



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:58 PM UTC

PDB ID : 7AKK / pdb\_00007akk  
Title : Structure of a complement factor-receptor complex  
Authors : Fernandez, F.J.; Santos-Lopez, J.; Martinez-Barricarte, R.; Querol-Garcia, J.; Navas-Yuste, S.; Savko, M.; Shepard, W.E.; Rodriguez de Cordoba, S.; Vega, M.C.  
Deposited on : 2020-10-01  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

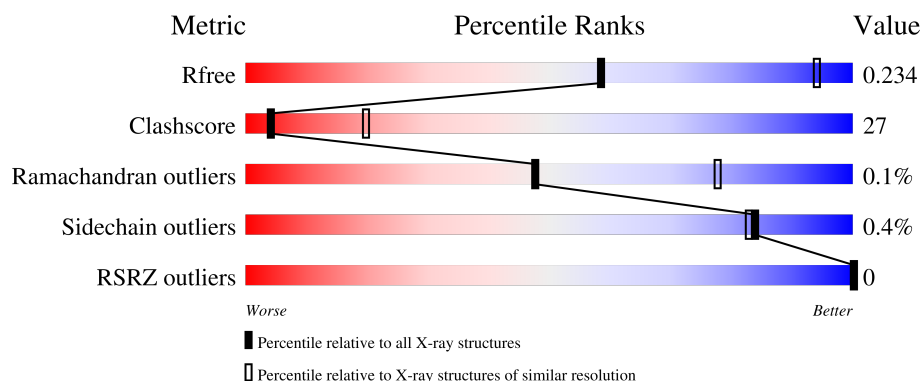
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



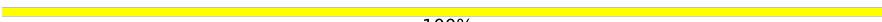
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1001 (3.44-3.36)                                      |
| Clashscore            | 190562                      | 1022 (3.44-3.36)                                      |
| Ramachandran outliers | 187476                      | 1012 (3.44-3.36)                                      |
| Sidechain outliers    | 187428                      | 1012 (3.44-3.36)                                      |
| RSRZ outliers         | 180081                      | 1001 (3.44-3.36)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | B     | 645    |                  |
| 1   | C     | 645    |                  |
| 2   | A     | 898    |                  |
| 2   | E     | 898    |                  |
| 3   | D     | 195    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 3   | H     | 195    | <br>56% 38% 5% |
| 4   | I     | 3      | <br>100%       |
| 5   | J     | 4      | <br>50% 50%    |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24012 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 Complement C3 beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | B     | 645      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5024  | 3198 | 851 | 960 | 15 |         |         |       |
| 1   | C     | 645      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5024  | 3198 | 851 | 960 | 15 |         |         |       |

- Molecule 2 is a protein called Complement C3b alpha' chain.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | A     | 842      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6736  | 4276 | 1128 | 1295 | 37 |         |         |       |
| 2   | E     | 504      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 4084  | 2585 | 684  | 789  | 26 |         |         |       |

There are 34 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | ?       | -        | ARG    | deletion | UNP P01024 |
| A     | ?       | -        | SER    | deletion | UNP P01024 |
| A     | ?       | -        | SER    | deletion | UNP P01024 |
| A     | ?       | -        | LYS    | deletion | UNP P01024 |
| A     | ?       | -        | ILE    | deletion | UNP P01024 |
| A     | ?       | -        | THR    | deletion | UNP P01024 |
| A     | ?       | -        | HIS    | deletion | UNP P01024 |
| A     | ?       | -        | ARG    | deletion | UNP P01024 |
| A     | ?       | -        | ILE    | deletion | UNP P01024 |
| A     | ?       | -        | HIS    | deletion | UNP P01024 |
| A     | ?       | -        | TRP    | deletion | UNP P01024 |
| A     | ?       | -        | GLU    | deletion | UNP P01024 |
| A     | ?       | -        | SER    | deletion | UNP P01024 |
| A     | ?       | -        | ALA    | deletion | UNP P01024 |
| A     | ?       | -        | SER    | deletion | UNP P01024 |
| A     | ?       | -        | LEU    | deletion | UNP P01024 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | ?       | -        | LEU    | deletion | UNP P01024 |
| E     | ?       | -        | ARG    | deletion | UNP P01024 |
| E     | ?       | -        | SER    | deletion | UNP P01024 |
| E     | ?       | -        | SER    | deletion | UNP P01024 |
| E     | ?       | -        | LYS    | deletion | UNP P01024 |
| E     | ?       | -        | ILE    | deletion | UNP P01024 |
| E     | ?       | -        | THR    | deletion | UNP P01024 |
| E     | ?       | -        | HIS    | deletion | UNP P01024 |
| E     | ?       | -        | ARG    | deletion | UNP P01024 |
| E     | ?       | -        | ILE    | deletion | UNP P01024 |
| E     | ?       | -        | HIS    | deletion | UNP P01024 |
| E     | ?       | -        | TRP    | deletion | UNP P01024 |
| E     | ?       | -        | GLU    | deletion | UNP P01024 |
| E     | ?       | -        | SER    | deletion | UNP P01024 |
| E     | ?       | -        | ALA    | deletion | UNP P01024 |
| E     | ?       | -        | SER    | deletion | UNP P01024 |
| E     | ?       | -        | LEU    | deletion | UNP P01024 |
| E     | ?       | -        | LEU    | deletion | UNP P01024 |

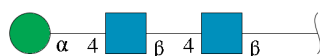
- Molecule 3 is a protein called Integrin alpha-M.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | D     | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1499  | 951 | 267 | 278 | 3 |         |         |       |
| 3   | H     | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1499  | 951 | 267 | 278 | 3 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | 128     | SER      | CYS    | engineered mutation | UNP P11215 |
| D     | 316     | GLY      | ILE    | engineered mutation | UNP P11215 |
| H     | 128     | SER      | CYS    | engineered mutation | UNP P11215 |
| H     | 316     | GLY      | ILE    | engineered mutation | UNP P11215 |

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



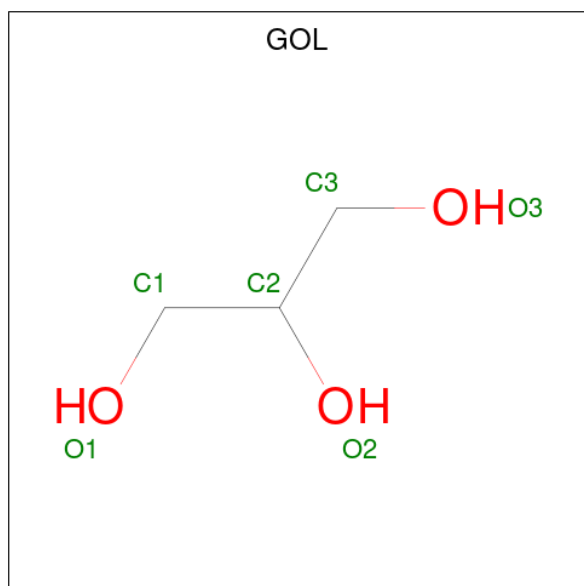
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4   | I     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5   | J     | 4        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |         |       |

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

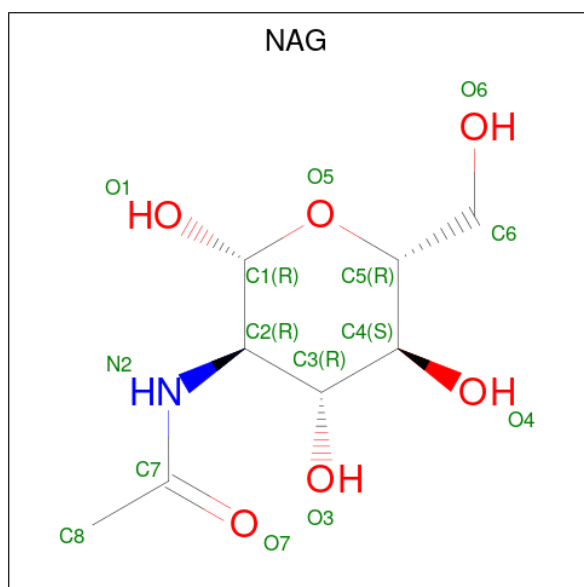
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 7   | A     | 1        | Total K<br>1 1 | 0       | 0       |
| 7   | C     | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 8   | H     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms                   | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------|---------|---------|
| 9   | E     | 1        | Total C N O<br>14 8 1 5 | 0       | 0       |

- Molecule 10 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 10  | B     | 6        | Total O<br>6 6 | 0       | 0       |
| 10  | A     | 7        | Total O<br>7 7 | 0       | 0       |

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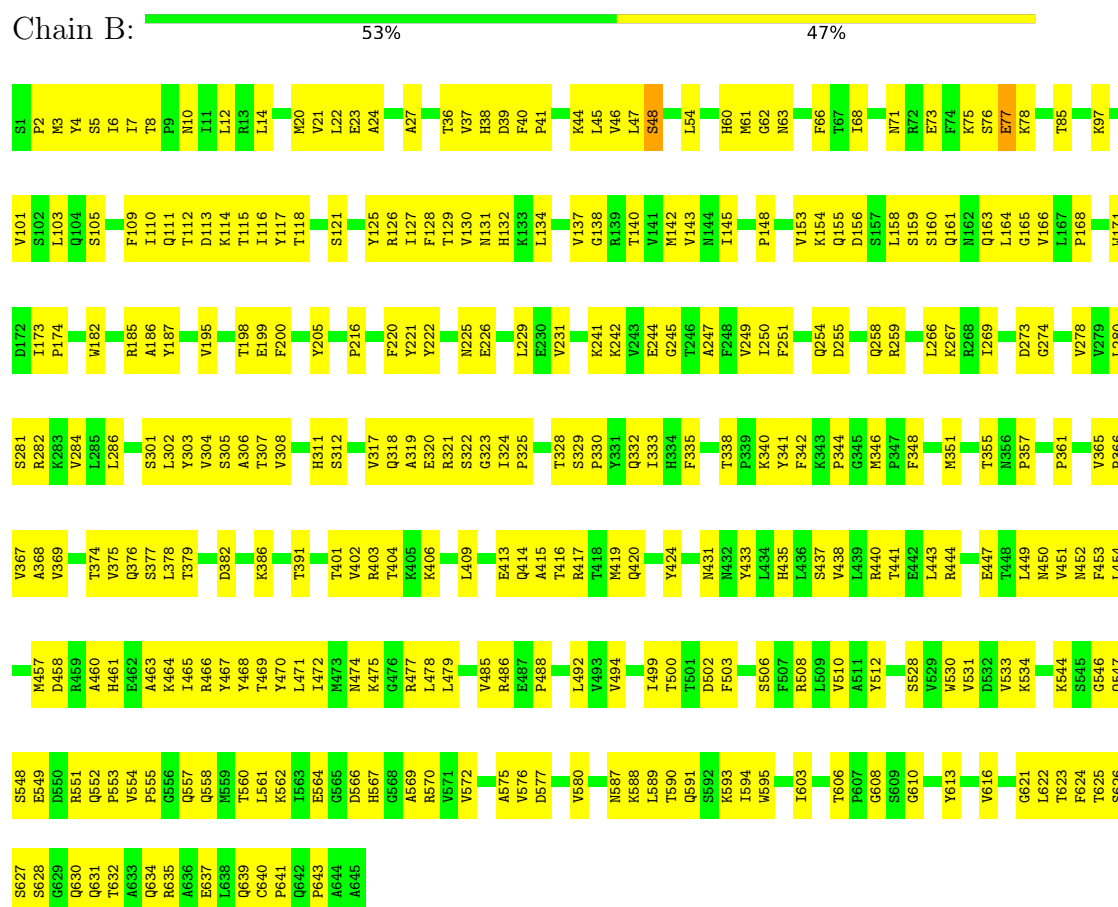
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 10  | D     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 10  | C     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 10  | E     | 2        | Total<br>2 | O<br>2 | 0       | 0       |



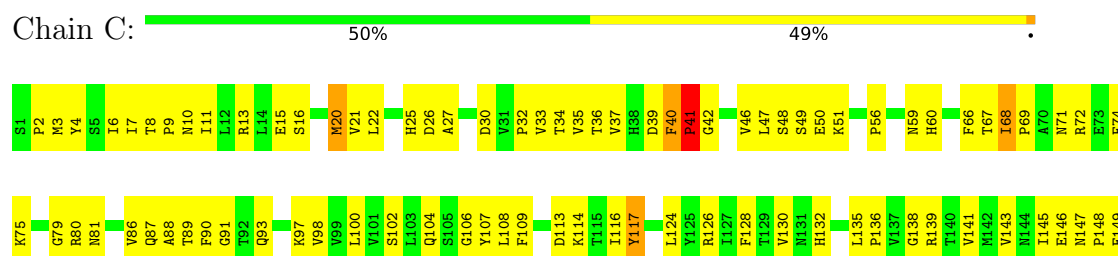
### 3 Residue-property plots

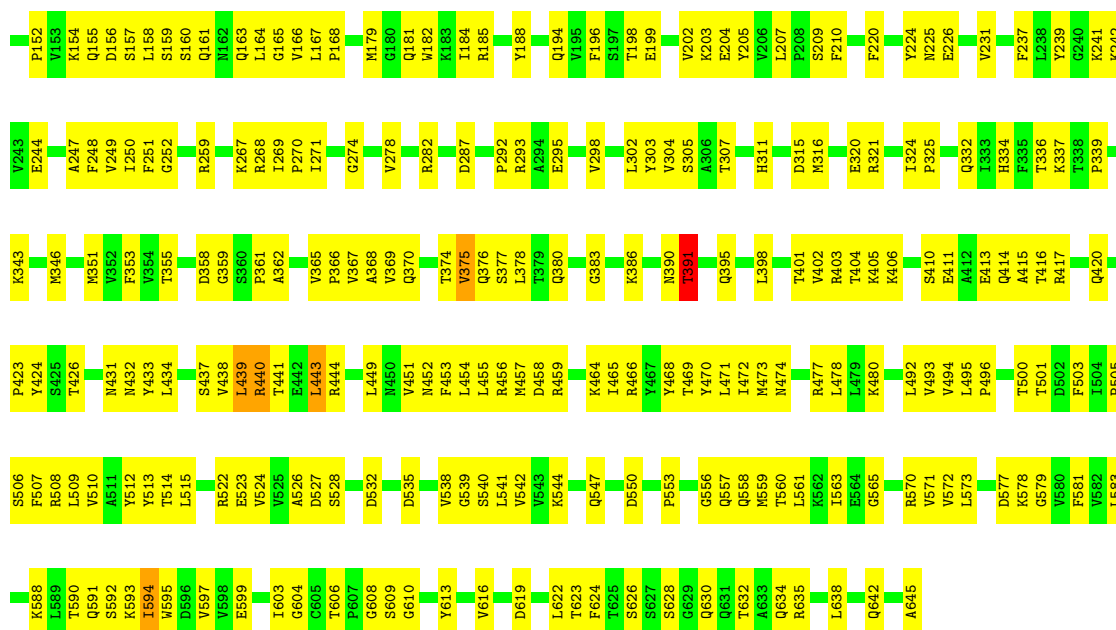
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Complement C3 beta chain



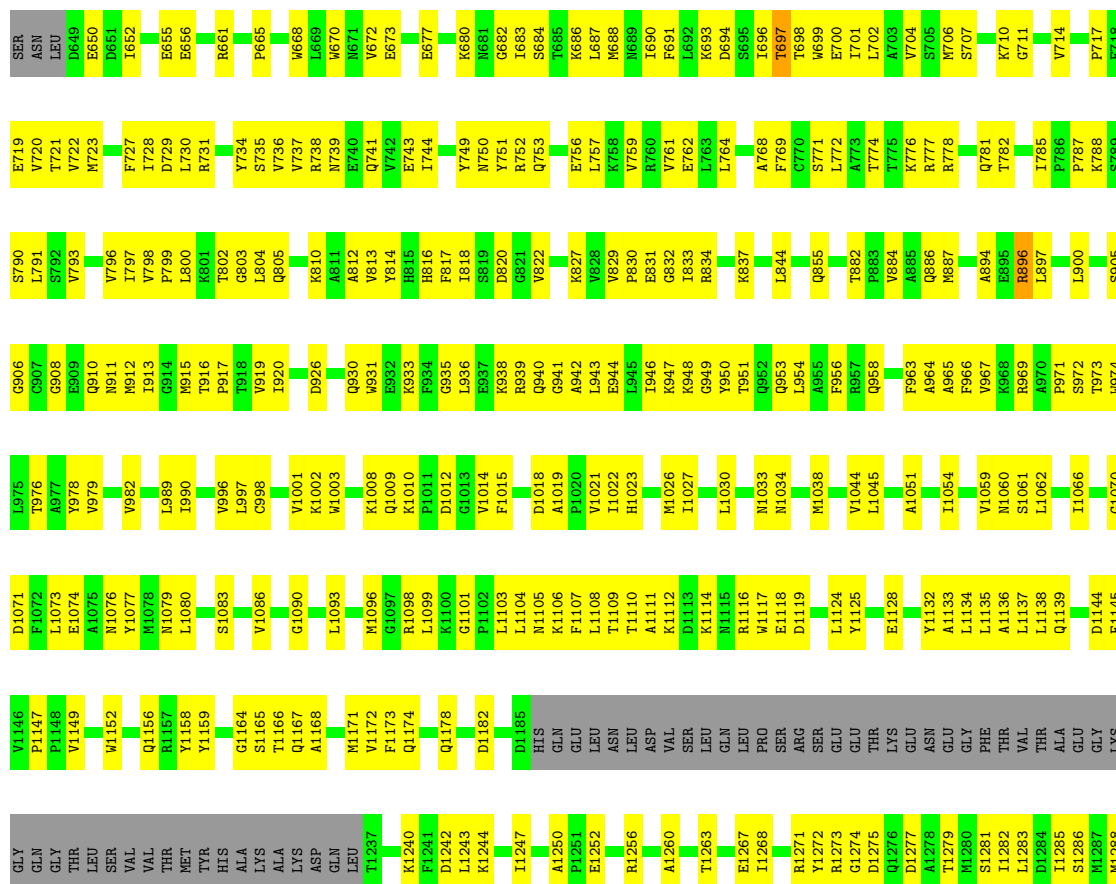
#### • Molecule 1: Complement C3 beta chain

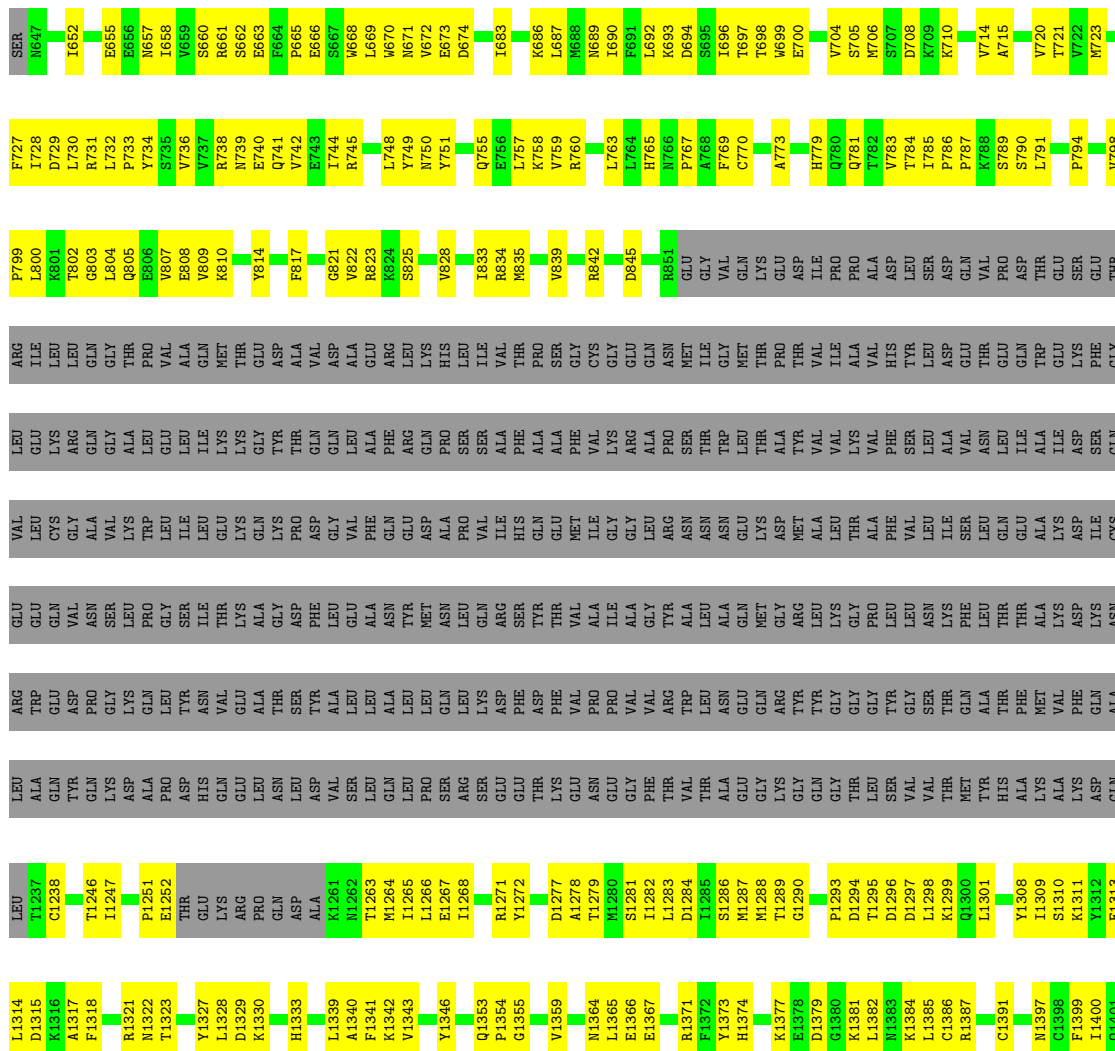


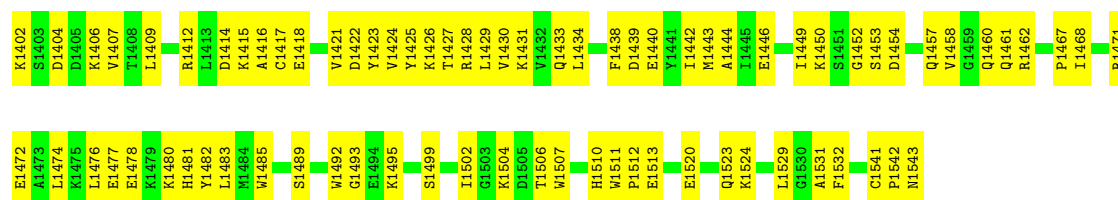


• Molecule 2: Complement C3b alpha' chain

Chain A: 47% 46% 6%

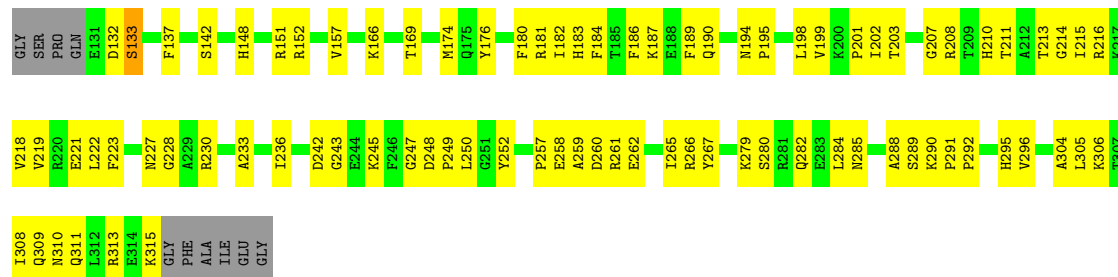






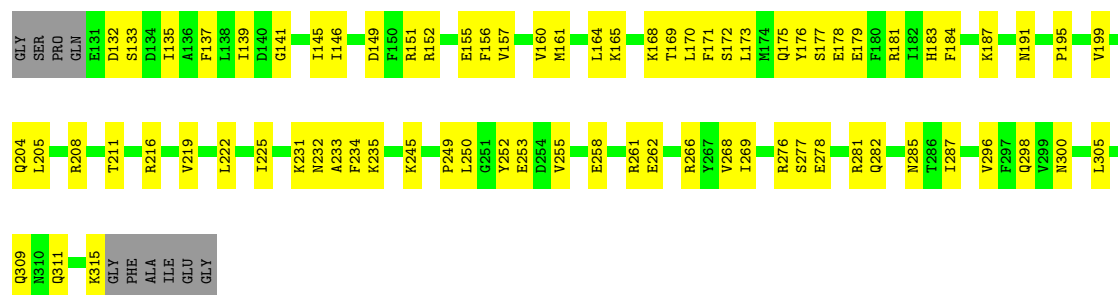
• Molecule 3: Integrin alpha-M

Chain D: 52% 43% 5%



• Molecule 3: Integrin alpha-M

Chain H: 56% 38% 5%



• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



• Molecule 5: beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 50% 50%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 111.29Å 150.73Å 111.30Å<br>90.00° 92.80° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 53.77 – 3.40<br>53.77 – 3.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (53.77-3.40)<br>99.3 (53.77-3.40)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.34                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.38 (at 3.40Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.13_2998                                            | Depositor        |
| R, $R_{free}$                                                           | 0.192 , 0.229<br>0.192 , 0.234                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2520 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 105.3                                                       | Xtriage          |
| Anisotropy                                                              | 0.249                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 90.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction                                             | 0.109 for l,k,-h<br>0.117 for h,-k,-l<br>0.326 for l,-k,h   | Xtriage          |
| Reported twinning fraction                                              | 0.500 for l,-k,h                                            | Depositor        |
| Outliers                                                                | 0 of 50383 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 24012                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 112.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MG, GOL, MAN, BMA, K

