | 1.81                     | 0.45              |
| 1:B:140:GLY:O    | 1:B:144:GLU:HG2  | 2.16                     | 0.45              |
| 1:F:31:ASN:HB2   | 3:G:476:HOH:O    | 2.17                     | 0.45              |
| 1:F:93:LYS:HD3   | 3:F:511:HOH:O    | 2.17                     | 0.45              |
| 1:D:43:LYS:HZ3   | 1:D:68:ALA:HB3   | 1.82                     | 0.44              |
| 1:B:151:LYS:HE2  | 1:B:295:GLU:OE2  | 2.17                     | 0.44              |
| 1:F:255:GLN:HE22 | 1:F:267:LEU:H    | 1.64                     | 0.44              |
| 1:I:265:TYR:CE2  | 1:I:283:LEU:HD11 | 2.51                     | 0.44              |
| 1:A:252:LYS:HE3  | 1:A:256:ARG:CZ   | 2.46                     | 0.44              |
| 1:H:62:LEU:HD13  | 1:H:95:TRP:HB2   | 1.98                     | 0.44              |
| 1:G:80:ASN:HA    | 1:G:83:ARG:HB2   | 1.99                     | 0.44              |
| 1:E:59:ILE:HB    | 1:E:60:PRO:HD3   | 1.98                     | 0.44              |
| 1:G:120:SER:HB3  | 1:G:123:ASN:ND2  | 2.33                     | 0.44              |
| 1:A:159:LEU:HG   | 1:A:163:LYS:HE3  | 1.99                     | 0.44              |
| 1:E:262:ARG:CG   | 1:E:264:GLU:HG3  | 2.44                     | 0.44              |
| 1:H:21:THR:HG22  | 1:H:21:THR:O     | 2.17                     | 0.44              |
| 1:H:122:LEU:CD2  | 1:H:149:ILE:HD13 | 2.47                     | 0.44              |
| 1:C:218:HIS:HB3  | 3:C:500:HOH:O    | 2.18                     | 0.44              |
| 1:C:54:PHE:CE2   | 1:C:56:SER:HB3   | 2.52                     | 0.44              |
| 1:A:146:ILE:HD12 | 1:A:158:ALA:HB1  | 1.99                     | 0.44              |
| 1:I:256:ARG:HG2  | 1:I:271:VAL:HG13 | 1.99                     | 0.44              |
| 1:H:57:GLU:HB2   | 1:H:101:ARG:HH22 | 1.80                     | 0.44              |
| 1:E:41:GLN:O     | 1:E:44:GLU:N     | 2.49                     | 0.44              |
| 1:B:30:LEU:N     | 1:B:30:LEU:HD12  | 2.33                     | 0.44              |
| 1:C:54:PHE:CZ    | 1:C:56:SER:HB3   | 2.52                     | 0.44              |
| 1:D:94:ASP:OD1   | 1:D:94:ASP:N     | 2.49                     | 0.44              |
| 1:H:76:ALA:HB1   | 1:H:80:ASN:ND2   | 2.32                     | 0.44              |
| 1:B:51:ALA:HB3   | 1:B:233:LEU:CD2  | 2.47                     | 0.44              |
| 1:F:85:LYS:CE    | 1:F:219:ARG:HH12 | 2.30                     | 0.44              |
| 1:D:256:ARG:HD2  | 1:D:256:ARG:HA   | 1.71                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:161:TRP:HE3  | 1:E:162:LEU:HD12 | 1.82                     | 0.44              |
| 1:A:8:GLN:CG     | 1:A:9:HIS:N      | 2.80                     | 0.44              |
| 1:E:300:THR:HG23 | 1:E:309:LYS:HE2  | 2.00                     | 0.44              |
| 1:H:142:PHE:O    | 1:H:145:GLN:HB3  | 2.17                     | 0.44              |
| 1:B:225:VAL:HG23 | 1:B:285:ALA:HB2  | 2.00                     | 0.44              |
| 1:E:71:LEU:O     | 1:E:234:LYS:HE3  | 2.18                     | 0.44              |
| 1:D:174:LYS:HE2  | 3:D:466:HOH:O    | 2.16                     | 0.44              |
| 1:H:2:ILE:HD11   | 1:H:53:VAL:CG2   | 2.43                     | 0.44              |
| 1:C:119:LYS:HE3  | 3:C:489:HOH:O    | 2.17                     | 0.44              |
| 1:C:303:LEU:HG   | 1:C:309:LYS:CA   | 2.46                     | 0.44              |
| 1:I:78:THR:O     | 1:I:81:GLU:HB2   | 2.18                     | 0.44              |
| 1:E:90:ALA:HB2   | 1:E:95:TRP:CD2   | 2.53                     | 0.44              |
| 1:E:107:TYR:CD1  | 1:E:117:LEU:HD11 | 2.52                     | 0.44              |
| 1:A:162:LEU:HB3  | 1:A:306:ALA:CB   | 2.48                     | 0.44              |
| 1:H:266:PRO:HA   | 3:H:479:HOH:O    | 2.17                     | 0.44              |
| 1:B:90:ALA:O     | 1:B:93:LYS:HE2   | 2.18                     | 0.44              |
| 1:I:81:GLU:OE1   | 1:I:268:ASN:ND2  | 2.51                     | 0.44              |
| 1:G:5:TYR:CD2    | 1:G:38:LEU:HD12  | 2.53                     | 0.44              |
| 1:F:279:PRO:O    | 1:F:282:LYS:HB2  | 2.17                     | 0.44              |
| 1:H:2:ILE:HG13   | 1:H:242:ALA:HA   | 2.00                     | 0.44              |
| 1:E:151:LYS:NZ   | 1:E:295:GLU:OE1  | 2.47                     | 0.44              |
