



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:53 AM UTC

PDB ID : 6HYE / pdb\_00006hye  
Title : PDX1.2/PDX1.3 complex (PDX1.3:K97A)  
Authors : Robinson, G.C.; Kaufmann, M.; Roux, C.; Martinez-Font, J.; Hothorn, M.;  
Thore, S.; Fitzpatrick, T.B.  
Deposited on : 2018-10-20  
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

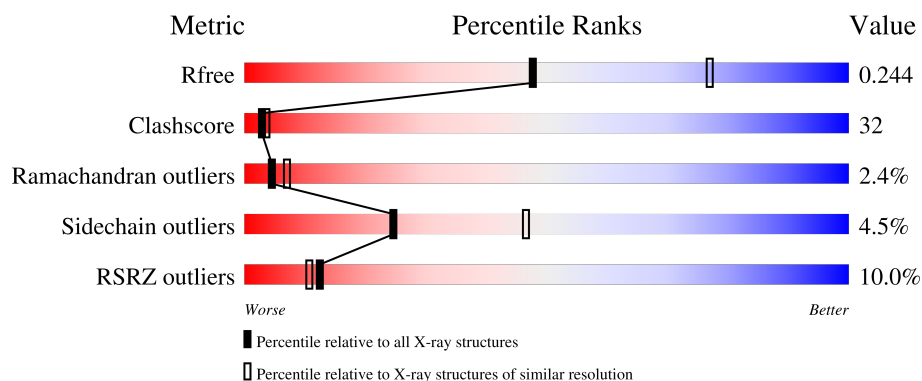
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 Å.

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



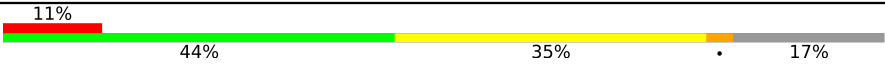
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 7383 (2.54-2.50)                                      |
| Clashscore            | 190562                      | 8079 (2.54-2.50)                                      |
| Ramachandran outliers | 187476                      | 7944 (2.54-2.50)                                      |
| Sidechain outliers    | 187428                      | 7946 (2.54-2.50)                                      |
| RSRZ outliers         | 180081                      | 7387 (2.54-2.50)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 1   | A     | 314    | <div> <div>3%</div> <div> <div>52%</div> <div>29%</div> <div>•</div> <div>16%</div> </div> </div>  |
| 1   | C     | 314    | <div> <div>6%</div> <div> <div>53%</div> <div>26%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 1   | E     | 314    | <div> <div>4%</div> <div> <div>49%</div> <div>28%</div> <div>•</div> <div>18%</div> </div> </div>  |
| 1   | G     | 314    | <div> <div>4%</div> <div> <div>53%</div> <div>27%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 2   | B     | 315    | <div> <div>10%</div> <div> <div>48%</div> <div>34%</div> <div>•</div> <div>15%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | D     | 315    |  |
| 2   | F     | 315    |  |
| 2   | H     | 315    |  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14893 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 Pyridoxal 5'-phosphate synthase-like subunit PDX1.2.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 264      | Total | C    | N   | O   | S  | 0       | 264     | 0     |
|     |       |          | 1861  | 1165 | 326 | 356 | 14 |         |         |       |
| 1   | C     | 261      | Total | C    | N   | O   | S  | 0       | 261     | 0     |
|     |       |          | 1848  | 1156 | 325 | 353 | 14 |         |         |       |
| 1   | E     | 258      | Total | C    | N   | O   | S  | 0       | 258     | 0     |
|     |       |          | 1812  | 1134 | 317 | 347 | 14 |         |         |       |
| 1   | G     | 262      | Total | C    | N   | O   | S  | 0       | 262     | 0     |
|     |       |          | 1848  | 1158 | 327 | 349 | 14 |         |         |       |

- Molecule 2 is a protein called Pyridoxal 5'-phosphate synthase subunit PDX1.3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 268      | Total | C    | N   | O   | S  | 0       | 268     | 0     |
|     |       |          | 1914  | 1201 | 339 | 356 | 18 |         |         |       |
| 2   | D     | 260      | Total | C    | N   | O   | S  | 0       | 260     | 0     |
|     |       |          | 1838  | 1151 | 327 | 342 | 18 |         |         |       |
| 2   | F     | 257      | Total | C    | N   | O   | S  | 0       | 257     | 0     |
|     |       |          | 1809  | 1130 | 323 | 339 | 17 |         |         |       |
| 2   | H     | 261      | Total | C    | N   | O   | S  | 0       | 261     | 0     |
|     |       |          | 1848  | 1158 | 329 | 343 | 18 |         |         |       |

There are 28 discrepancies between the modelled and reference sequences:

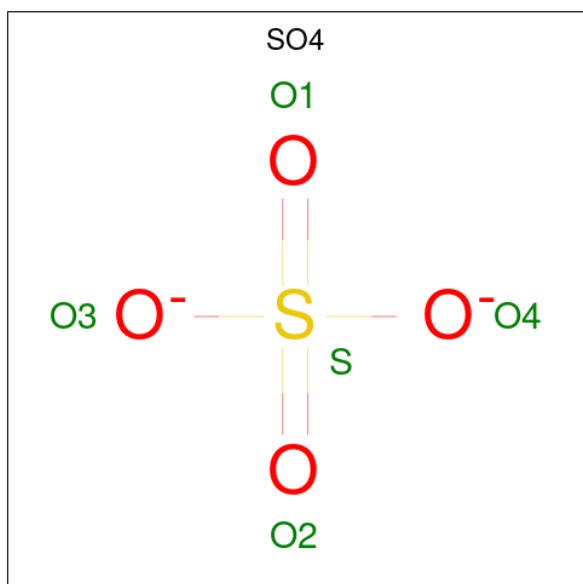
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 97      | ALA      | LYS    | engineered mutation | UNP Q8L940 |
| B     | 310     | HIS      | -      | expression tag      | UNP Q8L940 |
| B     | 311     | HIS      | -      | expression tag      | UNP Q8L940 |
| B     | 312     | HIS      | -      | expression tag      | UNP Q8L940 |
| B     | 313     | HIS      | -      | expression tag      | UNP Q8L940 |
| B     | 314     | HIS      | -      | expression tag      | UNP Q8L940 |
| B     | 315     | HIS      | -      | expression tag      | UNP Q8L940 |
| D     | 97      | ALA      | LYS    | engineered mutation | UNP Q8L940 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | 310     | HIS      | -      | expression tag      | UNP Q8L940 |
| D     | 311     | HIS      | -      | expression tag      | UNP Q8L940 |
| D     | 312     | HIS      | -      | expression tag      | UNP Q8L940 |
| D     | 313     | HIS      | -      | expression tag      | UNP Q8L940 |
| D     | 314     | HIS      | -      | expression tag      | UNP Q8L940 |
| D     | 315     | HIS      | -      | expression tag      | UNP Q8L940 |
| F     | 97      | ALA      | LYS    | engineered mutation | UNP Q8L940 |
| F     | 310     | HIS      | -      | expression tag      | UNP Q8L940 |
| F     | 311     | HIS      | -      | expression tag      | UNP Q8L940 |
| F     | 312     | HIS      | -      | expression tag      | UNP Q8L940 |
| F     | 313     | HIS      | -      | expression tag      | UNP Q8L940 |
| F     | 314     | HIS      | -      | expression tag      | UNP Q8L940 |
| F     | 315     | HIS      | -      | expression tag      | UNP Q8L940 |
| H     | 97      | ALA      | LYS    | engineered mutation | UNP Q8L940 |
| H     | 310     | HIS      | -      | expression tag      | UNP Q8L940 |
| H     | 311     | HIS      | -      | expression tag      | UNP Q8L940 |
| H     | 312     | HIS      | -      | expression tag      | UNP Q8L940 |
| H     | 313     | HIS      | -      | expression tag      | UNP Q8L940 |
| H     | 314     | HIS      | -      | expression tag      | UNP Q8L940 |
| H     | 315     | HIS      | -      | expression tag      | UNP Q8L940 |

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

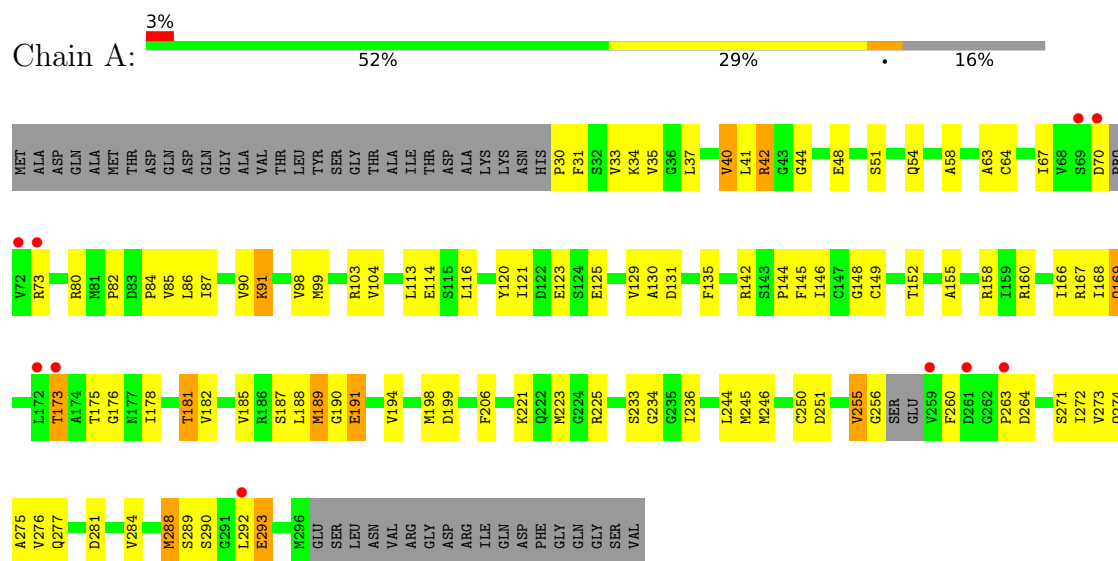
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 4   | C     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 4   | E     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 4   | G     | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 4   | B     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 4   | D     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 4   | F     | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 4   | H     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |

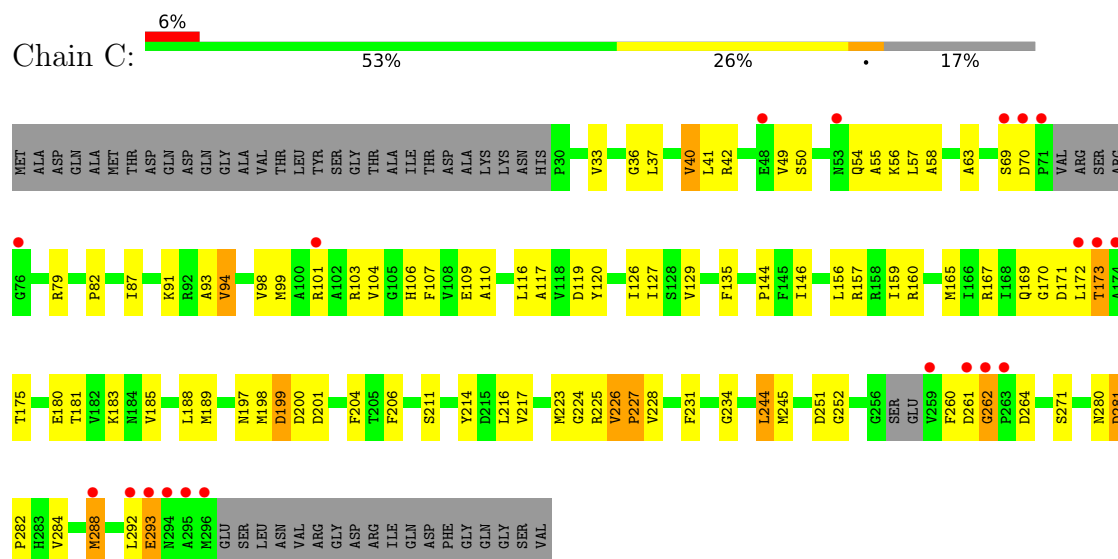
### 3 Residue-property plots [i](#)

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

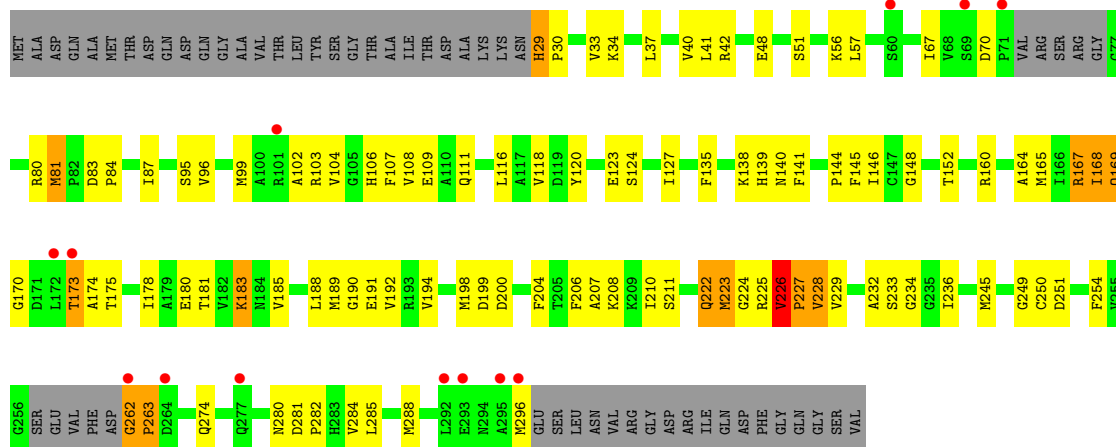
- Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2



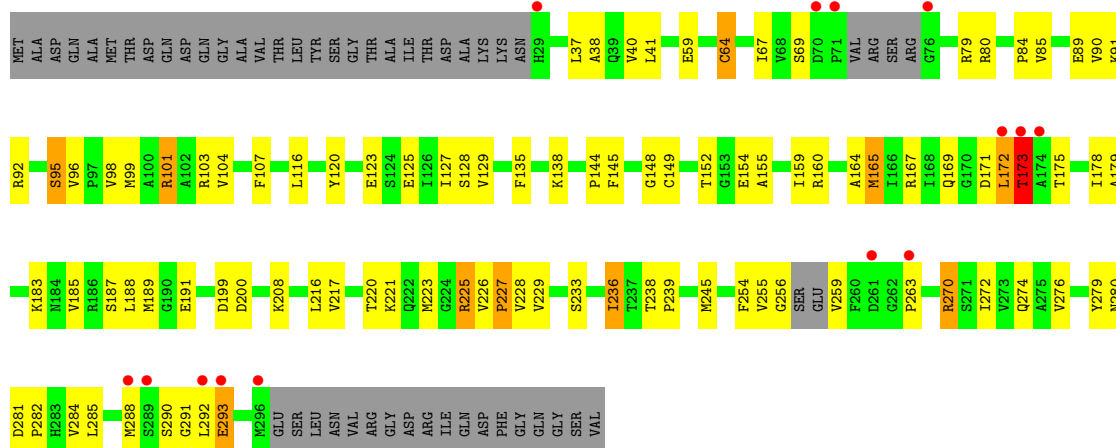
- Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2



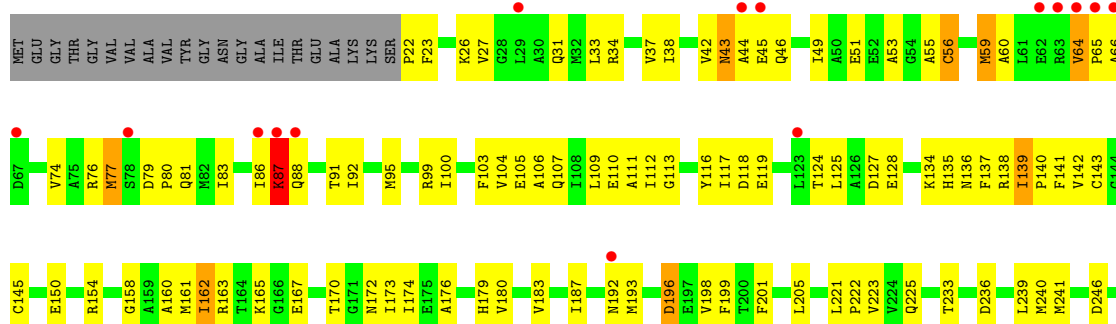
- Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2



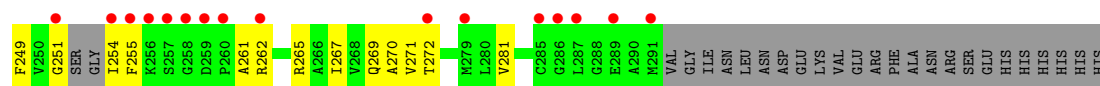
• Molecule 1: Pyridoxal 5'-phosphate synthase-like subunit PDX1.2



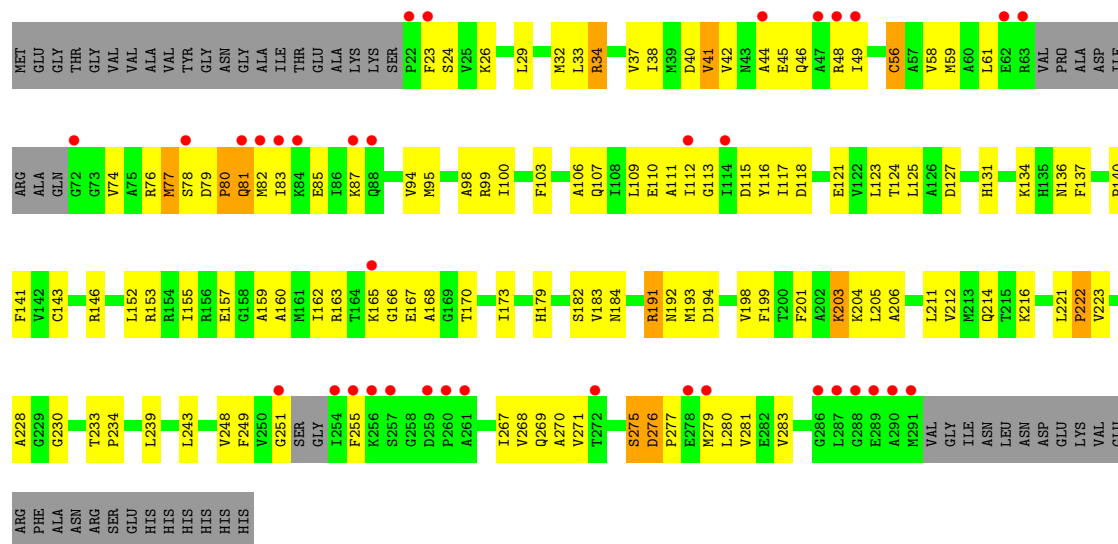
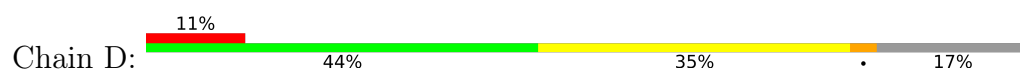
• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3