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | B     | 0.60         | 0/5126         | 0.86        | 2/6966 (0.0%)   |
| 1   | C     | 0.59         | 1/5126 (0.0%)  | 0.87        | 5/6966 (0.1%)   |
| 2   | A     | 0.51         | 0/6871         | 0.77        | 4/9303 (0.0%)   |
| 2   | E     | 0.56         | 0/4164         | 0.79        | 0/5629          |
| 3   | D     | 0.50         | 0/1527         | 0.77        | 1/2054 (0.0%)   |
| 3   | H     | 0.60         | 0/1527         | 0.86        | 0/2054          |
| All | All   | 0.56         | 1/24341 (0.0%) | 0.82        | 12/32972 (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   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 2   | A     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | C     | 117 | TYR  | C-N   | 5.80 | 1.45        | 1.33     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | A     | 697 | THR  | CA-CB-OG1 | -8.72 | 96.52       | 109.60   |
| 1   | C     | 41  | PRO  | CA-N-CD   | -7.24 | 101.87      | 112.00   |
| 3   | D     | 133 | SER  | N-CA-C    | 6.58  | 118.78      | 107.93   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | C     | 20   | MET  | CB-CG-SD | -5.78 | 95.36       | 112.70   |
| 1   | C     | 391  | THR  | CA-C-N   | -5.35 | 112.89      | 120.49   |
| 1   | C     | 391  | THR  | C-N-CA   | -5.35 | 112.89      | 120.49   |
| 1   | B     | 48   | SER  | CA-C-N   | -5.34 | 111.93      | 122.02   |
| 1   | B     | 48   | SER  | C-N-CA   | -5.34 | 111.93      | 122.02   |
| 2   | A     | 1061 | SER  | CA-C-N   | 5.11  | 129.64      | 121.62   |
| 2   | A     | 1061 | SER  | C-N-CA   | 5.11  | 129.64      | 121.62   |
| 2   | A     | 896  | ARG  | CG-CD-NE | 5.10  | 123.22      | 112.00   |
| 1   | C     | 50   | GLU  | N-CA-C   | 5.00  | 116.76      | 110.91   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | A     | 817 | PHE  | Peptide |
| 1   | B     | 640 | CYS  | Peptide |
| 1   | C     | 40  | PHE  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 5024  | 0        | 5084     | 287     | 0            |
| 1   | C     | 5024  | 0        | 5084     | 339     | 1            |
| 2   | A     | 6736  | 0        | 6668     | 374     | 2            |
| 2   | E     | 4084  | 0        | 4022     | 257     | 0            |
| 3   | D     | 1499  | 0        | 1509     | 67      | 1            |
| 3   | H     | 1499  | 0        | 1511     | 73      | 2            |
| 4   | I     | 39    | 0        | 33       | 2       | 0            |
| 5   | J     | 50    | 0        | 43       | 1       | 0            |
| 6   | B     | 6     | 0        | 8        | 0       | 0            |
| 6   | C     | 6     | 0        | 8        | 0       | 0            |
| 6   | E     | 6     | 0        | 8        | 1       | 0            |
| 7   | A     | 1     | 0        | 0        | 0       | 0            |
| 7   | C     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 1     | 0        | 0        | 0       | 0            |
| 8   | H     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | E     | 14    | 0        | 13       | 0       | 0            |
| 10  | A     | 7     | 0        | 0        | 0       | 0            |
| 10  | B     | 6     | 0        | 0        | 0       | 0            |
| 10  | C     | 4     | 0        | 0        | 0       | 0            |
| 10  | D     | 2     | 0        | 0        | 0       | 0            |
| 10  | E     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 24012 | 0        | 23991    | 1313    | 3            |

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 27.

