



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:04 PM GMT

PDB ID : 1RSC  
Title : STRUCTURE OF AN EFFECTOR INDUCED INACTIVATED STATE OF  
RIBULOSE BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE  
: THE BINARY COMPLEX BETWEEN ENZYME AND XYLULOSE BIS-  
PHOSPHATE  
Authors : Newman, J.; Gutteridge, S.  
Deposited on : 1994-03-29  
Resolution : 2.30 Å(reported)

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

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

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

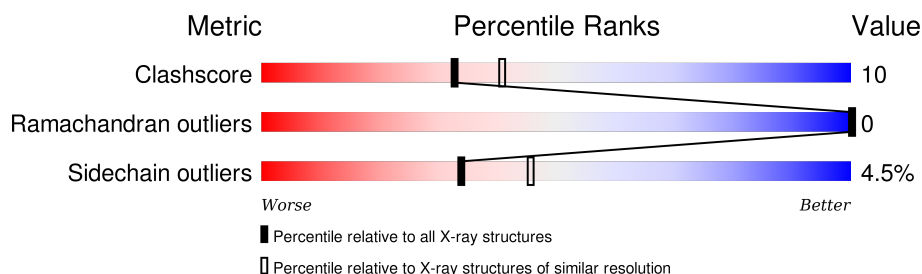
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 4452 (2.30-2.30)                                      |
| Ramachandran outliers | 100387                      | 4410 (2.30-2.30)                                      |
| Sidechain outliers    | 100360                      | 4409 (2.30-2.30)                                      |










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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 472    |                  |
| 1   | B     | 472    |                  |
| 1   | C     | 472    |                  |
| 1   | D     | 472    |                  |
| 1   | E     | 472    |                  |
| 1   | F     | 472    |                  |
| 1   | G     | 472    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | H     | 472    |  73%23%... |
| 2   | I     | 111    |  77%22%.   |
| 2   | J     | 111    |  76%23%.   |
| 2   | K     | 111    |  79%19%.   |
| 2   | L     | 111    |  77%22%.   |
| 2   | M     | 111    |  74%24%.   |
| 2   | N     | 111    |  79%19%.   |
| 2   | O     | 111    |  74%24%.   |
| 2   | P     | 111    |  75%23%.   |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36846 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 RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | B     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | C     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | D     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | E     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | F     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | G     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |
| 1   | H     | 467      | Total | C    | N   | O   | S  | 72      | 0       | 0     |
|     |       |          | 3653  | 2324 | 638 | 673 | 18 |         |         |       |

- Molecule 2 is a protein called RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN).

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | M     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |
| 2   | I     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |
| 2   | N     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |
| 2   | J     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |
| 2   | O     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |

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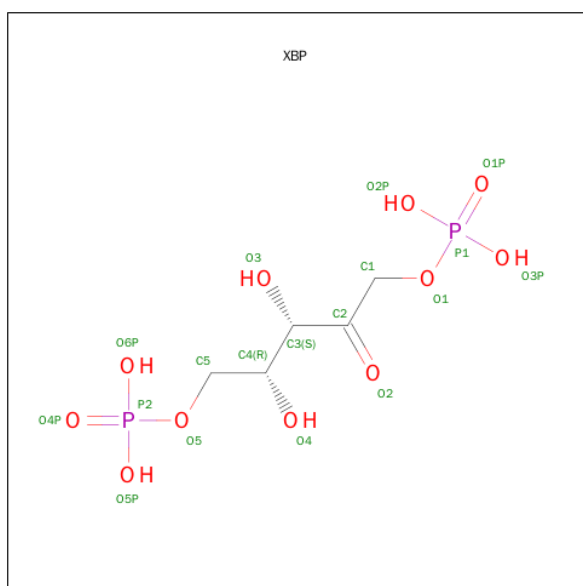
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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | K     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |
| 2   | P     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |
| 2   | L     | 109      | Total | C   | N   | O   | S | 58      | 0       | 0     |
|     |       |          | 909   | 583 | 154 | 165 | 7 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| M     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| I     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| N     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| J     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| O     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| K     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| P     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |
| L     | 109     | GLU      | GLN    | CONFLICT | UNP P04716 |

- Molecule 3 is SUGAR (XYLULOSE-1,5-BISPHOSPHATE) (three-letter code: XBP) (formula:  $C_5H_{12}O_{11}P_2$ ).



| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |
| 3   | B     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 3   | C     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |
| 3   | D     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |
| 3   | E     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |
| 3   | F     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |
| 3   | G     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |
| 3   | H     | 1        | Total | C | O  | P | 0       | 0       |
|     |       |          | 18    | 5 | 11 | 2 |         |         |

- Molecule 4 is water.

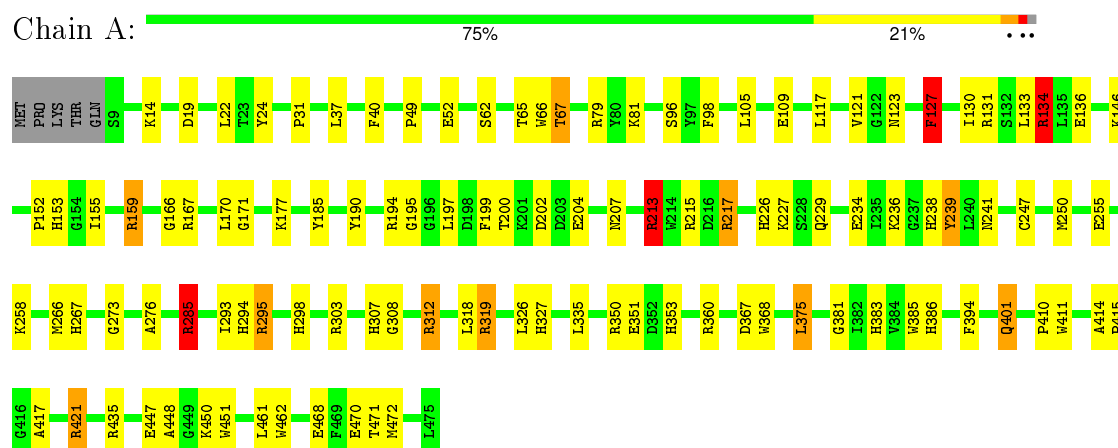
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 148      | Total | O   | 0       | 0       |
|     |       |          | 148   | 148 |         |         |
| 4   | B     | 9        | Total | O   | 0       | 0       |
|     |       |          | 9     | 9   |         |         |
| 4   | C     | 8        | Total | O   | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 4   | D     | 4        | Total | O   | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 4   | G     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 4   | J     | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 4   | M     | 35       | Total | O   | 0       | 0       |
|     |       |          | 35    | 35  |         |         |

### 3 Residue-property plots

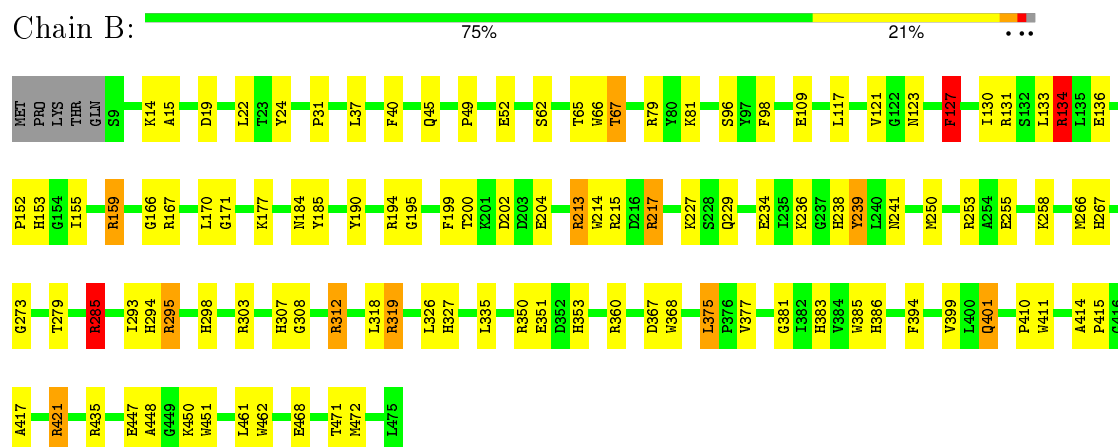
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

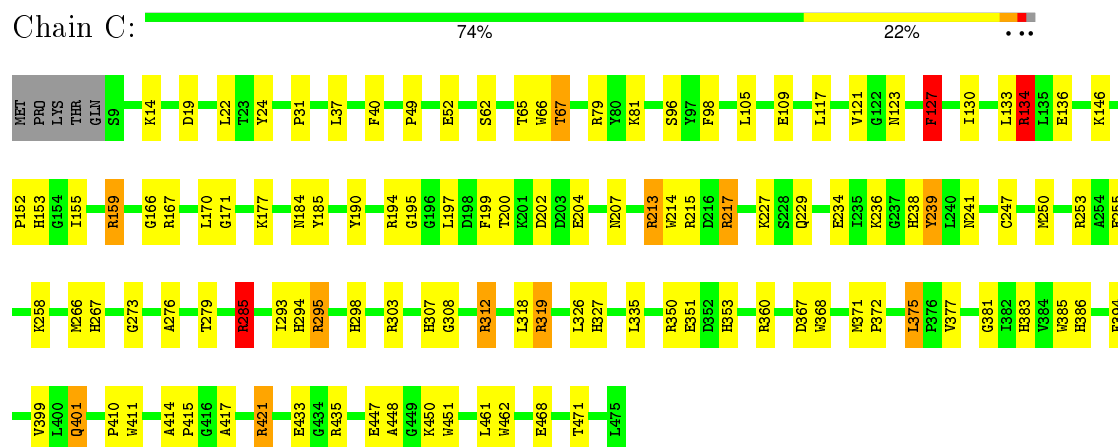
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



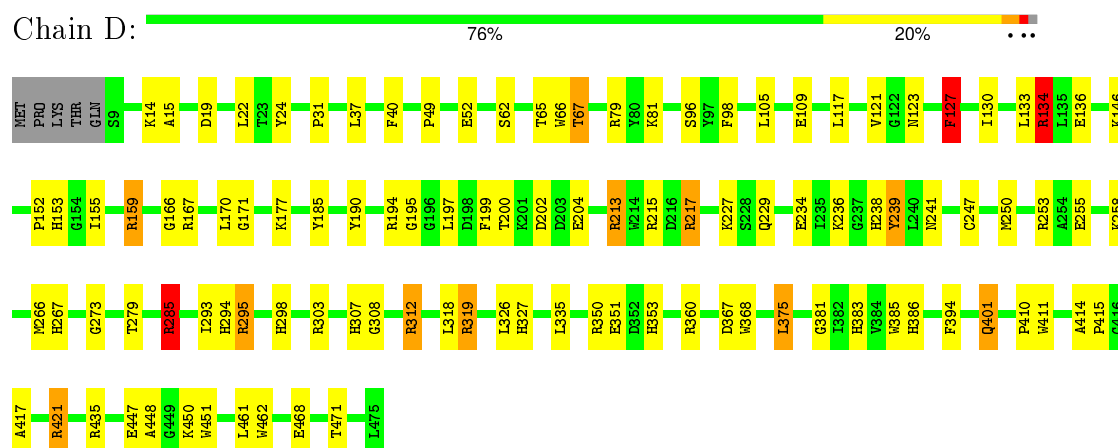
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



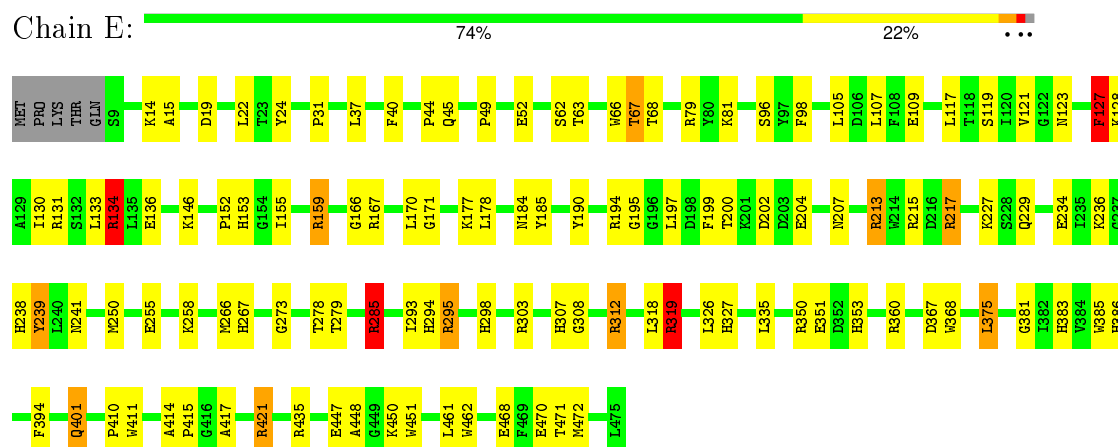
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



- Molecule 1: RIBULOSE 1,5 BISPSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



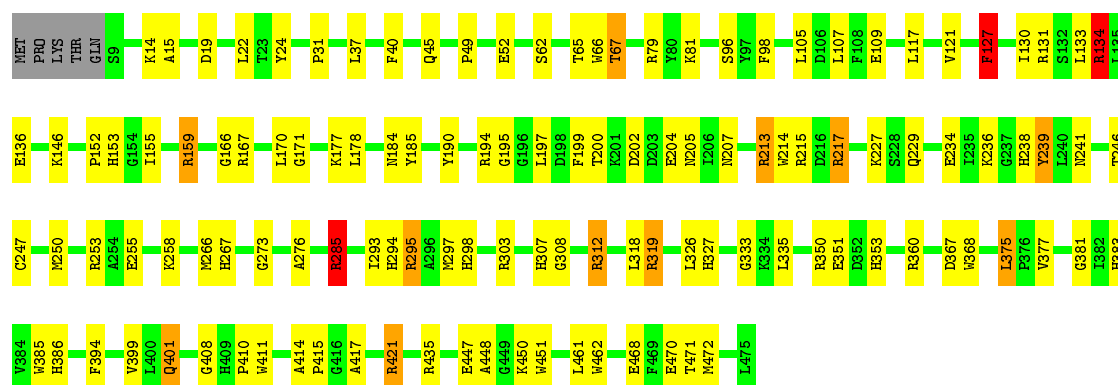
- Molecule 1: RIBULOSE 1,5 BISPSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



- Molecule 1: RIBULOSE 1,5 BISPSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

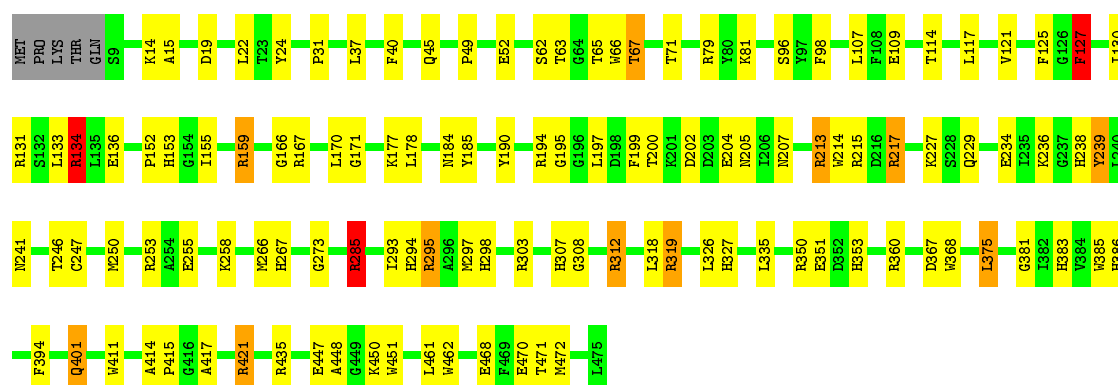


Chain F:  73% 23% ...