| 1:B:13:ALA:HA    | 1:B:16:VAL:HG12  | 2.00                     | 0.44              |
| 1:G:205:GLY:O    | 1:G:207:GLN:N    | 2.51                     | 0.44              |
| 1:G:223:ALA:HB3  | 1:G:286:PRO:HD3  | 2.00                     | 0.44              |
| 1:E:174:LYS:HB2  | 1:E:177:VAL:HG23 | 1.99                     | 0.44              |
| 1:I:45:GLU:HB2   | 1:I:49:SER:HB2   | 1.99                     | 0.43              |
| 1:I:255:GLN:HB2  | 1:I:271:VAL:HG21 | 1.99                     | 0.43              |
| 1:A:9:HIS:NE2    | 1:A:11:GLU:HB3   | 2.33                     | 0.43              |
| 1:D:117:LEU:HD22 | 1:D:214:ASN:CB   | 2.48                     | 0.43              |
| 1:C:140:GLY:O    | 1:C:144:GLU:HG2  | 2.19                     | 0.43              |
| 1:C:256:ARG:HH12 | 1:C:272:VAL:HB   | 1.82                     | 0.43              |
| 1:G:298:HIS:O    | 1:G:302:LEU:HG   | 2.18                     | 0.43              |
| 1:G:9:HIS:HB3    | 1:G:12:ALA:CB    | 2.46                     | 0.43              |
| 1:D:72:GLU:OE2   | 1:D:234:LYS:HG2  | 2.18                     | 0.43              |
| 1:H:252:LYS:O    | 1:H:256:ARG:HG3  | 2.18                     | 0.43              |
| 1:G:145:GLN:O    | 1:G:149:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:6:ASN:HB2    | 1:C:30:LEU:HD22  | 2.00                     | 0.43              |
| 1:D:217:ARG:HH11 | 1:D:217:ARG:HG2  | 1.84                     | 0.43              |
| 1:C:5:TYR:CE1    | 1:C:51:ALA:HB2   | 2.53                     | 0.43              |
| 1:E:130:LYS:O    | 1:E:132:ARG:HG3  | 2.19                     | 0.43              |
| 1:C:155:GLU:OE2  | 1:C:298:HIS:HE1  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:255:GLN:HE22 | 1:E:267:LEU:N    | 2.14                     | 0.43              |
| 1:D:130:LYS:HE3  | 1:D:131:ASN:ND2  | 2.34                     | 0.43              |
| 1:A:101:ARG:HG2  | 1:A:101:ARG:O    | 2.19                     | 0.43              |
| 1:B:292:THR:O    | 1:B:296:LYS:HG3  | 2.18                     | 0.43              |
| 1:B:101:ARG:HG3  | 1:B:264:GLU:HG2  | 2.01                     | 0.43              |
| 1:C:248:PHE:CE2  | 1:C:254:GLY:HA2  | 2.54                     | 0.43              |
| 1:C:108:ASP:OD2  | 1:C:110:ARG:HB2  | 2.18                     | 0.43              |
| 1:D:223:ALA:HB3  | 1:D:286:PRO:HD3  | 2.01                     | 0.43              |
| 1:E:57:GLU:HG2   | 1:E:58:GLN:HG2   | 2.00                     | 0.43              |
| 1:F:1:ASP:HA     | 1:F:26:ILE:HG23  | 2.00                     | 0.43              |
| 1:C:12:ALA:HB1   | 1:C:258:LEU:CD1  | 2.49                     | 0.43              |
| 1:G:130:LYS:HA   | 1:G:168:TYR:CB   | 2.46                     | 0.43              |
| 1:H:9:HIS:CD2    | 1:H:10:LYS:N     | 2.87                     | 0.43              |
| 1:I:255:GLN:HG3  | 1:I:268:ASN:HB2  | 2.01                     | 0.43              |
| 1:E:42:ILE:HD12  | 1:E:65:LEU:HD11  | 2.01                     | 0.43              |
| 1:D:183:GLU:OE1  | 1:D:211:THR:HG22 | 2.19                     | 0.43              |
| 1:F:144:GLU:OE1  | 1:F:144:GLU:HA   | 2.19                     | 0.43              |
| 1:F:232:VAL:HG13 | 1:F:242:ALA:HB1  | 2.01                     | 0.43              |
| 1:I:6:ASN:ND2    | 1:I:8:GLN:H      | 2.17                     | 0.43              |
| 1:I:22:ARG:HG3   | 1:I:22:ARG:HH11  | 1.84                     | 0.43              |
| 1:D:265:TYR:CD1  | 1:D:265:TYR:N    | 2.86                     | 0.43              |
| 1:E:45:GLU:H     | 1:E:45:GLU:HG2   | 1.66                     | 0.43              |
| 1:A:106:VAL:CG2  | 1:A:192:ILE:HG12 | 2.48                     | 0.43              |
| 1:I:34:LYS:CG    | 1:I:37:GLN:HG3   | 2.48                     | 0.43              |
| 1:H:20:PHE:CE2   | 1:H:26:ILE:HB    | 2.54                     | 0.43              |
| 1:D:55:TYR:CE1   | 1:D:249:LEU:HD13 | 2.54                     | 0.43              |
| 1:I:20:PHE:CE2   | 1:I:26:ILE:HB    | 2.54                     | 0.43              |
| 1:E:112:LEU:HD12 | 1:E:116:ASP:HB2  | 2.01                     | 0.43              |
| 1:A:182:VAL:HG12 | 1:A:211:THR:HG22 | 2.01                     | 0.43              |
| 1:I:180:GLN:O    | 1:I:184:ASN:ND2  | 2.51                     | 0.43              |
| 1:G:267:LEU:HD23 | 1:G:267:LEU:HA   | 1.86                     | 0.43              |
| 1:D:255:GLN:HB2  | 1:D:271:VAL:HG21 | 2.00                     | 0.42              |