All (1313) 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:C:370:GLN:HG3  | 1:C:401:THR:HB   | 1.14                     | 1.12              |
| 1:C:369:VAL:H    | 1:C:375:VAL:CG2  | 1.65                     | 1.09              |
| 1:C:369:VAL:H    | 1:C:375:VAL:HG21 | 0.94                     | 1.07              |
| 1:C:369:VAL:HG22 | 1:C:375:VAL:HG11 | 1.34                     | 1.07              |
| 1:B:155:GLN:HE21 | 2:E:804:LEU:HD13 | 1.13                     | 1.06              |
| 2:A:697:THR:HG22 | 2:A:698:THR:H    | 1.20                     | 1.06              |
| 1:C:369:VAL:N    | 1:C:375:VAL:HG21 | 1.75                     | 1.01              |
| 2:E:658:ILE:HB   | 2:E:810:LYS:HD3  | 1.44                     | 0.98              |
| 1:B:155:GLN:NE2  | 2:E:804:LEU:HD13 | 1.77                     | 0.97              |
| 2:A:1457:GLN:OE1 | 2:A:1460:GLN:NE2 | 2.00                     | 0.94              |
| 1:B:113:ASP:OD1  | 1:B:117:TYR:OH   | 1.84                     | 0.94              |
| 1:C:367:VAL:HA   | 1:C:404:THR:HA   | 1.47                     | 0.94              |
| 1:C:10:ASN:HD22  | 1:C:635:ARG:HH11 | 1.15                     | 0.92              |
| 1:C:370:GLN:HG3  | 1:C:401:THR:CB   | 1.98                     | 0.92              |
| 1:C:591:GLN:OE1  | 2:E:714:VAL:N    | 2.02                     | 0.92              |
| 2:A:661:ARG:NH2  | 2:A:820:ASP:OD1  | 2.03                     | 0.92              |
| 3:H:133:SER:HB2  | 3:H:169:THR:HA   | 1.52                     | 0.90              |
| 1:C:557:GLN:O    | 2:E:692:LEU:HG   | 1.73                     | 0.88              |
| 2:A:1354:PRO:HB3 | 2:A:1374:HIS:HB2 | 1.56                     | 0.88              |
| 1:B:164:LEU:HD23 | 1:B:570:ARG:HG3  | 1.55                     | 0.88              |
| 2:E:1353:GLN:NE2 | 2:E:1354:PRO:O   | 2.07                     | 0.87              |
| 2:A:680:LYS:N    | 2:A:683:ILE:O    | 2.07                     | 0.87              |
| 1:C:453:PHE:HB2  | 1:C:493:VAL:HG23 | 1.54                     | 0.87              |
| 2:A:697:THR:CG2  | 2:A:698:THR:H    | 1.88                     | 0.86              |
| 1:C:26:ASP:OD2   | 1:C:522:ARG:NH2  | 2.07                     | 0.86              |
| 2:E:1425:TYR:OH  | 2:E:1454:ASP:OD2 | 1.94                     | 0.85              |
| 2:A:697:THR:HG22 | 2:A:698:THR:N    | 1.92                     | 0.85              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:161:GLN:NE2   | 3:H:262:GLU:OE1  | 2.10                     | 0.85              |
| 3:D:184:PHE:HD2   | 3:D:189:PHE:HB2  | 1.42                     | 0.85              |
| 3:D:279:LYS:HA    | 3:D:282:GLN:HG2  | 1.59                     | 0.85              |
| 2:A:743:GLU:HB2   | 2:A:796:VAL:HG12 | 1.58                     | 0.84              |
| 1:C:126:ARG:NH2   | 1:C:573:LEU:O    | 2.10                     | 0.84              |
| 1:C:606:THR:HB    | 1:C:619:ASP:HB3  | 1.57                     | 0.84              |
| 1:B:36:THR:HB     | 1:B:38:HIS:HE1   | 1.40                     | 0.84              |
| 1:B:37:VAL:N      | 1:B:47:LEU:O     | 2.09                     | 0.84              |
| 1:C:386:LYS:HZ3   | 1:C:439:LEU:HA   | 1.40                     | 0.84              |
| 1:B:437:SER:O     | 1:B:452:ASN:ND2  | 2.11                     | 0.82              |
| 2:E:1287:MET:HE3  | 2:E:1293:PRO:HD3 | 1.58                     | 0.82              |
| 1:B:506:SER:HB2   | 1:B:530:TRP:HE1  | 1.44                     | 0.82              |
| 2:E:1438:PHE:HD1  | 2:E:1467:PRO:HA  | 1.43                     | 0.82              |
| 1:C:15:GLU:N      | 1:C:68:ILE:O     | 2.13                     | 0.81              |
| 2:A:759:VAL:HG22  | 2:A:813:VAL:HG12 | 1.61                     | 0.81              |
| 2:E:1271:ARG:NH1  | 2:E:1333:HIS:O   | 2.12                     | 0.81              |
| 1:B:36:THR:HB     | 1:B:38:HIS:CE1   | 2.15                     | 0.81              |
| 1:C:33:VAL:HG12   | 1:C:90:PHE:HA    | 1.62                     | 0.81              |
| 1:C:40:PHE:CD2    | 1:C:41:PRO:HD2   | 2.15                     | 0.81              |
| 2:E:786:PRO:HG2   | 2:E:789:SER:HB2  | 1.63                     | 0.81              |
| 2:E:1355:GLY:HA3  | 2:E:1373:TYR:CZ  | 2.15                     | 0.81              |
| 2:A:739:ASN:H     | 2:A:799:PRO:HG2  | 1.45                     | 0.80              |
| 1:C:606:THR:HG22  | 1:C:608:GLY:H    | 1.47                     | 0.80              |
| 1:B:2:PRO:HB3     | 1:B:27:ALA:HB2   | 1.63                     | 0.80              |
| 1:C:378:LEU:O     | 1:C:380:GLN:NE2  | 2.15                     | 0.80              |
| 1:C:426:THR:HG21  | 1:C:431:ASN:H    | 1.45                     | 0.80              |
| 3:H:137:PHE:HE1   | 3:H:171:PHE:HD1  | 1.25                     | 0.80              |
| 2:A:973:THR:OG1   | 2:A:1008:LYS:NZ  | 2.15                     | 0.80              |
| 2:A:1352:ILE:HG13 | 2:A:1374:HIS:HE2 | 1.47                     | 0.79              |
| 2:E:1277:ASP:OD1  | 2:E:1333:HIS:ND1 | 2.15                     | 0.79              |
| 2:A:1252:GLU:OE2  | 2:A:1263:THR:OG1 | 1.98                     | 0.79              |
| 1:C:179:MET:HE3   | 1:C:203:LYS:HD2  | 1.65                     | 0.79              |
| 3:D:184:PHE:CD2   | 3:D:189:PHE:HB2  | 2.17                     | 0.79              |
| 1:C:369:VAL:CG2   | 1:C:375:VAL:HG11 | 2.12                     | 0.79              |
| 3:H:276:ARG:NH2   | 3:H:277:SER:OG   | 2.15                     | 0.79              |
| 1:B:114:LYS:NZ    | 1:B:116:ILE:O    | 2.15                     | 0.78              |
| 2:A:1409:LEU:HB2  | 2:A:1528:ASP:HB3 | 1.64                     | 0.78              |
| 1:C:6:ILE:HD13    | 1:C:20:MET:HE2   | 1.65                     | 0.78              |
| 2:A:946:ILE:HD13  | 2:A:990:ILE:HD11 | 1.66                     | 0.78              |
| 2:A:1286:SER:O    | 2:A:1373:TYR:OH  | 2.02                     | 0.78              |
| 1:B:109:PHE:O     | 1:B:128:PHE:HD1  | 1.68                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:510:VAL:HG12 | 1:C:528:SER:HB2   | 1.66                     | 0.77              |
| 1:C:343:LYS:NZ   | 1:C:527:ASP:OD1   | 2.14                     | 0.77              |
| 2:A:696:ILE:O    | 2:A:697:THR:OG1   | 2.03                     | 0.77              |
| 2:A:1462:ARG:NH1 | 2:A:1496:PRO:O    | 2.18                     | 0.77              |
| 1:C:224:TYR:HA   | 1:C:282:ARG:HH22  | 1.50                     | 0.77              |
| 2:E:1283:LEU:HG  | 2:E:1359:VAL:HG22 | 1.67                     | 0.76              |
| 2:A:1171:MET:SD  | 2:A:1174:GLN:NE2  | 2.59                     | 0.76              |
| 2:A:1503:GLY:N   | 2:A:1506:THR:OG1  | 2.18                     | 0.76              |
| 1:C:451:VAL:HB   | 1:C:495:LEU:HB3   | 1.67                     | 0.76              |
| 2:E:741:GLN:HG3  | 2:E:798:VAL:HG22  | 1.67                     | 0.76              |
| 1:C:40:PHE:CG    | 1:C:41:PRO:HD2    | 2.21                     | 0.76              |
| 1:B:12:LEU:HB2   | 1:B:101:VAL:HG12  | 1.66                     | 0.76              |
| 1:B:198:THR:HG23 | 1:B:587:ASN:HB3   | 1.68                     | 0.76              |
| 1:B:320:GLU:OE2  | 1:B:322:SER:OG    | 2.04                     | 0.76              |
| 2:A:1429:LEU:O   | 2:A:1479:LYS:N    | 2.19                     | 0.76              |
| 1:B:302:LEU:HB2  | 1:B:324:ILE:HB    | 1.66                     | 0.76              |
| 2:A:777:ARG:NH2  | 2:A:1395:GLU:O    | 2.17                     | 0.76              |
| 2:E:661:ARG:NH2  | 2:E:728:ILE:O     | 2.18                     | 0.76              |
| 2:A:1290:GLY:O   | 2:A:1345:GLN:NE2  | 2.15                     | 0.76              |
| 2:A:1083:SER:OG  | 2:A:1119:ASP:OD1  | 2.04                     | 0.75              |
| 2:A:964:ALA:HB2  | 2:A:971:PRO:HA    | 1.68                     | 0.75              |
| 1:C:558:GLN:NE2  | 2:E:689:ASN:OD1   | 2.20                     | 0.75              |
| 1:C:403:ARG:NH1  | 1:C:411:GLU:O     | 2.18                     | 0.75              |
| 1:C:547:GLN:HE21 | 1:C:559:MET:HG3   | 1.50                     | 0.75              |
| 1:C:443:LEU:HD21 | 1:C:449:LEU:HD22  | 1.69                     | 0.74              |
| 2:E:1399:PHE:HZ  | 2:E:1402:LYS:HB2  | 1.51                     | 0.74              |
| 2:A:976:THR:HG21 | 2:A:1003:TRP:HZ3  | 1.53                     | 0.74              |
| 1:B:451:VAL:O    | 1:B:494:VAL:HA    | 1.86                     | 0.74              |
| 2:E:1481:HIS:HB2 | 2:E:1511:TRP:HB3  | 1.68                     | 0.74              |
| 1:B:606:THR:HG22 | 1:B:608:GLY:H     | 1.52                     | 0.73              |
| 2:A:963:PHE:HB2  | 2:A:976:THR:HA    | 1.68                     | 0.73              |
| 2:A:1308:TYR:HB3 | 2:A:1327:TYR:HB2  | 1.71                     | 0.73              |
| 1:C:209:SER:OG   | 1:C:315:ASP:OD2   | 2.04                     | 0.73              |
| 2:E:1407:VAL:O   | 2:E:1412:ARG:NH1  | 2.21                     | 0.73              |
| 1:C:152:PRO:HB2  | 1:C:155:GLN:HE21  | 1.53                     | 0.73              |
| 1:C:226:GLU:HA   | 1:C:282:ARG:HD2   | 1.70                     | 0.73              |
| 1:B:444:ARG:N    | 1:B:447:GLU:OE2   | 2.17                     | 0.73              |
| 2:A:782:THR:HG23 | 2:A:814:TYR:HE1   | 1.53                     | 0.73              |
| 2:A:1495:LYS:HG2 | 2:A:1498:LEU:HD11 | 1.70                     | 0.73              |
| 1:B:76:SER:HB3   | 2:E:767:PRO:CB    | 2.19                     | 0.73              |
| 1:C:128:PHE:HD2  | 2:E:706:MET:SD    | 2.12                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1318:PHE:N    | 2:E:1321:ARG:HH12 | 1.87                     | 0.73              |
| 2:A:668:TRP:HH2   | 2:A:690:ILE:HD12  | 1.52                     | 0.73              |
| 1:B:546:GLY:HA2   | 1:B:562:LYS:HE2   | 1.70                     | 0.72              |
| 2:A:1294:ASP:HB2  | 2:A:1342:LYS:HB2  | 1.69                     | 0.72              |
| 1:C:32:PRO:O      | 1:C:91:GLY:N      | 2.22                     | 0.72              |
| 1:C:561:LEU:O     | 2:E:687:LEU:HA    | 1.90                     | 0.72              |
| 1:C:591:GLN:HB2   | 2:E:714:VAL:HB    | 1.71                     | 0.72              |
| 1:B:361:PRO:HB3   | 1:B:382:ASP:C     | 2.14                     | 0.72              |
| 2:A:1460:GLN:OE1  | 2:A:1462:ARG:NH2  | 2.22                     | 0.72              |
| 2:E:1524:LYS:H    | 2:E:1524:LYS:HD2  | 1.54                     | 0.72              |
| 2:A:1474:LEU:HB3  | 2:A:1476:LEU:HG   | 1.72                     | 0.72              |
| 1:B:435:HIS:HB3   | 1:B:454:LEU:HB3   | 1.72                     | 0.72              |
| 1:C:10:ASN:HD22   | 1:C:635:ARG:NH1   | 1.88                     | 0.72              |
| 1:C:148:PRO:HD3   | 1:C:182:TRP:NE1   | 2.05                     | 0.72              |
| 1:B:129:THR:OG1   | 1:B:165:GLY:HA2   | 1.89                     | 0.72              |
| 2:E:1310:SER:N    | 2:E:1313:GLU:OE2  | 2.23                     | 0.72              |
| 1:C:369:VAL:HG22  | 1:C:375:VAL:CG1   | 2.16                     | 0.71              |
| 1:B:245:GLY:O     | 1:B:311:HIS:NE2   | 2.24                     | 0.71              |
| 3:H:266:ARG:NH1   | 3:H:287:ILE:O     | 2.23                     | 0.71              |
| 1:C:542:VAL:HG11  | 1:C:544:LYS:HE3   | 1.73                     | 0.71              |
| 2:A:673:GLU:HB3   | 2:A:686:LYS:HD3   | 1.71                     | 0.71              |
| 1:C:2:PRO:HA      | 1:C:25:HIS:O      | 1.90                     | 0.71              |
| 1:C:440:ARG:HH11  | 1:C:440:ARG:HG3   | 1.56                     | 0.71              |
| 2:A:1502:ILE:HG23 | 2:A:1506:THR:HG21 | 1.72                     | 0.71              |
| 3:H:137:PHE:HE1   | 3:H:171:PHE:CD1   | 2.09                     | 0.71              |
| 2:A:1407:VAL:O    | 2:A:1412:ARG:NH1  | 2.24                     | 0.71              |
| 3:D:219:VAL:HA    | 3:D:223:PHE:HB2   | 1.71                     | 0.70              |
| 2:A:1070:GLY:HA3  | 2:A:1096:MET:HE1  | 1.73                     | 0.70              |
| 3:H:141:GLY:HA3   | 3:H:175:GLN:HE21  | 1.56                     | 0.70              |
| 1:C:113:ASP:OD1   | 1:C:117:TYR:OH    | 2.08                     | 0.70              |
| 3:H:179:GLU:OE1   | 3:H:181:ARG:NH2   | 2.23                     | 0.70              |
| 1:B:155:GLN:HE21  | 2:E:804:LEU:CD1   | 1.98                     | 0.70              |
| 1:C:332:GLN:HB2   | 1:C:355:THR:OG1   | 1.92                     | 0.70              |
| 1:C:10:ASN:ND2    | 1:C:635:ARG:HH11  | 1.90                     | 0.70              |
| 1:C:47:LEU:HD23   | 1:C:66:PHE:HB2    | 1.74                     | 0.70              |
| 2:E:699:TRP:HB2   | 2:E:720:VAL:HG23  | 1.73                     | 0.70              |
| 2:A:655:GLU:OE1   | 2:A:778:ARG:NH2   | 2.22                     | 0.70              |
| 1:B:281:SER:HB2   | 1:B:284:VAL:HG23  | 1.73                     | 0.70              |
| 2:E:763:LEU:HA    | 2:E:809:VAL:HG12  | 1.73                     | 0.70              |
| 2:A:1008:LYS:HE2  | 2:A:1018:ASP:HB2  | 1.74                     | 0.70              |
| 1:C:13:ARG:O      | 1:C:16:SER:OG     | 2.08                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:351:MET:HE1  | 1:B:386:LYS:HG3  | 1.73                     | 0.70              |
| 1:B:155:GLN:NE2  | 2:E:804:LEU:CD1  | 2.52                     | 0.69              |
| 1:B:438:VAL:HG13 | 1:B:449:LEU:HD11 | 1.73                     | 0.69              |
| 1:C:440:ARG:NH1  | 1:C:440:ARG:HB3  | 2.06                     | 0.69              |
| 2:A:1077:TYR:OH  | 2:A:1107:PHE:HB2 | 1.93                     | 0.69              |
| 1:B:438:VAL:HG22 | 1:B:450:ASN:O    | 1.92                     | 0.69              |
| 1:C:148:PRO:HD3  | 1:C:182:TRP:CE2  | 2.28                     | 0.69              |
| 1:C:642:GLN:HB3  | 1:C:645:ALA:HB3  | 1.74                     | 0.69              |
| 2:E:1399:PHE:CZ  | 2:E:1402:LYS:HB2 | 2.28                     | 0.69              |
| 1:C:368:ALA:N    | 1:C:403:ARG:O    | 2.19                     | 0.69              |
| 2:E:1374:HIS:HB3 | 2:E:1377:LYS:HB2 | 1.73                     | 0.69              |
| 2:A:677:GLU:O    | 2:A:684:SER:OG   | 2.08                     | 0.68              |
| 3:D:195:PRO:O    | 3:D:198:LEU:N    | 2.26                     | 0.68              |
| 2:A:979:VAL:O    | 2:A:982:VAL:HG12 | 1.93                     | 0.68              |
| 1:B:569:ALA:HB2  | 2:A:707:SER:HB2  | 1.74                     | 0.68              |
| 1:C:440:ARG:NE   | 1:C:440:ARG:HA   | 2.08                     | 0.68              |
| 2:A:802:THR:HG22 | 2:A:803:GLY:H    | 1.57                     | 0.68              |
| 1:C:440:ARG:HH11 | 1:C:440:ARG:CG   | 2.07                     | 0.68              |
| 1:C:346:MET:HE1  | 1:C:454:LEU:HD23 | 1.75                     | 0.68              |
| 2:A:1135:LEU:O   | 2:A:1139:GLN:NE2 | 2.20                     | 0.67              |
| 2:A:1383:ASN:HB2 | 2:A:1394:ALA:O   | 1.94                     | 0.67              |
| 2:E:1288:MET:HG3 | 2:E:1373:TYR:HE1 | 1.59                     | 0.67              |
| 2:A:1304:GLY:HA3 | 2:A:1307:ARG:HD2 | 1.76                     | 0.67              |
| 2:E:661:ARG:N    | 2:E:821:GLY:O    | 2.22                     | 0.67              |
| 2:A:729:ASP:OD1  | 2:A:731:ARG:NH1  | 2.28                     | 0.67              |
| 2:A:761:VAL:HG21 | 2:A:793:VAL:HG21 | 1.76                     | 0.67              |
| 1:C:304:VAL:O    | 1:C:320:GLU:HA   | 1.94                     | 0.67              |
| 1:C:470:TYR:C    | 1:C:471:LEU:HD12 | 2.19                     | 0.67              |
| 1:B:97:LYS:NZ    | 1:B:632:THR:O    | 2.24                     | 0.67              |
| 1:C:181:GLN:HE21 | 1:C:199:GLU:HB3  | 1.59                     | 0.67              |
| 1:B:333:ILE:HD13 | 1:B:402:VAL:HG12 | 1.77                     | 0.67              |
| 1:C:455:LEU:HB2  | 1:C:468:TYR:OH   | 1.94                     | 0.67              |
| 3:H:195:PRO:O    | 3:H:199:VAL:HG23 | 1.95                     | 0.67              |
| 2:A:1242:ASP:OD1 | 2:A:1244:LYS:NZ  | 2.28                     | 0.67              |
| 1:B:303:TYR:HA   | 1:B:322:SER:HA   | 1.76                     | 0.67              |
| 2:A:1454:ASP:OD1 | 2:A:1455:GLU:N   | 2.28                     | 0.67              |
| 1:C:443:LEU:HD12 | 1:C:444:ARG:H    | 1.60                     | 0.67              |
| 3:D:176:TYR:OH   | 3:D:211:THR:HG22 | 1.95                     | 0.66              |
| 2:A:912:MET:HA   | 2:A:915:MET:HB3  | 1.75                     | 0.66              |
| 1:C:104:GLN:HB3  | 1:C:132:HIS:CE1  | 2.30                     | 0.66              |
| 3:H:305:LEU:HG   | 3:H:309:GLN:HB2  | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:6:ILE:HB      | 1:B:20:MET:HE3    | 1.76                     | 0.66              |
| 2:A:749:TYR:HD2   | 2:A:751:TYR:CE2   | 2.12                     | 0.66              |
| 1:C:160:SER:HB3   | 1:C:167:LEU:HD21  | 1.78                     | 0.66              |
| 2:A:943:LEU:HD21  | 2:A:989:LEU:HB3   | 1.78                     | 0.66              |
| 2:A:1242:ASP:OD2  | 2:A:1271:ARG:NH2  | 2.28                     | 0.66              |
| 2:E:1272:TYR:HD2  | 2:E:1333:HIS:HB3  | 1.61                     | 0.66              |
| 1:C:242:LYS:HB3   | 1:C:274:GLY:HA3   | 1.78                     | 0.65              |
| 1:C:90:PHE:N      | 1:C:93:GLN:O      | 2.24                     | 0.65              |
| 1:B:635:ARG:NE    | 1:B:637:GLU:O     | 2.27                     | 0.65              |
| 2:A:696:ILE:C     | 2:A:697:THR:HG1   | 2.03                     | 0.65              |
| 2:A:1112:LYS:HE3  | 2:A:1118:GLU:HB3  | 1.77                     | 0.65              |
| 1:C:370:GLN:CG    | 1:C:401:THR:HB    | 2.10                     | 0.65              |
| 2:E:1309:ILE:HB   | 2:E:1314:LEU:HD13 | 1.79                     | 0.65              |
| 1:C:10:ASN:ND2    | 1:C:635:ARG:HD3   | 2.12                     | 0.65              |
| 2:E:1492:TRP:HD1  | 2:E:1499:SER:HB2  | 1.61                     | 0.65              |
| 2:E:739:ASN:O     | 2:E:740:GLU:HG3   | 1.96                     | 0.65              |
| 1:B:474:ASN:O     | 1:B:477:ARG:NH1   | 2.30                     | 0.65              |
| 2:A:976:THR:HG21  | 2:A:1003:TRP:CZ3  | 2.32                     | 0.65              |
| 3:H:178:GLU:HB3   | 3:H:208:ARG:H     | 1.59                     | 0.65              |
| 3:H:216:ARG:HD2   | 3:H:255:VAL:HG12  | 1.79                     | 0.65              |
| 1:B:438:VAL:HG11  | 1:B:449:LEU:HD21  | 1.77                     | 0.65              |
| 2:A:905:SER:O     | 2:A:911:ASN:N     | 2.29                     | 0.65              |
| 1:C:247:ALA:HB2   | 1:C:271:ILE:HD11  | 1.78                     | 0.65              |
| 1:B:78:LYS:HG3    | 2:E:1489:SER:O    | 1.96                     | 0.65              |
| 2:A:704:VAL:HG22  | 2:A:714:VAL:HG22  | 1.79                     | 0.65              |
| 1:B:311:HIS:HB3   | 2:A:1312:TYR:CD1  | 2.33                     | 0.64              |
| 2:E:1412:ARG:HB3  | 2:E:1532:PHE:CE2  | 2.32                     | 0.64              |
| 2:A:947:LYS:O     | 2:A:951:THR:OG1   | 2.08                     | 0.64              |
| 2:E:1424:VAL:HG22 | 2:E:1485:TRP:HB2  | 1.79                     | 0.64              |
| 1:B:244:GLU:HB3   | 1:B:311:HIS:ND1   | 2.11                     | 0.64              |
| 2:A:750:ASN:ND2   | 2:A:785:ILE:O     | 2.31                     | 0.64              |
| 2:A:943:LEU:HA    | 2:A:946:ILE:HD12  | 1.79                     | 0.64              |
| 3:H:225:ILE:H     | 3:H:225:ILE:HD12  | 1.63                     | 0.64              |
| 1:B:4:TYR:HB2     | 1:B:627:SER:HB3   | 1.79                     | 0.64              |
| 3:H:156:PHE:O     | 3:H:160:VAL:HG23  | 1.98                     | 0.64              |
| 1:B:528:SER:OG    | 1:B:608:GLY:O     | 2.16                     | 0.64              |
| 1:C:369:VAL:HA    | 1:C:402:VAL:HG22  | 1.80                     | 0.64              |
| 1:C:590:THR:O     | 1:C:594:ILE:HG13  | 1.98                     | 0.64              |
| 3:H:161:MET:HE1   | 3:H:184:PHE:HZ    | 1.63                     | 0.64              |
| 1:B:312:SER:OG    | 2:A:790:SER:OG    | 2.16                     | 0.63              |
| 2:A:1492:TRP:HB2  | 2:A:1501:ILE:HD11 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:247:ALA:HB3   | 1:B:269:ILE:HG13  | 1.79                     | 0.63              |
| 1:B:577:ASP:CG    | 2:A:697:THR:HG21  | 2.23                     | 0.63              |
| 1:C:439:LEU:N     | 1:C:439:LEU:HD23  | 2.13                     | 0.63              |
| 1:C:609:SER:OG    | 1:C:610:GLY:N     | 2.32                     | 0.63              |
| 1:B:266:LEU:O     | 1:B:267:LYS:HD2   | 1.98                     | 0.63              |
| 1:B:128:PHE:HA    | 1:B:165:GLY:O     | 1.98                     | 0.63              |
| 2:A:1401:GLN:HE22 | 2:A:1405:ASP:HB2  | 1.62                     | 0.63              |
| 1:C:572:VAL:HG22  | 2:E:704:VAL:HB    | 1.80                     | 0.63              |
| 2:A:753:GLN:O     | 2:A:788:LYS:NZ    | 2.22                     | 0.63              |
| 1:C:75:LYS:HB3    | 1:C:79:GLY:HA3    | 1.81                     | 0.63              |
| 1:C:316:MET:HE1   | 2:E:1365:LEU:HB2  | 1.81                     | 0.63              |
| 2:E:1474:LEU:HB3  | 2:E:1476:LEU:HG   | 1.81                     | 0.63              |
| 2:E:741:GLN:CD    | 2:E:1382:LEU:HD12 | 2.24                     | 0.63              |
| 2:A:1071:ASP:OD1  | 2:A:1098:ARG:NH1  | 2.31                     | 0.62              |
| 1:C:225:ASN:O     | 1:C:282:ARG:NH1   | 2.31                     | 0.62              |
| 3:H:168:LYS:HE3   | 3:H:168:LYS:HA    | 1.80                     | 0.62              |
| 2:A:696:ILE:HA    | 2:A:722:VAL:HG12  | 1.79                     | 0.62              |
| 2:A:739:ASN:N     | 2:A:799:PRO:HG2   | 2.14                     | 0.62              |
| 1:C:75:LYS:HD2    | 1:C:80:ARG:HG2    | 1.79                     | 0.62              |
| 1:C:102:SER:HB2   | 1:C:638:LEU:HD22  | 1.81                     | 0.62              |
| 1:C:108:LEU:HB2   | 1:C:196:PHE:HD2   | 1.64                     | 0.62              |
| 2:E:1480:LYS:HB3  | 2:E:1510:HIS:ND1  | 2.14                     | 0.62              |
| 1:C:528:SER:HB3   | 1:C:616:VAL:HG13  | 1.80                     | 0.62              |
| 1:B:282:ARG:O     | 1:B:286:LEU:HG    | 1.99                     | 0.62              |
| 1:B:558:GLN:HG2   | 2:A:691:PHE:HD1   | 1.64                     | 0.62              |
| 2:A:668:TRP:CH2   | 2:A:690:ILE:HD12  | 2.35                     | 0.62              |
| 1:C:224:TYR:HA    | 1:C:282:ARG:NH2   | 2.15                     | 0.62              |
| 2:E:770:CYS:HB3   | 2:E:798:VAL:HB    | 1.80                     | 0.62              |
| 1:B:479:LEU:HD21  | 1:B:502:ASP:HB3   | 1.80                     | 0.62              |
| 2:E:729:ASP:OD2   | 2:E:731:ARG:NH1   | 2.30                     | 0.62              |
| 2:A:796:VAL:N     | 2:A:1353:GLN:OE1  | 2.24                     | 0.62              |
| 2:A:1021:VAL:HG23 | 2:A:1023:HIS:H    | 1.64                     | 0.62              |
| 1:C:204:GLU:HB3   | 2:E:734:TYR:CE2   | 2.35                     | 0.62              |
| 2:E:760:ARG:HG2   | 6:E:1602:GOL:H11  | 1.82                     | 0.62              |
| 2:E:1317:ALA:C    | 2:E:1321:ARG:HH12 | 2.08                     | 0.62              |
| 2:A:1073:LEU:O    | 2:A:1077:TYR:N    | 2.33                     | 0.61              |
| 2:A:1134:LEU:HA   | 2:A:1137:LEU:HD12 | 1.82                     | 0.61              |
| 1:C:6:ILE:HG12    | 1:C:22:LEU:HD23   | 1.81                     | 0.61              |
| 2:E:1450:LYS:NZ   | 2:E:1541:CYS:SG   | 2.73                     | 0.61              |
| 1:B:76:SER:HB3    | 2:E:767:PRO:HB2   | 1.81                     | 0.61              |
| 1:B:577:ASP:OD1   | 2:A:697:THR:HG21  | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:334:HIS:HB2   | 1:C:353:PHE:HB3   | 1.81                     | 0.61              |
| 2:E:1288:MET:HG3  | 2:E:1373:TYR:CE1  | 2.35                     | 0.61              |
| 2:E:1427:THR:O    | 2:E:1482:TYR:N    | 2.26                     | 0.61              |
| 3:D:279:LYS:HA    | 3:D:282:GLN:CG    | 2.30                     | 0.61              |
| 1:C:37:VAL:HG11   | 1:C:68:ILE:HD11   | 1.83                     | 0.61              |
| 1:B:125:TYR:HE2   | 1:B:143:VAL:HG11  | 1.65                     | 0.61              |
| 2:E:1311:LYS:O    | 2:E:1315:ASP:N    | 2.33                     | 0.61              |
| 2:A:749:TYR:HD2   | 2:A:751:TYR:HE2   | 1.46                     | 0.61              |
| 1:C:7:ILE:HA      | 1:C:623:THR:O     | 2.00                     | 0.61              |
| 1:C:241:LYS:HG3   | 2:E:751:TYR:CE1   | 2.36                     | 0.61              |
| 1:C:541:LEU:HD23  | 2:E:715:ALA:HB2   | 1.81                     | 0.61              |
| 1:C:571:VAL:O     | 2:E:672:VAL:HA    | 2.00                     | 0.61              |
| 2:E:770:CYS:HB2   | 2:E:800:LEU:HD21  | 1.82                     | 0.61              |
| 1:B:111:GLN:HB2   | 1:B:589:LEU:HD22  | 1.83                     | 0.61              |
| 3:D:174:MET:HB2   | 3:D:222:LEU:HD11  | 1.83                     | 0.61              |
| 3:D:285:ASN:OD1   | 3:D:296:VAL:HG21  | 2.00                     | 0.61              |
| 1:C:369:VAL:N     | 1:C:375:VAL:CG2   | 2.47                     | 0.61              |
| 1:C:433:TYR:HB2   | 1:C:456:ARG:HB3   | 1.82                     | 0.61              |
| 2:A:906:GLY:HA3   | 2:A:910:GLN:HB2   | 1.83                     | 0.61              |
| 1:C:72:ARG:HH21   | 1:C:72:ARG:HG3    | 1.66                     | 0.61              |
| 1:B:23:GLU:HA     | 1:B:60:HIS:O      | 2.01                     | 0.60              |
| 1:B:440:ARG:NH2   | 1:B:441:THR:O     | 2.34                     | 0.60              |
| 2:A:736:VAL:O     | 2:A:829:VAL:N     | 2.34                     | 0.60              |
| 1:C:630:GLN:CD    | 1:C:630:GLN:H     | 2.09                     | 0.60              |
| 2:E:757:LEU:O     | 2:E:784:THR:HA    | 2.01                     | 0.60              |
| 1:B:590:THR:OG1   | 1:B:593:LYS:HG2   | 2.02                     | 0.60              |
| 2:A:1285:ILE:HD12 | 2:A:1324:LEU:HD23 | 1.83                     | 0.60              |
| 1:B:36:THR:HG23   | 1:B:48:SER:CB     | 2.31                     | 0.60              |
| 1:B:572:VAL:HG12  | 2:A:672:VAL:HG22  | 1.84                     | 0.60              |
| 2:E:1434:LEU:HD23 | 2:E:1439:ASP:HB3  | 1.83                     | 0.60              |
| 2:A:1289:THR:OG1  | 2:A:1353:GLN:N    | 2.34                     | 0.60              |
| 1:B:6:ILE:C       | 1:B:7:ILE:HG13    | 2.26                     | 0.60              |
| 1:B:365:VAL:O     | 1:B:379:THR:HG23  | 2.02                     | 0.60              |
| 3:D:279:LYS:HA    | 3:D:282:GLN:HE21  | 1.67                     | 0.60              |
| 1:C:143:VAL:O     | 1:C:155:GLN:HA    | 2.02                     | 0.60              |
| 2:E:1238:CYS:SG   | 2:E:1371:ARG:NH2  | 2.66                     | 0.60              |
| 3:H:133:SER:O     | 3:H:170:LEU:N     | 2.34                     | 0.60              |
| 2:A:894:ALA:HA    | 2:A:897:LEU:HD13  | 1.83                     | 0.60              |
| 1:C:72:ARG:HG3    | 1:C:72:ARG:NH2    | 2.17                     | 0.60              |
| 2:A:944:GLU:OE1   | 2:A:948:LYS:NZ    | 2.35                     | 0.60              |
| 1:C:46:VAL:HG11   | 1:C:68:ILE:HG23   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:403:ARG:HG2   | 1:C:416:THR:HB    | 1.83                     | 0.60              |
| 1:B:465:ILE:O     | 1:B:486:ARG:HD3   | 2.02                     | 0.59              |
| 1:C:570:ARG:NH2   | 2:E:674:ASP:OD2   | 2.34                     | 0.59              |
| 1:C:590:THR:HG22  | 1:C:592:SER:H     | 1.66                     | 0.59              |
| 2:E:1317:ALA:C    | 2:E:1321:ARG:NH1  | 2.60                     | 0.59              |
| 2:E:1428:ARG:NH2  | 2:E:1446:GLU:OE2  | 2.32                     | 0.59              |
| 1:B:77:GLU:OE2    | 1:B:77:GLU:HA     | 2.00                     | 0.59              |
| 1:B:220:PHE:HB3   | 1:B:357:PRO:HG3   | 1.83                     | 0.59              |
| 2:E:1427:THR:HB   | 2:E:1444:ALA:C    | 2.28                     | 0.59              |
| 3:D:181:ARG:HD2   | 3:D:183:HIS:CE1   | 2.38                     | 0.59              |
| 3:D:221:GLU:O     | 3:D:227:ASN:ND2   | 2.29                     | 0.59              |
| 1:C:207:LEU:HD13  | 1:C:577:ASP:OD2   | 2.02                     | 0.59              |
| 1:C:369:VAL:HG22  | 1:C:375:VAL:HG21  | 1.83                     | 0.59              |
| 2:E:1418:GLU:O    | 2:E:1421:VAL:HG22 | 2.03                     | 0.59              |
| 3:D:195:PRO:O     | 3:D:199:VAL:HG23  | 2.03                     | 0.59              |
| 1:C:46:VAL:CG1    | 1:C:69:PRO:HD2    | 2.33                     | 0.59              |
| 2:E:755:GLN:C     | 2:E:787:PRO:HG3   | 2.28                     | 0.59              |
| 1:B:367:VAL:HG12  | 1:B:404:THR:HA    | 1.83                     | 0.59              |
| 1:C:558:GLN:HA    | 2:E:690:ILE:O     | 2.03                     | 0.59              |
| 1:C:104:GLN:HB3   | 1:C:132:HIS:HE1   | 1.67                     | 0.59              |
| 2:E:745:ARG:NH2   | 2:E:1284:ASP:OD1  | 2.36                     | 0.59              |
| 2:E:1438:PHE:CD1  | 2:E:1467:PRO:HA   | 2.30                     | 0.59              |
| 1:B:166:VAL:HG12  | 1:B:168:PRO:HD3   | 1.85                     | 0.58              |
| 1:B:301:SER:HB2   | 1:B:323:GLY:C     | 2.27                     | 0.58              |
| 1:C:432:ASN:ND2   | 1:C:457:MET:SD    | 2.76                     | 0.58              |
| 1:B:4:TYR:HD2     | 1:B:627:SER:CB    | 2.16                     | 0.58              |
| 3:H:253:GLU:OE2   | 3:H:253:GLU:N     | 2.32                     | 0.58              |
| 1:B:126:ARG:CZ    | 1:B:572:VAL:HB    | 2.34                     | 0.58              |
| 2:E:1431:LYS:HB3  | 2:E:1442:ILE:HD12 | 1.85                     | 0.58              |
| 1:B:63:ASN:HD22   | 4:I:1:NAG:C7      | 2.16                     | 0.58              |
| 2:E:738:ARG:HD3   | 2:E:802:THR:HG23  | 1.85                     | 0.58              |
| 1:C:334:HIS:HB3   | 1:C:336:THR:HG23  | 1.86                     | 0.58              |
| 2:E:839:VAL:HG22  | 2:E:842:ARG:HD2   | 1.85                     | 0.58              |
| 2:A:1429:LEU:HD23 | 2:A:1477:GLU:C    | 2.28                     | 0.58              |
| 1:C:106:GLY:HA2   | 1:C:132:HIS:ND1   | 2.18                     | 0.58              |
| 1:C:8:THR:HG22    | 1:C:20:MET:HG3    | 1.86                     | 0.58              |
| 1:C:247:ALA:HB3   | 1:C:269:ILE:HG13  | 1.86                     | 0.58              |
| 2:E:1414:ASP:O    | 2:E:1418:GLU:HG3  | 2.03                     | 0.58              |
| 3:H:139:ILE:HD11  | 3:H:175:GLN:HG3   | 1.83                     | 0.58              |
| 3:D:133:SER:H     | 3:D:230:ARG:HH21  | 1.52                     | 0.58              |
| 1:C:353:PHE:HE1   | 1:C:383:GLY:HA3   | 1.69                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:453:PHE:O    | 1:C:492:LEU:HA    | 2.04                     | 0.58              |
| 3:D:267:TYR:CD1  | 3:D:295:HIS:HA    | 2.39                     | 0.58              |
| 2:A:1283:LEU:O   | 2:A:1325:ILE:HA   | 2.04                     | 0.57              |
| 1:C:239:TYR:OH   | 2:E:751:TYR:OH    | 2.18                     | 0.57              |
| 2:E:1492:TRP:O   | 2:E:1499:SER:N    | 2.34                     | 0.57              |
| 1:B:131:ASN:HB3  | 1:B:137:VAL:HG11  | 1.85                     | 0.57              |
| 1:B:153:VAL:HG21 | 1:B:182:TRP:HZ3   | 1.70                     | 0.57              |
| 1:B:255:ASP:N    | 1:B:258:GLN:O     | 2.28                     | 0.57              |
| 3:D:279:LYS:HA   | 3:D:282:GLN:NE2   | 2.18                     | 0.57              |
| 1:B:112:THR:HB   | 1:B:117:TYR:OH    | 2.04                     | 0.57              |
| 2:E:1279:THR:HA  | 2:E:1330:LYS:HD2  | 1.85                     | 0.57              |
| 2:A:750:ASN:O    | 2:A:788:LYS:N     | 2.38                     | 0.57              |
| 2:A:1275:ASP:O   | 2:A:1333:HIS:NE2  | 2.38                     | 0.57              |
| 2:A:1418:GLU:O   | 2:A:1421:VAL:HG22 | 2.04                     | 0.57              |
| 1:C:7:ILE:HG23   | 1:C:623:THR:O     | 2.04                     | 0.57              |
| 2:E:794:PRO:HG3  | 2:E:1286:SER:HB2  | 1.87                     | 0.57              |
| 1:B:486:ARG:HH12 | 1:B:488:PRO:HA    | 1.69                     | 0.57              |
| 1:C:126:ARG:NH1  | 2:E:670:TRP:O     | 2.35                     | 0.57              |
| 1:C:376:GLN:HG3  | 1:C:405:LYS:HB3   | 1.85                     | 0.57              |
| 2:E:1427:THR:OG1 | 2:E:1443:MET:HE3  | 2.04                     | 0.57              |
| 1:B:402:VAL:O    | 1:B:416:THR:HA    | 2.05                     | 0.57              |
| 2:A:812:ALA:HB1  | 2:A:818:ILE:O     | 2.05                     | 0.57              |
| 2:A:973:THR:HA   | 2:A:976:THR:HB    | 1.86                     | 0.57              |
| 3:H:152:ARG:NH1  | 3:H:300:ASN:HB3   | 2.20                     | 0.57              |
| 2:A:673:GLU:HB3  | 2:A:686:LYS:CD    | 2.35                     | 0.57              |
| 1:B:444:ARG:HH21 | 1:B:534:LYS:HE2   | 1.70                     | 0.57              |
| 1:B:4:TYR:O      | 1:B:627:SER:N     | 2.34                     | 0.56              |
| 1:B:7:ILE:HB     | 1:B:21:VAL:CG2    | 2.35                     | 0.56              |
| 2:A:1101:GLY:O   | 2:A:1104:LEU:HB3  | 2.05                     | 0.56              |
| 3:D:258:GLU:O    | 3:D:262:GLU:HG2   | 2.05                     | 0.56              |
| 3:H:137:PHE:CE1  | 3:H:161:MET:HE2   | 2.41                     | 0.56              |
| 2:A:884:VAL:HG12 | 2:A:886:GLN:H     | 1.69                     | 0.56              |
| 2:A:1060:ASN:ND2 | 1:C:287:ASP:O     | 2.36                     | 0.56              |
| 1:C:386:LYS:NZ   | 1:C:439:LEU:HA    | 2.14                     | 0.56              |
| 2:A:958:GLN:NE2  | 2:A:967:VAL:O     | 2.37                     | 0.56              |
| 2:E:1511:TRP:HD1 | 2:E:1512:PRO:O    | 1.89                     | 0.56              |
| 1:B:469:THR:HB   | 1:B:512:TYR:CE1   | 2.40                     | 0.56              |
| 1:B:510:VAL:HG12 | 1:B:528:SER:CB    | 2.35                     | 0.56              |
| 1:C:47:LEU:HG    | 1:C:49:SER:H      | 1.71                     | 0.56              |
| 3:H:141:GLY:HA3  | 3:H:175:GLN:NE2   | 2.20                     | 0.56              |
| 2:A:774:THR:HG1  | 2:A:777:ARG:H     | 1.52                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:33:VAL:HA    | 1:C:89:THR:O      | 2.04                     | 0.56              |
| 2:A:1038:MET:HE1 | 2:A:1076:ASN:HB2  | 1.87                     | 0.56              |
| 2:A:1281:SER:C   | 2:A:1282:ILE:HD12 | 2.31                     | 0.56              |
| 3:H:216:ARG:HA   | 3:H:219:VAL:HG22  | 1.88                     | 0.56              |
| 2:A:996:VAL:HG23 | 2:A:997:LEU:HD13  | 1.88                     | 0.56              |
| 1:C:321:ARG:HG2  | 1:C:324:ILE:HD11  | 1.86                     | 0.56              |
| 2:A:1429:LEU:HG  | 2:A:1478:GLU:HA   | 1.88                     | 0.56              |
| 2:E:655:GLU:HG2  | 2:E:810:LYS:HD2   | 1.88                     | 0.56              |
| 1:B:14:LEU:HD12  | 1:B:103:LEU:HD13  | 1.88                     | 0.56              |
| 1:B:23:GLU:OE2   | 1:B:512:TYR:OH    | 2.19                     | 0.56              |
| 1:C:368:ALA:HB1  | 1:C:375:VAL:HG22  | 1.88                     | 0.56              |
| 1:B:229:LEU:HB3  | 1:B:280:LEU:HB3   | 1.88                     | 0.56              |
| 2:A:1492:TRP:HB3 | 2:A:1499:SER:HB2  | 1.87                     | 0.56              |
| 1:C:438:VAL:C    | 1:C:439:LEU:HD23  | 2.31                     | 0.56              |
| 1:B:185:ARG:HD3  | 1:B:195:VAL:HG11  | 1.88                     | 0.55              |
| 2:A:1256:ARG:HB3 | 2:A:1260:ALA:O    | 2.06                     | 0.55              |
| 2:A:1504:LYS:HE2 | 1:C:80:ARG:HH12   | 1.71                     | 0.55              |
| 1:C:7:ILE:HB     | 1:C:21:VAL:CG1    | 2.36                     | 0.55              |
| 1:C:334:HIS:N    | 1:C:353:PHE:O     | 2.39                     | 0.55              |
| 2:E:833:ILE:HG23 | 2:E:834:ARG:H     | 1.72                     | 0.55              |
| 2:E:1297:ASP:O   | 2:E:1301:LEU:HG   | 2.07                     | 0.55              |
| 2:E:1399:PHE:CE2 | 2:E:1400:ILE:O    | 2.59                     | 0.55              |
| 1:C:3:MET:HE2    | 1:C:626:SER:CB    | 2.36                     | 0.55              |
| 1:C:154:LYS:HE2  | 1:C:156:ASP:OD2   | 2.06                     | 0.55              |
| 3:H:160:VAL:O    | 3:H:164:LEU:HB2   | 2.07                     | 0.55              |
| 1:B:404:THR:OG1  | 1:B:414:GLN:OE1   | 2.18                     | 0.55              |
| 2:A:829:VAL:HG12 | 2:A:830:PRO:O     | 2.07                     | 0.55              |
| 1:C:128:PHE:CD2  | 2:E:706:MET:SD    | 2.98                     | 0.55              |
| 2:A:1315:ASP:OD1 | 2:A:1316:LYS:N    | 2.39                     | 0.55              |
| 1:C:535:ASP:HB3  | 1:C:595:TRP:CD1   | 2.42                     | 0.55              |
| 1:B:71:ASN:OD1   | 1:B:73:GLU:HG2    | 2.07                     | 0.55              |
| 1:B:110:ILE:HD11 | 1:B:186:ALA:HB3   | 1.89                     | 0.55              |
| 2:A:833:ILE:HG13 | 2:A:834:ARG:O     | 2.07                     | 0.55              |
| 2:A:1165:SER:O   | 2:A:1165:SER:OG   | 2.18                     | 0.55              |
| 2:E:786:PRO:HG2  | 2:E:789:SER:CB    | 2.35                     | 0.55              |
| 3:D:236:ILE:HG13 | 3:D:265:ILE:HB    | 1.89                     | 0.55              |
| 1:C:542:VAL:CG1  | 1:C:544:LYS:HE3   | 2.36                     | 0.55              |
| 1:C:248:PHE:HB2  | 1:C:307:THR:HB    | 1.89                     | 0.55              |
| 1:C:292:PRO:HB2  | 1:C:293:ARG:CZ    | 2.37                     | 0.55              |
| 2:E:1457:GLN:N   | 2:E:1460:GLN:OE1  | 2.37                     | 0.55              |
| 2:A:677:GLU:OE1  | 2:A:677:GLU:N     | 2.37                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:1045:LEU:HD11 | 2:A:1066:ILE:HG23 | 1.89                     | 0.55              |
| 2:A:1357:VAL:O    | 2:A:1370:THR:HA   | 2.07                     | 0.55              |
| 3:D:132:ASP:HB3   | 3:D:233:ALA:HA    | 1.88                     | 0.55              |
| 1:C:107:TYR:HA    | 1:C:196:PHE:CE2   | 2.41                     | 0.55              |
| 1:C:109:PHE:HB2   | 1:C:128:PHE:HB2   | 1.89                     | 0.55              |
| 2:E:696:ILE:HG23  | 2:E:723:MET:HA    | 1.88                     | 0.55              |
| 3:H:137:PHE:CE1   | 3:H:171:PHE:HD1   | 2.15                     | 0.55              |
| 1:B:5:SER:HB2     | 1:B:624:PHE:CE1   | 2.42                     | 0.54              |
| 1:B:603:ILE:HG13  | 1:B:621:GLY:HA3   | 1.90                     | 0.54              |
| 2:A:749:TYR:CD2   | 2:A:751:TYR:HE2   | 2.25                     | 0.54              |
| 2:A:1271:ARG:HH22 | 2:A:1273:ARG:NH1  | 2.05                     | 0.54              |
| 1:C:179:MET:HB3   | 1:C:202:VAL:O     | 2.07                     | 0.54              |
| 1:C:469:THR:HB    | 1:C:512:TYR:CE1   | 2.42                     | 0.54              |
| 3:H:151:ARG:O     | 3:H:155:GLU:HG2   | 2.07                     | 0.54              |
| 1:B:220:PHE:CZ    | 1:B:330:PRO:HB3   | 2.43                     | 0.54              |
| 2:A:698:THR:HA    | 2:A:720:VAL:O     | 2.07                     | 0.54              |
| 2:A:1382:LEU:HD12 | 2:A:1382:LEU:H    | 1.72                     | 0.54              |
| 2:A:1511:TRP:CD2  | 2:A:1529:LEU:HD13 | 2.43                     | 0.54              |
| 1:C:166:VAL:O     | 1:C:167:LEU:HD23  | 2.07                     | 0.54              |
| 2:A:919:VAL:HG11  | 2:A:982:VAL:HG22  | 1.89                     | 0.54              |
| 2:A:1466:SER:HB2  | 2:A:1502:ILE:HD12 | 1.89                     | 0.54              |
| 2:E:791:LEU:HG    | 2:E:1322:ASN:HD21 | 1.72                     | 0.54              |
| 1:B:554:VAL:HB    | 1:B:557:GLN:HB2   | 1.89                     | 0.54              |
| 2:A:942:ALA:O     | 2:A:946:ILE:N     | 2.34                     | 0.54              |
| 1:C:544:LYS:O     | 1:C:561:LEU:HD12  | 2.07                     | 0.54              |
| 2:E:1327:TYR:C    | 2:E:1328:LEU:HD23 | 2.33                     | 0.54              |
| 1:B:251:PHE:HA    | 1:B:304:VAL:HG22  | 1.90                     | 0.54              |
| 1:C:149:GLU:OE1   | 1:C:149:GLU:N     | 2.34                     | 0.54              |
| 1:C:343:LYS:HZ1   | 1:C:609:SER:HB2   | 1.72                     | 0.54              |
| 1:C:472:ILE:HD12  | 1:C:480:LYS:HB3   | 1.90                     | 0.54              |
| 2:A:1240:LYS:HG3  | 2:A:1272:TYR:CE1  | 2.42                     | 0.54              |
| 1:C:302:LEU:HB2   | 1:C:324:ILE:HB    | 1.89                     | 0.54              |
| 2:A:938:LYS:O     | 2:A:941:GLY:N     | 2.41                     | 0.54              |
| 1:C:540:SER:OG    | 2:E:683:ILE:HD11  | 2.07                     | 0.54              |
| 1:B:254:GLN:OE1   | 1:B:259:ARG:NH2   | 2.41                     | 0.54              |
| 2:A:1145:PHE:HE1  | 3:D:207:GLY:HA2   | 1.72                     | 0.54              |
| 2:A:1352:ILE:HG13 | 2:A:1374:HIS:NE2  | 2.18                     | 0.54              |
| 1:C:124:LEU:HB3   | 2:E:670:TRP:NE1   | 2.23                     | 0.54              |
| 1:C:410:SER:OG    | 1:C:413:GLU:HG3   | 2.07                     | 0.54              |
| 2:E:1442:ILE:HG22 | 2:E:1461:GLN:OE1  | 2.08                     | 0.54              |
| 1:B:624:PHE:H     | 1:B:632:THR:HG23  | 1.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:974:TRP:CZ2   | 2:A:1027:ILE:HA   | 2.43                     | 0.53              |
| 1:C:494:VAL:O     | 1:C:496:PRO:HD3   | 2.08                     | 0.53              |
| 1:C:526:ALA:HB3   | 1:C:613:TYR:HA    | 1.89                     | 0.53              |
| 1:C:624:PHE:H     | 1:C:632:THR:CG2   | 2.22                     | 0.53              |
| 2:E:1290:GLY:HA2  | 2:E:1346:TYR:CE2  | 2.43                     | 0.53              |
| 2:E:1308:TYR:CZ   | 2:E:1310:SER:HA   | 2.43                     | 0.53              |
| 1:C:6:ILE:HD13    | 1:C:20:MET:CE     | 2.37                     | 0.53              |
| 1:C:15:GLU:HG2    | 1:C:69:PRO:HA     | 1.89                     | 0.53              |
| 1:C:156:ASP:HB3   | 1:C:158:LEU:HD11  | 1.89                     | 0.53              |
| 2:A:1009:GLN:HG3  | 2:A:1015:PHE:CZ   | 2.43                     | 0.53              |
| 1:C:248:PHE:HD1   | 1:C:307:THR:O     | 1.90                     | 0.53              |
| 2:A:1293:PRO:HB3  | 2:A:1341:PHE:CE1  | 2.44                     | 0.53              |
| 2:A:1407:VAL:HG23 | 2:A:1412:ARG:CZ   | 2.38                     | 0.53              |
| 1:C:292:PRO:HB2   | 1:C:293:ARG:NH1   | 2.24                     | 0.53              |
| 1:C:403:ARG:NH1   | 1:C:414:GLN:HB2   | 2.23                     | 0.53              |
| 3:H:175:GLN:HB2   | 3:H:183:HIS:CD2   | 2.44                     | 0.53              |
| 1:B:249:VAL:O     | 1:B:266:LEU:HA    | 2.09                     | 0.53              |
| 1:B:377:SER:OG    | 1:B:378:LEU:N     | 2.39                     | 0.53              |
| 2:A:776:LYS:NZ    | 2:A:1505:ASP:OD1  | 2.30                     | 0.53              |
| 2:A:802:THR:HG21  | 2:A:830:PRO:HG3   | 1.88                     | 0.53              |
| 3:D:186:PHE:HB2   | 3:D:228:GLY:HA3   | 1.90                     | 0.53              |
| 3:D:213:THR:OG1   | 3:D:250:LEU:HB2   | 2.08                     | 0.53              |
| 1:C:74:PHE:O      | 1:C:75:LYS:HG2    | 2.09                     | 0.53              |
| 1:C:547:GLN:NE2   | 1:C:559:MET:HG3   | 2.23                     | 0.53              |
| 2:E:1263:THR:HA   | 2:E:1343:VAL:O    | 2.09                     | 0.53              |
| 2:A:912:MET:SD    | 2:A:982:VAL:HG11  | 2.48                     | 0.53              |
| 1:C:46:VAL:HG12   | 1:C:68:ILE:HD12   | 1.89                     | 0.53              |
| 1:C:46:VAL:HG12   | 1:C:69:PRO:HD2    | 1.90                     | 0.53              |
| 1:C:220:PHE:HA    | 1:C:325:PRO:HD2   | 1.91                     | 0.53              |
| 2:E:1385:LEU:O    | 2:E:1391:CYS:HA   | 2.08                     | 0.53              |
| 2:E:1404:ASP:OD1  | 2:E:1406:LYS:HG2  | 2.08                     | 0.53              |
| 2:E:1492:TRP:CD1  | 2:E:1499:SER:HB2  | 2.41                     | 0.53              |
| 2:A:771:SER:HB3   | 2:A:797:ILE:HG22  | 1.90                     | 0.53              |
| 2:A:1267:GLU:C    | 2:A:1268:ILE:HG13 | 2.33                     | 0.53              |
| 1:C:210:PHE:HA    | 1:C:237:PHE:HA    | 1.91                     | 0.53              |
| 2:A:1428:ARG:NH1  | 2:A:1446:GLU:OE2  | 2.41                     | 0.53              |
| 1:C:437:SER:O     | 1:C:452:ASN:ND2   | 2.39                     | 0.53              |
| 2:E:807:VAL:O     | 2:E:823:ARG:HA    | 2.08                     | 0.53              |
| 1:C:440:ARG:NH1   | 1:C:440:ARG:CB    | 2.71                     | 0.53              |
| 2:E:1366:GLU:OE1  | 2:E:1366:GLU:N    | 2.42                     | 0.53              |
| 1:B:549:GLU:OE1   | 1:B:549:GLU:N     | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:588:LYS:O     | 1:C:593:LYS:NZ    | 2.26                     | 0.53              |
| 1:B:576:VAL:O     | 2:A:700:GLU:N     | 2.38                     | 0.52              |
| 2:E:1429:LEU:HG   | 2:E:1478:GLU:HA   | 1.91                     | 0.52              |
| 2:A:813:VAL:CG2   | 2:A:818:ILE:HB    | 2.38                     | 0.52              |
| 2:A:1465:ILE:HD11 | 2:A:1501:ILE:HG23 | 1.92                     | 0.52              |
| 3:D:257:PRO:O     | 3:D:261:ARG:HG3   | 2.10                     | 0.52              |
| 1:C:474:ASN:O     | 1:C:477:ARG:HG3   | 2.10                     | 0.52              |
| 3:H:216:ARG:NE    | 3:H:258:GLU:OE1   | 2.36                     | 0.52              |
| 3:H:278:GLU:O     | 3:H:281:ARG:HG2   | 2.10                     | 0.52              |
| 1:B:6:ILE:HB      | 1:B:20:MET:CE     | 2.40                     | 0.52              |
| 2:A:1377:LYS:HD2  | 2:A:1377:LYS:N    | 2.24                     | 0.52              |
| 3:D:210:HIS:NE2   | 3:D:247:GLY:O     | 2.42                     | 0.52              |
| 1:C:128:PHE:HZ    | 1:C:572:VAL:HG21  | 1.75                     | 0.52              |
| 1:C:268:ARG:HH12  | 2:E:1328:LEU:C    | 2.17                     | 0.52              |
| 1:C:316:MET:SD    | 2:E:1365:LEU:HD22 | 2.50                     | 0.52              |
| 1:C:366:PRO:HA    | 1:C:377:SER:O     | 2.09                     | 0.52              |
| 2:E:1266:LEU:O    | 2:E:1340:ALA:HA   | 2.09                     | 0.52              |
| 3:H:151:ARG:NH2   | 3:H:155:GLU:OE2   | 2.42                     | 0.52              |
| 1:B:242:LYS:HD3   | 1:B:273:ASP:O     | 2.10                     | 0.52              |
| 1:B:474:ASN:OD1   | 1:B:477:ARG:NH2   | 2.41                     | 0.52              |
| 2:A:1457:GLN:O    | 2:A:1460:GLN:HG3  | 2.09                     | 0.52              |
| 2:E:765:HIS:ND1   | 2:E:773:ALA:O     | 2.26                     | 0.52              |
| 1:B:216:PRO:HA    | 1:B:231:VAL:HA    | 1.90                     | 0.52              |
| 1:C:295:GLU:O     | 1:C:298:VAL:HG12  | 2.09                     | 0.52              |
| 2:E:1520:GLU:HA   | 2:E:1523:GLN:HG3  | 1.91                     | 0.52              |
| 2:E:1247:ILE:HG13 | 2:E:1265:ILE:O    | 2.09                     | 0.52              |
| 2:E:1416:ALA:O    | 2:E:1421:VAL:HG21 | 2.10                     | 0.52              |
| 1:B:109:PHE:HB2   | 1:B:128:PHE:HB2   | 1.91                     | 0.52              |
| 1:B:148:PRO:HD3   | 1:B:182:TRP:CD1   | 2.44                     | 0.52              |
| 2:A:1450:LYS:HG2  | 2:A:1451:SER:O    | 2.10                     | 0.52              |
| 2:A:1528:ASP:O    | 2:A:1532:PHE:N    | 2.41                     | 0.52              |
| 1:C:270:PRO:O     | 1:C:271:ILE:HD13  | 2.10                     | 0.52              |
| 1:C:451:VAL:O     | 1:C:494:VAL:HA    | 2.09                     | 0.52              |
| 2:E:1426:LYS:HA   | 2:E:1483:LEU:HA   | 1.91                     | 0.52              |
| 2:A:1349:VAL:HG22 | 2:A:1350:GLU:H    | 1.74                     | 0.52              |
| 1:C:128:PHE:HA    | 1:C:165:GLY:O     | 2.09                     | 0.52              |
| 1:C:343:LYS:HZ3   | 1:C:527:ASP:CG    | 2.12                     | 0.52              |
| 1:B:36:THR:HA     | 1:B:48:SER:HA     | 1.90                     | 0.52              |
| 1:B:566:ASP:CG    | 2:A:710:LYS:HG2   | 2.35                     | 0.52              |
| 2:A:1074:GLU:HG3  | 2:A:1103:LEU:HD13 | 1.92                     | 0.52              |
| 2:A:1159:TYR:HA   | 2:A:1173:PHE:HZ   | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:353:PHE:CE1   | 1:C:383:GLY:HA3   | 2.44                     | 0.52              |
| 2:E:808:GLU:HG3   | 2:E:822:VAL:O     | 2.10                     | 0.52              |
| 3:H:178:GLU:HB3   | 3:H:208:ARG:N     | 2.23                     | 0.52              |
| 3:H:276:ARG:HE    | 3:H:277:SER:N     | 2.07                     | 0.52              |
| 1:B:3:MET:HG3     | 1:B:628:SER:OG    | 2.09                     | 0.52              |
| 2:A:1467:PRO:HD2  | 2:A:1470:CYS:SG   | 2.50                     | 0.52              |
| 1:B:97:LYS:HD3    | 1:B:631:GLN:OE1   | 2.11                     | 0.51              |
| 2:A:706:MET:HG3   | 2:A:711:GLY:O     | 2.09                     | 0.51              |
| 2:A:1409:LEU:HB2  | 2:A:1528:ASP:CB   | 2.37                     | 0.51              |
| 2:A:1535:SER:O    | 2:A:1539:PHE:HB2  | 2.11                     | 0.51              |
| 1:B:126:ARG:HG3   | 2:A:670:TRP:CZ2   | 2.45                     | 0.51              |
| 1:C:181:GLN:NE2   | 1:C:199:GLU:HB3   | 2.25                     | 0.51              |
| 1:C:426:THR:HG21  | 1:C:431:ASN:N     | 2.20                     | 0.51              |
| 1:B:332:GLN:HB2   | 1:B:355:THR:OG1   | 2.11                     | 0.51              |
| 2:E:658:ILE:O     | 2:E:810:LYS:HE2   | 2.11                     | 0.51              |
| 2:E:799:PRO:HB2   | 2:E:828:VAL:HG11  | 1.92                     | 0.51              |
| 3:H:178:GLU:HB3   | 3:H:208:ARG:HB2   | 1.92                     | 0.51              |
| 2:A:969:ARG:NH1   | 2:A:1022:ILE:HD11 | 2.25                     | 0.51              |
| 2:E:1333:HIS:HD1  | 2:E:1333:HIS:H    | 1.57                     | 0.51              |
| 2:A:813:VAL:HG22  | 2:A:818:ILE:HB    | 1.92                     | 0.51              |
| 3:D:213:THR:OG1   | 3:D:248:ASP:OD1   | 2.19                     | 0.51              |
| 3:D:305:LEU:HG    | 3:D:306:LYS:N     | 2.26                     | 0.51              |
| 1:C:138:GLY:O     | 1:C:139:ARG:NH1   | 2.35                     | 0.51              |
| 1:C:434:LEU:HB2   | 1:C:513:TYR:CE2   | 2.46                     | 0.51              |
| 1:B:37:VAL:O      | 1:B:46:VAL:N      | 2.43                     | 0.51              |
| 1:B:333:ILE:HB    | 1:B:417:ARG:HB2   | 1.93                     | 0.51              |
| 1:B:453:PHE:O     | 1:B:492:LEU:HA    | 2.10                     | 0.51              |
| 3:D:201:PRO:O     | 3:D:203:THR:HG23  | 2.11                     | 0.51              |
| 1:C:81:ASN:HB3    | 1:C:100:LEU:HD11  | 1.93                     | 0.51              |
| 1:B:424:TYR:OH    | 1:B:613:TYR:HB3   | 2.11                     | 0.51              |
| 3:D:148:HIS:CE1   | 3:D:151:ARG:HH21  | 2.29                     | 0.51              |
| 3:D:148:HIS:HE2   | 3:D:152:ARG:HE    | 1.59                     | 0.51              |
| 2:E:1318:PHE:N    | 2:E:1321:ARG:NH1  | 2.57                     | 0.51              |
| 2:A:831:GLU:O     | 2:A:833:ILE:HG23  | 2.10                     | 0.51              |
| 2:A:1093:LEU:O    | 2:A:1098:ARG:N    | 2.43                     | 0.51              |
| 2:A:1430:VAL:HG21 | 2:A:1444:ALA:HB2  | 1.93                     | 0.51              |
| 1:C:114:LYS:HB2   | 1:C:117:TYR:CZ    | 2.45                     | 0.51              |
| 1:C:207:LEU:HD11  | 2:E:666:GLU:HG2   | 1.93                     | 0.51              |
| 1:B:221:TYR:CE1   | 1:B:225:ASN:HB3   | 2.46                     | 0.51              |
| 2:E:1281:SER:C    | 2:E:1282:ILE:HD12 | 2.36                     | 0.51              |
| 1:B:348:PHE:CE2   | 1:B:419:MET:HE1   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:463:ALA:HA    | 1:B:488:PRO:HB3   | 1.93                     | 0.50              |
| 1:C:6:ILE:HA      | 1:C:21:VAL:O      | 2.11                     | 0.50              |
| 1:C:353:PHE:CE2   | 1:C:355:THR:HG22  | 2.45                     | 0.50              |
| 3:H:276:ARG:HH21  | 3:H:277:SER:HG    | 1.53                     | 0.50              |
| 1:B:226:GLU:H     | 1:B:226:GLU:CD    | 2.14                     | 0.50              |
| 2:A:738:ARG:HH11  | 2:A:830:PRO:HB3   | 1.76                     | 0.50              |
| 2:A:1133:ALA:HA   | 2:A:1136:ALA:HB3  | 1.93                     | 0.50              |
| 2:A:1309:ILE:HD11 | 2:A:1326:ILE:HG12 | 1.93                     | 0.50              |
| 3:D:176:TYR:HB2   | 3:D:180:PHE:CD2   | 2.46                     | 0.50              |
| 1:C:2:PRO:HG3     | 1:C:26:ASP:O      | 2.10                     | 0.50              |
| 1:B:27:ALA:O      | 1:B:60:HIS:NE2    | 2.45                     | 0.50              |
| 1:B:577:ASP:OD2   | 2:A:697:THR:HG21  | 2.10                     | 0.50              |
| 2:A:855:GLN:HG3   | 2:A:855:GLN:O     | 2.12                     | 0.50              |
| 2:A:1412:ARG:NH2  | 2:A:1509:GLU:OE2  | 2.42                     | 0.50              |
| 1:C:367:VAL:O     | 1:C:376:GLN:HA    | 2.11                     | 0.50              |
| 1:C:376:GLN:HG3   | 1:C:405:LYS:CB    | 2.41                     | 0.50              |
| 1:C:613:TYR:CE2   | 1:C:630:GLN:HB3   | 2.46                     | 0.50              |
| 2:E:1288:MET:O    | 2:E:1289:THR:C    | 2.54                     | 0.50              |
| 2:A:972:SER:OG    | 2:A:973:THR:N     | 2.44                     | 0.50              |
| 2:A:1331:VAL:HG23 | 2:A:1337:ASP:HB2  | 1.93                     | 0.50              |
| 1:C:591:GLN:O     | 1:C:594:ILE:HB    | 2.11                     | 0.50              |
| 2:E:662:SER:OG    | 2:E:694:ASP:OD2   | 2.26                     | 0.50              |
| 2:E:1313:GLU:OE1  | 2:E:1313:GLU:N    | 2.39                     | 0.50              |
| 2:A:896:ARG:HD3   | 2:A:1159:TYR:CZ   | 2.47                     | 0.50              |
| 2:A:1281:SER:O    | 2:A:1282:ILE:HD12 | 2.12                     | 0.50              |
| 2:A:1477:GLU:OE1  | 2:A:1480:LYS:NZ   | 2.42                     | 0.50              |
| 1:C:116:ILE:HG12  | 1:C:205:TYR:CE1   | 2.46                     | 0.50              |
| 1:C:353:PHE:CE1   | 1:C:361:PRO:HB3   | 2.47                     | 0.50              |
| 1:C:376:GLN:HE21  | 1:C:405:LYS:HB3   | 1.77                     | 0.50              |
| 3:H:132:ASP:O     | 3:H:234:PHE:N     | 2.42                     | 0.50              |
| 1:B:182:TRP:HB2   | 1:B:200:PHE:CE1   | 2.47                     | 0.50              |
| 1:B:182:TRP:O     | 1:B:199:GLU:HA    | 2.11                     | 0.50              |
| 1:B:475:LYS:HB2   | 1:B:477:ARG:NH1   | 2.27                     | 0.50              |
| 1:B:639:GLN:N     | 1:B:639:GLN:OE1   | 2.45                     | 0.50              |
| 3:D:166:LYS:O     | 3:D:169:THR:HG23  | 2.11                     | 0.50              |
| 3:H:165:LYS:HD3   | 3:H:165:LYS:C     | 2.35                     | 0.50              |
| 1:B:131:ASN:HB3   | 1:B:137:VAL:CG1   | 2.42                     | 0.50              |
| 1:B:506:SER:HA    | 1:B:533:VAL:HG23  | 1.94                     | 0.50              |
| 1:B:510:VAL:HG12  | 1:B:528:SER:HB2   | 1.94                     | 0.50              |
| 1:B:553:PRO:HG2   | 2:A:720:VAL:HG13  | 1.94                     | 0.50              |
| 2:A:735:SER:CB    | 2:A:827:LYS:HB2   | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:894:ALA:HB2   | 2:A:930:GLN:OE1   | 2.12                     | 0.50              |
| 2:A:964:ALA:HB2   | 2:A:971:PRO:CA    | 2.41                     | 0.50              |
| 2:A:998:CYS:O     | 2:A:1059:VAL:HG21 | 2.11                     | 0.50              |
| 2:A:1294:ASP:OD2  | 2:A:1297:ASP:N    | 2.44                     | 0.50              |
| 1:C:128:PHE:CZ    | 1:C:572:VAL:HG21  | 2.46                     | 0.50              |
| 1:C:556:GLY:N     | 2:E:692:LEU:O     | 2.34                     | 0.50              |
| 2:E:673:GLU:HB3   | 2:E:686:LYS:HE3   | 1.93                     | 0.50              |
| 2:E:1424:VAL:O    | 2:E:1449:ILE:HB   | 2.12                     | 0.50              |
| 3:H:133:SER:HB2   | 3:H:169:THR:CA    | 2.34                     | 0.50              |
| 1:B:577:ASP:OD1   | 2:A:697:THR:CG2   | 2.60                     | 0.50              |
| 2:A:1294:ASP:N    | 2:A:1342:LYS:O    | 2.45                     | 0.50              |
| 1:C:148:PRO:HD3   | 1:C:182:TRP:CD1   | 2.46                     | 0.50              |
| 2:E:1308:TYR:OH   | 2:E:1310:SER:HA   | 2.11                     | 0.50              |
| 2:A:764:LEU:HD11  | 2:A:810:LYS:HD2   | 1.94                     | 0.50              |