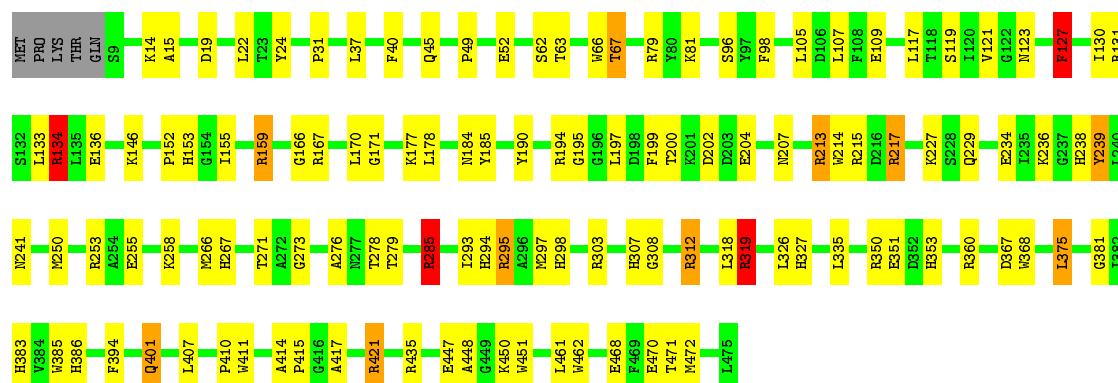
- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain G:  74% 22% ...



- Molecule 1: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain H:  73% 23% ...



- Molecule 2: RIBULOSE 1,5 BISPHTHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain M:  74% 24%




- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain I:  77% 22%



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain N:  79% 19%



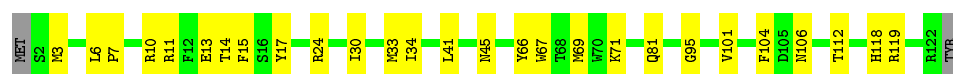
- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain J:  76% 23%




- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain O:  74% 24%



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain K:  79% 19%



- Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain P:  75% 23%



● Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)



## 4 Data and refinement statistics

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

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 224.40Å 112.60Å 200.30Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | (Not available) – 2.30                          | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-2.30)          | Depositor |
| $R_{merge}$  | (Not available)                                 | Depositor |
| $R_{sym}$  | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR  | Depositor |
| R, $R_{free}$  | 0.255 , (Not available)                         | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 36846   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 30.0  | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.32         | 1/3745 (0.0%)  | 0.51        | 1/5071 (0.0%)  |
| 1   | B     | 0.32         | 1/3745 (0.0%)  | 0.51        | 1/5071 (0.0%)  |
| 1   | C     | 0.32         | 1/3745 (0.0%)  | 0.52        | 1/5071 (0.0%)  |
| 1   | D     | 0.32         | 1/3745 (0.0%)  | 0.51        | 1/5071 (0.0%)  |
| 1   | E     | 0.32         | 1/3745 (0.0%)  | 0.52        | 1/5071 (0.0%)  |
| 1   | F     | 0.32         | 1/3745 (0.0%)  | 0.52        | 1/5071 (0.0%)  |
| 1   | G     | 0.32         | 1/3745 (0.0%)  | 0.52        | 1/5071 (0.0%)  |
| 1   | H     | 0.32         | 1/3745 (0.0%)  | 0.51        | 1/5071 (0.0%)  |
| 2   | I     | 0.30         | 0/936          | 0.46        | 0/1267         |
| 2   | J     | 0.30         | 0/936          | 0.46        | 0/1267         |
| 2   | K     | 0.30         | 0/936          | 0.46        | 0/1267         |
| 2   | L     | 0.30         | 0/936          | 0.46        | 0/1267         |
| 2   | M     | 0.30         | 0/936          | 0.46        | 0/1267         |
| 2   | N     | 0.30         | 0/936          | 0.46        | 0/1267         |
| 2   | O     | 0.30         | 0/936          | 0.47        | 0/1267         |
| 2   | P     | 0.31         | 0/936          | 0.47        | 0/1267         |
| All | All   | 0.32         | 8/37448 (0.0%) | 0.51        | 8/50704 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 9                   |
| 1   | B     | 0                   | 9                   |
| 1   | C     | 0                   | 9                   |
| 1   | D     | 0                   | 9                   |
| 1   | E     | 0                   | 9                   |
| 1   | F     | 0                   | 9                   |
| 1   | G     | 0                   | 9                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | H     | 0                   | 9                   |
| 2   | I     | 0                   | 1                   |
| 2   | J     | 0                   | 1                   |
| 2   | K     | 0                   | 1                   |
| 2   | L     | 0                   | 1                   |
| 2   | M     | 0                   | 1                   |
| 2   | N     | 0                   | 1                   |
| 2   | O     | 0                   | 1                   |
| 2   | P     | 0                   | 1                   |
| All | All   | 0                   | 80                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 127 | PHE  | CA-CB | -6.84 | 1.39        | 1.53     |
| 1   | H     | 127 | PHE  | CA-CB | -6.76 | 1.39        | 1.53     |
| 1   | C     | 127 | PHE  | CA-CB | -6.76 | 1.39        | 1.53     |
| 1   | A     | 127 | PHE  | CA-CB | -6.75 | 1.39        | 1.53     |
| 1   | B     | 127 | PHE  | CA-CB | -6.75 | 1.39        | 1.53     |
| 1   | D     | 127 | PHE  | CA-CB | -6.75 | 1.39        | 1.53     |
| 1   | F     | 127 | PHE  | CA-CB | -6.74 | 1.39        | 1.53     |
| 1   | E     | 127 | PHE  | CA-CB | -6.70 | 1.39        | 1.53     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 217 | ARG  | NE-CZ-NH2 | -5.57 | 117.51      | 120.30   |
| 1   | B     | 217 | ARG  | NE-CZ-NH2 | -5.57 | 117.52      | 120.30   |
| 1   | D     | 217 | ARG  | NE-CZ-NH2 | -5.54 | 117.53      | 120.30   |
| 1   | E     | 217 | ARG  | NE-CZ-NH2 | -5.53 | 117.53      | 120.30   |
| 1   | H     | 217 | ARG  | NE-CZ-NH2 | -5.52 | 117.54      | 120.30   |
| 1   | A     | 217 | ARG  | NE-CZ-NH2 | -5.51 | 117.55      | 120.30   |
| 1   | F     | 217 | ARG  | NE-CZ-NH2 | -5.47 | 117.56      | 120.30   |
| 1   | G     | 217 | ARG  | NE-CZ-NH2 | -5.38 | 117.61      | 120.30   |

There are no chirality outliers.

All (80) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 134 | ARG  | Sidechain |
| 1   | A     | 159 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 194 | ARG  | Sidechain |
| 1   | A     | 213 | ARG  | Sidechain |
| 1   | A     | 217 | ARG  | Sidechain |
| 1   | A     | 285 | ARG  | Sidechain |
| 1   | A     | 312 | ARG  | Sidechain |
| 1   | A     | 319 | ARG  | Sidechain |
| 1   | A     | 421 | ARG  | Sidechain |
| 1   | B     | 134 | ARG  | Sidechain |
| 1   | B     | 159 | ARG  | Sidechain |
| 1   | B     | 194 | ARG  | Sidechain |
| 1   | B     | 213 | ARG  | Sidechain |
| 1   | B     | 217 | ARG  | Sidechain |
| 1   | B     | 285 | ARG  | Sidechain |
| 1   | B     | 312 | ARG  | Sidechain |
| 1   | B     | 319 | ARG  | Sidechain |
| 1   | B     | 421 | ARG  | Sidechain |
| 1   | C     | 134 | ARG  | Sidechain |
| 1   | C     | 159 | ARG  | Sidechain |
| 1   | C     | 194 | ARG  | Sidechain |
| 1   | C     | 213 | ARG  | Sidechain |
| 1   | C     | 217 | ARG  | Sidechain |
| 1   | C     | 285 | ARG  | Sidechain |
| 1   | C     | 312 | ARG  | Sidechain |
| 1   | C     | 319 | ARG  | Sidechain |
| 1   | C     | 421 | ARG  | Sidechain |
| 1   | D     | 134 | ARG  | Sidechain |
| 1   | D     | 159 | ARG  | Sidechain |
| 1   | D     | 194 | ARG  | Sidechain |
| 1   | D     | 213 | ARG  | Sidechain |
| 1   | D     | 217 | ARG  | Sidechain |
| 1   | D     | 285 | ARG  | Sidechain |
| 1   | D     | 312 | ARG  | Sidechain |
| 1   | D     | 319 | ARG  | Sidechain |
| 1   | D     | 421 | ARG  | Sidechain |
| 1   | E     | 134 | ARG  | Sidechain |
| 1   | E     | 159 | ARG  | Sidechain |
| 1   | E     | 194 | ARG  | Sidechain |
| 1   | E     | 213 | ARG  | Sidechain |
| 1   | E     | 217 | ARG  | Sidechain |
| 1   | E     | 285 | ARG  | Sidechain |
| 1   | E     | 312 | ARG  | Sidechain |
| 1   | E     | 319 | ARG  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | E     | 421 | ARG  | Sidechain |
| 1   | F     | 134 | ARG  | Sidechain |
| 1   | F     | 159 | ARG  | Sidechain |
| 1   | F     | 194 | ARG  | Sidechain |
| 1   | F     | 213 | ARG  | Sidechain |
| 1   | F     | 217 | ARG  | Sidechain |
| 1   | F     | 285 | ARG  | Sidechain |
| 1   | F     | 312 | ARG  | Sidechain |
| 1   | F     | 319 | ARG  | Sidechain |
| 1   | F     | 421 | ARG  | Sidechain |
| 1   | G     | 134 | ARG  | Sidechain |
| 1   | G     | 159 | ARG  | Sidechain |
| 1   | G     | 194 | ARG  | Sidechain |
| 1   | G     | 213 | ARG  | Sidechain |
| 1   | G     | 217 | ARG  | Sidechain |
| 1   | G     | 285 | ARG  | Sidechain |
| 1   | G     | 312 | ARG  | Sidechain |
| 1   | G     | 319 | ARG  | Sidechain |
| 1   | G     | 421 | ARG  | Sidechain |
| 1   | H     | 134 | ARG  | Sidechain |
| 1   | H     | 159 | ARG  | Sidechain |
| 1   | H     | 194 | ARG  | Sidechain |
| 1   | H     | 213 | ARG  | Sidechain |
| 1   | H     | 217 | ARG  | Sidechain |
| 1   | H     | 285 | ARG  | Sidechain |
| 1   | H     | 312 | ARG  | Sidechain |
| 1   | H     | 319 | ARG  | Sidechain |
| 1   | H     | 421 | ARG  | Sidechain |
| 2   | I     | 66  | TYR  | Sidechain |
| 2   | J     | 66  | TYR  | Sidechain |
| 2   | K     | 66  | TYR  | Sidechain |
| 2   | L     | 66  | TYR  | Sidechain |
| 2   | M     | 66  | TYR  | Sidechain |
| 2   | N     | 66  | TYR  | Sidechain |
| 2   | O     | 66  | TYR  | Sidechain |
| 2   | P     | 66  | TYR  | Sidechain |

## 5.2 Too-close contacts

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



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3653  | 0        | 3568     | 93      | 0            |
| 1   | B     | 3653  | 0        | 3568     | 90      | 0            |
| 1   | C     | 3653  | 0        | 3568     | 88      | 1            |
| 1   | D     | 3653  | 0        | 3568     | 82      | 0            |
| 1   | E     | 3653  | 0        | 3568     | 102     | 0            |
| 1   | F     | 3653  | 0        | 3568     | 105     | 0            |
| 1   | G     | 3653  | 0        | 3568     | 113     | 0            |
| 1   | H     | 3653  | 0        | 3568     | 117     | 0            |
| 2   | I     | 909   | 0        | 860      | 14      | 1            |
| 2   | J     | 909   | 0        | 860      | 15      | 1            |
| 2   | K     | 909   | 0        | 860      | 11      | 30           |
| 2   | L     | 909   | 0        | 860      | 14      | 0            |
| 2   | M     | 909   | 0        | 860      | 16      | 1            |
| 2   | N     | 909   | 0        | 860      | 13      | 0            |
| 2   | O     | 909   | 0        | 860      | 16      | 30           |
| 2   | P     | 909   | 0        | 860      | 16      | 0            |
| 3   | A     | 18    | 0        | 8        | 2       | 0            |
| 3   | B     | 18    | 0        | 8        | 2       | 0            |
| 3   | C     | 18    | 0        | 8        | 2       | 0            |
| 3   | D     | 18    | 0        | 8        | 2       | 0            |
| 3   | E     | 18    | 0        | 8        | 2       | 0            |
| 3   | F     | 18    | 0        | 8        | 1       | 0            |
| 3   | G     | 18    | 0        | 8        | 1       | 0            |
| 3   | H     | 18    | 0        | 8        | 2       | 0            |
| 4   | A     | 148   | 0        | 0        | 3       | 0            |
| 4   | B     | 9     | 0        | 0        | 0       | 0            |
| 4   | C     | 8     | 0        | 0        | 0       | 0            |
| 4   | D     | 4     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 35    | 0        | 0        | 1       | 0            |
| All | All   | 36846 | 0        | 35488    | 721     | 32           |