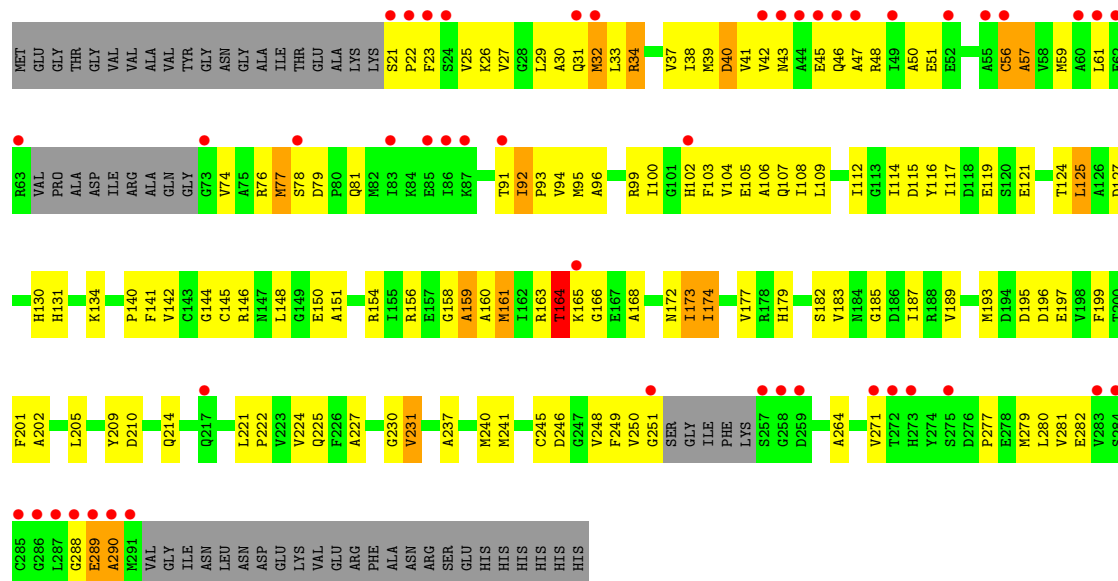




• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3

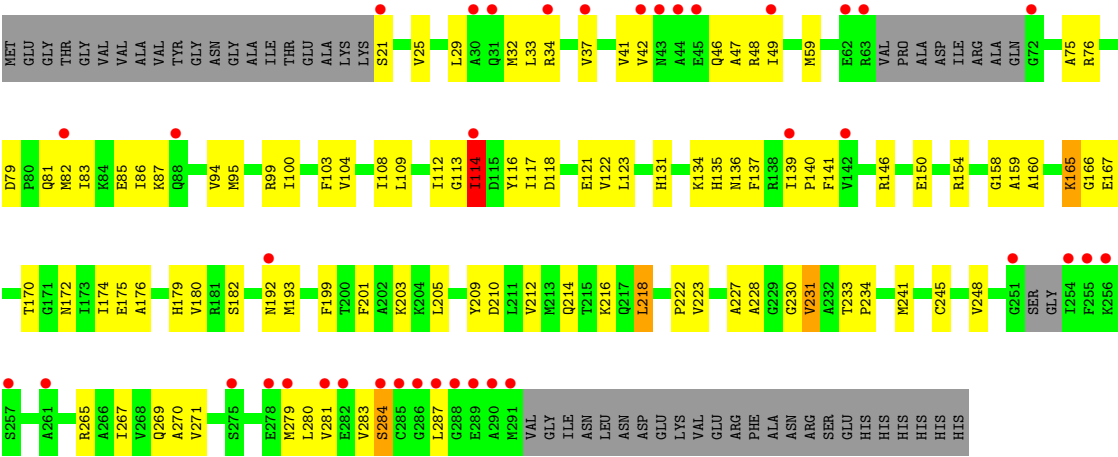


• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3



• Molecule 2: Pyridoxal 5'-phosphate synthase subunit PDX1.3





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | H 3                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 177.46Å 177.46Å 115.77Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 92.47 – 2.53<br>92.47 – 2.53                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (92.47-2.53)<br>100.0 (92.47-2.53)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.18                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.45 (at 2.55Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0135                                             | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.281<br>0.239 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2169 reflections (4.78%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 32.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.885                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 38.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.029 for h,-h-k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 14893                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 30.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.54         | 0/1885      | 0.89        | 3/2559 (0.1%)   |
| 1   | C     | 0.52         | 0/1872      | 1.00        | 7/2540 (0.3%)   |
| 1   | E     | 0.54         | 0/1834      | 0.97        | 9/2491 (0.4%)   |
| 1   | G     | 0.54         | 0/1872      | 0.90        | 1/2544 (0.0%)   |
| 2   | B     | 0.47         | 0/1940      | 0.83        | 1/2631 (0.0%)   |
| 2   | D     | 0.47         | 0/1862      | 0.83        | 0/2523          |
| 2   | F     | 0.46         | 0/1831      | 0.83        | 1/2483 (0.0%)   |
| 2   | H     | 0.48         | 0/1872      | 0.83        | 2/2538 (0.1%)   |
| All | All   | 0.50         | 0/14968     | 0.89        | 24/20309 (0.1%) |

There are no bond length outliers.

All (24) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | C     | 262[A] | GLY  | CA-C-N  | 11.39 | 134.08      | 119.84   |
| 1   | C     | 262[A] | GLY  | C-N-CA  | 11.39 | 134.08      | 119.84   |
| 1   | E     | 81[A]  | MET  | CA-C-N  | -7.85 | 112.26      | 120.03   |
| 1   | E     | 81[A]  | MET  | C-N-CA  | -7.85 | 112.26      | 120.03   |
| 1   | E     | 262[A] | GLY  | CA-C-N  | 7.09  | 128.71      | 119.84   |
| 1   | E     | 262[A] | GLY  | C-N-CA  | 7.09  | 128.71      | 119.84   |
| 1   | C     | 281[A] | ASP  | CA-C-N  | 6.36  | 126.56      | 119.32   |
| 1   | C     | 281[A] | ASP  | C-N-CA  | 6.36  | 126.56      | 119.32   |
| 2   | F     | 164[B] | THR  | CB-CA-C | -6.34 | 101.25      | 110.06   |
| 1   | G     | 217[A] | VAL  | N-CA-C  | -6.29 | 104.51      | 110.42   |
| 1   | E     | 29[A]  | HIS  | CA-C-N  | 6.13  | 125.75      | 119.56   |
| 1   | E     | 29[A]  | HIS  | C-N-CA  | 6.13  | 125.75      | 119.56   |
| 2   | H     | 165[B] | LYS  | N-CA-C  | -5.89 | 104.94      | 111.36   |
| 2   | H     | 212[B] | VAL  | N-CA-C  | -5.81 | 104.67      | 110.30   |
| 1   | E     | 226[A] | VAL  | CA-C-N  | 5.63  | 126.87      | 119.84   |
| 1   | E     | 226[A] | VAL  | C-N-CA  | 5.63  | 126.87      | 119.84   |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | A     | 191[A] | GLU  | N-CA-C  | -5.38 | 105.50      | 111.36   |
| 1   | C     | 264[A] | ASP  | CA-C-N  | 5.16  | 124.95      | 119.28   |
| 1   | C     | 264[A] | ASP  | C-N-CA  | 5.16  | 124.95      | 119.28   |
| 2   | B     | 162[B] | ILE  | CB-CA-C | -5.07 | 106.02      | 111.59   |
| 1   | C     | 94[A]  | VAL  | N-CA-C  | 5.06  | 114.86      | 107.88   |
| 1   | E     | 124[A] | SER  | N-CA-C  | 5.02  | 116.70      | 108.52   |
| 1   | A     | 264[A] | ASP  | CA-C-N  | 5.00  | 124.79      | 119.28   |
| 1   | A     | 264[A] | ASP  | C-N-CA  | 5.00  | 124.79      | 119.28   |

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     | 1861  | 0        | 1639     | 113     | 0            |
| 1   | C     | 1848  | 0        | 1635     | 89      | 0            |
| 1   | E     | 1812  | 0        | 1603     | 97      | 0            |
| 1   | G     | 1848  | 0        | 1638     | 92      | 0            |
| 2   | B     | 1914  | 0        | 1775     | 162     | 0            |
| 2   | D     | 1838  | 0        | 1676     | 135     | 0            |
| 2   | F     | 1809  | 0        | 1617     | 150     | 0            |
| 2   | H     | 1848  | 0        | 1687     | 101     | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 3   | B     | 5     | 0        | 0        | 0       | 0            |
| 3   | C     | 5     | 0        | 0        | 0       | 0            |
| 3   | D     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 10    | 0        | 0        | 0       | 0            |
| 3   | H     | 10    | 0        | 0        | 0       | 0            |
| 4   | A     | 11    | 0        | 0        | 1       | 0            |
| 4   | B     | 9     | 0        | 0        | 0       | 0            |
| 4   | C     | 9     | 0        | 0        | 1       | 0            |
| 4   | D     | 7     | 0        | 0        | 0       | 0            |
| 4   | E     | 12    | 0        | 0        | 0       | 0            |
| 4   | F     | 6     | 0        | 0        | 0       | 0            |
| 4   | G     | 6     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | H     | 15    | 0        | 0        | 0       | 0            |
| All | All   | 14893 | 0        | 13270    | 912     | 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 32.