| 2:A:813:VAL:HG23  | 2:A:816:HIS:HB2   | 1.92                     | 0.50              |
| 2:A:916:THR:HA    | 2:A:919:VAL:HG12  | 1.94                     | 0.50              |
| 2:A:1135:LEU:O    | 2:A:1139:GLN:HG2  | 2.12                     | 0.50              |
| 1:C:362:ALA:HB1   | 1:C:365:VAL:HG21  | 1.93                     | 0.50              |
| 1:C:573:LEU:HD12  | 2:E:671:ASN:HB3   | 1.93                     | 0.50              |
| 2:E:1268:ILE:HD12 | 2:E:1339:LEU:HD11 | 1.93                     | 0.50              |
| 1:B:7:ILE:HB      | 1:B:21:VAL:HG23   | 1.93                     | 0.49              |
| 2:A:956:PHE:HB2   | 2:A:967:VAL:HG13  | 1.92                     | 0.49              |
| 2:A:1408:THR:H    | 2:A:1411:GLU:HB2  | 1.77                     | 0.49              |
| 2:A:1408:THR:HG23 | 2:A:1411:GLU:HG3  | 1.94                     | 0.49              |
| 3:D:289:SER:OG    | 3:D:295:HIS:HD2   | 1.95                     | 0.49              |
| 1:C:204:GLU:HB3   | 2:E:734:TYR:CD2   | 2.47                     | 0.49              |
| 2:E:696:ILE:HG21  | 2:E:723:MET:HG3   | 1.94                     | 0.49              |
| 2:E:1412:ARG:HB3  | 2:E:1532:PHE:HE2  | 1.73                     | 0.49              |
| 1:B:14:LEU:HD22   | 1:B:68:ILE:HG21   | 1.93                     | 0.49              |
| 2:A:1152:TRP:O    | 2:A:1156:GLN:HG2  | 2.12                     | 0.49              |
| 3:D:142:SER:HB3   | 3:D:208:ARG:O     | 2.12                     | 0.49              |
| 1:C:339:PRO:HB3   | 1:C:608:GLY:HA3   | 1.95                     | 0.49              |
| 1:C:542:VAL:O     | 1:C:563:ILE:HA    | 2.13                     | 0.49              |
| 2:E:1264:MET:O    | 2:E:1343:VAL:HG22 | 2.12                     | 0.49              |
| 3:H:146:ILE:HG12  | 3:H:149:ASP:CG    | 2.37                     | 0.49              |
| 2:E:1364:ASN:CG   | 2:E:1367:GLU:HG2  | 2.36                     | 0.49              |
| 2:E:1429:LEU:HB3  | 2:E:1478:GLU:HA   | 1.95                     | 0.49              |
| 1:B:308:VAL:N     | 1:B:317:VAL:O     | 2.30                     | 0.49              |
| 2:A:1457:GLN:HB2  | 2:A:1460:GLN:HE21 | 1.77                     | 0.49              |
| 3:D:266:ARG:NH2   | 3:D:289:SER:HB3   | 2.28                     | 0.49              |
| 1:C:395:GLN:O     | 1:C:423:PRO:HG3   | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:452:ASN:HB3   | 1:C:492:LEU:HD11  | 1.94                     | 0.49              |
| 1:C:577:ASP:OD1   | 1:C:579:GLY:N     | 2.33                     | 0.49              |
| 1:B:39:ASP:CG     | 1:B:44:LYS:HG2    | 2.37                     | 0.49              |
| 2:A:1083:SER:HA   | 2:A:1086:VAL:HB   | 1.95                     | 0.49              |
| 2:A:1144:ASP:O    | 2:A:1147:PRO:HD2  | 2.11                     | 0.49              |
| 2:E:1246:THR:O    | 2:E:1267:GLU:HB3  | 2.12                     | 0.49              |
| 2:E:1318:PHE:HA   | 2:E:1321:ARG:NH1  | 2.27                     | 0.49              |
| 3:H:175:GLN:CD    | 3:H:205:LEU:HD13  | 2.38                     | 0.49              |
| 1:B:346:MET:N     | 1:B:391:THR:OG1   | 2.46                     | 0.49              |
| 1:B:560:THR:HG22  | 2:A:687:LEU:HD12  | 1.94                     | 0.49              |
| 2:A:1012:ASP:OD1  | 2:A:1012:ASP:N    | 2.45                     | 0.49              |
| 2:A:1086:VAL:CG1  | 2:A:1107:PHE:HA   | 2.43                     | 0.49              |
| 2:A:1324:LEU:HD21 | 2:A:1326:ILE:HD11 | 1.95                     | 0.49              |
| 1:C:366:PRO:O     | 1:C:404:THR:OG1   | 2.25                     | 0.49              |
| 1:B:10:ASN:ND2    | 1:B:621:GLY:HA2   | 2.28                     | 0.49              |
| 1:B:130:VAL:HB    | 1:B:134:LEU:HA    | 1.95                     | 0.49              |
| 1:B:475:LYS:HB2   | 1:B:477:ARG:HH12  | 1.77                     | 0.49              |
| 2:A:1405:ASP:CG   | 2:A:1406:LYS:H    | 2.20                     | 0.49              |
| 1:C:251:PHE:HD1   | 1:C:304:VAL:HG13  | 1.78                     | 0.49              |
| 2:E:779:HIS:CE1   | 2:E:781:GLN:HE22  | 2.30                     | 0.49              |
| 1:B:304:VAL:N     | 1:B:321:ARG:O     | 2.36                     | 0.49              |
| 3:D:187:LYS:O     | 3:D:190:GLN:N     | 2.45                     | 0.49              |
| 1:C:3:MET:N       | 1:C:25:HIS:O      | 2.40                     | 0.49              |
| 1:C:406:LYS:O     | 1:C:414:GLN:NE2   | 2.46                     | 0.49              |
| 2:E:817:PHE:C     | 3:H:282:GLN:HE21  | 2.21                     | 0.49              |
| 1:C:107:TYR:HA    | 1:C:196:PHE:HE2   | 1.78                     | 0.49              |
| 1:C:135:LEU:HD22  | 2:E:708:ASP:O     | 2.13                     | 0.49              |
| 1:C:572:VAL:CG2   | 2:E:704:VAL:HB    | 2.43                     | 0.49              |
| 2:E:665:PRO:HG2   | 2:E:668:TRP:CD1   | 2.48                     | 0.49              |
| 1:B:36:THR:HG23   | 1:B:48:SER:HB3    | 1.95                     | 0.48              |
| 1:B:330:PRO:HG2   | 1:B:409:LEU:HD21  | 1.95                     | 0.48              |
| 1:B:403:ARG:HA    | 1:B:415:ALA:O     | 2.12                     | 0.48              |
| 1:B:575:ALA:CB    | 2:A:701:ILE:HG12  | 2.42                     | 0.48              |
| 2:A:700:GLU:HG3   | 2:A:717:PRO:HB3   | 1.95                     | 0.48              |
| 2:A:1240:LYS:HG3  | 2:A:1272:TYR:HE1  | 1.78                     | 0.48              |
| 1:C:443:LEU:HD12  | 1:C:444:ARG:N     | 2.26                     | 0.48              |
| 2:E:748:LEU:HD12  | 2:E:748:LEU:H     | 1.77                     | 0.48              |
| 2:E:1429:LEU:HD23 | 2:E:1477:GLU:C    | 2.38                     | 0.48              |
| 3:H:135:ILE:O     | 3:H:171:PHE:HA    | 2.13                     | 0.48              |
| 3:H:137:PHE:CE1   | 3:H:171:PHE:CD1   | 2.96                     | 0.48              |
| 2:A:727:PHE:CE1   | 2:A:749:TYR:HB2   | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:730:LEU:HD23 | 2:A:822:VAL:HG12 | 1.95                     | 0.48              |
| 3:D:305:LEU:O    | 3:D:309:GLN:HB2  | 2.13                     | 0.48              |
| 1:C:139:ARG:O    | 1:C:159:SER:HA   | 2.13                     | 0.48              |
| 2:E:839:VAL:HG22 | 2:E:842:ARG:CG   | 2.44                     | 0.48              |
| 1:B:361:PRO:HB3  | 1:B:382:ASP:O    | 2.13                     | 0.48              |
| 1:B:624:PHE:H    | 1:B:632:THR:CG2  | 2.26                     | 0.48              |
| 3:D:258:GLU:HG3  | 3:D:259:ALA:N    | 2.27                     | 0.48              |
| 1:B:138:GLY:HA2  | 1:B:160:SER:OG   | 2.13                     | 0.48              |
| 1:B:242:LYS:HB3  | 1:B:274:GLY:HA3  | 1.95                     | 0.48              |
| 1:B:340:LYS:O    | 1:B:340:LYS:HG3  | 2.14                     | 0.48              |
| 2:A:910:GLN:HA   | 2:A:913:ILE:HB   | 1.95                     | 0.48              |
| 2:A:1427:THR:OG1 | 2:A:1428:ARG:N   | 2.44                     | 0.48              |
| 1:C:126:ARG:NE   | 1:C:572:VAL:HB   | 2.29                     | 0.48              |
| 2:E:657:ASN:CG   | 3:H:252:TYR:HD1  | 2.22                     | 0.48              |
| 1:B:311:HIS:HB3  | 2:A:1312:TYR:CE1 | 2.48                     | 0.48              |
| 1:B:566:ASP:OD2  | 2:A:710:LYS:HG2  | 2.13                     | 0.48              |
| 2:A:1116:ARG:NH2 | 2:A:1118:GLU:OE1 | 2.46                     | 0.48              |
| 2:A:1430:VAL:CG2 | 2:A:1444:ALA:HB2 | 2.44                     | 0.48              |
| 2:A:1482:TYR:HD1 | 2:A:1510:HIS:HA  | 1.78                     | 0.48              |
| 1:C:106:GLY:O    | 1:C:194:GLN:NE2  | 2.47                     | 0.48              |
| 1:C:346:MET:N    | 1:C:391:THR:OG1  | 2.46                     | 0.48              |
| 1:C:624:PHE:H    | 1:C:632:THR:HG23 | 1.79                     | 0.48              |
| 2:E:1481:HIS:HB2 | 2:E:1511:TRP:O   | 2.14                     | 0.48              |
| 1:B:63:ASN:ND2   | 4:I:1:NAG:C7     | 2.76                     | 0.48              |
| 1:B:78:LYS:HB3   | 2:E:1489:SER:HB2 | 1.95                     | 0.48              |
| 1:B:374:THR:HG22 | 1:B:375:VAL:HG23 | 1.96                     | 0.48              |
| 2:A:1033:ASN:OD1 | 2:A:1034:ASN:N   | 2.46                     | 0.48              |
| 1:C:403:ARG:HA   | 1:C:415:ALA:O    | 2.13                     | 0.48              |
| 2:E:784:THR:C    | 2:E:785:ILE:HD12 | 2.38                     | 0.48              |
| 2:E:1417:CYS:SG  | 2:E:1542:PRO:HD2 | 2.54                     | 0.48              |
| 1:B:6:ILE:CG1    | 1:B:625:THR:HB   | 2.43                     | 0.48              |
| 1:B:7:ILE:HA     | 1:B:623:THR:O    | 2.14                     | 0.48              |
| 1:B:8:THR:HG23   | 1:B:20:MET:HG3   | 1.95                     | 0.48              |
| 1:B:23:GLU:OE2   | 1:B:469:THR:HG21 | 2.14                     | 0.48              |
| 1:B:307:THR:HA   | 1:B:318:GLN:HA   | 1.96                     | 0.48              |
| 1:B:457:MET:SD   | 1:B:461:HIS:HB2  | 2.53                     | 0.48              |
| 2:A:728:ILE:HG13 | 2:A:820:ASP:OD2  | 2.13                     | 0.48              |
| 2:A:736:VAL:HG23 | 2:A:737:VAL:O    | 2.13                     | 0.48              |
| 2:A:908:GLY:HA3  | 2:A:965:ALA:HB1  | 1.96                     | 0.48              |
| 3:D:245:LYS:HB2  | 3:D:252:TYR:CE2  | 2.48                     | 0.48              |
| 1:C:453:PHE:HE1  | 1:C:495:LEU:HB2  | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1364:ASN:ND2  | 2:E:1367:GLU:OE1  | 2.46                     | 0.48              |
| 1:B:250:ILE:O     | 1:B:304:VAL:HG13  | 2.13                     | 0.48              |
| 2:A:911:ASN:HD21  | 2:A:949:GLY:C     | 2.21                     | 0.48              |
| 1:C:252:GLY:HA3   | 1:C:303:TYR:CZ    | 2.49                     | 0.48              |
| 1:C:500:THR:O     | 1:C:503:PHE:HD1   | 1.97                     | 0.48              |
| 3:H:139:ILE:CD1   | 3:H:175:GLN:HG3   | 2.44                     | 0.48              |
| 1:B:6:ILE:HG12    | 1:B:625:THR:O     | 2.14                     | 0.48              |
| 2:A:1010:LYS:HD2  | 2:A:1014:VAL:HB   | 1.96                     | 0.48              |
| 3:D:280:SER:O     | 3:D:284:LEU:HG    | 2.14                     | 0.48              |
| 2:E:1294:ASP:HB2  | 2:E:1342:LYS:HB2  | 1.95                     | 0.48              |
| 1:B:341:TYR:CD2   | 1:B:610:GLY:HA2   | 2.49                     | 0.48              |
| 2:A:1015:PHE:CE2  | 2:A:1044:VAL:HG11 | 2.49                     | 0.48              |
| 2:A:1158:TYR:CE2  | 2:A:1172:VAL:HG21 | 2.49                     | 0.48              |
| 3:D:186:PHE:O     | 3:D:190:GLN:N     | 2.47                     | 0.48              |
| 2:E:834:ARG:HD3   | 2:E:834:ARG:HA    | 1.44                     | 0.48              |
| 1:B:48:SER:O      | 1:B:48:SER:OG     | 2.29                     | 0.47              |
| 2:A:887:MET:HE1   | 2:A:933:LYS:NZ    | 2.29                     | 0.47              |
| 2:A:943:LEU:HG    | 2:A:990:ILE:HG13  | 1.95                     | 0.47              |
| 2:A:1250:ALA:HB3  | 2:A:1263:THR:HB   | 1.96                     | 0.47              |
| 2:A:1332:SER:N    | 2:A:1337:ASP:OD2  | 2.46                     | 0.47              |
| 1:C:2:PRO:HB3     | 1:C:27:ALA:HB2    | 1.95                     | 0.47              |
| 1:C:9:PRO:HD3     | 1:C:478:LEU:CD1   | 2.44                     | 0.47              |
| 1:C:35:VAL:HG22   | 1:C:88:ALA:CB     | 2.44                     | 0.47              |
| 1:C:426:THR:CG2   | 1:C:431:ASN:H     | 2.24                     | 0.47              |
| 2:E:1371:ARG:HA   | 2:E:1371:ARG:HD3  | 1.58                     | 0.47              |
| 2:E:1452:GLY:N    | 2:E:1454:ASP:OD1  | 2.35                     | 0.47              |
| 1:B:478:LEU:HD21  | 1:B:622:LEU:HD21  | 1.95                     | 0.47              |
| 2:A:1372:PHE:HB2  | 2:A:1380:GLY:HA3  | 1.96                     | 0.47              |
| 2:A:1412:ARG:NE   | 2:A:1509:GLU:OE1  | 2.45                     | 0.47              |
| 1:C:126:ARG:CZ    | 1:C:572:VAL:HB    | 2.44                     | 0.47              |
| 1:C:268:ARG:NH2   | 2:E:1329:ASP:OD1  | 2.45                     | 0.47              |
| 1:C:578:LYS:HA    | 1:C:581:PHE:HD2   | 1.79                     | 0.47              |
| 2:E:1293:PRO:HA   | 2:E:1342:LYS:O    | 2.14                     | 0.47              |
| 2:E:1427:THR:N    | 2:E:1482:TYR:O    | 2.44                     | 0.47              |
| 2:E:1429:LEU:CG   | 2:E:1478:GLU:HA   | 2.44                     | 0.47              |
| 3:H:268:VAL:O     | 3:H:269:ILE:HD13  | 2.14                     | 0.47              |
| 1:B:307:THR:HG23  | 1:B:318:GLN:HG2   | 1.95                     | 0.47              |
| 1:B:351:MET:HE3   | 1:B:440:ARG:HG2   | 1.95                     | 0.47              |
| 2:A:743:GLU:HA    | 2:A:796:VAL:HA    | 1.96                     | 0.47              |
| 2:A:1306:ASP:HA   | 2:A:1329:ASP:CG   | 2.40                     | 0.47              |
| 2:A:1429:LEU:HD13 | 2:A:1443:MET:HE2  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1272:TYR:O    | 2:E:1333:HIS:HA   | 2.14                     | 0.47              |
| 2:E:1423:TYR:HB2  | 2:E:1425:TYR:CZ   | 2.50                     | 0.47              |
| 2:E:1439:ASP:OD2  | 2:E:1468:ILE:HA   | 2.14                     | 0.47              |
| 5:J:2:NAG:O3      | 5:J:4:BMA:H5      | 2.14                     | 0.47              |
| 1:B:118:THR:HB    | 2:A:734:TYR:OH    | 2.14                     | 0.47              |
| 1:B:325:PRO:HG3   | 1:B:357:PRO:HB2   | 1.95                     | 0.47              |
| 2:A:969:ARG:HH12  | 2:A:1022:ILE:HD11 | 1.79                     | 0.47              |
| 1:C:508:ARG:CZ    | 1:C:604:GLY:HA3   | 2.44                     | 0.47              |
| 1:B:555:PRO:HB3   | 2:A:694:ASP:HA    | 1.95                     | 0.47              |
| 2:A:964:ALA:HB3   | 2:A:966:PHE:O     | 2.14                     | 0.47              |
| 2:A:1288:MET:HG3  | 2:A:1373:TYR:CE2  | 2.49                     | 0.47              |
| 1:C:7:ILE:O       | 1:C:21:VAL:HG12   | 2.13                     | 0.47              |
| 1:C:250:ILE:HG23  | 1:C:305:SER:HB3   | 1.97                     | 0.47              |
| 1:C:370:GLN:N     | 1:C:401:THR:O     | 2.38                     | 0.47              |
| 1:B:116:ILE:HG12  | 1:B:205:TYR:HE2   | 1.80                     | 0.47              |
| 1:B:266:LEU:C     | 1:B:267:LYS:HD2   | 2.40                     | 0.47              |
| 2:A:1077:TYR:O    | 2:A:1080:LEU:HG   | 2.15                     | 0.47              |
| 2:A:1145:PHE:CE1  | 3:D:207:GLY:HA2   | 2.50                     | 0.47              |
| 2:A:1288:MET:HE2  | 2:A:1373:TYR:CE2  | 2.49                     | 0.47              |
| 1:B:71:ASN:HB3    | 3:H:249:PRO:HB2   | 1.96                     | 0.47              |
| 1:B:222:TYR:HB3   | 1:B:225:ASN:HB2   | 1.95                     | 0.47              |
| 1:B:500:THR:O     | 1:B:503:PHE:HD1   | 1.97                     | 0.47              |
| 2:A:761:VAL:HG13  | 2:A:781:GLN:HB2   | 1.96                     | 0.47              |
| 2:A:769:PHE:HA    | 2:A:798:VAL:O     | 2.14                     | 0.47              |
| 2:A:912:MET:HE1   | 2:A:982:VAL:HG11  | 1.96                     | 0.47              |
| 2:A:1086:VAL:HG13 | 2:A:1107:PHE:HA   | 1.97                     | 0.47              |
| 1:C:231:VAL:HB    | 1:C:278:VAL:CG1   | 2.45                     | 0.47              |
| 1:C:417:ARG:HD2   | 1:C:417:ARG:HA    | 1.77                     | 0.47              |
| 1:C:432:ASN:ND2   | 1:C:523:GLU:OE2   | 2.48                     | 0.47              |
| 1:C:553:PRO:HD2   | 2:E:721:THR:O     | 2.15                     | 0.47              |
| 2:E:658:ILE:HG21  | 2:E:810:LYS:HB3   | 1.97                     | 0.47              |
| 2:E:668:TRP:CE3   | 2:E:669:LEU:HB2   | 2.49                     | 0.47              |
| 1:B:126:ARG:HG3   | 2:A:670:TRP:HZ2   | 1.78                     | 0.47              |
| 1:B:472:ILE:HD13  | 1:B:503:PHE:HE2   | 1.79                     | 0.47              |
| 1:B:551:ARG:HD3   | 1:B:552:GLN:H     | 1.79                     | 0.47              |
| 2:A:1111:ALA:HB1  | 2:A:1114:LYS:HA   | 1.96                     | 0.47              |
| 2:E:1433:GLN:HB3  | 2:E:1440:GLU:HB2  | 1.97                     | 0.47              |
| 3:D:216:ARG:HD2   | 3:D:250:LEU:HD13  | 1.96                     | 0.47              |
| 2:E:1272:TYR:CD2  | 2:E:1333:HIS:HB3  | 2.45                     | 0.47              |
| 3:H:176:TYR:CE1   | 3:H:211:THR:HA    | 2.49                     | 0.47              |
| 2:A:804:LEU:O     | 2:A:805:GLN:NE2   | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:1242:ASP:HB2  | 2:A:1271:ARG:HB3  | 1.96                     | 0.47              |
| 3:H:211:THR:H     | 3:H:245:LYS:HG3   | 1.79                     | 0.47              |
| 1:B:36:THR:HG21   | 1:B:45:LEU:HD22   | 1.98                     | 0.46              |
| 2:A:741:GLN:HB2   | 2:A:798:VAL:HG12  | 1.97                     | 0.46              |
| 2:A:1272:TYR:CE2  | 2:A:1274:GLY:HA3  | 2.50                     | 0.46              |
| 2:A:1309:ILE:HD11 | 2:A:1326:ILE:HA   | 1.97                     | 0.46              |
| 2:A:1511:TRP:CG   | 2:A:1529:LEU:HD13 | 2.50                     | 0.46              |
| 3:D:242:ASP:OD1   | 3:D:242:ASP:N     | 2.48                     | 0.46              |
| 2:E:805:GLN:O     | 2:E:825:SER:HA    | 2.15                     | 0.46              |
| 2:E:1446:GLU:O    | 2:E:1458:VAL:HG23 | 2.15                     | 0.46              |
| 2:A:682:GLY:C     | 2:A:683:ILE:HG13  | 2.41                     | 0.46              |
| 2:A:1021:VAL:HG23 | 2:A:1023:HIS:N    | 2.29                     | 0.46              |
| 2:A:1110:THR:OG1  | 2:A:1117:TRP:NE1  | 2.48                     | 0.46              |
| 2:E:1428:ARG:HA   | 2:E:1481:HIS:HA   | 1.96                     | 0.46              |
| 1:B:544:LYS:HD3   | 1:B:564:GLU:OE2   | 2.14                     | 0.46              |
| 3:D:310:ASN:HA    | 3:D:313:ARG:HB3   | 1.97                     | 0.46              |
| 1:C:10:ASN:O      | 1:C:11:ILE:HD13   | 2.16                     | 0.46              |
| 2:E:1430:VAL:HG21 | 2:E:1444:ALA:HB2  | 1.97                     | 0.46              |
| 1:B:547:GLN:C     | 1:B:549:GLU:H     | 2.22                     | 0.46              |
| 1:B:591:GLN:O     | 1:B:594:ILE:HB    | 2.15                     | 0.46              |
| 2:A:900:LEU:O     | 2:A:917:PRO:HB2   | 2.16                     | 0.46              |
| 1:C:40:PHE:HE1    | 1:C:98:VAL:HG11   | 1.78                     | 0.46              |
| 1:C:239:TYR:HE1   | 1:C:241:LYS:HB2   | 1.80                     | 0.46              |
| 1:C:405:LYS:HD2   | 1:C:405:LYS:HA    | 1.79                     | 0.46              |
| 1:C:628:SER:HB2   | 1:C:630:GLN:OE1   | 2.14                     | 0.46              |
| 2:E:760:ARG:HB2   | 2:E:814:TYR:OH    | 2.15                     | 0.46              |
| 2:E:1301:LEU:HD11 | 2:E:1341:PHE:HB3  | 1.96                     | 0.46              |
| 2:E:1422:ASP:OD2  | 2:E:1453:SER:N    | 2.47                     | 0.46              |
| 2:A:696:ILE:C     | 2:A:697:THR:OG1   | 2.52                     | 0.46              |
| 2:A:1090:GLY:O    | 2:A:1099:LEU:HD22 | 2.15                     | 0.46              |
| 2:A:1482:TYR:CD1  | 2:A:1510:HIS:HA   | 2.51                     | 0.46              |
| 3:D:305:LEU:HD23  | 3:D:305:LEU:H     | 1.80                     | 0.46              |
| 1:C:147:ASN:HB2   | 1:C:148:PRO:HD2   | 1.97                     | 0.46              |
| 1:C:441:THR:O     | 1:C:441:THR:HG22  | 2.14                     | 0.46              |
| 2:E:817:PHE:HA    | 3:H:282:GLN:HG3   | 1.98                     | 0.46              |
| 1:B:251:PHE:CE2   | 1:B:280:LEU:HB2   | 2.50                     | 0.46              |
| 2:A:1079:ASN:O    | 2:A:1080:LEU:HD23 | 2.16                     | 0.46              |
| 1:C:578:LYS:HD3   | 2:E:700:GLU:HB2   | 1.98                     | 0.46              |
| 2:E:808:GLU:HA    | 2:E:822:VAL:O     | 2.16                     | 0.46              |
| 3:H:135:ILE:HD13  | 3:H:169:THR:HB    | 1.98                     | 0.46              |
| 1:B:222:TYR:CE1   | 1:B:328:THR:HA    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:661:ARG:HB3   | 2:A:694:ASP:HB3   | 1.97                     | 0.46              |
| 2:A:912:MET:HE3   | 2:A:912:MET:HB3   | 1.56                     | 0.46              |
| 2:A:1400:ILE:HD11 | 2:A:1505:ASP:O    | 2.16                     | 0.46              |
| 1:C:36:THR:HG23   | 1:C:48:SER:HB2    | 1.97                     | 0.46              |
| 1:C:559:MET:HG2   | 1:C:560:THR:N     | 2.30                     | 0.46              |
| 2:E:1524:LYS:H    | 2:E:1524:LYS:CD   | 2.27                     | 0.46              |
| 2:A:1277:ASP:CG   | 2:A:1332:SER:HA   | 2.41                     | 0.46              |
| 1:C:506:SER:OG    | 1:C:599:GLU:OE2   | 2.22                     | 0.46              |
| 1:C:507:PHE:HE1   | 1:C:509:LEU:HB2   | 1.80                     | 0.46              |
| 1:B:7:ILE:HG12    | 1:B:624:PHE:HD1   | 1.81                     | 0.46              |
| 1:B:547:GLN:HG2   | 1:B:549:GLU:OE2   | 2.16                     | 0.46              |
| 2:A:1311:LYS:O    | 2:A:1315:ASP:N    | 2.41                     | 0.46              |
| 1:C:11:ILE:HD13   | 1:C:11:ILE:HA     | 1.74                     | 0.46              |
| 1:C:251:PHE:CD1   | 1:C:304:VAL:HG13  | 2.51                     | 0.46              |
| 1:C:353:PHE:CZ    | 1:C:361:PRO:HB3   | 2.51                     | 0.46              |
| 3:H:133:SER:O     | 3:H:169:THR:HA    | 2.16                     | 0.46              |
| 1:B:6:ILE:HG12    | 1:B:625:THR:HB    | 1.98                     | 0.46              |
| 1:B:443:LEU:HD23  | 1:B:447:GLU:OE2   | 2.15                     | 0.46              |
| 1:B:561:LEU:O     | 2:A:687:LEU:HD13  | 2.15                     | 0.46              |
| 1:B:628:SER:HB2   | 1:B:630:GLN:OE1   | 2.16                     | 0.46              |
| 2:A:1396:GLU:O    | 2:A:1469:LYS:NZ   | 2.40                     | 0.46              |
| 2:A:1424:VAL:HG22 | 2:A:1485:TRP:HB2  | 1.98                     | 0.46              |
| 1:C:453:PHE:HE1   | 1:C:495:LEU:CB    | 2.29                     | 0.46              |
| 2:E:1298:LEU:HD22 | 2:E:1314:LEU:HD11 | 1.99                     | 0.46              |
| 2:E:1513:GLU:OE1  | 2:E:1513:GLU:N    | 2.49                     | 0.46              |
| 1:B:125:TYR:CE2   | 1:B:143:VAL:HG11  | 2.49                     | 0.45              |
| 1:B:567:HIS:HD2   | 2:A:677:GLU:O     | 1.98                     | 0.45              |
| 2:A:738:ARG:NH1   | 2:A:831:GLU:OE2   | 2.49                     | 0.45              |
| 2:A:972:SER:HA    | 2:A:1019:ALA:HB3  | 1.98                     | 0.45              |
| 3:D:243:GLY:O     | 3:D:280:SER:HA    | 2.16                     | 0.45              |
| 1:C:337:LYS:NZ    | 1:C:532:ASP:OD2   | 2.49                     | 0.45              |
| 1:C:366:PRO:HD2   | 1:C:406:LYS:HE2   | 1.98                     | 0.45              |
| 2:E:1409:LEU:HD11 | 2:E:1531:ALA:CB   | 2.46                     | 0.45              |
| 2:A:830:PRO:O     | 2:A:832:GLY:N     | 2.50                     | 0.45              |
| 2:A:1158:TYR:CD2  | 2:A:1172:VAL:HG21 | 2.51                     | 0.45              |
| 2:A:1279:THR:HG1  | 2:A:1362:TYR:HE1  | 1.63                     | 0.45              |
| 2:A:1483:LEU:C    | 2:A:1484:MET:HG3  | 2.41                     | 0.45              |
| 3:D:311:GLN:O     | 3:D:315:LYS:HD2   | 2.17                     | 0.45              |
| 1:C:514:THR:HA    | 1:C:523:GLU:O     | 2.16                     | 0.45              |
| 2:E:1355:GLY:HA3  | 2:E:1373:TYR:CE1  | 2.48                     | 0.45              |
| 3:H:141:GLY:CA    | 3:H:175:GLN:HE21  | 2.27                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:348:PHE:CZ    | 1:B:419:MET:HE1   | 2.50                     | 0.45              |
| 1:C:136:PRO:CG    | 2:E:708:ASP:HA    | 2.45                     | 0.45              |
| 2:E:1387:ARG:NH1  | 2:E:1493:GLY:HA2  | 2.32                     | 0.45              |
| 1:C:147:ASN:HA    | 1:C:182:TRP:CD2   | 2.52                     | 0.45              |
| 1:C:390:ASN:OD1   | 1:C:390:ASN:N     | 2.48                     | 0.45              |
| 1:B:470:TYR:C     | 1:B:471:LEU:HD12  | 2.42                     | 0.45              |
| 1:C:458:ASP:OD1   | 1:C:459:ARG:N     | 2.50                     | 0.45              |
| 1:C:579:GLY:O     | 1:C:583:LEU:HD12  | 2.17                     | 0.45              |
| 2:E:1384:LYS:NZ   | 2:E:1386:CYS:SG   | 2.75                     | 0.45              |
| 1:B:78:LYS:HA     | 1:B:78:LYS:HD3    | 1.71                     | 0.45              |
| 1:B:154:LYS:HG3   | 1:B:171:TRP:CD1   | 2.51                     | 0.45              |
| 2:A:1358:LYS:HE3  | 2:A:1368:SER:CB   | 2.47                     | 0.45              |
| 2:A:1494:GLU:OE1  | 2:A:1495:LYS:HG3  | 2.16                     | 0.45              |
| 3:D:182:ILE:H     | 3:D:182:ILE:HD12  | 1.82                     | 0.45              |
| 2:E:1296:ASP:HA   | 2:E:1299:LYS:HD3  | 1.99                     | 0.45              |
| 2:E:1318:PHE:HA   | 2:E:1321:ARG:HH11 | 1.82                     | 0.45              |
| 1:B:458:ASP:OD2   | 1:B:460:ALA:HB3   | 2.16                     | 0.45              |
| 1:B:468:TYR:CE2   | 1:B:486:ARG:HD2   | 2.52                     | 0.45              |
| 1:B:508:ARG:HH21  | 1:B:606:THR:C     | 2.25                     | 0.45              |
| 1:B:555:PRO:HB2   | 2:A:661:ARG:HD3   | 1.99                     | 0.45              |
| 2:A:1104:LEU:HG   | 2:A:1108:LEU:HD12 | 1.98                     | 0.45              |
| 2:A:1309:ILE:HD13 | 2:A:1309:ILE:HA   | 1.79                     | 0.45              |
| 2:A:1441:TYR:CE1  | 2:A:1476:LEU:HD12 | 2.52                     | 0.45              |
| 1:C:86:VAL:HG12   | 1:C:97:LYS:O      | 2.17                     | 0.45              |
| 2:E:663:GLU:HB2   | 2:E:693:LYS:HD3   | 1.99                     | 0.45              |
| 2:E:736:VAL:HG23  | 2:E:828:VAL:HG13  | 1.98                     | 0.45              |
| 2:E:745:ARG:HH21  | 2:E:1323:THR:HB   | 1.82                     | 0.45              |
| 2:E:803:GLY:O     | 2:E:828:VAL:HG23  | 2.17                     | 0.45              |
| 2:E:1399:PHE:CD2  | 2:E:1400:ILE:O    | 2.70                     | 0.45              |
| 3:H:231:LYS:HG2   | 3:H:232:ASN:N     | 2.32                     | 0.45              |
| 3:H:285:ASN:OD1   | 3:H:296:VAL:HG21  | 2.17                     | 0.45              |
| 1:B:145:ILE:HG21  | 1:B:171:TRP:CE3   | 2.52                     | 0.45              |
| 1:B:464:LYS:O     | 1:B:466:ARG:HG2   | 2.17                     | 0.45              |
| 2:A:650:GLU:O     | 2:A:652:ILE:HG22  | 2.16                     | 0.45              |
| 1:C:46:VAL:HG13   | 1:C:69:PRO:HD2    | 1.98                     | 0.45              |
| 1:C:539:GLY:N     | 2:E:710:LYS:HD3   | 2.31                     | 0.45              |
| 3:H:252:TYR:HA    | 3:H:255:VAL:HG22  | 1.98                     | 0.45              |
| 1:B:4:TYR:O       | 1:B:626:SER:HA    | 2.16                     | 0.45              |
| 1:B:54:LEU:HD22   | 1:B:62:GLY:N      | 2.31                     | 0.45              |
| 1:B:244:GLU:OE1   | 1:B:244:GLU:HA    | 2.16                     | 0.45              |
| 2:A:1096:MET:O    | 2:A:1098:ARG:HG3  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:181:GLN:HE21  | 1:C:199:GLU:CB    | 2.26                     | 0.45              |
| 2:A:844:LEU:HD23  | 2:A:844:LEU:H     | 1.82                     | 0.45              |
| 2:A:974:TRP:O     | 2:A:978:TYR:HB3   | 2.17                     | 0.45              |
| 3:H:161:MET:HE1   | 3:H:184:PHE:CZ    | 2.48                     | 0.45              |
| 3:H:282:GLN:OE1   | 3:H:285:ASN:HB2   | 2.17                     | 0.45              |
| 1:B:351:MET:CE    | 1:B:386:LYS:HG3   | 2.46                     | 0.44              |
| 2:A:1145:PHE:O    | 2:A:1149:VAL:HG23 | 2.17                     | 0.44              |
| 2:A:1428:ARG:HD3  | 2:A:1481:HIS:NE2  | 2.32                     | 0.44              |
| 3:D:176:TYR:CE1   | 3:D:211:THR:HA    | 2.52                     | 0.44              |
| 1:C:343:LYS:HZ1   | 1:C:609:SER:CB    | 2.29                     | 0.44              |
| 1:C:547:GLN:OE1   | 1:C:550:ASP:HB2   | 2.17                     | 0.44              |
| 2:E:750:ASN:HD22  | 2:E:785:ILE:HG22  | 1.82                     | 0.44              |
| 2:E:1428:ARG:HH21 | 2:E:1446:GLU:CD   | 2.25                     | 0.44              |
| 1:B:530:TRP:CD1   | 1:B:531:VAL:N     | 2.85                     | 0.44              |
| 2:A:757:LEU:N     | 2:A:785:ILE:O     | 2.43                     | 0.44              |
| 2:A:768:ALA:O     | 2:A:800:LEU:N     | 2.49                     | 0.44              |
| 2:A:1134:LEU:O    | 2:A:1138:LEU:HG   | 2.17                     | 0.44              |
| 1:C:424:TYR:OH    | 1:C:526:ALA:N     | 2.45                     | 0.44              |
| 2:E:750:ASN:HB2   | 2:E:785:ILE:HG21  | 1.99                     | 0.44              |
| 2:E:1428:ARG:HD3  | 2:E:1481:HIS:CD2  | 2.52                     | 0.44              |
| 1:B:401:THR:HA    | 1:B:417:ARG:O     | 2.17                     | 0.44              |
| 2:A:665:PRO:HD2   | 2:A:693:LYS:HG3   | 1.98                     | 0.44              |
| 2:E:1461:GLN:O    | 2:E:1462:ARG:NH1  | 2.50                     | 0.44              |
| 3:H:258:GLU:HA    | 3:H:261:ARG:HG2   | 1.98                     | 0.44              |
| 1:B:109:PHE:O     | 1:B:128:PHE:CD1   | 2.58                     | 0.44              |
| 1:B:115:THR:CG2   | 1:B:588:LYS:HG3   | 2.48                     | 0.44              |
| 1:B:241:LYS:HD3   | 1:B:241:LYS:HA    | 1.66                     | 0.44              |
| 1:B:474:ASN:OD1   | 1:B:477:ARG:NH1   | 2.49                     | 0.44              |
| 2:A:702:LEU:HD11  | 2:A:714:VAL:HG13  | 1.99                     | 0.44              |
| 2:A:950:TYR:O     | 2:A:954:LEU:HG    | 2.18                     | 0.44              |
| 2:A:1352:ILE:O    | 2:A:1374:HIS:NE2  | 2.50                     | 0.44              |
| 2:E:1310:SER:O    | 2:E:1314:LEU:HB2  | 2.17                     | 0.44              |
| 1:B:126:ARG:NH1   | 1:B:572:VAL:HB    | 2.31                     | 0.44              |
| 1:B:547:GLN:C     | 1:B:549:GLU:N     | 2.76                     | 0.44              |
| 2:A:752:ARG:O     | 2:A:787:PRO:HB3   | 2.18                     | 0.44              |
| 2:A:1128:GLU:HG2  | 2:A:1132:TYR:CE2  | 2.53                     | 0.44              |
| 1:C:6:ILE:HD11    | 1:C:88:ALA:HB3    | 1.98                     | 0.44              |
| 2:E:1353:GLN:HG2  | 2:E:1354:PRO:N    | 2.31                     | 0.44              |
| 2:E:1471:ARG:HG3  | 2:E:1472:GLU:HG2  | 2.00                     | 0.44              |
| 1:B:47:LEU:HD23   | 1:B:66:PHE:HD2    | 1.83                     | 0.44              |
| 1:B:467:TYR:HB3   | 1:B:485:VAL:HA    | 1.98                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:479:LEU:HD21  | 1:B:502:ASP:CB   | 2.45                     | 0.44              |
| 3:D:137:PHE:CE2   | 3:D:157:VAL:HG13 | 2.53                     | 0.44              |
| 1:C:145:ILE:O     | 1:C:152:PRO:HA   | 2.17                     | 0.44              |
| 1:C:398:LEU:O     | 1:C:420:GLN:HG3  | 2.18                     | 0.44              |
| 2:A:702:LEU:HD11  | 2:A:714:VAL:CG1  | 2.48                     | 0.44              |
| 2:A:790:SER:OG    | 2:A:790:SER:O    | 2.32                     | 0.44              |
| 2:A:1523:GLN:HB3  | 2:A:1527:GLN:OE1 | 2.18                     | 0.44              |
| 1:C:34:THR:HG22   | 1:C:51:LYS:HG3   | 1.99                     | 0.44              |
| 1:C:36:THR:O      | 1:C:87:GLN:N     | 2.47                     | 0.44              |
| 1:C:164:LEU:O     | 1:C:166:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:167:LEU:HD23  | 1:C:167:LEU:HA   | 1.63                     | 0.44              |
| 2:E:683:ILE:HD13  | 2:E:683:ILE:HA   | 1.78                     | 0.44              |
| 2:E:697:THR:HG22  | 2:E:698:THR:O    | 2.17                     | 0.44              |
| 3:H:145:ILE:O     | 3:H:204:GLN:NE2  | 2.47                     | 0.44              |
| 1:B:121:SER:OG    | 1:B:173:ILE:HD12 | 2.18                     | 0.44              |
| 1:B:335:PHE:HD1   | 1:B:338:THR:HG21 | 1.83                     | 0.44              |
| 1:B:530:TRP:CD1   | 1:B:530:TRP:C    | 2.95                     | 0.44              |
| 2:A:1413:LEU:O    | 2:A:1417:CYS:N   | 2.45                     | 0.44              |
| 2:A:1449:ILE:CG2  | 2:A:1536:MET:HG2 | 2.48                     | 0.44              |
| 1:C:75:LYS:HG3    | 1:C:80:ARG:O     | 2.17                     | 0.44              |
| 1:C:147:ASN:HA    | 1:C:182:TRP:CE3  | 2.53                     | 0.44              |
| 2:E:740:GLU:O     | 2:E:742:VAL:HG13 | 2.18                     | 0.44              |
| 1:B:205:TYR:CD1   | 1:B:205:TYR:C    | 2.95                     | 0.44              |
| 2:A:673:GLU:OE1   | 2:A:686:LYS:NZ   | 2.48                     | 0.44              |
| 2:A:1178:GLN:NE2  | 2:A:1182:ASP:OD1 | 2.51                     | 0.44              |
| 1:C:8:THR:HG1     | 1:C:623:THR:HG1  | 1.60                     | 0.44              |
| 2:E:758:LYS:HA    | 2:E:783:VAL:O    | 2.18                     | 0.44              |
| 2:E:817:PHE:CA    | 3:H:282:GLN:HG3  | 2.48                     | 0.44              |
| 1:B:438:VAL:CG2   | 1:B:451:VAL:HA   | 2.48                     | 0.43              |
| 2:A:697:THR:O     | 2:A:722:VAL:N    | 2.49                     | 0.43              |
| 2:A:761:VAL:CG1   | 2:A:781:GLN:HB2  | 2.48                     | 0.43              |
| 2:A:1086:VAL:CG2  | 2:A:1106:LYS:HE3 | 2.48                     | 0.43              |
| 1:C:11:ILE:HD11   | 1:C:100:LEU:HD23 | 2.00                     | 0.43              |
| 1:C:146:GLU:OE2   | 1:C:185:ARG:HG3  | 2.18                     | 0.43              |
| 1:C:207:LEU:CD1   | 2:E:666:GLU:HG2  | 2.48                     | 0.43              |
| 2:E:669:LEU:HD12  | 2:E:669:LEU:HA   | 1.69                     | 0.43              |
| 2:E:833:ILE:O     | 2:E:835:MET:HE2  | 2.18                     | 0.43              |
| 1:B:307:THR:HG21  | 2:A:1362:TYR:O   | 2.18                     | 0.43              |
| 1:B:548:SER:N     | 1:B:549:GLU:OE1  | 2.51                     | 0.43              |
| 2:A:1432:VAL:HG23 | 2:A:1478:GLU:HG2 | 1.99                     | 0.43              |
| 1:C:184:ILE:N     | 1:C:198:THR:O    | 2.50                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:343:LYS:NZ    | 1:C:609:SER:HB2  | 2.33                     | 0.43              |
| 3:H:234:PHE:CZ    | 3:H:315:LYS:HG2  | 2.53                     | 0.43              |
| 1:B:140:THR:HA    | 1:B:159:SER:HA   | 2.00                     | 0.43              |
| 1:B:302:LEU:H     | 1:B:324:ILE:N    | 2.15                     | 0.43              |
| 1:B:333:ILE:HD12  | 1:B:402:VAL:O    | 2.18                     | 0.43              |
| 2:A:1341:PHE:HD1  | 2:A:1342:LYS:O   | 2.01                     | 0.43              |
| 2:A:1490:ASP:HB3  | 2:A:1501:ILE:HB  | 2.00                     | 0.43              |
| 1:C:249:VAL:HG22  | 1:C:267:LYS:O    | 2.18                     | 0.43              |
| 2:E:660:SER:OG    | 2:E:808:GLU:OE2  | 2.16                     | 0.43              |
| 2:E:781:GLN:OE1   | 2:E:781:GLN:N    | 2.50                     | 0.43              |
| 2:E:1251:PRO:O    | 2:E:1252:GLU:HB3 | 2.17                     | 0.43              |
| 2:E:1397:ASN:H    | 2:E:1504:LYS:HD2 | 1.83                     | 0.43              |
| 1:B:622:LEU:HA    | 1:B:622:LEU:HD23 | 1.53                     | 0.43              |
| 1:B:634:GLN:HB2   | 2:E:1543:ASN:HB3 | 2.00                     | 0.43              |
| 1:C:32:PRO:HG2    | 1:C:91:GLY:HA2   | 1.99                     | 0.43              |
| 1:C:39:ASP:OD1    | 1:C:42:GLY:HA3   | 2.19                     | 0.43              |
| 1:C:540:SER:O     | 1:C:565:GLY:HA2  | 2.18                     | 0.43              |
| 1:B:304:VAL:O     | 1:B:320:GLU:HA   | 2.17                     | 0.43              |
| 1:B:366:PRO:HA    | 1:B:377:SER:O    | 2.19                     | 0.43              |
| 1:B:553:PRO:HB2   | 2:A:721:THR:O    | 2.19                     | 0.43              |
| 1:B:560:THR:CG2   | 2:A:687:LEU:HD12 | 2.48                     | 0.43              |
| 2:A:1243:LEU:N    | 2:A:1244:LYS:HZ3 | 2.16                     | 0.43              |
| 2:A:1309:ILE:CD1  | 2:A:1326:ILE:HA  | 2.47                     | 0.43              |
| 1:C:473:MET:CE    | 1:C:603:ILE:HD11 | 2.49                     | 0.43              |
| 1:C:570:ARG:HA    | 2:E:674:ASP:OD1  | 2.19                     | 0.43              |
| 2:E:730:LEU:CB    | 2:E:822:VAL:HG11 | 2.48                     | 0.43              |
| 3:H:172:SER:OG    | 3:H:222:LEU:HD22 | 2.19                     | 0.43              |
| 1:B:24:ALA:HB3    | 1:B:60:HIS:HB3   | 2.00                     | 0.43              |
| 1:B:40:PHE:HD1    | 1:B:85:THR:OG1   | 2.01                     | 0.43              |
| 1:B:440:ARG:NH2   | 1:B:441:THR:C    | 2.76                     | 0.43              |
| 2:A:785:ILE:HG23  | 2:A:791:LEU:HB2  | 2.00                     | 0.43              |
| 2:A:1080:LEU:O    | 2:A:1106:LYS:HE2 | 2.19                     | 0.43              |
| 3:D:279:LYS:CA    | 3:D:282:GLN:HG2  | 2.38                     | 0.43              |
| 2:E:730:LEU:HG    | 2:E:732:LEU:HD21 | 2.01                     | 0.43              |
| 1:B:229:LEU:HD12  | 1:B:229:LEU:HA   | 1.84                     | 0.43              |
| 1:B:368:ALA:HB2   | 1:B:376:GLN:HA   | 2.00                     | 0.43              |
| 1:B:369:VAL:HG12  | 1:B:402:VAL:HG22 | 2.01                     | 0.43              |
| 2:E:1409:LEU:HD11 | 2:E:1531:ALA:HB3 | 2.00                     | 0.43              |
| 3:H:175:GLN:HB2   | 3:H:183:HIS:NE2  | 2.32                     | 0.43              |
| 1:B:340:LYS:HD2   | 1:B:420:GLN:O    | 2.18                     | 0.43              |
| 1:B:547:GLN:HG3   | 1:B:560:THR:HB   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:655:GLU:HB2   | 2:A:762:GLU:OE2   | 2.19                     | 0.43              |
| 2:A:939:ARG:HE    | 2:A:989:LEU:CD2   | 2.31                     | 0.43              |
| 2:A:1071:ASP:HA   | 2:A:1098:ARG:HH22 | 1.84                     | 0.43              |
| 2:A:1372:PHE:CB   | 2:A:1380:GLY:HA3  | 2.48                     | 0.43              |
| 3:D:133:SER:H     | 3:D:230:ARG:NH2   | 2.15                     | 0.43              |
| 1:C:3:MET:HE2     | 1:C:626:SER:OG    | 2.19                     | 0.43              |
| 1:B:156:ASP:HB3   | 1:B:158:LEU:HD11  | 2.01                     | 0.43              |
| 1:B:406:LYS:HB3   | 1:B:409:LEU:HD22  | 2.00                     | 0.43              |
| 2:A:1070:GLY:O    | 2:A:1073:LEU:HB2  | 2.19                     | 0.43              |
| 3:D:194:ASN:O     | 3:D:198:LEU:HG    | 2.19                     | 0.43              |
| 1:B:335:PHE:HB3   | 1:B:338:THR:OG1   | 2.19                     | 0.42              |
| 1:B:528:SER:HB3   | 1:B:616:VAL:HG13  | 2.00                     | 0.42              |
| 2:A:1316:LYS:HD3  | 2:A:1316:LYS:HA   | 1.94                     | 0.42              |
| 3:D:183:HIS:CE1   | 3:D:202:ILE:HG23  | 2.53                     | 0.42              |
| 1:C:138:GLY:HA3   | 1:C:161:GLN:N     | 2.34                     | 0.42              |
| 2:E:733:PRO:HG2   | 2:E:736:VAL:CG1   | 2.49                     | 0.42              |
| 2:A:913:ILE:HD11  | 2:A:1026:MET:SD   | 2.58                     | 0.42              |
| 3:D:306:LYS:H     | 3:D:306:LYS:HG2   | 1.63                     | 0.42              |
| 1:C:369:VAL:HG12  | 1:C:402:VAL:HG22  | 2.00                     | 0.42              |
| 1:C:464:LYS:O     | 1:C:466:ARG:HG2   | 2.19                     | 0.42              |
| 2:E:1502:ILE:HG23 | 2:E:1506:THR:HB   | 2.01                     | 0.42              |
| 1:B:269:ILE:HD13  | 1:B:278:VAL:HG21  | 2.00                     | 0.42              |
| 2:A:1125:TYR:N    | 2:A:1125:TYR:CD1  | 2.87                     | 0.42              |
| 2:A:1304:GLY:O    | 2:A:1307:ARG:HB2  | 2.19                     | 0.42              |
| 2:A:1507:TRP:CD1  | 2:A:1507:TRP:C    | 2.97                     | 0.42              |
| 1:C:108:LEU:HD21  | 1:C:188:TYR:CZ    | 2.54                     | 0.42              |
| 1:C:358:ASP:OD1   | 1:C:359:GLY:N     | 2.52                     | 0.42              |
| 2:E:1415:LYS:HB3  | 2:E:1485:TRP:HZ2  | 1.84                     | 0.42              |
| 1:B:105:SER:C     | 1:B:132:HIS:CE1   | 2.98                     | 0.42              |
| 2:A:1294:ASP:HB2  | 2:A:1342:LYS:CB   | 2.44                     | 0.42              |
| 2:A:1334:SER:OG   | 2:A:1335:GLU:N    | 2.53                     | 0.42              |
| 3:D:216:ARG:HD2   | 3:D:250:LEU:CD1   | 2.49                     | 0.42              |
| 3:D:290:LYS:HD3   | 3:D:292:PRO:HD3   | 2.00                     | 0.42              |
| 1:C:141:VAL:HG22  | 1:C:188:TYR:CD1   | 2.54                     | 0.42              |
| 1:C:248:PHE:CE2   | 2:E:1282:ILE:HD11 | 2.54                     | 0.42              |
| 1:C:524:VAL:O     | 1:C:613:TYR:HB3   | 2.19                     | 0.42              |
| 2:E:759:VAL:HB    | 2:E:783:VAL:HG23  | 2.02                     | 0.42              |
| 1:B:164:LEU:HD12  | 1:B:164:LEU:HA    | 1.75                     | 0.42              |
| 2:A:917:PRO:HA    | 2:A:920:ILE:HG22  | 2.01                     | 0.42              |
| 2:A:1474:LEU:HB3  | 2:A:1476:LEU:CG   | 2.47                     | 0.42              |
| 1:C:440:ARG:NH1   | 1:C:440:ARG:CG    | 2.72                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:544:LYS:HG3   | 1:B:562:LYS:HD2   | 2.01                     | 0.42              |
| 2:A:1138:LEU:HB2  | 2:A:1139:GLN:NE2  | 2.34                     | 0.42              |
| 3:D:176:TYR:HB2   | 3:D:180:PHE:HD2   | 1.83                     | 0.42              |
| 1:C:451:VAL:O     | 1:C:495:LEU:N     | 2.44                     | 0.42              |
| 1:C:526:ALA:C     | 1:C:616:VAL:HG21  | 2.44                     | 0.42              |
| 1:C:538:VAL:CG1   | 2:E:710:LYS:HG2   | 2.49                     | 0.42              |
| 1:C:541:LEU:HD22  | 2:E:705:SER:HB3   | 2.02                     | 0.42              |
| 3:H:250:LEU:HD23  | 3:H:250:LEU:HA    | 1.92                     | 0.42              |
| 1:B:71:ASN:CG     | 1:B:73:GLU:HG2    | 2.44                     | 0.42              |
| 2:A:735:SER:HA    | 2:A:827:LYS:HB2   | 2.02                     | 0.42              |
| 2:A:772:LEU:HD11  | 2:A:1353:GLN:N    | 2.35                     | 0.42              |
| 2:A:943:LEU:HD12  | 2:A:946:ILE:HD12  | 2.01                     | 0.42              |
| 2:A:1311:LYS:HD2  | 2:A:1315:ASP:HB3  | 2.01                     | 0.42              |
| 2:A:1400:ILE:HG13 | 2:A:1506:THR:O    | 2.20                     | 0.42              |
| 3:D:304:ALA:O     | 3:D:308:ILE:HG12  | 2.20                     | 0.42              |
| 1:C:440:ARG:HH11  | 1:C:440:ARG:CB    | 2.30                     | 0.42              |
| 2:E:741:GLN:HG3   | 2:E:798:VAL:CG2   | 2.44                     | 0.42              |
| 1:B:6:ILE:O       | 1:B:6:ILE:HG13    | 2.19                     | 0.42              |
| 1:B:40:PHE:HA     | 1:B:41:PRO:HA     | 1.85                     | 0.42              |
| 1:B:173:ILE:HA    | 1:B:174:PRO:HD3   | 1.87                     | 0.42              |
| 2:A:774:THR:N     | 2:A:777:ARG:O     | 2.47                     | 0.42              |
| 2:A:1001:VAL:HG11 | 2:A:1062:LEU:HD13 | 2.00                     | 0.42              |
| 2:A:1164:GLY:O    | 2:A:1166:THR:N    | 2.49                     | 0.42              |
| 2:A:1355:GLY:HA3  | 2:A:1373:TYR:CE2  | 2.55                     | 0.42              |
| 3:D:182:ILE:HG23  | 3:D:222:LEU:HD21  | 2.01                     | 0.42              |
| 1:C:332:GLN:OE1   | 1:C:355:THR:OG1   | 2.36                     | 0.42              |
| 2:E:745:ARG:NH2   | 2:E:1323:THR:HB   | 2.35                     | 0.42              |
| 3:H:172:SER:HA    | 3:H:184:PHE:CE1   | 2.54                     | 0.42              |
| 2:A:1105:ASN:ND2  | 2:A:1109:THR:OG1  | 2.53                     | 0.42              |
| 2:A:1247:ILE:HD12 | 2:A:1288:MET:HE1  | 2.02                     | 0.42              |
| 2:A:1543:ASN:HB3  | 1:C:634:GLN:HB2   | 2.02                     | 0.42              |
| 1:C:368:ALA:O     | 1:C:402:VAL:HG13  | 2.20                     | 0.42              |
| 1:C:465:ILE:HD11  | 1:C:515:LEU:HD13  | 2.02                     | 0.42              |
| 2:E:730:LEU:HD11  | 2:E:744:ILE:HD12  | 2.02                     | 0.42              |
| 2:E:1482:TYR:CD1  | 2:E:1510:HIS:HA   | 2.55                     | 0.42              |
| 3:H:157:VAL:CG1   | 3:H:161:MET:HE3   | 2.50                     | 0.42              |
| 3:H:233:ALA:O     | 3:H:235:LYS:HG3   | 2.20                     | 0.42              |
| 1:B:437:SER:OG    | 1:B:452:ASN:HB2   | 2.20                     | 0.42              |
| 1:B:561:LEU:HB3   | 2:A:688:MET:HB2   | 2.01                     | 0.42              |
| 2:A:837:LYS:HD2   | 2:A:837:LYS:O     | 2.20                     | 0.42              |
| 2:A:990:ILE:HD12  | 2:A:990:ILE:H     | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:214:GLY:O     | 3:D:218:VAL:HG23  | 2.20                     | 0.42              |
| 3:D:266:ARG:CZ    | 3:D:289:SER:HB3   | 2.50                     | 0.42              |
| 1:C:434:LEU:HD12  | 1:C:454:LEU:O     | 2.19                     | 0.42              |
| 1:C:622:LEU:HD23  | 1:C:622:LEU:HA    | 1.68                     | 0.42              |
| 1:B:305:SER:HA    | 1:B:319:ALA:O     | 2.19                     | 0.41              |
| 1:B:328:THR:O     | 1:B:413:GLU:HG2   | 2.20                     | 0.41              |
| 2:A:1124:LEU:HD22 | 2:A:1168:ALA:HB3  | 2.02                     | 0.41              |
| 2:A:1421:VAL:O    | 2:A:1421:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:247:ALA:CB    | 1:C:271:ILE:HD11  | 2.49                     | 0.41              |
| 2:E:714:VAL:HG12  | 2:E:715:ALA:N     | 2.35                     | 0.41              |
| 2:E:730:LEU:HB3   | 2:E:822:VAL:HG11  | 2.01                     | 0.41              |
| 2:E:1329:ASP:O    | 2:E:1330:LYS:HG2  | 2.20                     | 0.41              |
| 3:H:276:ARG:HE    | 3:H:276:ARG:C     | 2.27                     | 0.41              |
| 3:H:298:GLN:HG2   | 3:H:300:ASN:OD1   | 2.20                     | 0.41              |
| 1:B:413:GLU:O     | 1:B:414:GLN:C     | 2.62                     | 0.41              |
| 1:B:595:TRP:CE3   | 1:B:595:TRP:HA    | 2.56                     | 0.41              |
| 2:A:774:THR:OG1   | 2:A:777:ARG:N     | 2.39                     | 0.41              |
| 2:A:1083:SER:HB2  | 2:A:1117:TRP:HD1  | 1.85                     | 0.41              |
| 2:A:1358:LYS:HG2  | 2:A:1360:TYR:CD2  | 2.54                     | 0.41              |
| 2:A:1428:ARG:HG3  | 2:A:1481:HIS:CG   | 2.55                     | 0.41              |
| 1:C:244:GLU:O     | 1:C:311:HIS:ND1   | 2.53                     | 0.41              |
| 2:E:652:ILE:HB    | 2:E:814:TYR:CE1   | 2.55                     | 0.41              |
| 2:E:1278:ALA:O    | 2:E:1330:LYS:HD2  | 2.19                     | 0.41              |
| 3:H:187:LYS:O     | 3:H:191:ASN:ND2   | 2.53                     | 0.41              |
| 2:A:670:TRP:O     | 2:A:670:TRP:CD1   | 2.74                     | 0.41              |
| 2:A:743:GLU:HG2   | 2:A:744:ILE:N     | 2.35                     | 0.41              |
| 2:A:935:GLY:O     | 2:A:936:LEU:HB2   | 2.20                     | 0.41              |
| 1:C:74:PHE:O      | 1:C:75:LYS:HE2    | 2.19                     | 0.41              |
| 1:C:163:GLN:HG2   | 1:C:166:VAL:O     | 2.20                     | 0.41              |
| 1:C:224:TYR:O     | 1:C:224:TYR:CG    | 2.72                     | 0.41              |
| 1:C:292:PRO:O     | 1:C:293:ARG:HG3   | 2.19                     | 0.41              |
| 1:C:367:VAL:HG12  | 1:C:404:THR:CB    | 2.50                     | 0.41              |
| 2:E:769:PHE:CE1   | 2:E:799:PRO:HA    | 2.55                     | 0.41              |
| 2:E:1511:TRP:CZ3  | 2:E:1529:LEU:HD22 | 2.55                     | 0.41              |
| 1:B:142:MET:HB2   | 1:B:187:TYR:CZ    | 2.56                     | 0.41              |
| 1:B:306:ALA:O     | 1:B:319:ALA:N     | 2.39                     | 0.41              |
| 1:B:641:PRO:HB2   | 1:B:643:PRO:HD2   | 2.02                     | 0.41              |
| 2:A:1051:ALA:O    | 2:A:1054:ILE:HB   | 2.20                     | 0.41              |
| 1:C:376:GLN:NE2   | 1:C:405:LYS:HB3   | 2.35                     | 0.41              |
| 1:C:593:LYS:O     | 1:C:597:VAL:HG23  | 2.21                     | 0.41              |
| 2:A:699:TRP:O     | 2:A:719:GLU:HA    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:1026:MET:O    | 2:A:1167:GLN:HG2  | 2.20                     | 0.41              |
| 1:C:40:PHE:CE1    | 1:C:98:VAL:HG11   | 2.55                     | 0.41              |
| 1:C:505:PRO:HD3   | 1:C:595:TRP:CZ3   | 2.56                     | 0.41              |
| 1:C:630:GLN:CD    | 1:C:630:GLN:N     | 2.76                     | 0.41              |
| 2:E:748:LEU:O     | 2:E:790:SER:HB2   | 2.21                     | 0.41              |
| 2:E:1309:ILE:HG22 | 2:E:1313:GLU:CG   | 2.51                     | 0.41              |
| 1:B:125:TYR:HD2   | 1:B:127:ILE:HD11  | 1.85                     | 0.41              |
| 1:B:329:SER:OG    | 1:B:413:GLU:O     | 2.25                     | 0.41              |
| 2:A:696:ILE:CG2   | 2:A:723:MET:HA    | 2.51                     | 0.41              |
| 2:A:1293:PRO:HB3  | 2:A:1341:PHE:HE1  | 1.86                     | 0.41              |
| 2:A:1407:VAL:HG23 | 2:A:1412:ARG:NH2  | 2.36                     | 0.41              |
| 2:A:1439:ASP:OD2  | 2:A:1471:ARG:HB2  | 2.21                     | 0.41              |
| 3:D:215:ILE:O     | 3:D:219:VAL:HG23  | 2.21                     | 0.41              |
| 1:C:27:ALA:O      | 1:C:60:HIS:NE2    | 2.54                     | 0.41              |
| 1:C:56:PRO:O      | 1:C:59:ASN:N      | 2.39                     | 0.41              |
| 2:E:750:ASN:CB    | 2:E:785:ILE:HG21  | 2.51                     | 0.41              |
| 2:E:1295:THR:O    | 2:E:1299:LYS:HG3  | 2.21                     | 0.41              |
| 2:E:1426:LYS:HA   | 2:E:1482:TYR:O    | 2.20                     | 0.41              |
| 1:B:163:GLN:HG2   | 1:B:166:VAL:O     | 2.20                     | 0.41              |
| 1:B:624:PHE:O     | 1:B:631:GLN:HA    | 2.21                     | 0.41              |
| 2:A:1428:ARG:HA   | 2:A:1481:HIS:HA   | 2.03                     | 0.41              |
| 2:E:833:ILE:HG23  | 2:E:834:ARG:N     | 2.34                     | 0.41              |
| 2:E:839:VAL:HG22  | 2:E:842:ARG:CD    | 2.49                     | 0.41              |
| 2:E:1379:ASP:N    | 2:E:1379:ASP:OD1  | 2.54                     | 0.41              |
| 1:B:22:LEU:HB3    | 1:B:54:LEU:HD11   | 2.03                     | 0.41              |
| 1:B:443:LEU:HA    | 1:B:447:GLU:OE2   | 2.21                     | 0.41              |
| 2:A:940:GLN:OE1   | 2:A:944:GLU:HG2   | 2.21                     | 0.41              |
| 2:A:1074:GLU:O    | 2:A:1103:LEU:HD21 | 2.21                     | 0.41              |
| 2:A:1133:ALA:O    | 2:A:1137:LEU:N    | 2.54                     | 0.41              |
| 1:C:440:ARG:HH11  | 1:C:440:ARG:HB3   | 1.80                     | 0.41              |
| 2:E:741:GLN:OE1   | 2:E:1382:LEU:N    | 2.44                     | 0.41              |
| 2:E:1377:LYS:HD3  | 2:E:1381:LYS:O    | 2.21                     | 0.41              |
| 1:B:7:ILE:CG1     | 1:B:624:PHE:HD1   | 2.34                     | 0.41              |
| 1:B:333:ILE:O     | 1:B:417:ARG:NE    | 2.54                     | 0.41              |
| 1:B:577:ASP:O     | 1:B:580:VAL:HG23  | 2.20                     | 0.41              |
| 2:A:1240:LYS:HD2  | 2:A:1240:LYS:HA   | 1.85                     | 0.41              |
| 2:A:1317:ALA:C    | 2:A:1319:SER:H    | 2.29                     | 0.41              |
| 2:A:1412:ARG:HG2  | 2:A:1507:TRP:CH2  | 2.55                     | 0.41              |
| 3:D:279:LYS:HA    | 3:D:282:GLN:CD    | 2.46                     | 0.41              |
| 1:C:4:TYR:O       | 1:C:626:SER:HA    | 2.21                     | 0.41              |
| 1:C:67:THR:O      | 1:C:69:PRO:HD3    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:126:ARG:HG2  | 1:C:168:PRO:HA    | 2.03                     | 0.41              |
| 1:C:351:MET:CE   | 1:C:440:ARG:HB2   | 2.51                     | 0.41              |
| 2:E:740:GLU:O    | 2:E:799:PRO:HD2   | 2.21                     | 0.41              |
| 2:E:845:ASP:OD1  | 2:E:845:ASP:N     | 2.53                     | 0.41              |
| 2:E:1329:ASP:C   | 2:E:1330:LYS:HG2  | 2.46                     | 0.41              |
| 2:E:1495:LYS:H   | 2:E:1495:LYS:HG2  | 1.75                     | 0.41              |
| 3:H:173:LEU:HB2  | 3:H:184:PHE:CE2   | 2.56                     | 0.41              |
| 1:B:222:TYR:HE1  | 1:B:328:THR:HA    | 1.86                     | 0.41              |
| 2:A:782:THR:HG23 | 2:A:814:TYR:CE1   | 2.44                     | 0.41              |
| 2:A:882:THR:HG23 | 2:A:882:THR:O     | 2.21                     | 0.41              |
| 2:A:1002:LYS:HE2 | 2:A:1002:LYS:HB3  | 1.89                     | 0.41              |
| 2:A:1010:LYS:C   | 2:A:1012:ASP:H    | 2.29                     | 0.41              |
| 2:A:1358:LYS:HE3 | 2:A:1368:SER:HB3  | 2.02                     | 0.41              |
| 1:C:259:ARG:HD3  | 1:C:303:TYR:CE1   | 2.56                     | 0.41              |
| 2:E:727:PHE:CE1  | 2:E:749:TYR:HB2   | 2.56                     | 0.41              |
| 1:B:140:THR:HA   | 1:B:158:LEU:O     | 2.20                     | 0.40              |
| 1:B:259:ARG:HD3  | 1:B:303:TYR:CD1   | 2.56                     | 0.40              |
| 1:B:321:ARG:HA   | 1:B:321:ARG:HD2   | 1.73                     | 0.40              |
| 1:B:342:PHE:CE1  | 1:B:344:PRO:HG3   | 2.57                     | 0.40              |
| 1:B:450:ASN:HB3  | 1:B:494:VAL:HG11  | 2.03                     | 0.40              |
| 2:A:756:GLU:HA   | 2:A:785:ILE:O     | 2.21                     | 0.40              |
| 2:A:1027:ILE:O   | 2:A:1030:LEU:HD13 | 2.21                     | 0.40              |
| 2:A:1470:CYS:O   | 2:A:1471:ARG:C    | 2.64                     | 0.40              |
| 3:D:260:ASP:OD1  | 3:D:266:ARG:NH2   | 2.53                     | 0.40              |
| 3:D:288:ALA:CB   | 3:D:296:VAL:HG22  | 2.51                     | 0.40              |
| 1:B:2:PRO:HB3    | 1:B:27:ALA:CB     | 2.41                     | 0.40              |
| 1:B:61:MET:HE2   | 1:B:61:MET:HB3    | 1.83                     | 0.40              |
| 1:B:449:LEU:HB3  | 1:B:499:ILE:HD11  | 2.02                     | 0.40              |
| 2:A:911:ASN:O    | 2:A:915:MET:N     | 2.54                     | 0.40              |
| 2:A:926:ASP:HA   | 2:A:931:TRP:CD1   | 2.56                     | 0.40              |
| 2:A:1372:PHE:HB2 | 2:A:1379:ASP:O    | 2.22                     | 0.40              |
| 3:D:291:PRO:O    | 3:D:295:HIS:ND1   | 2.55                     | 0.40              |
| 1:C:559:MET:HE2  | 1:C:559:MET:HB3   | 1.93                     | 0.40              |
| 2:E:817:PHE:CZ   | 3:H:281:ARG:HD2   | 2.56                     | 0.40              |
| 1:B:431:ASN:HA   | 1:B:433:TYR:CE2   | 2.57                     | 0.40              |
| 2:A:916:THR:HB   | 2:A:917:PRO:HD3   | 2.03                     | 0.40              |
| 2:A:1243:LEU:O   | 2:A:1371:ARG:NE   | 2.55                     | 0.40              |
| 1:C:30:ASP:OD1   | 1:C:30:ASP:N      | 2.54                     | 0.40              |
| 1:C:141:VAL:O    | 1:C:157:SER:HA    | 2.22                     | 0.40              |
| 1:C:353:PHE:HD1  | 1:C:383:GLY:O     | 2.05                     | 0.40              |
| 2:E:769:PHE:CD1  | 2:E:799:PRO:HA    | 2.57                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:116:ILE:HG12 | 1:B:205:TYR:CE2   | 2.56                     | 0.40              |
| 1:B:138:GLY:HA3  | 1:B:161:GLN:OE1   | 2.21                     | 0.40              |
| 1:C:100:LEU:HD21 | 1:C:638:LEU:HD23  | 2.03                     | 0.40              |
| 1:C:443:LEU:HD13 | 1:C:443:LEU:HA    | 1.94                     | 0.40              |
| 3:H:311:GLN:O    | 3:H:315:LYS:HE3   | 2.20                     | 0.40              |
| 1:B:335:PHE:O    | 1:B:338:THR:OG1   | 2.31                     | 0.40              |
| 2:A:911:ASN:HB3  | 2:A:953:GLN:OE1   | 2.21                     | 0.40              |
| 2:A:1520:GLU:HA  | 2:A:1523:GLN:HG3  | 2.02                     | 0.40              |
| 1:C:130:VAL:HA   | 1:C:135:LEU:O     | 2.21                     | 0.40              |
| 1:C:403:ARG:HH11 | 1:C:414:GLN:HB2   | 1.85                     | 0.40              |
| 1:C:471:LEU:HB2  | 1:C:510:VAL:HG22  | 2.03                     | 0.40              |
| 1:C:501:THR:HB   | 1:C:538:VAL:HG13  | 2.04                     | 0.40              |
| 2:E:1373:TYR:C   | 2:E:1373:TYR:CD1  | 3.00                     | 0.40              |
| 2:E:1421:VAL:O   | 2:E:1421:VAL:HG23 | 2.20                     | 0.40              |
| 2:E:1507:TRP:CD1 | 2:E:1507:TRP:C    | 2.99                     | 0.40              |