| 1:F:11:GLU:HG3   | 1:F:261:VAL:CG1  | 2.49                     | 0.42              |
| 1:B:43:LYS:HZ1   | 1:B:64:THR:HB    | 1.84                     | 0.42              |
| 1:D:80:ASN:HA    | 1:D:83:ARG:HD3   | 1.99                     | 0.42              |
| 1:I:99:SER:HA    | 1:I:267:LEU:HD13 | 2.01                     | 0.42              |
| 1:H:117:LEU:CD1  | 1:H:117:LEU:N    | 2.82                     | 0.42              |
| 1:A:38:LEU:O     | 1:A:41:GLN:HB3   | 2.19                     | 0.42              |
| 1:I:303:LEU:HD23 | 1:I:308:MET:SD   | 2.59                     | 0.42              |
| 1:F:7:GLY:HA2    | 1:F:33:ALA:O     | 2.19                     | 0.42              |
| 1:D:115:LYS:HD2  | 1:D:116:ASP:OD1  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:ARG:HD2  | 1:A:145:GLN:HB2  | 2.01                     | 0.42              |
| 1:B:40:GLY:O     | 1:B:44:GLU:HG2   | 2.19                     | 0.42              |
| 1:A:217:ARG:NH1  | 1:A:278:GLU:OE1  | 2.52                     | 0.42              |
| 1:A:59:ILE:N     | 1:A:60:PRO:CD    | 2.82                     | 0.42              |
| 1:F:16:VAL:HG11  | 1:F:249:LEU:CD2  | 2.49                     | 0.42              |
| 1:H:113:SER:O    | 1:H:117:LEU:HD13 | 2.20                     | 0.42              |
| 1:C:26:ILE:HG13  | 1:C:241:GLU:OE1  | 2.19                     | 0.42              |
| 1:D:256:ARG:NE   | 3:D:411:HOH:O    | 2.51                     | 0.42              |
| 1:A:309:LYS:HG3  | 1:A:309:LYS:O    | 2.19                     | 0.42              |
| 1:I:234:LYS:HD2  | 1:I:234:LYS:C    | 2.39                     | 0.42              |
| 1:C:3:THR:O      | 1:C:51:ALA:HA    | 2.19                     | 0.42              |
| 1:A:203:GLU:HG3  | 1:A:204:LYS:N    | 2.34                     | 0.42              |
| 1:D:152:LEU:O    | 1:D:153:LYS:HD3  | 2.19                     | 0.42              |
| 1:C:256:ARG:HH12 | 1:C:272:VAL:H    | 1.58                     | 0.42              |
| 1:C:306:ALA:HB3  | 1:C:308:MET:HE3  | 2.01                     | 0.42              |
| 1:G:67:ALA:HA    | 1:G:92:LYS:HZ2   | 1.84                     | 0.42              |
| 1:C:27:LYS:HD3   | 1:C:27:LYS:N     | 2.35                     | 0.42              |
| 1:C:228:SER:HB3  | 3:C:476:HOH:O    | 2.18                     | 0.42              |
| 1:F:104:VAL:HG12 | 1:F:215:PHE:CE2  | 2.55                     | 0.42              |
| 1:B:90:ALA:HB2   | 1:B:95:TRP:CE2   | 2.55                     | 0.42              |
| 1:G:69:ASN:O     | 1:G:234:LYS:HG3  | 2.20                     | 0.42              |
| 1:D:252:LYS:HG3  | 1:D:253:GLU:N    | 2.34                     | 0.42              |
| 1:D:303:LEU:CD2  | 1:D:308:MET:HE1  | 2.50                     | 0.42              |
| 1:H:180:GLN:HA   | 1:H:183:GLU:HB3  | 2.00                     | 0.42              |
| 1:H:93:LYS:HE3   | 3:H:466:HOH:O    | 2.19                     | 0.42              |
| 1:D:58:GLN:HG3   | 1:D:60:PRO:HD2   | 2.00                     | 0.42              |
| 1:E:18:ASP:O     | 1:E:22:ARG:HG3   | 2.19                     | 0.42              |
| 1:D:193:ASN:HB3  | 1:D:195:TYR:CE1  | 2.54                     | 0.42              |
| 1:F:84:GLY:O     | 1:F:85:LYS:C     | 2.57                     | 0.42              |
| 1:G:2:ILE:CG1    | 1:G:28:VAL:HG22  | 2.50                     | 0.42              |
| 1:G:146:ILE:O    | 1:G:150:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:267:LEU:HD23 | 1:A:267:LEU:HA   | 1.91                     | 0.42              |
| 1:H:45:GLU:HB2   | 1:H:49:SER:HB2   | 2.02                     | 0.42              |
| 1:D:12:ALA:O     | 1:D:16:VAL:HG23  | 2.19                     | 0.42              |
| 1:D:245:PHE:O    | 1:D:249:LEU:HG   | 2.20                     | 0.42              |
| 1:E:6:ASN:ND2    | 1:E:8:GLN:H      | 2.17                     | 0.42              |
| 1:I:8:GLN:HE21   | 1:I:8:GLN:HB2    | 1.67                     | 0.42              |
| 1:B:24:THR:HB    | 1:B:26:ILE:HG13  | 2.02                     | 0.42              |
| 1:F:83:ARG:HD3   | 3:F:457:HOH:O    | 2.20                     | 0.42              |
| 1:B:52:ASP:HA    | 1:B:236:SER:HB2  | 2.01                     | 0.42              |
| 1:B:106:VAL:CG2  | 1:B:211:THR:HG23 | 2.45                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:400:ZRC:O3A  | 2:D:400:ZRC:O31  | 2.38                     | 0.42              |