All (912) 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) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:173[B]:ILE:HD11 | 2:F:240[B]:MET:CE   | 1.40                     | 1.48              |
| 2:F:146[B]:ARG:NH2  | 2:F:150[B]:GLU:OE2  | 1.63                     | 1.30              |
| 2:B:150[B]:GLU:OE2  | 2:B:165[B]:LYS:HE3  | 1.08                     | 1.24              |
| 2:F:173[B]:ILE:CD1  | 2:F:240[B]:MET:HE3  | 1.68                     | 1.23              |
| 1:A:48[A]:GLU:HA    | 1:A:67[A]:ILE:CG2   | 1.74                     | 1.18              |
| 2:F:201[B]:PHE:CE2  | 2:F:205[B]:LEU:HD11 | 1.81                     | 1.15              |
| 2:F:173[B]:ILE:CD1  | 2:F:240[B]:MET:CE   | 2.24                     | 1.14              |
| 2:B:150[B]:GLU:OE2  | 2:B:165[B]:LYS:CE   | 1.94                     | 1.13              |
| 1:A:48[A]:GLU:HA    | 1:A:67[A]:ILE:HG22  | 1.14                     | 1.11              |
| 1:E:169[A]:GLN:HA   | 1:E:169[A]:GLN:OE1  | 1.36                     | 1.10              |
| 2:D:40[B]:ASP:O     | 2:D:41[B]:VAL:HG13  | 1.49                     | 1.10              |
| 1:C:185[A]:VAL:HG21 | 1:C:245[A]:MET:CE   | 1.80                     | 1.10              |
| 2:D:275[B]:SER:O    | 2:D:277[B]:PRO:HD3  | 1.52                     | 1.07              |
| 2:B:64[B]:VAL:HG13  | 2:B:65[B]:PRO:HD2   | 1.38                     | 1.06              |
| 1:A:274[A]:GLN:OE1  | 1:A:288[A]:MET:HE2  | 1.59                     | 1.03              |
| 2:F:173[B]:ILE:HD11 | 2:F:240[B]:MET:HE2  | 1.41                     | 1.02              |
| 2:F:164[B]:THR:O    | 2:F:164[B]:THR:CG2  | 2.03                     | 1.02              |
| 2:F:165[B]:LYS:O    | 2:F:179[B]:HIS:ND1  | 1.92                     | 1.01              |
| 1:G:99[A]:MET:HG2   | 1:G:120[A]:TYR:HB2  | 1.37                     | 1.01              |
| 1:A:185[A]:VAL:HG21 | 1:A:245[A]:MET:CE   | 1.91                     | 1.00              |
| 1:G:69[A]:SER:CB    | 1:G:101[A]:ARG:NH1  | 2.25                     | 1.00              |
| 2:B:59[B]:MET:HE1   | 2:B:118[B]:ASP:CB   | 1.90                     | 0.99              |
| 1:C:54[A]:GLN:HG2   | 1:C:260[A]:PHE:CE2  | 1.98                     | 0.99              |
| 1:G:256[A]:GLY:O    | 1:G:259[A]:VAL:N    | 1.95                     | 0.98              |
| 2:D:46[B]:GLN:HG2   | 2:D:255[B]:PHE:CE1  | 1.98                     | 0.98              |
| 2:D:276[B]:ASP:OD1  | 2:D:279[B]:MET:N    | 1.96                     | 0.97              |
| 2:F:29[B]:LEU:O     | 2:F:116[B]:TYR:OH   | 1.83                     | 0.97              |
| 2:H:192[B]:ASN:OD1  | 2:H:192[B]:ASN:O    | 1.83                     | 0.96              |
| 1:C:146[A]:ILE:HD12 | 1:C:165[A]:MET:HG2  | 1.44                     | 0.96              |
| 2:B:59[B]:MET:HE1   | 2:B:118[B]:ASP:HB3  | 1.44                     | 0.96              |
| 2:D:276[B]:ASP:CG   | 2:D:279[B]:MET:HB2  | 1.89                     | 0.96              |
| 1:C:185[A]:VAL:HG21 | 1:C:245[A]:MET:HE1  | 1.47                     | 0.95              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:H:160[B]:ALA:O    | 2:H:223[B]:VAL:HB   | 1.67                     | 0.95              |
| 1:E:280[A]:ASN:O    | 1:E:282[A]:PRO:HD3  | 1.67                     | 0.94              |
| 1:E:99[A]:MET:HG2   | 1:E:120[A]:TYR:HB2  | 1.49                     | 0.94              |
| 1:E:274[A]:GLN:HG3  | 1:E:288[A]:MET:HE2  | 1.48                     | 0.94              |
| 1:C:146[A]:ILE:CD1  | 1:C:165[A]:MET:HG2  | 1.96                     | 0.94              |
| 1:G:185[A]:VAL:HG21 | 1:G:245[A]:MET:CE   | 1.97                     | 0.94              |
| 2:B:239[B]:LEU:HD12 | 2:H:103[B]:PHE:CZ   | 2.03                     | 0.94              |
| 1:C:146[A]:ILE:HD12 | 1:C:165[A]:MET:SD   | 2.08                     | 0.94              |
| 1:A:185[A]:VAL:HG21 | 1:A:245[A]:MET:HE1  | 1.50                     | 0.93              |
| 1:C:146[A]:ILE:HD12 | 1:C:165[A]:MET:CG   | 1.98                     | 0.93              |
| 2:D:82[B]:MET:O     | 2:D:82[B]:MET:SD    | 2.26                     | 0.93              |
| 2:F:124[B]:THR:O    | 2:F:125[B]:LEU:O    | 1.86                     | 0.93              |
| 1:A:225[A]:ARG:NH2  | 1:A:251[A]:ASP:OD2  | 2.02                     | 0.93              |
| 1:E:274[A]:GLN:HG3  | 1:E:288[A]:MET:CE   | 1.99                     | 0.92              |
| 1:A:99[A]:MET:SD    | 1:A:146[A]:ILE:CD1  | 2.57                     | 0.92              |
| 2:F:164[B]:THR:O    | 2:F:164[B]:THR:HG22 | 1.70                     | 0.91              |
| 1:G:281[A]:ASP:CG   | 1:G:284[A]:VAL:HG23 | 1.94                     | 0.91              |
| 2:D:275[B]:SER:O    | 2:D:277[B]:PRO:CD   | 2.19                     | 0.91              |
| 1:A:48[A]:GLU:CG    | 1:A:67[A]:ILE:HG21  | 2.02                     | 0.90              |
| 2:B:201[B]:PHE:CE2  | 2:B:205[B]:LEU:HD11 | 2.07                     | 0.90              |
| 1:A:99[A]:MET:HG2   | 1:A:120[A]:TYR:HB2  | 1.52                     | 0.90              |
| 2:F:173[B]:ILE:HD11 | 2:F:240[B]:MET:HE3  | 0.90                     | 0.89              |
| 2:B:172[B]:ASN:OD1  | 2:B:174[B]:ILE:HG22 | 1.72                     | 0.89              |
| 2:D:276[B]:ASP:OD2  | 2:D:279[B]:MET:HB2  | 1.72                     | 0.89              |
| 1:G:125[A]:GLU:HG3  | 1:G:169[A]:GLN:OE1  | 1.72                     | 0.89              |
| 1:A:48[A]:GLU:CA    | 1:A:67[A]:ILE:HG22  | 2.00                     | 0.89              |
| 2:F:42[B]:VAL:HG12  | 2:F:61[B]:LEU:O     | 1.74                     | 0.88              |
| 1:A:37[A]:LEU:O     | 1:A:40[A]:VAL:HG13  | 1.72                     | 0.88              |
| 1:A:73[A]:ARG:CB    | 1:A:173[A]:THR:CG2  | 2.51                     | 0.87              |
| 2:H:95[B]:MET:HG2   | 2:H:116[B]:TYR:HB2  | 1.56                     | 0.87              |
| 2:B:160[B]:ALA:O    | 2:B:223[B]:VAL:HB   | 1.75                     | 0.87              |
| 2:F:174[B]:ILE:HG12 | 2:F:174[B]:ILE:O    | 1.74                     | 0.87              |
| 2:F:201[B]:PHE:HE2  | 2:F:205[B]:LEU:HD11 | 1.37                     | 0.87              |
| 2:D:276[B]:ASP:CG   | 2:D:279[B]:MET:CB   | 2.48                     | 0.86              |
| 1:A:125[A]:GLU:CD   | 1:A:169[A]:GLN:HG2  | 2.00                     | 0.86              |
| 2:D:40[B]:ASP:O     | 2:D:41[B]:VAL:CG1   | 2.24                     | 0.86              |
| 2:D:80[B]:PRO:O     | 2:D:83[B]:ILE:N     | 2.07                     | 0.86              |
| 2:F:79[B]:ASP:OD1   | 2:F:81[B]:GLN:N     | 2.08                     | 0.85              |
| 1:C:99[A]:MET:HG2   | 1:C:120[A]:TYR:HB2  | 1.56                     | 0.85              |
| 1:E:80[A]:ARG:HG2   | 1:E:103[A]:ARG:CZ   | 2.07                     | 0.85              |
| 1:E:169[A]:GLN:NE2  | 1:E:170[A]:GLY:H    | 1.75                     | 0.85              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:E:185[A]:VAL:HG21 | 1:E:245[A]:MET:HE1  | 1.56                     | 0.85              |
| 1:G:270[A]:ARG:NH1  | 1:G:274[A]:GLN:NE2  | 2.25                     | 0.85              |
| 2:H:146[B]:ARG:NH2  | 2:H:150[B]:GLU:OE2  | 2.09                     | 0.84              |
| 1:A:73[A]:ARG:CB    | 1:A:173[A]:THR:HG23 | 2.07                     | 0.84              |
| 2:F:164[B]:THR:O    | 2:F:164[B]:THR:HG23 | 1.77                     | 0.84              |
| 2:H:37[B]:VAL:CG2   | 2:H:271[B]:VAL:HG21 | 2.08                     | 0.84              |
| 2:B:64[B]:VAL:HG13  | 2:B:65[B]:PRO:CD    | 2.08                     | 0.84              |
| 2:D:214[B]:GLN:NE2  | 2:D:222[B]:PRO:HB3  | 1.92                     | 0.84              |
| 1:E:48[A]:GLU:HG2   | 1:E:67[A]:ILE:HG21  | 1.60                     | 0.83              |
| 1:E:99[A]:MET:SD    | 1:E:146[A]:ILE:HD11 | 2.17                     | 0.83              |
| 1:A:245[A]:MET:HE3  | 1:A:245[A]:MET:HA   | 1.60                     | 0.83              |
| 1:G:84[A]:PRO:HB3   | 1:G:116[A]:LEU:HD11 | 1.60                     | 0.83              |
| 2:D:82[B]:MET:HA    | 2:D:85[B]:GLU:OE1   | 1.77                     | 0.83              |
| 2:H:59[B]:MET:HE1   | 2:H:118[B]:ASP:HB2  | 1.59                     | 0.83              |
| 1:E:274[A]:GLN:CG   | 1:E:288[A]:MET:HE2  | 2.07                     | 0.82              |
| 1:C:185[A]:VAL:HG21 | 1:C:245[A]:MET:HE2  | 1.61                     | 0.82              |
| 1:E:232[A]:ALA:CB   | 1:E:245[A]:MET:HE2  | 2.08                     | 0.82              |
| 1:E:99[A]:MET:SD    | 1:E:146[A]:ILE:CD1  | 2.68                     | 0.81              |
| 1:A:48[A]:GLU:CA    | 1:A:67[A]:ILE:CG2   | 2.57                     | 0.81              |
| 1:E:48[A]:GLU:HG2   | 1:E:67[A]:ILE:CG2   | 2.11                     | 0.81              |
| 2:B:221[B]:LEU:O    | 2:B:223[B]:VAL:N    | 2.13                     | 0.81              |
| 1:G:281[A]:ASP:OD2  | 1:G:284[A]:VAL:CG2  | 2.29                     | 0.81              |
| 1:A:99[A]:MET:CE    | 1:A:146[A]:ILE:HD11 | 2.11                     | 0.81              |
| 2:H:227[B]:ALA:HB2  | 2:H:245[B]:CYS:SG   | 2.20                     | 0.81              |
| 1:E:169[A]:GLN:CD   | 1:E:170[A]:GLY:H    | 1.88                     | 0.80              |
| 1:G:69[A]:SER:CB    | 1:G:101[A]:ARG:HH11 | 1.94                     | 0.80              |
| 2:B:42[B]:VAL:HG23  | 2:B:42[B]:VAL:O     | 1.80                     | 0.80              |
| 2:F:76[B]:ARG:HG2   | 2:F:99[B]:ARG:CZ    | 2.11                     | 0.80              |
| 2:B:34[B]:ARG:HH22  | 2:D:32[B]:MET:HE3   | 1.46                     | 0.80              |
| 2:F:117[B]:ILE:CG2  | 2:F:141[B]:PHE:CE2  | 2.65                     | 0.80              |
| 1:E:185[A]:VAL:HG21 | 1:E:245[A]:MET:CE   | 2.11                     | 0.80              |
| 1:G:172[A]:LEU:O    | 1:G:173[A]:THR:O    | 2.00                     | 0.80              |
| 2:F:201[B]:PHE:CE2  | 2:F:205[B]:LEU:CD1  | 2.62                     | 0.80              |
| 2:F:199[B]:PHE:CD1  | 2:F:209[B]:TYR:CE1  | 2.70                     | 0.80              |
| 1:E:181[A]:THR:OG1  | 1:E:234[A]:GLY:O    | 2.00                     | 0.79              |
| 1:A:190[A]:GLY:O    | 1:A:194[A]:VAL:HG23 | 1.83                     | 0.79              |
| 2:D:192[B]:ASN:O    | 2:D:192[B]:ASN:OD1  | 2.00                     | 0.79              |
| 2:D:239[B]:LEU:HD12 | 2:F:103[B]:PHE:CZ   | 2.16                     | 0.79              |
| 2:F:95[B]:MET:HG2   | 2:F:116[B]:TYR:HB2  | 1.65                     | 0.79              |
| 2:F:115[B]:ASP:O    | 2:F:140[B]:PRO:HD2  | 1.83                     | 0.79              |
| 1:A:274[A]:GLN:OE1  | 1:A:288[A]:MET:CE   | 2.31                     | 0.78              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:C:180[A]:GLU:OE1  | 1:C:183[A]:LYS:HE3  | 1.83                     | 0.78              |
| 2:D:117[B]:ILE:HG21 | 2:D:141[B]:PHE:CE2  | 2.18                     | 0.78              |
| 2:B:167[B]:GLU:OE1  | 2:B:170[B]:THR:OG1  | 2.02                     | 0.78              |
| 2:F:199[B]:PHE:CE1  | 2:F:209[B]:TYR:CZ   | 2.71                     | 0.78              |
| 2:B:34[B]:ARG:CZ    | 2:D:32[B]:MET:HG2   | 2.13                     | 0.78              |
| 2:B:265[B]:ARG:HE   | 2:B:269[B]:GLN:NE2  | 1.83                     | 0.77              |
| 2:D:117[B]:ILE:CG2  | 2:D:141[B]:PHE:CE2  | 2.67                     | 0.77              |
| 1:C:146[A]:ILE:CD1  | 1:C:165[A]:MET:HE2  | 2.14                     | 0.77              |
| 2:F:117[B]:ILE:HG21 | 2:F:141[B]:PHE:CE2  | 2.19                     | 0.77              |
| 2:B:110[B]:GLU:CD   | 2:B:139[B]:ILE:HG22 | 2.09                     | 0.77              |
| 2:H:116[B]:TYR:CD2  | 2:H:140[B]:PRO:HG2  | 2.19                     | 0.77              |
| 1:A:187[A]:SER:O    | 1:A:191[A]:GLU:HG3  | 1.83                     | 0.77              |
| 1:G:281[A]:ASP:OD2  | 1:G:284[A]:VAL:HG23 | 1.85                     | 0.77              |
| 2:F:173[B]:ILE:HG13 | 2:F:173[B]:ILE:O    | 1.84                     | 0.77              |
| 2:B:239[B]:LEU:CD1  | 2:H:103[B]:PHE:CZ   | 2.67                     | 0.77              |
| 2:F:117[B]:ILE:HG21 | 2:F:141[B]:PHE:HE2  | 1.49                     | 0.77              |
| 2:B:110[B]:GLU:HG3  | 2:B:139[B]:ILE:CG2  | 2.15                     | 0.77              |
| 1:A:189[A]:MET:HA   | 1:A:189[A]:MET:HE2  | 1.67                     | 0.76              |
| 2:H:59[B]:MET:HE1   | 2:H:118[B]:ASP:CB   | 2.15                     | 0.76              |
| 2:B:22[B]:PRO:O     | 2:B:26[B]:LYS:HG3   | 1.86                     | 0.76              |
| 2:D:134[B]:LYS:HB3  | 2:D:141[B]:PHE:CD1  | 2.21                     | 0.76              |
| 2:H:122[B]:VAL:HG12 | 2:H:122[B]:VAL:O    | 1.84                     | 0.76              |
| 1:A:73[A]:ARG:CB    | 1:A:173[A]:THR:HG22 | 2.15                     | 0.76              |
| 1:E:29[A]:HIS:O     | 1:E:33[A]:VAL:HG23  | 1.86                     | 0.76              |
| 1:A:120[A]:TYR:CD1  | 1:A:144[A]:PRO:HG2  | 2.21                     | 0.75              |
| 1:G:185[A]:VAL:HG21 | 1:G:245[A]:MET:HE2  | 1.66                     | 0.75              |
| 2:B:239[B]:LEU:HD12 | 2:H:103[B]:PHE:CE1  | 2.22                     | 0.75              |
| 2:D:95[B]:MET:HG2   | 2:D:116[B]:TYR:HB2  | 1.69                     | 0.75              |
| 1:C:103[A]:ARG:HG2  | 1:C:127[A]:ILE:HG22 | 1.67                     | 0.74              |
| 2:D:82[B]:MET:SD    | 2:D:82[B]:MET:C     | 2.71                     | 0.74              |
| 2:H:135[B]:HIS:O    | 2:H:137[B]:PHE:N    | 2.20                     | 0.74              |
| 1:A:181[A]:THR:OG1  | 1:A:234[A]:GLY:O    | 2.05                     | 0.74              |
| 2:D:115[B]:ASP:O    | 2:D:140[B]:PRO:HD2  | 1.87                     | 0.74              |
| 1:C:271[A]:SER:OG   | 1:C:292[A]:LEU:HD21 | 1.86                     | 0.74              |
| 1:C:288[A]:MET:HE3  | 1:C:288[A]:MET:HA   | 1.69                     | 0.74              |
| 2:B:134[B]:LYS:HG2  | 2:B:141[B]:PHE:CG   | 2.23                     | 0.74              |
| 2:B:34[B]:ARG:NH2   | 2:D:32[B]:MET:HG2   | 2.03                     | 0.73              |
| 2:F:117[B]:ILE:CG2  | 2:F:141[B]:PHE:HE2  | 2.01                     | 0.73              |
| 1:G:185[A]:VAL:HG21 | 1:G:245[A]:MET:HE1  | 1.69                     | 0.73              |
| 2:B:42[B]:VAL:O     | 2:B:43[B]:ASN:HB3   | 1.89                     | 0.73              |
| 1:A:67[A]:ILE:HG23  | 1:A:67[A]:ILE:O     | 1.89                     | 0.73              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:H:280[B]:LEU:O    | 2:H:284[B]:SER:OG   | 2.07                     | 0.73              |
| 1:A:42[A]:ARG:HD2   | 1:C:36[A]:GLY:O     | 1.88                     | 0.72              |
| 1:A:125[A]:GLU:OE2  | 1:A:169[A]:GLN:HG2  | 1.90                     | 0.72              |
| 2:F:134[B]:LYS:HG2  | 2:F:141[B]:PHE:CD1  | 2.24                     | 0.72              |
| 1:A:173[A]:THR:HB   | 1:A:175[A]:THR:HG23 | 1.70                     | 0.72              |
| 2:F:173[B]:ILE:CG1  | 2:F:240[B]:MET:CE   | 2.69                     | 0.71              |
| 1:G:236[A]:ILE:N    | 1:G:236[A]:ILE:HD13 | 2.05                     | 0.71              |
| 2:B:281[B]:VAL:HG21 | 2:H:112[B]:ILE:HG23 | 1.72                     | 0.71              |
| 1:G:173[A]:THR:HB   | 1:G:175[A]:THR:HG23 | 1.73                     | 0.71              |
| 1:A:148[A]:GLY:HA2  | 1:A:167[A]:ARG:O    | 1.91                     | 0.71              |
| 2:F:144[B]:GLY:HA2  | 2:F:163[B]:ARG:O    | 1.89                     | 0.70              |
| 1:A:185[A]:VAL:HG21 | 1:A:245[A]:MET:HE2  | 1.71                     | 0.70              |
| 2:D:40[B]:ASP:C     | 2:D:41[B]:VAL:HG13  | 2.16                     | 0.70              |
| 1:A:40[A]:VAL:HG12  | 1:C:33[A]:VAL:HG22  | 1.72                     | 0.70              |
| 2:F:21[B]:SER:O     | 2:F:25[B]:VAL:HG23  | 1.90                     | 0.70              |
| 1:E:138[A]:LYS:HG2  | 1:E:145[A]:PHE:CD2  | 2.26                     | 0.70              |
| 2:B:135[B]:HIS:C    | 2:B:137[B]:PHE:H    | 1.99                     | 0.70              |
| 1:G:91[A]:LYS:HA    | 1:G:98[A]:VAL:HG21  | 1.72                     | 0.70              |
| 1:C:104[A]:VAL:HB   | 1:C:129[A]:VAL:HG13 | 1.73                     | 0.69              |
| 2:H:139[B]:ILE:HG23 | 2:H:140[B]:PRO:HD2  | 1.71                     | 0.69              |
| 1:G:154[A]:GLU:OE2  | 1:G:169[A]:GLN:NE2  | 2.24                     | 0.69              |
| 1:G:281[A]:ASP:CG   | 1:G:284[A]:VAL:CG2  | 2.65                     | 0.69              |
| 2:F:93[B]:PRO:HA    | 2:F:115[B]:ASP:OD2  | 1.93                     | 0.69              |
| 1:E:169[A]:GLN:CD   | 1:E:170[A]:GLY:N    | 2.50                     | 0.69              |
| 1:G:187[A]:SER:O    | 1:G:191[A]:GLU:HG3  | 1.91                     | 0.69              |
| 2:B:145[B]:CYS:SG   | 2:B:163[B]:ARG:O    | 2.47                     | 0.69              |
| 2:D:77[B]:MET:HG2   | 2:D:78[B]:SER:N     | 2.06                     | 0.69              |
| 2:D:160[B]:ALA:O    | 2:D:223[B]:VAL:HB   | 1.93                     | 0.69              |
| 2:B:59[B]:MET:HE1   | 2:B:118[B]:ASP:OD2  | 1.93                     | 0.69              |
| 1:A:281[A]:ASP:OD2  | 1:A:284[A]:VAL:HG23 | 1.93                     | 0.68              |
| 1:C:79[A]:ARG:O     | 1:C:127[A]:ILE:HG23 | 1.92                     | 0.68              |
| 1:C:185[A]:VAL:CG2  | 1:C:245[A]:MET:HE1  | 2.22                     | 0.68              |
| 1:E:99[A]:MET:CE    | 1:E:146[A]:ILE:HD11 | 2.23                     | 0.68              |
| 1:C:54[A]:GLN:HG2   | 1:C:260[A]:PHE:CZ   | 2.28                     | 0.68              |
| 2:B:59[B]:MET:HE1   | 2:B:118[B]:ASP:CG   | 2.17                     | 0.68              |
| 2:B:110[B]:GLU:OE2  | 2:B:139[B]:ILE:HG22 | 1.93                     | 0.68              |
| 2:F:43[B]:ASN:OD1   | 2:F:45[B]:GLU:CB    | 2.41                     | 0.68              |
| 2:F:124[B]:THR:O    | 2:F:125[B]:LEU:C    | 2.35                     | 0.68              |
| 2:H:87[B]:LYS:HA    | 2:H:94[B]:VAL:HG21  | 1.74                     | 0.68              |
| 2:B:142[B]:VAL:HG13 | 2:B:161[B]:MET:O    | 1.94                     | 0.68              |
| 1:G:90[A]:VAL:HG23  | 1:G:91[A]:LYS:N     | 2.09                     | 0.68              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:B:134[B]:LYS:HG2  | 2:B:141[B]:PHE:CD2  | 2.29                     | 0.68              |
| 1:G:149[A]:CYS:N    | 1:G:169[A]:GLN:HG3  | 2.10                     | 0.67              |
| 1:E:284[A]:VAL:O    | 1:E:288[A]:MET:HB2  | 1.94                     | 0.67              |
| 2:H:109[B]:LEU:HA   | 2:H:112[B]:ILE:HD11 | 1.76                     | 0.67              |
| 2:B:221[B]:LEU:C    | 2:B:223[B]:VAL:H    | 2.02                     | 0.67              |
| 1:E:232[A]:ALA:HB1  | 1:E:245[A]:MET:HE2  | 1.75                     | 0.67              |
| 1:C:180[A]:GLU:OE1  | 1:C:183[A]:LYS:CE   | 2.43                     | 0.67              |
| 1:A:33[A]:VAL:O     | 1:A:37[A]:LEU:HG    | 1.95                     | 0.67              |
| 1:E:262[A]:GLY:O    | 1:E:263[A]:PRO:CB   | 2.42                     | 0.67              |
| 1:A:244[A]:LEU:HD12 | 1:G:107[A]:PHE:CZ   | 2.30                     | 0.66              |
| 1:E:232[A]:ALA:HB2  | 1:E:245[A]:MET:HE2  | 1.76                     | 0.66              |
| 2:H:201[B]:PHE:CE2  | 2:H:205[B]:LEU:HD11 | 2.31                     | 0.66              |
| 1:G:104[A]:VAL:HG13 | 1:G:135[A]:PHE:CD1  | 2.31                     | 0.66              |
| 2:F:227[B]:ALA:HB2  | 2:F:245[B]:CYS:SG   | 2.35                     | 0.66              |
| 2:D:42[B]:VAL:HA    | 2:D:61[B]:LEU:O     | 1.95                     | 0.66              |
| 2:D:214[B]:GLN:NE2  | 2:D:222[B]:PRO:CB   | 2.59                     | 0.66              |
| 2:D:239[B]:LEU:HD12 | 2:F:103[B]:PHE:CE1  | 2.29                     | 0.66              |
| 2:D:203[B]:LYS:O    | 2:D:206[B]:ALA:N    | 2.27                     | 0.66              |
| 2:F:154[B]:ARG:HE   | 2:F:154[B]:ARG:HA   | 1.60                     | 0.66              |
| 2:H:135[B]:HIS:C    | 2:H:137[B]:PHE:H    | 2.04                     | 0.66              |
| 1:A:99[A]:MET:SD    | 1:A:146[A]:ILE:HD11 | 2.32                     | 0.66              |
| 1:A:152[A]:THR:OG1  | 1:A:188[A]:LEU:HD12 | 1.95                     | 0.66              |
| 2:F:158[B]:GLY:O    | 2:F:159[B]:ALA:C    | 2.38                     | 0.66              |
| 1:C:199[A]:ASP:OD1  | 1:C:199[A]:ASP:C    | 2.39                     | 0.66              |
| 1:G:69[A]:SER:CB    | 1:G:101[A]:ARG:HH12 | 2.08                     | 0.66              |
| 1:A:48[A]:GLU:HB2   | 1:A:256[A]:GLY:HA2  | 1.78                     | 0.65              |
| 1:A:281[A]:ASP:CG   | 1:A:284[A]:VAL:HG23 | 2.21                     | 0.65              |
| 2:D:239[B]:LEU:CD1  | 2:F:103[B]:PHE:CZ   | 2.80                     | 0.65              |
| 2:H:230[B]:GLY:O    | 2:H:231[B]:VAL:C    | 2.38                     | 0.65              |
| 2:B:87[B]:LYS:HE3   | 2:B:113[B]:GLY:O    | 1.96                     | 0.65              |
| 2:B:59[B]:MET:CE    | 2:B:118[B]:ASP:HB3  | 2.22                     | 0.65              |
| 1:A:189[A]:MET:HA   | 1:A:189[A]:MET:CE   | 2.27                     | 0.65              |
| 1:G:245[A]:MET:HE3  | 1:G:245[A]:MET:HA   | 1.79                     | 0.65              |
| 1:C:292[A]:LEU:O    | 1:C:293[A]:GLU:CB   | 2.45                     | 0.64              |
| 2:F:165[B]:LYS:O    | 2:F:179[B]:HIS:CE1  | 2.50                     | 0.64              |
| 1:C:50[A]:SER:HA    | 1:C:69[A]:SER:O     | 1.97                     | 0.64              |
| 2:F:146[B]:ARG:CZ   | 2:F:150[B]:GLU:OE2  | 2.45                     | 0.64              |
| 2:B:145[B]:CYS:O    | 2:B:165[B]:LYS:N    | 2.25                     | 0.64              |
| 1:G:281[A]:ASP:OD2  | 1:G:284[A]:VAL:HG21 | 1.97                     | 0.64              |
| 2:D:40[B]:ASP:HB2   | 2:D:251[B]:GLY:HA2  | 1.80                     | 0.64              |
| 2:D:33[B]:LEU:HD22  | 2:D:56[B]:CYS:SG    | 2.37                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:56[B]:CYS:O     | 2:F:57[B]:ALA:HB2   | 1.96                     | 0.64              |
| 2:H:199[B]:PHE:CE1  | 2:H:209[B]:TYR:CZ   | 2.86                     | 0.64              |
| 2:D:165[B]:LYS:HE3  | 2:D:168[B]:ALA:HB2  | 1.80                     | 0.64              |
| 1:A:135[A]:PHE:CE2  | 1:A:158[A]:ARG:CZ   | 2.82                     | 0.63              |
| 2:F:173[B]:ILE:CD1  | 2:F:240[B]:MET:HE2  | 2.14                     | 0.63              |
| 2:B:60[B]:ALA:HB1   | 2:B:86[B]:ILE:HD12  | 1.80                     | 0.63              |
| 2:B:173[B]:ILE:HG23 | 2:B:173[B]:ILE:O    | 1.97                     | 0.63              |
| 1:G:167[A]:ARG:HG3  | 1:G:167[A]:ARG:HH11 | 1.63                     | 0.63              |
| 2:D:127[B]:ASP:C    | 2:D:127[B]:ASP:OD1  | 2.38                     | 0.63              |
| 2:F:225[B]:GLN:O    | 2:F:246[B]:ASP:HB2  | 1.99                     | 0.63              |
| 1:G:125[A]:GLU:CG   | 1:G:169[A]:GLN:OE1  | 2.46                     | 0.63              |
| 2:H:134[B]:LYS:HG2  | 2:H:141[B]:PHE:CG   | 2.33                     | 0.63              |
| 1:E:191[A]:GLU:CG   | 1:E:206[A]:PHE:HZ   | 2.12                     | 0.63              |
| 2:B:110[B]:GLU:HG3  | 2:B:139[B]:ILE:HG22 | 1.81                     | 0.63              |
| 2:D:87[B]:LYS:HA    | 2:D:94[B]:VAL:HG21  | 1.80                     | 0.63              |
| 2:B:100[B]:ILE:HB   | 2:B:125[B]:LEU:HD12 | 1.80                     | 0.62              |
| 2:H:122[B]:VAL:O    | 2:H:122[B]:VAL:CG1  | 2.47                     | 0.62              |
| 1:A:99[A]:MET:HE1   | 1:A:146[A]:ILE:HD11 | 1.80                     | 0.62              |
| 2:B:135[B]:HIS:O    | 2:B:137[B]:PHE:N    | 2.32                     | 0.62              |
| 2:F:166[B]:GLY:HA2  | 2:F:179[B]:HIS:CE1  | 2.35                     | 0.62              |
| 2:B:60[B]:ALA:CB    | 2:B:86[B]:ILE:HD12  | 2.29                     | 0.62              |
| 1:C:169[A]:GLN:HG3  | 1:C:170[A]:GLY:H    | 1.63                     | 0.62              |
| 2:B:281[B]:VAL:HG22 | 2:H:108[B]:ILE:HG23 | 1.82                     | 0.62              |
| 2:F:277[B]:PRO:O    | 2:F:281[B]:VAL:HG23 | 1.99                     | 0.62              |
| 2:H:267[B]:ILE:O    | 2:H:270[B]:ALA:HB3  | 1.99                     | 0.62              |
| 2:F:163[B]:ARG:O    | 2:F:163[B]:ARG:HG3  | 1.97                     | 0.62              |
| 1:A:48[A]:GLU:CG    | 1:A:67[A]:ILE:CG2   | 2.78                     | 0.62              |
| 2:H:79[B]:ASP:OD1   | 2:H:81[B]:GLN:N     | 2.25                     | 0.62              |
| 2:B:110[B]:GLU:CG   | 2:B:139[B]:ILE:HG22 | 2.30                     | 0.62              |
| 2:B:127[B]:ASP:C    | 2:B:127[B]:ASP:OD1  | 2.42                     | 0.61              |
| 2:B:193[B]:MET:HE1  | 2:B:201[B]:PHE:CD1  | 2.35                     | 0.61              |
| 2:F:199[B]:PHE:CE1  | 2:F:209[B]:TYR:CE1  | 2.88                     | 0.61              |
| 1:C:79[A]:ARG:O     | 1:C:127[A]:ILE:CG2  | 2.48                     | 0.61              |
| 1:E:225[A]:ARG:NH2  | 1:E:251[A]:ASP:OD2  | 2.32                     | 0.61              |
| 2:B:110[B]:GLU:HG3  | 2:B:139[B]:ILE:HG21 | 1.82                     | 0.61              |
| 2:H:108[B]:ILE:O    | 2:H:112[B]:ILE:HG12 | 2.00                     | 0.61              |
| 2:B:23[B]:PHE:O     | 2:B:27[B]:VAL:HG23  | 1.99                     | 0.61              |
| 1:C:169[A]:GLN:HG3  | 1:C:170[A]:GLY:N    | 2.15                     | 0.61              |
| 1:E:233[A]:SER:HB2  | 1:E:254[A]:PHE:HB2  | 1.82                     | 0.61              |
| 2:H:175[B]:GLU:O    | 2:H:176[B]:ALA:C    | 2.44                     | 0.61              |
| 1:C:93[A]:ALA:O     | 1:C:94[A]:VAL:CG1   | 2.48                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:G:189[A]:MET:HE3  | 1:G:189[A]:MET:HA   | 1.82                     | 0.61              |
| 1:G:272[A]:ILE:O    | 1:G:276[A]:VAL:HG23 | 2.01                     | 0.61              |
| 2:B:201[B]:PHE:HE2  | 2:B:205[B]:LEU:HD11 | 1.62                     | 0.61              |
| 2:F:112[B]:ILE:O    | 2:F:112[B]:ILE:HG22 | 2.00                     | 0.61              |
| 2:D:80[B]:PRO:O     | 2:D:81[B]:GLN:C     | 2.41                     | 0.60              |
| 2:H:179[B]:HIS:O    | 2:H:182[B]:SER:N    | 2.34                     | 0.60              |
| 2:B:79[B]:ASP:OD1   | 2:B:80[B]:PRO:HD2   | 2.02                     | 0.60              |
| 2:F:230[B]:GLY:O    | 2:F:231[B]:VAL:C    | 2.45                     | 0.60              |
| 2:H:79[B]:ASP:OD1   | 2:H:79[B]:ASP:C     | 2.45                     | 0.60              |
| 1:G:226[A]:VAL:O    | 1:G:228[A]:VAL:N    | 2.34                     | 0.60              |
| 2:B:55[B]:ALA:O     | 2:B:92[B]:ILE:HD12  | 2.01                     | 0.60              |
| 2:D:166[B]:GLY:HA2  | 2:D:179[B]:HIS:CE1  | 2.36                     | 0.60              |
| 2:F:94[B]:VAL:N     | 2:F:115[B]:ASP:OD2  | 2.29                     | 0.60              |
| 2:B:241[B]:MET:SD   | 2:B:271[B]:VAL:HG13 | 2.42                     | 0.60              |
| 2:B:34[B]:ARG:NH1   | 2:D:32[B]:MET:HG2   | 2.17                     | 0.59              |
| 2:B:95[B]:MET:HG2   | 2:B:116[B]:TYR:HB2  | 1.82                     | 0.59              |
| 1:C:171[A]:ASP:OD2  | 1:C:175[A]:THR:HG21 | 2.02                     | 0.59              |
| 2:F:96[B]:ALA:HB2   | 2:F:114[B]:ILE:CD1  | 2.32                     | 0.59              |
| 2:D:201[B]:PHE:CE2  | 2:D:205[B]:LEU:HD11 | 2.37                     | 0.59              |
| 2:F:59[B]:MET:CE    | 2:F:95[B]:MET:SD    | 2.91                     | 0.59              |
| 1:C:185[A]:VAL:O    | 1:C:189[A]:MET:HG2  | 2.03                     | 0.59              |
| 1:A:198[A]:MET:HE1  | 1:A:206[A]:PHE:CD1  | 2.37                     | 0.59              |
| 1:E:168[A]:ILE:HG22 | 1:E:233[A]:SER:H    | 1.67                     | 0.59              |
| 2:B:119[B]:GLU:OE1  | 2:B:134[B]:LYS:NZ   | 2.36                     | 0.59              |
| 2:F:195[B]:ASP:O    | 2:F:197[B]:GLU:N    | 2.36                     | 0.59              |
| 2:H:76[B]:ARG:HG2   | 2:H:99[B]:ARG:CZ    | 2.32                     | 0.59              |
| 1:C:146[A]:ILE:HD12 | 1:C:165[A]:MET:CE   | 2.32                     | 0.59              |
| 2:B:37[B]:VAL:CG2   | 2:B:271[B]:VAL:HG21 | 2.33                     | 0.59              |
| 2:D:117[B]:ILE:HG22 | 2:D:141[B]:PHE:CE2  | 2.37                     | 0.59              |
| 2:F:29[B]:LEU:C     | 2:F:116[B]:TYR:OH   | 2.46                     | 0.59              |
| 2:F:288[B]:GLY:O    | 2:F:289[B]:GLU:C    | 2.46                     | 0.59              |
| 2:H:160[B]:ALA:O    | 2:H:223[B]:VAL:CB   | 2.47                     | 0.58              |
| 2:D:81[B]:GLN:O     | 2:D:85[B]:GLU:HG3   | 2.03                     | 0.58              |
| 2:H:121[B]:GLU:CD   | 2:H:165[B]:LYS:HG2  | 2.27                     | 0.58              |
| 2:B:100[B]:ILE:HA   | 2:B:119[B]:GLU:HG2  | 1.85                     | 0.58              |
| 2:B:265[B]:ARG:HE   | 2:B:269[B]:GLN:CD   | 2.12                     | 0.58              |
| 2:F:96[B]:ALA:HB2   | 2:F:114[B]:ILE:HD11 | 1.86                     | 0.58              |
| 2:F:154[B]:ARG:HA   | 2:F:154[B]:ARG:NE   | 2.18                     | 0.58              |
| 2:H:179[B]:HIS:O    | 2:H:180[B]:VAL:C    | 2.47                     | 0.58              |
| 2:D:165[B]:LYS:O    | 2:D:179[B]:HIS:ND1  | 2.37                     | 0.58              |
| 2:D:275[B]:SER:C    | 2:D:277[B]:PRO:HD3  | 2.26                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:279[B]:MET:O    | 2:F:280[B]:LEU:C    | 2.46                     | 0.58              |
| 1:C:146[A]:ILE:HD12 | 1:C:165[A]:MET:HE2  | 1.86                     | 0.58              |
| 1:E:81[A]:MET:HB2   | 1:E:109[A]:GLU:CD   | 2.29                     | 0.58              |
| 1:A:181[A]:THR:O    | 1:A:185[A]:VAL:HG23 | 2.04                     | 0.58              |
| 1:E:191[A]:GLU:HG3  | 1:E:206[A]:PHE:HZ   | 1.68                     | 0.58              |
| 2:D:193[B]:MET:HE1  | 2:D:201[B]:PHE:CD1  | 2.38                     | 0.58              |
| 2:B:117[B]:ILE:HG21 | 2:B:141[B]:PHE:CE2  | 2.39                     | 0.58              |
| 1:C:56[A]:LYS:O     | 1:C:57[A]:LEU:C     | 2.44                     | 0.57              |
| 1:E:30[A]:PRO:O     | 1:E:34[A]:LYS:HG3   | 2.04                     | 0.57              |
| 2:D:80[B]:PRO:O     | 2:D:82[B]:MET:N     | 2.37                     | 0.57              |
| 2:H:37[B]:VAL:HG23  | 2:H:271[B]:VAL:HG21 | 1.83                     | 0.57              |
| 2:B:110[B]:GLU:CG   | 2:B:139[B]:ILE:CG2  | 2.82                     | 0.57              |
| 1:E:198[A]:MET:HE1  | 1:E:206[A]:PHE:CD1  | 2.40                     | 0.57              |
| 1:G:90[A]:VAL:O     | 1:G:91[A]:LYS:C     | 2.47                     | 0.57              |
| 1:G:155[A]:ALA:O    | 1:G:159[A]:ILE:HG13 | 2.04                     | 0.57              |
| 2:F:174[B]:ILE:O    | 2:F:174[B]:ILE:CG1  | 2.51                     | 0.57              |
| 1:C:225[A]:ARG:NH2  | 1:C:251[A]:ASP:OD2  | 2.33                     | 0.57              |
| 1:G:90[A]:VAL:CG2   | 1:G:91[A]:LYS:N     | 2.67                     | 0.57              |
| 2:F:37[B]:VAL:HG22  | 2:F:271[B]:VAL:HG21 | 1.85                     | 0.57              |
| 1:A:82[A]:PRO:HG2   | 1:A:87[A]:ILE:HD11  | 1.85                     | 0.57              |
| 1:G:85[A]:VAL:O     | 1:G:89[A]:GLU:HG3   | 2.04                     | 0.57              |
| 1:G:200[A]:ASP:OD1  | 1:G:221[A]:LYS:HE2  | 2.04                     | 0.57              |
| 2:D:191[B]:ARG:O    | 2:D:216[B]:LYS:NZ   | 2.38                     | 0.57              |
| 2:D:276[B]:ASP:CG   | 2:D:279[B]:MET:HB3  | 2.27                     | 0.57              |
| 2:F:96[B]:ALA:CB    | 2:F:114[B]:ILE:CD1  | 2.82                     | 0.57              |
| 2:F:279[B]:MET:O    | 2:F:282[B]:GLU:N    | 2.36                     | 0.57              |
| 1:A:185[A]:VAL:O    | 1:A:189[A]:MET:HG2  | 2.05                     | 0.57              |
| 2:B:172[B]:ASN:CG   | 2:B:174[B]:ILE:HG22 | 2.29                     | 0.57              |
| 2:D:103[B]:PHE:O    | 2:D:107[B]:GLN:HG3  | 2.04                     | 0.57              |
| 1:C:171[A]:ASP:OD2  | 1:C:175[A]:THR:OG1  | 2.22                     | 0.57              |
| 2:B:37[B]:VAL:HG22  | 2:B:271[B]:VAL:HG21 | 1.86                     | 0.57              |
| 1:A:292[A]:LEU:O    | 1:A:293[A]:GLU:CB   | 2.53                     | 0.56              |
| 1:C:288[A]:MET:HA   | 1:C:288[A]:MET:CE   | 2.32                     | 0.56              |
| 1:G:292[A]:LEU:O    | 1:G:293[A]:GLU:CB   | 2.52                     | 0.56              |
| 2:D:184[B]:ASN:ND2  | 2:D:243[B]:LEU:O    | 2.38                     | 0.56              |
| 1:E:222[A]:GLN:O    | 1:E:224[A]:GLY:N    | 2.38                     | 0.56              |
| 2:B:80[B]:PRO:O     | 2:B:83[B]:ILE:N     | 2.37                     | 0.56              |
| 2:B:281[B]:VAL:HG11 | 2:H:112[B]:ILE:HG22 | 1.86                     | 0.56              |
| 2:H:265[B]:ARG:NH1  | 2:H:269[B]:GLN:NE2  | 2.53                     | 0.56              |
| 2:F:59[B]:MET:HE2   | 2:F:95[B]:MET:SD    | 2.45                     | 0.56              |
| 2:F:127[B]:ASP:C    | 2:F:127[B]:ASP:OD1  | 2.49                     | 0.56              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:E:199[A]:ASP:OD1  | 1:E:199[A]:ASP:C    | 2.49                     | 0.56              |
| 1:G:80[A]:ARG:HG2   | 1:G:103[A]:ARG:CZ   | 2.35                     | 0.56              |
| 2:B:79[B]:ASP:OD1   | 2:B:79[B]:ASP:C     | 2.49                     | 0.56              |
| 2:D:106[B]:ALA:O    | 2:D:107[B]:GLN:C    | 2.49                     | 0.56              |
| 2:D:134[B]:LYS:HG2  | 2:D:141[B]:PHE:CD1  | 2.40                     | 0.56              |
| 2:D:146[B]:ARG:HG2  | 2:D:179[B]:HIS:NE2  | 2.21                     | 0.56              |
| 2:H:209[B]:TYR:O    | 2:H:210[B]:ASP:C    | 2.48                     | 0.56              |
| 1:A:87[A]:ILE:CD1   | 1:A:113[A]:LEU:CD2  | 2.83                     | 0.56              |
| 1:E:168[A]:ILE:HG12 | 1:E:185[A]:VAL:HG23 | 1.87                     | 0.56              |
| 1:G:41[A]:LEU:HD22  | 1:G:64[A]:CYS:SG    | 2.45                     | 0.56              |
| 2:F:41[B]:VAL:HG11  | 2:F:47[B]:ALA:HA    | 1.87                     | 0.56              |
| 1:A:48[A]:GLU:HA    | 1:A:67[A]:ILE:HG23  | 1.79                     | 0.56              |
| 1:E:173[A]:THR:HB   | 1:E:175[A]:THR:HG23 | 1.88                     | 0.56              |
| 2:B:79[B]:ASP:OD1   | 2:B:80[B]:PRO:N     | 2.39                     | 0.56              |
| 2:H:42[B]:VAL:HG22  | 2:H:46[B]:GLN:OE1   | 2.05                     | 0.56              |
| 2:D:134[B]:LYS:HD2  | 2:D:141[B]:PHE:CB   | 2.36                     | 0.56              |
| 2:F:38[B]:ILE:HD13  | 2:F:95[B]:MET:HE1   | 1.87                     | 0.56              |
| 1:G:223[A]:MET:HE1  | 1:G:227[A]:PRO:HA   | 1.88                     | 0.55              |
| 2:B:60[B]:ALA:CB    | 2:B:86[B]:ILE:CD1   | 2.83                     | 0.55              |
| 1:C:280[A]:ASN:O    | 1:C:282[A]:PRO:HD3  | 2.06                     | 0.55              |
| 1:E:174[A]:ALA:HB1  | 1:E:296[A]:MET:HE1  | 1.89                     | 0.55              |
| 2:F:195[B]:ASP:C    | 2:F:197[B]:GLU:H    | 2.14                     | 0.55              |
| 1:E:67[A]:ILE:HG23  | 1:E:67[A]:ILE:O     | 2.06                     | 0.55              |
| 1:E:37[A]:LEU:O     | 1:E:120[A]:TYR:OH   | 2.25                     | 0.55              |
| 1:G:238[A]:THR:O    | 1:G:239[A]:PRO:C    | 2.49                     | 0.55              |
| 1:C:104[A]:VAL:HG13 | 1:C:135[A]:PHE:CD1  | 2.42                     | 0.55              |
| 2:B:38[B]:ILE:HD13  | 2:B:95[B]:MET:HE1   | 1.89                     | 0.55              |
| 2:B:76[B]:ARG:O     | 2:B:77[B]:MET:C     | 2.50                     | 0.55              |
| 2:B:281[B]:VAL:CG2  | 2:H:112[B]:ILE:HG23 | 2.36                     | 0.55              |
| 2:H:199[B]:PHE:CD1  | 2:H:209[B]:TYR:CE1  | 2.94                     | 0.55              |
| 1:E:108[A]:VAL:O    | 1:E:109[A]:GLU:C    | 2.49                     | 0.55              |
| 1:A:67[A]:ILE:CG2   | 1:A:67[A]:ILE:O     | 2.54                     | 0.55              |
| 2:F:38[B]:ILE:HD13  | 2:F:95[B]:MET:CE    | 2.36                     | 0.55              |
| 1:A:99[A]:MET:SD    | 1:A:146[A]:ILE:HD12 | 2.47                     | 0.55              |
| 2:H:139[B]:ILE:CG2  | 2:H:140[B]:PRO:HD2  | 2.37                     | 0.55              |
| 1:C:93[A]:ALA:C     | 1:C:94[A]:VAL:HG13  | 2.32                     | 0.55              |
| 2:H:103[B]:PHE:CE1  | 2:H:104[B]:VAL:HG23 | 2.42                     | 0.55              |
| 2:B:112[B]:ILE:HG22 | 2:B:112[B]:ILE:O    | 2.06                     | 0.54              |
| 2:B:162[B]:ILE:HG22 | 2:B:163[B]:ARG:N    | 2.22                     | 0.54              |
| 1:A:131[A]:ASP:OD1  | 1:A:131[A]:ASP:C    | 2.49                     | 0.54              |
| 1:C:126[A]:ILE:HD12 | 1:C:126[A]:ILE:N    | 2.22                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:C:156[A]:LEU:CD1  | 1:C:217[A]:VAL:HG22 | 2.37                     | 0.54              |
| 1:E:138[A]:LYS:HG2  | 1:E:145[A]:PHE:CG   | 2.41                     | 0.54              |
| 2:B:80[B]:PRO:O     | 2:B:81[B]:GLN:C     | 2.50                     | 0.54              |
| 2:D:110[B]:GLU:O    | 2:D:113[B]:GLY:N    | 2.39                     | 0.54              |
| 1:A:34[A]:LYS:HB3   | 1:A:144[A]:PRO:HB3  | 1.87                     | 0.54              |
| 1:A:199[A]:ASP:C    | 1:A:199[A]:ASP:OD1  | 2.50                     | 0.54              |
| 1:E:41[A]:LEU:O     | 1:E:42[A]:ARG:C     | 2.50                     | 0.54              |
| 2:B:79[B]:ASP:OD1   | 2:B:80[B]:PRO:CD    | 2.55                     | 0.54              |
| 2:H:241[B]:MET:SD   | 2:H:271[B]:VAL:HG13 | 2.47                     | 0.54              |
| 1:C:204[A]:PHE:CD1  | 1:C:214[A]:TYR:CE1  | 2.95                     | 0.54              |
| 2:B:87[B]:LYS:CD    | 2:B:113[B]:GLY:O    | 2.55                     | 0.54              |
| 1:C:58[A]:ALA:O     | 1:C:63[A]:ALA:CB    | 2.56                     | 0.54              |
| 2:B:139[B]:ILE:HG13 | 2:B:140[B]:PRO:HD2  | 1.89                     | 0.54              |
| 2:B:176[B]:ALA:O    | 2:B:180[B]:VAL:HG23 | 2.06                     | 0.54              |
| 2:D:23[B]:PHE:HA    | 2:D:26[B]:LYS:HD2   | 1.89                     | 0.54              |
| 2:D:167[B]:GLU:OE1  | 2:D:170[B]:THR:HG21 | 2.08                     | 0.54              |
| 1:C:223[A]:MET:HE1  | 1:C:227[A]:PRO:HA   | 1.89                     | 0.54              |
| 1:E:164[A]:ALA:O    | 1:E:228[A]:VAL:HB   | 2.08                     | 0.54              |
| 2:F:33[B]:LEU:O     | 2:F:34[B]:ARG:C     | 2.50                     | 0.54              |
| 2:H:113[B]:GLY:O    | 2:H:114[B]:ILE:C    | 2.50                     | 0.54              |
| 1:G:226[A]:VAL:C    | 1:G:228[A]:VAL:H    | 2.15                     | 0.54              |
| 2:F:115[B]:ASP:O    | 2:F:140[B]:PRO:CD   | 2.53                     | 0.54              |
| 1:C:260[A]:PHE:C    | 1:C:262[A]:GLY:H    | 2.16                     | 0.54              |
| 2:B:87[B]:LYS:HD2   | 2:B:113[B]:GLY:O    | 2.08                     | 0.53              |
| 2:D:280[B]:LEU:HA   | 2:D:283[B]:VAL:HG22 | 1.89                     | 0.53              |
| 1:A:54[A]:GLN:HG2   | 1:A:260[A]:PHE:CE2  | 2.43                     | 0.53              |
| 1:C:49[A]:VAL:HG11  | 1:C:55[A]:ALA:HA    | 1.89                     | 0.53              |
| 2:D:106[B]:ALA:O    | 2:D:109[B]:LEU:N    | 2.41                     | 0.53              |
| 2:D:239[B]:LEU:HD11 | 2:F:103[B]:PHE:CE2  | 2.43                     | 0.53              |
| 2:F:37[B]:VAL:CG2   | 2:F:271[B]:VAL:HG21 | 2.38                     | 0.53              |
| 2:F:195[B]:ASP:C    | 2:F:197[B]:GLU:N    | 2.66                     | 0.53              |
| 2:D:41[B]:VAL:HG21  | 2:D:58[B]:VAL:HB    | 1.89                     | 0.53              |
| 2:D:134[B]:LYS:HG2  | 2:D:141[B]:PHE:CE1  | 2.44                     | 0.53              |
| 2:D:221[B]:LEU:C    | 2:D:223[B]:VAL:H    | 2.17                     | 0.53              |
| 2:F:160[B]:ALA:O    | 2:F:161[B]:MET:HB2  | 2.09                     | 0.53              |
| 1:A:168[A]:ILE:CG1  | 1:A:233[A]:SER:H    | 2.20                     | 0.53              |
| 2:F:199[B]:PHE:CE1  | 2:F:209[B]:TYR:OH   | 2.62                     | 0.53              |
| 1:C:157[A]:ARG:NH1  | 1:C:211[A]:SER:O    | 2.32                     | 0.53              |
| 2:B:160[B]:ALA:O    | 2:B:223[B]:VAL:CB   | 2.53                     | 0.53              |
| 2:H:146[B]:ARG:NH2  | 2:H:150[B]:GLU:CD   | 2.66                     | 0.53              |
| 2:B:76[B]:ARG:O     | 2:B:77[B]:MET:O     | 2.26                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:B:142[B]:VAL:HA   | 2:B:161[B]:MET:O    | 2.09                     | 0.53              |
| 2:D:146[B]:ARG:HG2  | 2:D:179[B]:HIS:CE1  | 2.44                     | 0.53              |
| 1:A:114[A]:GLU:OE2  | 1:A:142[A]:ARG:N    | 2.40                     | 0.53              |
| 1:G:270[A]:ARG:HH11 | 1:G:274[A]:GLN:NE2  | 2.04                     | 0.53              |
| 2:D:59[B]:MET:HE1   | 2:D:118[B]:ASP:HB2  | 1.90                     | 0.53              |
| 1:E:102[A]:ALA:C    | 1:E:127[A]:ILE:HD11 | 2.34                     | 0.53              |
| 1:G:220[A]:THR:HG23 | 1:G:225[A]:ARG:O    | 2.08                     | 0.53              |
| 2:F:40[B]:ASP:HB2   | 2:F:251[B]:GLY:HA2  | 1.89                     | 0.53              |
| 1:E:56[A]:LYS:O     | 1:E:57[A]:LEU:C     | 2.51                     | 0.53              |
| 2:B:86[B]:ILE:C     | 2:B:88[B]:GLN:H     | 2.16                     | 0.53              |
| 2:H:82[B]:MET:O     | 2:H:83[B]:ILE:C     | 2.52                     | 0.53              |
| 2:B:139[B]:ILE:HG13 | 2:B:140[B]:PRO:CD   | 2.39                     | 0.52              |
| 2:B:201[B]:PHE:CE2  | 2:B:205[B]:LEU:CD1  | 2.85                     | 0.52              |
| 2:D:162[B]:ILE:HG12 | 2:D:223[B]:VAL:HG21 | 1.91                     | 0.52              |
| 2:H:59[B]:MET:CE    | 2:H:118[B]:ASP:OD2  | 2.57                     | 0.52              |
| 1:E:274[A]:GLN:CB   | 1:E:288[A]:MET:HE2  | 2.39                     | 0.52              |
| 1:G:290[A]:SER:O    | 1:G:291[A]:GLY:C    | 2.51                     | 0.52              |