All (3) 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:A:756:GLU:OE2  | 3:H:300:ASN:ND2[2_747] | 1.93                     | 0.27              |
| 2:A:1428:ARG:NH2 | 3:H:191:ASN:O[1_455]   | 2.07                     | 0.13              |
| 3:D:249:PRO:O    | 1:C:71:ASN:ND2[2_657]  | 2.08                     | 0.12              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | B     | 643/645 (100%) | 609 (95%) | 34 (5%)  | 0        | 100         | 100 |
| 1   | C     | 643/645 (100%) | 617 (96%) | 25 (4%)  | 1 (0%)   | 43          | 71  |
| 2   | A     | 836/898 (93%)  | 743 (89%) | 92 (11%) | 1 (0%)   | 48          | 78  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | E     | 498/898 (56%)   | 441 (89%)  | 57 (11%) | 0        | 100         | 100 |
| 3   | D     | 183/195 (94%)   | 169 (92%)  | 14 (8%)  | 0        | 100         | 100 |
| 3   | H     | 183/195 (94%)   | 173 (94%)  | 9 (5%)   | 1 (0%)   | 24          | 54  |
| All | All   | 2986/3476 (86%) | 2752 (92%) | 231 (8%) | 3 (0%)   | 48          | 78  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 41  | PRO  |
| 2   | A     | 656 | GLU  |
| 3   | H     | 177 | SER  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | B     | 567/567 (100%)  | 565 (100%)  | 2 (0%)   | 84          | 83  |
| 1   | C     | 567/567 (100%)  | 559 (99%)   | 8 (1%)   | 59          | 70  |
| 2   | A     | 745/794 (94%)   | 745 (100%)  | 0        | 100         | 100 |
| 2   | E     | 463/794 (58%)   | 463 (100%)  | 0        | 100         | 100 |
| 3   | D     | 166/172 (96%)   | 166 (100%)  | 0        | 100         | 100 |
| 3   | H     | 166/172 (96%)   | 166 (100%)  | 0        | 100         | 100 |
| All | All   | 2674/3066 (87%) | 2664 (100%) | 10 (0%)  | 84          | 83  |