| 1:D:144:GLU:CG   | 1:D:224:LEU:HD21 | 2.49                     | 0.42              |
| 1:A:75:PRO:CD    | 1:A:243:LYS:HZ2  | 2.32                     | 0.42              |
| 1:D:86:GLY:HA2   | 1:D:287:GLN:HG2  | 2.00                     | 0.42              |
| 1:E:57:GLU:O     | 1:E:101:ARG:NH2  | 2.52                     | 0.42              |
| 1:D:199:ALA:O    | 1:D:203:GLU:OE1  | 2.37                     | 0.42              |
| 1:H:174:LYS:HD3  | 1:H:174:LYS:HA   | 1.83                     | 0.42              |
| 1:H:301:ARG:HA   | 1:H:304:GLU:OE1  | 2.19                     | 0.42              |
| 1:I:291:THR:HA   | 1:I:295:GLU:OE1  | 2.20                     | 0.42              |
| 1:H:176:SER:O    | 1:H:180:GLN:NE2  | 2.53                     | 0.42              |
| 1:E:112:LEU:HD12 | 1:E:116:ASP:CB   | 2.50                     | 0.42              |
| 1:B:17:ALA:O     | 1:B:20:PHE:HB3   | 2.20                     | 0.42              |
| 1:D:265:TYR:CZ   | 1:D:283:LEU:HD11 | 2.56                     | 0.41              |
| 1:H:42:ILE:HD12  | 1:H:65:LEU:HD11  | 2.02                     | 0.41              |
| 1:H:130:LYS:O    | 1:H:132:ARG:HG3  | 2.20                     | 0.41              |
| 1:C:198:HIS:HB3  | 1:C:275:PHE:CD2  | 2.54                     | 0.41              |
| 1:F:173:ALA:HB3  | 1:F:174:LYS:HE3  | 2.01                     | 0.41              |
| 1:E:71:LEU:C     | 1:E:234:LYS:HG3  | 2.40                     | 0.41              |
| 1:A:279:PRO:HD2  | 1:A:282:LYS:HZ1  | 1.83                     | 0.41              |
| 1:H:117:LEU:HD23 | 1:H:214:ASN:HB2  | 2.02                     | 0.41              |
| 1:G:143:LEU:O    | 1:G:147:VAL:HG23 | 2.19                     | 0.41              |
| 1:A:76:ALA:O     | 1:A:80:ASN:HB2   | 2.20                     | 0.41              |
| 1:A:206:VAL:HA   | 1:A:209:VAL:HG22 | 2.01                     | 0.41              |
| 1:I:92:LYS:HB2   | 1:I:94:ASP:OD2   | 2.20                     | 0.41              |
| 1:C:121:VAL:CG2  | 1:C:216:VAL:HG21 | 2.50                     | 0.41              |
| 1:B:106:VAL:CG2  | 1:B:211:THR:CG2  | 2.98                     | 0.41              |
| 1:C:130:LYS:O    | 1:C:132:ARG:HG3  | 2.19                     | 0.41              |
| 1:C:233:LEU:N    | 1:C:233:LEU:HD12 | 2.35                     | 0.41              |
| 1:I:109:THR:O    | 1:I:109:THR:CG2  | 2.68                     | 0.41              |
| 1:G:234:LYS:NZ   | 1:G:234:LYS:CB   | 2.79                     | 0.41              |
| 1:B:59:ILE:N     | 1:B:60:PRO:CD    | 2.84                     | 0.41              |
| 1:E:152:LEU:HD21 | 1:E:288:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:106:VAL:HG22 | 1:A:192:ILE:HG12 | 2.02                     | 0.41              |
| 1:E:109:THR:HG21 | 1:E:212:ARG:CG   | 2.50                     | 0.41              |
| 1:D:59:ILE:N     | 1:D:60:PRO:CD    | 2.84                     | 0.41              |
| 1:F:217:ARG:HG2  | 1:F:217:ARG:HH11 | 1.85                     | 0.41              |
| 1:D:134:GLY:HA2  | 1:D:170:LYS:O    | 2.20                     | 0.41              |
| 1:D:225:VAL:HG23 | 1:D:285:ALA:HB2  | 2.02                     | 0.41              |
| 1:B:131:ASN:CA   | 1:B:170:LYS:HE3  | 2.51                     | 0.41              |
| 1:G:69:ASN:C     | 1:G:71:LEU:H     | 2.24                     | 0.41              |
| 1:C:79:ILE:HD12  | 1:C:93:LYS:CG    | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:178:ALA:CB   | 1:F:192:ILE:HD11 | 2.50                     | 0.41              |
| 1:G:233:LEU:CD1  | 1:G:233:LEU:H    | 2.33                     | 0.41              |
| 1:F:255:GLN:NE2  | 1:F:268:ASN:H    | 2.19                     | 0.41              |
| 1:I:298:HIS:HD2  | 3:I:456:HOH:O    | 2.02                     | 0.41              |
| 1:C:90:ALA:HB2   | 1:C:95:TRP:CD2   | 2.55                     | 0.41              |
| 1:C:149:ILE:O    | 1:C:153:LYS:N    | 2.47                     | 0.41              |
| 1:C:55:TYR:CD1   | 1:C:249:LEU:HD13 | 2.56                     | 0.41              |
| 1:H:2:ILE:O      | 1:H:28:VAL:HA    | 2.20                     | 0.41              |
| 1:C:236:SER:OG   | 1:C:239:LYS:HE2  | 2.21                     | 0.41              |
| 1:C:48:ARG:HD2   | 3:C:472:HOH:O    | 2.21                     | 0.41              |
| 1:E:252:LYS:HE2  | 1:E:268:ASN:OD1  | 2.20                     | 0.41              |
