



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:07 AM EDT

PDB ID : 1SOJ / pdb\_00001soj  
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B IN COMPLEX WITH IBMX  
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.  
Deposited on : 2004-03-15  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

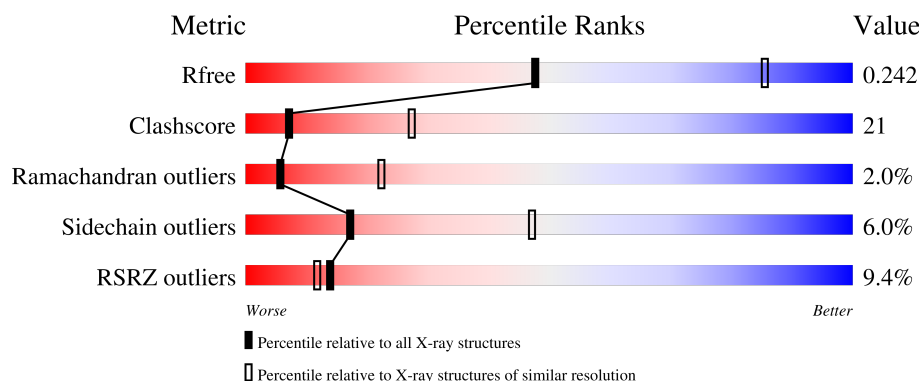
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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

| Mol | Chain | Length | Quality of chain     |
|-----|-------|--------|----------------------|
| 1   | A     | 420    | <br>6% 56% 28% 13%   |
| 1   | B     | 420    | <br>8% 53% 32% 5% 9% |
| 1   | C     | 420    | <br>6% 53% 29% 13%   |
| 1   | D     | 420    | <br>9% 53% 32% 5% 9% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 420    |                  |
| 1   | F     | 420    |                  |
| 1   | G     | 420    |                  |
| 1   | H     | 420    |                  |
| 1   | I     | 420    |                  |
| 1   | J     | 420    |                  |
| 1   | K     | 420    |                  |
| 1   | L     | 420    |                  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36048 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2907  | 1862 | 496 | 535 | 14 |         |         |       |
| 1   | B     | 381      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 1922 | 519 | 562 | 14 |         |         |       |
| 1   | C     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2907  | 1862 | 496 | 535 | 14 |         |         |       |
| 1   | D     | 381      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 1922 | 519 | 562 | 14 |         |         |       |
| 1   | E     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2907  | 1862 | 496 | 535 | 14 |         |         |       |
| 1   | F     | 381      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 1922 | 519 | 562 | 14 |         |         |       |
| 1   | G     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2907  | 1862 | 496 | 535 | 14 |         |         |       |
| 1   | H     | 381      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 1922 | 519 | 562 | 14 |         |         |       |
| 1   | I     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2907  | 1862 | 496 | 535 | 14 |         |         |       |
| 1   | J     | 381      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 1922 | 519 | 562 | 14 |         |         |       |
| 1   | K     | 364      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2907  | 1862 | 496 | 535 | 14 |         |         |       |
| 1   | L     | 381      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3017  | 1922 | 519 | 562 | 14 |         |         |       |

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

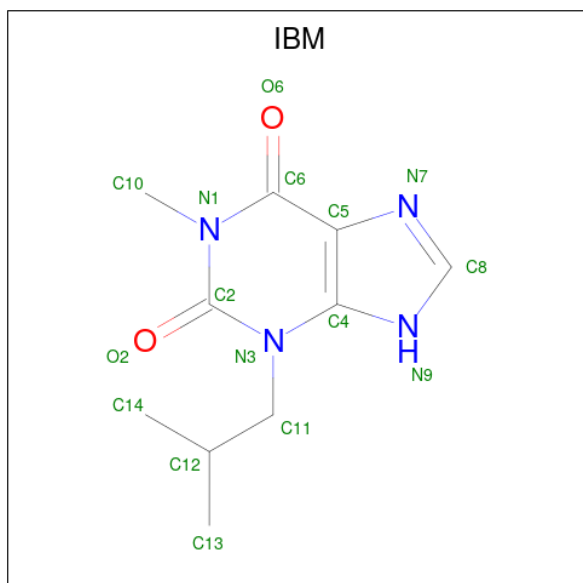
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | B     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | C     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | D     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | E     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | F     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | G     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | H     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | I     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | J     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | K     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | L     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 3 is 3-ISOBUTYL-1-METHYLNANTHINE (CCD ID: IBM) (formula:  $C_{10}H_{14}N_4O_2$ ).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |
| 3   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 10 | 4 | 2 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 4   | B     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 4   | C     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 4   | D     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 4   | E     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 4   | F     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 4   | G     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 4   | H     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |

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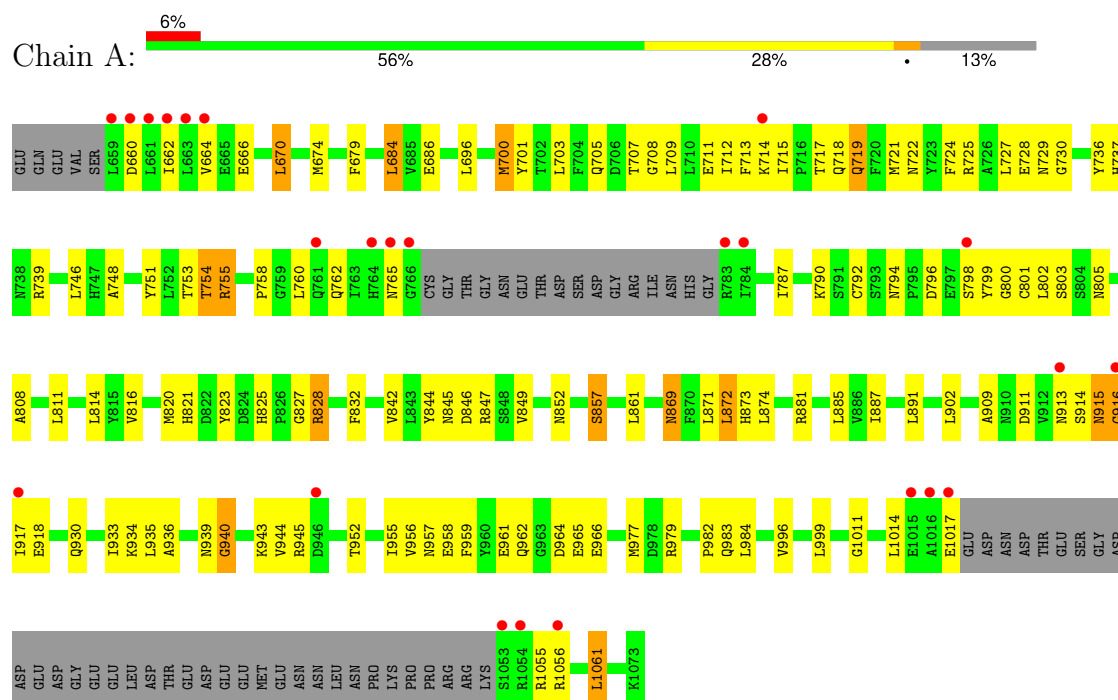
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | I     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 4   | J     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 4   | K     | 24       | Total<br>24 | O<br>24 | 0       | 0       |
| 4   | L     | 24       | Total<br>24 | O<br>24 | 0       | 0       |

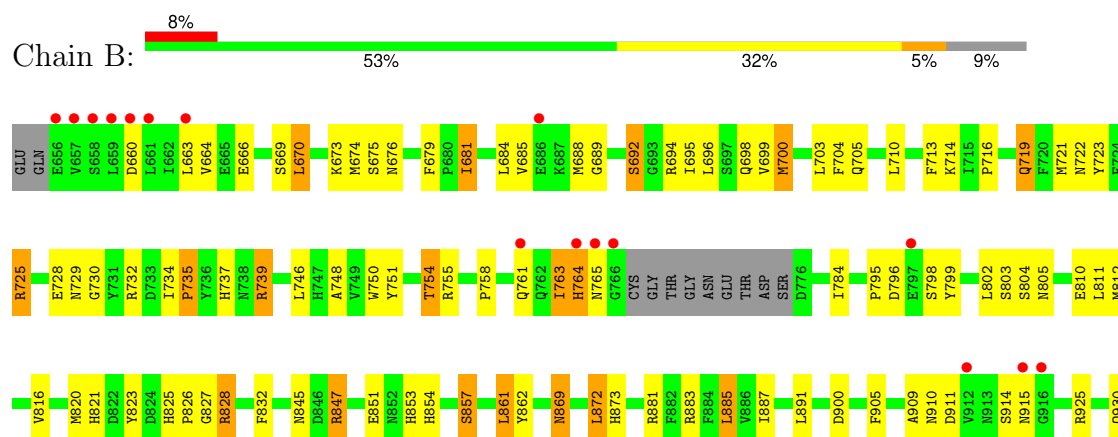
### 3 Residue-property plots

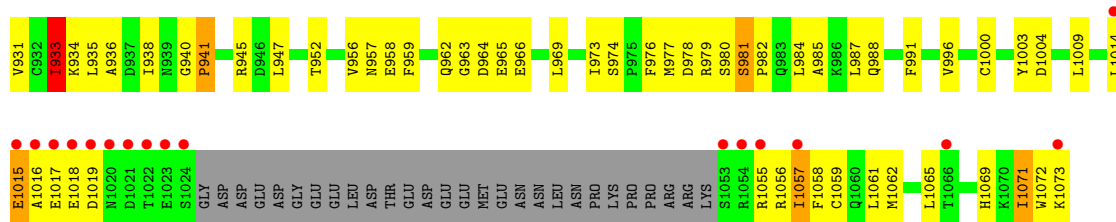
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

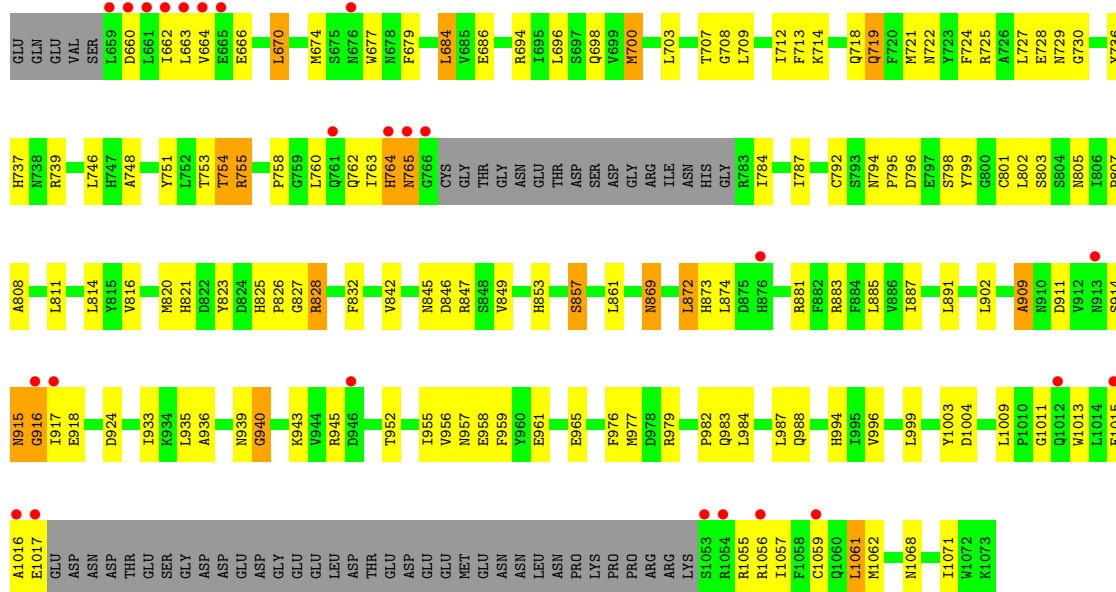


#### • Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

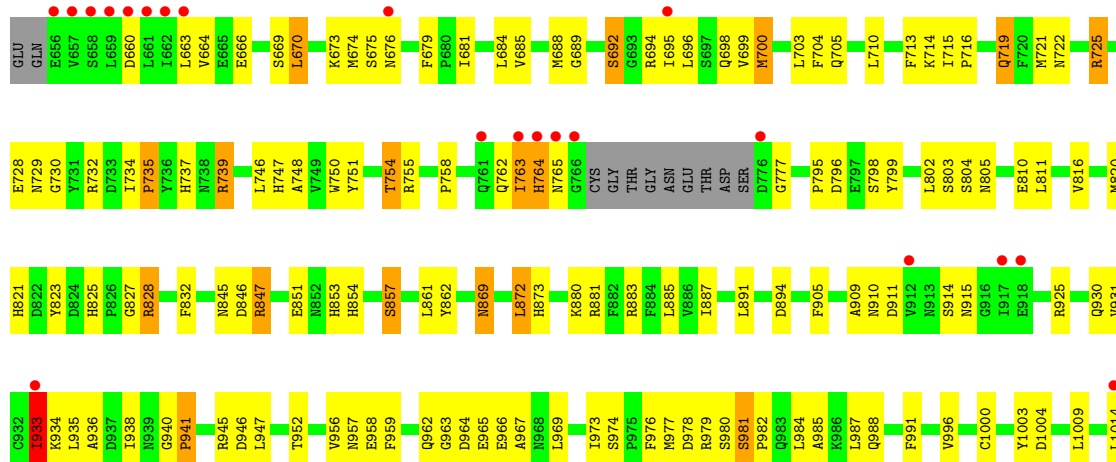


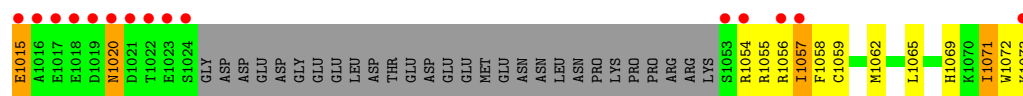


• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

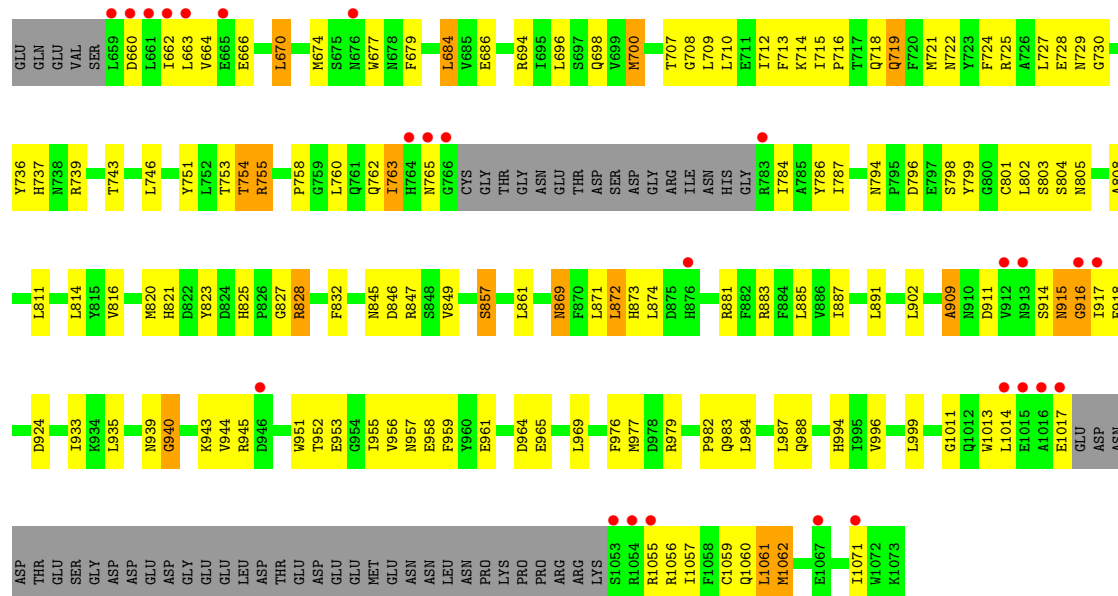


• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

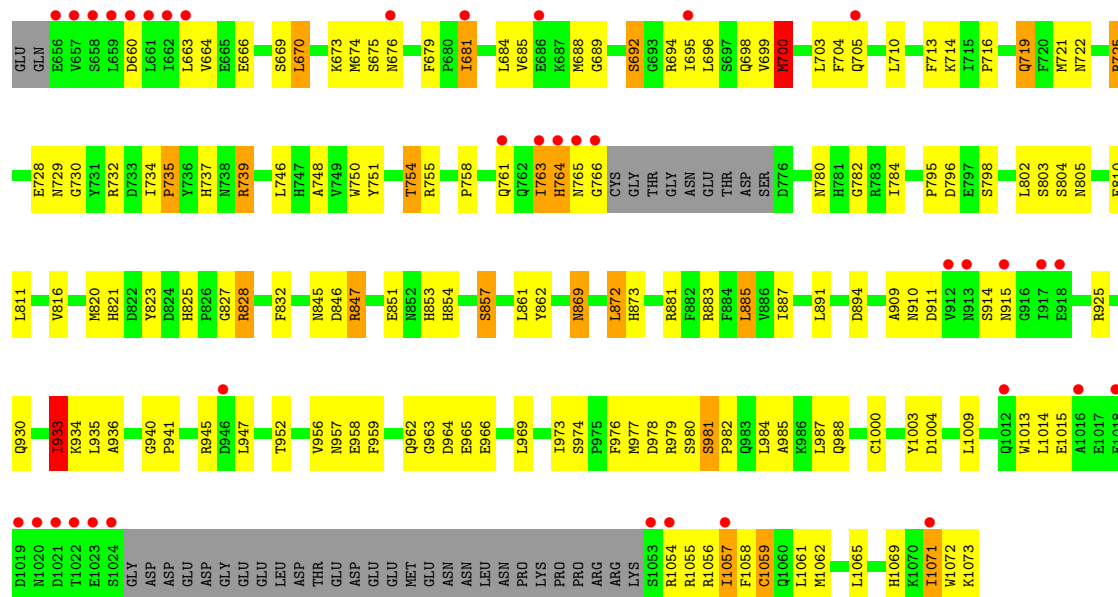




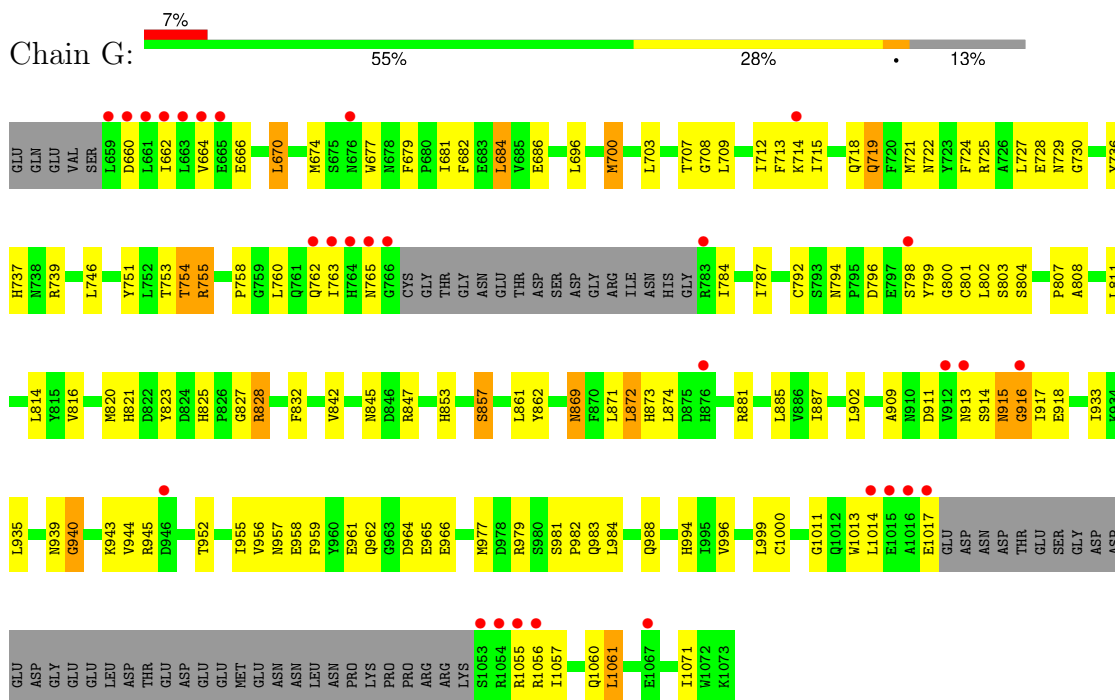
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



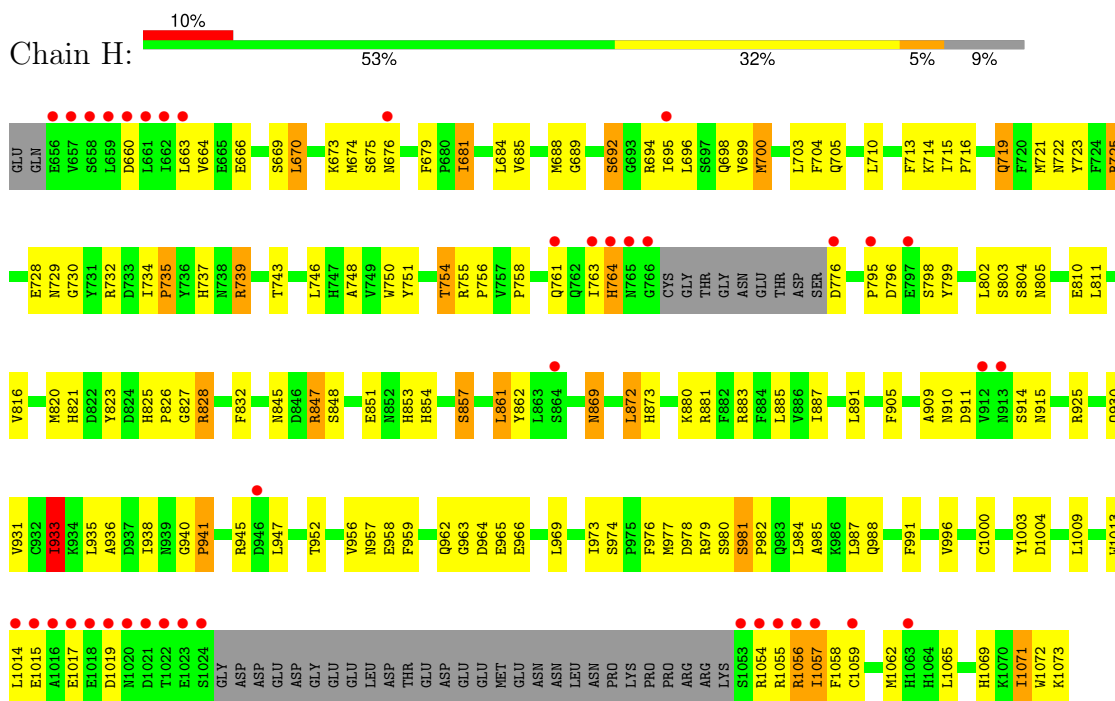
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



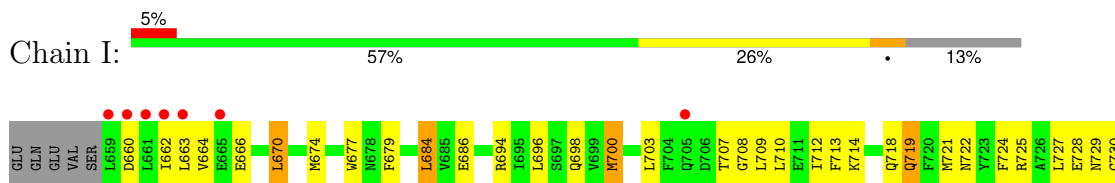
- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