| 2:B:183[B]:VAL:O    | 2:B:187[B]:ILE:HG13 | 2.09                     | 0.52              |
| 2:B:134[B]:LYS:HE3  | 2:B:143[B]:CYS:SG   | 2.50                     | 0.52              |
| 2:H:233[B]:THR:O    | 2:H:234[B]:PRO:C    | 2.53                     | 0.52              |
| 2:B:60[B]:ALA:HB2   | 2:B:86[B]:ILE:CD1   | 2.39                     | 0.52              |
| 1:A:80[A]:ARG:HG2   | 1:A:103[A]:ARG:CZ   | 2.40                     | 0.52              |
| 1:E:168[A]:ILE:HG23 | 1:E:169[A]:GLN:N    | 2.24                     | 0.52              |
| 1:G:152[A]:THR:HA   | 1:G:188[A]:LEU:CD1  | 2.40                     | 0.52              |
| 2:B:86[B]:ILE:C     | 2:B:88[B]:GLN:N     | 2.65                     | 0.52              |
| 2:H:134[B]:LYS:HG2  | 2:H:141[B]:PHE:CD1  | 2.44                     | 0.52              |
| 1:A:129[A]:VAL:HG12 | 1:A:130[A]:ALA:N    | 2.25                     | 0.52              |
| 2:D:33[B]:LEU:O     | 2:D:34[B]:ARG:C     | 2.52                     | 0.52              |
| 2:H:116[B]:TYR:HD2  | 2:H:140[B]:PRO:HG2  | 1.73                     | 0.52              |
| 1:C:119[A]:ASP:O    | 1:C:144[A]:PRO:HD2  | 2.10                     | 0.52              |
| 2:B:162[B]:ILE:CG2  | 2:B:163[B]:ARG:N    | 2.72                     | 0.52              |
| 2:B:239[B]:LEU:HA   | 2:H:104[B]:VAL:HG21 | 1.92                     | 0.52              |
| 2:F:185[B]:GLY:O    | 2:F:189[B]:VAL:HG23 | 2.10                     | 0.52              |
| 2:F:193[B]:MET:HE1  | 2:F:201[B]:PHE:CD1  | 2.45                     | 0.52              |
| 1:C:198[A]:MET:HE1  | 1:C:206[A]:PHE:CD1  | 2.45                     | 0.52              |
| 2:F:199[B]:PHE:HE1  | 2:F:209[B]:TYR:CZ   | 2.27                     | 0.52              |
| 2:H:167[B]:GLU:HG2  | 2:H:170[B]:THR:CG2  | 2.40                     | 0.52              |
| 1:A:99[A]:MET:SD    | 1:A:146[A]:ILE:HD13 | 2.48                     | 0.51              |
| 1:C:49[A]:VAL:HG21  | 1:C:55[A]:ALA:HB2   | 1.92                     | 0.51              |
| 1:G:171[A]:ASP:O    | 1:G:172[A]:LEU:O    | 2.27                     | 0.51              |
| 2:F:124[B]:THR:O    | 2:F:124[B]:THR:HG22 | 2.10                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:C:223[A]:MET:CE   | 1:C:227[A]:PRO:HA   | 2.41                     | 0.51              |
| 2:B:74[B]:VAL:HG12  | 2:B:76[B]:ARG:HG3   | 1.91                     | 0.51              |
| 2:B:86[B]:ILE:O     | 2:B:88[B]:GLN:N     | 2.43                     | 0.51              |
| 2:B:265[B]:ARG:NH2  | 2:B:269[B]:GLN:HG3  | 2.25                     | 0.51              |
| 1:G:138[A]:LYS:HG2  | 1:G:145[A]:PHE:CG   | 2.45                     | 0.51              |
| 2:D:134[B]:LYS:HG2  | 2:D:141[B]:PHE:CG   | 2.46                     | 0.51              |
| 1:A:245[A]:MET:CE   | 1:A:245[A]:MET:HA   | 2.37                     | 0.51              |
| 2:B:196[B]:ASP:OD1  | 2:B:196[B]:ASP:N    | 2.43                     | 0.51              |
| 2:H:214[B]:GLN:NE2  | 2:H:222[B]:PRO:HB3  | 2.24                     | 0.51              |
| 1:E:180[A]:GLU:OE1  | 1:E:183[A]:LYS:NZ   | 2.43                     | 0.51              |
| 1:E:225[A]:ARG:NH1  | 1:E:226[A]:VAL:O    | 2.44                     | 0.51              |
| 1:E:274[A]:GLN:HG3  | 1:E:288[A]:MET:HE1  | 1.90                     | 0.51              |
| 2:B:79[B]:ASP:O     | 2:B:80[B]:PRO:C     | 2.53                     | 0.51              |
| 2:D:134[B]:LYS:HD2  | 2:D:141[B]:PHE:HB3  | 1.92                     | 0.51              |
| 2:F:121[B]:GLU:CD   | 2:F:121[B]:GLU:H    | 2.19                     | 0.51              |
| 1:A:125[A]:GLU:CD   | 1:A:169[A]:GLN:CG   | 2.81                     | 0.51              |
| 2:B:51[B]:GLU:C     | 2:B:53[B]:ALA:H     | 2.17                     | 0.51              |
| 2:F:43[B]:ASN:OD1   | 2:F:45[B]:GLU:N     | 2.44                     | 0.51              |
| 1:C:37[A]:LEU:O     | 1:C:40[A]:VAL:HG13  | 2.11                     | 0.51              |
| 2:B:117[B]:ILE:CG2  | 2:B:141[B]:PHE:CE2  | 2.93                     | 0.51              |
| 2:F:39[B]:MET:HE1   | 2:F:264[B]:ALA:HB1  | 1.93                     | 0.51              |
| 1:C:224[A]:GLY:O    | 1:C:225[A]:ARG:HB2  | 2.11                     | 0.50              |
| 1:E:180[A]:GLU:CD   | 1:E:183[A]:LYS:HZ3  | 2.19                     | 0.50              |
| 2:B:76[B]:ARG:C     | 2:B:77[B]:MET:O     | 2.50                     | 0.50              |
| 2:H:48[B]:ARG:O     | 2:H:49[B]:ILE:C     | 2.53                     | 0.50              |
| 1:A:30[A]:PRO:O     | 1:A:34[A]:LYS:HG3   | 2.12                     | 0.50              |
| 1:G:173[A]:THR:HB   | 1:G:175[A]:THR:CG2  | 2.40                     | 0.50              |
| 2:B:42[B]:VAL:O     | 2:B:42[B]:VAL:CG2   | 2.53                     | 0.50              |
| 2:D:276[B]:ASP:O    | 2:D:277[B]:PRO:C    | 2.53                     | 0.50              |
| 2:B:87[B]:LYS:CE    | 2:B:113[B]:GLY:O    | 2.59                     | 0.50              |
| 2:D:80[B]:PRO:C     | 2:D:82[B]:MET:N     | 2.69                     | 0.50              |
| 1:C:116[A]:LEU:O    | 1:C:117[A]:ALA:HB3  | 2.11                     | 0.50              |
| 1:C:126[A]:ILE:HD11 | 1:C:169[A]:GLN:NE2  | 2.27                     | 0.50              |
| 1:E:190[A]:GLY:O    | 1:E:194[A]:VAL:HG23 | 2.12                     | 0.50              |
| 1:G:67[A]:ILE:HD12  | 1:G:99[A]:MET:HE2   | 1.93                     | 0.50              |
| 2:H:37[B]:VAL:HG22  | 2:H:271[B]:VAL:HG21 | 1.90                     | 0.50              |
| 1:A:37[A]:LEU:O     | 1:A:40[A]:VAL:CG1   | 2.52                     | 0.50              |
| 1:C:93[A]:ALA:O     | 1:C:94[A]:VAL:HG12  | 2.12                     | 0.50              |
| 1:E:165[A]:MET:HG3  | 1:E:229[A]:VAL:HB   | 1.93                     | 0.50              |
| 2:B:46[B]:GLN:HB3   | 2:B:255[B]:PHE:CZ   | 2.47                     | 0.50              |
| 1:G:90[A]:VAL:O     | 1:G:92[A]:ARG:N     | 2.45                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:106[B]:ALA:O    | 2:F:109[B]:LEU:N    | 2.44                     | 0.50              |
| 2:F:32[B]:MET:HE2   | 2:F:32[B]:MET:HA    | 1.93                     | 0.50              |
| 1:C:58[A]:ALA:O     | 1:C:63[A]:ALA:HB2   | 2.11                     | 0.50              |
| 1:C:82[A]:PRO:HG2   | 1:C:87[A]:ILE:HD11  | 1.94                     | 0.50              |
| 2:B:239[B]:LEU:CD1  | 2:H:103[B]:PHE:CE1  | 2.93                     | 0.50              |
| 2:B:272[B]:THR:HG22 | 2:B:272[B]:THR:O    | 2.11                     | 0.49              |
| 1:C:281[A]:ASP:CG   | 1:C:284[A]:VAL:HG23 | 2.37                     | 0.49              |
| 2:B:76[B]:ARG:HG2   | 2:B:99[B]:ARG:CZ    | 2.41                     | 0.49              |
| 2:D:40[B]:ASP:HA    | 2:D:59[B]:MET:HB3   | 1.94                     | 0.49              |
| 2:H:167[B]:GLU:CD   | 2:H:170[B]:THR:HG21 | 2.36                     | 0.49              |
| 2:D:136[B]:ASN:C    | 2:D:137[B]:PHE:CD1  | 2.90                     | 0.49              |
| 2:F:142[B]:VAL:HG22 | 2:F:161[B]:MET:HB3  | 1.94                     | 0.49              |
| 1:A:87[A]:ILE:CD1   | 1:A:113[A]:LEU:HD21 | 2.43                     | 0.49              |
| 1:G:120[A]:TYR:CD1  | 1:G:144[A]:PRO:HG2  | 2.48                     | 0.49              |
| 1:A:185[A]:VAL:CG2  | 1:A:245[A]:MET:HE1  | 2.33                     | 0.49              |
| 1:A:67[A]:ILE:HD12  | 1:A:99[A]:MET:HB3   | 1.94                     | 0.49              |
| 1:G:59[A]:GLU:HG3   | 1:G:96[A]:VAL:HG22  | 1.94                     | 0.49              |
| 2:B:281[B]:VAL:HG11 | 2:H:112[B]:ILE:CG2  | 2.42                     | 0.49              |
| 1:G:199[A]:ASP:OD1  | 1:G:199[A]:ASP:C    | 2.56                     | 0.49              |
| 2:B:167[B]:GLU:OE1  | 2:B:170[B]:THR:CB   | 2.61                     | 0.49              |
| 2:B:221[B]:LEU:C    | 2:B:223[B]:VAL:N    | 2.65                     | 0.49              |
| 2:D:76[B]:ARG:O     | 2:D:77[B]:MET:O     | 2.31                     | 0.49              |
| 2:D:76[B]:ARG:C     | 2:D:77[B]:MET:O     | 2.53                     | 0.49              |
| 2:H:167[B]:GLU:OE1  | 2:H:170[B]:THR:HG21 | 2.13                     | 0.49              |
| 1:A:149[A]:CYS:SG   | 1:A:155[A]:ALA:HB2  | 2.52                     | 0.49              |
| 1:E:168[A]:ILE:HD11 | 1:E:185[A]:VAL:HA   | 1.95                     | 0.49              |
| 2:B:173[B]:ILE:CG1  | 2:B:240[B]:MET:HE3  | 2.43                     | 0.49              |
| 1:A:167[A]:ARG:O    | 1:A:167[A]:ARG:HG3  | 2.13                     | 0.49              |
| 1:E:169[A]:GLN:NE2  | 1:E:170[A]:GLY:N    | 2.52                     | 0.49              |
| 2:D:37[B]:VAL:HG22  | 2:D:271[B]:VAL:HG21 | 1.94                     | 0.49              |
| 2:D:74[B]:VAL:HG13  | 2:D:124[B]:THR:HG21 | 1.94                     | 0.49              |
| 1:A:221[A]:LYS:C    | 1:A:223[A]:MET:N    | 2.71                     | 0.48              |
| 2:D:38[B]:ILE:HD13  | 2:D:95[B]:MET:HE3   | 1.95                     | 0.48              |
| 2:D:134[B]:LYS:CB   | 2:D:141[B]:PHE:CD1  | 2.95                     | 0.48              |
| 2:F:164[B]:THR:HG22 | 2:F:227[B]:ALA:HA   | 1.95                     | 0.48              |
| 2:H:41[B]:VAL:HG11  | 2:H:47[B]:ALA:HA    | 1.94                     | 0.48              |
| 1:C:41[A]:LEU:O     | 1:C:42[A]:ARG:C     | 2.56                     | 0.48              |
| 1:E:120[A]:TYR:CD1  | 1:E:144[A]:PRO:HG2  | 2.48                     | 0.48              |
| 2:B:192[B]:ASN:CG   | 2:B:192[B]:ASN:O    | 2.55                     | 0.48              |
| 2:H:214[B]:GLN:HE21 | 2:H:222[B]:PRO:HB3  | 1.78                     | 0.48              |
| 1:C:199[A]:ASP:OD1  | 1:C:201[A]:ASP:N    | 2.45                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:D:76[B]:ARG:HG2   | 2:D:99[B]:ARG:CZ    | 2.43                     | 0.48              |
| 2:F:76[B]:ARG:HG2   | 2:F:99[B]:ARG:NE    | 2.29                     | 0.48              |
| 2:F:96[B]:ALA:HB3   | 2:F:114[B]:ILE:HD13 | 1.96                     | 0.48              |
| 1:E:245[A]:MET:HE3  | 1:E:245[A]:MET:HA   | 1.94                     | 0.48              |
| 2:B:135[B]:HIS:C    | 2:B:137[B]:PHE:N    | 2.64                     | 0.48              |
| 2:F:100[B]:ILE:HA   | 2:F:119[B]:GLU:HG2  | 1.95                     | 0.48              |
| 2:H:193[B]:MET:O    | 2:H:216[B]:LYS:NZ   | 2.42                     | 0.48              |
| 2:B:64[B]:VAL:HG12  | 2:B:66[B]:ALA:H     | 1.79                     | 0.48              |
| 2:D:233[B]:THR:O    | 2:D:234[B]:PRO:C    | 2.57                     | 0.48              |
| 1:A:31[A]:PHE:O     | 1:A:35[A]:VAL:HG23  | 2.14                     | 0.48              |
| 1:E:185[A]:VAL:CG2  | 1:E:245[A]:MET:HE1  | 2.37                     | 0.48              |
| 2:B:46[B]:GLN:O     | 2:B:49[B]:ILE:N     | 2.46                     | 0.48              |
| 2:D:143[B]:CYS:SG   | 2:D:159[B]:ALA:HB2  | 2.54                     | 0.48              |
| 2:F:145[B]:CYS:HB2  | 2:F:150[B]:GLU:HB3  | 1.96                     | 0.48              |
| 1:C:126[A]:ILE:HD12 | 1:C:172[A]:LEU:HD22 | 1.96                     | 0.48              |
| 1:G:38[A]:ALA:O     | 1:G:229[A]:VAL:HG21 | 2.13                     | 0.48              |
| 2:B:42[B]:VAL:O     | 2:B:43[B]:ASN:CB    | 2.58                     | 0.48              |
| 2:D:134[B]:LYS:HE2  | 2:D:157[B]:GLU:O    | 2.13                     | 0.48              |
| 1:A:91[A]:LYS:HA    | 1:A:98[A]:VAL:HG21  | 1.96                     | 0.48              |
| 1:G:172[A]:LEU:C    | 1:G:173[A]:THR:O    | 2.56                     | 0.48              |
| 2:B:267[B]:ILE:O    | 2:B:270[B]:ALA:HB3  | 2.14                     | 0.48              |
| 2:F:104[B]:VAL:HG12 | 2:F:104[B]:VAL:O    | 2.12                     | 0.48              |
| 2:B:38[B]:ILE:HD12  | 2:B:249[B]:PHE:CZ   | 2.49                     | 0.48              |
| 2:B:60[B]:ALA:HB2   | 2:B:86[B]:ILE:HD13  | 1.95                     | 0.47              |
| 2:F:172[B]:ASN:CG   | 2:F:174[B]:ILE:HG22 | 2.39                     | 0.47              |
| 2:H:21[B]:SER:O     | 2:H:25[B]:VAL:HG23  | 2.14                     | 0.47              |
| 2:B:106[B]:ALA:O    | 2:B:107[B]:GLN:C    | 2.57                     | 0.47              |
| 2:D:48[B]:ARG:O     | 2:D:49[B]:ILE:C     | 2.56                     | 0.47              |
| 1:A:54[A]:GLN:HB3   | 1:A:260[A]:PHE:CZ   | 2.48                     | 0.47              |
| 1:A:178[A]:ILE:O    | 1:A:178[A]:ILE:CG1  | 2.63                     | 0.47              |
| 1:A:58[A]:ALA:O     | 1:A:63[A]:ALA:HB3   | 2.14                     | 0.47              |
| 1:G:59[A]:GLU:OE2   | 1:G:95[A]:SER:N     | 2.33                     | 0.47              |
| 2:B:37[B]:VAL:O     | 2:B:37[B]:VAL:HG12  | 2.14                     | 0.47              |
| 1:G:125[A]:GLU:CD   | 1:G:169[A]:GLN:OE1  | 2.57                     | 0.47              |
| 2:B:60[B]:ALA:HB1   | 2:B:86[B]:ILE:CD1   | 2.42                     | 0.47              |
| 1:E:139[A]:HIS:C    | 1:E:141[A]:PHE:H    | 2.23                     | 0.47              |
| 1:E:222[A]:GLN:C    | 1:E:224[A]:GLY:H    | 2.22                     | 0.47              |
| 2:D:79[B]:ASP:O     | 2:D:82[B]:MET:HB3   | 2.14                     | 0.47              |
| 2:D:275[B]:SER:O    | 2:D:277[B]:PRO:HD2  | 2.11                     | 0.47              |
| 1:A:246[A]:MET:CE   | 1:A:250[A]:CYS:O    | 2.62                     | 0.47              |
| 1:C:91[A]:LYS:HA    | 1:C:98[A]:VAL:HG21  | 1.96                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:C:93[A]:ALA:C     | 1:C:94[A]:VAL:CG1   | 2.87                     | 0.47              |
| 1:C:226[A]:VAL:C    | 1:C:228[A]:VAL:H    | 2.23                     | 0.47              |
| 2:D:100[B]:ILE:HD11 | 2:D:121[B]:GLU:HB3  | 1.97                     | 0.47              |
| 2:D:276[B]:ASP:OD1  | 2:D:279[B]:MET:CB   | 2.62                     | 0.47              |
| 2:F:79[B]:ASP:OD1   | 2:F:79[B]:ASP:C     | 2.58                     | 0.47              |
| 2:F:106[B]:ALA:O    | 2:F:107[B]:GLN:C    | 2.58                     | 0.47              |
| 2:F:161[B]:MET:HG3  | 2:F:224[B]:VAL:HB   | 1.96                     | 0.47              |
| 2:H:131[B]:HIS:CE1  | 2:H:154[B]:ARG:CZ   | 2.98                     | 0.47              |
| 1:A:41[A]:LEU:O     | 1:A:42[A]:ARG:C     | 2.57                     | 0.47              |
| 1:A:135[A]:PHE:CE2  | 1:A:158[A]:ARG:NH2  | 2.83                     | 0.47              |
| 1:A:135[A]:PHE:CD2  | 1:A:158[A]:ARG:NH2  | 2.83                     | 0.47              |
| 1:E:189[A]:MET:HE3  | 1:E:249[A]:GLY:HA3  | 1.96                     | 0.47              |
| 1:G:148[A]:GLY:HA2  | 1:G:167[A]:ARG:O    | 2.14                     | 0.47              |
| 2:D:117[B]:ILE:HG22 | 2:D:141[B]:PHE:CD2  | 2.50                     | 0.47              |
| 2:F:56[B]:CYS:O     | 2:F:56[B]:CYS:SG    | 2.73                     | 0.47              |
| 2:F:131[B]:HIS:CE1  | 2:F:154[B]:ARG:NH1  | 2.82                     | 0.47              |
| 1:A:152[A]:THR:HA   | 1:A:188[A]:LEU:CD1  | 2.45                     | 0.47              |
| 2:D:276[B]:ASP:OD1  | 2:D:276[B]:ASP:C    | 2.58                     | 0.47              |
| 2:H:117[B]:ILE:HG21 | 2:H:141[B]:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:58[A]:ALA:O     | 1:A:63[A]:ALA:CB    | 2.62                     | 0.47              |
| 1:C:197[A]:ASN:OD1  | 1:C:197[A]:ASN:O    | 2.33                     | 0.47              |
| 2:F:22[B]:PRO:O     | 2:F:26[B]:LYS:HG3   | 2.15                     | 0.47              |
| 2:F:33[B]:LEU:HD22  | 2:F:56[B]:CYS:SG    | 2.55                     | 0.47              |
| 2:D:173[B]:ILE:HG22 | 2:D:230[B]:GLY:C    | 2.40                     | 0.46              |
| 2:D:276[B]:ASP:OD1  | 2:D:276[B]:ASP:O    | 2.33                     | 0.46              |
| 1:C:159[A]:ILE:HG22 | 1:C:216[A]:LEU:HD11 | 1.97                     | 0.46              |
| 2:B:103[B]:PHE:CE1  | 2:B:104[B]:VAL:HG23 | 2.50                     | 0.46              |
| 2:D:134[B]:LYS:HD2  | 2:D:141[B]:PHE:CG   | 2.50                     | 0.46              |
| 2:D:179[B]:HIS:O    | 2:D:182[B]:SER:HB3  | 2.15                     | 0.46              |
| 1:A:244[A]:LEU:HD12 | 1:G:107[A]:PHE:CE1  | 2.49                     | 0.46              |
| 1:C:204[A]:PHE:CE1  | 1:C:214[A]:TYR:CE1  | 3.04                     | 0.46              |
| 2:B:134[B]:LYS:CG   | 2:B:141[B]:PHE:CG   | 2.98                     | 0.46              |
| 1:C:107[A]:PHE:O    | 1:C:110[A]:ALA:HB3  | 2.16                     | 0.46              |
| 1:E:48[A]:GLU:HA    | 1:E:67[A]:ILE:CG2   | 2.44                     | 0.46              |
| 2:F:148[B]:LEU:HD13 | 2:F:183[B]:VAL:HG13 | 1.97                     | 0.46              |
| 2:H:59[B]:MET:HE3   | 2:H:118[B]:ASP:OD2  | 2.16                     | 0.46              |
| 1:A:86[A]:LEU:HD12  | 1:A:86[A]:LEU:O     | 2.15                     | 0.46              |
| 1:C:93[A]:ALA:O     | 1:C:94[A]:VAL:HG13  | 2.16                     | 0.46              |
| 1:C:126[A]:ILE:N    | 1:C:126[A]:ILE:CD1  | 2.79                     | 0.46              |
| 2:B:167[B]:GLU:OE1  | 2:B:170[B]:THR:HG21 | 2.16                     | 0.46              |
| 2:B:251[B]:GLY:C    | 2:B:254[B]:ILE:N    | 2.73                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:214[B]:GLN:NE2  | 2:F:222[B]:PRO:HB3  | 2.31                     | 0.46              |
| 1:A:42[A]:ARG:HH12  | 1:A:225[A]:ARG:HH12 | 1.64                     | 0.46              |
| 1:A:67[A]:ILE:HD12  | 1:A:99[A]:MET:CB    | 2.45                     | 0.46              |
| 1:A:121[A]:ILE:HG21 | 1:A:145[A]:PHE:CE2  | 2.51                     | 0.46              |
| 1:E:152[A]:THR:HA   | 1:E:188[A]:LEU:CD1  | 2.45                     | 0.46              |
| 2:D:136[B]:ASN:O    | 2:D:137[B]:PHE:CD1  | 2.69                     | 0.46              |
| 1:E:160[A]:ARG:HA   | 1:E:160[A]:ARG:HD2  | 1.64                     | 0.46              |
| 2:B:51[B]:GLU:OE2   | 2:B:91[B]:THR:OG1   | 2.31                     | 0.46              |
| 2:F:145[B]:CYS:SG   | 2:F:151[B]:ALA:HB2  | 2.55                     | 0.46              |
| 1:A:48[A]:GLU:CB    | 1:A:67[A]:ILE:CG2   | 2.93                     | 0.46              |
| 1:A:70[A]:ASP:CB    | 4:A:510:HOH:O       | 2.64                     | 0.46              |
| 1:A:246[A]:MET:HG3  | 1:A:276[A]:VAL:HG13 | 1.98                     | 0.46              |
| 2:H:41[B]:VAL:HG23  | 2:H:86[B]:ILE:CD1   | 2.46                     | 0.46              |
| 2:D:77[B]:MET:CG    | 2:D:78[B]:SER:N     | 2.75                     | 0.46              |
| 2:F:154[B]:ARG:NE   | 2:F:154[B]:ARG:CA   | 2.78                     | 0.46              |
| 2:F:237[B]:ALA:O    | 2:F:241[B]:MET:HG2  | 2.16                     | 0.46              |
| 1:E:199[A]:ASP:OD1  | 1:E:200[A]:ASP:N    | 2.48                     | 0.45              |
| 2:B:38[B]:ILE:CD1   | 2:B:95[B]:MET:HE1   | 2.46                     | 0.45              |
| 2:B:134[B]:LYS:HG2  | 2:B:141[B]:PHE:CD1  | 2.50                     | 0.45              |
| 2:D:268[B]:VAL:O    | 2:D:269[B]:GLN:C    | 2.59                     | 0.45              |
| 1:C:103[A]:ARG:HG2  | 1:C:127[A]:ILE:CG2  | 2.43                     | 0.45              |
| 1:E:146[A]:ILE:HG12 | 1:E:165[A]:MET:SD   | 2.56                     | 0.45              |
| 1:C:106[A]:HIS:CE1  | 1:C:109[A]:GLU:HG3  | 2.51                     | 0.45              |
| 1:E:168[A]:ILE:HG12 | 1:E:185[A]:VAL:CG2  | 2.46                     | 0.45              |
| 1:G:37[A]:LEU:O     | 1:G:40[A]:VAL:HG22  | 2.16                     | 0.45              |
| 2:D:40[B]:ASP:C     | 2:D:41[B]:VAL:CG1   | 2.84                     | 0.45              |
| 2:H:199[B]:PHE:CE1  | 2:H:209[B]:TYR:OH   | 2.69                     | 0.45              |
| 2:H:279[B]:MET:O    | 2:H:283[B]:VAL:HG22 | 2.16                     | 0.45              |
| 1:C:156[A]:LEU:HD12 | 1:C:217[A]:VAL:HG22 | 1.99                     | 0.45              |
| 2:B:59[B]:MET:CE    | 2:B:118[B]:ASP:OD2  | 2.61                     | 0.45              |
| 1:C:204[A]:PHE:CE1  | 1:C:214[A]:TYR:CZ   | 3.05                     | 0.45              |
| 2:B:112[B]:ILE:O    | 2:B:112[B]:ILE:CG2  | 2.64                     | 0.45              |
| 2:B:241[B]:MET:CG   | 2:B:271[B]:VAL:HG13 | 2.47                     | 0.45              |
| 2:D:134[B]:LYS:HG2  | 2:D:141[B]:PHE:CZ   | 2.52                     | 0.45              |
| 2:F:134[B]:LYS:HG2  | 2:F:141[B]:PHE:CG   | 2.52                     | 0.45              |
| 2:H:37[B]:VAL:CG2   | 2:H:271[B]:VAL:CG2  | 2.90                     | 0.45              |
| 1:A:236[A]:ILE:HD13 | 1:A:236[A]:ILE:N    | 2.31                     | 0.45              |
| 1:E:232[A]:ALA:HB2  | 1:E:250[A]:CYS:SG   | 2.57                     | 0.45              |
| 1:G:167[A]:ARG:HG3  | 1:G:167[A]:ARG:NH1  | 2.31                     | 0.45              |
| 2:B:64[B]:VAL:CG1   | 2:B:65[B]:PRO:CD    | 2.88                     | 0.45              |
| 2:B:261[B]:ALA:O    | 2:B:262[B]:ARG:C    | 2.59                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:23[B]:PHE:HE1   | 2:F:158[B]:GLY:O    | 2.00                     | 0.45              |
| 2:H:109[B]:LEU:O    | 2:H:112[B]:ILE:CG1  | 2.65                     | 0.45              |
| 1:A:33[A]:VAL:O     | 1:A:33[A]:VAL:HG12  | 2.16                     | 0.45              |
| 1:E:204[A]:PHE:O    | 1:E:207[A]:ALA:HB3  | 2.16                     | 0.45              |
| 1:E:210[A]:ILE:O    | 1:E:211[A]:SER:C    | 2.59                     | 0.45              |
| 2:H:33[B]:LEU:O     | 2:H:34[B]:ARG:C     | 2.59                     | 0.45              |
| 2:H:167[B]:GLU:HG2  | 2:H:170[B]:THR:HG23 | 1.98                     | 0.45              |
| 1:C:126[A]:ILE:O    | 1:C:126[A]:ILE:HG22 | 2.17                     | 0.45              |
| 2:D:152[B]:LEU:CD1  | 2:D:212[B]:VAL:HG22 | 2.47                     | 0.45              |
| 2:F:150[B]:GLU:O    | 2:F:154[B]:ARG:HG2  | 2.17                     | 0.45              |
| 1:E:148[A]:GLY:HA2  | 1:E:167[A]:ARG:O    | 2.17                     | 0.45              |
| 2:B:128[B]:GLU:HG2  | 2:B:128[B]:GLU:O    | 2.11                     | 0.45              |
| 2:F:26[B]:LYS:O     | 2:F:27[B]:VAL:C     | 2.59                     | 0.45              |
| 2:F:183[B]:VAL:O    | 2:F:187[B]:ILE:HG13 | 2.17                     | 0.45              |
| 2:B:51[B]:GLU:C     | 2:B:53[B]:ALA:N     | 2.75                     | 0.44              |
| 2:D:134[B]:LYS:HG2  | 2:D:141[B]:PHE:CD2  | 2.52                     | 0.44              |
| 2:F:249[B]:PHE:C    | 2:F:250[B]:VAL:HG23 | 2.41                     | 0.44              |
| 1:C:173[A]:THR:HG23 | 1:C:175[A]:THR:CG2  | 2.47                     | 0.44              |
| 2:D:193[B]:MET:O    | 2:D:216[B]:LYS:NZ   | 2.50                     | 0.44              |
| 2:F:59[B]:MET:HE1   | 2:F:95[B]:MET:SD    | 2.57                     | 0.44              |
| 2:F:173[B]:ILE:CG1  | 2:F:240[B]:MET:HE2  | 2.43                     | 0.44              |
| 1:A:281[A]:ASP:OD2  | 1:A:284[A]:VAL:CG2  | 2.65                     | 0.44              |
| 1:G:67[A]:ILE:O     | 1:G:67[A]:ILE:HG23  | 2.17                     | 0.44              |
| 2:B:109[B]:LEU:O    | 2:B:110[B]:GLU:C    | 2.61                     | 0.44              |
| 2:B:272[B]:THR:O    | 2:B:272[B]:THR:CG2  | 2.65                     | 0.44              |
| 2:H:100[B]:ILE:HG23 | 2:H:131[B]:HIS:CD2  | 2.52                     | 0.44              |
| 2:H:146[B]:ARG:HG2  | 2:H:179[B]:HIS:CE1  | 2.52                     | 0.44              |
| 2:H:158[B]:GLY:O    | 2:H:159[B]:ALA:C    | 2.60                     | 0.44              |
| 1:G:104[A]:VAL:HA   | 1:G:123[A]:GLU:HG2  | 1.99                     | 0.44              |
| 1:G:284[A]:VAL:O    | 1:G:288[A]:MET:HG2  | 2.18                     | 0.44              |
| 2:B:33[B]:LEU:HD23  | 2:B:56[B]:CYS:SG    | 2.57                     | 0.44              |
| 2:B:179[B]:HIS:O    | 2:B:180[B]:VAL:C    | 2.59                     | 0.44              |
| 2:D:29[B]:LEU:O     | 2:D:116[B]:TYR:OH   | 2.35                     | 0.44              |
| 2:F:221[B]:LEU:HD23 | 2:F:221[B]:LEU:HA   | 1.86                     | 0.44              |
| 1:A:166[A]:ILE:HG22 | 1:A:167[A]:ARG:N    | 2.33                     | 0.44              |
| 1:E:226[A]:VAL:O    | 1:E:228[A]:VAL:N    | 2.49                     | 0.44              |
| 1:G:79[A]:ARG:O     | 1:G:127[A]:ILE:HB   | 2.18                     | 0.44              |
| 2:D:110[B]:GLU:C    | 2:D:112[B]:ILE:H    | 2.25                     | 0.44              |
| 2:D:134[B]:LYS:CG   | 2:D:141[B]:PHE:CD1  | 3.00                     | 0.44              |
| 1:C:40[A]:VAL:O     | 1:C:40[A]:VAL:HG23  | 2.15                     | 0.44              |
| 2:D:267[B]:ILE:O    | 2:D:270[B]:ALA:HB3  | 2.18                     | 0.44              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:F:76[B]:ARG:HD3   | 2:F:99[B]:ARG:NH2   | 2.32                     | 0.44              |
| 2:H:192[B]:ASN:OD1  | 2:H:192[B]:ASN:C    | 2.56                     | 0.44              |
| 2:B:44[B]:ALA:O     | 2:B:45[B]:GLU:C     | 2.60                     | 0.44              |
| 2:B:241[B]:MET:HG3  | 2:B:271[B]:VAL:HG13 | 1.99                     | 0.44              |
| 2:F:99[B]:ARG:O     | 2:F:100[B]:ILE:C    | 2.61                     | 0.44              |
| 1:E:87[A]:ILE:O     | 1:E:87[A]:ILE:HG22  | 2.16                     | 0.44              |
| 1:E:108[A]:VAL:O    | 1:E:111[A]:GLN:N    | 2.51                     | 0.44              |
| 1:G:255[A]:VAL:O    | 1:G:255[A]:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:125[A]:GLU:HG3  | 1:A:169[A]:GLN:OE1  | 2.17                     | 0.43              |
| 1:E:178[A]:ILE:HD13 | 1:E:236[A]:ILE:HA   | 1.99                     | 0.43              |
| 2:D:46[B]:GLN:HG2   | 2:D:255[B]:PHE:CZ   | 2.49                     | 0.43              |
| 2:D:99[B]:ARG:HG2   | 2:D:123[B]:LEU:HB3  | 2.00                     | 0.43              |
| 2:D:194[B]:ASP:C    | 2:D:194[B]:ASP:OD1  | 2.61                     | 0.43              |
| 2:D:221[B]:LEU:HD23 | 2:D:221[B]:LEU:HA   | 1.84                     | 0.43              |
| 2:F:30[B]:ALA:HA    | 2:F:116[B]:TYR:OH   | 2.18                     | 0.43              |
| 2:F:102[B]:HIS:CG   | 2:F:105[B]:GLU:HG3  | 2.53                     | 0.43              |
| 1:G:279[A]:TYR:O    | 1:G:285[A]:LEU:HD11 | 2.17                     | 0.43              |
| 2:B:33[B]:LEU:O     | 2:B:34[B]:ARG:C     | 2.60                     | 0.43              |
| 2:B:76[B]:ARG:HG2   | 2:B:99[B]:ARG:NH1   | 2.33                     | 0.43              |
| 2:D:76[B]:ARG:O     | 2:D:77[B]:MET:C     | 2.62                     | 0.43              |
| 1:G:164[A]:ALA:O    | 1:G:165[A]:MET:HB2  | 2.19                     | 0.43              |
| 1:G:280[A]:ASN:O    | 1:G:282[A]:PRO:HD3  | 2.18                     | 0.43              |
| 2:B:77[B]:MET:HB2   | 2:B:105[B]:GLU:CD   | 2.44                     | 0.43              |
| 2:D:153[B]:ARG:NH1  | 2:D:206[B]:ALA:O    | 2.40                     | 0.43              |
| 2:F:32[B]:MET:HA    | 2:F:32[B]:MET:CE    | 2.49                     | 0.43              |
| 2:H:114[B]:ILE:HD12 | 2:H:114[B]:ILE:HA   | 1.90                     | 0.43              |
| 1:A:44[A]:GLY:HA3   | 1:A:64[A]:CYS:SG    | 2.58                     | 0.43              |
| 1:A:272[A]:ILE:O    | 1:A:275[A]:ALA:HB3  | 2.18                     | 0.43              |
| 2:B:139[B]:ILE:HA   | 2:B:140[B]:PRO:HD3  | 1.78                     | 0.43              |
| 2:D:98[B]:ALA:O     | 2:D:99[B]:ARG:C     | 2.61                     | 0.43              |
| 2:D:239[B]:LEU:CD1  | 2:F:103[B]:PHE:CE2  | 3.01                     | 0.43              |
| 2:F:165[B]:LYS:HD2  | 2:F:165[B]:LYS:HA   | 1.64                     | 0.43              |
| 2:F:279[B]:MET:O    | 2:F:281[B]:VAL:N    | 2.52                     | 0.43              |
| 2:F:289[B]:GLU:O    | 2:F:290[B]:ALA:O    | 2.37                     | 0.43              |
| 1:E:274[A]:GLN:HB2  | 1:E:288[A]:MET:HE2  | 2.00                     | 0.43              |
| 2:F:56[B]:CYS:O     | 2:F:57[B]:ALA:CB    | 2.62                     | 0.43              |
| 1:A:255[A]:VAL:O    | 1:A:255[A]:VAL:HG23 | 2.18                     | 0.43              |
| 2:B:106[B]:ALA:O    | 2:B:109[B]:LEU:N    | 2.48                     | 0.43              |
| 2:H:134[B]:LYS:O    | 2:H:135[B]:HIS:C    | 2.61                     | 0.43              |
| 1:A:123[A]:GLU:CD   | 1:A:135[A]:PHE:HD1  | 2.26                     | 0.43              |
| 2:D:203[B]:LYS:O    | 2:D:204[B]:LYS:C    | 2.61                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:H:75[B]:ALA:HB1   | 2:H:123[B]:LEU:HD22 | 2.00                     | 0.43              |
| 1:C:107[A]:PHE:O    | 1:C:110[A]:ALA:N    | 2.52                     | 0.43              |
| 2:D:37[B]:VAL:HG21  | 2:D:268[B]:VAL:HA   | 2.00                     | 0.43              |
| 2:H:192[B]:ASN:O    | 2:H:192[B]:ASN:CG   | 2.59                     | 0.43              |
| 1:E:285[A]:LEU:HA   | 1:E:285[A]:LEU:HD23 | 1.78                     | 0.43              |
| 2:F:48[B]:ARG:C     | 2:F:50[B]:ALA:N     | 2.76                     | 0.43              |
| 1:A:104[A]:VAL:HA   | 1:A:123[A]:GLU:HG2  | 2.01                     | 0.42              |
| 1:E:223[A]:MET:C    | 1:E:225[A]:ARG:N    | 2.76                     | 0.42              |
| 1:G:152[A]:THR:OG1  | 1:G:191[A]:GLU:OE1  | 2.37                     | 0.42              |
| 2:D:134[B]:LYS:CG   | 2:D:141[B]:PHE:CG   | 3.02                     | 0.42              |
| 2:D:221[B]:LEU:C    | 2:D:223[B]:VAL:N    | 2.75                     | 0.42              |
| 2:F:74[B]:VAL:HG13  | 2:F:124[B]:THR:HG21 | 2.01                     | 0.42              |
| 2:F:179[B]:HIS:O    | 2:F:182[B]:SER:HB3  | 2.19                     | 0.42              |
| 2:H:109[B]:LEU:O    | 2:H:112[B]:ILE:HG12 | 2.19                     | 0.42              |
| 2:H:287[B]:LEU:HD23 | 2:H:287[B]:LEU:HA   | 1.87                     | 0.42              |
| 1:A:86[A]:LEU:O     | 1:A:87[A]:ILE:C     | 2.59                     | 0.42              |
| 1:A:175[A]:THR:O    | 1:A:176[A]:GLY:C    | 2.62                     | 0.42              |
| 1:E:116[A]:LEU:HD11 | 1:E:118[A]:VAL:HG13 | 2.01                     | 0.42              |
| 1:E:223[A]:MET:O    | 1:E:224[A]:GLY:C    | 2.62                     | 0.42              |
| 1:G:171[A]:ASP:C    | 1:G:172[A]:LEU:O    | 2.61                     | 0.42              |
| 1:G:292[A]:LEU:HD12 | 1:G:292[A]:LEU:HA   | 1.80                     | 0.42              |
| 2:D:281[B]:VAL:HG22 | 2:F:108[B]:ILE:HG23 | 2.00                     | 0.42              |
| 2:F:127[B]:ASP:OD2  | 2:F:130[B]:HIS:HB2  | 2.19                     | 0.42              |
| 2:H:29[B]:LEU:O     | 2:H:116[B]:TYR:OH   | 2.37                     | 0.42              |
| 2:H:203[B]:LYS:HE2  | 2:H:203[B]:LYS:HB3  | 1.86                     | 0.42              |
| 1:A:90[A]:VAL:O     | 1:A:91[A]:LYS:C     | 2.62                     | 0.42              |
| 1:C:244[A]:LEU:HD11 | 1:E:107[A]:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:99[A]:MET:SD    | 1:E:146[A]:ILE:HD12 | 2.57                     | 0.42              |
| 1:G:128[A]:SER:O    | 1:G:129[A]:VAL:C    | 2.62                     | 0.42              |
| 2:D:198[B]:VAL:O    | 2:D:199[B]:PHE:C    | 2.61                     | 0.42              |
| 2:H:82[B]:MET:O     | 2:H:85[B]:GLU:N     | 2.52                     | 0.42              |
| 2:D:183[B]:VAL:O    | 2:D:184[B]:ASN:C    | 2.62                     | 0.42              |
| 2:H:41[B]:VAL:CG2   | 2:H:86[B]:ILE:HD13  | 2.49                     | 0.42              |
| 2:H:59[B]:MET:HE1   | 2:H:118[B]:ASP:CG   | 2.43                     | 0.42              |
| 1:E:208[A]:LYS:HB3  | 1:E:208[A]:LYS:HE2  | 1.86                     | 0.42              |
| 2:B:110[B]:GLU:O    | 2:B:111[B]:ALA:C    | 2.63                     | 0.42              |
| 2:B:111[B]:ALA:O    | 2:B:113[B]:GLY:N    | 2.53                     | 0.42              |
| 2:B:128[B]:GLU:O    | 2:B:128[B]:GLU:CG   | 2.67                     | 0.42              |
| 2:B:225[B]:GLN:O    | 2:B:246[B]:ASP:HB2  | 2.19                     | 0.42              |
| 2:B:239[B]:LEU:HD11 | 2:H:103[B]:PHE:CE2  | 2.54                     | 0.42              |
| 2:D:44[B]:ALA:O     | 2:D:45[B]:GLU:C     | 2.63                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:D:228[B]:ALA:HB2  | 2:D:249[B]:PHE:HB2  | 2.02                     | 0.42              |
| 2:F:76[B]:ARG:O     | 2:F:77[B]:MET:C     | 2.62                     | 0.42              |
| 2:H:37[B]:VAL:HG22  | 2:H:248[B]:VAL:HG22 | 2.01                     | 0.42              |
| 1:C:199[A]:ASP:O    | 1:C:200[A]:ASP:C    | 2.62                     | 0.42              |
| 1:G:178[A]:ILE:O    | 1:G:179[A]:ALA:C    | 2.61                     | 0.42              |
| 2:B:64[B]:VAL:CG1   | 2:B:65[B]:PRO:N     | 2.81                     | 0.42              |
| 2:F:100[B]:ILE:HA   | 2:F:119[B]:GLU:CG   | 2.50                     | 0.42              |
| 1:E:281[A]:ASP:OD1  | 1:E:284[A]:VAL:N    | 2.47                     | 0.42              |
| 1:G:167[A]:ARG:NH1  | 1:G:167[A]:ARG:CG   | 2.80                     | 0.42              |
| 1:G:208[A]:LYS:HE2  | 1:G:208[A]:LYS:HB3  | 1.84                     | 0.42              |
| 2:B:124[B]:THR:O    | 2:B:125[B]:LEU:C    | 2.62                     | 0.42              |
| 2:B:192[B]:ASN:O    | 2:B:192[B]:ASN:OD1  | 2.37                     | 0.42              |
| 2:F:51[B]:GLU:HG3   | 2:F:92[B]:ILE:HG12  | 2.01                     | 0.42              |
| 2:F:108[B]:ILE:O    | 2:F:112[B]:ILE:HG13 | 2.18                     | 0.42              |
| 2:F:117[B]:ILE:HG22 | 2:F:141[B]:PHE:CE2  | 2.51                     | 0.42              |
| 1:A:166[A]:ILE:CG2  | 1:A:167[A]:ARG:N    | 2.82                     | 0.42              |
| 1:C:181[A]:THR:OG1  | 1:C:234[A]:GLY:O    | 2.28                     | 0.42              |
| 1:E:83[A]:ASP:HA    | 1:E:84[A]:PRO:HD3   | 1.96                     | 0.42              |
| 1:G:64[A]:CYS:SG    | 1:G:64[A]:CYS:O     | 2.77                     | 0.42              |
| 2:B:33[B]:LEU:CD2   | 2:B:56[B]:CYS:SG    | 3.08                     | 0.42              |
| 2:F:112[B]:ILE:O    | 2:F:112[B]:ILE:CG2  | 2.67                     | 0.42              |
| 1:C:171[A]:ASP:OD2  | 1:C:175[A]:THR:CG2  | 2.68                     | 0.42              |
| 1:G:90[A]:VAL:C     | 1:G:92[A]:ARG:N     | 2.76                     | 0.42              |
| 1:G:149[A]:CYS:SG   | 1:G:155[A]:ALA:HB2  | 2.60                     | 0.42              |
| 1:G:188[A]:LEU:O    | 1:G:189[A]:MET:C    | 2.63                     | 0.42              |
| 2:D:38[B]:ILE:HD13  | 2:D:95[B]:MET:CE    | 2.50                     | 0.42              |
| 1:A:86[A]:LEU:HD12  | 1:A:86[A]:LEU:C     | 2.45                     | 0.42              |
| 1:A:271[A]:SER:HA   | 1:A:288[A]:MET:HG3  | 2.01                     | 0.42              |
| 1:A:273[A]:VAL:O    | 1:A:277[A]:GLN:HG3  | 2.20                     | 0.42              |
| 1:G:167[A]:ARG:HH11 | 1:G:167[A]:ARG:CG   | 2.28                     | 0.42              |
| 2:F:23[B]:PHE:O     | 2:F:26[B]:LYS:N     | 2.53                     | 0.42              |
| 2:B:31[B]:GLN:C     | 2:B:33[B]:LEU:H     | 2.27                     | 0.41              |
| 2:B:135[B]:HIS:CE1  | 2:B:158[B]:GLY:HA2  | 2.54                     | 0.41              |
| 1:C:225[A]:ARG:HG2  | 1:C:226[A]:VAL:N    | 2.35                     | 0.41              |
| 1:C:231[A]:PHE:CZ   | 1:C:252[A]:GLY:HA3  | 2.55                     | 0.41              |
| 2:B:198[B]:VAL:O    | 2:B:199[B]:PHE:C    | 2.62                     | 0.41              |
| 1:A:121[A]:ILE:O    | 1:A:145[A]:PHE:HA   | 2.20                     | 0.41              |
| 1:A:160[A]:ARG:HA   | 1:A:160[A]:ARG:HD2  | 1.80                     | 0.41              |
| 1:C:42[A]:ARG:HG2   | 1:C:251[A]:ASP:HB3  | 2.02                     | 0.41              |
| 1:C:160[A]:ARG:HD2  | 1:C:160[A]:ARG:HA   | 1.86                     | 0.41              |
| 1:G:90[A]:VAL:CG2   | 1:G:91[A]:LYS:H     | 2.33                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:G:185[A]:VAL:CG2  | 1:G:245[A]:MET:HE1  | 2.43                     | 0.41              |
| 1:A:189[A]:MET:CE   | 1:A:189[A]:MET:CA   | 2.94                     | 0.41              |
| 1:E:226[A]:VAL:C    | 1:E:228[A]:VAL:H    | 2.27                     | 0.41              |
| 1:G:148[A]:GLY:HA3  | 1:G:169[A]:GLN:HG2  | 2.02                     | 0.41              |
| 2:B:233[B]:THR:O    | 2:B:236[B]:ASP:HB2  | 2.19                     | 0.41              |
| 1:A:84[A]:PRO:HB3   | 1:A:116[A]:LEU:HD11 | 2.03                     | 0.41              |
| 1:E:138[A]:LYS:HG2  | 1:E:145[A]:PHE:CE2  | 2.55                     | 0.41              |
| 1:G:41[A]:LEU:CD2   | 1:G:64[A]:CYS:SG    | 3.08                     | 0.41              |
| 2:D:155[B]:ILE:HG22 | 2:D:211[B]:LEU:HD11 | 2.01                     | 0.41              |
| 2:F:31[B]:GLN:C     | 2:F:33[B]:LEU:H     | 2.27                     | 0.41              |
| 1:E:191[A]:GLU:HG2  | 1:E:206[A]:PHE:HZ   | 1.84                     | 0.41              |
| 1:G:274[A]:GLN:HB3  | 1:G:288[A]:MET:HE3  | 2.01                     | 0.41              |
| 2:D:131[B]:HIS:HB2  | 2:D:157[B]:GLU:OE1  | 2.21                     | 0.41              |
| 2:D:192[B]:ASN:O    | 2:D:192[B]:ASN:CG   | 2.62                     | 0.41              |
| 2:D:201[B]:PHE:CE2  | 2:D:205[B]:LEU:CD1  | 3.01                     | 0.41              |
| 2:F:96[B]:ALA:HB3   | 2:F:114[B]:ILE:CD1  | 2.49                     | 0.41              |
| 2:F:173[B]:ILE:O    | 2:F:177[B]:VAL:HG23 | 2.21                     | 0.41              |
| 2:H:172[B]:ASN:OD1  | 2:H:174[B]:ILE:HG22 | 2.20                     | 0.41              |
| 1:C:101[A]:ARG:NH2  | 4:C:502:HOH:O       | 2.53                     | 0.41              |
| 1:E:188[A]:LEU:O    | 1:E:192[A]:VAL:HG23 | 2.21                     | 0.41              |
| 2:B:150[B]:GLU:O    | 2:B:154[B]:ARG:HG2  | 2.21                     | 0.41              |
| 2:D:134[B]:LYS:HE2  | 2:D:134[B]:LYS:HB2  | 1.92                     | 0.41              |
| 2:D:162[B]:ILE:HG12 | 2:D:223[B]:VAL:CG2  | 2.50                     | 0.41              |
| 2:F:199[B]:PHE:O    | 2:F:202[B]:ALA:HB3  | 2.20                     | 0.41              |
| 1:E:222[A]:GLN:C    | 1:E:224[A]:GLY:N    | 2.77                     | 0.41              |
| 2:B:281[B]:VAL:CG1  | 2:H:112[B]:ILE:CG2  | 2.99                     | 0.41              |
| 2:D:121[B]:GLU:CD   | 2:D:121[B]:GLU:H    | 2.28                     | 0.41              |
| 2:F:165[B]:LYS:HE2  | 2:F:168[B]:ALA:HB2  | 2.01                     | 0.41              |
| 2:H:218[B]:LEU:HD23 | 2:H:218[B]:LEU:HA   | 1.82                     | 0.41              |
| 1:A:178[A]:ILE:O    | 1:A:182[A]:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:246[A]:MET:CG   | 1:A:276[A]:VAL:HG13 | 2.51                     | 0.41              |
| 1:C:146[A]:ILE:CG1  | 1:C:165[A]:MET:HG2  | 2.48                     | 0.41              |
| 1:E:106[A]:HIS:CG   | 1:E:109[A]:GLU:HG3  | 2.55                     | 0.41              |
| 1:G:226[A]:VAL:HA   | 1:G:227[A]:PRO:HD3  | 1.89                     | 0.41              |
| 2:D:46[B]:GLN:CG    | 2:D:255[B]:PHE:CE1  | 2.88                     | 0.41              |
| 2:F:156[B]:ARG:HA   | 2:F:156[B]:ARG:HD2  | 1.84                     | 0.41              |
| 2:F:158[B]:GLY:O    | 2:F:159[B]:ALA:O    | 2.39                     | 0.41              |
| 2:H:166[B]:GLY:HA3  | 2:H:228[B]:ALA:O    | 2.20                     | 0.41              |
| 1:E:104[A]:VAL:HA   | 1:E:123[A]:GLU:HG2  | 2.03                     | 0.41              |
| 1:E:123[A]:GLU:CD   | 1:E:135[A]:PHE:HD1  | 2.29                     | 0.41              |
| 2:F:42[B]:VAL:HG22  | 2:F:46[B]:GLN:OE1   | 2.21                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:H:201[B]:PHE:CE2  | 2:H:205[B]:LEU:CD1  | 3.03                     | 0.41              |
| 1:G:199[A]:ASP:OD1  | 1:G:200[A]:ASP:N    | 2.54                     | 0.40              |
| 2:D:100[B]:ILE:HG23 | 2:D:131[B]:HIS:CD2  | 2.56                     | 0.40              |
| 2:F:279[B]:MET:C    | 2:F:281[B]:VAL:N    | 2.78                     | 0.40              |
| 1:E:180[A]:GLU:CD   | 1:E:183[A]:LYS:NZ   | 2.80                     | 0.40              |
| 1:G:160[A]:ARG:HD3  | 1:G:216[A]:LEU:HD12 | 2.04                     | 0.40              |
| 2:B:110[B]:GLU:OE2  | 2:B:138[B]:ARG:N    | 2.54                     | 0.40              |
| 2:D:155[B]:ILE:HG13 | 2:D:162[B]:ILE:HD11 | 2.04                     | 0.40              |
| 2:F:117[B]:ILE:HB   | 2:F:141[B]:PHE:CE2  | 2.57                     | 0.40              |
| 1:E:223[A]:MET:SD   | 1:E:227[A]:PRO:HB3  | 2.62                     | 0.40              |
| 2:B:111[B]:ALA:C    | 2:B:113[B]:GLY:N    | 2.79                     | 0.40              |
| 2:H:103[B]:PHE:CD1  | 2:H:104[B]:VAL:HG23 | 2.57                     | 0.40              |
| 2:F:77[B]:MET:HG2   | 2:F:78[B]:SER:N     | 2.37                     | 0.40              |
| 2:H:32[B]:MET:O     | 2:H:32[B]:MET:SD    | 2.79                     | 0.40              |
| 2:H:103[B]:PHE:CD1  | 2:H:104[B]:VAL:N    | 2.90                     | 0.40              |
| 1:A:31[A]:PHE:HA    | 1:A:34[A]:LYS:HE3   | 2.03                     | 0.40              |
| 1:E:170[A]:GLY:HA3  | 1:E:234[A]:GLY:HA3  | 2.04                     | 0.40              |
| 1:G:233[A]:SER:HB2  | 1:G:254[A]:PHE:HB2  | 2.04                     | 0.40              |
| 2:B:221[B]:LEU:HD23 | 2:B:221[B]:LEU:HA   | 1.89                     | 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     | 258/314 (82%) | 232 (90%) | 23 (9%)  | 3 (1%)   | 10          | 19 |
| 1   | C     | 255/314 (81%) | 227 (89%) | 23 (9%)  | 5 (2%)   | 6           | 9  |
| 1   | E     | 252/314 (80%) | 228 (90%) | 18 (7%)  | 6 (2%)   | 4           | 7  |
| 1   | G     | 256/314 (82%) | 232 (91%) | 18 (7%)  | 6 (2%)   | 5           | 7  |
| 2   | B     | 264/315 (84%) | 230 (87%) | 29 (11%) | 5 (2%)   | 6           | 10 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | D     | 254/315 (81%)   | 213 (84%)  | 30 (12%) | 11 (4%)  | 2           | 2  |
| 2   | F     | 251/315 (80%)   | 219 (87%)  | 22 (9%)  | 10 (4%)  | 2           | 2  |
| 2   | H     | 255/315 (81%)   | 224 (88%)  | 28 (11%) | 3 (1%)   | 10          | 19 |
| All | All   | 2045/2516 (81%) | 1805 (88%) | 191 (9%) | 49 (2%)  | 4           | 7  |