| 1:A:8:GLN:HG2    | 1:A:9:HIS:H      | 1.86                     | 0.41              |
| 1:F:38:LEU:O     | 1:F:42:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:237:GLN:CD   | 1:B:237:GLN:H    | 2.22                     | 0.41              |
| 1:D:107:TYR:CD1  | 1:D:117:LEU:HD21 | 2.55                     | 0.41              |
| 1:B:103:ARG:NH2  | 3:B:403:HOH:O    | 2.40                     | 0.41              |
| 1:D:18:ASP:O     | 1:D:22:ARG:HG3   | 2.20                     | 0.41              |
| 1:E:83:ARG:HG3   | 1:E:83:ARG:HH11  | 1.84                     | 0.41              |
| 1:C:268:ASN:HA   | 1:C:269:PRO:HD2  | 1.94                     | 0.41              |
| 1:D:65:LEU:CD2   | 1:D:65:LEU:N     | 2.84                     | 0.41              |
| 1:E:268:ASN:ND2  | 1:E:269:PRO:HD2  | 2.36                     | 0.41              |
| 1:F:240:ASP:O    | 1:F:244:LYS:HG3  | 2.20                     | 0.41              |
| 1:C:101:ARG:O    | 1:C:225:VAL:HA   | 2.21                     | 0.41              |
| 1:C:225:VAL:HG23 | 1:C:285:ALA:HB2  | 2.02                     | 0.41              |
| 1:C:268:ASN:ND2  | 1:C:270:HIS:H    | 2.18                     | 0.41              |
| 1:C:236:SER:OG   | 1:C:239:LYS:HG3  | 2.20                     | 0.41              |
| 1:G:70:LEU:C     | 1:G:234:LYS:HG2  | 2.41                     | 0.41              |
| 1:G:164:GLY:O    | 1:G:168:TYR:CE1  | 2.74                     | 0.41              |
| 1:H:6:ASN:O      | 1:H:32:SER:HA    | 2.19                     | 0.41              |
| 1:G:2:ILE:CD1    | 1:G:28:VAL:HG22  | 2.47                     | 0.41              |
| 1:C:5:TYR:HE2    | 1:C:41:GLN:HG2   | 1.86                     | 0.41              |
| 1:A:51:ALA:HB3   | 1:A:233:LEU:HD22 | 2.02                     | 0.41              |
| 1:H:137:PRO:HA   | 1:H:142:PHE:CD2  | 2.56                     | 0.41              |
| 1:G:265:TYR:CE2  | 1:G:277:LEU:HB3  | 2.55                     | 0.41              |
| 1:A:71:LEU:HB2   | 1:A:94:ASP:HB2   | 2.02                     | 0.41              |
| 1:D:51:ALA:HB3   | 1:D:233:LEU:CD2  | 2.51                     | 0.41              |
| 1:C:92:LYS:O     | 1:C:93:LYS:CB    | 2.69                     | 0.41              |
| 1:F:85:LYS:HB3   | 1:F:86:GLY:H     | 1.55                     | 0.41              |
| 1:C:303:LEU:HG   | 1:C:309:LYS:H    | 1.86                     | 0.41              |
| 1:I:255:GLN:HG3  | 1:I:268:ASN:CB   | 2.51                     | 0.41              |
| 1:H:111:LYS:HD2  | 1:H:188:ASP:OD1  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:147:VAL:HG11 | 1:B:291:THR:HG23 | 2.03                     | 0.41              |
| 1:G:104:VAL:CG1  | 1:G:105:VAL:N    | 2.83                     | 0.41              |
| 1:H:60:PRO:HA    | 1:H:63:ALA:HB3   | 2.01                     | 0.41              |
| 1:H:74:LEU:HA    | 1:H:75:PRO:HD3   | 1.91                     | 0.41              |
| 1:D:184:ASN:HB2  | 1:D:186:GLU:CG   | 2.51                     | 0.41              |
| 1:D:103:ARG:HD3  | 3:D:431:HOH:O    | 2.21                     | 0.41              |
| 1:B:202:ARG:HH22 | 1:B:274:THR:C    | 2.25                     | 0.41              |
| 1:E:151:LYS:CE   | 1:E:295:GLU:OE1  | 2.68                     | 0.41              |
| 1:D:124:TYR:HB2  | 3:D:501:HOH:O    | 2.21                     | 0.41              |
| 1:F:46:GLY:O     | 1:F:48:ARG:N     | 2.54                     | 0.41              |
| 1:H:144:GLU:OE2  | 1:H:291:THR:HG21 | 2.20                     | 0.41              |
| 1:I:136:VAL:O    | 1:I:139:SER:HB3  | 2.20                     | 0.41              |
| 1:D:175:ASN:HD22 | 1:D:192:ILE:HG22 | 1.86                     | 0.41              |
| 1:B:2:ILE:HG22   | 1:B:52:ASP:OD1   | 2.20                     | 0.41              |
| 1:E:262:ARG:HE   | 1:E:264:GLU:CD   | 2.24                     | 0.41              |
| 1:G:3:THR:HB     | 1:G:50:PRO:O     | 2.20                     | 0.41              |
| 1:D:181:ALA:HA   | 1:D:186:GLU:OE1  | 2.20                     | 0.41              |
| 1:H:218:HIS:O    | 1:H:219:ARG:HB2  | 2.21                     | 0.41              |
| 1:C:166:LYS:HD3  | 1:C:166:LYS:C    | 2.40                     | 0.41              |
| 1:D:106:VAL:HG21 | 1:D:179:LEU:CD1  | 2.51                     | 0.41              |
| 1:H:143:LEU:HD11 | 1:H:299:ALA:HB3  | 2.03                     | 0.41              |
| 1:B:71:LEU:HD12  | 1:B:94:ASP:OD2   | 2.21                     | 0.41              |