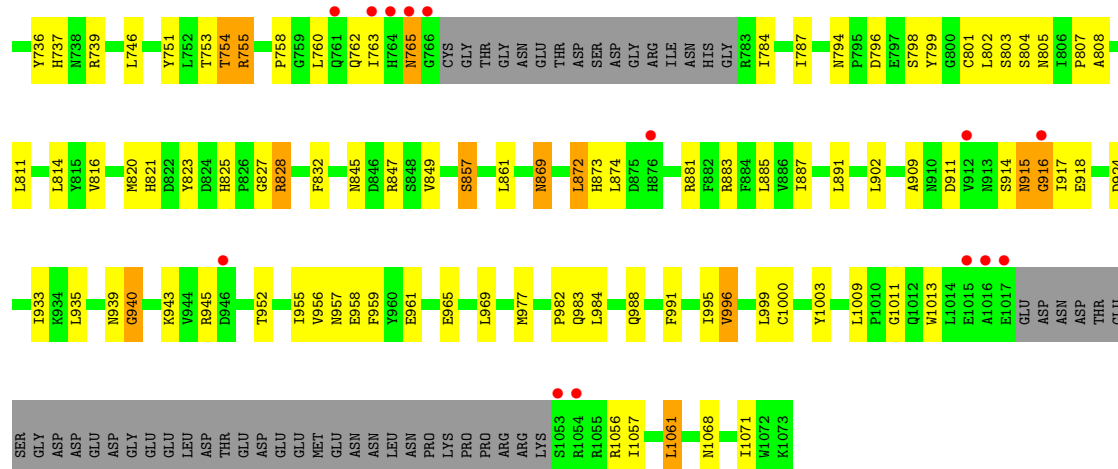


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

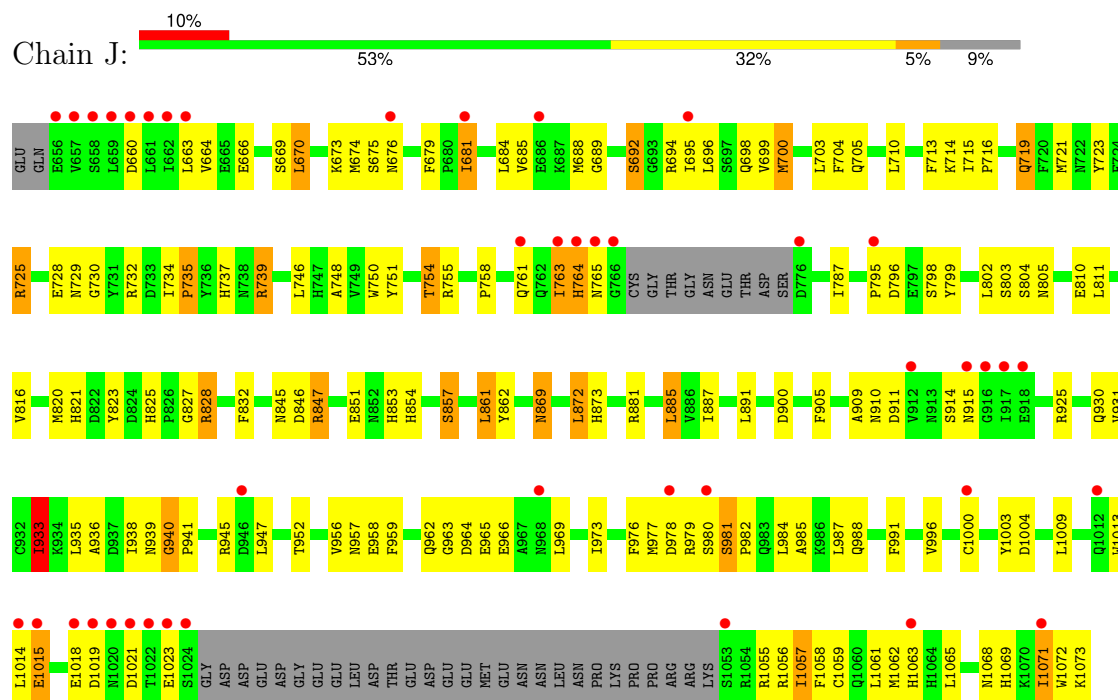


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

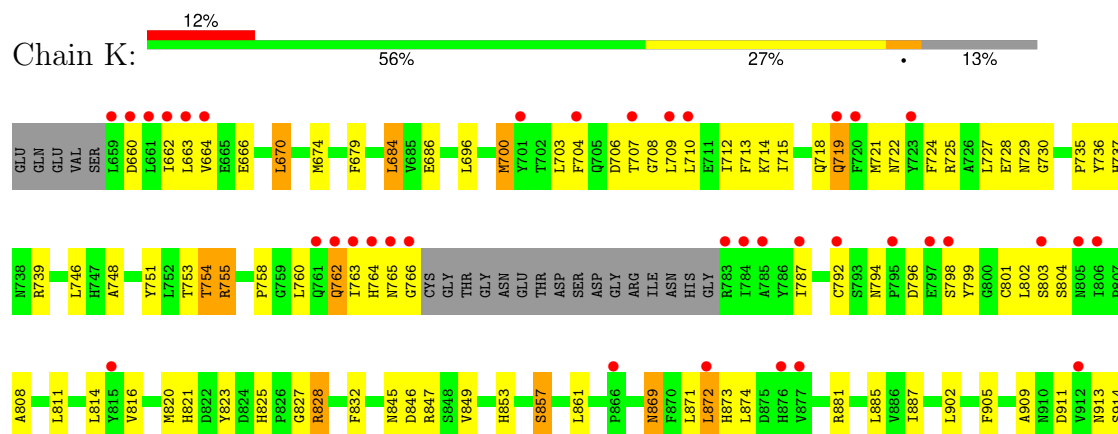


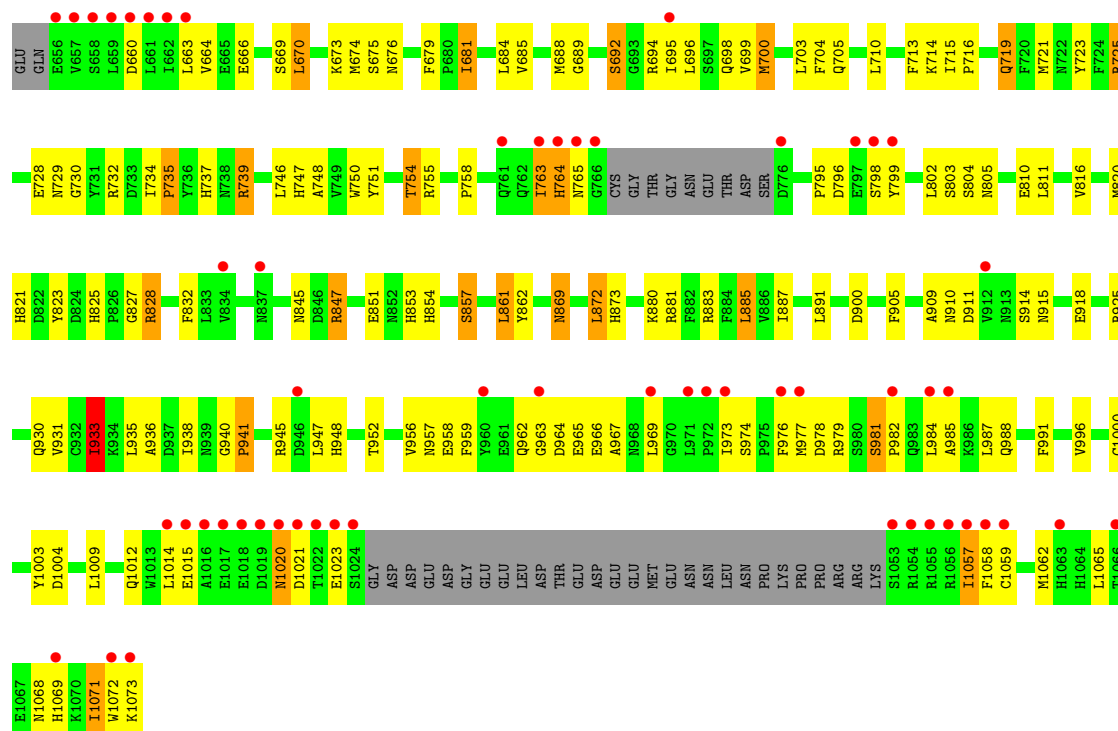


• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 275.05Å 147.08Å 253.49Å<br>90.00° 109.84° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 30.00 – 2.90<br>30.00 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.7 (30.00-2.90)<br>96.6 (30.00-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.14 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | CNX                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.231 , 0.249<br>0.228 , 0.242                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10128 reflections (4.98%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.691                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 54.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 36048                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 48.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.57         | 0/2982         | 0.91        | 5/4053 (0.1%)   |
| 1   | B     | 0.52         | 0/3092         | 0.89        | 7/4203 (0.2%)   |
| 1   | C     | 0.56         | 0/2982         | 0.90        | 6/4053 (0.1%)   |
| 1   | D     | 0.59         | 0/3092         | 0.89        | 7/4203 (0.2%)   |
| 1   | E     | 0.61         | 0/2982         | 0.91        | 8/4053 (0.2%)   |
| 1   | F     | 0.61         | 1/3092 (0.0%)  | 0.90        | 7/4203 (0.2%)   |
| 1   | G     | 0.55         | 0/2982         | 0.90        | 9/4053 (0.2%)   |
| 1   | H     | 0.53         | 0/3092         | 0.88        | 6/4203 (0.1%)   |
| 1   | I     | 0.57         | 0/2982         | 0.91        | 4/4053 (0.1%)   |
| 1   | J     | 0.58         | 0/3092         | 0.90        | 8/4203 (0.2%)   |
| 1   | K     | 0.52         | 0/2982         | 0.90        | 4/4053 (0.1%)   |
| 1   | L     | 0.53         | 0/3092         | 0.89        | 6/4203 (0.1%)   |
| All | All   | 0.56         | 1/36444 (0.0%) | 0.90        | 77/49536 (0.2%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 700 | MET  | SD-CE | -6.35 | 1.63        | 1.79     |