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

All (721) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:462:TRP:HE1 | 1:H:67:THR:HG21 | 1.07                     | 1.17              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:E:462:TRP:HE1 | 1:F:67:THR:HG21 | 0.98                     | 1.14              |
| 1:C:462:TRP:HE1 | 1:D:67:THR:HG21 | 1.12                     | 1.14              |
| 1:G:67:THR:HG21 | 1:H:462:TRP:HE1 | 1.02                     | 1.11              |
| 1:A:462:TRP:HE1 | 1:B:67:THR:HG21 | 1.01                     | 1.09              |
| 1:E:67:THR:HG21 | 1:F:462:TRP:HE1 | 1.02                     | 1.09              |
| 1:A:67:THR:HG21 | 1:B:462:TRP:HE1 | 1.11                     | 1.09              |
| 1:C:67:THR:HG21 | 1:D:462:TRP:HE1 | 1.15                     | 1.05              |
| 1:H:295:ARG:HD3 | 3:H:476:XBP:O4P | 1.60                     | 1.01              |
| 1:F:295:ARG:HD3 | 3:F:476:XBP:O4P | 1.61                     | 1.01              |
| 1:G:295:ARG:HD3 | 3:G:476:XBP:O4P | 1.60                     | 1.01              |
| 1:D:295:ARG:HD3 | 3:D:476:XBP:O4P | 1.60                     | 1.01              |
| 1:B:295:ARG:HD3 | 3:B:476:XBP:O4P | 1.60                     | 1.00              |
| 1:E:295:ARG:HD3 | 3:E:476:XBP:O4P | 1.61                     | 1.00              |
| 1:C:295:ARG:HD3 | 3:C:476:XBP:O4P | 1.60                     | 1.00              |
| 1:G:67:THR:HG21 | 1:H:462:TRP:NE1 | 1.75                     | 1.00              |
| 1:A:295:ARG:HD3 | 3:A:476:XBP:O4P | 1.60                     | 0.99              |
| 1:E:462:TRP:NE1 | 1:F:67:THR:HG21 | 1.76                     | 0.99              |
| 1:E:67:THR:HG21 | 1:F:462:TRP:NE1 | 1.79                     | 0.98              |
| 1:G:462:TRP:NE1 | 1:H:67:THR:HG21 | 1.79                     | 0.98              |
| 1:A:462:TRP:NE1 | 1:B:67:THR:HG21 | 1.78                     | 0.96              |
| 1:C:462:TRP:NE1 | 1:D:67:THR:HG21 | 1.90                     | 0.87              |
| 1:A:67:THR:HG21 | 1:B:462:TRP:NE1 | 1.89                     | 0.86              |
| 1:G:335:LEU:CD2 | 1:H:127:PHE:CD1 | 2.62                     | 0.83              |
| 1:C:250:MET:CE  | 1:C:267:HIS:NE2 | 2.44                     | 0.81              |
| 1:F:250:MET:CE  | 1:F:267:HIS:NE2 | 2.44                     | 0.81              |
| 1:E:250:MET:CE  | 1:E:267:HIS:NE2 | 2.44                     | 0.81              |
| 1:E:67:THR:CG2  | 1:F:462:TRP:HE1 | 1.91                     | 0.80              |
| 1:A:250:MET:CE  | 1:A:267:HIS:NE2 | 2.44                     | 0.80              |
| 1:H:250:MET:CE  | 1:H:267:HIS:NE2 | 2.44                     | 0.80              |
| 1:B:250:MET:CE  | 1:B:267:HIS:NE2 | 2.44                     | 0.80              |
| 1:G:250:MET:CE  | 1:G:267:HIS:NE2 | 2.44                     | 0.80              |
| 1:D:250:MET:CE  | 1:D:267:HIS:NE2 | 2.44                     | 0.80              |
| 1:C:67:THR:HG21 | 1:D:462:TRP:NE1 | 1.94                     | 0.79              |
| 1:G:66:TRP:CD1  | 1:H:381:GLY:HA2 | 2.20                     | 0.76              |
| 2:O:41:LEU:HD11 | 2:O:69:MET:HG3  | 1.69                     | 0.74              |
| 2:L:41:LEU:HD11 | 2:L:69:MET:HG3  | 1.69                     | 0.74              |
| 2:J:41:LEU:HD11 | 2:J:69:MET:HG3  | 1.69                     | 0.74              |
| 2:N:41:LEU:HD11 | 2:N:69:MET:HG3  | 1.69                     | 0.74              |
| 2:I:41:LEU:HD11 | 2:I:69:MET:HG3  | 1.69                     | 0.73              |
| 2:K:41:LEU:HD11 | 2:K:69:MET:HG3  | 1.69                     | 0.73              |
| 2:M:41:LEU:HD11 | 2:M:69:MET:HG3  | 1.69                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:250:MET:HE2  | 1:D:267:HIS:NE2  | 2.05                     | 0.72              |
| 2:P:41:LEU:HD11  | 2:P:69:MET:HG3   | 1.70                     | 0.72              |
| 1:H:250:MET:HE2  | 1:H:267:HIS:NE2  | 2.05                     | 0.72              |
| 1:G:15:ALA:HB1   | 1:H:461:LEU:HD21 | 1.71                     | 0.72              |
| 1:E:250:MET:HE2  | 1:E:267:HIS:NE2  | 2.04                     | 0.71              |
| 1:B:250:MET:HE2  | 1:B:267:HIS:NE2  | 2.04                     | 0.71              |
| 1:E:127:PHE:CD1  | 1:F:335:LEU:CD2  | 2.73                     | 0.71              |
| 1:G:335:LEU:HD21 | 1:H:127:PHE:CD1  | 2.24                     | 0.70              |
| 1:E:462:TRP:HE1  | 1:F:67:THR:CG2   | 1.91                     | 0.70              |
| 1:G:127:PHE:CD1  | 1:H:335:LEU:CD2  | 2.73                     | 0.70              |
| 1:F:250:MET:HE2  | 1:F:267:HIS:NE2  | 2.06                     | 0.69              |
| 1:G:250:MET:HE2  | 1:G:267:HIS:NE2  | 2.05                     | 0.69              |
| 1:C:250:MET:HE2  | 1:C:267:HIS:NE2  | 2.06                     | 0.69              |
| 1:E:273:GLY:HA3  | 1:F:273:GLY:HA3  | 1.75                     | 0.69              |
| 1:G:303:ARG:NH2  | 1:H:130:ILE:O    | 2.26                     | 0.69              |
| 1:G:335:LEU:HD23 | 1:H:127:PHE:CD1  | 2.26                     | 0.69              |
| 1:A:250:MET:HE1  | 1:A:267:HIS:CE1  | 2.28                     | 0.69              |
| 1:F:234:GLU:OE1  | 1:F:421:ARG:NH2  | 2.27                     | 0.68              |
| 1:D:234:GLU:OE1  | 1:D:421:ARG:NH2  | 2.27                     | 0.68              |
| 1:A:462:TRP:HE1  | 1:B:67:THR:CG2   | 1.93                     | 0.68              |
| 1:G:127:PHE:CD1  | 1:H:335:LEU:HD23 | 2.28                     | 0.68              |
| 1:G:234:GLU:OE1  | 1:G:421:ARG:NH2  | 2.27                     | 0.68              |
| 1:G:253:ARG:NH2  | 1:H:109:GLU:OE2  | 2.20                     | 0.68              |
| 1:G:462:TRP:HE1  | 1:H:67:THR:CG2   | 1.96                     | 0.68              |
| 1:A:234:GLU:OE1  | 1:A:421:ARG:NH2  | 2.27                     | 0.67              |
| 1:C:234:GLU:OE1  | 1:C:421:ARG:NH2  | 2.27                     | 0.67              |
| 1:H:234:GLU:OE1  | 1:H:421:ARG:NH2  | 2.27                     | 0.67              |
| 1:E:234:GLU:OE1  | 1:E:421:ARG:NH2  | 2.27                     | 0.67              |
| 1:G:273:GLY:HA3  | 1:H:273:GLY:HA3  | 1.76                     | 0.67              |
| 1:E:383:HIS:H    | 1:E:386:HIS:HD2  | 1.44                     | 0.66              |
| 1:E:127:PHE:CD1  | 1:F:335:LEU:HD21 | 2.31                     | 0.66              |
| 1:B:234:GLU:OE1  | 1:B:421:ARG:NH2  | 2.27                     | 0.66              |
| 1:D:383:HIS:H    | 1:D:386:HIS:HD2  | 1.44                     | 0.66              |
| 1:A:383:HIS:H    | 1:A:386:HIS:HD2  | 1.44                     | 0.66              |
| 1:C:383:HIS:H    | 1:C:386:HIS:HD2  | 1.44                     | 0.65              |
| 1:B:383:HIS:H    | 1:B:386:HIS:HD2  | 1.44                     | 0.65              |
| 1:G:383:HIS:H    | 1:G:386:HIS:HD2  | 1.44                     | 0.65              |
| 1:A:155:ILE:HG12 | 1:A:375:LEU:HD13 | 1.79                     | 0.65              |
| 1:E:155:ILE:HG12 | 1:E:375:LEU:HD13 | 1.79                     | 0.65              |
| 1:D:155:ILE:HG12 | 1:D:375:LEU:HD13 | 1.78                     | 0.65              |
| 1:H:383:HIS:H    | 1:H:386:HIS:HD2  | 1.44                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:30:ILE:O     | 2:P:34:ILE:HG12  | 1.97                     | 0.65              |
| 1:H:155:ILE:HG12 | 1:H:375:LEU:HD13 | 1.78                     | 0.65              |
| 1:G:155:ILE:HG12 | 1:G:375:LEU:HD13 | 1.78                     | 0.65              |
| 1:F:383:HIS:H    | 1:F:386:HIS:HD2  | 1.44                     | 0.65              |
| 2:J:30:ILE:O     | 2:J:34:ILE:HG12  | 1.97                     | 0.65              |
| 1:B:155:ILE:HG12 | 1:B:375:LEU:HD13 | 1.78                     | 0.64              |
| 2:I:30:ILE:O     | 2:I:34:ILE:HG12  | 1.97                     | 0.64              |
| 1:G:335:LEU:CD2  | 1:H:127:PHE:HD1  | 2.10                     | 0.64              |
| 2:M:30:ILE:O     | 2:M:34:ILE:HG12  | 1.97                     | 0.64              |
| 1:C:155:ILE:HG12 | 1:C:375:LEU:HD13 | 1.79                     | 0.64              |
| 2:L:30:ILE:O     | 2:L:34:ILE:HG12  | 1.97                     | 0.64              |
| 2:N:30:ILE:O     | 2:N:34:ILE:HG12  | 1.97                     | 0.64              |
| 1:F:155:ILE:HG12 | 1:F:375:LEU:HD13 | 1.79                     | 0.64              |
| 2:K:30:ILE:O     | 2:K:34:ILE:HG12  | 1.97                     | 0.63              |
| 1:E:335:LEU:CD2  | 1:F:127:PHE:CD1  | 2.81                     | 0.63              |
| 1:G:381:GLY:HA2  | 1:H:66:TRP:CD1   | 2.33                     | 0.63              |
| 1:A:335:LEU:CD2  | 1:B:127:PHE:CD1  | 2.82                     | 0.63              |
| 2:O:30:ILE:O     | 2:O:34:ILE:HG12  | 1.98                     | 0.63              |
| 1:A:273:GLY:HA3  | 1:B:273:GLY:HA3  | 1.80                     | 0.61              |
| 1:E:350:ARG:NH2  | 1:E:394:PHE:O    | 2.34                     | 0.61              |
| 1:H:350:ARG:NH2  | 1:H:394:PHE:O    | 2.34                     | 0.61              |
| 1:A:127:PHE:CD1  | 1:B:335:LEU:CD2  | 2.83                     | 0.61              |
| 1:F:350:ARG:NH2  | 1:F:394:PHE:O    | 2.34                     | 0.61              |
| 1:G:350:ARG:NH2  | 1:G:394:PHE:O    | 2.34                     | 0.61              |
| 1:A:350:ARG:NH2  | 1:A:394:PHE:O    | 2.34                     | 0.61              |
| 1:C:350:ARG:NH2  | 1:C:394:PHE:O    | 2.34                     | 0.60              |
| 1:G:66:TRP:CH2   | 1:H:383:HIS:HD2  | 2.18                     | 0.60              |
| 1:C:273:GLY:HA3  | 1:D:273:GLY:HA3  | 1.83                     | 0.60              |
| 1:E:127:PHE:CD1  | 1:F:335:LEU:HD23 | 2.37                     | 0.60              |
| 1:B:350:ARG:NH2  | 1:B:394:PHE:O    | 2.34                     | 0.60              |
| 1:A:250:MET:HE1  | 1:A:267:HIS:NE2  | 2.16                     | 0.59              |
| 1:D:350:ARG:NH2  | 1:D:394:PHE:O    | 2.34                     | 0.59              |
| 3:E:476:XBP:O2P  | 1:F:65:THR:OG1   | 2.15                     | 0.59              |
| 1:E:130:ILE:O    | 1:F:303:ARG:NH2  | 2.34                     | 0.59              |
| 1:G:461:LEU:HD21 | 1:H:15:ALA:HB1   | 1.85                     | 0.59              |
| 1:G:177:LYS:HB2  | 1:H:63:THR:HA    | 1.85                     | 0.58              |
| 1:A:65:THR:OG1   | 3:B:476:XBP:O2P  | 2.17                     | 0.58              |
| 1:G:107:LEU:HD22 | 1:H:178:LEU:HD12 | 1.85                     | 0.58              |
| 1:G:107:LEU:HD22 | 1:H:178:LEU:CD1  | 2.34                     | 0.58              |
| 1:G:470:GLU:O    | 1:H:45:GLN:NE2   | 2.37                     | 0.58              |
| 1:G:130:ILE:O    | 1:H:303:ARG:NH2  | 2.36                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:131:ARG:O    | 1:H:472:MET:HG3  | 2.04                     | 0.58              |
| 1:G:178:LEU:CD1  | 1:H:107:LEU:HD22 | 2.34                     | 0.58              |
| 1:G:319:ARG:NH2  | 1:G:351:GLU:O    | 2.34                     | 0.57              |
| 1:G:297:MET:HA   | 1:H:121:VAL:O    | 2.05                     | 0.57              |
| 1:C:319:ARG:NH2  | 1:C:351:GLU:O    | 2.35                     | 0.57              |
| 1:B:229:GLN:NE2  | 1:B:236:LYS:H    | 2.03                     | 0.57              |
| 1:E:229:GLN:NE2  | 1:E:236:LYS:H    | 2.03                     | 0.56              |
| 1:C:229:GLN:NE2  | 1:C:236:LYS:H    | 2.03                     | 0.56              |
| 1:A:229:GLN:NE2  | 1:A:236:LYS:H    | 2.03                     | 0.56              |
| 1:B:411:TRP:CD1  | 2:I:3:MET:HB3    | 2.41                     | 0.56              |
| 1:E:234:GLU:CD   | 1:E:421:ARG:HH22 | 2.09                     | 0.56              |
| 1:E:335:LEU:HD23 | 1:F:127:PHE:CD1  | 2.39                     | 0.56              |
| 1:H:411:TRP:CD1  | 2:L:3:MET:HB3    | 2.41                     | 0.56              |
| 1:D:411:TRP:CD1  | 2:J:3:MET:HB3    | 2.41                     | 0.56              |
| 1:D:318:LEU:O    | 1:D:318:LEU:HG   | 2.06                     | 0.56              |
| 1:C:335:LEU:CD2  | 1:D:127:PHE:CD1  | 2.89                     | 0.56              |
| 1:D:229:GLN:NE2  | 1:D:236:LYS:H    | 2.03                     | 0.56              |
| 1:F:229:GLN:NE2  | 1:F:236:LYS:H    | 2.03                     | 0.56              |
| 1:C:234:GLU:CD   | 1:C:421:ARG:HH22 | 2.09                     | 0.56              |
| 1:F:411:TRP:CD1  | 2:K:3:MET:HB3    | 2.41                     | 0.56              |
| 1:E:411:TRP:CD1  | 2:O:3:MET:HB3    | 2.41                     | 0.56              |
| 1:H:229:GLN:NE2  | 1:H:236:LYS:H    | 2.03                     | 0.56              |
| 1:C:411:TRP:CD1  | 2:N:3:MET:HB3    | 2.41                     | 0.56              |
| 1:E:123:ASN:ND2  | 1:F:204:GLU:OE2  | 2.38                     | 0.56              |
| 1:G:229:GLN:NE2  | 1:G:236:LYS:H    | 2.03                     | 0.56              |
| 1:A:319:ARG:NH2  | 1:A:351:GLU:O    | 2.35                     | 0.56              |
| 1:H:234:GLU:CD   | 1:H:421:ARG:HH22 | 2.10                     | 0.56              |
| 1:C:127:PHE:CD1  | 1:D:335:LEU:CD2  | 2.89                     | 0.56              |
| 1:B:318:LEU:HG   | 1:B:318:LEU:O    | 2.06                     | 0.56              |
| 1:A:250:MET:HE2  | 1:A:267:HIS:NE2  | 2.21                     | 0.55              |
| 1:E:127:PHE:HD1  | 1:F:335:LEU:CD2  | 2.17                     | 0.55              |
| 1:C:318:LEU:O    | 1:C:318:LEU:HG   | 2.06                     | 0.55              |
| 1:B:234:GLU:CD   | 1:B:421:ARG:HH22 | 2.10                     | 0.55              |
| 3:A:476:XBP:O2P  | 1:B:65:THR:OG1   | 2.15                     | 0.55              |
| 1:E:381:GLY:HA2  | 1:F:66:TRP:CD1   | 2.40                     | 0.55              |
| 1:A:123:ASN:ND2  | 1:B:204:GLU:OE2  | 2.39                     | 0.55              |
| 1:G:45:GLN:NE2   | 1:H:470:GLU:O    | 2.40                     | 0.55              |
| 1:A:411:TRP:CD1  | 2:M:3:MET:HB3    | 2.41                     | 0.55              |
| 1:F:318:LEU:O    | 1:F:318:LEU:HG   | 2.06                     | 0.55              |
| 1:A:335:LEU:HD23 | 1:B:127:PHE:CD1  | 2.42                     | 0.55              |
| 1:A:127:PHE:CD1  | 1:B:335:LEU:HD21 | 2.42                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:411:TRP:CD1  | 2:P:3:MET:HB3    | 2.41                     | 0.55              |
| 1:F:234:GLU:CD   | 1:F:421:ARG:HH22 | 2.10                     | 0.55              |
| 1:B:319:ARG:NH2  | 1:B:351:GLU:O    | 2.35                     | 0.55              |
| 1:A:318:LEU:HG   | 1:A:318:LEU:O    | 2.06                     | 0.55              |
| 1:G:127:PHE:CD1  | 1:H:335:LEU:HD21 | 2.42                     | 0.55              |
| 1:D:234:GLU:CD   | 1:D:421:ARG:HH22 | 2.10                     | 0.55              |
| 1:H:318:LEU:O    | 1:H:318:LEU:HG   | 2.06                     | 0.55              |
| 1:E:62:SER:O     | 1:F:177:LYS:HB2  | 2.07                     | 0.55              |
| 1:A:381:GLY:HA2  | 1:B:66:TRP:CD1   | 2.42                     | 0.54              |
| 1:G:67:THR:CG2   | 1:H:462:TRP:HE1  | 1.95                     | 0.54              |
| 1:D:250:MET:HE2  | 1:D:267:HIS:CD2  | 2.43                     | 0.54              |
| 1:D:319:ARG:NH2  | 1:D:351:GLU:O    | 2.35                     | 0.54              |
| 1:E:472:MET:HG3  | 1:F:131:ARG:O    | 2.07                     | 0.54              |