All (10) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 75  | LYS  |
| 1   | B     | 77  | GLU  |
| 1   | C     | 68  | ILE  |
| 1   | C     | 374 | THR  |
| 1   | C     | 375 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 391 | THR  |
| 1   | C     | 439 | LEU  |
| 1   | C     | 440 | ARG  |
| 1   | C     | 443 | LEU  |
| 1   | C     | 594 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 10   | ASN  |
| 1   | B     | 144  | ASN  |
| 1   | B     | 155  | GLN  |
| 1   | B     | 318  | GLN  |
| 1   | B     | 420  | GLN  |
| 1   | B     | 461  | HIS  |
| 1   | B     | 567  | HIS  |
| 2   | A     | 724  | GLN  |
| 2   | A     | 805  | GLN  |
| 2   | A     | 815  | HIS  |
| 2   | A     | 867  | GLN  |
| 2   | A     | 1049 | GLN  |
| 2   | A     | 1105 | ASN  |
| 2   | A     | 1174 | GLN  |
| 2   | A     | 1276 | GLN  |
| 2   | A     | 1344 | HIS  |
| 2   | A     | 1383 | ASN  |
| 2   | A     | 1461 | GLN  |
| 2   | A     | 1510 | HIS  |
| 2   | A     | 1518 | GLN  |
| 2   | A     | 1543 | ASN  |
| 3   | D     | 175  | GLN  |
| 3   | D     | 190  | GLN  |
| 3   | D     | 232  | ASN  |
| 3   | D     | 282  | GLN  |
| 3   | D     | 295  | HIS  |
| 1   | C     | 10   | ASN  |
| 1   | C     | 93   | GLN  |
| 1   | C     | 144  | ASN  |
| 1   | C     | 155  | GLN  |
| 1   | C     | 162  | ASN  |
| 1   | C     | 181  | GLN  |
| 1   | C     | 193  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 254  | GLN  |
| 1   | C     | 376  | GLN  |
| 1   | C     | 420  | GLN  |
| 1   | C     | 558  | GLN  |
| 1   | C     | 631  | GLN  |
| 2   | E     | 681  | ASN  |
| 2   | E     | 689  | ASN  |
| 2   | E     | 724  | GLN  |
| 2   | E     | 779  | HIS  |
| 2   | E     | 816  | HIS  |
| 2   | E     | 1300 | GLN  |
| 2   | E     | 1345 | GLN  |
| 2   | E     | 1348 | ASN  |
| 2   | E     | 1383 | ASN  |
| 2   | E     | 1457 | GLN  |
| 2   | E     | 1525 | GLN  |
| 3   | H     | 175  | GLN  |
| 3   | H     | 191  | ASN  |
| 3   | H     | 311  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