All (77) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 909 | ALA  | N-CA-C | 8.06 | 119.76      | 110.97   |
| 1   | F     | 909 | ALA  | N-CA-C | 7.93 | 119.61      | 110.97   |
| 1   | J     | 909 | ALA  | N-CA-C | 7.87 | 119.55      | 110.97   |
| 1   | B     | 909 | ALA  | N-CA-C | 7.84 | 119.51      | 110.97   |
| 1   | H     | 909 | ALA  | N-CA-C | 7.79 | 119.46      | 110.97   |
| 1   | L     | 909 | ALA  | N-CA-C | 7.57 | 119.22      | 110.97   |
| 1   | G     | 715 | ILE  | N-CA-C | 6.94 | 113.88      | 107.56   |
| 1   | A     | 715 | ILE  | N-CA-C | 6.65 | 113.61      | 107.56   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | L     | 933 | ILE  | CB-CA-C | -6.64 | 103.17      | 112.14   |
| 1   | F     | 933 | ILE  | CB-CA-C | -6.61 | 103.22      | 112.14   |
| 1   | B     | 933 | ILE  | CB-CA-C | -6.50 | 103.36      | 112.14   |
| 1   | D     | 933 | ILE  | CB-CA-C | -6.49 | 103.38      | 112.14   |
| 1   | J     | 933 | ILE  | CB-CA-C | -6.46 | 103.42      | 112.14   |
| 1   | H     | 933 | ILE  | CB-CA-C | -6.40 | 103.50      | 112.14   |
| 1   | L     | 725 | ARG  | N-CA-C  | -6.35 | 104.28      | 111.14   |
| 1   | C     | 821 | HIS  | N-CA-C  | 6.28  | 118.93      | 111.71   |
| 1   | K     | 715 | ILE  | N-CA-C  | 6.14  | 113.14      | 107.56   |
| 1   | G     | 821 | HIS  | N-CA-C  | 6.08  | 118.70      | 111.71   |
| 1   | I     | 821 | HIS  | N-CA-C  | 6.07  | 118.69      | 111.71   |
| 1   | E     | 821 | HIS  | N-CA-C  | 6.07  | 118.69      | 111.71   |
| 1   | K     | 821 | HIS  | N-CA-C  | 6.02  | 118.64      | 111.71   |
| 1   | J     | 725 | ARG  | N-CA-C  | -6.02 | 104.64      | 111.14   |
| 1   | B     | 725 | ARG  | N-CA-C  | -5.96 | 104.71      | 111.14   |
| 1   | D     | 725 | ARG  | N-CA-C  | -5.88 | 104.79      | 111.14   |
| 1   | J     | 821 | HIS  | N-CA-C  | 5.85  | 119.52      | 112.38   |
| 1   | H     | 795 | PRO  | N-CA-CB | 5.80  | 109.34      | 103.25   |
| 1   | H     | 821 | HIS  | N-CA-C  | 5.79  | 119.44      | 112.38   |
| 1   | F     | 725 | ARG  | N-CA-C  | -5.75 | 104.94      | 111.14   |
| 1   | L     | 795 | PRO  | N-CA-CB | 5.74  | 109.28      | 103.25   |
| 1   | E     | 755 | ARG  | CA-C-N  | 5.73  | 126.02      | 119.83   |
| 1   | E     | 755 | ARG  | C-N-CA  | 5.73  | 126.02      | 119.83   |
| 1   | A     | 755 | ARG  | CA-C-N  | 5.69  | 125.97      | 119.83   |
| 1   | A     | 755 | ARG  | C-N-CA  | 5.69  | 125.97      | 119.83   |
| 1   | B     | 795 | PRO  | N-CA-CB | 5.69  | 109.22      | 103.25   |
| 1   | C     | 755 | ARG  | CA-C-N  | 5.68  | 125.96      | 119.83   |
| 1   | C     | 755 | ARG  | C-N-CA  | 5.68  | 125.96      | 119.83   |
| 1   | H     | 725 | ARG  | N-CA-C  | -5.63 | 105.06      | 111.14   |
| 1   | L     | 821 | HIS  | N-CA-C  | 5.60  | 119.22      | 112.38   |
| 1   | F     | 821 | HIS  | N-CA-C  | 5.57  | 119.18      | 112.38   |
| 1   | J     | 795 | PRO  | N-CA-CB | 5.57  | 109.10      | 103.25   |
| 1   | L     | 735 | PRO  | N-CA-C  | 5.56  | 121.15      | 113.65   |
| 1   | D     | 821 | HIS  | N-CA-C  | 5.55  | 119.15      | 112.38   |
| 1   | H     | 735 | PRO  | N-CA-C  | 5.54  | 121.13      | 113.65   |
| 1   | B     | 821 | HIS  | N-CA-C  | 5.54  | 119.13      | 112.38   |
| 1   | D     | 795 | PRO  | N-CA-CB | 5.52  | 109.05      | 103.25   |
| 1   | F     | 795 | PRO  | N-CA-CB | 5.49  | 109.01      | 103.25   |
| 1   | B     | 735 | PRO  | N-CA-C  | 5.41  | 120.95      | 113.65   |
| 1   | G     | 994 | HIS  | N-CA-C  | 5.38  | 119.95      | 112.90   |
| 1   | F     | 784 | ILE  | CB-CA-C | -5.32 | 105.48      | 111.23   |
| 1   | E     | 994 | HIS  | N-CA-C  | 5.24  | 119.77      | 112.90   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | I     | 755  | ARG  | CA-C-N  | 5.22  | 125.47      | 119.83   |
| 1   | I     | 755  | ARG  | C-N-CA  | 5.22  | 125.47      | 119.83   |
| 1   | K     | 755  | ARG  | CA-C-N  | 5.22  | 125.47      | 119.83   |
| 1   | K     | 755  | ARG  | C-N-CA  | 5.22  | 125.47      | 119.83   |
| 1   | I     | 996  | VAL  | CB-CA-C | -5.22 | 105.09      | 112.14   |
| 1   | E     | 909  | ALA  | N-CA-C  | 5.22  | 119.56      | 112.04   |
| 1   | J     | 735  | PRO  | N-CA-C  | 5.22  | 120.69      | 113.65   |
| 1   | A     | 821  | HIS  | N-CA-C  | 5.18  | 118.70      | 112.38   |
| 1   | E     | 996  | VAL  | CB-CA-C | -5.17 | 105.16      | 112.14   |
| 1   | D     | 735  | PRO  | N-CA-C  | 5.16  | 120.62      | 113.65   |
| 1   | J     | 681  | ILE  | CB-CA-C | -5.16 | 105.36      | 111.97   |
| 1   | D     | 777  | GLY  | N-CA-C  | 5.15  | 120.34      | 114.67   |
| 1   | G     | 755  | ARG  | CA-C-N  | 5.15  | 125.39      | 119.83   |
| 1   | G     | 755  | ARG  | C-N-CA  | 5.15  | 125.39      | 119.83   |
| 1   | F     | 735  | PRO  | N-CA-C  | 5.13  | 120.57      | 113.65   |
| 1   | C     | 909  | ALA  | N-CA-C  | 5.12  | 119.42      | 112.04   |
| 1   | C     | 996  | VAL  | CB-CA-C | -5.11 | 105.24      | 112.14   |
| 1   | G     | 996  | VAL  | CB-CA-C | -5.11 | 105.25      | 112.14   |
| 1   | G     | 1060 | GLN  | N-CA-C  | 5.11  | 117.24      | 111.11   |
| 1   | G     | 981  | SER  | CA-C-N  | 5.09  | 125.07      | 120.03   |
| 1   | G     | 981  | SER  | C-N-CA  | 5.09  | 125.07      | 120.03   |
| 1   | C     | 994  | HIS  | N-CA-C  | 5.08  | 119.55      | 112.90   |
| 1   | E     | 1060 | GLN  | N-CA-C  | 5.07  | 117.20      | 111.11   |
| 1   | A     | 996  | VAL  | CB-CA-C | -5.06 | 105.31      | 112.14   |
| 1   | J     | 787  | ILE  | CB-CA-C | -5.03 | 104.56      | 111.49   |
| 1   | B     | 784  | ILE  | CB-CA-C | -5.02 | 105.81      | 111.23   |
| 1   | E     | 1062 | MET  | N-CA-C  | -5.01 | 105.89      | 111.36   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2907  | 0        | 2772     | 114     | 0            |
| 1   | B     | 3017  | 0        | 2834     | 143     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 2907  | 0        | 2772     | 130     | 0            |
| 1   | D     | 3017  | 0        | 2834     | 141     | 0            |
| 1   | E     | 2907  | 0        | 2772     | 122     | 0            |
| 1   | F     | 3017  | 0        | 2834     | 132     | 0            |
| 1   | G     | 2907  | 0        | 2772     | 115     | 0            |
| 1   | H     | 3017  | 0        | 2834     | 133     | 0            |
| 1   | I     | 2907  | 0        | 2772     | 114     | 0            |
| 1   | J     | 3017  | 0        | 2834     | 152     | 0            |
| 1   | K     | 2907  | 0        | 2772     | 116     | 0            |
| 1   | L     | 3017  | 0        | 2834     | 131     | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 16    | 0        | 14       | 0       | 0            |
| 3   | B     | 16    | 0        | 14       | 0       | 0            |
| 3   | C     | 16    | 0        | 14       | 0       | 0            |
| 3   | D     | 16    | 0        | 14       | 0       | 0            |
| 3   | E     | 16    | 0        | 14       | 0       | 0            |
| 3   | F     | 16    | 0        | 14       | 0       | 0            |
| 3   | G     | 16    | 0        | 14       | 0       | 0            |
| 3   | H     | 16    | 0        | 14       | 0       | 0            |
| 3   | I     | 16    | 0        | 14       | 0       | 0            |
| 3   | J     | 16    | 0        | 14       | 0       | 0            |
| 3   | K     | 16    | 0        | 14       | 0       | 0            |
| 3   | L     | 16    | 0        | 14       | 0       | 0            |
| 4   | A     | 24    | 0        | 0        | 1       | 0            |
| 4   | B     | 24    | 0        | 0        | 3       | 0            |
| 4   | C     | 24    | 0        | 0        | 1       | 0            |
| 4   | D     | 24    | 0        | 0        | 1       | 0            |
| 4   | E     | 23    | 0        | 0        | 2       | 0            |
| 4   | F     | 25    | 0        | 0        | 1       | 0            |
| 4   | G     | 23    | 0        | 0        | 1       | 0            |
| 4   | H     | 25    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | I     | 24    | 0        | 0        | 1       | 0            |
| 4   | J     | 24    | 0        | 0        | 0       | 0            |
| 4   | K     | 24    | 0        | 0        | 1       | 0            |
| 4   | L     | 24    | 0        | 0        | 1       | 0            |
| All | All   | 36048 | 0        | 33804    | 1450    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (1450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:719:GLN:H     | 1:A:719:GLN:HE21 | 1.04                     | 1.00              |
| 1:E:825:HIS:HD2   | 1:E:827:GLY:H    | 1.10                     | 1.00              |
| 1:I:719:GLN:H     | 1:I:719:GLN:HE21 | 1.06                     | 0.98              |
| 1:K:762:GLN:HE22  | 1:K:804:SER:HB2  | 1.28                     | 0.98              |
| 1:K:719:GLN:H     | 1:K:719:GLN:HE21 | 1.06                     | 0.98              |
| 1:E:719:GLN:H     | 1:E:719:GLN:HE21 | 1.05                     | 0.97              |
| 1:G:719:GLN:H     | 1:G:719:GLN:HE21 | 1.05                     | 0.96              |
| 1:G:1014:LEU:HD12 | 1:G:1056:ARG:HB3 | 1.45                     | 0.96              |
| 1:I:825:HIS:HD2   | 1:I:827:GLY:H    | 1.09                     | 0.96              |
| 1:C:825:HIS:HD2   | 1:C:827:GLY:H    | 1.10                     | 0.95              |
| 1:L:719:GLN:HE21  | 1:L:719:GLN:N    | 1.64                     | 0.95              |
| 1:B:719:GLN:HE21  | 1:B:719:GLN:N    | 1.63                     | 0.95              |
| 1:C:719:GLN:H     | 1:C:719:GLN:HE21 | 1.10                     | 0.95              |
| 1:D:719:GLN:HE21  | 1:D:719:GLN:N    | 1.65                     | 0.94              |
| 1:F:719:GLN:HE21  | 1:F:719:GLN:N    | 1.63                     | 0.94              |
| 1:G:825:HIS:HD2   | 1:G:827:GLY:H    | 1.11                     | 0.94              |
| 1:H:719:GLN:HE21  | 1:H:719:GLN:N    | 1.64                     | 0.94              |
| 1:J:719:GLN:HE21  | 1:J:719:GLN:N    | 1.64                     | 0.94              |
| 1:B:719:GLN:H     | 1:B:719:GLN:NE2  | 1.64                     | 0.94              |
| 1:F:719:GLN:H     | 1:F:719:GLN:NE2  | 1.65                     | 0.94              |
| 1:A:825:HIS:HD2   | 1:A:827:GLY:H    | 1.09                     | 0.94              |
| 1:L:719:GLN:H     | 1:L:719:GLN:NE2  | 1.66                     | 0.93              |
| 1:L:911:ASP:H     | 1:L:914:SER:HB3  | 1.34                     | 0.93              |
| 1:H:719:GLN:H     | 1:H:719:GLN:NE2  | 1.66                     | 0.93              |
| 1:J:719:GLN:H     | 1:J:719:GLN:NE2  | 1.65                     | 0.93              |
| 1:B:911:ASP:H     | 1:B:914:SER:HB3  | 1.33                     | 0.92              |
| 1:D:719:GLN:H     | 1:D:719:GLN:NE2  | 1.67                     | 0.92              |
| 1:F:911:ASP:H     | 1:F:914:SER:HB3  | 1.33                     | 0.92              |
| 1:K:825:HIS:HD2   | 1:K:827:GLY:H    | 1.10                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:911:ASP:H     | 1:D:914:SER:HB3   | 1.36                     | 0.90              |
| 1:A:762:GLN:HE21  | 1:A:801:CYS:H     | 1.19                     | 0.90              |
| 1:H:911:ASP:H     | 1:H:914:SER:HB3   | 1.34                     | 0.89              |
| 1:J:911:ASP:H     | 1:J:914:SER:HB3   | 1.34                     | 0.89              |
| 1:H:828:ARG:HG2   | 1:H:832:PHE:CD2   | 2.08                     | 0.89              |
| 1:K:762:GLN:HA    | 1:K:762:GLN:HE21  | 1.37                     | 0.88              |
| 1:F:828:ARG:HG2   | 1:F:832:PHE:CD2   | 2.08                     | 0.88              |
| 1:K:730:GLY:HA3   | 1:K:823:TYR:CE1   | 2.08                     | 0.88              |
| 1:A:730:GLY:HA3   | 1:A:823:TYR:CE1   | 2.09                     | 0.87              |
| 1:J:828:ARG:HG2   | 1:J:832:PHE:CD2   | 2.09                     | 0.87              |
| 1:B:828:ARG:HG2   | 1:B:832:PHE:CD2   | 2.09                     | 0.86              |
| 1:E:730:GLY:HA3   | 1:E:823:TYR:CE1   | 2.11                     | 0.86              |
| 1:G:730:GLY:HA3   | 1:G:823:TYR:CE1   | 2.11                     | 0.86              |
| 1:I:754:THR:HG21  | 1:I:755:ARG:HH21  | 1.38                     | 0.86              |
| 1:F:758:PRO:HG2   | 1:F:1057:ILE:HD13 | 1.56                     | 0.86              |
| 1:D:828:ARG:HG2   | 1:D:832:PHE:CD2   | 2.10                     | 0.86              |
| 1:L:828:ARG:HG2   | 1:L:832:PHE:CD2   | 2.11                     | 0.85              |
| 1:G:754:THR:HG21  | 1:G:755:ARG:HH21  | 1.39                     | 0.85              |
| 1:C:754:THR:HG21  | 1:C:755:ARG:HH21  | 1.39                     | 0.85              |
| 1:J:758:PRO:HG2   | 1:J:1057:ILE:HD13 | 1.59                     | 0.85              |
| 1:A:754:THR:HG21  | 1:A:755:ARG:HH21  | 1.41                     | 0.84              |
| 1:D:700:MET:HE3   | 1:D:746:LEU:CD2   | 2.07                     | 0.84              |
| 1:A:719:GLN:HE21  | 1:A:719:GLN:N     | 1.74                     | 0.84              |
| 1:C:730:GLY:HA3   | 1:C:823:TYR:CE1   | 2.11                     | 0.84              |
| 1:D:825:HIS:HD2   | 1:D:827:GLY:H     | 1.25                     | 0.84              |
| 1:I:730:GLY:HA3   | 1:I:823:TYR:CE1   | 2.11                     | 0.84              |
| 1:K:754:THR:HG21  | 1:K:755:ARG:HH21  | 1.39                     | 0.84              |
| 1:C:754:THR:HG22  | 1:C:755:ARG:HE    | 1.44                     | 0.83              |
| 1:G:719:GLN:HE21  | 1:G:719:GLN:N     | 1.75                     | 0.83              |
| 1:H:825:HIS:HD2   | 1:H:827:GLY:H     | 1.25                     | 0.83              |
| 1:E:719:GLN:HE21  | 1:E:719:GLN:N     | 1.75                     | 0.83              |
| 1:I:754:THR:HG22  | 1:I:755:ARG:HE    | 1.43                     | 0.83              |
| 1:E:754:THR:HG21  | 1:E:755:ARG:HH21  | 1.41                     | 0.83              |
| 1:F:700:MET:HE3   | 1:F:746:LEU:CD2   | 2.07                     | 0.83              |
| 1:B:700:MET:HE3   | 1:B:746:LEU:CD2   | 2.08                     | 0.83              |
| 1:I:719:GLN:HE21  | 1:I:719:GLN:N     | 1.76                     | 0.83              |
| 1:F:825:HIS:HD2   | 1:F:827:GLY:H     | 1.25                     | 0.82              |
| 1:K:719:GLN:HE21  | 1:K:719:GLN:N     | 1.75                     | 0.82              |
| 1:J:700:MET:HE3   | 1:J:746:LEU:CD2   | 2.09                     | 0.82              |
| 1:B:1014:LEU:HD12 | 1:B:1056:ARG:HB3  | 1.61                     | 0.82              |
| 1:A:754:THR:HG22  | 1:A:755:ARG:HE    | 1.44                     | 0.82              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:825:HIS:HD2  | 1:L:827:GLY:H     | 1.25                     | 0.82              |
| 1:H:700:MET:HE3  | 1:H:746:LEU:CD2   | 2.10                     | 0.81              |
| 1:L:700:MET:HE3  | 1:L:746:LEU:CD2   | 2.10                     | 0.81              |
| 1:G:754:THR:HG22 | 1:G:755:ARG:HE    | 1.45                     | 0.81              |
| 1:C:828:ARG:HG2  | 1:C:832:PHE:CD2   | 2.16                     | 0.81              |
| 1:A:705:GLN:HE22 | 1:J:1056:ARG:HH21 | 1.25                     | 0.81              |
| 1:G:828:ARG:HG2  | 1:G:832:PHE:CD2   | 2.16                     | 0.81              |
| 1:C:887:ILE:HD13 | 1:D:845:ASN:HB3   | 1.63                     | 0.80              |
| 1:J:825:HIS:HD2  | 1:J:827:GLY:H     | 1.24                     | 0.80              |
| 1:A:762:GLN:HE21 | 1:A:801:CYS:N     | 1.79                     | 0.80              |
| 1:A:887:ILE:HD13 | 1:B:845:ASN:HB3   | 1.63                     | 0.80              |
| 1:C:719:GLN:HE21 | 1:C:719:GLN:N     | 1.79                     | 0.80              |
| 1:K:754:THR:HG22 | 1:K:755:ARG:HE    | 1.44                     | 0.80              |
| 1:B:825:HIS:HD2  | 1:B:827:GLY:H     | 1.26                     | 0.80              |
| 1:C:959:PHE:HB3  | 1:C:977:MET:HG2   | 1.64                     | 0.79              |
| 1:E:828:ARG:HG2  | 1:E:832:PHE:CD2   | 2.17                     | 0.79              |
| 1:L:739:ARG:HH11 | 1:L:739:ARG:HG2   | 1.48                     | 0.79              |
| 1:E:754:THR:HG22 | 1:E:755:ARG:HE    | 1.47                     | 0.79              |
| 1:I:737:HIS:HD2  | 1:I:958:GLU:OE2   | 1.66                     | 0.78              |
| 1:A:828:ARG:HG2  | 1:A:832:PHE:CD2   | 2.18                     | 0.78              |
| 1:A:959:PHE:HB3  | 1:A:977:MET:HG2   | 1.65                     | 0.77              |
| 1:D:739:ARG:HG2  | 1:D:739:ARG:HH11  | 1.50                     | 0.77              |
| 1:G:719:GLN:H    | 1:G:719:GLN:NE2   | 1.82                     | 0.77              |
| 1:E:737:HIS:HD2  | 1:E:958:GLU:OE2   | 1.67                     | 0.77              |
| 1:K:762:GLN:NE2  | 1:K:804:SER:HB2   | 1.98                     | 0.77              |
| 1:K:828:ARG:HG2  | 1:K:832:PHE:CD2   | 2.20                     | 0.77              |
| 1:I:883:ARG:NH1  | 1:J:846:ASP:OD2   | 2.18                     | 0.77              |
| 1:G:959:PHE:HB3  | 1:G:977:MET:HG2   | 1.65                     | 0.77              |
| 1:D:758:PRO:HG2  | 1:D:1057:ILE:HD13 | 1.66                     | 0.77              |
| 1:A:737:HIS:HD2  | 1:A:958:GLU:OE2   | 1.66                     | 0.76              |
| 1:G:913:ASN:ND2  | 1:K:1056:ARG:HH21 | 1.83                     | 0.76              |
| 1:J:739:ARG:HH11 | 1:J:739:ARG:HG2   | 1.48                     | 0.76              |
| 1:B:739:ARG:HG2  | 1:B:739:ARG:HH11  | 1.50                     | 0.76              |
| 1:F:730:GLY:HA3  | 1:F:823:TYR:CE1   | 2.21                     | 0.76              |
| 1:L:730:GLY:HA3  | 1:L:823:TYR:CE1   | 2.20                     | 0.76              |
| 1:K:887:ILE:HD13 | 1:L:845:ASN:HB3   | 1.64                     | 0.76              |
| 1:E:719:GLN:H    | 1:E:719:GLN:NE2   | 1.83                     | 0.76              |
| 1:E:959:PHE:HB3  | 1:E:977:MET:HG2   | 1.67                     | 0.76              |
| 1:C:737:HIS:HD2  | 1:C:958:GLU:OE2   | 1.67                     | 0.75              |
| 1:I:828:ARG:HG2  | 1:I:832:PHE:CD2   | 2.19                     | 0.75              |
| 1:J:730:GLY:HA3  | 1:J:823:TYR:CE1   | 2.21                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:754:THR:HG21  | 1:D:755:ARG:HH21  | 1.51                     | 0.75              |
| 1:K:737:HIS:HD2   | 1:K:958:GLU:OE2   | 1.68                     | 0.75              |
| 1:H:739:ARG:HG2   | 1:H:739:ARG:HH11  | 1.51                     | 0.75              |
| 1:K:696:LEU:HB3   | 1:K:728:GLU:HG2   | 1.68                     | 0.75              |
| 1:B:915:ASN:CG    | 1:C:945:ARG:NH1   | 2.45                     | 0.75              |
| 1:E:1014:LEU:HD12 | 1:E:1056:ARG:HB3  | 1.69                     | 0.74              |
| 1:K:719:GLN:H     | 1:K:719:GLN:NE2   | 1.83                     | 0.74              |
| 1:D:730:GLY:HA3   | 1:D:823:TYR:CE1   | 2.22                     | 0.74              |
| 1:J:754:THR:HG21  | 1:J:755:ARG:HH21  | 1.52                     | 0.74              |
| 1:I:696:LEU:HB3   | 1:I:728:GLU:HG2   | 1.70                     | 0.74              |
| 1:H:730:GLY:HA3   | 1:H:823:TYR:CE1   | 2.22                     | 0.74              |
| 1:H:754:THR:HG21  | 1:H:755:ARG:HH21  | 1.53                     | 0.74              |
| 1:I:959:PHE:HB3   | 1:I:977:MET:HG2   | 1.69                     | 0.73              |
| 1:G:1014:LEU:HD12 | 1:G:1056:ARG:CB   | 2.18                     | 0.73              |
| 1:F:739:ARG:HG2   | 1:F:739:ARG:HH11  | 1.51                     | 0.73              |
| 1:F:911:ASP:N     | 1:F:914:SER:HB3   | 2.03                     | 0.73              |
| 1:B:1057:ILE:HD12 | 1:B:1058:PHE:N    | 2.03                     | 0.73              |
| 1:A:705:GLN:NE2   | 1:J:1056:ARG:HH21 | 1.87                     | 0.73              |
| 1:F:754:THR:HG21  | 1:F:755:ARG:HH21  | 1.52                     | 0.73              |
| 1:E:887:ILE:HD13  | 1:F:845:ASN:HB3   | 1.71                     | 0.73              |
| 1:B:754:THR:HG21  | 1:B:755:ARG:HH21  | 1.54                     | 0.72              |
| 1:C:696:LEU:HB3   | 1:C:728:GLU:HG2   | 1.70                     | 0.72              |
| 1:A:719:GLN:H     | 1:A:719:GLN:NE2   | 1.82                     | 0.72              |
| 1:B:911:ASP:N     | 1:B:914:SER:HB3   | 2.02                     | 0.72              |
| 1:L:911:ASP:N     | 1:L:914:SER:HB3   | 2.04                     | 0.72              |
| 1:B:730:GLY:HA3   | 1:B:823:TYR:CE1   | 2.24                     | 0.72              |
| 1:H:696:LEU:HB3   | 1:H:728:GLU:HG2   | 1.70                     | 0.72              |
| 1:F:1057:ILE:HD12 | 1:F:1058:PHE:N    | 2.03                     | 0.72              |
| 1:K:959:PHE:HB3   | 1:K:977:MET:HG2   | 1.70                     | 0.72              |
| 1:J:911:ASP:N     | 1:J:914:SER:HB3   | 2.03                     | 0.72              |
| 1:A:696:LEU:HB3   | 1:A:728:GLU:HG2   | 1.71                     | 0.72              |
| 1:G:737:HIS:HD2   | 1:G:958:GLU:OE2   | 1.71                     | 0.72              |
| 1:G:1017:GLU:HB3  | 1:G:1055:ARG:HD3  | 1.72                     | 0.72              |
| 1:D:700:MET:HE3   | 1:D:746:LEU:HD22  | 1.72                     | 0.72              |
| 1:E:696:LEU:HB3   | 1:E:728:GLU:HG2   | 1.71                     | 0.72              |
| 1:F:696:LEU:HB3   | 1:F:728:GLU:HG2   | 1.71                     | 0.72              |
| 1:F:1059:CYS:HB3  | 1:F:1062:MET:HB2  | 1.72                     | 0.71              |
| 1:D:911:ASP:N     | 1:D:914:SER:HB3   | 2.05                     | 0.71              |
| 1:L:696:LEU:HB3   | 1:L:728:GLU:HG2   | 1.70                     | 0.71              |
| 1:G:696:LEU:HB3   | 1:G:728:GLU:HG2   | 1.72                     | 0.71              |
| 1:H:956:VAL:HG11  | 1:H:984:LEU:HD13  | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:1057:ILE:HD12 | 1:J:1058:PHE:N    | 2.06                     | 0.71              |
| 1:B:696:LEU:HB3   | 1:B:728:GLU:HG2   | 1.71                     | 0.71              |
| 1:B:700:MET:HE3   | 1:B:746:LEU:HD22  | 1.73                     | 0.71              |
| 1:C:1017:GLU:H    | 1:C:1055:ARG:HD3  | 1.55                     | 0.71              |
| 1:L:956:VAL:HG11  | 1:L:984:LEU:HD13  | 1.72                     | 0.71              |
| 1:E:1017:GLU:HB3  | 1:E:1055:ARG:HD3  | 1.73                     | 0.70              |
| 1:D:956:VAL:HG11  | 1:D:984:LEU:HD13  | 1.72                     | 0.70              |
| 1:B:956:VAL:HG11  | 1:B:984:LEU:HD13  | 1.73                     | 0.70              |
| 1:L:754:THR:HG21  | 1:L:755:ARG:HH21  | 1.56                     | 0.70              |
| 1:H:1013:TRP:CE3  | 1:H:1057:ILE:HG22 | 2.27                     | 0.70              |
| 1:I:891:LEU:HD13  | 1:J:847:ARG:NH2   | 2.06                     | 0.70              |
| 1:H:911:ASP:N     | 1:H:914:SER:HB3   | 2.04                     | 0.69              |
| 1:I:719:GLN:H     | 1:I:719:GLN:NE2   | 1.84                     | 0.69              |
| 1:F:700:MET:HE3   | 1:F:746:LEU:HD22  | 1.71                     | 0.69              |
| 1:H:945:ARG:HH12  | 1:H:1071:ILE:HG21 | 1.57                     | 0.69              |
| 1:F:956:VAL:HG11  | 1:F:984:LEU:HD13  | 1.73                     | 0.69              |
| 1:J:696:LEU:HB3   | 1:J:728:GLU:HG2   | 1.73                     | 0.69              |
| 1:B:674:MET:HE1   | 1:B:699:VAL:HG13  | 1.75                     | 0.69              |
| 1:D:696:LEU:HB3   | 1:D:728:GLU:HG2   | 1.73                     | 0.69              |
| 1:J:956:VAL:HG11  | 1:J:984:LEU:HD13  | 1.73                     | 0.69              |
| 1:J:959:PHE:HA    | 1:J:977:MET:HE2   | 1.75                     | 0.69              |
| 1:I:762:GLN:NE2   | 1:I:801:CYS:H     | 1.91                     | 0.68              |
| 1:L:959:PHE:HA    | 1:L:977:MET:HE2   | 1.75                     | 0.68              |
| 1:C:719:GLN:H     | 1:C:719:GLN:NE2   | 1.87                     | 0.68              |
| 1:L:853:HIS:O     | 1:L:857:SER:HB2   | 1.94                     | 0.68              |
| 1:F:853:HIS:O     | 1:F:857:SER:HB2   | 1.93                     | 0.68              |
| 1:J:700:MET:HE3   | 1:J:746:LEU:HD22  | 1.76                     | 0.68              |
| 1:A:816:VAL:CG1   | 1:A:820:MET:HE3   | 2.24                     | 0.68              |
| 1:F:945:ARG:HH12  | 1:F:1071:ILE:HG21 | 1.59                     | 0.68              |
| 1:H:1056:ARG:HH11 | 1:H:1056:ARG:HB3  | 1.58                     | 0.67              |
| 1:K:816:VAL:CG1   | 1:K:820:MET:HE3   | 2.25                     | 0.67              |
| 1:H:853:HIS:O     | 1:H:857:SER:HB2   | 1.94                     | 0.67              |
| 1:H:959:PHE:HA    | 1:H:977:MET:HE2   | 1.76                     | 0.67              |
| 1:H:816:VAL:O     | 1:H:820:MET:HG2   | 1.95                     | 0.67              |
| 1:I:891:LEU:CD1   | 1:J:847:ARG:CZ    | 2.73                     | 0.67              |
| 1:B:853:HIS:O     | 1:B:857:SER:HB2   | 1.94                     | 0.67              |
| 1:E:816:VAL:HG12  | 1:E:820:MET:HE3   | 1.76                     | 0.67              |
| 1:D:853:HIS:O     | 1:D:857:SER:HB2   | 1.94                     | 0.67              |
| 1:L:700:MET:HE3   | 1:L:746:LEU:HD22  | 1.77                     | 0.67              |
| 1:I:816:VAL:CG1   | 1:I:820:MET:HE3   | 2.25                     | 0.67              |
| 1:E:816:VAL:CG1   | 1:E:820:MET:HE3   | 2.25                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:674:MET:HE1  | 1:F:699:VAL:HG13  | 1.77                     | 0.66              |
| 1:C:845:ASN:HB3  | 1:D:887:ILE:HD13  | 1.77                     | 0.66              |
| 1:H:689:GLY:O    | 1:H:692:SER:HB3   | 1.95                     | 0.66              |
| 1:B:915:ASN:ND2  | 1:C:945:ARG:HH11  | 1.92                     | 0.66              |
| 1:D:816:VAL:O    | 1:D:820:MET:HG2   | 1.96                     | 0.66              |
| 1:D:945:ARG:HH12 | 1:D:1071:ILE:HG21 | 1.60                     | 0.66              |
| 1:L:734:ILE:HB   | 1:L:735:PRO:HD2   | 1.77                     | 0.66              |
| 1:F:816:VAL:O    | 1:F:820:MET:HG2   | 1.96                     | 0.66              |
| 1:B:689:GLY:O    | 1:B:692:SER:HB3   | 1.95                     | 0.66              |
| 1:B:761:GLN:HG2  | 1:B:763:ILE:H     | 1.60                     | 0.66              |
| 1:J:853:HIS:O    | 1:J:857:SER:HB2   | 1.96                     | 0.66              |
| 1:J:945:ARG:HH12 | 1:J:1071:ILE:HG21 | 1.59                     | 0.66              |
| 1:G:739:ARG:HG2  | 4:G:1423:HOH:O    | 1.95                     | 0.65              |
| 1:H:700:MET:HE3  | 1:H:746:LEU:HD22  | 1.77                     | 0.65              |
| 1:L:816:VAL:O    | 1:L:820:MET:HG2   | 1.96                     | 0.65              |
| 1:A:825:HIS:CD2  | 1:A:827:GLY:H     | 2.02                     | 0.65              |
| 1:G:816:VAL:CG1  | 1:G:820:MET:HE3   | 2.26                     | 0.65              |
| 1:J:734:ILE:HB   | 1:J:735:PRO:HD2   | 1.77                     | 0.65              |
| 1:B:979:ARG:O    | 1:B:982:PRO:HD3   | 1.96                     | 0.65              |
| 1:L:734:ILE:HD11 | 1:L:737:HIS:HB2   | 1.79                     | 0.65              |
| 1:L:945:ARG:HH12 | 1:L:1071:ILE:HG21 | 1.60                     | 0.65              |
| 1:F:734:ILE:HB   | 1:F:735:PRO:HD2   | 1.78                     | 0.65              |