All (49) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | E     | 263[A] | PRO  |
| 1   | G     | 172[A] | LEU  |
| 1   | G     | 173[A] | THR  |
| 2   | B     | 77[B]  | MET  |
| 2   | B     | 136[B] | ASN  |
| 2   | D     | 77[B]  | MET  |
| 2   | D     | 276[B] | ASP  |
| 2   | F     | 77[B]  | MET  |
| 2   | F     | 125[B] | LEU  |
| 2   | F     | 290[B] | ALA  |
| 2   | H     | 136[B] | ASN  |
| 1   | C     | 293[A] | GLU  |
| 1   | E     | 223[A] | MET  |
| 2   | F     | 57[B]  | ALA  |
| 2   | F     | 161[B] | MET  |
| 2   | F     | 231[B] | VAL  |
| 2   | F     | 289[B] | GLU  |
| 2   | H     | 231[B] | VAL  |
| 1   | E     | 227[A] | PRO  |
| 1   | G     | 227[A] | PRO  |
| 1   | G     | 293[A] | GLU  |
| 2   | B     | 43[B]  | ASN  |
| 2   | D     | 81[B]  | GLN  |
| 2   | F     | 159[B] | ALA  |
| 2   | F     | 196[B] | ASP  |
| 1   | A     | 293[A] | GLU  |
| 1   | E     | 222[A] | GLN  |
| 1   | G     | 165[A] | MET  |
| 2   | B     | 87[B]  | LYS  |
| 2   | B     | 222[B] | PRO  |
| 2   | D     | 111[B] | ALA  |
| 2   | D     | 125[B] | LEU  |
| 2   | D     | 203[B] | LYS  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | F     | 34[B]  | ARG  |
| 1   | A     | 42[A]  | ARG  |
| 1   | C     | 227[A] | PRO  |
| 1   | E     | 70[A]  | ASP  |
| 1   | E     | 140[A] | ASN  |
| 1   | G     | 263[A] | PRO  |
| 2   | D     | 34[B]  | ARG  |
| 2   | D     | 80[B]  | PRO  |
| 2   | D     | 191[B] | ARG  |
| 1   | A     | 263[A] | PRO  |
| 1   | C     | 261[A] | ASP  |
| 2   | D     | 41[B]  | VAL  |
| 1   | C     | 70[A]  | ASP  |
| 2   | D     | 222[B] | PRO  |
| 2   | H     | 114[B] | ILE  |
| 1   | C     | 40[A]  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 177/256 (69%)   | 165 (93%)  | 12 (7%)  | 14          | 28 |
| 1   | C     | 179/256 (70%)   | 172 (96%)  | 7 (4%)   | 28          | 52 |
| 1   | E     | 172/256 (67%)   | 161 (94%)  | 11 (6%)  | 16          | 31 |
| 1   | G     | 175/256 (68%)   | 167 (95%)  | 8 (5%)   | 24          | 45 |
| 2   | B     | 182/244 (75%)   | 176 (97%)  | 6 (3%)   | 33          | 58 |
| 2   | D     | 173/244 (71%)   | 168 (97%)  | 5 (3%)   | 37          | 63 |
| 2   | F     | 168/244 (69%)   | 158 (94%)  | 10 (6%)  | 17          | 34 |
| 2   | H     | 174/244 (71%)   | 170 (98%)  | 4 (2%)   | 44          | 70 |
| All | All   | 1400/2000 (70%) | 1337 (96%) | 63 (4%)  | 24          | 46 |