| 1:G:15:ALA:HB1   | 1:H:461:LEU:CD2  | 2.37                     | 0.54              |
| 1:E:250:MET:CE   | 1:E:267:HIS:CE1  | 2.91                     | 0.54              |
| 1:A:234:GLU:CD   | 1:A:421:ARG:HH22 | 2.09                     | 0.54              |
| 1:G:472:MET:HG3  | 1:H:131:ARG:O    | 2.07                     | 0.54              |
| 1:G:318:LEU:HG   | 1:G:318:LEU:O    | 2.06                     | 0.54              |
| 1:G:234:GLU:CD   | 1:G:421:ARG:HH22 | 2.10                     | 0.54              |
| 1:F:319:ARG:NH2  | 1:F:351:GLU:O    | 2.35                     | 0.54              |
| 1:G:127:PHE:HD1  | 1:H:335:LEU:CD2  | 2.18                     | 0.54              |
| 1:E:318:LEU:HG   | 1:E:318:LEU:O    | 2.06                     | 0.54              |
| 1:B:250:MET:CE   | 1:B:267:HIS:CE1  | 2.91                     | 0.53              |
| 1:D:250:MET:CE   | 1:D:267:HIS:CE1  | 2.91                     | 0.53              |
| 1:C:250:MET:CE   | 1:C:267:HIS:CE1  | 2.91                     | 0.53              |
| 1:H:250:MET:CE   | 1:H:267:HIS:CE1  | 2.91                     | 0.53              |
| 2:O:104:PHE:HZ   | 1:G:184:ASN:HD21 | 1.55                     | 0.53              |
| 1:G:109:GLU:OE1  | 1:H:207:ASN:HB3  | 2.08                     | 0.53              |
| 1:F:250:MET:CE   | 1:F:267:HIS:CE1  | 2.91                     | 0.53              |
| 1:G:177:LYS:HB2  | 1:H:62:SER:O     | 2.08                     | 0.53              |
| 1:A:335:LEU:HD21 | 1:B:127:PHE:CD1  | 2.44                     | 0.53              |
| 1:C:123:ASN:ND2  | 1:D:204:GLU:OE2  | 2.42                     | 0.53              |
| 1:E:303:ARG:NH2  | 1:F:130:ILE:O    | 2.42                     | 0.53              |
| 1:C:250:MET:HE2  | 1:C:267:HIS:CE1  | 2.44                     | 0.53              |
| 1:E:131:ARG:O    | 1:F:472:MET:HG3  | 2.10                     | 0.52              |
| 1:E:250:MET:HE2  | 1:E:267:HIS:CD2  | 2.43                     | 0.52              |
| 1:G:250:MET:CE   | 1:G:267:HIS:CE1  | 2.91                     | 0.52              |
| 1:A:250:MET:CE   | 1:A:267:HIS:CE1  | 2.91                     | 0.52              |
| 1:B:184:ASN:HD21 | 2:J:104:PHE:HZ   | 1.56                     | 0.51              |
| 1:F:250:MET:HE2  | 1:F:267:HIS:CE1  | 2.45                     | 0.51              |
| 1:G:335:LEU:HD21 | 1:H:127:PHE:CE1  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:319:ARG:NH2  | 1:E:351:GLU:O    | 2.35                     | 0.51              |
| 1:E:295:ARG:HD2  | 1:E:327:HIS:HB2  | 1.93                     | 0.51              |
| 1:A:213:ARG:HD2  | 4:A:491:HOH:O    | 2.10                     | 0.51              |
| 1:H:31:PRO:HB3   | 1:H:37:LEU:HD21  | 1.93                     | 0.51              |
| 1:E:335:LEU:HD21 | 1:F:127:PHE:CD1  | 2.45                     | 0.51              |
| 2:N:104:PHE:HZ   | 1:E:184:ASN:HD21 | 1.56                     | 0.51              |
| 1:A:31:PRO:HB3   | 1:A:37:LEU:HD21  | 1.93                     | 0.51              |
| 1:G:66:TRP:CH2   | 1:H:383:HIS:CD2  | 2.99                     | 0.51              |
| 1:E:335:LEU:CD2  | 1:F:127:PHE:HD1  | 2.23                     | 0.51              |
| 1:G:31:PRO:HB3   | 1:G:37:LEU:HD21  | 1.93                     | 0.51              |
| 1:F:31:PRO:HB3   | 1:F:37:LEU:HD21  | 1.93                     | 0.51              |
| 1:D:31:PRO:HB3   | 1:D:37:LEU:HD21  | 1.93                     | 0.51              |
| 1:D:295:ARG:HD2  | 1:D:327:HIS:HB2  | 1.93                     | 0.51              |
| 1:G:246:THR:HG22 | 1:H:278:THR:HG22 | 1.93                     | 0.51              |
| 1:C:31:PRO:HB3   | 1:C:37:LEU:HD21  | 1.93                     | 0.51              |
| 1:E:448:ALA:HA   | 1:E:451:TRP:NE1  | 2.26                     | 0.51              |
| 1:E:202:ASP:OD1  | 1:E:238:HIS:HE1  | 1.94                     | 0.51              |
| 1:C:448:ALA:HA   | 1:C:451:TRP:NE1  | 2.26                     | 0.50              |
| 1:G:121:VAL:O    | 1:H:297:MET:HA   | 2.12                     | 0.50              |
| 1:B:295:ARG:HD2  | 1:B:327:HIS:HB2  | 1.93                     | 0.50              |
| 1:C:295:ARG:HD2  | 1:C:327:HIS:HB2  | 1.93                     | 0.50              |
| 1:A:295:ARG:HD2  | 1:A:327:HIS:HB2  | 1.93                     | 0.50              |
| 1:F:250:MET:CE   | 1:F:267:HIS:HE2  | 2.23                     | 0.50              |
| 1:D:250:MET:CE   | 1:D:267:HIS:HE2  | 2.24                     | 0.50              |
| 1:E:31:PRO:HB3   | 1:E:37:LEU:HD21  | 1.93                     | 0.50              |
| 1:D:202:ASP:OD1  | 1:D:238:HIS:HE1  | 1.94                     | 0.50              |
| 1:B:31:PRO:HB3   | 1:B:37:LEU:HD21  | 1.93                     | 0.50              |
| 1:H:202:ASP:OD1  | 1:H:238:HIS:HE1  | 1.94                     | 0.50              |
| 1:A:202:ASP:OD1  | 1:A:238:HIS:HE1  | 1.94                     | 0.50              |
| 1:A:303:ARG:NH2  | 1:B:130:ILE:O    | 2.44                     | 0.50              |
| 1:F:448:ALA:HA   | 1:F:451:TRP:NE1  | 2.26                     | 0.50              |
| 1:B:448:ALA:HA   | 1:B:451:TRP:NE1  | 2.26                     | 0.50              |
| 1:G:448:ALA:HA   | 1:G:451:TRP:NE1  | 2.27                     | 0.50              |
| 1:F:295:ARG:HD2  | 1:F:327:HIS:HB2  | 1.93                     | 0.50              |
| 1:A:153:HIS:HE1  | 4:A:526:HOH:O    | 1.94                     | 0.50              |
| 1:B:202:ASP:OD1  | 1:B:238:HIS:HE1  | 1.94                     | 0.50              |
| 1:H:295:ARG:HD2  | 1:H:327:HIS:HB2  | 1.93                     | 0.50              |
| 1:E:414:ALA:HB3  | 1:E:415:PRO:HD3  | 1.94                     | 0.50              |
| 1:H:448:ALA:HA   | 1:H:451:TRP:NE1  | 2.26                     | 0.50              |
| 1:E:461:LEU:HD21 | 1:F:15:ALA:HB1   | 1.93                     | 0.50              |
| 1:D:448:ALA:HA   | 1:D:451:TRP:NE1  | 2.27                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:381:GLY:HA2  | 1:D:66:TRP:CD1   | 2.47                     | 0.50              |
| 1:B:250:MET:HE2  | 1:B:267:HIS:CD2  | 2.46                     | 0.50              |
| 1:G:250:MET:HE2  | 1:G:267:HIS:CD2  | 2.47                     | 0.50              |
| 1:F:184:ASN:HD21 | 2:L:104:PHE:HZ   | 1.57                     | 0.50              |
| 1:C:202:ASP:OD1  | 1:C:238:HIS:HE1  | 1.94                     | 0.50              |
| 1:A:448:ALA:HA   | 1:A:451:TRP:NE1  | 2.26                     | 0.50              |
| 1:E:127:PHE:HD1  | 1:F:335:LEU:HD21 | 1.76                     | 0.49              |
| 1:H:414:ALA:HB3  | 1:H:415:PRO:HD3  | 1.94                     | 0.49              |
| 1:F:202:ASP:OD1  | 1:F:238:HIS:HE1  | 1.94                     | 0.49              |
| 2:O:69:MET:HE3   | 2:O:71:LYS:O     | 2.13                     | 0.49              |
| 1:A:127:PHE:CD1  | 1:B:335:LEU:HD23 | 2.47                     | 0.49              |
| 1:G:109:GLU:OE2  | 1:H:253:ARG:NH2  | 2.36                     | 0.49              |
| 1:E:105:LEU:HD21 | 1:H:146:LYS:HD2  | 1.94                     | 0.49              |
| 1:A:435:ARG:NH2  | 1:A:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:G:295:ARG:HD2  | 1:G:327:HIS:HB2  | 1.93                     | 0.49              |
| 1:F:435:ARG:NH2  | 1:F:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:G:202:ASP:OD1  | 1:G:238:HIS:HE1  | 1.94                     | 0.49              |
| 1:C:435:ARG:NH2  | 1:C:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:E:109:GLU:OE2  | 1:F:253:ARG:NH2  | 2.28                     | 0.49              |
| 1:C:414:ALA:HB3  | 1:C:415:PRO:HD3  | 1.95                     | 0.49              |
| 1:H:435:ARG:NH2  | 1:H:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:D:435:ARG:NH2  | 1:D:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:B:250:MET:CE   | 1:B:267:HIS:HE2  | 2.23                     | 0.49              |
| 1:A:335:LEU:CD2  | 1:B:127:PHE:HD1  | 2.25                     | 0.49              |
| 1:E:435:ARG:NH2  | 1:E:447:GLU:OE1  | 2.46                     | 0.49              |
| 1:C:117:LEU:O    | 1:C:121:VAL:HG22 | 2.13                     | 0.49              |
| 1:F:117:LEU:O    | 1:F:121:VAL:HG22 | 2.13                     | 0.49              |
| 1:D:250:MET:HE1  | 1:D:267:HIS:CE1  | 2.47                     | 0.49              |
| 1:B:414:ALA:HB3  | 1:B:415:PRO:HD3  | 1.94                     | 0.49              |
| 1:E:40:PHE:O     | 1:E:98:PHE:HA    | 2.13                     | 0.49              |
| 1:G:63:THR:HA    | 1:H:177:LYS:HB2  | 1.94                     | 0.49              |
| 1:B:117:LEU:O    | 1:B:121:VAL:HG22 | 2.13                     | 0.49              |
| 1:E:117:LEU:O    | 1:E:121:VAL:HG22 | 2.13                     | 0.49              |
| 1:G:435:ARG:NH2  | 1:G:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:A:67:THR:CG2   | 1:B:462:TRP:HE1  | 2.02                     | 0.49              |
| 1:H:250:MET:CE   | 1:H:267:HIS:HE2  | 2.23                     | 0.49              |
| 1:G:200:THR:OG1  | 1:G:238:HIS:HD2  | 1.96                     | 0.49              |
| 1:E:177:LYS:HB2  | 1:F:62:SER:O     | 2.13                     | 0.49              |
| 1:B:435:ARG:NH2  | 1:B:447:GLU:OE1  | 2.45                     | 0.49              |
| 1:C:204:GLU:OE2  | 1:D:123:ASN:ND2  | 2.46                     | 0.49              |
| 1:A:40:PHE:O     | 1:A:98:PHE:HA    | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:65:THR:OG1   | 3:D:476:XBP:O2P  | 2.21                     | 0.49              |
| 1:H:40:PHE:O     | 1:H:98:PHE:HA    | 2.13                     | 0.49              |
| 1:G:125:PHE:O    | 1:H:303:ARG:HD3  | 2.13                     | 0.48              |
| 1:F:200:THR:OG1  | 1:F:238:HIS:HD2  | 1.96                     | 0.48              |
| 1:A:117:LEU:O    | 1:A:121:VAL:HG22 | 2.13                     | 0.48              |
| 1:D:40:PHE:O     | 1:D:98:PHE:HA    | 2.13                     | 0.48              |
| 1:A:414:ALA:HB3  | 1:A:415:PRO:HD3  | 1.94                     | 0.48              |
| 1:C:127:PHE:CD1  | 1:D:335:LEU:HD21 | 2.48                     | 0.48              |
| 1:G:117:LEU:O    | 1:G:121:VAL:HG22 | 2.13                     | 0.48              |
| 1:H:200:THR:OG1  | 1:H:238:HIS:HD2  | 1.96                     | 0.48              |
| 1:A:461:LEU:HD21 | 1:B:15:ALA:HB1   | 1.93                     | 0.48              |
| 1:G:178:LEU:HD12 | 1:H:107:LEU:HD22 | 1.94                     | 0.48              |
| 1:B:319:ARG:HG2  | 1:B:368:TRP:CZ3  | 2.49                     | 0.48              |
| 1:C:40:PHE:O     | 1:C:98:PHE:HA    | 2.13                     | 0.48              |
| 1:F:40:PHE:O     | 1:F:98:PHE:HA    | 2.13                     | 0.48              |
| 2:J:69:MET:HE3   | 2:J:71:LYS:O     | 2.13                     | 0.48              |
| 1:D:319:ARG:HG2  | 1:D:368:TRP:CZ3  | 2.49                     | 0.48              |
| 1:D:414:ALA:HB3  | 1:D:415:PRO:HD3  | 1.95                     | 0.48              |
| 1:G:205:ASN:HB2  | 1:H:119:SER:OG   | 2.14                     | 0.48              |
| 1:H:250:MET:HE2  | 1:H:267:HIS:CD2  | 2.48                     | 0.48              |
| 1:F:229:GLN:HE21 | 1:F:236:LYS:H    | 1.62                     | 0.48              |
| 1:H:117:LEU:O    | 1:H:121:VAL:HG22 | 2.13                     | 0.48              |
| 1:A:319:ARG:HG2  | 1:A:368:TRP:CZ3  | 2.49                     | 0.48              |
| 1:G:318:LEU:HD22 | 1:G:326:LEU:HD13 | 1.96                     | 0.48              |
| 1:E:319:ARG:HG2  | 1:E:368:TRP:CZ3  | 2.49                     | 0.48              |
| 1:B:200:THR:OG1  | 1:B:238:HIS:HD2  | 1.96                     | 0.48              |
| 1:B:40:PHE:O     | 1:B:98:PHE:HA    | 2.13                     | 0.48              |
| 1:D:295:ARG:HG3  | 1:D:298:HIS:CD2  | 2.49                     | 0.48              |
| 1:H:319:ARG:NH2  | 1:H:351:GLU:O    | 2.35                     | 0.48              |
| 1:E:295:ARG:HG3  | 1:E:298:HIS:CD2  | 2.49                     | 0.48              |
| 1:C:295:ARG:HG3  | 1:C:298:HIS:CD2  | 2.49                     | 0.48              |
| 2:N:69:MET:HE3   | 2:N:71:LYS:O     | 2.14                     | 0.48              |
| 1:D:117:LEU:O    | 1:D:121:VAL:HG22 | 2.13                     | 0.48              |
| 1:E:250:MET:HE1  | 1:E:267:HIS:CE1  | 2.49                     | 0.48              |
| 1:G:250:MET:CE   | 1:G:267:HIS:HE2  | 2.24                     | 0.48              |
| 2:P:69:MET:HE3   | 2:P:72:LEU:HD23  | 1.95                     | 0.48              |
| 1:F:319:ARG:HG2  | 1:F:368:TRP:CZ3  | 2.49                     | 0.48              |
| 1:F:414:ALA:HB3  | 1:F:415:PRO:HD3  | 1.95                     | 0.48              |
| 1:G:40:PHE:O     | 1:G:98:PHE:HA    | 2.13                     | 0.48              |
| 1:E:134:ARG:HA   | 1:E:308:GLY:O    | 2.14                     | 0.48              |
| 1:B:295:ARG:HG3  | 1:B:298:HIS:CD2  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:69:MET:HE3   | 2:L:71:LYS:O     | 2.14                     | 0.48              |
| 2:I:69:MET:HE3   | 2:I:71:LYS:O     | 2.14                     | 0.48              |
| 1:C:319:ARG:HG2  | 1:C:368:TRP:CZ3  | 2.49                     | 0.48              |
| 1:A:472:MET:HG3  | 1:B:131:ARG:O    | 2.14                     | 0.48              |
| 1:G:414:ALA:HB3  | 1:G:415:PRO:HD3  | 1.95                     | 0.48              |
| 1:H:295:ARG:HG3  | 1:H:298:HIS:CD2  | 2.49                     | 0.47              |
| 1:G:295:ARG:HG3  | 1:G:298:HIS:CD2  | 2.49                     | 0.47              |
| 1:A:247:CYS:H    | 1:B:279:THR:HG1  | 1.62                     | 0.47              |
| 1:C:318:LEU:HD22 | 1:C:326:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:200:THR:OG1  | 1:A:238:HIS:HD2  | 1.96                     | 0.47              |
| 1:G:204:GLU:OE2  | 1:H:123:ASN:ND2  | 2.47                     | 0.47              |
| 1:C:109:GLU:OE2  | 1:D:253:ARG:NH2  | 2.32                     | 0.47              |
| 1:B:134:ARG:HA   | 1:B:308:GLY:O    | 2.14                     | 0.47              |
| 1:A:295:ARG:HG3  | 1:A:298:HIS:CD2  | 2.49                     | 0.47              |
| 1:C:250:MET:CE   | 1:C:267:HIS:HE2  | 2.23                     | 0.47              |
| 1:E:200:THR:OG1  | 1:E:238:HIS:HD2  | 1.96                     | 0.47              |
| 1:D:200:THR:OG1  | 1:D:238:HIS:HD2  | 1.96                     | 0.47              |
| 1:C:200:THR:OG1  | 1:C:238:HIS:HD2  | 1.96                     | 0.47              |
| 1:H:319:ARG:HG2  | 1:H:368:TRP:CZ3  | 2.49                     | 0.47              |
| 1:A:146:LYS:HD2  | 1:D:105:LEU:HD21 | 1.96                     | 0.47              |
| 1:E:49:PRO:HG2   | 1:E:52:GLU:HB3   | 1.96                     | 0.47              |
| 1:D:134:ARG:HA   | 1:D:308:GLY:O    | 2.14                     | 0.47              |
| 1:C:49:PRO:HG2   | 1:C:52:GLU:HB3   | 1.96                     | 0.47              |
| 1:A:177:LYS:HB2  | 1:B:62:SER:O     | 2.14                     | 0.47              |
| 1:B:49:PRO:HG2   | 1:B:52:GLU:HB3   | 1.96                     | 0.47              |
| 3:C:476:XPB:O2P  | 1:D:65:THR:OG1   | 2.22                     | 0.47              |
| 1:A:250:MET:CE   | 1:A:267:HIS:HE2  | 2.23                     | 0.47              |
| 1:H:250:MET:HE2  | 1:H:267:HIS:CE1  | 2.50                     | 0.47              |
| 1:D:19:ASP:HB2   | 1:D:22:LEU:HG    | 1.97                     | 0.47              |
| 2:N:119:ARG:HG3  | 2:N:119:ARG:HH11 | 1.79                     | 0.47              |