7 monosaccharides 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 |
| 4   | NAG  | I     | 1   | 1,4  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.50 | 0        |
| 4   | NAG  | I     | 2   | 4    | 14,14,15     | 0.75 | 0        | 17,19,21    | 1.15 | 2 (11%)  |
| 4   | MAN  | I     | 3   | 4    | 11,11,12     | 2.17 | 4 (36%)  | 15,15,17    | 1.42 | 2 (13%)  |
| 5   | NAG  | J     | 1   | 5,1  | 14,14,15     | 0.94 | 1 (7%)   | 17,19,21    | 0.57 | 0        |
| 5   | NAG  | J     | 2   | 5    | 14,14,15     | 0.85 | 1 (7%)   | 17,19,21    | 0.80 | 0        |
| 5   | MAN  | J     | 3   | 5    | 11,11,12     | 2.11 | 4 (36%)  | 15,15,17    | 1.78 | 2 (13%)  |
| 5   | BMA  | J     | 4   | 5    | 11,11,12     | 1.79 | 4 (36%)  | 15,15,17    | 1.06 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | I     | 1   | 1,4  | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | I     | 2   | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | MAN  | I     | 3   | 4    | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | NAG  | J     | 1   | 5,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | J     | 2   | 5    | -       | 3/6/23/26 | 0/1/1/1 |
| 5   | MAN  | J     | 3   | 5    | -       | 1/2/19/22 | 0/1/1/1 |
| 5   | BMA  | J     | 4   | 5    | -       | 0/2/19/22 | 0/1/1/1 |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | I     | 3   | MAN  | O5-C1 | 5.27  | 1.52        | 1.43     |
| 5   | J     | 3   | MAN  | C2-C3 | 4.64  | 1.59        | 1.52     |
| 5   | J     | 4   | BMA  | C4-C3 | 3.12  | 1.60        | 1.52     |
| 5   | J     | 1   | NAG  | O5-C1 | 2.85  | 1.48        | 1.43     |
| 5   | J     | 4   | BMA  | C2-C3 | 2.77  | 1.56        | 1.52     |
| 5   | J     | 4   | BMA  | O5-C1 | 2.76  | 1.48        | 1.43     |
| 5   | J     | 3   | MAN  | O5-C5 | 2.76  | 1.48        | 1.43     |
| 4   | I     | 3   | MAN  | C1-C2 | 2.72  | 1.58        | 1.52     |
| 4   | I     | 3   | MAN  | O3-C3 | -2.60 | 1.36        | 1.43     |
| 5   | J     | 2   | NAG  | O5-C1 | -2.59 | 1.39        | 1.43     |
| 5   | J     | 3   | MAN  | C4-C5 | 2.50  | 1.58        | 1.53     |
| 5   | J     | 4   | BMA  | C1-C2 | 2.31  | 1.57        | 1.52     |
| 5   | J     | 3   | MAN  | C1-C2 | 2.21  | 1.57        | 1.52     |
| 4   | I     | 3   | MAN  | O4-C4 | 2.12  | 1.48        | 1.43     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | J     | 3   | MAN  | C1-O5-C5 | 5.24  | 119.21      | 112.19   |
| 4   | I     | 3   | MAN  | C1-O5-C5 | 2.75  | 115.87      | 112.19   |
| 4   | I     | 3   | MAN  | C1-C2-C3 | 2.74  | 113.63      | 109.64   |
| 5   | J     | 3   | MAN  | C1-C2-C3 | 2.68  | 113.55      | 109.64   |
| 4   | I     | 2   | NAG  | O4-C4-C5 | -2.33 | 103.58      | 109.32   |
| 4   | I     | 2   | NAG  | O5-C1-C2 | -2.08 | 108.08      | 111.29   |