| 1:K:816:VAL:HG12 | 1:K:820:MET:HE3   | 1.79                     | 0.65              |
| 1:A:816:VAL:HG12 | 1:A:820:MET:HE3   | 1.78                     | 0.65              |
| 1:D:734:ILE:HD11 | 1:D:737:HIS:HB2   | 1.78                     | 0.65              |
| 1:G:887:ILE:HD13 | 1:H:845:ASN:HB3   | 1.78                     | 0.65              |
| 1:H:734:ILE:HD11 | 1:H:737:HIS:HB2   | 1.79                     | 0.65              |
| 1:J:674:MET:HE1  | 1:J:699:VAL:HG13  | 1.77                     | 0.65              |
| 1:L:674:MET:HE1  | 1:L:699:VAL:HG13  | 1.77                     | 0.65              |
| 1:B:734:ILE:HD11 | 1:B:737:HIS:HB2   | 1.79                     | 0.65              |
| 1:D:689:GLY:O    | 1:D:692:SER:HB3   | 1.97                     | 0.65              |
| 1:B:959:PHE:HA   | 1:B:977:MET:HE2   | 1.79                     | 0.64              |
| 1:I:816:VAL:HG12 | 1:I:820:MET:HE3   | 1.79                     | 0.64              |
| 1:I:825:HIS:CD2  | 1:I:827:GLY:H     | 2.01                     | 0.64              |
| 1:B:816:VAL:O    | 1:B:820:MET:HG2   | 1.97                     | 0.64              |
| 1:B:945:ARG:HH12 | 1:B:1071:ILE:HG21 | 1.61                     | 0.64              |
| 1:A:845:ASN:HB3  | 1:B:887:ILE:HD13  | 1.79                     | 0.64              |
| 1:A:945:ARG:NH1  | 1:D:915:ASN:CG    | 2.55                     | 0.64              |
| 1:C:816:VAL:CG1  | 1:C:820:MET:HE3   | 2.28                     | 0.64              |
| 1:D:754:THR:HG22 | 1:D:755:ARG:HE    | 1.62                     | 0.64              |
| 1:E:1017:GLU:H   | 1:E:1055:ARG:HD3  | 1.62                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:689:GLY:O     | 1:F:692:SER:HB3   | 1.97                     | 0.64              |
| 1:E:1014:LEU:HD12 | 1:E:1056:ARG:CB   | 2.27                     | 0.64              |
| 1:H:674:MET:HE1   | 1:H:699:VAL:HG13  | 1.78                     | 0.64              |
| 1:J:739:ARG:HG2   | 1:J:739:ARG:NH1   | 2.11                     | 0.64              |
| 1:K:700:MET:HE3   | 1:K:746:LEU:CD1   | 2.28                     | 0.64              |
| 1:H:979:ARG:O     | 1:H:982:PRO:HD3   | 1.96                     | 0.64              |
| 1:H:739:ARG:HG2   | 1:H:739:ARG:NH1   | 2.13                     | 0.64              |
| 1:D:959:PHE:HA    | 1:D:977:MET:HE2   | 1.79                     | 0.64              |
| 1:I:887:ILE:HD13  | 1:J:845:ASN:HB3   | 1.80                     | 0.64              |
| 1:A:739:ARG:HG2   | 4:A:1123:HOH:O    | 1.98                     | 0.63              |
| 1:B:734:ILE:HB    | 1:B:735:PRO:HD2   | 1.79                     | 0.63              |
| 1:F:734:ILE:HD11  | 1:F:737:HIS:HB2   | 1.80                     | 0.63              |
| 1:L:739:ARG:HG2   | 1:L:739:ARG:NH1   | 2.10                     | 0.63              |
| 1:J:1013:TRP:CZ3  | 1:J:1055:ARG:HB3  | 2.33                     | 0.63              |
| 1:K:825:HIS:CD2   | 1:K:827:GLY:H     | 2.03                     | 0.63              |
| 1:G:816:VAL:HG12  | 1:G:820:MET:HE3   | 1.80                     | 0.63              |
| 1:J:816:VAL:O     | 1:J:820:MET:HG2   | 1.99                     | 0.63              |
| 1:F:959:PHE:HA    | 1:F:977:MET:HE2   | 1.78                     | 0.63              |
| 1:I:762:GLN:HA    | 1:I:805:ASN:HD21  | 1.62                     | 0.63              |
| 1:J:689:GLY:O     | 1:J:692:SER:HB3   | 1.98                     | 0.63              |
| 1:L:689:GLY:O     | 1:L:692:SER:HB3   | 1.98                     | 0.63              |
| 1:I:707:THR:HG23  | 1:I:787:ILE:HD12  | 1.81                     | 0.63              |
| 1:B:739:ARG:HG2   | 1:B:739:ARG:NH1   | 2.12                     | 0.63              |
| 1:E:902:LEU:HD11  | 1:E:999:LEU:HA    | 1.81                     | 0.63              |
| 1:F:739:ARG:HG2   | 1:F:739:ARG:NH1   | 2.14                     | 0.63              |
| 1:L:979:ARG:O     | 1:L:982:PRO:HD3   | 1.98                     | 0.63              |
| 1:A:902:LEU:HD11  | 1:A:999:LEU:HA    | 1.80                     | 0.63              |
| 1:L:758:PRO:HG2   | 1:L:1057:ILE:HG13 | 1.80                     | 0.63              |
| 1:E:707:THR:HG23  | 1:E:787:ILE:HD12  | 1.81                     | 0.62              |
| 1:D:674:MET:HE1   | 1:D:699:VAL:HG13  | 1.80                     | 0.62              |
| 1:A:762:GLN:HA    | 1:A:805:ASN:HD21  | 1.63                     | 0.62              |
| 1:I:883:ARG:HH12  | 1:J:846:ASP:CG    | 2.07                     | 0.62              |
| 1:J:734:ILE:HD11  | 1:J:737:HIS:HB2   | 1.82                     | 0.62              |
| 1:A:945:ARG:HD3   | 1:D:915:ASN:HD21  | 1.63                     | 0.62              |
| 1:L:825:HIS:CD2   | 1:L:827:GLY:H     | 2.14                     | 0.62              |
| 1:I:902:LEU:HD11  | 1:I:999:LEU:HA    | 1.81                     | 0.62              |
| 1:C:816:VAL:HG12  | 1:C:820:MET:HE3   | 1.80                     | 0.62              |
| 1:K:902:LEU:HD11  | 1:K:999:LEU:HA    | 1.81                     | 0.62              |
| 1:B:934:LYS:HD3   | 4:B:1135:HOH:O    | 1.99                     | 0.62              |
| 1:C:1056:ARG:HG3  | 1:C:1056:ARG:HH11 | 1.64                     | 0.62              |
| 1:G:700:MET:HE3   | 1:G:746:LEU:CD1   | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:911:ASP:HB3   | 1:K:914:SER:HB3   | 1.82                     | 0.62              |
| 1:C:911:ASP:HB3   | 1:C:914:SER:HB3   | 1.82                     | 0.62              |
| 1:L:692:SER:O     | 1:L:695:ILE:HG13  | 2.00                     | 0.62              |
| 1:B:825:HIS:CD2   | 1:B:827:GLY:H     | 2.15                     | 0.61              |
| 1:G:913:ASN:HD22  | 1:K:1056:ARG:HH21 | 1.47                     | 0.61              |
| 1:C:707:THR:HG23  | 1:C:787:ILE:HD12  | 1.80                     | 0.61              |
| 1:C:718:GLN:HG3   | 1:C:722:ASN:HD21  | 1.65                     | 0.61              |
| 1:D:1000:CYS:HB3  | 1:D:1062:MET:HE1  | 1.82                     | 0.61              |
| 1:G:902:LEU:HD11  | 1:G:999:LEU:HA    | 1.82                     | 0.61              |
| 1:C:700:MET:HE3   | 1:C:746:LEU:CD1   | 2.30                     | 0.61              |
| 1:H:734:ILE:HB    | 1:H:735:PRO:HD2   | 1.80                     | 0.61              |
| 1:I:825:HIS:HD2   | 1:I:827:GLY:N     | 1.91                     | 0.61              |
| 1:C:902:LEU:HD11  | 1:C:999:LEU:HA    | 1.83                     | 0.61              |
| 1:A:917:ILE:O     | 1:A:918:GLU:HB2   | 2.01                     | 0.61              |
| 1:G:707:THR:HG23  | 1:G:787:ILE:HD12  | 1.83                     | 0.61              |
| 1:L:719:GLN:HE21  | 1:L:719:GLN:H     | 0.81                     | 0.61              |
| 1:A:945:ARG:CD    | 1:D:915:ASN:HD21  | 2.13                     | 0.61              |
| 1:C:825:HIS:CD2   | 1:C:827:GLY:H     | 2.03                     | 0.61              |
| 1:H:692:SER:O     | 1:H:695:ILE:HG13  | 2.00                     | 0.61              |
| 1:K:707:THR:HG23  | 1:K:787:ILE:HD12  | 1.83                     | 0.61              |
| 1:E:700:MET:HE3   | 1:E:746:LEU:CD1   | 2.31                     | 0.60              |
| 1:J:692:SER:O     | 1:J:695:ILE:HG13  | 2.01                     | 0.60              |
| 1:J:1058:PHE:CE1  | 1:J:1063:HIS:CE1  | 2.88                     | 0.60              |
| 1:A:707:THR:HG23  | 1:A:787:ILE:HD12  | 1.82                     | 0.60              |
| 1:A:911:ASP:HB3   | 1:A:914:SER:HB3   | 1.83                     | 0.60              |
| 1:E:825:HIS:CD2   | 1:E:827:GLY:H     | 2.03                     | 0.60              |
| 1:E:845:ASN:HB3   | 1:F:887:ILE:HD13  | 1.82                     | 0.60              |
| 1:I:891:LEU:HD12  | 1:J:847:ARG:NH1   | 2.16                     | 0.60              |
| 1:J:825:HIS:CD2   | 1:J:827:GLY:H     | 2.13                     | 0.60              |
| 1:J:1057:ILE:HD12 | 1:J:1058:PHE:H    | 1.65                     | 0.60              |
| 1:A:945:ARG:HH11  | 1:D:915:ASN:ND2   | 1.99                     | 0.60              |
| 1:A:825:HIS:HD2   | 1:A:827:GLY:N     | 1.92                     | 0.60              |
| 1:J:754:THR:HG22  | 1:J:755:ARG:HE    | 1.67                     | 0.60              |
| 1:F:692:SER:O     | 1:F:695:ILE:HG13  | 2.02                     | 0.60              |
| 1:J:725:ARG:HG3   | 1:J:725:ARG:HH11  | 1.67                     | 0.60              |
| 1:I:911:ASP:HB3   | 1:I:914:SER:HB3   | 1.83                     | 0.60              |
| 1:J:1003:TYR:CD2  | 1:J:1009:LEU:HG   | 2.36                     | 0.60              |
| 1:K:719:GLN:HA    | 1:K:722:ASN:HD22  | 1.67                     | 0.60              |
| 1:K:679:PHE:HZ    | 1:K:684:LEU:HD12  | 1.67                     | 0.60              |
| 1:D:734:ILE:HB    | 1:D:735:PRO:HD2   | 1.82                     | 0.60              |
| 1:F:1000:CYS:HB3  | 1:F:1062:MET:HE1  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:911:ASP:HB3  | 1:G:914:SER:HB3   | 1.82                     | 0.60              |
| 1:I:891:LEU:HD12 | 1:J:847:ARG:CZ    | 2.32                     | 0.60              |
| 1:I:845:ASN:HB3  | 1:J:887:ILE:HD13  | 1.83                     | 0.59              |
| 1:E:911:ASP:HB3  | 1:E:914:SER:HB3   | 1.84                     | 0.59              |
| 1:A:707:THR:CG2  | 1:A:709:LEU:HG    | 2.33                     | 0.59              |
| 1:D:692:SER:O    | 1:D:695:ILE:HG13  | 2.02                     | 0.59              |
| 1:D:1069:HIS:CE1 | 1:D:1073:LYS:HZ2  | 2.21                     | 0.59              |
| 1:F:754:THR:HG22 | 1:F:755:ARG:HE    | 1.67                     | 0.59              |
| 1:E:718:GLN:HG3  | 1:E:722:ASN:HD21  | 1.67                     | 0.59              |
| 1:H:754:THR:HG22 | 1:H:755:ARG:HE    | 1.67                     | 0.59              |
| 1:L:700:MET:HE3  | 1:L:746:LEU:HD21  | 1.85                     | 0.59              |
| 1:B:692:SER:O    | 1:B:695:ILE:HG13  | 2.02                     | 0.59              |
| 1:G:825:HIS:CD2  | 1:G:827:GLY:H     | 2.04                     | 0.59              |
| 1:F:1003:TYR:CD2 | 1:F:1009:LEU:HG   | 2.38                     | 0.59              |
| 1:L:754:THR:HG22 | 1:L:755:ARG:HE    | 1.68                     | 0.59              |
| 1:B:725:ARG:HG3  | 1:B:725:ARG:HH11  | 1.67                     | 0.59              |
| 1:H:679:PHE:HZ   | 1:H:684:LEU:HD12  | 1.68                     | 0.59              |
| 1:L:725:ARG:HG3  | 1:L:725:ARG:HH11  | 1.66                     | 0.59              |
| 1:K:707:THR:CG2  | 1:K:709:LEU:HG    | 2.32                     | 0.58              |
| 1:F:979:ARG:O    | 1:F:982:PRO:HD3   | 2.02                     | 0.58              |
| 1:H:751:TYR:CZ   | 1:H:755:ARG:HG3   | 2.37                     | 0.58              |
| 1:K:730:GLY:HA3  | 1:K:823:TYR:HE1   | 1.64                     | 0.58              |
| 1:C:917:ILE:O    | 1:C:918:GLU:HB2   | 2.03                     | 0.58              |
| 1:D:739:ARG:HG2  | 1:D:739:ARG:NH1   | 2.13                     | 0.58              |
| 1:F:748:ALA:HB3  | 1:F:936:ALA:HB1   | 1.86                     | 0.58              |
| 1:B:1069:HIS:CE1 | 1:B:1073:LYS:HZ2  | 2.21                     | 0.58              |
| 1:D:979:ARG:O    | 1:D:982:PRO:HD3   | 2.03                     | 0.58              |
| 1:G:917:ILE:O    | 1:G:918:GLU:HB2   | 2.03                     | 0.58              |
| 1:H:825:HIS:CD2  | 1:H:827:GLY:H     | 2.14                     | 0.58              |
| 1:B:941:PRO:O    | 1:B:1065:LEU:HD12 | 2.03                     | 0.58              |
| 1:C:707:THR:CG2  | 1:C:709:LEU:HG    | 2.34                     | 0.58              |
| 1:C:1017:GLU:HB3 | 1:C:1055:ARG:HD3  | 1.84                     | 0.58              |
| 1:D:700:MET:HE3  | 1:D:746:LEU:HD21  | 1.84                     | 0.58              |
| 1:I:700:MET:HE3  | 1:I:746:LEU:CD1   | 2.34                     | 0.58              |
| 1:I:754:THR:CG2  | 1:I:755:ARG:HH21  | 2.15                     | 0.58              |
| 1:L:1003:TYR:CD2 | 1:L:1009:LEU:HG   | 2.39                     | 0.58              |
| 1:A:700:MET:HE3  | 1:A:746:LEU:CD1   | 2.33                     | 0.58              |
| 1:B:754:THR:HG22 | 1:B:755:ARG:HE    | 1.69                     | 0.58              |
| 1:E:909:ALA:HB2  | 1:E:917:ILE:HD11  | 1.85                     | 0.58              |
| 1:F:669:SER:HB3  | 1:F:673:LYS:NZ    | 2.19                     | 0.58              |
| 1:J:962:GLN:O    | 1:J:966:GLU:HG3   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:1058:PHE:HE1  | 1:J:1063:HIS:ND1  | 2.01                     | 0.58              |
| 1:C:883:ARG:NH1   | 1:D:846:ASP:OD2   | 2.36                     | 0.58              |
| 1:E:917:ILE:O     | 1:E:918:GLU:HB2   | 2.04                     | 0.58              |
| 1:E:1071:ILE:HG21 | 1:J:915:ASN:ND2   | 2.19                     | 0.58              |
| 1:B:915:ASN:HD21  | 1:C:945:ARG:CD    | 2.16                     | 0.58              |
| 1:I:707:THR:CG2   | 1:I:709:LEU:HG    | 2.34                     | 0.58              |
| 1:H:725:ARG:HH11  | 1:H:725:ARG:HG3   | 1.67                     | 0.57              |
| 1:H:1000:CYS:HB3  | 1:H:1062:MET:HE1  | 1.86                     | 0.57              |
| 1:B:660:ASP:O     | 1:B:664:VAL:HG23  | 2.04                     | 0.57              |
| 1:F:962:GLN:O     | 1:F:966:GLU:HG3   | 2.03                     | 0.57              |
| 1:H:669:SER:HB3   | 1:H:673:LYS:NZ    | 2.19                     | 0.57              |
| 1:K:909:ALA:HB2   | 1:K:917:ILE:HD11  | 1.85                     | 0.57              |
| 1:E:679:PHE:HZ    | 1:E:684:LEU:HD12  | 1.69                     | 0.57              |
| 1:F:1057:ILE:HD12 | 1:F:1058:PHE:H    | 1.67                     | 0.57              |
| 1:K:825:HIS:HD2   | 1:K:827:GLY:N     | 1.93                     | 0.57              |
| 1:L:748:ALA:HB3   | 1:L:936:ALA:HB1   | 1.86                     | 0.57              |
| 1:E:719:GLN:HA    | 1:E:722:ASN:HD22  | 1.68                     | 0.57              |
| 1:G:718:GLN:HG3   | 1:G:722:ASN:HD21  | 1.69                     | 0.57              |
| 1:G:719:GLN:HA    | 1:G:722:ASN:HD22  | 1.69                     | 0.57              |
| 1:G:909:ALA:HB2   | 1:G:917:ILE:HD11  | 1.85                     | 0.57              |
| 1:I:1056:ARG:HG3  | 1:I:1056:ARG:HH11 | 1.69                     | 0.57              |
| 1:K:718:GLN:HG3   | 1:K:722:ASN:HD21  | 1.68                     | 0.57              |
| 1:B:1003:TYR:CD2  | 1:B:1009:LEU:HG   | 2.40                     | 0.57              |
| 1:E:707:THR:CG2   | 1:E:709:LEU:HG    | 2.35                     | 0.57              |
| 1:G:679:PHE:HZ    | 1:G:684:LEU:HD12  | 1.69                     | 0.57              |
| 1:G:1013:TRP:CE3  | 1:G:1057:ILE:HG22 | 2.40                     | 0.57              |
| 1:B:674:MET:C     | 1:B:676:ASN:H     | 2.13                     | 0.57              |
| 1:E:751:TYR:CE2   | 1:E:755:ARG:HG3   | 2.40                     | 0.57              |
| 1:L:679:PHE:HZ    | 1:L:684:LEU:HD12  | 1.70                     | 0.57              |
| 1:F:825:HIS:CD2   | 1:F:827:GLY:H     | 2.15                     | 0.57              |
| 1:H:700:MET:HE3   | 1:H:746:LEU:HD21  | 1.85                     | 0.57              |
| 1:B:700:MET:HE3   | 1:B:746:LEU:HD21  | 1.84                     | 0.57              |
| 1:B:751:TYR:CZ    | 1:B:755:ARG:HG3   | 2.40                     | 0.57              |
| 1:D:725:ARG:HG3   | 1:D:725:ARG:HH11  | 1.69                     | 0.57              |
| 1:H:1003:TYR:CD2  | 1:H:1009:LEU:HG   | 2.39                     | 0.57              |
| 1:I:718:GLN:HG3   | 1:I:722:ASN:HD21  | 1.69                     | 0.57              |
| 1:L:828:ARG:HG2   | 1:L:832:PHE:CG    | 2.40                     | 0.57              |
| 1:B:1000:CYS:HB3  | 1:B:1062:MET:HE1  | 1.85                     | 0.57              |
| 1:H:660:ASP:O     | 1:H:664:VAL:HG23  | 2.05                     | 0.57              |
| 1:I:802:LEU:HD22  | 1:I:802:LEU:H     | 1.70                     | 0.57              |
| 1:I:1013:TRP:CE3  | 1:I:1057:ILE:HG22 | 2.40                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:952:THR:HG23 | 1:D:988:GLN:NE2   | 2.20                     | 0.56              |
| 1:F:725:ARG:HG3  | 1:F:725:ARG:HH11  | 1.70                     | 0.56              |
| 1:F:804:SER:C    | 1:F:805:ASN:HD22  | 2.13                     | 0.56              |
| 1:H:748:ALA:HB3  | 1:H:936:ALA:HB1   | 1.87                     | 0.56              |
| 1:J:979:ARG:O    | 1:J:982:PRO:HD3   | 2.05                     | 0.56              |
| 1:L:1012:GLN:O   | 1:L:1057:ILE:HG12 | 2.05                     | 0.56              |
| 1:D:804:SER:C    | 1:D:805:ASN:HD22  | 2.13                     | 0.56              |
| 1:K:845:ASN:HB3  | 1:L:887:ILE:HD13  | 1.86                     | 0.56              |
| 1:D:669:SER:HB3  | 1:D:673:LYS:NZ    | 2.20                     | 0.56              |
| 1:F:700:MET:HE3  | 1:F:746:LEU:HD21  | 1.84                     | 0.56              |
| 1:G:802:LEU:HD22 | 1:G:802:LEU:H     | 1.71                     | 0.56              |
| 1:H:719:GLN:HE21 | 1:H:719:GLN:H     | 0.81                     | 0.56              |
| 1:H:945:ARG:NH1  | 1:H:1071:ILE:HG21 | 2.20                     | 0.56              |
| 1:K:762:GLN:HE21 | 1:K:762:GLN:CA    | 2.13                     | 0.56              |
| 1:K:917:ILE:O    | 1:K:918:GLU:HB2   | 2.04                     | 0.56              |
| 1:C:719:GLN:HA   | 1:C:722:ASN:HD22  | 1.70                     | 0.56              |
| 1:L:669:SER:HB3  | 1:L:673:LYS:NZ    | 2.20                     | 0.56              |
| 1:D:679:PHE:HZ   | 1:D:684:LEU:HD12  | 1.69                     | 0.56              |
| 1:D:941:PRO:O    | 1:D:1065:LEU:HD12 | 2.06                     | 0.56              |
| 1:H:915:ASN:CG   | 1:K:945:ARG:NH1   | 2.63                     | 0.56              |
| 1:F:945:ARG:NH1  | 1:F:1071:ILE:HG21 | 2.20                     | 0.56              |
| 1:L:1000:CYS:HB3 | 1:L:1062:MET:HE1  | 1.86                     | 0.56              |
| 1:A:1061:LEU:C   | 1:A:1061:LEU:HD12 | 2.31                     | 0.56              |
| 1:D:674:MET:C    | 1:D:676:ASN:H     | 2.13                     | 0.56              |
| 1:I:969:LEU:HD23 | 1:L:873:HIS:CD2   | 2.41                     | 0.56              |
| 1:L:674:MET:C    | 1:L:676:ASN:H     | 2.14                     | 0.56              |
| 1:L:962:GLN:O    | 1:L:966:GLU:HG3   | 2.06                     | 0.56              |
| 1:C:679:PHE:HZ   | 1:C:684:LEU:HD12  | 1.71                     | 0.56              |
| 1:C:909:ALA:HB2  | 1:C:917:ILE:HD11  | 1.88                     | 0.56              |
| 1:C:1061:LEU:C   | 1:C:1061:LEU:HD12 | 2.31                     | 0.56              |
| 1:D:962:GLN:O    | 1:D:966:GLU:HG3   | 2.05                     | 0.56              |
| 1:E:802:LEU:HD22 | 1:E:802:LEU:H     | 1.70                     | 0.56              |
| 1:J:1069:HIS:CE1 | 1:J:1073:LYS:HZ2  | 2.24                     | 0.56              |
| 1:K:935:LEU:O    | 1:K:935:LEU:HD23  | 2.06                     | 0.56              |
| 1:L:941:PRO:O    | 1:L:1065:LEU:HD12 | 2.05                     | 0.56              |
| 1:G:845:ASN:HB3  | 1:H:887:ILE:HD13  | 1.88                     | 0.56              |
| 1:H:732:ARG:HD2  | 1:H:825:HIS:O     | 2.06                     | 0.56              |
| 1:I:679:PHE:HZ   | 1:I:684:LEU:HD12  | 1.71                     | 0.56              |
| 1:J:700:MET:HE3  | 1:J:746:LEU:HD21  | 1.84                     | 0.56              |
| 1:G:754:THR:CG2  | 1:G:755:ARG:HH21  | 2.16                     | 0.56              |
| 1:I:909:ALA:HB2  | 1:I:917:ILE:HD11  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:669:SER:HB3  | 1:B:673:LYS:NZ    | 2.21                     | 0.55              |
| 1:C:935:LEU:HD23 | 1:C:935:LEU:O     | 2.06                     | 0.55              |
| 1:C:1013:TRP:CE3 | 1:C:1057:ILE:HG22 | 2.40                     | 0.55              |
| 1:D:862:TYR:OH   | 1:D:869:ASN:ND2   | 2.38                     | 0.55              |
| 1:H:828:ARG:HG2  | 1:H:832:PHE:CG    | 2.40                     | 0.55              |
| 1:J:674:MET:C    | 1:J:676:ASN:H     | 2.13                     | 0.55              |
| 1:J:945:ARG:NH1  | 1:J:1071:ILE:HG21 | 2.21                     | 0.55              |
| 1:K:713:PHE:CD2  | 1:K:874:LEU:HD21  | 2.41                     | 0.55              |
| 1:L:660:ASP:O    | 1:L:664:VAL:HG23  | 2.05                     | 0.55              |
| 1:A:679:PHE:HZ   | 1:A:684:LEU:HD12  | 1.71                     | 0.55              |
| 1:A:754:THR:CG2  | 1:A:755:ARG:HH21  | 2.17                     | 0.55              |
| 1:D:1003:TYR:CD2 | 1:D:1009:LEU:HG   | 2.40                     | 0.55              |
| 1:L:751:TYR:CZ   | 1:L:755:ARG:HG3   | 2.41                     | 0.55              |
| 1:B:679:PHE:HZ   | 1:B:684:LEU:HD12  | 1.71                     | 0.55              |
| 1:D:751:TYR:CZ   | 1:D:755:ARG:HG3   | 2.42                     | 0.55              |
| 1:E:869:ASN:C    | 1:E:869:ASN:HD22  | 2.14                     | 0.55              |
| 1:F:674:MET:C    | 1:F:676:ASN:H     | 2.14                     | 0.55              |
| 1:I:730:GLY:HA3  | 1:I:823:TYR:HE1   | 1.68                     | 0.55              |
| 1:J:941:PRO:O    | 1:J:1065:LEU:HD12 | 2.06                     | 0.55              |
| 1:C:1017:GLU:HB3 | 1:C:1055:ARG:HB2  | 1.88                     | 0.55              |
| 1:F:660:ASP:O    | 1:F:664:VAL:HG23  | 2.07                     | 0.55              |
| 1:G:708:GLY:O    | 1:G:712:ILE:HG13  | 2.06                     | 0.55              |
| 1:A:730:GLY:HA3  | 1:A:823:TYR:HE1   | 1.66                     | 0.55              |
| 1:C:869:ASN:C    | 1:C:869:ASN:HD22  | 2.14                     | 0.55              |
| 1:D:825:HIS:CD2  | 1:D:827:GLY:H     | 2.14                     | 0.55              |
| 1:F:828:ARG:HG2  | 1:F:832:PHE:CG    | 2.42                     | 0.55              |
| 1:G:707:THR:CG2  | 1:G:709:LEU:HG    | 2.37                     | 0.55              |
| 1:B:828:ARG:HG2  | 1:B:832:PHE:CG    | 2.41                     | 0.55              |
| 1:C:751:TYR:CE2  | 1:C:755:ARG:HG3   | 2.42                     | 0.55              |
| 1:F:679:PHE:HZ   | 1:F:684:LEU:HD12  | 1.72                     | 0.55              |
| 1:I:719:GLN:HA   | 1:I:722:ASN:HD22  | 1.70                     | 0.55              |
| 1:J:669:SER:HB3  | 1:J:673:LYS:NZ    | 2.22                     | 0.55              |
| 1:K:760:LEU:HD23 | 1:K:801:CYS:N     | 2.22                     | 0.55              |
| 1:L:945:ARG:NH1  | 1:L:1071:ILE:HG21 | 2.22                     | 0.55              |
| 1:A:802:LEU:H    | 1:A:802:LEU:HD22  | 1.72                     | 0.55              |
| 1:E:751:TYR:CZ   | 1:E:755:ARG:HG3   | 2.42                     | 0.55              |
| 1:F:763:ILE:O    | 1:F:764:HIS:CB    | 2.53                     | 0.55              |
| 1:F:911:ASP:H    | 1:F:914:SER:CB    | 2.15                     | 0.55              |
| 1:B:748:ALA:HB3  | 1:B:936:ALA:HB1   | 1.89                     | 0.55              |
| 1:E:847:ARG:CZ   | 1:F:891:LEU:HD13  | 2.37                     | 0.55              |
| 1:H:674:MET:C    | 1:H:676:ASN:H     | 2.13                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:962:GLN:O     | 1:H:966:GLU:HG3   | 2.07                     | 0.55              |
| 1:J:660:ASP:O     | 1:J:664:VAL:HG23  | 2.07                     | 0.55              |
| 1:K:1061:LEU:C    | 1:K:1061:LEU:HD12 | 2.31                     | 0.55              |
| 1:L:1020:ASN:CG   | 1:L:1021:ASP:H    | 2.15                     | 0.55              |
| 1:B:881:ARG:HG3   | 1:B:881:ARG:HH11  | 1.72                     | 0.55              |
| 1:B:1014:LEU:HD12 | 1:B:1056:ARG:CB   | 2.36                     | 0.55              |
| 1:E:708:GLY:O     | 1:E:712:ILE:HG13  | 2.07                     | 0.55              |
| 1:I:847:ARG:CZ    | 1:J:891:LEU:HD13  | 2.37                     | 0.55              |
| 1:A:718:GLN:HG3   | 1:A:722:ASN:HD21  | 1.71                     | 0.55              |
| 1:D:881:ARG:HH11  | 1:D:881:ARG:HG3   | 1.72                     | 0.55              |
| 1:I:1061:LEU:HD12 | 1:I:1061:LEU:C    | 2.32                     | 0.55              |
| 1:K:802:LEU:H     | 1:K:802:LEU:HD22  | 1.72                     | 0.55              |
| 1:G:842:VAL:HA    | 1:H:883:ARG:HH22  | 1.71                     | 0.54              |
| 1:I:917:ILE:O     | 1:I:918:GLU:HB2   | 2.05                     | 0.54              |
| 1:J:862:TYR:OH    | 1:J:869:ASN:ND2   | 2.40                     | 0.54              |
| 1:B:862:TYR:OH    | 1:B:869:ASN:ND2   | 2.37                     | 0.54              |
| 1:D:737:HIS:HD2   | 1:D:958:GLU:OE2   | 1.90                     | 0.54              |
| 1:E:1061:LEU:C    | 1:E:1061:LEU:HD12 | 2.32                     | 0.54              |
| 1:G:945:ARG:HD3   | 1:L:915:ASN:HD21  | 1.72                     | 0.54              |
| 1:C:754:THR:CG2   | 1:C:755:ARG:HH21  | 2.15                     | 0.54              |
| 1:L:763:ILE:O     | 1:L:764:HIS:CB    | 2.55                     | 0.54              |
| 1:C:825:HIS:HD2   | 1:C:827:GLY:N     | 1.93                     | 0.54              |
| 1:G:1061:LEU:HD12 | 1:G:1061:LEU:C    | 2.33                     | 0.54              |
| 1:I:751:TYR:CE2   | 1:I:755:ARG:HG3   | 2.42                     | 0.54              |
| 1:K:869:ASN:C     | 1:K:869:ASN:HD22  | 2.15                     | 0.54              |
| 1:A:751:TYR:CE2   | 1:A:755:ARG:HG3   | 2.42                     | 0.54              |
| 1:D:945:ARG:NH1   | 1:D:1071:ILE:HG21 | 2.22                     | 0.54              |
| 1:E:825:HIS:HD2   | 1:E:827:GLY:N     | 1.93                     | 0.54              |
| 1:F:862:TYR:OH    | 1:F:869:ASN:ND2   | 2.39                     | 0.54              |
| 1:G:751:TYR:CE2   | 1:G:755:ARG:HG3   | 2.41                     | 0.54              |
| 1:J:804:SER:C     | 1:J:805:ASN:HD22  | 2.15                     | 0.54              |
| 1:A:721:MET:O     | 1:A:725:ARG:HG3   | 2.08                     | 0.54              |
| 1:E:762:GLN:HA    | 1:E:805:ASN:HD21  | 1.73                     | 0.54              |
| 1:H:862:TYR:OH    | 1:H:869:ASN:ND2   | 2.39                     | 0.54              |
| 1:I:708:GLY:O     | 1:I:712:ILE:HG13  | 2.07                     | 0.54              |
| 1:J:751:TYR:CZ    | 1:J:755:ARG:HG3   | 2.42                     | 0.54              |
| 1:K:708:GLY:O     | 1:K:712:ILE:HG13  | 2.08                     | 0.54              |
| 1:K:847:ARG:CZ    | 1:L:891:LEU:HD13  | 2.37                     | 0.54              |
| 1:G:935:LEU:HD23  | 1:G:935:LEU:O     | 2.08                     | 0.54              |
| 1:J:684:LEU:HD23  | 1:J:688:MET:HG3   | 1.89                     | 0.54              |
| 1:B:804:SER:C     | 1:B:805:ASN:HD22  | 2.16                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:713:PHE:CD2  | 1:C:874:LEU:HD21  | 2.43                     | 0.54              |
| 1:C:881:ARG:HG3  | 1:C:881:ARG:HH11  | 1.73                     | 0.54              |
| 1:D:748:ALA:HB3  | 1:D:936:ALA:HB1   | 1.90                     | 0.54              |
| 1:I:700:MET:HE3  | 1:I:746:LEU:CD2   | 2.38                     | 0.54              |
| 1:B:962:GLN:O    | 1:B:966:GLU:HG3   | 2.07                     | 0.54              |