| 1:G:134:ARG:HA   | 1:G:308:GLY:O    | 2.15                     | 0.47              |
| 1:F:295:ARG:HG3  | 1:F:298:HIS:CD2  | 2.49                     | 0.47              |
| 2:M:69:MET:HE3   | 2:M:71:LYS:O     | 2.14                     | 0.47              |
| 1:C:335:LEU:HD21 | 1:D:127:PHE:CD1  | 2.50                     | 0.47              |
| 1:A:318:LEU:HD22 | 1:A:326:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:152:PRO:HB2  | 1:A:153:HIS:CD2  | 2.49                     | 0.47              |
| 1:E:152:PRO:HB2  | 1:E:153:HIS:CD2  | 2.49                     | 0.47              |
| 1:D:152:PRO:HB2  | 1:D:153:HIS:CD2  | 2.49                     | 0.47              |
| 2:K:119:ARG:HH11 | 2:K:119:ARG:HG3  | 1.79                     | 0.47              |
| 2:M:119:ARG:HG3  | 2:M:119:ARG:HH11 | 1.79                     | 0.47              |
| 1:B:318:LEU:HD22 | 1:B:326:LEU:HD13 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:166:GLY:HA2  | 2:K:112:THR:O    | 2.15                     | 0.47              |
| 1:H:19:ASP:HB2   | 1:H:22:LEU:HG    | 1.96                     | 0.47              |
| 1:E:119:SER:OG   | 1:F:205:ASN:HB2  | 2.14                     | 0.47              |
| 1:F:134:ARG:HA   | 1:F:308:GLY:O    | 2.14                     | 0.47              |
| 1:H:49:PRO:HG2   | 1:H:52:GLU:HB3   | 1.96                     | 0.47              |
| 1:G:166:GLY:HA2  | 2:P:112:THR:O    | 2.15                     | 0.47              |
| 1:A:19:ASP:HB2   | 1:A:22:LEU:HG    | 1.96                     | 0.47              |
| 1:C:250:MET:HE1  | 1:C:276:ALA:HB1  | 1.96                     | 0.47              |
| 1:D:229:GLN:HE21 | 1:D:236:LYS:H    | 1.62                     | 0.47              |
| 1:H:229:GLN:HE21 | 1:H:236:LYS:H    | 1.62                     | 0.47              |
| 1:F:318:LEU:HD22 | 1:F:326:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:318:LEU:HD22 | 1:E:326:LEU:HD13 | 1.96                     | 0.47              |
| 1:A:447:GLU:O    | 1:A:450:LYS:HB2  | 2.15                     | 0.47              |
| 1:D:447:GLU:O    | 1:D:450:LYS:HB2  | 2.15                     | 0.47              |
| 1:C:134:ARG:HA   | 1:C:308:GLY:O    | 2.14                     | 0.47              |
| 1:B:152:PRO:HB2  | 1:B:153:HIS:CD2  | 2.49                     | 0.47              |
| 2:L:119:ARG:HH11 | 2:L:119:ARG:HG3  | 1.79                     | 0.47              |
| 1:G:152:PRO:HB2  | 1:G:153:HIS:CD2  | 2.49                     | 0.47              |
| 1:H:152:PRO:HB2  | 1:H:153:HIS:CD2  | 2.49                     | 0.47              |
| 1:E:66:TRP:CD1   | 1:F:381:GLY:HA2  | 2.50                     | 0.47              |
| 1:H:166:GLY:HA2  | 2:L:112:THR:O    | 2.15                     | 0.47              |
| 1:A:49:PRO:HG2   | 1:A:52:GLU:HB3   | 1.96                     | 0.47              |
| 2:I:119:ARG:HH11 | 2:I:119:ARG:HG3  | 1.79                     | 0.47              |
| 1:G:319:ARG:HG2  | 1:G:368:TRP:CZ3  | 2.49                     | 0.47              |
| 1:B:229:GLN:HE21 | 1:B:236:LYS:H    | 1.62                     | 0.47              |
| 1:C:229:GLN:HE21 | 1:C:236:LYS:H    | 1.62                     | 0.47              |
| 1:F:447:GLU:O    | 1:F:450:LYS:HB2  | 2.15                     | 0.47              |
| 1:B:166:GLY:HA2  | 2:I:112:THR:O    | 2.15                     | 0.47              |
| 1:C:19:ASP:HB2   | 1:C:22:LEU:HG    | 1.96                     | 0.47              |
| 1:G:65:THR:OG1   | 3:H:476:XBP:O2P  | 2.14                     | 0.47              |
| 2:K:69:MET:HE3   | 2:K:71:LYS:O     | 2.14                     | 0.47              |
| 1:G:229:GLN:HE21 | 1:G:236:LYS:H    | 1.62                     | 0.47              |
| 1:G:185:TYR:OH   | 1:G:202:ASP:HA   | 2.15                     | 0.47              |
| 1:G:49:PRO:HG2   | 1:G:52:GLU:HB3   | 1.96                     | 0.47              |
| 1:E:447:GLU:O    | 1:E:450:LYS:HB2  | 2.15                     | 0.47              |
| 1:B:447:GLU:O    | 1:B:450:LYS:HB2  | 2.15                     | 0.47              |
| 1:G:19:ASP:HB2   | 1:G:22:LEU:HG    | 1.96                     | 0.47              |
| 1:E:159:ARG:NH2  | 1:E:167:ARG:O    | 2.46                     | 0.47              |
| 1:E:19:ASP:HB2   | 1:E:22:LEU:HG    | 1.97                     | 0.47              |
| 1:A:130:ILE:O    | 1:B:303:ARG:NH2  | 2.44                     | 0.47              |
| 1:A:134:ARG:HA   | 1:A:308:GLY:O    | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:159:ARG:NH2  | 1:H:167:ARG:O    | 2.47                     | 0.46              |
| 1:C:152:PRO:HB2  | 1:C:153:HIS:CD2  | 2.49                     | 0.46              |
| 2:O:119:ARG:HH11 | 2:O:119:ARG:HG3  | 1.79                     | 0.46              |
| 1:F:152:PRO:HB2  | 1:F:153:HIS:CD2  | 2.49                     | 0.46              |
| 1:H:134:ARG:HA   | 1:H:308:GLY:O    | 2.14                     | 0.46              |
| 1:A:127:PHE:HD1  | 1:B:335:LEU:CD2  | 2.28                     | 0.46              |
| 1:G:447:GLU:O    | 1:G:450:LYS:HB2  | 2.15                     | 0.46              |
| 1:B:19:ASP:HB2   | 1:B:22:LEU:HG    | 1.97                     | 0.46              |
| 1:E:207:ASN:HB3  | 1:F:109:GLU:OE1  | 2.15                     | 0.46              |
| 1:C:166:GLY:HA2  | 2:N:112:THR:O    | 2.15                     | 0.46              |
| 2:P:119:ARG:HH11 | 2:P:119:ARG:HG3  | 1.80                     | 0.46              |
| 1:E:166:GLY:HA2  | 2:O:112:THR:O    | 2.15                     | 0.46              |
| 1:E:229:GLN:HE21 | 1:E:236:LYS:H    | 1.62                     | 0.46              |
| 1:E:185:TYR:OH   | 1:E:202:ASP:HA   | 2.16                     | 0.46              |
| 1:A:166:GLY:HA2  | 2:M:112:THR:O    | 2.15                     | 0.46              |
| 2:J:119:ARG:HG3  | 2:J:119:ARG:HH11 | 1.79                     | 0.46              |
| 1:D:318:LEU:HD22 | 1:D:326:LEU:HD13 | 1.96                     | 0.46              |
| 1:H:447:GLU:O    | 1:H:450:LYS:HB2  | 2.15                     | 0.46              |
| 1:F:19:ASP:HB2   | 1:F:22:LEU:HG    | 1.96                     | 0.46              |
| 1:H:318:LEU:HD22 | 1:H:326:LEU:HD13 | 1.96                     | 0.46              |
| 1:D:185:TYR:OH   | 1:D:202:ASP:HA   | 2.16                     | 0.46              |
| 1:F:49:PRO:HG2   | 1:F:52:GLU:HB3   | 1.96                     | 0.46              |
| 1:A:229:GLN:HE21 | 1:A:236:LYS:H    | 1.62                     | 0.46              |
| 1:C:185:TYR:OH   | 1:C:202:ASP:HA   | 2.16                     | 0.46              |
| 1:F:185:TYR:OH   | 1:F:202:ASP:HA   | 2.16                     | 0.46              |
| 1:F:250:MET:HE1  | 1:F:276:ALA:HB1  | 1.97                     | 0.46              |
| 1:C:335:LEU:HD23 | 1:D:127:PHE:CD1  | 2.50                     | 0.46              |
| 1:H:185:TYR:OH   | 1:H:202:ASP:HA   | 2.16                     | 0.46              |
| 1:A:185:TYR:OH   | 1:A:202:ASP:HA   | 2.16                     | 0.46              |
| 1:D:49:PRO:HG2   | 1:D:52:GLU:HB3   | 1.96                     | 0.46              |
| 1:B:185:TYR:OH   | 1:B:202:ASP:HA   | 2.16                     | 0.45              |
| 1:G:383:HIS:HD2  | 1:H:66:TRP:CH2   | 2.34                     | 0.45              |
| 1:C:447:GLU:O    | 1:C:450:LYS:HB2  | 2.15                     | 0.45              |
| 1:C:66:TRP:CD1   | 1:D:381:GLY:HA2  | 2.51                     | 0.45              |
| 1:D:166:GLY:HA2  | 2:J:112:THR:O    | 2.15                     | 0.45              |
| 1:G:62:SER:O     | 1:H:177:LYS:HB2  | 2.16                     | 0.45              |
| 1:E:45:GLN:NE2   | 1:F:470:GLU:O    | 2.48                     | 0.45              |
| 1:C:461:LEU:HD21 | 1:D:15:ALA:HB1   | 1.99                     | 0.45              |
| 1:F:295:ARG:HG3  | 1:F:298:HIS:CG   | 2.52                     | 0.45              |
| 1:E:295:ARG:HG3  | 1:E:298:HIS:CG   | 2.52                     | 0.45              |
| 1:A:295:ARG:HG3  | 1:A:298:HIS:CG   | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:178:LEU:HD13 | 1:H:107:LEU:HD22 | 1.98                     | 0.45              |
| 1:E:383:HIS:HD2  | 1:F:66:TRP:CH2   | 2.35                     | 0.45              |
| 1:A:204:GLU:OE2  | 1:B:123:ASN:ND2  | 2.50                     | 0.45              |
| 1:D:295:ARG:HG3  | 1:D:298:HIS:CG   | 2.52                     | 0.45              |
| 1:B:295:ARG:HG3  | 1:B:298:HIS:CG   | 2.52                     | 0.45              |
| 1:D:293:ILE:HG21 | 1:D:318:LEU:HD13 | 1.99                     | 0.45              |
| 1:F:250:MET:HE2  | 1:F:267:HIS:CD2  | 2.51                     | 0.45              |
| 1:H:293:ILE:HG21 | 1:H:318:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:295:ARG:HG3  | 1:C:298:HIS:CG   | 2.52                     | 0.44              |
| 1:G:295:ARG:HG3  | 1:G:298:HIS:CG   | 2.52                     | 0.44              |
| 1:B:293:ILE:HG21 | 1:B:318:LEU:HD13 | 1.99                     | 0.44              |
| 1:G:293:ILE:HG21 | 1:G:318:LEU:HD13 | 1.99                     | 0.44              |
| 1:H:295:ARG:HG3  | 1:H:298:HIS:CG   | 2.52                     | 0.44              |
| 1:E:250:MET:CE   | 1:E:267:HIS:HE2  | 2.23                     | 0.44              |
| 1:A:293:ILE:HG21 | 1:A:318:LEU:HD13 | 1.99                     | 0.44              |
| 1:F:293:ILE:HG21 | 1:F:318:LEU:HD13 | 1.99                     | 0.44              |
| 1:E:293:ILE:HG21 | 1:E:318:LEU:HD13 | 2.00                     | 0.44              |
| 1:A:105:LEU:HD21 | 1:D:146:LYS:HD2  | 1.99                     | 0.44              |
| 1:A:250:MET:HE3  | 1:A:276:ALA:HB1  | 2.00                     | 0.44              |
| 1:G:66:TRP:CG    | 1:H:381:GLY:HA2  | 2.52                     | 0.44              |
| 1:C:127:PHE:CD1  | 1:D:335:LEU:HD23 | 2.52                     | 0.44              |
| 1:C:293:ILE:HG21 | 1:C:318:LEU:HD13 | 1.99                     | 0.44              |
| 1:G:250:MET:HE2  | 1:G:267:HIS:CE1  | 2.52                     | 0.44              |
| 1:G:381:GLY:HA2  | 1:H:66:TRP:CG    | 2.52                     | 0.44              |
| 1:E:239:TYR:HE2  | 1:E:401:GLN:HE22 | 1.66                     | 0.44              |
| 1:H:383:HIS:CE1  | 1:H:385:TRP:HB2  | 2.53                     | 0.44              |
| 1:A:130:ILE:HD13 | 1:A:130:ILE:HA   | 1.86                     | 0.44              |
| 1:C:253:ARG:NH2  | 1:D:109:GLU:OE2  | 2.35                     | 0.44              |
| 1:H:130:ILE:HD13 | 1:H:130:ILE:HA   | 1.86                     | 0.44              |
| 1:G:207:ASN:HB3  | 1:H:109:GLU:OE1  | 2.18                     | 0.44              |
| 1:G:383:HIS:CE1  | 1:G:385:TRP:HB2  | 2.53                     | 0.44              |
| 1:C:152:PRO:O    | 1:C:285:ARG:HD3  | 2.18                     | 0.44              |
| 1:A:159:ARG:NH2  | 1:A:167:ARG:O    | 2.47                     | 0.44              |
| 1:C:239:TYR:HE2  | 1:C:401:GLN:HE22 | 1.66                     | 0.44              |
| 2:O:14:THR:O     | 2:O:15:PHE:HB2   | 2.18                     | 0.44              |
| 1:D:383:HIS:CE1  | 1:D:385:TRP:HB2  | 2.53                     | 0.44              |
| 1:C:383:HIS:CE1  | 1:C:385:TRP:HB2  | 2.53                     | 0.44              |
| 1:B:383:HIS:CE1  | 1:B:385:TRP:HB2  | 2.53                     | 0.44              |
| 1:F:383:HIS:CE1  | 1:F:385:TRP:HB2  | 2.53                     | 0.44              |
| 1:D:152:PRO:O    | 1:D:285:ARG:HD3  | 2.18                     | 0.44              |
| 1:G:152:PRO:O    | 1:G:285:ARG:HD3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:195:GLY:HA3  | 1:A:417:ALA:HB3  | 2.00                     | 0.44              |
| 1:F:195:GLY:HA3  | 1:F:417:ALA:HB3  | 2.00                     | 0.44              |
| 1:F:152:PRO:O    | 1:F:285:ARG:HD3  | 2.18                     | 0.43              |
| 1:B:159:ARG:NH2  | 1:B:167:ARG:O    | 2.47                     | 0.43              |
| 1:E:178:LEU:CD1  | 1:F:107:LEU:HD22 | 2.48                     | 0.43              |
| 1:A:131:ARG:O    | 1:B:472:MET:HG3  | 2.18                     | 0.43              |
| 1:C:293:ILE:HG21 | 1:C:318:LEU:CD1  | 2.49                     | 0.43              |
| 1:B:152:PRO:O    | 1:B:285:ARG:HD3  | 2.18                     | 0.43              |
| 1:E:470:GLU:O    | 1:F:45:GLN:NE2   | 2.50                     | 0.43              |
| 1:C:130:ILE:HD13 | 1:C:130:ILE:HA   | 1.86                     | 0.43              |
| 1:D:159:ARG:NH2  | 1:D:167:ARG:O    | 2.47                     | 0.43              |
| 1:A:383:HIS:CE1  | 1:A:385:TRP:HB2  | 2.53                     | 0.43              |
| 1:B:293:ILE:HG21 | 1:B:318:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:293:ILE:HG21 | 1:A:318:LEU:CD1  | 2.49                     | 0.43              |
| 1:G:293:ILE:HG21 | 1:G:318:LEU:CD1  | 2.48                     | 0.43              |
| 2:P:33:MET:HE1   | 2:P:101:VAL:HG12 | 1.99                     | 0.43              |
| 1:A:62:SER:O     | 1:B:177:LYS:HB2  | 2.18                     | 0.43              |
| 1:E:63:THR:HA    | 1:F:177:LYS:HB2  | 1.99                     | 0.43              |
| 2:M:14:THR:O     | 2:M:15:PHE:HB2   | 2.19                     | 0.43              |
| 2:N:14:THR:O     | 2:N:15:PHE:HB2   | 2.19                     | 0.43              |
| 1:D:195:GLY:HA3  | 1:D:417:ALA:HB3  | 2.00                     | 0.43              |
| 2:O:11:ARG:HG3   | 2:O:17:TYR:CE1   | 2.54                     | 0.43              |
| 2:P:14:THR:O     | 2:P:15:PHE:HB2   | 2.19                     | 0.43              |
| 2:J:14:THR:O     | 2:J:15:PHE:HB2   | 2.19                     | 0.43              |
| 1:G:114:THR:HG23 | 1:H:271:THR:C    | 2.39                     | 0.43              |
| 1:H:152:PRO:O    | 1:H:285:ARG:HD3  | 2.18                     | 0.43              |
| 1:C:239:TYR:HB3  | 1:C:266:MET:HB2  | 2.01                     | 0.43              |
| 2:L:14:THR:O     | 2:L:15:PHE:HB2   | 2.19                     | 0.43              |
| 2:K:14:THR:O     | 2:K:15:PHE:HB2   | 2.19                     | 0.43              |
| 2:J:11:ARG:HG3   | 2:J:17:TYR:CE1   | 2.54                     | 0.43              |
| 2:O:6:LEU:HA     | 2:O:7:PRO:HD3    | 1.92                     | 0.43              |
| 1:E:279:THR:HG1  | 1:F:247:CYS:H    | 1.67                     | 0.43              |
| 1:C:195:GLY:HA3  | 1:C:417:ALA:HB3  | 2.00                     | 0.43              |
| 1:B:239:TYR:HB3  | 1:B:266:MET:HB2  | 2.01                     | 0.43              |
| 2:I:19:PRO:HA    | 2:I:20:PRO:HD3   | 1.90                     | 0.43              |
| 1:E:195:GLY:HA3  | 1:E:417:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:66:TRP:CD1   | 1:B:381:GLY:HA2  | 2.54                     | 0.43              |
| 1:E:128:LYS:HD2  | 1:F:333:GLY:O    | 2.18                     | 0.43              |
| 1:D:293:ILE:HG21 | 1:D:318:LEU:CD1  | 2.49                     | 0.43              |
| 1:E:239:TYR:HB3  | 1:E:266:MET:HB2  | 2.01                     | 0.43              |
| 2:M:19:PRO:HA    | 2:M:20:PRO:HD3   | 1.90                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:11:ARG:HG3   | 2:N:17:TYR:CE1   | 2.54                     | 0.43              |
| 2:I:11:ARG:HG3   | 2:I:17:TYR:CE1   | 2.54                     | 0.43              |
| 2:P:19:PRO:HA    | 2:P:20:PRO:HD3   | 1.91                     | 0.43              |
| 1:G:195:GLY:HA3  | 1:G:417:ALA:HB3  | 2.00                     | 0.43              |
| 1:E:383:HIS:CE1  | 1:E:385:TRP:HB2  | 2.54                     | 0.43              |