| 1:A:57:GLU:HG2   | 1:A:101:ARG:HH12 | 1.86                     | 0.40              |
| 1:C:304:GLU:CG   | 1:C:309:LYS:HG3  | 2.51                     | 0.40              |
| 1:H:106:VAL:HG12 | 1:H:192:ILE:CD1  | 2.51                     | 0.40              |
| 1:G:9:HIS:HB2    | 1:G:262:ARG:HD2  | 2.03                     | 0.40              |
| 1:H:117:LEU:HD23 | 1:H:214:ASN:CG   | 2.42                     | 0.40              |
| 1:I:90:ALA:HB2   | 1:I:95:TRP:CD2   | 2.55                     | 0.40              |
| 1:H:178:ALA:O    | 1:H:182:VAL:HG23 | 2.21                     | 0.40              |
| 1:G:111:LYS:HD2  | 3:G:455:HOH:O    | 2.20                     | 0.40              |
| 1:G:256:ARG:NH1  | 1:G:256:ARG:CB   | 2.85                     | 0.40              |
| 1:A:217:ARG:HB3  | 1:A:284:GLU:OE2  | 2.20                     | 0.40              |
| 1:C:52:ASP:HB3   | 1:C:242:ALA:HB2  | 2.03                     | 0.40              |
| 1:G:182:VAL:HG12 | 1:G:211:THR:HG22 | 2.04                     | 0.40              |
| 1:I:20:PHE:HZ    | 1:I:26:ILE:HD12  | 1.86                     | 0.40              |
| 1:H:59:ILE:H     | 1:H:60:PRO:HD2   | 1.85                     | 0.40              |
| 1:G:39:ALA:HA    | 1:G:65:LEU:HD11  | 2.03                     | 0.40              |
| 1:H:149:ILE:HG12 | 1:H:221:PRO:HB3  | 2.03                     | 0.40              |
| 1:I:112:LEU:C    | 1:I:112:LEU:HD12 | 2.41                     | 0.40              |
| 1:A:206:VAL:O    | 1:A:209:VAL:HG22 | 2.21                     | 0.40              |
| 1:I:74:LEU:HA    | 1:I:75:PRO:HD3   | 1.87                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:10:LYS:O     | 1:C:14:GLN:HG2   | 2.21                     | 0.40              |
| 2:C:400:ZRC:O2A  | 2:C:400:ZRC:O23  | 2.39                     | 0.40              |
| 1:I:35:GLY:HA3   | 1:I:57:GLU:OE2   | 2.21                     | 0.40              |
| 1:H:2:ILE:CG2    | 1:H:28:VAL:HG12  | 2.51                     | 0.40              |
| 1:G:202:ARG:NH2  | 1:G:274:THR:CG2  | 2.74                     | 0.40              |
| 1:C:52:ASP:CA    | 1:C:236:SER:HB2  | 2.45                     | 0.40              |
| 1:H:33:ALA:HB3   | 1:H:38:LEU:CG    | 2.49                     | 0.40              |
| 1:D:127:PRO:HG3  | 1:D:168:TYR:CZ   | 2.55                     | 0.40              |
| 1:B:21:THR:O     | 1:B:25:GLY:N     | 2.46                     | 0.40              |
| 1:B:297:GLU:O    | 1:B:301:ARG:HG2  | 2.21                     | 0.40              |
| 1:C:251:GLY:O    | 1:C:255:GLN:HG2  | 2.22                     | 0.40              |
| 1:I:255:GLN:HB3  | 1:I:271:VAL:HG21 | 2.03                     | 0.40              |
| 1:D:180:GLN:HE21 | 1:D:184:ASN:CG   | 2.23                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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     | 307/309 (99%)   | 288 (94%)  | 19 (6%)  | 0        | 100         | 100 |
| 1   | B     | 307/309 (99%)   | 288 (94%)  | 17 (6%)  | 2 (1%)   | 26          | 6   |
| 1   | C     | 307/309 (99%)   | 283 (92%)  | 20 (6%)  | 4 (1%)   | 15          | 2   |
| 1   | D     | 307/309 (99%)   | 291 (95%)  | 14 (5%)  | 2 (1%)   | 26          | 6   |
| 1   | E     | 307/309 (99%)   | 291 (95%)  | 12 (4%)  | 4 (1%)   | 15          | 2   |
| 1   | F     | 307/309 (99%)   | 292 (95%)  | 13 (4%)  | 2 (1%)   | 26          | 6   |
| 1   | G     | 307/309 (99%)   | 281 (92%)  | 23 (8%)  | 3 (1%)   | 19          | 3   |
| 1   | H     | 307/309 (99%)   | 287 (94%)  | 18 (6%)  | 2 (1%)   | 26          | 6   |
| 1   | I     | 307/309 (99%)   | 291 (95%)  | 15 (5%)  | 1 (0%)   | 46          | 19  |
| All | All   | 2763/2781 (99%) | 2592 (94%) | 151 (6%) | 20 (1%)  | 26          | 6   |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 195 | TYR  |
| 1   | F     | 85  | LYS  |
| 1   | C     | 46  | GLY  |
| 1   | D     | 252 | LYS  |
| 1   | F     | 47  | SER  |
| 1   | G     | 8   | GLN  |
| 1   | G     | 206 | VAL  |
| 1   | H     | 308 | MET  |
| 1   | I     | 23  | ALA  |
| 1   | E     | 114 | GLU  |
| 1   | B     | 93  | LYS  |
| 1   | C     | 47  | SER  |
| 1   | C     | 114 | GLU  |
| 1   | E     | 217 | ARG  |
| 1   | B     | 217 | ARG  |
| 1   | E     | 35  | GLY  |
| 1   | H     | 2   | ILE  |
| 1   | E     | 42  | ILE  |
| 1   | G     | 2   | ILE  |
| 1   | D     | 192 | 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     | 245/245 (100%) | 233 (95%) | 12 (5%)  | 31          | 5  |