| 1:D:660:ASP:O    | 1:D:664:VAL:HG23  | 2.07                     | 0.54              |
| 1:F:934:LYS:HD3  | 4:F:1335:HOH:O    | 2.08                     | 0.54              |
| 1:K:713:PHE:HD2  | 1:K:874:LEU:HD21  | 1.72                     | 0.54              |
| 1:K:751:TYR:CE2  | 1:K:755:ARG:HG3   | 2.43                     | 0.54              |
| 1:F:941:PRO:O    | 1:F:1065:LEU:HD12 | 2.08                     | 0.53              |
| 1:A:790:LYS:NZ   | 1:J:1014:LEU:HD23 | 2.23                     | 0.53              |
| 1:B:719:GLN:HE21 | 1:B:719:GLN:H     | 0.79                     | 0.53              |
| 1:G:700:MET:HE3  | 1:G:746:LEU:CD2   | 2.38                     | 0.53              |
| 1:H:804:SER:C    | 1:H:805:ASN:HD22  | 2.16                     | 0.53              |
| 1:I:869:ASN:HD22 | 1:I:869:ASN:C     | 2.14                     | 0.53              |
| 1:L:684:LEU:HD23 | 1:L:688:MET:HG3   | 1.91                     | 0.53              |
| 1:L:735:PRO:HG2  | 1:L:958:GLU:HB2   | 1.90                     | 0.53              |
| 1:A:737:HIS:CD2  | 1:A:958:GLU:OE2   | 2.56                     | 0.53              |
| 1:C:730:GLY:HA3  | 1:C:823:TYR:HE1   | 1.69                     | 0.53              |
| 1:G:760:LEU:HD23 | 1:G:801:CYS:N     | 2.23                     | 0.53              |
| 1:J:761:GLN:HG2  | 1:J:763:ILE:H     | 1.72                     | 0.53              |
| 1:K:753:THR:HA   | 1:K:802:LEU:HD23  | 1.90                     | 0.53              |
| 1:L:862:TYR:OH   | 1:L:869:ASN:ND2   | 2.39                     | 0.53              |
| 1:B:684:LEU:HD23 | 1:B:688:MET:HG3   | 1.89                     | 0.53              |
| 1:B:945:ARG:NH1  | 1:B:1071:ILE:HG21 | 2.23                     | 0.53              |
| 1:C:708:GLY:O    | 1:C:712:ILE:HG13  | 2.08                     | 0.53              |
| 1:C:802:LEU:H    | 1:C:802:LEU:HD22  | 1.73                     | 0.53              |
| 1:C:1017:GLU:CB  | 1:C:1055:ARG:HD3  | 2.39                     | 0.53              |
| 1:F:751:TYR:CZ   | 1:F:755:ARG:HG3   | 2.44                     | 0.53              |
| 1:H:737:HIS:HD2  | 1:H:958:GLU:OE2   | 1.91                     | 0.53              |
| 1:I:765:ASN:HA   | 1:I:804:SER:HB3   | 1.90                     | 0.53              |
| 1:H:941:PRO:O    | 1:H:1065:LEU:HD12 | 2.08                     | 0.53              |
| 1:I:721:MET:O    | 1:I:725:ARG:HG3   | 2.08                     | 0.53              |
| 1:J:748:ALA:HB3  | 1:J:936:ALA:HB1   | 1.90                     | 0.53              |
| 1:A:847:ARG:CZ   | 1:B:891:LEU:HD13  | 2.39                     | 0.53              |
| 1:B:911:ASP:H    | 1:B:914:SER:CB    | 2.14                     | 0.53              |
| 1:E:730:GLY:HA3  | 1:E:823:TYR:HE1   | 1.69                     | 0.53              |
| 1:H:915:ASN:HD21 | 1:K:945:ARG:CD    | 2.22                     | 0.53              |
| 1:L:732:ARG:HD2  | 1:L:825:HIS:O     | 2.08                     | 0.53              |
| 1:C:739:ARG:HG2  | 4:C:1223:HOH:O    | 2.08                     | 0.53              |
| 1:F:735:PRO:HG2  | 1:F:958:GLU:HB2   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:1059:CYS:HB3  | 1:F:1062:MET:CB  | 2.38                     | 0.53              |
| 1:H:1014:LEU:HD21 | 1:H:1058:PHE:HB2 | 1.91                     | 0.53              |
| 1:J:679:PHE:HZ    | 1:J:684:LEU:HD12 | 1.73                     | 0.53              |
| 1:J:828:ARG:HG2   | 1:J:832:PHE:CG   | 2.43                     | 0.53              |
| 1:L:959:PHE:CA    | 1:L:977:MET:HE2  | 2.38                     | 0.53              |
| 1:A:869:ASN:C     | 1:A:869:ASN:HD22 | 2.16                     | 0.53              |
| 1:C:760:LEU:HD23  | 1:C:801:CYS:N    | 2.24                     | 0.53              |
| 1:H:881:ARG:HG3   | 1:H:881:ARG:HH11 | 1.72                     | 0.53              |
| 1:C:751:TYR:CZ    | 1:C:755:ARG:HG3  | 2.44                     | 0.53              |
| 1:F:952:THR:HG23  | 1:F:988:GLN:NE2  | 2.24                     | 0.53              |
| 1:G:881:ARG:HG3   | 1:G:881:ARG:HH11 | 1.74                     | 0.53              |
| 1:J:704:PHE:HB3   | 1:J:710:LEU:HG   | 1.91                     | 0.53              |
| 1:A:719:GLN:HA    | 1:A:722:ASN:HD22 | 1.73                     | 0.53              |
| 1:E:753:THR:HA    | 1:E:802:LEU:HD23 | 1.91                     | 0.53              |
| 1:F:881:ARG:HG3   | 1:F:881:ARG:HH11 | 1.73                     | 0.53              |
| 1:G:753:THR:HA    | 1:G:802:LEU:HD23 | 1.91                     | 0.53              |
| 1:H:915:ASN:HD21  | 1:K:945:ARG:HD3  | 1.74                     | 0.53              |
| 1:H:959:PHE:CA    | 1:H:977:MET:HE2  | 2.39                     | 0.53              |
| 1:I:713:PHE:CD2   | 1:I:874:LEU:HD21 | 2.44                     | 0.53              |
| 1:J:763:ILE:O     | 1:J:764:HIS:CB   | 2.57                     | 0.53              |
| 1:K:721:MET:O     | 1:K:725:ARG:HG3  | 2.09                     | 0.53              |
| 1:G:700:MET:HE3   | 1:G:746:LEU:HD11 | 1.91                     | 0.52              |
| 1:H:828:ARG:NH1   | 1:H:965:GLU:OE1  | 2.43                     | 0.52              |
| 1:J:737:HIS:HD2   | 1:J:958:GLU:OE2  | 1.91                     | 0.52              |
| 1:J:1059:CYS:HB2  | 1:J:1062:MET:HB2 | 1.91                     | 0.52              |
| 1:L:881:ARG:HG3   | 1:L:881:ARG:HH11 | 1.74                     | 0.52              |
| 1:A:909:ALA:HB2   | 1:A:917:ILE:HD11 | 1.89                     | 0.52              |
| 1:F:685:VAL:HG22  | 1:F:695:ILE:CD1  | 2.39                     | 0.52              |
| 1:I:754:THR:HG22  | 1:I:755:ARG:NE   | 2.21                     | 0.52              |
| 1:C:763:ILE:C     | 1:C:765:ASN:H    | 2.17                     | 0.52              |
| 1:C:1017:GLU:N    | 1:C:1055:ARG:HD3 | 2.22                     | 0.52              |
| 1:D:762:GLN:HA    | 1:D:762:GLN:OE1  | 2.10                     | 0.52              |
| 1:F:737:HIS:HD2   | 1:F:958:GLU:OE2  | 1.93                     | 0.52              |
| 1:H:684:LEU:HD23  | 1:H:688:MET:HG3  | 1.92                     | 0.52              |
| 1:J:816:VAL:HG12  | 1:J:820:MET:HE3  | 1.92                     | 0.52              |
| 1:E:1017:GLU:CB   | 1:E:1055:ARG:HD3 | 2.38                     | 0.52              |
| 1:D:828:ARG:HG2   | 1:D:832:PHE:CG   | 2.43                     | 0.52              |
| 1:E:662:ILE:O     | 1:E:666:GLU:HG3  | 2.08                     | 0.52              |
| 1:E:763:ILE:H     | 1:E:805:ASN:ND2  | 2.07                     | 0.52              |
| 1:F:1014:LEU:HD13 | 1:F:1056:ARG:NH2 | 2.25                     | 0.52              |
| 1:H:816:VAL:HG12  | 1:H:820:MET:HE3  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:737:HIS:HD2   | 1:L:958:GLU:OE2  | 1.92                     | 0.52              |
| 1:G:751:TYR:CZ    | 1:G:755:ARG:HG3  | 2.44                     | 0.52              |
| 1:J:732:ARG:HD2   | 1:J:825:HIS:O    | 2.10                     | 0.52              |
| 1:C:700:MET:HE3   | 1:C:746:LEU:CD2  | 2.40                     | 0.52              |
| 1:C:753:THR:HA    | 1:C:802:LEU:HD23 | 1.91                     | 0.52              |
| 1:E:713:PHE:CD2   | 1:E:874:LEU:HD21 | 2.45                     | 0.52              |
| 1:I:891:LEU:CD1   | 1:J:847:ARG:NH2  | 2.70                     | 0.52              |
| 1:K:707:THR:HG22  | 1:K:709:LEU:HG   | 1.91                     | 0.52              |
| 1:B:737:HIS:HD2   | 1:B:958:GLU:OE2  | 1.93                     | 0.52              |
| 1:C:1056:ARG:HG3  | 1:C:1056:ARG:NH1 | 2.25                     | 0.52              |
| 1:L:704:PHE:HB3   | 1:L:710:LEU:HG   | 1.92                     | 0.52              |
| 1:D:684:LEU:HD23  | 1:D:688:MET:HG3  | 1.90                     | 0.52              |
| 1:I:662:ILE:O     | 1:I:666:GLU:HG3  | 2.10                     | 0.52              |
| 1:J:959:PHE:CA    | 1:J:977:MET:HE2  | 2.39                     | 0.52              |
| 1:A:707:THR:HG22  | 1:A:709:LEU:HG   | 1.92                     | 0.52              |
| 1:A:753:THR:HA    | 1:A:802:LEU:HD23 | 1.92                     | 0.52              |
| 1:E:700:MET:HE3   | 1:E:746:LEU:CD2  | 2.40                     | 0.52              |
| 1:B:915:ASN:HD21  | 1:C:945:ARG:HD3  | 1.75                     | 0.51              |
| 1:D:1014:LEU:HD12 | 1:D:1056:ARG:CB  | 2.40                     | 0.51              |
| 1:E:700:MET:HE3   | 1:E:746:LEU:HD11 | 1.92                     | 0.51              |
| 1:J:911:ASP:H     | 1:J:914:SER:CB   | 2.15                     | 0.51              |
| 1:A:700:MET:HE3   | 1:A:746:LEU:CD2  | 2.39                     | 0.51              |
| 1:F:732:ARG:HD2   | 1:F:825:HIS:O    | 2.11                     | 0.51              |
| 1:K:764:HIS:O     | 1:K:766:GLY:N    | 2.43                     | 0.51              |
| 1:D:828:ARG:NH1   | 1:D:965:GLU:OE1  | 2.44                     | 0.51              |
| 1:G:911:ASP:HB3   | 1:G:914:SER:CB   | 2.41                     | 0.51              |
| 1:J:881:ARG:HG3   | 1:J:881:ARG:HH11 | 1.75                     | 0.51              |
| 1:K:700:MET:HE3   | 1:K:746:LEU:HD11 | 1.91                     | 0.51              |
| 1:B:816:VAL:HG12  | 1:B:820:MET:HE3  | 1.92                     | 0.51              |
| 1:G:721:MET:O     | 1:G:725:ARG:HG3  | 2.10                     | 0.51              |
| 1:J:1058:PHE:CD1  | 1:J:1063:HIS:CE1 | 2.98                     | 0.51              |
| 1:C:1017:GLU:HB3  | 1:C:1055:ARG:CD  | 2.41                     | 0.51              |
| 1:E:760:LEU:HD23  | 1:E:801:CYS:N    | 2.26                     | 0.51              |
| 1:E:1017:GLU:HB3  | 1:E:1055:ARG:CD  | 2.41                     | 0.51              |
| 1:I:751:TYR:CZ    | 1:I:755:ARG:HG3  | 2.46                     | 0.51              |
| 1:L:911:ASP:H     | 1:L:914:SER:CB   | 2.16                     | 0.51              |
| 1:A:751:TYR:CZ    | 1:A:755:ARG:HG3  | 2.45                     | 0.51              |
| 1:A:935:LEU:O     | 1:A:935:LEU:HD23 | 2.11                     | 0.51              |
| 1:D:704:PHE:HB3   | 1:D:710:LEU:HG   | 1.91                     | 0.51              |
| 1:D:732:ARG:HD2   | 1:D:825:HIS:O    | 2.10                     | 0.51              |
| 1:I:737:HIS:CD2   | 1:I:958:GLU:OE2  | 2.56                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:754:THR:CG2   | 1:K:755:ARG:HH21 | 2.18                     | 0.51              |
| 1:E:881:ARG:HG3   | 1:E:881:ARG:HH11 | 1.76                     | 0.51              |
| 1:E:935:LEU:HD23  | 1:E:935:LEU:O    | 2.11                     | 0.51              |
| 1:H:704:PHE:HB3   | 1:H:710:LEU:HG   | 1.92                     | 0.51              |
| 1:K:700:MET:HE3   | 1:K:746:LEU:CD2  | 2.40                     | 0.51              |
| 1:K:881:ARG:HG3   | 1:K:881:ARG:HH11 | 1.76                     | 0.51              |
| 1:F:684:LEU:HD23  | 1:F:688:MET:HG3  | 1.92                     | 0.51              |
| 1:I:753:THR:HA    | 1:I:802:LEU:HD23 | 1.92                     | 0.51              |
| 1:A:713:PHE:CD2   | 1:A:874:LEU:HD21 | 2.46                     | 0.51              |
| 1:C:721:MET:O     | 1:C:725:ARG:HG3  | 2.10                     | 0.51              |
| 1:F:704:PHE:HB3   | 1:F:710:LEU:HG   | 1.92                     | 0.51              |
| 1:I:869:ASN:C     | 1:I:869:ASN:ND2  | 2.69                     | 0.51              |
| 1:J:1000:CYS:HB3  | 1:J:1062:MET:HE1 | 1.92                     | 0.51              |
| 1:K:911:ASP:HB3   | 1:K:914:SER:CB   | 2.40                     | 0.51              |
| 1:L:804:SER:C     | 1:L:805:ASN:HD22 | 2.19                     | 0.51              |
| 1:C:713:PHE:HD2   | 1:C:874:LEU:HD21 | 1.76                     | 0.51              |
| 1:L:816:VAL:HG12  | 1:L:820:MET:HE3  | 1.92                     | 0.51              |
| 1:A:881:ARG:HG3   | 1:A:881:ARG:HH11 | 1.76                     | 0.50              |
| 1:B:828:ARG:NH1   | 1:B:965:GLU:OE1  | 2.44                     | 0.50              |
| 1:I:881:ARG:HG3   | 1:I:881:ARG:HH11 | 1.76                     | 0.50              |
| 1:K:751:TYR:CZ    | 1:K:755:ARG:HG3  | 2.45                     | 0.50              |
| 1:A:754:THR:HG22  | 1:A:755:ARG:NE   | 2.22                     | 0.50              |
| 1:D:763:ILE:O     | 1:D:764:HIS:CB   | 2.58                     | 0.50              |
| 1:K:762:GLN:HA    | 1:K:762:GLN:NE2  | 2.18                     | 0.50              |
| 1:A:708:GLY:O     | 1:A:712:ILE:HG13 | 2.12                     | 0.50              |
| 1:B:952:THR:HG23  | 1:B:988:GLN:NE2  | 2.27                     | 0.50              |
| 1:C:662:ILE:O     | 1:C:666:GLU:HG3  | 2.10                     | 0.50              |
| 1:A:1014:LEU:HD12 | 1:A:1056:ARG:CB  | 2.42                     | 0.50              |
| 1:C:700:MET:HE3   | 1:C:746:LEU:HD11 | 1.93                     | 0.50              |
| 1:C:869:ASN:C     | 1:C:869:ASN:ND2  | 2.69                     | 0.50              |
| 1:E:1071:ILE:CG2  | 1:J:915:ASN:ND2  | 2.75                     | 0.50              |
| 1:H:685:VAL:HG22  | 1:H:695:ILE:CD1  | 2.41                     | 0.50              |
| 1:H:803:SER:HA    | 1:H:811:LEU:HD11 | 1.94                     | 0.50              |
| 1:J:685:VAL:HG22  | 1:J:695:ILE:CD1  | 2.41                     | 0.50              |
| 1:L:1069:HIS:ND1  | 1:L:1073:LYS:NZ  | 2.55                     | 0.50              |
| 1:B:735:PRO:HG2   | 1:B:958:GLU:HB2  | 1.94                     | 0.50              |
| 1:D:735:PRO:HG2   | 1:D:958:GLU:HB2  | 1.92                     | 0.50              |
| 1:E:713:PHE:HD2   | 1:E:874:LEU:HD21 | 1.77                     | 0.50              |
| 1:D:719:GLN:HE21  | 1:D:719:GLN:H    | 0.81                     | 0.50              |
| 1:F:828:ARG:NH1   | 1:F:965:GLU:OE1  | 2.44                     | 0.50              |
| 1:F:959:PHE:CA    | 1:F:977:MET:HE2  | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:735:PRO:HG2  | 1:J:958:GLU:HB2  | 1.92                     | 0.50              |
| 1:J:739:ARG:HH11 | 1:J:739:ARG:CG   | 2.23                     | 0.50              |
| 1:L:735:PRO:HG2  | 1:L:958:GLU:CB   | 2.41                     | 0.50              |
| 1:L:976:PHE:CD2  | 1:L:987:LEU:HB2  | 2.47                     | 0.50              |
| 1:A:911:ASP:HB3  | 1:A:914:SER:CB   | 2.41                     | 0.50              |
| 1:L:828:ARG:NH1  | 1:L:965:GLU:OE1  | 2.45                     | 0.50              |
| 1:L:964:ASP:OD2  | 1:L:979:ARG:NH1  | 2.45                     | 0.50              |
| 1:B:915:ASN:CG   | 1:C:945:ARG:HH11 | 2.14                     | 0.50              |
| 1:D:816:VAL:HG12 | 1:D:820:MET:HE3  | 1.93                     | 0.50              |
| 1:D:965:GLU:O    | 1:D:969:LEU:HG   | 2.11                     | 0.50              |
| 1:E:721:MET:O    | 1:E:725:ARG:HG3  | 2.11                     | 0.50              |
| 1:F:761:GLN:HG2  | 1:F:763:ILE:H    | 1.76                     | 0.50              |
| 1:F:1013:TRP:CZ3 | 1:F:1055:ARG:HB3 | 2.47                     | 0.50              |
| 1:I:707:THR:HG22 | 1:I:709:LEU:HG   | 1.94                     | 0.50              |
| 1:L:985:ALA:HA   | 1:L:1072:TRP:CE3 | 2.47                     | 0.50              |
| 1:C:891:LEU:HD13 | 1:D:847:ARG:NH2  | 2.26                     | 0.50              |
| 1:C:911:ASP:HB3  | 1:C:914:SER:CB   | 2.41                     | 0.50              |
| 1:D:911:ASP:H    | 1:D:914:SER:CB   | 2.18                     | 0.50              |
| 1:G:730:GLY:HA3  | 1:G:823:TYR:HE1  | 1.68                     | 0.50              |
| 1:K:660:ASP:O    | 1:K:664:VAL:HG23 | 2.12                     | 0.50              |
| 1:C:737:HIS:CD2  | 1:C:958:GLU:OE2  | 2.58                     | 0.49              |
| 1:H:763:ILE:O    | 1:H:764:HIS:CB   | 2.60                     | 0.49              |
| 1:H:911:ASP:H    | 1:H:914:SER:CB   | 2.16                     | 0.49              |
| 1:J:684:LEU:HD23 | 1:J:684:LEU:O    | 2.11                     | 0.49              |
| 1:A:662:ILE:O    | 1:A:666:GLU:HG3  | 2.11                     | 0.49              |
| 1:C:754:THR:HG22 | 1:C:755:ARG:NE   | 2.21                     | 0.49              |
| 1:B:803:SER:HA   | 1:B:811:LEU:HD11 | 1.93                     | 0.49              |
| 1:H:761:GLN:HG2  | 1:H:763:ILE:H    | 1.76                     | 0.49              |
| 1:E:739:ARG:HG2  | 4:E:1323:HOH:O   | 2.11                     | 0.49              |
| 1:A:760:LEU:HD23 | 1:A:801:CYS:N    | 2.27                     | 0.49              |
| 1:A:956:VAL:HG11 | 1:A:984:LEU:HD13 | 1.94                     | 0.49              |
| 1:B:704:PHE:HB3  | 1:B:710:LEU:HG   | 1.93                     | 0.49              |
| 1:C:754:THR:CG2  | 1:C:755:ARG:HE   | 2.21                     | 0.49              |
| 1:K:736:TYR:CD1  | 1:K:955:ILE:HG13 | 2.47                     | 0.49              |
| 1:B:732:ARG:HD2  | 1:B:825:HIS:O    | 2.12                     | 0.49              |
| 1:G:713:PHE:CD2  | 1:G:874:LEU:HD21 | 2.48                     | 0.49              |
| 1:I:713:PHE:HD2  | 1:I:874:LEU:HD21 | 1.76                     | 0.49              |
| 1:B:1015:GLU:O   | 1:B:1055:ARG:HD2 | 2.12                     | 0.49              |
| 1:I:700:MET:HE3  | 1:I:746:LEU:HD11 | 1.94                     | 0.49              |
| 1:E:911:ASP:HB3  | 1:E:914:SER:CB   | 2.42                     | 0.49              |
| 1:E:1059:CYS:SG  | 1:E:1062:MET:HB2 | 2.53                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:794:ASN:HB3   | 1:K:799:TYR:HB2  | 1.94                     | 0.49              |
| 1:K:956:VAL:HG11  | 1:K:984:LEU:HD13 | 1.95                     | 0.49              |
| 1:L:685:VAL:HG22  | 1:L:695:ILE:CD1  | 2.42                     | 0.49              |
| 1:C:660:ASP:O     | 1:C:664:VAL:HG23 | 2.13                     | 0.49              |
| 1:I:911:ASP:HB3   | 1:I:914:SER:CB   | 2.42                     | 0.49              |
| 1:K:662:ILE:O     | 1:K:666:GLU:HG3  | 2.12                     | 0.49              |
| 1:L:803:SER:HA    | 1:L:811:LEU:HD11 | 1.95                     | 0.49              |
| 1:A:736:TYR:CD1   | 1:A:955:ILE:HG13 | 2.48                     | 0.49              |
| 1:D:959:PHE:CA    | 1:D:977:MET:HE2  | 2.41                     | 0.49              |
| 1:G:660:ASP:O     | 1:G:664:VAL:HG23 | 2.13                     | 0.49              |
| 1:I:935:LEU:O     | 1:I:935:LEU:HD23 | 2.12                     | 0.49              |
| 1:A:660:ASP:O     | 1:A:664:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:915:ASN:OD1   | 1:C:945:ARG:NH1  | 2.46                     | 0.48              |
| 1:E:707:THR:HG22  | 1:E:709:LEU:HG   | 1.94                     | 0.48              |
| 1:A:700:MET:HE3   | 1:A:746:LEU:HD11 | 1.95                     | 0.48              |
| 1:B:810:GLU:OE1   | 1:B:925:ARG:HD2  | 2.13                     | 0.48              |
| 1:C:736:TYR:CD1   | 1:C:955:ILE:HG13 | 2.48                     | 0.48              |
| 1:B:685:VAL:HG22  | 1:B:695:ILE:CD1  | 2.43                     | 0.48              |
| 1:C:816:VAL:O     | 1:C:820:MET:HG2  | 2.13                     | 0.48              |
| 1:D:934:LYS:HD3   | 4:D:1235:HOH:O   | 2.14                     | 0.48              |
| 1:F:1014:LEU:HD21 | 1:F:1058:PHE:HB2 | 1.95                     | 0.48              |
| 1:G:869:ASN:C     | 1:G:869:ASN:HD22 | 2.20                     | 0.48              |
| 1:K:729:ASN:HA    | 1:K:739:ARG:NH2  | 2.27                     | 0.48              |
| 1:A:729:ASN:HA    | 1:A:739:ARG:NH2  | 2.28                     | 0.48              |
| 1:B:991:PHE:CE2   | 1:B:996:VAL:HG23 | 2.48                     | 0.48              |
| 1:E:869:ASN:C     | 1:E:869:ASN:ND2  | 2.68                     | 0.48              |
| 1:G:662:ILE:O     | 1:G:666:GLU:HG3  | 2.12                     | 0.48              |
| 1:G:794:ASN:HB3   | 1:G:799:TYR:HB2  | 1.95                     | 0.48              |
| 1:H:1069:HIS:CE1  | 1:H:1073:LYS:HZ2 | 2.29                     | 0.48              |
| 1:J:1058:PHE:HE1  | 1:J:1063:HIS:CE1 | 2.30                     | 0.48              |
| 1:K:729:ASN:HA    | 1:K:739:ARG:HH21 | 1.78                     | 0.48              |
| 1:B:959:PHE:CA    | 1:B:977:MET:HE2  | 2.42                     | 0.48              |
| 1:B:964:ASP:OD2   | 1:B:979:ARG:NH1  | 2.46                     | 0.48              |
| 1:C:956:VAL:HG11  | 1:C:984:LEU:HD13 | 1.94                     | 0.48              |
| 1:E:754:THR:CG2   | 1:E:755:ARG:HH21 | 2.18                     | 0.48              |
| 1:F:735:PRO:HG2   | 1:F:958:GLU:CB   | 2.44                     | 0.48              |
| 1:J:1058:PHE:CE1  | 1:J:1063:HIS:ND1 | 2.80                     | 0.48              |
| 1:C:846:ASP:OD2   | 1:D:883:ARG:NH1  | 2.47                     | 0.48              |
| 1:K:869:ASN:C     | 1:K:869:ASN:ND2  | 2.70                     | 0.48              |
| 1:C:707:THR:HG22  | 1:C:709:LEU:HG   | 1.94                     | 0.48              |
| 1:D:685:VAL:HG22  | 1:D:695:ILE:CD1  | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:965:GLU:O     | 1:F:969:LEU:HG    | 2.13                     | 0.48              |
| 1:H:985:ALA:HA    | 1:H:1072:TRP:CE3  | 2.49                     | 0.48              |
| 1:J:828:ARG:NH1   | 1:J:965:GLU:OE1   | 2.46                     | 0.48              |
| 1:L:952:THR:HG23  | 1:L:988:GLN:NE2   | 2.28                     | 0.48              |
| 1:B:985:ALA:HA    | 1:B:1072:TRP:CE3  | 2.49                     | 0.48              |
| 1:D:803:SER:HA    | 1:D:811:LEU:HD11  | 1.96                     | 0.48              |
| 1:E:737:HIS:CD2   | 1:E:958:GLU:OE2   | 2.58                     | 0.48              |
| 1:H:735:PRO:HG2   | 1:H:958:GLU:HB2   | 1.95                     | 0.48              |
| 1:I:739:ARG:HG2   | 4:I:1523:HOH:O    | 2.13                     | 0.48              |
| 1:J:965:GLU:O     | 1:J:969:LEU:HG    | 2.13                     | 0.48              |
| 1:L:1059:CYS:HB3  | 1:L:1062:MET:HB2  | 1.96                     | 0.48              |
| 1:F:816:VAL:HG12  | 1:F:820:MET:HE3   | 1.95                     | 0.48              |
| 1:F:964:ASP:OD2   | 1:F:979:ARG:NH1   | 2.47                     | 0.48              |
| 1:G:825:HIS:HD2   | 1:G:827:GLY:N     | 1.94                     | 0.48              |
| 1:G:847:ARG:CZ    | 1:H:891:LEU:HD13  | 2.43                     | 0.48              |
| 1:H:716:PRO:HB2   | 1:H:719:GLN:HE22  | 1.79                     | 0.48              |
| 1:I:794:ASN:HB3   | 1:I:799:TYR:HB2   | 1.96                     | 0.48              |
| 1:L:965:GLU:O     | 1:L:969:LEU:HG    | 2.14                     | 0.48              |
| 1:A:869:ASN:C     | 1:A:869:ASN:ND2   | 2.71                     | 0.48              |
| 1:C:1059:CYS:SG   | 1:C:1062:MET:HB2  | 2.54                     | 0.48              |
| 1:D:739:ARG:HH11  | 1:D:739:ARG:CG    | 2.24                     | 0.48              |
| 1:E:883:ARG:NH1   | 1:F:846:ASP:OD2   | 2.46                     | 0.48              |
| 1:E:939:ASN:O     | 1:E:940:GLY:C     | 2.57                     | 0.48              |
| 1:G:913:ASN:ND2   | 1:K:1056:ARG:HE   | 2.12                     | 0.48              |
| 1:G:945:ARG:NH1   | 1:L:918:GLU:OE2   | 2.47                     | 0.48              |
| 1:H:964:ASP:OD2   | 1:H:979:ARG:NH1   | 2.47                     | 0.48              |
| 1:H:700:MET:HE3   | 1:H:746:LEU:CD1   | 2.44                     | 0.47              |
| 1:H:952:THR:HG23  | 1:H:988:GLN:NE2   | 2.29                     | 0.47              |
| 1:H:1013:TRP:CZ3  | 1:H:1057:ILE:HG22 | 2.48                     | 0.47              |
| 1:I:736:TYR:CD1   | 1:I:955:ILE:HG13  | 2.49                     | 0.47              |
| 1:E:891:LEU:CD1   | 1:F:847:ARG:CZ    | 2.93                     | 0.47              |
| 1:E:891:LEU:HD13  | 1:F:847:ARG:NH2   | 2.28                     | 0.47              |
| 1:E:1071:ILE:HG21 | 1:J:915:ASN:HD21  | 1.79                     | 0.47              |
| 1:L:674:MET:HE1   | 1:L:699:VAL:CG1   | 2.44                     | 0.47              |
| 1:B:965:GLU:O     | 1:B:969:LEU:HG    | 2.14                     | 0.47              |
| 1:E:729:ASN:HA    | 1:E:739:ARG:HH21  | 1.79                     | 0.47              |
| 1:E:915:ASN:O     | 1:E:916:GLY:C     | 2.58                     | 0.47              |
| 1:H:729:ASN:HA    | 1:H:739:ARG:HH22  | 1.79                     | 0.47              |
| 1:H:991:PHE:CE2   | 1:H:996:VAL:HG23  | 2.49                     | 0.47              |
| 1:H:1059:CYS:HB3  | 1:H:1062:MET:HB2  | 1.96                     | 0.47              |
| 1:I:762:GLN:HE22  | 1:I:801:CYS:H     | 1.60                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:735:PRO:HG2   | 1:J:958:GLU:CB   | 2.44                     | 0.47              |
| 1:K:787:ILE:HG23  | 1:K:808:ALA:CB   | 2.44                     | 0.47              |
| 1:L:670:LEU:O     | 1:L:674:MET:HG3  | 2.15                     | 0.47              |
| 1:A:724:PHE:O     | 1:A:728:GLU:HG3  | 2.13                     | 0.47              |
| 1:C:729:ASN:HA    | 1:C:739:ARG:NH2  | 2.28                     | 0.47              |
| 1:D:796:ASP:OD1   | 1:D:798:SER:N    | 2.39                     | 0.47              |
| 1:E:794:ASN:HB3   | 1:E:799:TYR:HB2  | 1.96                     | 0.47              |
| 1:H:816:VAL:CG1   | 1:H:820:MET:HE3  | 2.44                     | 0.47              |
| 1:H:1056:ARG:HB3  | 1:H:1056:ARG:NH1 | 2.28                     | 0.47              |
| 1:I:729:ASN:HA    | 1:I:739:ARG:NH2  | 2.29                     | 0.47              |
| 1:J:803:SER:HA    | 1:J:811:LEU:HD11 | 1.96                     | 0.47              |
| 1:L:810:GLU:OE1   | 1:L:925:ARG:HD2  | 2.15                     | 0.47              |
| 1:C:891:LEU:CD1   | 1:D:847:ARG:CZ   | 2.92                     | 0.47              |
| 1:G:754:THR:HG22  | 1:G:755:ARG:NE   | 2.22                     | 0.47              |
| 1:H:735:PRO:HG2   | 1:H:958:GLU:CB   | 2.45                     | 0.47              |
| 1:H:915:ASN:CG    | 1:K:945:ARG:HH11 | 2.23                     | 0.47              |
| 1:I:847:ARG:NH2   | 1:J:891:LEU:HD13 | 2.30                     | 0.47              |
| 1:B:735:PRO:HG2   | 1:B:958:GLU:CB   | 2.44                     | 0.47              |
| 1:C:883:ARG:HH12  | 1:D:846:ASP:CG   | 2.21                     | 0.47              |
| 1:D:700:MET:HE3   | 1:D:746:LEU:CD1  | 2.45                     | 0.47              |
| 1:D:716:PRO:HB2   | 1:D:719:GLN:HE22 | 1.80                     | 0.47              |
| 1:E:846:ASP:HB2   | 4:E:1334:HOH:O   | 2.14                     | 0.47              |
| 1:G:707:THR:HG22  | 1:G:709:LEU:HG   | 1.97                     | 0.47              |
| 1:I:760:LEU:HD23  | 1:I:801:CYS:N    | 2.30                     | 0.47              |
| 1:A:701:TYR:OH    | 1:J:1015:GLU:OE1 | 2.32                     | 0.47              |
| 1:B:872:LEU:HD13  | 1:B:873:HIS:CG   | 2.50                     | 0.47              |
| 1:D:735:PRO:HG2   | 1:D:958:GLU:CB   | 2.44                     | 0.47              |
| 1:E:952:THR:HG23  | 1:E:988:GLN:NE2  | 2.30                     | 0.47              |
| 1:F:1069:HIS:CE1  | 1:F:1073:LYS:HZ2 | 2.33                     | 0.47              |
| 1:G:796:ASP:OD1   | 1:G:798:SER:CB   | 2.63                     | 0.47              |
| 1:I:729:ASN:HA    | 1:I:739:ARG:HH21 | 1.79                     | 0.47              |