| 1:F:293:ILE:HG21 | 1:F:318:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:152:PRO:O    | 1:A:285:ARG:HD3  | 2.18                     | 0.43              |
| 1:A:207:ASN:HB3  | 1:B:109:GLU:OE1  | 2.18                     | 0.43              |
| 1:E:152:PRO:O    | 1:E:285:ARG:HD3  | 2.18                     | 0.43              |
| 2:J:33:MET:HE1   | 2:J:101:VAL:HG12 | 2.01                     | 0.43              |
| 1:B:195:GLY:HA3  | 1:B:417:ALA:HB3  | 2.00                     | 0.43              |
| 1:H:293:ILE:HG21 | 1:H:318:LEU:CD1  | 2.49                     | 0.42              |
| 1:D:204:GLU:OE1  | 1:D:294:HIS:CE1  | 2.72                     | 0.42              |
| 1:H:239:TYR:HE2  | 1:H:401:GLN:HE22 | 1.66                     | 0.42              |
| 2:I:14:THR:O     | 2:I:15:PHE:HB2   | 2.19                     | 0.42              |
| 1:D:171:GLY:HA2  | 1:D:199:PHE:O    | 2.19                     | 0.42              |
| 1:A:383:HIS:HD2  | 1:B:66:TRP:CH2   | 2.37                     | 0.42              |
| 1:B:204:GLU:OE1  | 1:B:294:HIS:CE1  | 2.72                     | 0.42              |
| 1:B:239:TYR:HE2  | 1:B:401:GLN:HE22 | 1.66                     | 0.42              |
| 2:L:11:ARG:HG3   | 2:L:17:TYR:CE1   | 2.54                     | 0.42              |
| 1:C:190:TYR:CZ   | 1:C:227:LYS:HE3  | 2.55                     | 0.42              |
| 1:E:107:LEU:HD22 | 1:F:178:LEU:CD1  | 2.50                     | 0.42              |
| 1:F:239:TYR:HE2  | 1:F:401:GLN:HE22 | 1.66                     | 0.42              |
| 1:E:171:GLY:HA2  | 1:E:199:PHE:O    | 2.19                     | 0.42              |
| 1:G:239:TYR:HE2  | 1:G:401:GLN:HE22 | 1.66                     | 0.42              |
| 1:F:204:GLU:OE1  | 1:F:294:HIS:CE1  | 2.72                     | 0.42              |
| 1:E:293:ILE:HG21 | 1:E:318:LEU:CD1  | 2.49                     | 0.42              |
| 1:H:195:GLY:HA3  | 1:H:417:ALA:HB3  | 2.00                     | 0.42              |
| 2:M:11:ARG:HG3   | 2:M:17:TYR:CE1   | 2.54                     | 0.42              |
| 1:A:171:GLY:HA2  | 1:A:199:PHE:O    | 2.19                     | 0.42              |
| 1:E:190:TYR:CZ   | 1:E:227:LYS:HE3  | 2.54                     | 0.42              |
| 2:P:11:ARG:HG3   | 2:P:17:TYR:CE1   | 2.54                     | 0.42              |
| 2:O:33:MET:HE1   | 2:O:101:VAL:HG12 | 2.01                     | 0.42              |
| 1:H:204:GLU:OE1  | 1:H:294:HIS:CE1  | 2.72                     | 0.42              |
| 2:O:95:GLY:O     | 2:O:118:HIS:HE1  | 2.03                     | 0.42              |
| 1:C:177:LYS:HB2  | 1:D:62:SER:O     | 2.20                     | 0.42              |
| 1:A:24:TYR:CE1   | 1:A:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:D:24:TYR:CE1   | 1:D:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:D:190:TYR:CZ   | 1:D:227:LYS:HE3  | 2.55                     | 0.42              |
| 1:B:24:TYR:CE1   | 1:B:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:G:190:TYR:CZ   | 1:G:227:LYS:HE3  | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:133:LEU:O    | 1:B:307:HIS:HA   | 2.20                     | 0.42              |
| 1:C:250:MET:HE2  | 1:C:267:HIS:CD2  | 2.53                     | 0.42              |
| 1:G:204:GLU:OE1  | 1:G:294:HIS:CE1  | 2.72                     | 0.42              |
| 1:H:239:TYR:HB3  | 1:H:266:MET:HB2  | 2.01                     | 0.42              |
| 1:B:136:GLU:OE1  | 1:B:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:C:136:GLU:OE1  | 1:C:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:D:136:GLU:OE1  | 1:D:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:H:24:TYR:CE1   | 1:H:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:H:190:TYR:CZ   | 1:H:227:LYS:HE3  | 2.55                     | 0.42              |
| 2:I:95:GLY:O     | 2:I:118:HIS:HE1  | 2.03                     | 0.42              |
| 1:G:71:THR:HG21  | 1:H:407:LEU:HD23 | 2.00                     | 0.42              |
| 1:C:133:LEU:O    | 1:C:307:HIS:HA   | 2.20                     | 0.42              |
| 1:E:204:GLU:OE1  | 1:E:294:HIS:CE1  | 2.73                     | 0.42              |
| 1:G:171:GLY:HA2  | 1:G:199:PHE:O    | 2.20                     | 0.42              |
| 2:K:11:ARG:HG3   | 2:K:17:TYR:CE1   | 2.54                     | 0.42              |
| 2:N:95:GLY:O     | 2:N:118:HIS:HE1  | 2.03                     | 0.42              |
| 1:E:136:GLU:OE1  | 1:E:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:G:136:GLU:OE1  | 1:G:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:A:239:TYR:HE2  | 1:A:401:GLN:HE22 | 1.66                     | 0.42              |
| 1:A:136:GLU:OE1  | 1:A:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:H:250:MET:HE1  | 1:H:276:ALA:HB1  | 2.02                     | 0.42              |
| 2:P:69:MET:HE3   | 2:P:71:LYS:O     | 2.19                     | 0.42              |
| 1:E:130:ILE:HA   | 1:E:130:ILE:HD13 | 1.87                     | 0.42              |
| 1:C:204:GLU:OE1  | 1:C:294:HIS:CE1  | 2.72                     | 0.42              |
| 1:A:470:GLU:O    | 1:B:45:GLN:NE2   | 2.53                     | 0.42              |
| 1:G:24:TYR:CE1   | 1:G:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:B:250:MET:HE1  | 1:B:267:HIS:CE1  | 2.55                     | 0.42              |
| 1:E:410:PRO:HD3  | 1:E:461:LEU:HD22 | 2.02                     | 0.42              |
| 1:A:204:GLU:OE1  | 1:A:294:HIS:CE1  | 2.72                     | 0.42              |
| 2:L:19:PRO:HA    | 2:L:20:PRO:HD3   | 1.90                     | 0.42              |
| 1:C:24:TYR:CE1   | 1:C:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:F:171:GLY:HA2  | 1:F:199:PHE:O    | 2.20                     | 0.42              |
| 1:D:239:TYR:HB3  | 1:D:266:MET:HB2  | 2.01                     | 0.42              |
| 1:F:24:TYR:CE1   | 1:F:81:LYS:HB2   | 2.55                     | 0.42              |
| 1:E:178:LEU:HD12 | 1:F:107:LEU:HD22 | 2.01                     | 0.42              |
| 1:G:197:LEU:HG   | 1:G:417:ALA:HB1  | 2.02                     | 0.42              |
| 1:H:136:GLU:OE1  | 1:H:312:ARG:NH2  | 2.53                     | 0.42              |
| 1:H:133:LEU:O    | 1:H:307:HIS:HA   | 2.20                     | 0.42              |
| 1:B:190:TYR:CZ   | 1:B:227:LYS:HE3  | 2.55                     | 0.42              |
| 1:B:171:GLY:HA2  | 1:B:199:PHE:O    | 2.19                     | 0.42              |
| 1:E:133:LEU:O    | 1:E:307:HIS:HA   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:136:GLU:OE1  | 1:F:312:ARG:NH2  | 2.53                     | 0.42              |
| 2:M:104:PHE:HZ   | 1:C:184:ASN:HD21 | 1.64                     | 0.42              |
| 1:A:190:TYR:CZ   | 1:A:227:LYS:HE3  | 2.55                     | 0.42              |
| 1:C:247:CYS:H    | 1:D:279:THR:HG1  | 1.67                     | 0.42              |
| 1:F:197:LEU:HG   | 1:F:417:ALA:HB1  | 2.02                     | 0.42              |
| 1:F:239:TYR:HB3  | 1:F:266:MET:HB2  | 2.01                     | 0.42              |
| 2:P:6:LEU:HA     | 2:P:7:PRO:HD3    | 1.92                     | 0.42              |
| 2:J:6:LEU:HA     | 2:J:7:PRO:HD3    | 1.92                     | 0.42              |
| 1:B:353:HIS:HD2  | 1:B:367:ASP:OD1  | 2.03                     | 0.42              |
| 1:G:461:LEU:CD2  | 1:H:15:ALA:HB1   | 2.49                     | 0.41              |
| 1:A:239:TYR:HB3  | 1:A:266:MET:HB2  | 2.01                     | 0.41              |
| 2:J:95:GLY:O     | 2:J:118:HIS:HE1  | 2.03                     | 0.41              |
| 1:E:146:LYS:HD2  | 1:H:105:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:133:LEU:O    | 1:A:307:HIS:HA   | 2.20                     | 0.41              |
| 1:G:239:TYR:HB3  | 1:G:266:MET:HB2  | 2.01                     | 0.41              |
| 1:D:239:TYR:HE2  | 1:D:401:GLN:HE22 | 1.66                     | 0.41              |
| 1:F:159:ARG:NH2  | 1:F:167:ARG:O    | 2.47                     | 0.41              |
| 1:E:353:HIS:HD2  | 1:E:367:ASP:OD1  | 2.03                     | 0.41              |
| 2:K:95:GLY:O     | 2:K:118:HIS:HE1  | 2.03                     | 0.41              |
| 2:M:45:ASN:HB2   | 2:M:67:TRP:CD2   | 2.55                     | 0.41              |
| 2:L:95:GLY:O     | 2:L:118:HIS:HE1  | 2.03                     | 0.41              |
| 1:F:133:LEU:O    | 1:F:307:HIS:HA   | 2.20                     | 0.41              |
| 2:I:13:GLU:HB3   | 2:I:14:THR:H     | 1.73                     | 0.41              |
| 2:J:45:ASN:HB2   | 2:J:67:TRP:CD2   | 2.56                     | 0.41              |
| 1:H:171:GLY:HA2  | 1:H:199:PHE:O    | 2.19                     | 0.41              |
| 1:H:353:HIS:HD2  | 1:H:367:ASP:OD1  | 2.03                     | 0.41              |
| 1:C:353:HIS:HD2  | 1:C:367:ASP:OD1  | 2.03                     | 0.41              |
| 1:A:226:HIS:HE1  | 4:A:487:HOH:O    | 2.03                     | 0.41              |
| 1:C:62:SER:O     | 1:D:177:LYS:HB2  | 2.21                     | 0.41              |
| 1:A:410:PRO:HD3  | 1:A:461:LEU:HD22 | 2.02                     | 0.41              |
| 1:E:278:THR:HG22 | 1:F:246:THR:HG22 | 2.02                     | 0.41              |
| 1:F:190:TYR:CZ   | 1:F:227:LYS:HE3  | 2.55                     | 0.41              |
| 1:D:133:LEU:O    | 1:D:307:HIS:HA   | 2.20                     | 0.41              |
| 2:O:10:ARG:O     | 2:O:11:ARG:HD2   | 2.21                     | 0.41              |
| 1:B:410:PRO:HD3  | 1:B:461:LEU:HD22 | 2.02                     | 0.41              |
| 1:C:171:GLY:HA2  | 1:C:199:PHE:O    | 2.19                     | 0.41              |
| 2:M:95:GLY:O     | 2:M:118:HIS:HE1  | 2.03                     | 0.41              |
| 1:G:133:LEU:O    | 1:G:307:HIS:HA   | 2.20                     | 0.41              |
| 1:D:410:PRO:HD3  | 1:D:461:LEU:HD22 | 2.02                     | 0.41              |
| 1:H:410:PRO:HD3  | 1:H:461:LEU:HD22 | 2.02                     | 0.41              |
| 1:G:127:PHE:CE1  | 1:H:335:LEU:HD21 | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:197:LEU:HG   | 1:E:417:ALA:HB1  | 2.03                     | 0.41              |
| 2:M:118:HIS:HD2  | 4:M:155:HOH:O    | 2.02                     | 0.41              |
| 2:I:45:ASN:HB2   | 2:I:67:TRP:CD2   | 2.56                     | 0.41              |
| 1:F:353:HIS:HD2  | 1:F:367:ASP:OD1  | 2.03                     | 0.41              |
| 1:G:159:ARG:NH2  | 1:G:167:ARG:O    | 2.47                     | 0.41              |
| 2:L:45:ASN:HB2   | 2:L:67:TRP:CD2   | 2.55                     | 0.41              |
| 2:M:33:MET:HE1   | 2:M:101:VAL:HG12 | 2.03                     | 0.41              |
| 1:C:410:PRO:HD3  | 1:C:461:LEU:HD22 | 2.02                     | 0.41              |
| 2:K:45:ASN:HB2   | 2:K:67:TRP:CD2   | 2.56                     | 0.41              |
| 1:E:24:TYR:CE1   | 1:E:81:LYS:HB2   | 2.55                     | 0.41              |
| 1:F:130:ILE:HD13 | 1:F:130:ILE:HA   | 1.86                     | 0.41              |
| 1:G:247:CYS:H    | 1:H:279:THR:HG1  | 1.69                     | 0.41              |
| 1:D:197:LEU:HG   | 1:D:417:ALA:HB1  | 2.02                     | 0.41              |
| 2:P:95:GLY:O     | 2:P:118:HIS:HE1  | 2.03                     | 0.41              |
| 1:E:15:ALA:HB1   | 1:F:461:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:353:HIS:HD2  | 1:A:367:ASP:OD1  | 2.03                     | 0.41              |
| 1:C:371:MET:HA   | 1:C:372:PRO:HD3  | 1.97                     | 0.41              |
| 1:B:250:MET:HE2  | 1:B:267:HIS:CE1  | 2.53                     | 0.41              |
| 1:G:214:TRP:CD2  | 1:G:253:ARG:HG2  | 2.56                     | 0.41              |
| 1:C:130:ILE:O    | 1:D:303:ARG:NH2  | 2.54                     | 0.41              |
| 1:H:197:LEU:HG   | 1:H:417:ALA:HB1  | 2.02                     | 0.41              |
| 2:I:104:PHE:HZ   | 1:H:184:ASN:HD21 | 1.63                     | 0.41              |
| 1:C:159:ARG:NH2  | 1:C:167:ARG:O    | 2.47                     | 0.41              |
| 2:M:6:LEU:HA     | 2:M:7:PRO:HD3    | 1.92                     | 0.41              |
| 1:E:121:VAL:O    | 1:F:297:MET:HA   | 2.21                     | 0.40              |
| 1:A:197:LEU:HG   | 1:A:417:ALA:HB1  | 2.02                     | 0.40              |
| 2:J:10:ARG:O     | 2:J:11:ARG:HD2   | 2.21                     | 0.40              |
| 2:L:10:ARG:O     | 2:L:11:ARG:HD2   | 2.21                     | 0.40              |
| 1:G:71:THR:CG2   | 1:H:407:LEU:HD23 | 2.51                     | 0.40              |
| 1:F:410:PRO:HD3  | 1:F:461:LEU:HD22 | 2.02                     | 0.40              |
| 1:G:353:HIS:HD2  | 1:G:367:ASP:OD1  | 2.04                     | 0.40              |
| 2:N:45:ASN:HB2   | 2:N:67:TRP:CD2   | 2.55                     | 0.40              |
| 2:N:6:LEU:HA     | 2:N:7:PRO:HD3    | 1.92                     | 0.40              |
| 1:C:105:LEU:HD21 | 1:F:146:LYS:HD2  | 2.03                     | 0.40              |
| 1:C:279:THR:HG1  | 1:D:247:CYS:H    | 1.69                     | 0.40              |
| 2:O:13:GLU:HB3   | 2:O:14:THR:H     | 1.73                     | 0.40              |
| 2:I:10:ARG:O     | 2:I:11:ARG:HD2   | 2.21                     | 0.40              |
| 2:P:10:ARG:O     | 2:P:11:ARG:HD2   | 2.21                     | 0.40              |
| 2:L:6:LEU:HA     | 2:L:7:PRO:HD3    | 1.92                     | 0.40              |
| 1:C:146:LYS:HD2  | 1:F:105:LEU:HD21 | 2.03                     | 0.40              |
| 1:B:377:VAL:HG22 | 1:B:399:VAL:HB   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:45:ASN:HB2   | 2:O:67:TRP:CD2   | 2.55                     | 0.40              |
| 2:P:45:ASN:HB2   | 2:P:67:TRP:CD2   | 2.56                     | 0.40              |
| 2:O:11:ARG:HH21  | 2:O:17:TYR:HA    | 1.87                     | 0.40              |
| 2:J:11:ARG:HH21  | 2:J:17:TYR:HA    | 1.87                     | 0.40              |
| 2:N:11:ARG:HH21  | 2:N:17:TYR:HA    | 1.87                     | 0.40              |
| 2:P:11:ARG:HH21  | 2:P:17:TYR:HA    | 1.87                     | 0.40              |
| 1:C:377:VAL:HG22 | 1:C:399:VAL:HB   | 2.03                     | 0.40              |
| 1:D:353:HIS:HD2  | 1:D:367:ASP:OD1  | 2.03                     | 0.40              |
| 1:E:68:THR:O     | 1:F:408:GLY:HA2  | 2.21                     | 0.40              |
| 1:H:214:TRP:CD2  | 1:H:253:ARG:HG2  | 2.57                     | 0.40              |
| 1:E:109:GLU:OE1  | 1:F:207:ASN:HB3  | 2.21                     | 0.40              |
| 1:C:197:LEU:HG   | 1:C:417:ALA:HB1  | 2.02                     | 0.40              |
| 2:K:11:ARG:HG3   | 2:K:17:TYR:CZ    | 2.57                     | 0.40              |
| 1:C:303:ARG:NH2  | 1:D:130:ILE:O    | 2.54                     | 0.40              |
| 1:E:44:PRO:HA    | 1:E:130:ILE:HD13 | 2.03                     | 0.40              |
| 1:B:130:ILE:HD13 | 1:B:130:ILE:HA   | 1.86                     | 0.40              |
| 1:F:214:TRP:CD2  | 1:F:253:ARG:HG2  | 2.57                     | 0.40              |
| 1:C:207:ASN:HB3  | 1:D:109:GLU:OE1  | 2.22                     | 0.40              |
| 1:C:214:TRP:CD2  | 1:C:253:ARG:HG2  | 2.57                     | 0.40              |
| 2:M:10:ARG:O     | 2:M:11:ARG:HD2   | 2.21                     | 0.40              |
| 1:F:377:VAL:HG22 | 1:F:399:VAL:HB   | 2.03                     | 0.40              |
| 1:A:109:GLU:OE2  | 1:B:253:ARG:NH2  | 2.35                     | 0.40              |
| 1:B:214:TRP:CD2  | 1:B:253:ARG:HG2  | 2.57                     | 0.40              |