| 1   | B     | 245/245 (100%) | 233 (95%) | 12 (5%)  | 31          | 5  |
| 1   | C     | 245/245 (100%) | 234 (96%) | 11 (4%)  | 34          | 6  |
| 1   | D     | 245/245 (100%) | 233 (95%) | 12 (5%)  | 31          | 5  |
| 1   | E     | 245/245 (100%) | 236 (96%) | 9 (4%)   | 41          | 10 |
| 1   | F     | 245/245 (100%) | 235 (96%) | 10 (4%)  | 37          | 7  |
| 1   | G     | 245/245 (100%) | 238 (97%) | 7 (3%)   | 50          | 16 |
| 1   | H     | 245/245 (100%) | 235 (96%) | 10 (4%)  | 37          | 7  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |
|-----|-------|------------------|------------|----------|-------------|
| 1   | I     | 245/245 (100%)   | 232 (95%)  | 13 (5%)  | 28 4        |
| All | All   | 2205/2205 (100%) | 2109 (96%) | 96 (4%)  | 35 7        |

All (96) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 45  | GLU  |
| 1   | A     | 60  | PRO  |
| 1   | A     | 80  | ASN  |
| 1   | A     | 101 | ARG  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 106 | VAL  |
| 1   | A     | 115 | LYS  |
| 1   | A     | 146 | ILE  |
| 1   | A     | 187 | ILE  |
| 1   | A     | 191 | LEU  |
| 1   | A     | 216 | VAL  |
| 1   | A     | 301 | ARG  |
| 1   | B     | 1   | ASP  |
| 1   | B     | 14  | GLN  |
| 1   | B     | 93  | LYS  |
| 1   | B     | 103 | ARG  |
| 1   | B     | 175 | ASN  |
| 1   | B     | 183 | GLU  |
| 1   | B     | 188 | ASP  |
| 1   | B     | 211 | THR  |
| 1   | B     | 237 | GLN  |
| 1   | B     | 239 | LYS  |
| 1   | B     | 253 | GLU  |
| 1   | B     | 278 | GLU  |
| 1   | C     | 8   | GLN  |
| 1   | C     | 18  | ASP  |
| 1   | C     | 103 | ARG  |
| 1   | C     | 174 | LYS  |
| 1   | C     | 188 | ASP  |
| 1   | C     | 207 | GLN  |
| 1   | C     | 211 | THR  |
| 1   | C     | 239 | LYS  |
| 1   | C     | 253 | GLU  |
| 1   | C     | 259 | THR  |
| 1   | C     | 268 | ASN  |
| 1   | D     | 53  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 103 | ARG  |
| 1   | D     | 115 | LYS  |
| 1   | D     | 132 | ARG  |
| 1   | D     | 167 | GLU  |
| 1   | D     | 214 | ASN  |
| 1   | D     | 216 | VAL  |
| 1   | D     | 240 | ASP  |
| 1   | D     | 256 | ARG  |
| 1   | D     | 264 | GLU  |
| 1   | D     | 268 | ASN  |
| 1   | D     | 287 | GLN  |
| 1   | E     | 103 | ARG  |
| 1   | E     | 139 | SER  |
| 1   | E     | 188 | ASP  |
| 1   | E     | 200 | PHE  |
| 1   | E     | 219 | ARG  |
| 1   | E     | 252 | LYS  |
| 1   | E     | 259 | THR  |
| 1   | E     | 268 | ASN  |
| 1   | E     | 280 | ILE  |
| 1   | F     | 8   | GLN  |
| 1   | F     | 11  | GLU  |
| 1   | F     | 111 | LYS  |
| 1   | F     | 114 | GLU  |
| 1   | F     | 115 | LYS  |
| 1   | F     | 174 | LYS  |
| 1   | F     | 191 | LEU  |
| 1   | F     | 240 | ASP  |
| 1   | F     | 280 | ILE  |
| 1   | F     | 287 | GLN  |
| 1   | G     | 55  | TYR  |
| 1   | G     | 94  | ASP  |
| 1   | G     | 103 | ARG  |
| 1   | G     | 168 | TYR  |
| 1   | G     | 278 | GLU  |
| 1   | G     | 288 | VAL  |
| 1   | G     | 294 | SER  |
| 1   | H     | 2   | ILE  |
| 1   | H     | 3   | THR  |
| 1   | H     | 103 | ARG  |
| 1   | H     | 117 | LEU  |
| 1   | H     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 192 | ILE  |
| 1   | H     | 233 | LEU  |
| 1   | H     | 256 | ARG  |
| 1   | H     | 287 | GLN  |
| 1   | H     | 301 | ARG  |
| 1   | I     | 30  | LEU  |
| 1   | I     | 36  | ASP  |
| 1   | I     | 57  | GLU  |
| 1   | I     | 71  | LEU  |
| 1   | I     | 72  | GLU  |
| 1   | I     | 80  | ASN  |
| 1   | I     | 188 | ASP  |
| 1   | I     | 212 | ARG  |
| 1   | I     | 213 | LEU  |
| 1   | I     | 253 | GLU  |
| 1   | I     | 264 | GLU  |
| 1   | I     | 287 | GLN  |
| 1   | I     | 301 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | GLN  |
| 1   | A     | 14  | GLN  |
| 1   | A     | 58  | GLN  |
| 1   | A     | 131 | ASN  |
| 1   | A     | 208 | ASN  |
| 1   | A     | 210 | HIS  |
| 1   | A     | 238 | ASN  |
| 1   | A     | 298 | HIS  |
| 1   | B     | 123 | ASN  |
| 1   | B     | 175 | ASN  |
| 1   | B     | 193 | ASN  |
| 1   | B     | 214 | ASN  |
| 1   | B     | 237 | GLN  |
| 1   | B     | 270 | HIS  |
| 1   | B     | 298 | HIS  |
| 1   | C     | 8   | GLN  |
| 1   | C     | 9   | HIS  |
| 1   | C     | 123 | ASN  |
| 1   | C     | 131 | ASN  |
| 1   | C     | 175 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 180 | GLN  |
| 1   | C     | 237 | GLN  |
| 1   | C     | 255 | GLN  |