| 1:J:810:GLU:OE1   | 1:J:925:ARG:HD2  | 2.14                     | 0.47              |
| 1:K:670:LEU:HD22  | 1:K:674:MET:SD   | 2.54                     | 0.47              |
| 1:K:727:LEU:HD21  | 1:K:820:MET:HB3  | 1.97                     | 0.47              |
| 1:A:1014:LEU:HD12 | 1:A:1056:ARG:HB3 | 1.97                     | 0.47              |
| 1:B:674:MET:HE1   | 1:B:699:VAL:CG1  | 2.44                     | 0.47              |
| 1:B:729:ASN:HA    | 1:B:739:ARG:HH22 | 1.80                     | 0.47              |
| 1:B:1014:LEU:HD21 | 1:B:1058:PHE:HB2 | 1.97                     | 0.47              |
| 1:C:729:ASN:HA    | 1:C:739:ARG:HH21 | 1.78                     | 0.47              |
| 1:F:915:ASN:CG    | 1:I:945:ARG:NH1  | 2.73                     | 0.47              |
| 1:A:939:ASN:O     | 1:A:940:GLY:C    | 2.58                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:684:LEU:HD23  | 1:B:684:LEU:O     | 2.14                     | 0.47              |
| 1:D:964:ASP:OD2   | 1:D:979:ARG:NH1   | 2.47                     | 0.47              |
| 1:E:729:ASN:HA    | 1:E:739:ARG:NH2   | 2.29                     | 0.47              |
| 1:G:816:VAL:O     | 1:G:820:MET:HG2   | 2.14                     | 0.47              |
| 1:L:985:ALA:HA    | 1:L:1072:TRP:HE3  | 1.79                     | 0.47              |
| 1:A:729:ASN:HA    | 1:A:739:ARG:HH21  | 1.79                     | 0.47              |
| 1:B:845:ASN:O     | 1:B:847:ARG:HG2   | 2.15                     | 0.47              |
| 1:B:981:SER:N     | 1:B:982:PRO:CD    | 2.78                     | 0.47              |
| 1:C:794:ASN:HB3   | 1:C:799:TYR:HB2   | 1.97                     | 0.47              |
| 1:D:985:ALA:HA    | 1:D:1072:TRP:CE3  | 2.49                     | 0.47              |
| 1:E:816:VAL:O     | 1:E:820:MET:HG2   | 2.15                     | 0.47              |
| 1:J:985:ALA:HA    | 1:J:1072:TRP:CE3  | 2.50                     | 0.47              |
| 1:A:790:LYS:HZ2   | 1:J:1014:LEU:HD23 | 1.78                     | 0.46              |
| 1:C:915:ASN:O     | 1:C:916:GLY:C     | 2.58                     | 0.46              |
| 1:D:1057:ILE:HD12 | 1:D:1058:PHE:N    | 2.30                     | 0.46              |
| 1:E:754:THR:HG22  | 1:E:755:ARG:NE    | 2.24                     | 0.46              |
| 1:E:956:VAL:HG11  | 1:E:984:LEU:HD13  | 1.97                     | 0.46              |
| 1:G:670:LEU:HD22  | 1:G:674:MET:SD    | 2.55                     | 0.46              |
| 1:G:1056:ARG:HG3  | 1:G:1056:ARG:HH11 | 1.80                     | 0.46              |
| 1:J:719:GLN:HE21  | 1:J:719:GLN:H     | 0.80                     | 0.46              |
| 1:A:1056:ARG:HG3  | 1:A:1056:ARG:HH11 | 1.80                     | 0.46              |
| 1:F:1069:HIS:ND1  | 1:F:1073:LYS:NZ   | 2.56                     | 0.46              |
| 1:G:729:ASN:HA    | 1:G:739:ARG:NH2   | 2.31                     | 0.46              |
| 1:H:965:GLU:O     | 1:H:969:LEU:HG    | 2.15                     | 0.46              |
| 1:L:729:ASN:HA    | 1:L:739:ARG:HH22  | 1.80                     | 0.46              |
| 1:A:1017:GLU:HB3  | 1:A:1055:ARG:CD   | 2.46                     | 0.46              |
| 1:D:930:GLN:O     | 1:D:933:ILE:HG13  | 2.16                     | 0.46              |
| 1:G:674:MET:CE    | 1:G:703:LEU:HD21  | 2.45                     | 0.46              |
| 1:I:670:LEU:HD22  | 1:I:674:MET:SD    | 2.56                     | 0.46              |
| 1:I:1056:ARG:HG3  | 1:I:1056:ARG:NH1  | 2.31                     | 0.46              |
| 1:L:991:PHE:CE2   | 1:L:996:VAL:HG23  | 2.50                     | 0.46              |
| 1:B:713:PHE:O     | 1:B:714:LYS:C     | 2.58                     | 0.46              |
| 1:B:915:ASN:OD1   | 1:C:945:ARG:CZ    | 2.64                     | 0.46              |
| 1:G:727:LEU:HD21  | 1:G:820:MET:HB3   | 1.97                     | 0.46              |
| 1:H:845:ASN:O     | 1:H:847:ARG:HG2   | 2.15                     | 0.46              |
| 1:H:981:SER:N     | 1:H:982:PRO:CD    | 2.79                     | 0.46              |
| 1:I:939:ASN:O     | 1:I:940:GLY:C     | 2.58                     | 0.46              |
| 1:J:938:ILE:HD12  | 1:J:996:VAL:HG22  | 1.97                     | 0.46              |
| 1:B:985:ALA:HA    | 1:B:1072:TRP:HE3  | 1.81                     | 0.46              |
| 1:E:846:ASP:OD2   | 1:F:883:ARG:NH1   | 2.48                     | 0.46              |
| 1:E:1071:ILE:CG2  | 1:J:915:ASN:HD22  | 2.29                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:976:PHE:CD2   | 1:F:987:LEU:HB2  | 2.50                     | 0.46              |
| 1:I:660:ASP:O     | 1:I:664:VAL:HG23 | 2.15                     | 0.46              |
| 1:I:915:ASN:O     | 1:I:916:GLY:C    | 2.58                     | 0.46              |
| 1:K:823:TYR:CE2   | 1:K:857:SER:HB3  | 2.51                     | 0.46              |
| 1:L:796:ASP:OD1   | 1:L:798:SER:N    | 2.43                     | 0.46              |
| 1:A:939:ASN:ND2   | 1:A:943:LYS:HE3  | 2.31                     | 0.46              |
| 1:C:1017:GLU:H    | 1:C:1055:ARG:CD  | 2.27                     | 0.46              |
| 1:F:729:ASN:HA    | 1:F:739:ARG:HH22 | 1.81                     | 0.46              |
| 1:G:762:GLN:CD    | 1:G:800:GLY:HA2  | 2.41                     | 0.46              |
| 1:B:974:SER:HB2   | 1:B:977:MET:SD   | 2.56                     | 0.46              |
| 1:D:872:LEU:HD13  | 1:D:873:HIS:CG   | 2.51                     | 0.46              |
| 1:E:787:ILE:HG23  | 1:E:808:ALA:CB   | 2.46                     | 0.46              |
| 1:J:952:THR:HG23  | 1:J:988:GLN:NE2  | 2.31                     | 0.46              |
| 1:L:725:ARG:HG3   | 1:L:725:ARG:NH1  | 2.30                     | 0.46              |
| 1:L:1014:LEU:HD21 | 1:L:1058:PHE:HB2 | 1.97                     | 0.46              |
| 1:G:1056:ARG:HE   | 1:K:913:ASN:ND2  | 2.13                     | 0.46              |
| 1:K:707:THR:HG21  | 1:K:709:LEU:HG   | 1.98                     | 0.46              |
| 1:B:716:PRO:HB2   | 1:B:719:GLN:HE22 | 1.81                     | 0.46              |
| 1:C:713:PHE:O     | 1:C:714:LYS:C    | 2.57                     | 0.46              |
| 1:G:763:ILE:C     | 1:G:765:ASN:H    | 2.23                     | 0.46              |
| 1:H:872:LEU:HD13  | 1:H:873:HIS:CG   | 2.51                     | 0.46              |
| 1:J:976:PHE:CD2   | 1:J:987:LEU:HB2  | 2.51                     | 0.46              |
| 1:L:973:ILE:HG21  | 1:L:978:ASP:HB2  | 1.97                     | 0.46              |
| 1:A:718:GLN:OE1   | 1:J:1021:ASP:HA  | 2.16                     | 0.45              |
| 1:D:754:THR:CG2   | 1:D:755:ARG:HH21 | 2.26                     | 0.45              |
| 1:D:973:ILE:HG21  | 1:D:978:ASP:HB2  | 1.98                     | 0.45              |
| 1:F:754:THR:CG2   | 1:F:755:ARG:HH21 | 2.25                     | 0.45              |
| 1:F:981:SER:N     | 1:F:982:PRO:CD   | 2.79                     | 0.45              |
| 1:G:736:TYR:CD1   | 1:G:955:ILE:HG13 | 2.50                     | 0.45              |
| 1:G:915:ASN:O     | 1:G:916:GLY:C    | 2.58                     | 0.45              |
| 1:I:956:VAL:HG11  | 1:I:984:LEU:HD13 | 1.97                     | 0.45              |
| 1:J:725:ARG:HG3   | 1:J:725:ARG:NH1  | 2.31                     | 0.45              |
| 1:K:846:ASP:HB2   | 4:K:1634:HOH:O   | 2.15                     | 0.45              |
| 1:K:871:LEU:HB3   | 1:K:874:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:700:MET:HE3   | 1:B:746:LEU:CD1  | 2.45                     | 0.45              |
| 1:B:915:ASN:HD21  | 1:C:945:ARG:HD2  | 1.81                     | 0.45              |
| 1:D:1020:ASN:HD22 | 1:D:1020:ASN:HA  | 1.59                     | 0.45              |
| 1:H:1057:ILE:HD12 | 1:H:1058:PHE:N   | 2.31                     | 0.45              |
| 1:I:816:VAL:O     | 1:I:820:MET:HG2  | 2.16                     | 0.45              |
| 1:J:700:MET:HE3   | 1:J:746:LEU:CD1  | 2.46                     | 0.45              |
| 1:A:727:LEU:HD21  | 1:A:820:MET:HB3  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:816:VAL:O     | 1:A:820:MET:HG2  | 2.15                     | 0.45              |
| 1:E:754:THR:CG2   | 1:E:755:ARG:HE   | 2.24                     | 0.45              |
| 1:G:713:PHE:O     | 1:G:714:LYS:C    | 2.58                     | 0.45              |
| 1:J:816:VAL:CG1   | 1:J:820:MET:HE3  | 2.47                     | 0.45              |
| 1:K:754:THR:CG2   | 1:K:755:ARG:HE   | 2.21                     | 0.45              |
| 1:A:915:ASN:O     | 1:A:916:GLY:C    | 2.59                     | 0.45              |
| 1:D:703:LEU:HD22  | 1:D:750:TRP:CE2  | 2.52                     | 0.45              |
| 1:D:810:GLU:OE1   | 1:D:925:ARG:HD2  | 2.16                     | 0.45              |
| 1:F:985:ALA:HA    | 1:F:1072:TRP:CE3 | 2.51                     | 0.45              |
| 1:G:939:ASN:ND2   | 1:G:943:LYS:HE3  | 2.32                     | 0.45              |
| 1:G:945:ARG:CD    | 1:L:915:ASN:HD21 | 2.28                     | 0.45              |
| 1:K:816:VAL:O     | 1:K:820:MET:HG2  | 2.16                     | 0.45              |
| 1:A:707:THR:HG21  | 1:A:709:LEU:HG   | 1.98                     | 0.45              |
| 1:B:976:PHE:CD2   | 1:B:987:LEU:HB2  | 2.51                     | 0.45              |
| 1:D:1014:LEU:HD12 | 1:D:1056:ARG:HB2 | 1.96                     | 0.45              |
| 1:G:787:ILE:HG23  | 1:G:808:ALA:CB   | 2.47                     | 0.45              |
| 1:G:956:VAL:HG11  | 1:G:984:LEU:HD13 | 1.98                     | 0.45              |
| 1:K:674:MET:CE    | 1:K:703:LEU:HD21 | 2.47                     | 0.45              |
| 1:K:939:ASN:O     | 1:K:940:GLY:C    | 2.60                     | 0.45              |
| 1:A:713:PHE:HD2   | 1:A:874:LEU:HD21 | 1.81                     | 0.45              |
| 1:A:957:ASN:O     | 1:A:961:GLU:HG3  | 2.16                     | 0.45              |
| 1:E:660:ASP:O     | 1:E:664:VAL:HG23 | 2.17                     | 0.45              |
| 1:F:1014:LEU:HD12 | 1:F:1056:ARG:HB3 | 1.99                     | 0.45              |
| 1:H:725:ARG:HG3   | 1:H:725:ARG:NH1  | 2.30                     | 0.45              |
| 1:J:670:LEU:O     | 1:J:674:MET:HG3  | 2.17                     | 0.45              |
| 1:L:816:VAL:CG1   | 1:L:820:MET:HE3  | 2.47                     | 0.45              |
| 1:L:938:ILE:HD12  | 1:L:996:VAL:HG22 | 1.97                     | 0.45              |
| 1:B:872:LEU:HD13  | 1:B:873:HIS:CD2  | 2.52                     | 0.45              |
| 1:C:764:HIS:O     | 1:C:765:ASN:O    | 2.35                     | 0.45              |
| 1:D:938:ILE:HD12  | 1:D:996:VAL:HG22 | 1.98                     | 0.45              |
| 1:E:957:ASN:O     | 1:E:961:GLU:HG3  | 2.17                     | 0.45              |
| 1:F:700:MET:HE3   | 1:F:746:LEU:CD1  | 2.47                     | 0.45              |
| 1:F:719:GLN:HE21  | 1:F:719:GLN:H    | 0.79                     | 0.45              |
| 1:F:739:ARG:HH11  | 1:F:739:ARG:CG   | 2.26                     | 0.45              |
| 1:G:869:ASN:C     | 1:G:869:ASN:ND2  | 2.73                     | 0.45              |
| 1:H:851:GLU:HA    | 1:H:854:HIS:HD2  | 1.82                     | 0.45              |
| 1:B:670:LEU:O     | 1:B:674:MET:HG3  | 2.16                     | 0.45              |
| 1:B:703:LEU:HD22  | 1:B:750:TRP:CE2  | 2.52                     | 0.45              |
| 1:C:784:ILE:HG21  | 1:C:807:PRO:HB3  | 1.97                     | 0.45              |
| 1:C:787:ILE:HG23  | 1:C:808:ALA:CB   | 2.47                     | 0.45              |
| 1:C:939:ASN:O     | 1:C:940:GLY:C    | 2.60                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:1055:ARG:HG2  | 1:D:1056:ARG:H   | 1.81                     | 0.45              |
| 1:H:976:PHE:CD2   | 1:H:987:LEU:HB2  | 2.51                     | 0.45              |
| 1:J:1059:CYS:HB2  | 1:J:1062:MET:CB  | 2.47                     | 0.45              |
| 1:A:762:GLN:NE2   | 1:A:800:GLY:HA2  | 2.31                     | 0.45              |
| 1:B:694:ARG:O     | 1:B:698:GLN:HG2  | 2.17                     | 0.45              |
| 1:H:985:ALA:HA    | 1:H:1072:TRP:HE3 | 1.81                     | 0.45              |
| 1:E:784:ILE:HG22  | 1:E:786:TYR:CE1  | 2.52                     | 0.45              |
| 1:F:796:ASP:OD1   | 1:F:798:SER:N    | 2.41                     | 0.45              |
| 1:F:851:GLU:HA    | 1:F:854:HIS:HD2  | 1.81                     | 0.45              |
| 1:J:754:THR:CG2   | 1:J:755:ARG:HH21 | 2.26                     | 0.45              |
| 1:L:694:ARG:O     | 1:L:698:GLN:HG2  | 2.17                     | 0.45              |
| 1:B:705:GLN:HG2   | 1:B:710:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:851:GLU:HA    | 1:B:854:HIS:HD2  | 1.82                     | 0.44              |
| 1:E:763:ILE:H     | 1:E:805:ASN:HD21 | 1.64                     | 0.44              |
| 1:E:796:ASP:OD1   | 1:E:798:SER:CB   | 2.66                     | 0.44              |
| 1:G:1056:ARG:HH21 | 1:K:913:ASN:HD22 | 1.65                     | 0.44              |
| 1:I:724:PHE:O     | 1:I:728:GLU:HG3  | 2.16                     | 0.44              |
| 1:J:872:LEU:HD13  | 1:J:873:HIS:CG   | 2.52                     | 0.44              |
| 1:L:981:SER:N     | 1:L:982:PRO:CD   | 2.79                     | 0.44              |
| 1:C:670:LEU:HD22  | 1:C:674:MET:SD   | 2.57                     | 0.44              |
| 1:C:707:THR:HG21  | 1:C:709:LEU:HG   | 1.98                     | 0.44              |
| 1:I:915:ASN:HD22  | 1:I:915:ASN:HA   | 1.65                     | 0.44              |
| 1:L:705:GLN:HG2   | 1:L:710:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:725:ARG:HG3   | 1:B:725:ARG:NH1  | 2.30                     | 0.44              |
| 1:B:1016:ALA:C    | 1:B:1018:GLU:H   | 2.25                     | 0.44              |
| 1:D:845:ASN:O     | 1:D:847:ARG:HG2  | 2.17                     | 0.44              |
| 1:E:939:ASN:ND2   | 1:E:943:LYS:HE3  | 2.33                     | 0.44              |
| 1:G:913:ASN:ND2   | 1:K:1056:ARG:NH2 | 2.60                     | 0.44              |
| 1:I:823:TYR:CE2   | 1:I:857:SER:HB3  | 2.52                     | 0.44              |
| 1:J:694:ARG:O     | 1:J:698:GLN:HG2  | 2.17                     | 0.44              |
| 1:J:973:ILE:HG21  | 1:J:978:ASP:HB2  | 1.99                     | 0.44              |
| 1:K:846:ASP:OD2   | 1:L:883:ARG:NH1  | 2.51                     | 0.44              |
| 1:L:930:GLN:O     | 1:L:933:ILE:HG13 | 2.17                     | 0.44              |
| 1:C:847:ARG:CZ    | 1:D:891:LEU:HD13 | 2.48                     | 0.44              |
| 1:D:694:ARG:O     | 1:D:698:GLN:HG2  | 2.17                     | 0.44              |
| 1:G:823:TYR:CE2   | 1:G:857:SER:HB3  | 2.53                     | 0.44              |
| 1:B:963:GLY:O     | 1:B:973:ILE:HD12 | 2.18                     | 0.44              |
| 1:D:981:SER:N     | 1:D:982:PRO:CD   | 2.79                     | 0.44              |
| 1:E:823:TYR:CE2   | 1:E:857:SER:HB3  | 2.52                     | 0.44              |
| 1:F:684:LEU:HD23  | 1:F:684:LEU:O    | 2.17                     | 0.44              |
| 1:G:762:GLN:HB3   | 1:G:765:ASN:CB   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:674:MET:C    | 1:H:676:ASN:N     | 2.76                     | 0.44              |
| 1:I:700:MET:HE3  | 1:I:746:LEU:HD21  | 2.00                     | 0.44              |
| 1:J:1003:TYR:HD2 | 1:J:1009:LEU:HG   | 1.81                     | 0.44              |
| 1:A:814:LEU:HD11 | 1:A:933:ILE:HB    | 2.00                     | 0.44              |
| 1:C:952:THR:O    | 1:C:956:VAL:HG22  | 2.18                     | 0.44              |
| 1:E:727:LEU:HD21 | 1:E:820:MET:HB3   | 2.00                     | 0.44              |
| 1:I:872:LEU:HD13 | 1:I:873:HIS:CD2   | 2.53                     | 0.44              |
| 1:I:957:ASN:O    | 1:I:961:GLU:HG3   | 2.18                     | 0.44              |
| 1:K:724:PHE:O    | 1:K:728:GLU:HG3   | 2.17                     | 0.44              |
| 1:L:721:MET:O    | 1:L:725:ARG:HG2   | 2.18                     | 0.44              |
| 1:L:905:PHE:CD1  | 1:L:931:VAL:HG21  | 2.52                     | 0.44              |
| 1:A:787:ILE:HG23 | 1:A:808:ALA:CB    | 2.48                     | 0.44              |
| 1:B:739:ARG:HH11 | 1:B:739:ARG:CG    | 2.23                     | 0.44              |
| 1:C:939:ASN:ND2  | 1:C:943:LYS:HE3   | 2.33                     | 0.44              |
| 1:D:674:MET:HE2  | 1:D:747:HIS:HD2   | 1.81                     | 0.44              |
| 1:D:684:LEU:HD23 | 1:D:684:LEU:O     | 2.18                     | 0.44              |
| 1:D:729:ASN:HA   | 1:D:739:ARG:HH22  | 1.82                     | 0.44              |
| 1:D:816:VAL:CG1  | 1:D:820:MET:HE3   | 2.48                     | 0.44              |
| 1:E:847:ARG:NH2  | 1:F:891:LEU:HD13  | 2.33                     | 0.44              |
| 1:H:751:TYR:CE2  | 1:H:755:ARG:HG3   | 2.52                     | 0.44              |
| 1:L:713:PHE:O    | 1:L:714:LYS:C     | 2.61                     | 0.44              |
| 1:A:670:LEU:HD22 | 1:A:674:MET:SD    | 2.58                     | 0.44              |
| 1:A:674:MET:CE   | 1:A:703:LEU:HD21  | 2.48                     | 0.44              |
| 1:D:670:LEU:O    | 1:D:674:MET:HG3   | 2.18                     | 0.44              |
| 1:D:976:PHE:CD2  | 1:D:987:LEU:HB2   | 2.53                     | 0.44              |
| 1:F:700:MET:CE   | 1:F:746:LEU:HD21  | 2.48                     | 0.44              |
| 1:F:803:SER:HA   | 1:F:811:LEU:HD11  | 1.99                     | 0.44              |
| 1:G:729:ASN:HA   | 1:G:739:ARG:HH21  | 1.82                     | 0.44              |
| 1:G:915:ASN:HD22 | 1:G:915:ASN:HA    | 1.65                     | 0.44              |
| 1:H:694:ARG:O    | 1:H:698:GLN:HG2   | 2.18                     | 0.44              |
| 1:H:721:MET:O    | 1:H:725:ARG:HG2   | 2.18                     | 0.44              |
| 1:H:974:SER:HB2  | 1:H:977:MET:SD    | 2.58                     | 0.44              |
| 1:H:1004:ASP:HA  | 1:H:1009:LEU:HD12 | 1.99                     | 0.44              |
| 1:I:872:LEU:HD13 | 1:I:873:HIS:CG    | 2.53                     | 0.44              |
| 1:J:845:ASN:O    | 1:J:847:ARG:HG2   | 2.17                     | 0.44              |
| 1:K:915:ASN:O    | 1:K:916:GLY:C     | 2.60                     | 0.44              |
| 1:F:805:ASN:HD22 | 1:F:805:ASN:N     | 2.16                     | 0.44              |
| 1:F:810:GLU:OE1  | 1:F:925:ARG:HD2   | 2.18                     | 0.44              |
| 1:F:930:GLN:O    | 1:F:933:ILE:HG13  | 2.18                     | 0.44              |
| 1:G:957:ASN:O    | 1:G:961:GLU:HG3   | 2.17                     | 0.44              |
| 1:H:825:HIS:CD2  | 1:H:826:PRO:HD2   | 2.53                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:796:ASP:OD1  | 1:J:798:SER:N     | 2.41                     | 0.44              |
| 1:J:964:ASP:OD2  | 1:J:979:ARG:NH1   | 2.51                     | 0.44              |
| 1:J:981:SER:N    | 1:J:982:PRO:CD    | 2.79                     | 0.44              |
| 1:K:764:HIS:O    | 1:K:804:SER:O     | 2.36                     | 0.44              |
| 1:L:681:ILE:H    | 1:L:681:ILE:HG13  | 1.45                     | 0.44              |
| 1:A:982:PRO:C    | 1:A:983:GLN:HG2   | 2.43                     | 0.43              |
| 1:E:713:PHE:O    | 1:E:714:LYS:C     | 2.61                     | 0.43              |
| 1:E:872:LEU:HD13 | 1:E:873:HIS:CG    | 2.53                     | 0.43              |
| 1:E:891:LEU:HD12 | 1:F:847:ARG:CZ    | 2.48                     | 0.43              |
| 1:F:872:LEU:HD13 | 1:F:873:HIS:CG    | 2.53                     | 0.43              |
| 1:F:973:ILE:HG21 | 1:F:978:ASP:HB2   | 1.98                     | 0.43              |
| 1:G:713:PHE:HD2  | 1:G:874:LEU:HD21  | 1.82                     | 0.43              |
| 1:G:724:PHE:O    | 1:G:728:GLU:HG3   | 2.17                     | 0.43              |
| 1:I:707:THR:HG21 | 1:I:709:LEU:HG    | 1.99                     | 0.43              |
| 1:J:713:PHE:O    | 1:J:714:LYS:C     | 2.61                     | 0.43              |
| 1:L:872:LEU:HD13 | 1:L:873:HIS:CG    | 2.53                     | 0.43              |
| 1:L:956:VAL:HG23 | 1:L:957:ASN:N     | 2.33                     | 0.43              |
| 1:A:847:ARG:NH2  | 1:B:891:LEU:HD13  | 2.32                     | 0.43              |
| 1:B:816:VAL:CG1  | 1:B:820:MET:HE3   | 2.47                     | 0.43              |
| 1:D:985:ALA:HA   | 1:D:1072:TRP:HE3  | 1.82                     | 0.43              |
| 1:G:765:ASN:HA   | 1:G:804:SER:HB3   | 2.00                     | 0.43              |
| 1:I:754:THR:CG2  | 1:I:755:ARG:HE    | 2.21                     | 0.43              |
| 1:J:991:PHE:CE2  | 1:J:996:VAL:HG23  | 2.54                     | 0.43              |
| 1:K:939:ASN:ND2  | 1:K:943:LYS:HE3   | 2.33                     | 0.43              |
| 1:K:1004:ASP:CB  | 1:K:1009:LEU:HD12 | 2.48                     | 0.43              |
| 1:L:670:LEU:HD22 | 1:L:674:MET:SD    | 2.58                     | 0.43              |
| 1:L:700:MET:HE3  | 1:L:746:LEU:CD1   | 2.48                     | 0.43              |
| 1:A:914:SER:OG   | 1:A:915:ASN:N     | 2.51                     | 0.43              |
| 1:B:881:ARG:HG3  | 1:B:881:ARG:NH1   | 2.33                     | 0.43              |
| 1:C:982:PRO:C    | 1:C:983:GLN:HG2   | 2.43                     | 0.43              |
| 1:D:725:ARG:HG3  | 1:D:725:ARG:NH1   | 2.32                     | 0.43              |
| 1:E:917:ILE:O    | 1:E:924:ASP:OD2   | 2.36                     | 0.43              |
| 1:F:1061:LEU:C   | 1:F:1061:LEU:HD12 | 2.43                     | 0.43              |
| 1:G:939:ASN:O    | 1:G:940:GLY:C     | 2.62                     | 0.43              |
| 1:H:810:GLU:OE1  | 1:H:925:ARG:HD2   | 2.18                     | 0.43              |
| 1:I:982:PRO:C    | 1:I:983:GLN:HG2   | 2.43                     | 0.43              |
| 1:J:670:LEU:HD22 | 1:J:674:MET:SD    | 2.58                     | 0.43              |
| 1:J:729:ASN:HA   | 1:J:739:ARG:HH22  | 1.83                     | 0.43              |
| 1:L:885:LEU:HD12 | 1:L:885:LEU:HA    | 1.78                     | 0.43              |
| 1:B:694:ARG:HA   | 1:B:728:GLU:OE2   | 2.18                     | 0.43              |
| 1:H:930:GLN:O    | 1:H:933:ILE:HG13  | 2.17                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:674:MET:HE1  | 1:J:699:VAL:CG1   | 2.45                     | 0.43              |
| 1:J:851:GLU:HA   | 1:J:854:HIS:HD2   | 1.83                     | 0.43              |
| 1:K:952:THR:HG23 | 1:K:988:GLN:NE2   | 2.34                     | 0.43              |
| 1:L:963:GLY:O    | 1:L:973:ILE:HD12  | 2.18                     | 0.43              |
| 1:C:677:TRP:NE1  | 1:C:943:LYS:HD3   | 2.34                     | 0.43              |
| 1:C:842:VAL:HA   | 1:D:883:ARG:HH22  | 1.83                     | 0.43              |
| 1:C:891:LEU:HD12 | 1:D:847:ARG:CZ    | 2.49                     | 0.43              |
| 1:D:881:ARG:HG3  | 1:D:881:ARG:NH1   | 2.34                     | 0.43              |
| 1:D:1004:ASP:HA  | 1:D:1009:LEU:HD12 | 2.00                     | 0.43              |
| 1:E:1013:TRP:CE3 | 1:E:1057:ILE:HG22 | 2.53                     | 0.43              |
| 1:F:985:ALA:HA   | 1:F:1072:TRP:HE3  | 1.84                     | 0.43              |
| 1:H:872:LEU:HD13 | 1:H:873:HIS:CD2   | 2.53                     | 0.43              |
| 1:L:974:SER:HB2  | 1:L:977:MET:SD    | 2.58                     | 0.43              |
| 1:B:956:VAL:HG23 | 1:B:957:ASN:N     | 2.34                     | 0.43              |
| 1:F:694:ARG:O    | 1:F:698:GLN:HG2   | 2.17                     | 0.43              |
| 1:F:694:ARG:HA   | 1:F:728:GLU:OE2   | 2.18                     | 0.43              |
| 1:G:964:ASP:OD2  | 1:G:979:ARG:NH1   | 2.52                     | 0.43              |
| 1:I:713:PHE:O    | 1:I:714:LYS:C     | 2.62                     | 0.43              |
| 1:K:982:PRO:C    | 1:K:983:GLN:HG2   | 2.43                     | 0.43              |
| 1:B:670:LEU:HD22 | 1:B:674:MET:SD    | 2.58                     | 0.43              |
| 1:C:823:TYR:CE2  | 1:C:857:SER:HB3   | 2.53                     | 0.43              |
| 1:C:853:HIS:O    | 1:C:857:SER:HB2   | 2.19                     | 0.43              |
| 1:D:754:THR:HG22 | 1:D:755:ARG:NE    | 2.31                     | 0.43              |
| 1:E:677:TRP:NE1  | 1:E:943:LYS:HD3   | 2.33                     | 0.43              |
| 1:E:724:PHE:O    | 1:E:728:GLU:HG3   | 2.18                     | 0.43              |
| 1:G:758:PRO:HD3  | 1:G:1011:GLY:H    | 1.83                     | 0.43              |
| 1:G:952:THR:HG23 | 1:G:988:GLN:NE2   | 2.34                     | 0.43              |
| 1:H:956:VAL:HG23 | 1:H:957:ASN:N     | 2.34                     | 0.43              |
| 1:I:787:ILE:HG23 | 1:I:808:ALA:CB    | 2.48                     | 0.43              |
| 1:I:803:SER:HA   | 1:I:811:LEU:HD11  | 2.00                     | 0.43              |
| 1:K:803:SER:HA   | 1:K:811:LEU:HD11  | 2.01                     | 0.43              |
| 1:L:684:LEU:HD23 | 1:L:684:LEU:O     | 2.19                     | 0.43              |
| 1:L:758:PRO:HG3  | 1:L:799:TYR:HE2   | 1.84                     | 0.43              |
| 1:A:700:MET:HE3  | 1:A:746:LEU:HD21  | 2.01                     | 0.43              |
| 1:D:805:ASN:HD22 | 1:D:805:ASN:N     | 2.16                     | 0.43              |
| 1:D:956:VAL:HG23 | 1:D:957:ASN:N     | 2.33                     | 0.43              |
| 1:F:681:ILE:H    | 1:F:681:ILE:HG13  | 1.45                     | 0.43              |
| 1:F:721:MET:O    | 1:F:725:ARG:HG2   | 2.18                     | 0.43              |
| 1:G:677:TRP:NE1  | 1:G:943:LYS:HD3   | 2.34                     | 0.43              |
| 1:H:684:LEU:HD23 | 1:H:684:LEU:O     | 2.19                     | 0.43              |
| 1:H:723:TYR:CE1  | 1:H:861:LEU:HD13  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:914:SER:OG   | 1:I:915:ASN:N     | 2.51                     | 0.43              |
| 1:K:847:ARG:NH2  | 1:L:891:LEU:HD13  | 2.33                     | 0.43              |
| 1:A:803:SER:HA   | 1:A:811:LEU:HD11  | 2.01                     | 0.43              |
| 1:A:823:TYR:CE2  | 1:A:857:SER:HB3   | 2.54                     | 0.43              |
| 1:B:684:LEU:CD2  | 1:B:688:MET:HG3   | 2.48                     | 0.43              |
| 1:B:755:ARG:HD2  | 4:B:1131:HOH:O    | 2.18                     | 0.43              |
| 1:B:973:ILE:HG21 | 1:B:978:ASP:HB2   | 2.01                     | 0.43              |
| 1:C:724:PHE:O    | 1:C:728:GLU:HG3   | 2.19                     | 0.43              |
| 1:C:758:PRO:HD3  | 1:C:1011:GLY:H    | 1.83                     | 0.43              |
| 1:H:963:GLY:O    | 1:H:973:ILE:HD12  | 2.19                     | 0.43              |
| 1:K:748:ALA:HB3  | 1:K:936:ALA:HB1   | 2.01                     | 0.43              |
| 1:K:1003:TYR:HD2 | 1:K:1009:LEU:HG   | 1.84                     | 0.43              |
| 1:A:945:ARG:NH1  | 1:D:915:ASN:ND2   | 2.65                     | 0.43              |
| 1:A:964:ASP:OD2  | 1:A:979:ARG:NH1   | 2.52                     | 0.43              |
| 1:D:705:GLN:HG2  | 1:D:710:LEU:HD12  | 2.00                     | 0.43              |