All (63) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 40[A]  | VAL  |
| 1   | A     | 51[A]  | SER  |
| 1   | A     | 85[A]  | VAL  |
| 1   | A     | 91[A]  | LYS  |
| 1   | A     | 169[A] | GLN  |
| 1   | A     | 173[A] | THR  |
| 1   | A     | 181[A] | THR  |
| 1   | A     | 189[A] | MET  |
| 1   | A     | 255[A] | VAL  |
| 1   | A     | 288[A] | MET  |
| 1   | A     | 289[A] | SER  |
| 1   | A     | 290[A] | SER  |
| 1   | C     | 167[A] | ARG  |
| 1   | C     | 173[A] | THR  |
| 1   | C     | 188[A] | LEU  |
| 1   | C     | 199[A] | ASP  |
| 1   | C     | 226[A] | VAL  |
| 1   | C     | 244[A] | LEU  |
| 1   | C     | 288[A] | MET  |
| 1   | E     | 40[A]  | VAL  |
| 1   | E     | 51[A]  | SER  |
| 1   | E     | 95[A]  | SER  |
| 1   | E     | 96[A]  | VAL  |
| 1   | E     | 167[A] | ARG  |
| 1   | E     | 168[A] | ILE  |
| 1   | E     | 169[A] | GLN  |
| 1   | E     | 173[A] | THR  |
| 1   | E     | 183[A] | LYS  |
| 1   | E     | 226[A] | VAL  |
| 1   | E     | 228[A] | VAL  |
| 1   | G     | 64[A]  | CYS  |
| 1   | G     | 95[A]  | SER  |
| 1   | G     | 101[A] | ARG  |
| 1   | G     | 173[A] | THR  |
| 1   | G     | 183[A] | LYS  |
| 1   | G     | 225[A] | ARG  |
| 1   | G     | 236[A] | ILE  |
| 1   | G     | 270[A] | ARG  |
| 2   | B     | 56[B]  | CYS  |
| 2   | B     | 59[B]  | MET  |
| 2   | B     | 64[B]  | VAL  |
| 2   | B     | 87[B]  | LYS  |
| 2   | B     | 139[B] | ILE  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | B     | 196[B] | ASP  |
| 2   | D     | 24[B]  | SER  |
| 2   | D     | 56[B]  | CYS  |
| 2   | D     | 163[B] | ARG  |
| 2   | D     | 248[B] | VAL  |
| 2   | D     | 275[B] | SER  |
| 2   | F     | 32[B]  | MET  |
| 2   | F     | 40[B]  | ASP  |
| 2   | F     | 56[B]  | CYS  |
| 2   | F     | 91[B]  | THR  |
| 2   | F     | 92[B]  | ILE  |
| 2   | F     | 164[B] | THR  |
| 2   | F     | 173[B] | ILE  |
| 2   | F     | 174[B] | ILE  |
| 2   | F     | 210[B] | ASP  |
| 2   | F     | 248[B] | VAL  |
| 2   | H     | 114[B] | ILE  |
| 2   | H     | 218[B] | LEU  |
| 2   | H     | 281[B] | VAL  |
| 2   | H     | 284[B] | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 54[A]  | GLN  |
| 1   | A     | 137[A] | ASN  |
| 1   | A     | 140[A] | ASN  |
| 1   | A     | 219[A] | GLN  |
| 1   | A     | 247[A] | GLN  |
| 1   | C     | 111[A] | GLN  |
| 1   | C     | 140[A] | ASN  |
| 1   | C     | 197[A] | ASN  |
| 1   | C     | 247[A] | GLN  |
| 1   | C     | 274[A] | GLN  |
| 1   | C     | 278[A] | HIS  |
| 1   | E     | 111[A] | GLN  |
| 1   | E     | 140[A] | ASN  |
| 1   | E     | 177[A] | ASN  |
| 1   | G     | 39[A]  | GLN  |
| 1   | G     | 111[A] | GLN  |
| 1   | G     | 137[A] | ASN  |
| 1   | G     | 140[A] | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | G     | 196[A] | ASN  |
| 1   | G     | 278[A] | HIS  |
| 2   | B     | 192[B] | ASN  |
| 2   | B     | 242[B] | GLN  |
| 2   | D     | 184[B] | ASN  |
| 2   | D     | 242[B] | GLN  |
| 2   | F     | 214[B] | GLN  |
| 2   | F     | 242[B] | GLN  |
| 2   | F     | 273[B] | HIS  |
| 2   | H     | 107[B] | GLN  |
| 2   | H     | 172[B] | ASN  |
| 2   | H     | 214[B] | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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 | $\# Z  > 2$ |
| 3   | SO4  | C     | 401 | -    | 4,4,4        | 0.40 | 0           | 6,6,6       | 0.58 | 0           |
| 3   | SO4  | A     | 401 | -    | 4,4,4        | 0.29 | 0           | 6,6,6       | 0.82 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | H     | 402 | -    | 4,4,4        | 0.51 | 0           | 6,6,6       | 0.70 | 0           |
| 3   | SO4  | B     | 401 | -    | 4,4,4        | 0.50 | 0           | 6,6,6       | 0.38 | 0           |
| 3   | SO4  | F     | 402 | -    | 4,4,4        | 0.52 | 0           | 6,6,6       | 0.44 | 0           |
| 3   | SO4  | H     | 401 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.48 | 0           |
| 3   | SO4  | F     | 401 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.58 | 0           |
| 3   | SO4  | D     | 401 | -    | 4,4,4        | 0.51 | 0           | 6,6,6       | 0.42 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9       |
|-----|-------|-----------------|--------|----------|-------|-----------------------|-------------|
| 1   | A     | 264/314 (84%)   | 0.19   | 10 (3%)  | 44 40 | 7, 11, 20, 35         | 264 (100%)  |
| 1   | C     | 261/314 (83%)   | 0.28   | 20 (7%)  | 19 17 | 7, 11, 24, 34         | 261 (100%)  |
| 1   | E     | 258/314 (82%)   | 0.25   | 13 (5%)  | 34 31 | 7, 12, 24, 34         | 258 (100%)  |
| 1   | G     | 262/314 (83%)   | 0.22   | 14 (5%)  | 32 29 | 7, 11, 21, 31         | 262 (100%)  |
| 2   | B     | 268/315 (85%)   | 0.84   | 31 (11%) | 9 8   | 8, 16, 32, 37         | 268 (100%)  |
| 2   | D     | 260/315 (82%)   | 0.99   | 36 (13%) | 6 5   | 10, 17, 38, 59        | 260 (100%)  |
| 2   | F     | 257/315 (81%)   | 1.12   | 47 (18%) | 3 3   | 11, 17, 36, 73        | 257 (100%)  |
| 2   | H     | 261/315 (82%)   | 0.96   | 38 (14%) | 6 5   | 9, 17, 31, 60         | 261 (100%)  |
| All | All   | 2091/2516 (83%) | 0.60   | 209 (9%) | 12 11 | 7, 14, 30, 73         | 2091 (100%) |