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 2:O:24:ARG:CZ  | 2:K:21:LEU:C[2_554]   | 0.17                     | 2.03              |
| 2:O:81:GLN:NE2 | 2:K:24:ARG:NH1[2_554] | 0.59                     | 1.61              |
| 2:O:81:GLN:CG  | 2:K:24:ARG:NH2[2_554] | 0.80                     | 1.40              |
| 2:O:81:GLN:NE2 | 2:K:24:ARG:CZ[2_554]  | 1.03                     | 1.17              |
| 2:O:24:ARG:NH1 | 2:K:21:LEU:CA[2_554]  | 1.05                     | 1.15              |
| 2:O:81:GLN:CD  | 2:K:24:ARG:CZ[2_554]  | 1.17                     | 1.03              |
| 2:O:24:ARG:NH2 | 2:K:21:LEU:C[2_554]   | 1.20                     | 1.00              |
| 2:O:24:ARG:CZ  | 2:K:22:SER:N[2_554]   | 1.20                     | 1.00              |
| 2:O:24:ARG:CZ  | 2:K:21:LEU:O[2_554]   | 1.33                     | 0.87              |
| 2:O:24:ARG:NE  | 2:K:21:LEU:O[2_554]   | 1.35                     | 0.85              |
| 2:O:24:ARG:NH1 | 2:K:21:LEU:C[2_554]   | 1.40                     | 0.80              |
| 2:O:24:ARG:NE  | 2:K:21:LEU:C[2_554]   | 1.41                     | 0.79              |