| 1:D:872:LEU:HD13 | 1:D:873:HIS:CD2   | 2.54                     | 0.43              |
| 1:F:716:PRO:HB2  | 1:F:719:GLN:HE22  | 1.84                     | 0.43              |
| 1:H:705:GLN:HG2  | 1:H:710:LEU:HD12  | 2.00                     | 0.43              |
| 1:H:905:PHE:CD1  | 1:H:931:VAL:HG21  | 2.54                     | 0.43              |
| 1:I:796:ASP:OD1  | 1:I:798:SER:CB    | 2.67                     | 0.43              |
| 1:J:716:PRO:HB2  | 1:J:719:GLN:HE22  | 1.83                     | 0.43              |
| 1:K:957:ASN:O    | 1:K:961:GLU:HG3   | 2.19                     | 0.43              |
| 1:L:845:ASN:O    | 1:L:847:ARG:HG2   | 2.19                     | 0.43              |
| 1:A:713:PHE:O    | 1:A:714:LYS:C     | 2.62                     | 0.42              |
| 1:A:794:ASN:HB3  | 1:A:799:TYR:HB2   | 2.00                     | 0.42              |
| 1:D:894:ASP:OD1  | 1:D:894:ASP:C     | 2.62                     | 0.42              |
| 1:E:707:THR:HG21 | 1:E:709:LEU:HG    | 2.00                     | 0.42              |
| 1:E:758:PRO:HD3  | 1:E:1011:GLY:H    | 1.84                     | 0.42              |
| 1:E:964:ASP:OD2  | 1:E:979:ARG:NH1   | 2.52                     | 0.42              |
| 1:F:705:GLN:HG2  | 1:F:710:LEU:HD12  | 2.02                     | 0.42              |
| 1:A:758:PRO:HD3  | 1:A:1011:GLY:H    | 1.84                     | 0.42              |
| 1:B:674:MET:C    | 1:B:676:ASN:N     | 2.75                     | 0.42              |
| 1:E:710:LEU:HD23 | 1:E:710:LEU:HA    | 1.87                     | 0.42              |
| 1:F:845:ASN:O    | 1:F:847:ARG:HG2   | 2.19                     | 0.42              |
| 1:G:803:SER:HA   | 1:G:811:LEU:HD11  | 2.01                     | 0.42              |
| 1:H:881:ARG:HG3  | 1:H:881:ARG:NH1   | 2.33                     | 0.42              |
| 1:I:727:LEU:HD21 | 1:I:820:MET:HB3   | 2.02                     | 0.42              |
| 1:J:705:GLN:HG2  | 1:J:710:LEU:HD12  | 2.00                     | 0.42              |
| 1:J:758:PRO:HG3  | 1:J:799:TYR:HE2   | 1.84                     | 0.42              |
| 1:K:737:HIS:CD2  | 1:K:958:GLU:OE2   | 2.59                     | 0.42              |
| 1:B:1004:ASP:HA  | 1:B:1009:LEU:HD12 | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:957:ASN:O     | 1:C:961:GLU:HG3   | 2.20                     | 0.42              |
| 1:D:851:GLU:HA    | 1:D:854:HIS:HD2   | 1.83                     | 0.42              |
| 1:D:952:THR:O     | 1:D:956:VAL:HG22  | 2.19                     | 0.42              |
| 1:F:754:THR:HG22  | 1:F:755:ARG:NE    | 2.34                     | 0.42              |
| 1:F:780:ASN:C     | 1:F:782:GLY:H     | 2.27                     | 0.42              |
| 1:I:677:TRP:NE1   | 1:I:943:LYS:HD3   | 2.34                     | 0.42              |
| 1:I:917:ILE:O     | 1:I:924:ASP:OD2   | 2.38                     | 0.42              |
| 1:J:674:MET:C     | 1:J:676:ASN:N     | 2.75                     | 0.42              |
| 1:J:684:LEU:CD2   | 1:J:688:MET:HG3   | 2.49                     | 0.42              |
| 1:B:721:MET:O     | 1:B:725:ARG:HG2   | 2.20                     | 0.42              |
| 1:B:796:ASP:OD1   | 1:B:798:SER:N     | 2.41                     | 0.42              |
| 1:C:796:ASP:OD1   | 1:C:798:SER:CB    | 2.68                     | 0.42              |
| 1:F:764:HIS:O     | 1:F:766:GLY:N     | 2.52                     | 0.42              |
| 1:F:952:THR:O     | 1:F:956:VAL:HG22  | 2.19                     | 0.42              |
| 1:G:1014:LEU:N    | 1:G:1056:ARG:O    | 2.53                     | 0.42              |
| 1:H:694:ARG:HA    | 1:H:728:GLU:OE2   | 2.19                     | 0.42              |
| 1:H:721:MET:O     | 1:H:722:ASN:C     | 2.61                     | 0.42              |
| 1:I:684:LEU:HD23  | 1:I:684:LEU:O     | 2.20                     | 0.42              |
| 1:J:663:LEU:HA    | 1:J:666:GLU:OE1   | 2.19                     | 0.42              |
| 1:J:703:LEU:HD22  | 1:J:750:TRP:CE2   | 2.54                     | 0.42              |
| 1:J:985:ALA:HA    | 1:J:1072:TRP:HE3  | 1.84                     | 0.42              |
| 1:K:663:LEU:C     | 1:K:663:LEU:HD23  | 2.44                     | 0.42              |
| 1:L:681:ILE:O     | 1:L:685:VAL:HG23  | 2.19                     | 0.42              |
| 1:E:663:LEU:C     | 1:E:663:LEU:HD23  | 2.45                     | 0.42              |
| 1:F:674:MET:HE1   | 1:F:699:VAL:CG1   | 2.46                     | 0.42              |
| 1:F:1014:LEU:HD13 | 1:F:1056:ARG:HH21 | 1.84                     | 0.42              |
| 1:J:700:MET:CE    | 1:J:746:LEU:HD21  | 2.50                     | 0.42              |
| 1:J:721:MET:O     | 1:J:725:ARG:HG2   | 2.19                     | 0.42              |
| 1:J:956:VAL:HG23  | 1:J:957:ASN:N     | 2.34                     | 0.42              |
| 1:L:1069:HIS:CE1  | 1:L:1073:LYS:HZ2  | 2.35                     | 0.42              |
| 1:A:871:LEU:HB3   | 1:A:874:LEU:HD12  | 2.01                     | 0.42              |
| 1:B:1061:LEU:HD12 | 1:B:1061:LEU:C    | 2.45                     | 0.42              |
| 1:D:758:PRO:HG3   | 1:D:799:TYR:HE2   | 1.84                     | 0.42              |
| 1:E:982:PRO:C     | 1:E:983:GLN:HG2   | 2.44                     | 0.42              |
| 1:F:816:VAL:CG1   | 1:F:820:MET:HE3   | 2.50                     | 0.42              |
| 1:H:915:ASN:ND2   | 1:K:945:ARG:HH11  | 2.18                     | 0.42              |
| 1:J:694:ARG:HA    | 1:J:728:GLU:OE2   | 2.19                     | 0.42              |
| 1:J:952:THR:O     | 1:J:956:VAL:HG22  | 2.20                     | 0.42              |
| 1:L:663:LEU:HA    | 1:L:666:GLU:OE1   | 2.20                     | 0.42              |
| 1:L:703:LEU:HD22  | 1:L:750:TRP:CE2   | 2.54                     | 0.42              |
| 1:L:755:ARG:HD2   | 4:L:1631:HOH:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:851:GLU:HA   | 1:L:854:HIS:HD2  | 1.85                     | 0.42              |
| 1:A:842:VAL:HA   | 1:B:883:ARG:HH22 | 1.84                     | 0.42              |
| 1:B:663:LEU:HA   | 1:B:666:GLU:OE1  | 2.19                     | 0.42              |
| 1:B:905:PHE:CD1  | 1:B:931:VAL:HG21 | 2.54                     | 0.42              |
| 1:C:803:SER:HA   | 1:C:811:LEU:HD11 | 2.02                     | 0.42              |
| 1:C:814:LEU:HD11 | 1:C:933:ILE:HB   | 2.02                     | 0.42              |
| 1:E:969:LEU:HD23 | 1:H:873:HIS:CD2  | 2.54                     | 0.42              |
| 1:F:725:ARG:HG3  | 1:F:725:ARG:NH1  | 2.33                     | 0.42              |
| 1:G:737:HIS:CD2  | 1:G:958:GLU:OE2  | 2.60                     | 0.42              |
| 1:G:814:LEU:HD11 | 1:G:933:ILE:HB   | 2.01                     | 0.42              |
| 1:G:862:TYR:OH   | 1:G:869:ASN:ND2  | 2.52                     | 0.42              |
| 1:H:710:LEU:HD23 | 1:H:715:ILE:HB   | 2.02                     | 0.42              |
| 1:H:938:ILE:HD12 | 1:H:996:VAL:HG22 | 2.01                     | 0.42              |
| 1:H:973:ILE:HG21 | 1:H:978:ASP:HB2  | 2.00                     | 0.42              |
| 1:I:991:PHE:CD1  | 1:I:995:ILE:HD12 | 2.54                     | 0.42              |
| 1:L:716:PRO:HB2  | 1:L:719:GLN:HE22 | 1.85                     | 0.42              |
| 1:A:872:LEU:HD12 | 1:A:873:HIS:H    | 1.85                     | 0.42              |
| 1:C:663:LEU:C    | 1:C:663:LEU:HD23 | 2.45                     | 0.42              |
| 1:D:674:MET:C    | 1:D:676:ASN:N    | 2.75                     | 0.42              |
| 1:D:710:LEU:HD23 | 1:D:715:ILE:HB   | 2.02                     | 0.42              |
| 1:D:880:LYS:HD2  | 1:D:880:LYS:HA   | 1.88                     | 0.42              |
| 1:D:980:SER:O    | 1:D:981:SER:HB2  | 2.19                     | 0.42              |
| 1:G:962:GLN:O    | 1:G:966:GLU:HG3  | 2.20                     | 0.42              |
| 1:I:969:LEU:HD23 | 1:L:873:HIS:HD2  | 1.82                     | 0.42              |
| 1:J:723:TYR:CE1  | 1:J:861:LEU:HD13 | 2.55                     | 0.42              |
| 1:L:1059:CYS:HB3 | 1:L:1062:MET:CB  | 2.49                     | 0.42              |
| 1:D:663:LEU:HA   | 1:D:666:GLU:OE1  | 2.20                     | 0.42              |
| 1:D:713:PHE:O    | 1:D:714:LYS:C    | 2.62                     | 0.42              |
| 1:H:695:ILE:HG22 | 1:H:743:THR:HG21 | 2.01                     | 0.42              |
| 1:J:930:GLN:O    | 1:J:933:ILE:HG13 | 2.20                     | 0.42              |
| 1:J:1015:GLU:CD  | 1:J:1019:ASP:HB2 | 2.45                     | 0.42              |
| 1:K:713:PHE:O    | 1:K:714:LYS:C    | 2.62                     | 0.42              |
| 1:K:872:LEU:HD12 | 1:K:873:HIS:H    | 1.85                     | 0.42              |
| 1:L:881:ARG:HG3  | 1:L:881:ARG:NH1  | 2.34                     | 0.42              |
| 1:B:758:PRO:HG3  | 1:B:799:TYR:HE2  | 1.85                     | 0.42              |
| 1:B:763:ILE:O    | 1:B:764:HIS:CB   | 2.67                     | 0.42              |
| 1:D:721:MET:O    | 1:D:722:ASN:C    | 2.63                     | 0.42              |
| 1:E:872:LEU:HD13 | 1:E:873:HIS:CD2  | 2.54                     | 0.42              |
| 1:E:914:SER:OG   | 1:E:915:ASN:N    | 2.52                     | 0.42              |
| 1:E:944:VAL:HG22 | 1:E:945:ARG:N    | 2.35                     | 0.42              |
| 1:F:974:SER:HB2  | 1:F:977:MET:SD   | 2.59                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:784:ILE:HG21 | 1:G:807:PRO:HB3   | 2.00                     | 0.42              |
| 1:I:663:LEU:HD23 | 1:I:663:LEU:C     | 2.45                     | 0.42              |
| 1:J:1004:ASP:HA  | 1:J:1009:LEU:HD12 | 2.01                     | 0.42              |
| 1:K:872:LEU:HD13 | 1:K:873:HIS:CG    | 2.54                     | 0.42              |
| 1:K:1004:ASP:HB2 | 1:K:1009:LEU:HD12 | 2.02                     | 0.42              |
| 1:L:1003:TYR:HD2 | 1:L:1009:LEU:HG   | 1.83                     | 0.42              |
| 1:A:952:THR:O    | 1:A:956:VAL:HG22  | 2.20                     | 0.41              |
| 1:B:952:THR:O    | 1:B:956:VAL:HG22  | 2.20                     | 0.41              |
| 1:C:694:ARG:O    | 1:C:698:GLN:HG2   | 2.20                     | 0.41              |
| 1:C:727:LEU:HD21 | 1:C:820:MET:HB3   | 2.02                     | 0.41              |
| 1:C:915:ASN:HD22 | 1:C:915:ASN:HA    | 1.63                     | 0.41              |
| 1:C:976:PHE:CG   | 1:C:987:LEU:HD13  | 2.55                     | 0.41              |
| 1:D:974:SER:HB2  | 1:D:977:MET:SD    | 2.60                     | 0.41              |
| 1:G:707:THR:HG21 | 1:G:709:LEU:HG    | 2.01                     | 0.41              |
| 1:J:963:GLY:O    | 1:J:973:ILE:HD12  | 2.19                     | 0.41              |
| 1:K:796:ASP:OD1  | 1:K:798:SER:CB    | 2.68                     | 0.41              |
| 1:L:754:THR:HG22 | 1:L:755:ARG:NE    | 2.35                     | 0.41              |
| 1:A:846:ASP:OD2  | 1:B:883:ARG:NH1   | 2.53                     | 0.41              |
| 1:C:825:HIS:CD2  | 1:C:826:PRO:HD2   | 2.55                     | 0.41              |
| 1:D:963:GLY:O    | 1:D:973:ILE:HD12  | 2.20                     | 0.41              |
| 1:D:991:PHE:CE2  | 1:D:996:VAL:HG23  | 2.54                     | 0.41              |
| 1:E:670:LEU:HD22 | 1:E:674:MET:SD    | 2.60                     | 0.41              |
| 1:F:894:ASP:C    | 1:F:894:ASP:OD1   | 2.64                     | 0.41              |
| 1:I:1068:ASN:O   | 1:I:1071:ILE:HG12 | 2.20                     | 0.41              |
| 1:J:710:LEU:HD23 | 1:J:715:ILE:HB    | 2.03                     | 0.41              |
| 1:L:1004:ASP:HA  | 1:L:1009:LEU:HD12 | 2.01                     | 0.41              |
| 1:A:891:LEU:HD13 | 1:B:847:ARG:NH2   | 2.35                     | 0.41              |
| 1:B:751:TYR:CE1  | 1:B:755:ARG:HG3   | 2.55                     | 0.41              |
| 1:D:905:PHE:CD1  | 1:D:931:VAL:HG21  | 2.55                     | 0.41              |
| 1:F:703:LEU:HD22 | 1:F:750:TRP:CE2   | 2.55                     | 0.41              |
| 1:F:963:GLY:O    | 1:F:973:ILE:HD12  | 2.20                     | 0.41              |
| 1:G:700:MET:HE3  | 1:G:746:LEU:HD21  | 2.02                     | 0.41              |
| 1:G:913:ASN:CG   | 1:K:1056:ARG:HE   | 2.28                     | 0.41              |
| 1:G:952:THR:O    | 1:G:956:VAL:HG22  | 2.20                     | 0.41              |
| 1:H:670:LEU:HD22 | 1:H:674:MET:SD    | 2.60                     | 0.41              |
| 1:H:755:ARG:HA   | 1:H:756:PRO:HD3   | 1.91                     | 0.41              |
| 1:L:694:ARG:HA   | 1:L:728:GLU:OE2   | 2.20                     | 0.41              |
| 1:C:674:MET:CE   | 1:C:703:LEU:HD21  | 2.50                     | 0.41              |
| 1:D:1059:CYS:HB3 | 1:D:1062:MET:CB   | 2.51                     | 0.41              |
| 1:H:663:LEU:HA   | 1:H:666:GLU:OE1   | 2.19                     | 0.41              |
| 1:H:703:LEU:HD22 | 1:H:750:TRP:CE2   | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:1068:ASN:O    | 1:K:1071:ILE:HG12 | 2.20                     | 0.41              |
| 1:L:674:MET:HE2   | 1:L:747:HIS:HD2   | 1.86                     | 0.41              |
| 1:L:751:TYR:CE2   | 1:L:755:ARG:HG3   | 2.55                     | 0.41              |
| 1:A:717:THR:OG1   | 1:J:1019:ASP:HA   | 2.20                     | 0.41              |
| 1:A:796:ASP:OD1   | 1:A:798:SER:CB    | 2.69                     | 0.41              |
| 1:B:751:TYR:CE2   | 1:B:755:ARG:HG3   | 2.55                     | 0.41              |
| 1:B:812:MET:O     | 1:B:816:VAL:HG23  | 2.20                     | 0.41              |
| 1:C:1003:TYR:HD2  | 1:C:1009:LEU:HG   | 1.85                     | 0.41              |
| 1:E:736:TYR:CD1   | 1:E:955:ILE:HG13  | 2.55                     | 0.41              |
| 1:F:674:MET:C     | 1:F:676:ASN:N     | 2.76                     | 0.41              |
| 1:F:721:MET:O     | 1:F:722:ASN:C     | 2.64                     | 0.41              |
| 1:G:853:HIS:O     | 1:G:857:SER:HB2   | 2.21                     | 0.41              |
| 1:H:674:MET:HE1   | 1:H:699:VAL:CG1   | 2.47                     | 0.41              |
| 1:H:796:ASP:OD1   | 1:H:798:SER:N     | 2.41                     | 0.41              |
| 1:I:710:LEU:HD23  | 1:I:710:LEU:HA    | 1.87                     | 0.41              |
| 1:J:1061:LEU:C    | 1:J:1061:LEU:HD12 | 2.46                     | 0.41              |
| 1:L:723:TYR:CE1   | 1:L:861:LEU:HD13  | 2.56                     | 0.41              |
| 1:L:1020:ASN:CG   | 1:L:1021:ASP:N    | 2.78                     | 0.41              |
| 1:A:902:LEU:HD12  | 1:A:902:LEU:HA    | 1.93                     | 0.41              |
| 1:B:723:TYR:CE1   | 1:B:861:LEU:HD13  | 2.56                     | 0.41              |
| 1:B:930:GLN:O     | 1:B:933:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:938:ILE:HD12  | 1:B:996:VAL:HG22  | 2.02                     | 0.41              |
| 1:E:872:LEU:HD12  | 1:E:873:HIS:H     | 1.83                     | 0.41              |
| 1:F:713:PHE:O     | 1:F:714:LYS:C     | 2.63                     | 0.41              |
| 1:F:881:ARG:HG3   | 1:F:881:ARG:NH1   | 2.35                     | 0.41              |
| 1:F:1003:TYR:HD2  | 1:F:1009:LEU:HG   | 1.82                     | 0.41              |
| 1:G:674:MET:HE1   | 1:G:703:LEU:HD21  | 2.03                     | 0.41              |
| 1:G:681:ILE:HG23  | 1:G:682:PHE:N     | 2.35                     | 0.41              |
| 1:G:1071:ILE:HG21 | 1:L:915:ASN:ND2   | 2.36                     | 0.41              |
| 1:H:980:SER:O     | 1:H:981:SER:HB2   | 2.19                     | 0.41              |
| 1:I:814:LEU:HD11  | 1:I:933:ILE:HB    | 2.02                     | 0.41              |
| 1:L:880:LYS:HD2   | 1:L:880:LYS:HA    | 1.87                     | 0.41              |
| 1:A:844:TYR:CE2   | 1:A:852:ASN:HB3   | 2.55                     | 0.41              |
| 1:D:721:MET:O     | 1:D:725:ARG:HG2   | 2.19                     | 0.41              |
| 1:E:953:GLU:O     | 1:E:957:ASN:ND2   | 2.54                     | 0.41              |
| 1:F:663:LEU:HA    | 1:F:666:GLU:OE1   | 2.21                     | 0.41              |
| 1:H:751:TYR:CE1   | 1:H:755:ARG:HG3   | 2.55                     | 0.41              |
| 1:I:674:MET:CE    | 1:I:703:LEU:HD21  | 2.50                     | 0.41              |
| 1:I:784:ILE:HG21  | 1:I:807:PRO:HB3   | 2.02                     | 0.41              |
| 1:K:762:GLN:NE2   | 1:K:804:SER:CB    | 2.78                     | 0.41              |
| 1:C:762:GLN:HA    | 1:C:805:ASN:HD21  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:917:ILE:O     | 1:C:924:ASP:OD2   | 2.38                     | 0.41              |
| 1:D:716:PRO:HB2   | 1:D:719:GLN:NE2   | 2.35                     | 0.41              |
| 1:F:670:LEU:O     | 1:F:674:MET:HG3   | 2.20                     | 0.41              |
| 1:G:944:VAL:HG22  | 1:G:945:ARG:N     | 2.36                     | 0.41              |
| 1:I:939:ASN:ND2   | 1:I:943:LYS:HE3   | 2.36                     | 0.41              |
| 1:I:952:THR:HG23  | 1:I:988:GLN:NE2   | 2.35                     | 0.41              |
| 1:I:1003:TYR:HD2  | 1:I:1009:LEU:HG   | 1.86                     | 0.41              |
| 1:J:754:THR:HG22  | 1:J:755:ARG:NE    | 2.34                     | 0.41              |
| 1:A:748:ALA:HB3   | 1:A:936:ALA:HB1   | 2.03                     | 0.41              |
| 1:B:681:ILE:H     | 1:B:681:ILE:HG13  | 1.46                     | 0.41              |
| 1:B:754:THR:HG22  | 1:B:755:ARG:NE    | 2.35                     | 0.41              |
| 1:B:885:LEU:HD12  | 1:B:885:LEU:HA    | 1.79                     | 0.41              |
| 1:B:980:SER:O     | 1:B:981:SER:HB2   | 2.20                     | 0.41              |
| 1:C:976:PHE:CD2   | 1:C:987:LEU:HB2   | 2.56                     | 0.41              |
| 1:C:979:ARG:O     | 1:C:982:PRO:HD3   | 2.21                     | 0.41              |
| 1:D:1014:LEU:HD21 | 1:D:1058:PHE:HB2  | 2.03                     | 0.41              |
| 1:D:1015:GLU:H    | 1:D:1015:GLU:HG3  | 1.76                     | 0.41              |
| 1:E:694:ARG:O     | 1:E:698:GLN:HG2   | 2.21                     | 0.41              |
| 1:E:715:ILE:HA    | 1:E:716:PRO:HD2   | 1.96                     | 0.41              |
| 1:E:803:SER:HA    | 1:E:811:LEU:HD11  | 2.02                     | 0.41              |
| 1:E:976:PHE:CG    | 1:E:987:LEU:HD13  | 2.56                     | 0.41              |
| 1:F:685:VAL:HG22  | 1:F:695:ILE:HD11  | 2.03                     | 0.41              |
| 1:F:1004:ASP:HA   | 1:F:1009:LEU:HD12 | 2.02                     | 0.41              |
| 1:G:871:LEU:HB3   | 1:G:874:LEU:HD12  | 2.02                     | 0.41              |
| 1:G:872:LEU:HD13  | 1:G:873:HIS:CG    | 2.56                     | 0.41              |
| 1:H:758:PRO:HG3   | 1:H:799:TYR:HE2   | 1.85                     | 0.41              |
| 1:I:872:LEU:HD12  | 1:I:873:HIS:H     | 1.85                     | 0.41              |
| 1:I:991:PHE:CE2   | 1:I:996:VAL:HG23  | 2.56                     | 0.41              |
| 1:J:881:ARG:HG3   | 1:J:881:ARG:NH1   | 2.35                     | 0.41              |
| 1:K:917:ILE:O     | 1:K:924:ASP:OD2   | 2.38                     | 0.41              |
| 1:L:967:ALA:HB2   | 1:L:973:ILE:HD11  | 2.03                     | 0.41              |
| 1:B:828:ARG:NH2   | 4:B:1129:HOH:O    | 2.54                     | 0.41              |
| 1:B:881:ARG:HG2   | 1:B:885:LEU:HD22  | 2.02                     | 0.41              |
| 1:C:795:PRO:HD2   | 1:C:799:TYR:CD1   | 2.56                     | 0.41              |
| 1:C:952:THR:HG23  | 1:C:988:GLN:NE2   | 2.36                     | 0.41              |
| 1:E:871:LEU:HB3   | 1:E:874:LEU:HD12  | 2.03                     | 0.41              |
| 1:J:900:ASP:OD1   | 1:J:900:ASP:N     | 2.54                     | 0.41              |
| 1:K:704:PHE:HB3   | 1:K:710:LEU:HG    | 2.03                     | 0.41              |
| 1:K:953:GLU:O     | 1:K:957:ASN:ND2   | 2.54                     | 0.41              |
| 1:L:710:LEU:HD23  | 1:L:715:ILE:HB    | 2.03                     | 0.41              |
| 1:A:913:ASN:HA    | 1:C:1056:ARG:HE   | 1.85                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:825:HIS:CD2   | 1:B:826:PRO:HD2   | 2.56                     | 0.40              |
| 1:C:872:LEU:HD13  | 1:C:873:HIS:CD2   | 2.57                     | 0.40              |
| 1:C:872:LEU:HD13  | 1:C:873:HIS:CG    | 2.56                     | 0.40              |
| 1:D:1003:TYR:HD2  | 1:D:1009:LEU:HG   | 1.85                     | 0.40              |
| 1:E:814:LEU:HD11  | 1:E:933:ILE:HB    | 2.02                     | 0.40              |
| 1:F:881:ARG:HG2   | 1:F:885:LEU:HD22  | 2.03                     | 0.40              |
| 1:G:914:SER:OG    | 1:G:915:ASN:N     | 2.49                     | 0.40              |
| 1:J:805:ASN:HD22  | 1:J:805:ASN:N     | 2.19                     | 0.40              |
| 1:J:885:LEU:HD12  | 1:J:885:LEU:HA    | 1.81                     | 0.40              |
| 1:J:905:PHE:CD1   | 1:J:931:VAL:HG21  | 2.56                     | 0.40              |
| 1:J:1015:GLU:OE1  | 1:J:1019:ASP:HB2  | 2.20                     | 0.40              |
| 1:K:988:GLN:OE1   | 1:K:988:GLN:HA    | 2.21                     | 0.40              |
| 1:A:711:GLU:OE2   | 1:J:1013:TRP:HB2  | 2.21                     | 0.40              |
| 1:A:962:GLN:O     | 1:A:966:GLU:HG3   | 2.22                     | 0.40              |
| 1:B:979:ARG:C     | 1:B:981:SER:H     | 2.30                     | 0.40              |
| 1:C:700:MET:HE3   | 1:C:746:LEU:HD21  | 2.03                     | 0.40              |
| 1:C:1015:GLU:HB3  | 1:C:1016:ALA:H    | 1.77                     | 0.40              |
| 1:D:694:ARG:HA    | 1:D:728:GLU:OE2   | 2.21                     | 0.40              |
| 1:D:751:TYR:CE2   | 1:D:755:ARG:HG3   | 2.56                     | 0.40              |
| 1:F:956:VAL:HG23  | 1:F:957:ASN:N     | 2.36                     | 0.40              |
| 1:G:982:PRO:C     | 1:G:983:GLN:HG2   | 2.46                     | 0.40              |
| 1:H:880:LYS:HA    | 1:H:880:LYS:HD2   | 1.86                     | 0.40              |
| 1:I:758:PRO:HD3   | 1:I:1011:GLY:H    | 1.86                     | 0.40              |
| 1:J:751:TYR:CE2   | 1:J:755:ARG:HG3   | 2.56                     | 0.40              |
| 1:K:758:PRO:HD3   | 1:K:1011:GLY:H    | 1.85                     | 0.40              |
| 1:K:853:HIS:O     | 1:K:857:SER:HB2   | 2.22                     | 0.40              |
| 1:L:948:HIS:CD2   | 1:L:1068:ASN:HB3  | 2.56                     | 0.40              |
| 1:L:952:THR:O     | 1:L:956:VAL:HG22  | 2.20                     | 0.40              |
| 1:C:748:ALA:HB3   | 1:C:936:ALA:HB1   | 2.03                     | 0.40              |
| 1:C:1068:ASN:O    | 1:C:1071:ILE:HG12 | 2.21                     | 0.40              |
| 1:D:1069:HIS:CE1  | 1:D:1073:LYS:NZ   | 2.89                     | 0.40              |
| 1:E:1071:ILE:HG22 | 1:J:915:ASN:HD22  | 1.85                     | 0.40              |
| 1:F:980:SER:O     | 1:F:981:SER:HB2   | 2.21                     | 0.40              |
| 1:H:713:PHE:O     | 1:H:714:LYS:C     | 2.64                     | 0.40              |
| 1:I:694:ARG:O     | 1:I:698:GLN:HG2   | 2.21                     | 0.40              |
| 1:I:802:LEU:HD22  | 1:I:802:LEU:N     | 2.36                     | 0.40              |
| 1:J:980:SER:O     | 1:J:981:SER:HB2   | 2.21                     | 0.40              |
| 1:J:1068:ASN:O    | 1:J:1071:ILE:HG12 | 2.21                     | 0.40              |
| 1:A:930:GLN:O     | 1:A:934:LYS:HG3   | 2.22                     | 0.40              |
| 1:A:944:VAL:HG22  | 1:A:945:ARG:N     | 2.37                     | 0.40              |
| 1:B:900:ASP:OD1   | 1:B:900:ASP:N     | 2.55                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1069:HIS:CE1 | 1:B:1073:LYS:NZ   | 2.90                     | 0.40              |
| 1:C:881:ARG:HG3  | 1:C:881:ARG:NH1   | 2.35                     | 0.40              |
| 1:D:1059:CYS:HB3 | 1:D:1062:MET:HB2  | 2.03                     | 0.40              |
| 1:E:700:MET:HE3  | 1:E:746:LEU:HD21  | 2.02                     | 0.40              |
| 1:E:804:SER:C    | 1:E:805:ASN:HD22  | 2.30                     | 0.40              |
| 1:H:670:LEU:O    | 1:H:674:MET:HG3   | 2.21                     | 0.40              |
| 1:H:681:ILE:O    | 1:H:685:VAL:HG23  | 2.21                     | 0.40              |
| 1:H:716:PRO:HB2  | 1:H:719:GLN:NE2   | 2.36                     | 0.40              |
| 1:H:754:THR:HG22 | 1:H:755:ARG:NE    | 2.35                     | 0.40              |
| 1:H:847:ARG:O    | 1:H:848:SER:C     | 2.64                     | 0.40              |
| 1:H:1019:ASP:OD2 | 1:H:1055:ARG:HA   | 2.21                     | 0.40              |
| 1:K:754:THR:HG22 | 1:K:755:ARG:NE    | 2.22                     | 0.40              |
| 1:K:814:LEU:HD11 | 1:K:933:ILE:HB    | 2.02                     | 0.40              |
| 1:K:905:PHE:CD1  | 1:K:931:VAL:HG21  | 2.56                     | 0.40              |
| 1:L:900:ASP:N    | 1:L:900:ASP:OD1   | 2.55                     | 0.40              |
| 1:B:721:MET:O    | 1:B:722:ASN:C     | 2.64                     | 0.40              |
| 1:B:1059:CYS:HB3 | 1:B:1062:MET:HB2  | 2.03                     | 0.40              |
| 1:C:1004:ASP:CB  | 1:C:1009:LEU:HD12 | 2.52                     | 0.40              |
| 1:D:945:ARG:O    | 1:D:946:ASP:C     | 2.65                     | 0.40              |
| 1:D:967:ALA:HB2  | 1:D:973:ILE:HD11  | 2.04                     | 0.40              |
| 1:E:712:ILE:HG13 | 1:E:712:ILE:H     | 1.77                     | 0.40              |
| 1:E:743:THR:O    | 1:E:746:LEU:HB3   | 2.22                     | 0.40              |
| 1:E:951:TRP:O    | 1:E:955:ILE:HD12  | 2.22                     | 0.40              |
| 1:G:754:THR:CG2  | 1:G:755:ARG:HE    | 2.22                     | 0.40              |
| 1:H:1004:ASP:CA  | 1:H:1009:LEU:HD12 | 2.51                     | 0.40              |
| 1:J:939:ASN:O    | 1:J:940:GLY:C     | 2.65                     | 0.40              |
| 1:K:735:PRO:HG2  | 1:K:958:GLU:HB2   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 358/420 (85%)   | 332 (93%)  | 21 (6%)  | 5 (1%)   | 9           | 30 |
| 1   | B     | 375/420 (89%)   | 337 (90%)  | 28 (8%)  | 10 (3%)  | 4           | 16 |
| 1   | C     | 358/420 (85%)   | 330 (92%)  | 22 (6%)  | 6 (2%)   | 7           | 26 |
| 1   | D     | 375/420 (89%)   | 334 (89%)  | 31 (8%)  | 10 (3%)  | 4           | 16 |
| 1   | E     | 358/420 (85%)   | 334 (93%)  | 18 (5%)  | 6 (2%)   | 7           | 26 |
| 1   | F     | 375/420 (89%)   | 335 (89%)  | 31 (8%)  | 9 (2%)   | 4           | 18 |
| 1   | G     | 358/420 (85%)   | 333 (93%)  | 22 (6%)  | 3 (1%)   | 16          | 44 |
| 1   | H     | 375/420 (89%)   | 339 (90%)  | 28 (8%)  | 8 (2%)   | 5           | 21 |
| 1   | I     | 358/420 (85%)   | 332 (93%)  | 20 (6%)  | 6 (2%)   | 7           | 26 |
| 1   | J     | 375/420 (89%)   | 338 (90%)  | 28 (8%)  | 9 (2%)   | 4           | 18 |
| 1   | K     | 358/420 (85%)   | 327 (91%)  | 25 (7%)  | 6 (2%)   | 7           | 26 |
| 1   | L     | 375/420 (89%)   | 334 (89%)  | 30 (8%)  | 11 (3%)  | 3           | 15 |
| All | All   | 4398/5040 (87%) | 4005 (91%) | 304 (7%) | 89 (2%)  | 6           | 22 |