All (209) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | F     | 289[B] | GLU  | 9.5  |
| 2   | F     | 291[B] | MET  | 8.4  |
| 2   | D     | 63[B]  | ARG  | 8.3  |
| 2   | H     | 288[B] | GLY  | 8.1  |
| 2   | D     | 289[B] | GLU  | 8.0  |
| 2   | F     | 257[B] | SER  | 7.8  |
| 2   | H     | 291[B] | MET  | 7.6  |
| 1   | E     | 262[A] | GLY  | 7.1  |
| 2   | F     | 287[B] | LEU  | 6.5  |
| 1   | A     | 172[A] | LEU  | 6.4  |
| 2   | H     | 289[B] | GLU  | 6.4  |
| 1   | C     | 71[A]  | PRO  | 6.4  |
| 2   | D     | 254[B] | ILE  | 6.1  |
| 2   | D     | 291[B] | MET  | 6.0  |
| 1   | E     | 292[A] | LEU  | 5.8  |
| 2   | H     | 287[B] | LEU  | 5.6  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | D     | 22[B]  | PRO  | 5.6  |
| 2   | B     | 257[B] | SER  | 5.5  |
| 2   | F     | 290[B] | ALA  | 5.5  |
| 2   | B     | 64[B]  | VAL  | 5.5  |
| 2   | H     | 290[B] | ALA  | 5.5  |
| 2   | F     | 272[B] | THR  | 5.5  |
| 1   | A     | 173[A] | THR  | 5.4  |
| 1   | C     | 172[A] | LEU  | 5.3  |
| 1   | C     | 173[A] | THR  | 5.3  |
| 2   | D     | 287[B] | LEU  | 5.2  |
| 2   | F     | 285[B] | CYS  | 5.2  |
| 2   | D     | 72[B]  | GLY  | 5.2  |
| 2   | H     | 257[B] | SER  | 5.2  |
| 2   | D     | 257[B] | SER  | 5.2  |
| 2   | D     | 81[B]  | GLN  | 5.1  |
| 2   | H     | 254[B] | ILE  | 5.1  |
| 2   | F     | 251[B] | GLY  | 5.1  |
| 2   | H     | 45[B]  | GLU  | 5.1  |
| 1   | E     | 173[A] | THR  | 5.0  |
| 2   | F     | 288[B] | GLY  | 5.0  |
| 1   | E     | 172[A] | LEU  | 5.0  |
| 2   | F     | 21[B]  | SER  | 5.0  |
| 2   | D     | 62[B]  | GLU  | 5.0  |
| 1   | G     | 173[A] | THR  | 4.9  |
| 2   | B     | 45[B]  | GLU  | 4.9  |
| 2   | B     | 88[B]  | GLN  | 4.9  |
| 1   | C     | 70[A]  | ASP  | 4.8  |
| 1   | G     | 71[A]  | PRO  | 4.8  |
| 2   | D     | 290[B] | ALA  | 4.7  |
| 2   | F     | 87[B]  | LYS  | 4.5  |
| 2   | B     | 254[B] | ILE  | 4.5  |
| 2   | B     | 66[B]  | ALA  | 4.4  |
| 1   | A     | 70[A]  | ASP  | 4.4  |
| 2   | D     | 84[B]  | LYS  | 4.4  |
| 1   | E     | 71[A]  | PRO  | 4.3  |
| 2   | B     | 65[B]  | PRO  | 4.3  |
| 2   | F     | 45[B]  | GLU  | 4.3  |
| 2   | D     | 288[B] | GLY  | 4.2  |
| 2   | H     | 21[B]  | SER  | 4.1  |
| 2   | D     | 87[B]  | LYS  | 4.1  |
| 1   | C     | 294[A] | ASN  | 4.0  |
| 1   | C     | 259[A] | VAL  | 4.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | B     | 259[B] | ASP  | 3.9  |
| 2   | F     | 63[B]  | ARG  | 3.9  |
| 2   | F     | 44[B]  | ALA  | 3.9  |
| 2   | B     | 256[B] | LYS  | 3.9  |
| 2   | F     | 275[B] | SER  | 3.9  |
| 2   | D     | 255[B] | PHE  | 3.8  |
| 1   | C     | 174[A] | ALA  | 3.8  |
| 1   | A     | 263[A] | PRO  | 3.8  |
| 1   | E     | 295[A] | ALA  | 3.8  |
| 2   | D     | 82[B]  | MET  | 3.7  |
| 2   | D     | 259[B] | ASP  | 3.7  |
| 1   | G     | 172[A] | LEU  | 3.6  |
| 2   | D     | 256[B] | LYS  | 3.6  |
| 2   | B     | 289[B] | GLU  | 3.5  |
| 2   | F     | 42[B]  | VAL  | 3.5  |
| 2   | F     | 32[B]  | MET  | 3.5  |
| 2   | F     | 43[B]  | ASN  | 3.5  |
| 2   | B     | 63[B]  | ARG  | 3.5  |
| 2   | B     | 291[B] | MET  | 3.4  |
| 2   | B     | 251[B] | GLY  | 3.4  |
| 2   | D     | 88[B]  | GLN  | 3.4  |
| 2   | H     | 43[B]  | ASN  | 3.4  |
| 2   | B     | 285[B] | CYS  | 3.3  |
| 1   | C     | 101[A] | ARG  | 3.3  |
| 2   | F     | 61[B]  | LEU  | 3.3  |
| 2   | F     | 46[B]  | GLN  | 3.2  |
| 1   | G     | 261[A] | ASP  | 3.2  |
| 1   | E     | 101[A] | ARG  | 3.2  |
| 2   | H     | 192[B] | ASN  | 3.2  |
| 1   | A     | 259[A] | VAL  | 3.1  |
| 1   | C     | 261[A] | ASP  | 3.1  |
| 2   | H     | 63[B]  | ARG  | 3.1  |
| 1   | A     | 69[A]  | SER  | 3.0  |
| 1   | C     | 53[A]  | ASN  | 3.0  |
| 2   | F     | 258[B] | GLY  | 3.0  |
| 1   | A     | 72[A]  | VAL  | 3.0  |
| 2   | H     | 139[B] | ILE  | 3.0  |
| 2   | D     | 272[B] | THR  | 3.0  |
| 2   | D     | 286[B] | GLY  | 3.0  |
| 2   | F     | 286[B] | GLY  | 3.0  |
| 2   | B     | 29[B]  | LEU  | 2.9  |
| 2   | F     | 52[B]  | GLU  | 2.9  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | H     | 72[B]  | GLY  | 2.9  |
| 2   | H     | 256[B] | LYS  | 2.9  |
| 1   | G     | 263[A] | PRO  | 2.9  |
| 1   | G     | 292[A] | LEU  | 2.9  |
| 2   | F     | 217[B] | GLN  | 2.9  |
| 2   | B     | 86[B]  | ILE  | 2.8  |
| 2   | F     | 56[B]  | CYS  | 2.8  |
| 1   | E     | 296[A] | MET  | 2.8  |
| 2   | F     | 47[B]  | ALA  | 2.8  |
| 2   | F     | 73[B]  | GLY  | 2.8  |
| 2   | B     | 287[B] | LEU  | 2.8  |
| 2   | D     | 47[B]  | ALA  | 2.8  |
| 2   | H     | 261[B] | ALA  | 2.8  |
| 1   | C     | 69[A]  | SER  | 2.8  |
| 2   | H     | 49[B]  | ILE  | 2.7  |
| 1   | C     | 292[A] | LEU  | 2.7  |
| 2   | F     | 273[B] | HIS  | 2.7  |
| 2   | B     | 286[B] | GLY  | 2.7  |
| 2   | H     | 142[B] | VAL  | 2.7  |
| 2   | H     | 281[B] | VAL  | 2.7  |
| 2   | B     | 272[B] | THR  | 2.7  |
| 1   | C     | 76[A]  | GLY  | 2.7  |
| 2   | B     | 67[B]  | ASP  | 2.6  |
| 2   | H     | 114[B] | ILE  | 2.6  |
| 2   | H     | 255[B] | PHE  | 2.6  |
| 2   | F     | 62[B]  | GLU  | 2.6  |
| 2   | D     | 112[B] | ILE  | 2.6  |
| 2   | B     | 279[B] | MET  | 2.6  |
| 1   | G     | 289[A] | SER  | 2.6  |
| 1   | G     | 29[A]  | HIS  | 2.6  |
| 2   | D     | 48[B]  | ARG  | 2.6  |
| 2   | D     | 114[B] | ILE  | 2.6  |
| 2   | D     | 23[B]  | PHE  | 2.6  |
| 2   | F     | 283[B] | VAL  | 2.6  |
| 2   | H     | 37[B]  | VAL  | 2.6  |
| 2   | H     | 34[B]  | ARG  | 2.6  |
| 2   | D     | 49[B]  | ILE  | 2.6  |
| 2   | B     | 255[B] | PHE  | 2.6  |
| 2   | B     | 260[B] | PRO  | 2.5  |
| 2   | D     | 279[B] | MET  | 2.5  |
| 2   | F     | 85[B]  | GLU  | 2.5  |
| 1   | C     | 295[A] | ALA  | 2.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | A     | 261[A] | ASP  | 2.5  |
| 2   | B     | 62[B]  | GLU  | 2.5  |
| 2   | B     | 87[B]  | LYS  | 2.5  |
| 2   | H     | 42[B]  | VAL  | 2.5  |
| 1   | C     | 293[A] | GLU  | 2.5  |
| 2   | F     | 49[B]  | ILE  | 2.5  |
| 2   | F     | 86[B]  | ILE  | 2.5  |
| 2   | F     | 284[B] | SER  | 2.5  |
| 2   | F     | 102[B] | HIS  | 2.5  |
| 2   | B     | 192[B] | ASN  | 2.4  |
| 2   | B     | 44[B]  | ALA  | 2.4  |
| 2   | F     | 165[B] | LYS  | 2.4  |
| 2   | D     | 83[B]  | ILE  | 2.4  |
| 1   | G     | 288[A] | MET  | 2.4  |
| 2   | F     | 22[B]  | PRO  | 2.4  |
| 2   | H     | 286[B] | GLY  | 2.4  |
| 2   | H     | 279[B] | MET  | 2.4  |
| 2   | D     | 260[B] | PRO  | 2.4  |
| 1   | G     | 76[A]  | GLY  | 2.4  |
| 1   | C     | 262[A] | GLY  | 2.3  |
| 1   | A     | 73[A]  | ARG  | 2.3  |
| 2   | F     | 31[B]  | GLN  | 2.3  |
| 2   | H     | 82[B]  | MET  | 2.3  |
| 2   | D     | 165[B] | LYS  | 2.3  |
| 2   | F     | 91[B]  | THR  | 2.3  |
| 2   | F     | 24[B]  | SER  | 2.3  |
| 2   | F     | 78[B]  | SER  | 2.3  |
| 2   | D     | 278[B] | GLU  | 2.3  |
| 2   | H     | 62[B]  | GLU  | 2.3  |
| 2   | D     | 261[B] | ALA  | 2.3  |
| 2   | H     | 251[B] | GLY  | 2.3  |
| 2   | H     | 275[B] | SER  | 2.3  |
| 2   | B     | 262[B] | ARG  | 2.3  |
| 1   | C     | 288[A] | MET  | 2.3  |
| 1   | C     | 296[A] | MET  | 2.3  |
| 1   | G     | 296[A] | MET  | 2.3  |
| 1   | C     | 48[A]  | GLU  | 2.3  |
| 2   | H     | 31[B]  | GLN  | 2.2  |
| 1   | E     | 60[A]  | SER  | 2.2  |
| 2   | H     | 44[B]  | ALA  | 2.2  |
| 2   | D     | 251[B] | GLY  | 2.2  |
| 2   | D     | 78[B]  | SER  | 2.2  |