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| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 2:O:81:GLN:CD  | 2:K:24:ARG:NH2[2_554] | 1.42                     | 0.78              |
| 2:O:24:ARG:NH2 | 2:K:21:LEU:O[2_554]   | 1.51                     | 0.69              |
| 2:O:24:ARG:CZ  | 2:K:21:LEU:CA[2_554]  | 1.56                     | 0.64              |
| 2:O:24:ARG:NE  | 2:K:22:SER:N[2_554]   | 1.67                     | 0.53              |
| 2:O:24:ARG:NH1 | 2:K:22:SER:N[2_554]   | 1.73                     | 0.47              |
| 2:O:81:GLN:CD  | 2:K:24:ARG:NH1[2_554] | 1.73                     | 0.47              |
| 2:O:81:GLN:NE2 | 2:K:24:ARG:NE[2_554]  | 1.89                     | 0.31              |
| 2:O:81:GLN:CG  | 2:K:24:ARG:CZ[2_554]  | 1.89                     | 0.31              |
| 2:O:24:ARG:NH2 | 2:K:22:SER:N[2_554]   | 1.97                     | 0.23              |
| 2:O:24:ARG:NH1 | 2:K:21:LEU:N[2_554]   | 1.99                     | 0.21              |
| 2:O:24:ARG:NH2 | 2:K:21:LEU:CA[2_554]  | 2.03                     | 0.17              |
| 2:O:81:GLN:CB  | 2:K:24:ARG:NH2[2_554] | 2.06                     | 0.14              |
| 2:O:24:ARG:NH2 | 2:K:22:SER:O[2_554]   | 2.07                     | 0.13              |
| 2:O:81:GLN:CD  | 2:K:24:ARG:NE[2_554]  | 2.09                     | 0.11              |
| 2:M:24:ARG:NH1 | 1:C:433:GLU:O[3_654]  | 2.11                     | 0.09              |
| 2:O:81:GLN:NE2 | 2:K:24:ARG:NH2[2_554] | 2.13                     | 0.07              |
| 2:O:24:ARG:NE  | 2:K:22:SER:CA[2_554]  | 2.14                     | 0.06              |
| 2:I:28:ALA:CB  | 2:J:24:ARG:CZ[3_655]  | 2.15                     | 0.05              |
| 2:O:24:ARG:NH2 | 2:K:21:LEU:CB[2_554]  | 2.18                     | 0.02              |
| 2:O:81:GLN:OE1 | 2:K:24:ARG:CZ[2_554]  | 2.19                     | 0.01              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 465/472 (98%) | 451 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | B     | 465/472 (98%) | 451 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | C     | 465/472 (98%) | 451 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | D     | 465/472 (98%) | 451 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | E     | 465/472 (98%) | 451 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | F     | 465/472 (98%) | 451 (97%) | 14 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | G     | 465/472 (98%)   | 451 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 1   | H     | 465/472 (98%)   | 451 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 2   | I     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | J     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | K     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | L     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | M     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | N     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | O     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| 2   | P     | 107/111 (96%)   | 98 (92%)   | 9 (8%)   | 0        | 100         | 100 |
| All | All   | 4576/4664 (98%) | 4392 (96%) | 184 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 377/383 (98%) | 357 (95%) | 20 (5%)  | 28          | 37 |
| 1   | B     | 377/383 (98%) | 357 (95%) | 20 (5%)  | 28          | 37 |
| 1   | C     | 377/383 (98%) | 357 (95%) | 20 (5%)  | 28          | 37 |
| 1   | D     | 377/383 (98%) | 357 (95%) | 20 (5%)  | 28          | 37 |
| 1   | E     | 377/383 (98%) | 356 (94%) | 21 (6%)  | 26          | 35 |
| 1   | F     | 377/383 (98%) | 357 (95%) | 20 (5%)  | 28          | 37 |
| 1   | G     | 377/383 (98%) | 357 (95%) | 20 (5%)  | 28          | 37 |
| 1   | H     | 377/383 (98%) | 356 (94%) | 21 (6%)  | 26          | 35 |
| 2   | I     | 99/104 (95%)  | 98 (99%)  | 1 (1%)   | 82          | 91 |
| 2   | J     | 99/104 (95%)  | 98 (99%)  | 1 (1%)   | 82          | 91 |
| 2   | K     | 99/104 (95%)  | 98 (99%)  | 1 (1%)   | 82          | 91 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | L     | 99/104 (95%)    | 98 (99%)   | 1 (1%)   | 82          | 91 |
| 2   | M     | 99/104 (95%)    | 98 (99%)   | 1 (1%)   | 82          | 91 |
| 2   | N     | 99/104 (95%)    | 98 (99%)   | 1 (1%)   | 82          | 91 |
| 2   | O     | 99/104 (95%)    | 98 (99%)   | 1 (1%)   | 82          | 91 |
| 2   | P     | 99/104 (95%)    | 98 (99%)   | 1 (1%)   | 82          | 91 |
| All | All   | 3808/3896 (98%) | 3638 (96%) | 170 (4%) | 34          | 46 |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | LYS  |
| 1   | A     | 67  | THR  |
| 1   | A     | 79  | ARG  |
| 1   | A     | 96  | SER  |
| 1   | A     | 127 | PHE  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 170 | LEU  |
| 1   | A     | 213 | ARG  |
| 1   | A     | 215 | ARG  |
| 1   | A     | 239 | TYR  |
| 1   | A     | 241 | ASN  |
| 1   | A     | 255 | GLU  |
| 1   | A     | 258 | LYS  |
| 1   | A     | 285 | ARG  |
| 1   | A     | 295 | ARG  |
| 1   | A     | 360 | ARG  |
| 1   | A     | 375 | LEU  |
| 1   | A     | 401 | GLN  |
| 1   | A     | 468 | GLU  |
| 1   | A     | 471 | THR  |
| 2   | M     | 106 | ASN  |
| 1   | B     | 14  | LYS  |
| 1   | B     | 67  | THR  |
| 1   | B     | 79  | ARG  |
| 1   | B     | 96  | SER  |
| 1   | B     | 127 | PHE  |
| 1   | B     | 134 | ARG  |
| 1   | B     | 170 | LEU  |
| 1   | B     | 213 | ARG  |
| 1   | B     | 215 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 239 | TYR  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 255 | GLU  |
| 1   | B     | 258 | LYS  |
| 1   | B     | 285 | ARG  |
| 1   | B     | 295 | ARG  |
| 1   | B     | 360 | ARG  |
| 1   | B     | 375 | LEU  |
| 1   | B     | 401 | GLN  |
| 1   | B     | 468 | GLU  |
| 1   | B     | 471 | THR  |
| 2   | I     | 106 | ASN  |
| 1   | C     | 14  | LYS  |
| 1   | C     | 67  | THR  |
| 1   | C     | 79  | ARG  |
| 1   | C     | 96  | SER  |
| 1   | C     | 127 | PHE  |
| 1   | C     | 134 | ARG  |
| 1   | C     | 170 | LEU  |
| 1   | C     | 213 | ARG  |
| 1   | C     | 215 | ARG  |
| 1   | C     | 239 | TYR  |
| 1   | C     | 241 | ASN  |
| 1   | C     | 255 | GLU  |
| 1   | C     | 258 | LYS  |
| 1   | C     | 285 | ARG  |
| 1   | C     | 295 | ARG  |
| 1   | C     | 360 | ARG  |
| 1   | C     | 375 | LEU  |
| 1   | C     | 401 | GLN  |
| 1   | C     | 468 | GLU  |
| 1   | C     | 471 | THR  |
| 2   | N     | 106 | ASN  |
| 1   | D     | 14  | LYS  |
| 1   | D     | 67  | THR  |
| 1   | D     | 79  | ARG  |
| 1   | D     | 96  | SER  |
| 1   | D     | 127 | PHE  |
| 1   | D     | 134 | ARG  |
| 1   | D     | 170 | LEU  |
| 1   | D     | 213 | ARG  |
| 1   | D     | 215 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 239 | TYR  |
| 1   | D     | 241 | ASN  |
| 1   | D     | 255 | GLU  |
| 1   | D     | 258 | LYS  |
| 1   | D     | 285 | ARG  |
| 1   | D     | 295 | ARG  |
| 1   | D     | 360 | ARG  |
| 1   | D     | 375 | LEU  |
| 1   | D     | 401 | GLN  |
| 1   | D     | 468 | GLU  |
| 1   | D     | 471 | THR  |
| 2   | J     | 106 | ASN  |
| 1   | E     | 14  | LYS  |
| 1   | E     | 67  | THR  |
| 1   | E     | 79  | ARG  |
| 1   | E     | 96  | SER  |
| 1   | E     | 127 | PHE  |
| 1   | E     | 134 | ARG  |
| 1   | E     | 170 | LEU  |
| 1   | E     | 213 | ARG  |
| 1   | E     | 215 | ARG  |
| 1   | E     | 239 | TYR  |
| 1   | E     | 241 | ASN  |
| 1   | E     | 255 | GLU  |
| 1   | E     | 258 | LYS  |
| 1   | E     | 285 | ARG  |
| 1   | E     | 295 | ARG  |
| 1   | E     | 319 | ARG  |
| 1   | E     | 360 | ARG  |
| 1   | E     | 375 | LEU  |
| 1   | E     | 401 | GLN  |
| 1   | E     | 468 | GLU  |
| 1   | E     | 471 | THR  |
| 2   | O     | 106 | ASN  |
| 1   | F     | 14  | LYS  |
| 1   | F     | 67  | THR  |
| 1   | F     | 79  | ARG  |
| 1   | F     | 96  | SER  |
| 1   | F     | 127 | PHE  |
| 1   | F     | 134 | ARG  |
| 1   | F     | 170 | LEU  |
| 1   | F     | 213 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 215 | ARG  |
| 1   | F     | 239 | TYR  |
| 1   | F     | 241 | ASN  |
| 1   | F     | 255 | GLU  |
| 1   | F     | 258 | LYS  |
| 1   | F     | 285 | ARG  |
| 1   | F     | 295 | ARG  |
| 1   | F     | 360 | ARG  |
| 1   | F     | 375 | LEU  |
| 1   | F     | 401 | GLN  |
| 1   | F     | 468 | GLU  |
| 1   | F     | 471 | THR  |
| 2   | K     | 106 | ASN  |
| 1   | G     | 14  | LYS  |
| 1   | G     | 67  | THR  |
| 1   | G     | 79  | ARG  |
| 1   | G     | 96  | SER  |
| 1   | G     | 127 | PHE  |
| 1   | G     | 134 | ARG  |
| 1   | G     | 170 | LEU  |
| 1   | G     | 213 | ARG  |
| 1   | G     | 215 | ARG  |
| 1   | G     | 239 | TYR  |
| 1   | G     | 241 | ASN  |
| 1   | G     | 255 | GLU  |
| 1   | G     | 258 | LYS  |
| 1   | G     | 285 | ARG  |
| 1   | G     | 295 | ARG  |
| 1   | G     | 360 | ARG  |
| 1   | G     | 375 | LEU  |
| 1   | G     | 401 | GLN  |
| 1   | G     | 468 | GLU  |
| 1   | G     | 471 | THR  |
| 2   | P     | 106 | ASN  |
| 1   | H     | 14  | LYS  |
| 1   | H     | 67  | THR  |
| 1   | H     | 79  | ARG  |
| 1   | H     | 96  | SER  |
| 1   | H     | 127 | PHE  |
| 1   | H     | 134 | ARG  |
| 1   | H     | 170 | LEU  |
| 1   | H     | 213 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 215 | ARG  |
| 1   | H     | 239 | TYR  |
| 1   | H     | 241 | ASN  |
| 1   | H     | 255 | GLU  |
| 1   | H     | 258 | LYS  |
| 1   | H     | 285 | ARG  |
| 1   | H     | 295 | ARG  |
| 1   | H     | 319 | ARG  |
| 1   | H     | 360 | ARG  |
| 1   | H     | 375 | LEU  |
| 1   | H     | 401 | GLN  |
| 1   | H     | 468 | GLU  |
| 1   | H     | 471 | THR  |
| 2   | L     | 106 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 153 | HIS  |
| 1   | A     | 156 | GLN  |
| 1   | A     | 226 | HIS  |
| 1   | A     | 229 | GLN  |
| 1   | A     | 238 | HIS  |
| 1   | A     | 241 | ASN  |
| 1   | A     | 277 | ASN  |
| 1   | A     | 304 | GLN  |
| 1   | A     | 353 | HIS  |
| 1   | A     | 386 | HIS  |
| 1   | A     | 401 | GLN  |
| 1   | A     | 420 | ASN  |
| 2   | M     | 106 | ASN  |
| 2   | M     | 118 | HIS  |
| 1   | B     | 153 | HIS  |
| 1   | B     | 229 | GLN  |
| 1   | B     | 238 | HIS  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 277 | ASN  |
| 1   | B     | 304 | GLN  |
| 1   | B     | 353 | HIS  |
| 1   | B     | 386 | HIS  |
| 1   | B     | 401 | GLN  |
| 1   | B     | 420 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 106 | ASN  |
| 2   | I     | 118 | HIS  |
| 1   | C     | 153 | HIS  |
| 1   | C     | 229 | GLN  |
| 1   | C     | 238 | HIS  |
| 1   | C     | 241 | ASN  |
| 1   | C     | 277 | ASN  |
| 1   | C     | 304 | GLN  |
| 1   | C     | 353 | HIS  |
| 1   | C     | 386 | HIS  |
| 1   | C     | 401 | GLN  |
| 1   | C     | 420 | ASN  |
| 2   | N     | 106 | ASN  |
| 2   | N     | 118 | HIS  |
| 1   | D     | 153 | HIS  |
| 1   | D     | 229 | GLN  |
| 1   | D     | 238 | HIS  |
| 1   | D     | 241 | ASN  |
| 1   | D     | 277 | ASN  |
| 1   | D     | 304 | GLN  |
| 1   | D     | 353 | HIS  |
| 1   | D     | 386 | HIS  |
| 1   | D     | 401 | GLN  |
| 1   | D     | 420 | ASN  |
| 2   | J     | 106 | ASN  |
| 2   | J     | 118 | HIS  |
| 1   | E     | 153 | HIS  |
| 1   | E     | 229 | GLN  |
| 1   | E     | 238 | HIS  |
| 1   | E     | 241 | ASN  |
| 1   | E     | 277 | ASN  |
| 1   | E     | 304 | GLN  |
| 1   | E     | 353 | HIS  |
| 1   | E     | 383 | HIS  |
| 1   | E     | 386 | HIS  |
| 1   | E     | 401 | GLN  |
| 1   | E     | 420 | ASN  |
| 2   | O     | 106 | ASN  |
| 2   | O     | 118 | HIS  |
| 1   | F     | 153 | HIS  |
| 1   | F     | 229 | GLN  |
| 1   | F     | 238 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 241 | ASN  |
| 1   | F     | 277 | ASN  |
| 1   | F     | 304 | GLN  |
| 1   | F     | 353 | HIS  |
| 1   | F     | 386 | HIS  |
| 1   | F     | 401 | GLN  |
| 1   | F     | 420 | ASN  |
| 2   | K     | 106 | ASN  |
| 2   | K     | 118 | HIS  |
| 1   | G     | 153 | HIS  |
| 1   | G     | 156 | GLN  |
| 1   | G     | 229 | GLN  |
| 1   | G     | 238 | HIS  |
| 1   | G     | 241 | ASN  |
| 1   | G     | 277 | ASN  |
| 1   | G     | 304 | GLN  |
| 1   | G     | 353 | HIS  |
| 1   | G     | 383 | HIS  |
| 1   | G     | 386 | HIS  |
| 1   | G     | 401 | GLN  |
| 1   | G     | 420 | ASN  |
| 2   | P     | 106 | ASN  |
| 2   | P     | 118 | HIS  |
| 1   | H     | 123 | ASN  |
| 1   | H     | 153 | HIS  |
| 1   | H     | 229 | GLN  |
| 1   | H     | 238 | HIS  |
| 1   | H     | 241 | ASN  |
| 1   | H     | 277 | ASN  |
| 1   | H     | 304 | GLN  |
| 1   | H     | 353 | HIS  |
| 1   | H     | 383 | HIS  |
| 1   | H     | 386 | HIS  |
| 1   | H     | 401 | GLN  |
| 1   | H     | 420 | ASN  |
| 2   | L     | 106 | ASN  |
| 2   | L     | 118 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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   | XBP  | A     | 476 | -    | 17,17,17     | 2.11 | 5 (29%)     | 15,25,25    | 1.20 | 0           |
| 3   | XBP  | B     | 476 | -    | 17,17,17     | 2.12 | 6 (35%)     | 15,25,25    | 1.20 | 0           |
| 3   | XBP  | C     | 476 | -    | 17,17,17     | 2.12 | 5 (29%)     | 15,25,25    | 1.20 | 0           |
| 3   | XBP  | D     | 476 | -    | 17,17,17     | 2.12 | 5 (29%)     | 15,25,25    | 1.19 | 0           |
| 3   | XBP  | E     | 476 | -    | 17,17,17     | 2.12 | 5 (29%)     | 15,25,25    | 1.19 | 0           |
| 3   | XBP  | F     | 476 | 1    | 17,17,17     | 2.12 | 5 (29%)     | 15,25,25    | 1.20 | 0           |
| 3   | XBP  | G     | 476 | 1    | 17,17,17     | 2.11 | 5 (29%)     | 15,25,25    | 1.20 | 0           |
| 3   | XBP  | H     | 476 | -    | 17,17,17     | 2.11 | 6 (35%)     | 15,25,25    | 1.20 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | XBP  | A     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | XBP  | B     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | XBP  | C     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | XBP  | D     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | XBP  | E     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | XBP  | F     | 476 | 1    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | XBP  | G     | 476 | 1    | -       | 0/20/20/20 | 0/0/0/0 |
| 3   | XBP  | H     | 476 | -    | -       | 0/20/20/20 | 0/0/0/0 |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | G     | 476 | XBP  | P2-O5  | -3.42 | 1.48        | 1.60     |
| 3   | B     | 476 | XBP  | P2-O5  | -3.39 | 1.48        | 1.60     |
| 3   | H     | 476 | XBP  | P2-O5  | -3.38 | 1.48        | 1.60     |
| 3   | D     | 476 | XBP  | P2-O5  | -3.38 | 1.48        | 1.60     |
| 3   | F     | 476 | XBP  | P2-O5  | -3.38 | 1.48        | 1.60     |
| 3   | A     | 476 | XBP  | P2-O5  | -3.38 | 1.48        | 1.60     |
| 3   | C     | 476 | XBP  | P2-O5  | -3.37 | 1.49        | 1.60     |
| 3   | E     | 476 | XBP  | P2-O5  | -3.30 | 1.49        | 1.60     |
| 3   | B     | 476 | XBP  | P1-O1  | -2.62 | 1.51        | 1.60     |
| 3   | D     | 476 | XBP  | P1-O1  | -2.62 | 1.51        | 1.60     |
| 3   | E     | 476 | XBP  | P1-O1  | -2.61 | 1.51        | 1.60     |
| 3   | C     | 476 | XBP  | P1-O1  | -2.61 | 1.51        | 1.60     |
| 3   | F     | 476 | XBP  | P1-O1  | -2.61 | 1.51        | 1.60     |
| 3   | A     | 476 | XBP  | P1-O1  | -2.60 | 1.51        | 1.60     |
| 3   | G     | 476 | XBP  | P1-O1  | -2.60 | 1.51        | 1.60     |
| 3   | H     | 476 | XBP  | P1-O1  | -2.59 | 1.51        | 1.60     |
| 3   | H     | 476 | XBP  | P2-O4P | 2.00  | 1.57        | 1.51     |
| 3   | B     | 476 | XBP  | P2-O4P | 2.01  | 1.57        | 1.51     |
| 3   | B     | 476 | XBP  | P2-O6P | 2.18  | 1.62        | 1.54     |
| 3   | E     | 476 | XBP  | P2-O6P | 2.20  | 1.62        | 1.54     |
| 3   | A     | 476 | XBP  | P2-O6P | 2.20  | 1.62        | 1.54     |
| 3   | F     | 476 | XBP  | P2-O6P | 2.21  | 1.62        | 1.54     |
| 3   | H     | 476 | XBP  | P2-O6P | 2.21  | 1.62        | 1.54     |
| 3   | G     | 476 | XBP  | P2-O6P | 2.21  | 1.62        | 1.54     |
| 3   | D     | 476 | XBP  | P2-O6P | 2.21  | 1.62        | 1.54     |
| 3   | C     | 476 | XBP  | P2-O6P | 2.21  | 1.62        | 1.54     |
| 3   | E     | 476 | XBP  | P1-O1P | 2.37  | 1.59        | 1.51     |
| 3   | H     | 476 | XBP  | P1-O1P | 2.41  | 1.59        | 1.51     |
| 3   | A     | 476 | XBP  | P1-O1P | 2.42  | 1.59        | 1.51     |
| 3   | B     | 476 | XBP  | P1-O1P | 2.42  | 1.59        | 1.51     |
| 3   | C     | 476 | XBP  | P1-O1P | 2.43  | 1.59        | 1.51     |
| 3   | F     | 476 | XBP  | P1-O1P | 2.43  | 1.59        | 1.51     |
| 3   | G     | 476 | XBP  | P1-O1P | 2.43  | 1.59        | 1.51     |
| 3   | D     | 476 | XBP  | P1-O1P | 2.44  | 1.59        | 1.51     |
| 3   | G     | 476 | XBP  | O1-C1  | 5.51  | 1.46        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | A     | 476 | XBP  | O1-C1 | 5.54 | 1.46        | 1.43     |
| 3   | H     | 476 | XBP  | O1-C1 | 5.54 | 1.46        | 1.43     |
| 3   | C     | 476 | XBP  | O1-C1 | 5.55 | 1.46        | 1.43     |
| 3   | B     | 476 | XBP  | O1-C1 | 5.60 | 1.46        | 1.43     |
| 3   | D     | 476 | XBP  | O1-C1 | 5.60 | 1.46        | 1.43     |
| 3   | F     | 476 | XBP  | O1-C1 | 5.62 | 1.46        | 1.43     |
| 3   | E     | 476 | XBP  | O1-C1 | 5.67 | 1.47        | 1.43     |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 476 | XBP  | 2       | 0            |
| 3   | B     | 476 | XBP  | 2       | 0            |
| 3   | C     | 476 | XBP  | 2       | 0            |
| 3   | D     | 476 | XBP  | 2       | 0            |
| 3   | E     | 476 | XBP  | 2       | 0            |
| 3   | F     | 476 | XBP  | 1       | 0            |
| 3   | G     | 476 | XBP  | 1       | 0            |
| 3   | H     | 476 | XBP  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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