| 1   | C     | 268 | ASN  |
| 1   | C     | 270 | HIS  |
| 1   | C     | 298 | HIS  |
| 1   | D     | 14  | GLN  |
| 1   | D     | 80  | ASN  |
| 1   | D     | 123 | ASN  |
| 1   | D     | 175 | ASN  |
| 1   | D     | 180 | GLN  |
| 1   | D     | 193 | ASN  |
| 1   | D     | 218 | HIS  |
| 1   | D     | 268 | ASN  |
| 1   | D     | 298 | HIS  |
| 1   | E     | 6   | ASN  |
| 1   | E     | 180 | GLN  |
| 1   | E     | 238 | ASN  |
| 1   | E     | 255 | GLN  |
| 1   | E     | 270 | HIS  |
| 1   | E     | 298 | HIS  |
| 1   | F     | 37  | GLN  |
| 1   | F     | 123 | ASN  |
| 1   | F     | 184 | ASN  |
| 1   | F     | 218 | HIS  |
| 1   | F     | 238 | ASN  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 270 | HIS  |
| 1   | F     | 298 | HIS  |
| 1   | G     | 31  | ASN  |
| 1   | G     | 58  | GLN  |
| 1   | G     | 69  | ASN  |
| 1   | G     | 123 | ASN  |
| 1   | G     | 175 | ASN  |
| 1   | G     | 184 | ASN  |
| 1   | G     | 208 | ASN  |
| 1   | G     | 237 | GLN  |
| 1   | G     | 255 | GLN  |
| 1   | G     | 298 | HIS  |
| 1   | G     | 305 | GLN  |
| 1   | H     | 9   | HIS  |
| 1   | H     | 14  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 37  | GLN  |
| 1   | H     | 41  | GLN  |
| 1   | H     | 80  | ASN  |
| 1   | H     | 175 | ASN  |
| 1   | H     | 180 | GLN  |
| 1   | H     | 208 | ASN  |
| 1   | H     | 214 | ASN  |
| 1   | H     | 255 | GLN  |
| 1   | H     | 268 | ASN  |
| 1   | H     | 270 | HIS  |
| 1   | H     | 287 | GLN  |
| 1   | H     | 298 | HIS  |
| 1   | I     | 6   | ASN  |
| 1   | I     | 8   | GLN  |
| 1   | I     | 31  | ASN  |
| 1   | I     | 69  | ASN  |
| 1   | I     | 80  | ASN  |
| 1   | I     | 175 | ASN  |
| 1   | I     | 184 | ASN  |
| 1   | I     | 193 | ASN  |
| 1   | I     | 207 | GLN  |
| 1   | I     | 238 | ASN  |
| 1   | I     | 298 | HIS  |
| 1   | I     | 305 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | ZRC  | A     | 400 | 1    | 3,23,25      | 1.20 | 1 (33%)  | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | B     | 400 | 1    | 3,23,25      | 0.81 | 0        | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | C     | 400 | 1    | 3,23,25      | 2.86 | 2 (66%)  | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | D     | 400 | 1    | 3,23,25      | 1.71 | 1 (33%)  | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | E     | 400 | 1    | 3,23,25      | 0.21 | 0        | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | F     | 400 | 1    | 3,23,25      | 1.68 | 1 (33%)  | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | G     | 400 | 1    | 3,23,25      | 2.20 | 1 (33%)  | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | H     | 400 | 1    | 3,23,25      | 2.24 | 1 (33%)  | 0,66,78     | 0.00 | -        |
| 2   | ZRC  | I     | 400 | 1    | 3,23,25      | 1.72 | 1 (33%)  | 0,66,78     | 0.00 | -        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | ZRC  | A     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | B     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | C     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | D     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | E     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | F     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | G     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | H     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |
| 2   | ZRC  | I     | 400 | 1    | -       | 0/0/89/99 | 0/0/5/5 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | A     | 400 | ZRC  | ZR3-O00 | 2.08 | 2.16        | 2.09     |
| 2   | C     | 400 | ZRC  | ZR1-O00 | 2.35 | 2.17        | 2.09     |
| 2   | I     | 400 | ZRC  | ZR1-O00 | 2.52 | 2.17        | 2.09     |
| 2   | F     | 400 | ZRC  | ZR3-O00 | 2.84 | 2.18        | 2.09     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | D     | 400 | ZRC  | ZR3-O00 | 2.95 | 2.19        | 2.09     |
| 2   | G     | 400 | ZRC  | ZR3-O00 | 3.32 | 2.20        | 2.09     |
| 2   | H     | 400 | ZRC  | ZR1-O00 | 3.65 | 2.21        | 2.09     |
| 2   | C     | 400 | ZRC  | ZR3-O00 | 4.35 | 2.24        | 2.09     |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 400 | ZRC  | 1       | 0            |
| 2   | C     | 400 | ZRC  | 1       | 0            |
| 2   | D     | 400 | ZRC  | 2       | 0            |
| 2   | H     | 400 | ZRC  | 1       | 0            |
| 2   | I     | 400 | ZRC  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.