There are no chirality outliers.

All (11) torsion outliers are listed below:

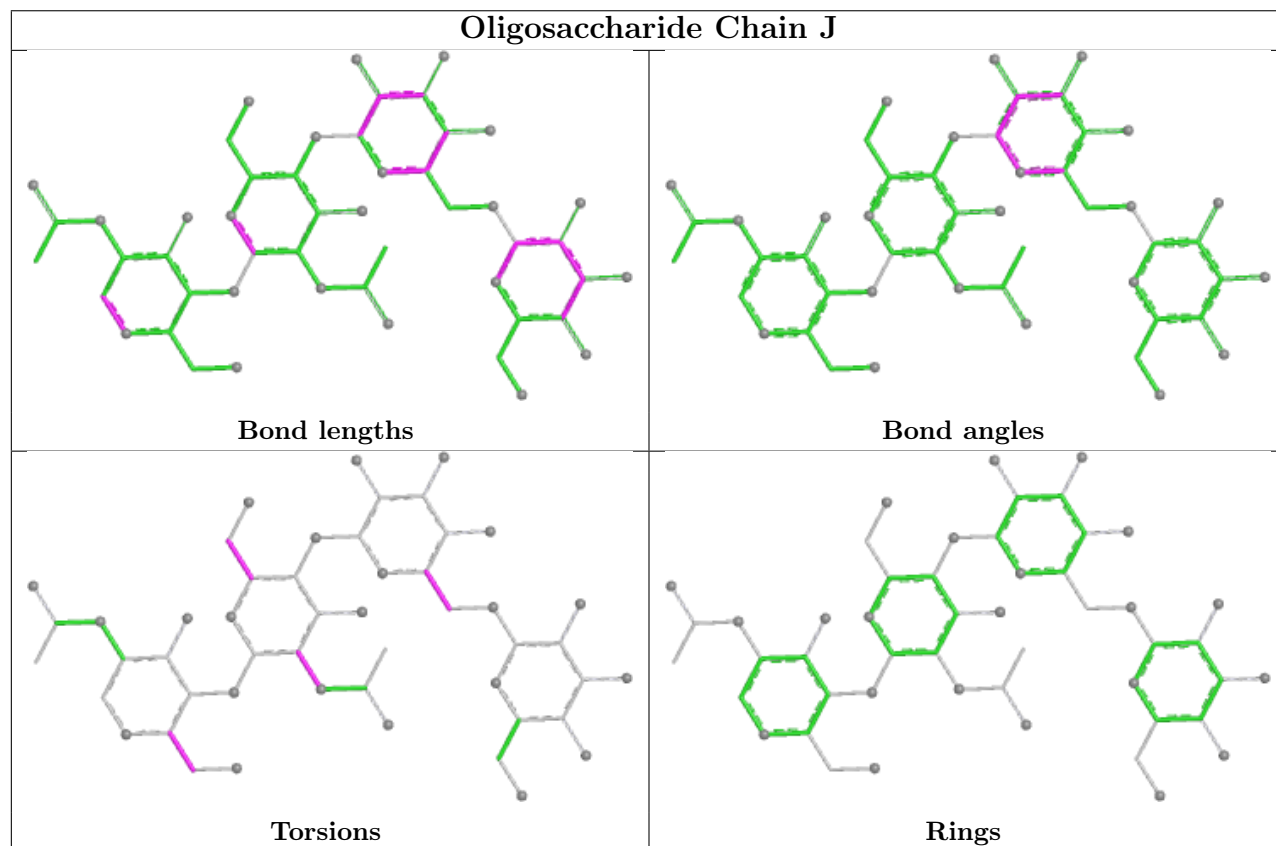
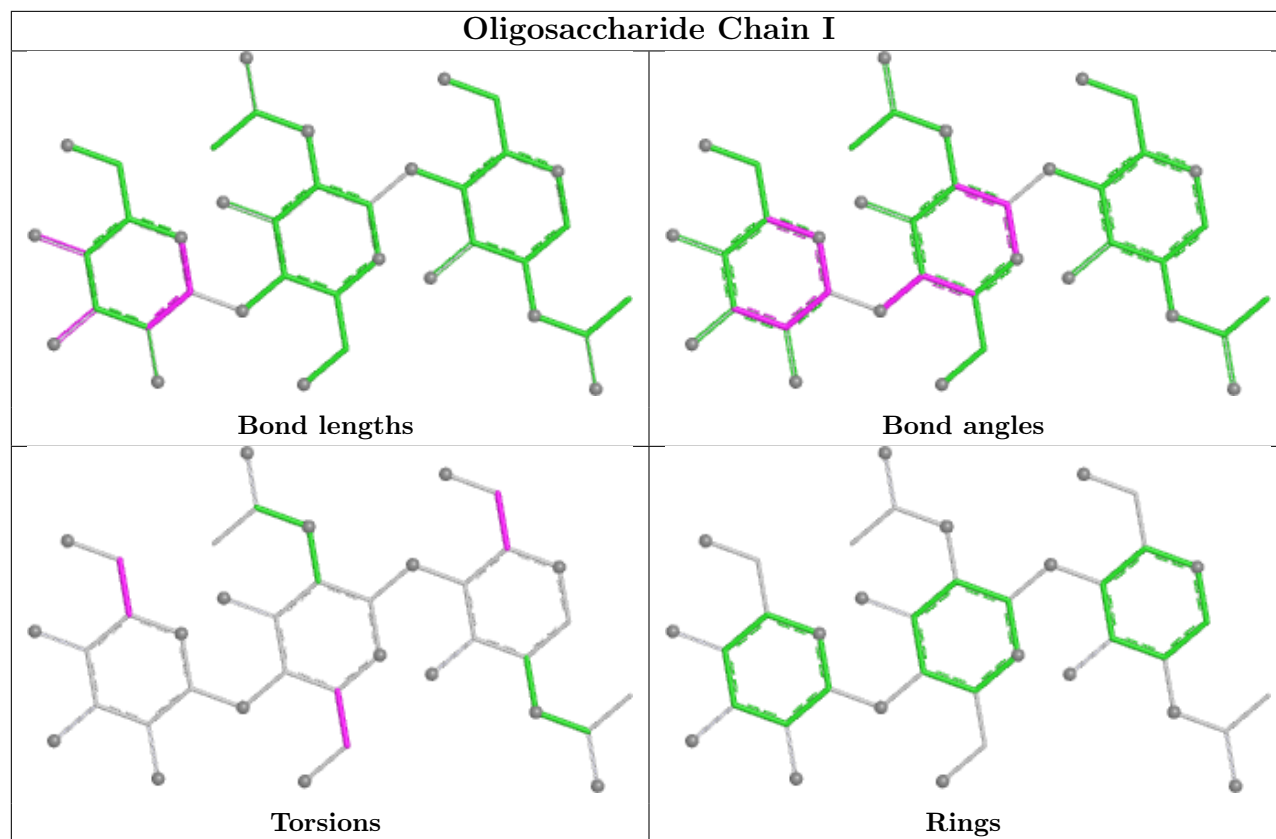
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | J     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | I     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | I     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | J     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | I     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | J     | 2   | NAG  | C4-C5-C6-O6 |
| 4   | I     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | J     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | I     | 3   | MAN  | O5-C5-C6-O6 |
| 5   | J     | 2   | NAG  | C1-C2-N2-C7 |
| 5   | J     | 3   | MAN  | C4-C5-C6-O6 |

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | I     | 1   | NAG  | 2       | 0            |
| 5   | J     | 2   | NAG  | 1       | 0            |
| 5   | J     | 4   | BMA  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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 |
| 6   | GOL  | E     | 1602 | -    | 5,5,5        | 1.15 | 0        | 5,5,5       | 1.08 | 0        |
| 6   | GOL  | B     | 1601 | -    | 5,5,5        | 1.78 | 2 (40%)  | 5,5,5       | 0.62 | 0        |
| 6   | GOL  | C     | 1601 | -    | 5,5,5        | 0.95 | 0        | 5,5,5       | 1.06 | 0        |
| 9   | NAG  | E     | 1601 | 2    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.80 | 1 (5%)   |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 6   | GOL  | E     | 1602 | -    | -       | 2/4/4/4   | -       |
| 6   | GOL  | B     | 1601 | -    | -       | 3/4/4/4   | -       |
| 6   | GOL  | C     | 1601 | -    | -       | 0/4/4/4   | -       |
| 9   | NAG  | E     | 1601 | 2    | -       | 0/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 6   | B     | 1601 | GOL  | C3-C2 | 3.15 | 1.63        | 1.51     |
| 6   | B     | 1601 | GOL  | C1-C2 | 2.23 | 1.60        | 1.51     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 9   | E     | 1601 | NAG  | C1-O5-C5 | 2.22 | 115.16      | 112.19   |

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 6   | B     | 1601 | GOL  | C1-C2-C3-O3 |
| 6   | E     | 1602 | GOL  | O1-C1-C2-C3 |
| 6   | E     | 1602 | GOL  | O1-C1-C2-O2 |
| 6   | B     | 1601 | GOL  | O2-C2-C3-O3 |
| 6   | B     | 1601 | GOL  | O1-C1-C2-O2 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | E     | 1602 | GOL  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1   | B     | 645/645 (100%)  | -1.59  | 0 100 100 | 47, 108, 152, 185     | 0     |
| 1   | C     | 645/645 (100%)  | -1.60  | 0 100 100 | 57, 104, 150, 179     | 0     |
| 2   | A     | 842/898 (93%)   | -1.54  | 0 100 100 | 55, 127, 164, 192     | 0     |
| 2   | E     | 504/898 (56%)   | -1.59  | 0 100 100 | 58, 111, 170, 204     | 0     |
| 3   | D     | 185/195 (94%)   | -1.54  | 0 100 100 | 78, 108, 133, 155     | 0     |
| 3   | H     | 185/195 (94%)   | -1.62  | 0 100 100 | 68, 93, 123, 145      | 0     |
| All | All   | 3006/3476 (86%) | -1.58  | 0 100 100 | 47, 111, 159, 204     | 0     |

There are no RSRZ outliers to report.

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

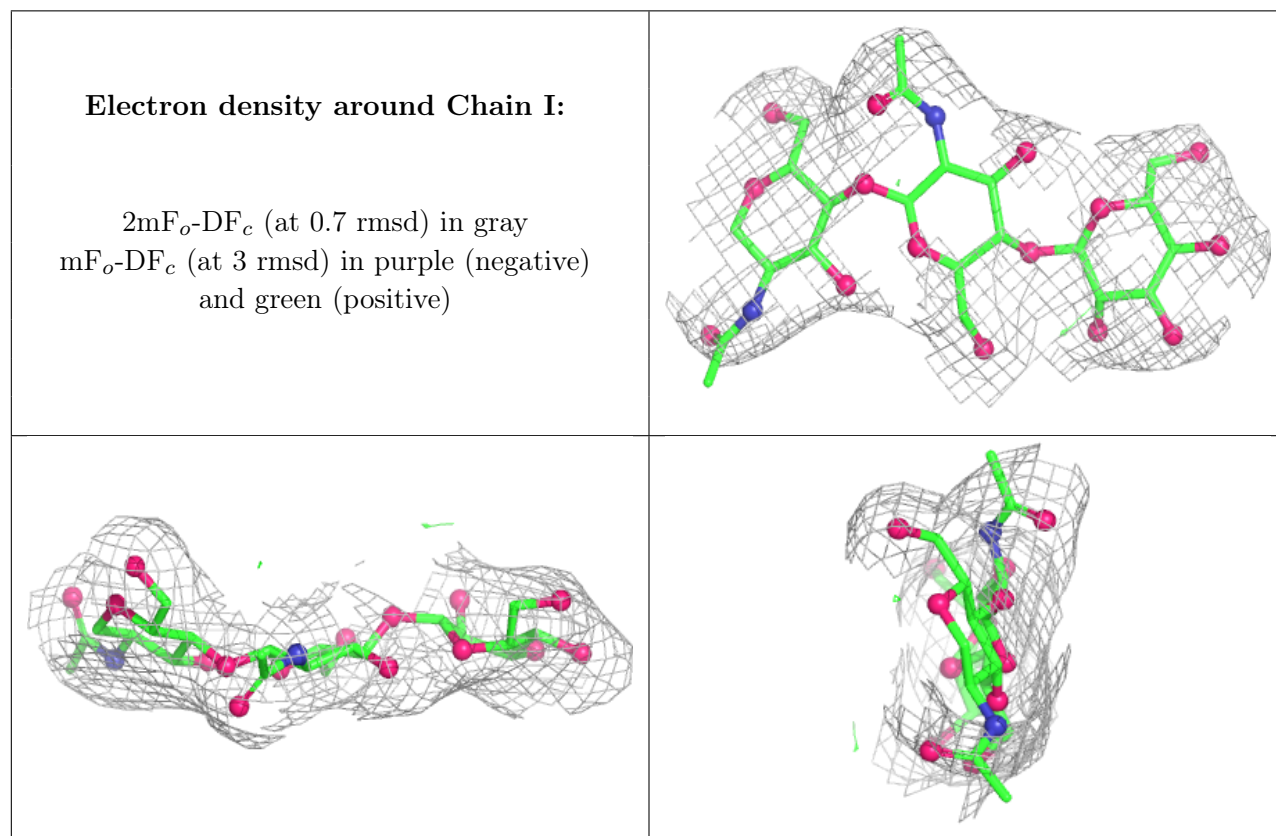
There are no non-standard protein/DNA/RNA residues in this entry.

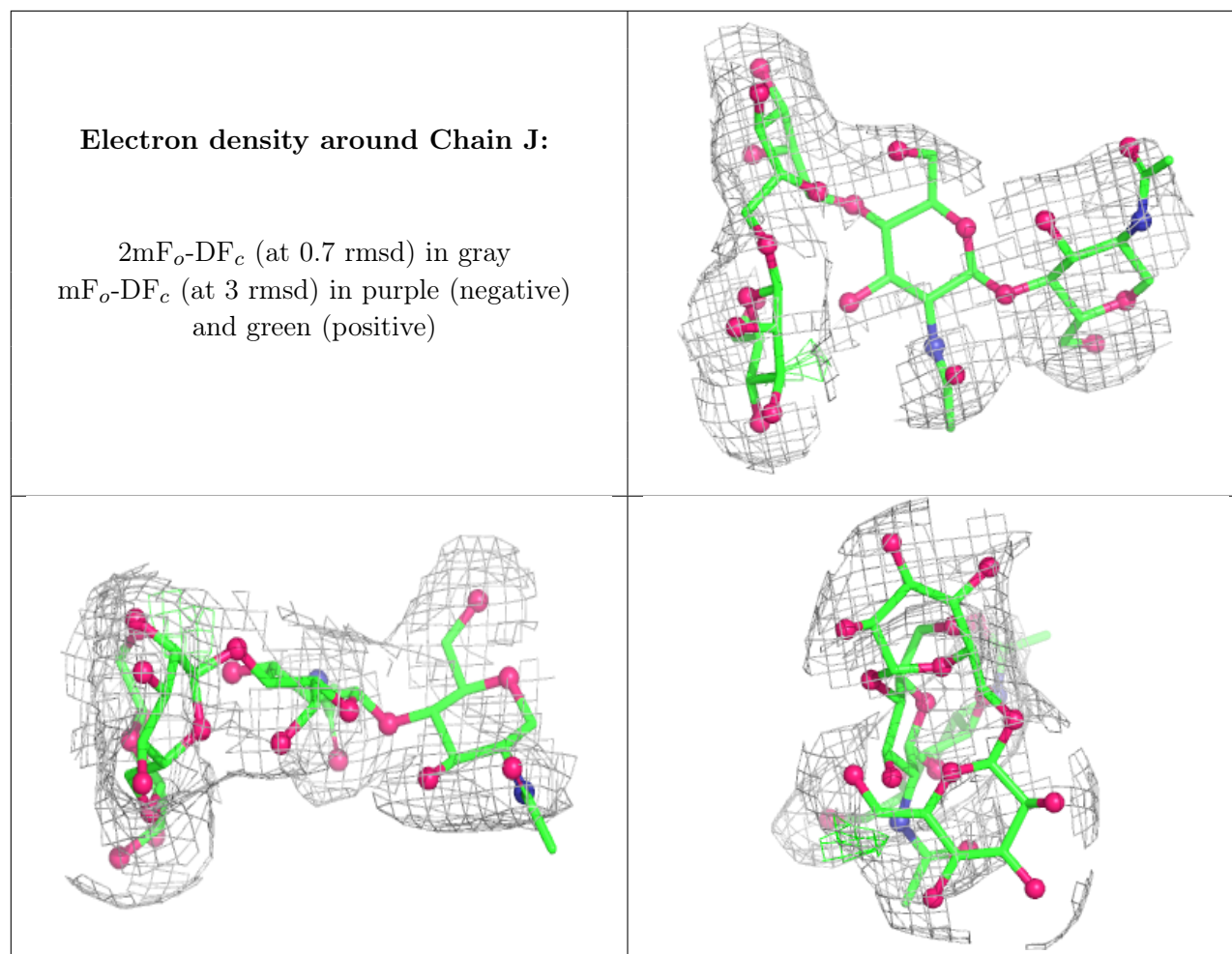
### 6.3 Carbohydrates [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|----------------------------|-------|
| 4   | NAG  | I     | 1   | 14/15 | -    | -   | 123,128,134,135            | 0     |
| 4   | NAG  | I     | 2   | 14/15 | -    | -   | 138,141,144,145            | 0     |
| 4   | MAN  | I     | 3   | 11/12 | -    | -   | 120,126,137,141            | 0     |
| 5   | NAG  | J     | 1   | 14/15 | -    | -   | 98,107,131,132             | 0     |
| 5   | NAG  | J     | 2   | 14/15 | -    | -   | 106,118,132,140            | 0     |
| 5   | MAN  | J     | 3   | 11/12 | -    | -   | 135,144,147,150            | 0     |
| 5   | BMA  | J     | 4   | 11/12 | -    | -   | 119,126,140,143            | 0     |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 9   | NAG  | E     | 1601 | 14/15 | 0.96 | 0.05 | 157,161,166,168             | 0     |
| 6   | GOL  | C     | 1601 | 6/6   | 0.99 | 0.04 | 81,91,93,93                 | 0     |
| 6   | GOL  | E     | 1602 | 6/6   | 0.99 | 0.08 | 69,73,75,76                 | 0     |
| 8   | MG   | D     | 2101 | 1/1   | 0.99 | 0.02 | 117,117,117,117             | 0     |
| 8   | MG   | H     | 2001 | 1/1   | 0.99 | 0.03 | 82,82,82,82                 | 0     |
| 6   | GOL  | B     | 1601 | 6/6   | 0.99 | 0.07 | 67,70,71,73                 | 0     |
| 7   | K    | C     | 1602 | 1/1   | 1.00 | 0.03 | 71,71,71,71                 | 0     |
| 7   | K    | A     | 1601 | 1/1   | 1.00 | 0.04 | 71,71,71,71                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.