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*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | G     | 293[A] | GLU  | 2.2  |
| 2   | F     | 23[B]  | PHE  | 2.2  |
| 2   | H     | 284[B] | SER  | 2.2  |
| 1   | E     | 264[A] | ASP  | 2.2  |
| 1   | G     | 70[A]  | ASP  | 2.2  |
| 1   | C     | 263[A] | PRO  | 2.2  |
| 2   | D     | 44[B]  | ALA  | 2.1  |
| 2   | F     | 55[B]  | ALA  | 2.1  |
| 1   | E     | 293[A] | GLU  | 2.1  |
| 2   | H     | 88[B]  | GLN  | 2.1  |
| 2   | F     | 83[B]  | ILE  | 2.1  |
| 2   | H     | 285[B] | CYS  | 2.1  |
| 2   | H     | 30[B]  | ALA  | 2.1  |
| 2   | B     | 258[B] | GLY  | 2.1  |
| 1   | E     | 69[A]  | SER  | 2.1  |
| 2   | H     | 278[B] | GLU  | 2.1  |
| 1   | E     | 277[A] | GLN  | 2.0  |
| 2   | B     | 123[B] | LEU  | 2.0  |
| 2   | H     | 282[B] | GLU  | 2.0  |
| 2   | B     | 78[B]  | SER  | 2.0  |
| 2   | F     | 271[B] | VAL  | 2.0  |
| 1   | A     | 292[A] | LEU  | 2.0  |
| 1   | G     | 174[A] | ALA  | 2.0  |
| 2   | F     | 60[B]  | ALA  | 2.0  |
| 2   | F     | 259[B] | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | SO4  | F     | 402 | 5/5   | 0.84 | 0.16 | 63,68,73,74                 | 0     |
| 3   | SO4  | D     | 401 | 5/5   | 0.88 | 0.18 | 55,59,62,63                 | 0     |
| 3   | SO4  | H     | 402 | 5/5   | 0.92 | 0.11 | 38,43,45,47                 | 0     |
| 3   | SO4  | B     | 401 | 5/5   | 0.95 | 0.09 | 42,42,43,45                 | 0     |
| 3   | SO4  | A     | 401 | 5/5   | 0.96 | 0.16 | 26,28,28,29                 | 0     |
| 3   | SO4  | C     | 401 | 5/5   | 0.97 | 0.08 | 25,27,29,29                 | 0     |
| 3   | SO4  | H     | 401 | 5/5   | 0.97 | 0.09 | 29,30,31,35                 | 0     |
| 3   | SO4  | F     | 401 | 5/5   | 0.97 | 0.07 | 28,29,30,33                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.