All (89) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 869  | ASN  |
| 1   | C     | 765  | ASN  |
| 1   | C     | 869  | ASN  |
| 1   | D     | 764  | HIS  |
| 1   | E     | 763  | ILE  |
| 1   | E     | 869  | ASN  |
| 1   | F     | 764  | HIS  |
| 1   | F     | 765  | ASN  |
| 1   | H     | 764  | HIS  |
| 1   | I     | 763  | ILE  |
| 1   | I     | 765  | ASN  |
| 1   | I     | 869  | ASN  |
| 1   | J     | 764  | HIS  |
| 1   | K     | 763  | ILE  |
| 1   | K     | 765  | ASN  |
| 1   | K     | 869  | ASN  |
| 1   | L     | 764  | HIS  |
| 1   | A     | 916  | GLY  |
| 1   | B     | 764  | HIS  |
| 1   | B     | 1071 | ILE  |
| 1   | C     | 916  | GLY  |
| 1   | D     | 763  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 765  | ASN  |
| 1   | D     | 1054 | ARG  |
| 1   | D     | 1071 | ILE  |
| 1   | E     | 765  | ASN  |
| 1   | E     | 916  | GLY  |
| 1   | F     | 1054 | ARG  |
| 1   | F     | 1071 | ILE  |
| 1   | G     | 869  | ASN  |
| 1   | G     | 916  | GLY  |
| 1   | H     | 1071 | ILE  |
| 1   | I     | 916  | GLY  |
| 1   | J     | 763  | ILE  |
| 1   | J     | 1023 | GLU  |
| 1   | J     | 1071 | ILE  |
| 1   | K     | 916  | GLY  |
| 1   | L     | 1020 | ASN  |
| 1   | L     | 1071 | ILE  |
| 1   | A     | 765  | ASN  |
| 1   | B     | 675  | SER  |
| 1   | C     | 764  | HIS  |
| 1   | J     | 675  | SER  |
| 1   | J     | 765  | ASN  |
| 1   | L     | 763  | ILE  |
| 1   | L     | 765  | ASN  |
| 1   | L     | 869  | ASN  |
| 1   | A     | 940  | GLY  |
| 1   | B     | 869  | ASN  |
| 1   | B     | 940  | GLY  |
| 1   | B     | 981  | SER  |
| 1   | D     | 869  | ASN  |
| 1   | D     | 981  | SER  |
| 1   | E     | 940  | GLY  |
| 1   | F     | 675  | SER  |
| 1   | F     | 869  | ASN  |
| 1   | F     | 981  | SER  |
| 1   | H     | 675  | SER  |
| 1   | H     | 869  | ASN  |
| 1   | H     | 981  | SER  |
| 1   | J     | 869  | ASN  |
| 1   | J     | 981  | SER  |
| 1   | K     | 940  | GLY  |
| 1   | L     | 675  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L     | 940  | GLY  |
| 1   | L     | 981  | SER  |
| 1   | L     | 1023 | GLU  |
| 1   | B     | 763  | ILE  |
| 1   | B     | 765  | ASN  |
| 1   | C     | 940  | GLY  |
| 1   | D     | 675  | SER  |
| 1   | D     | 940  | GLY  |
| 1   | F     | 763  | ILE  |
| 1   | H     | 940  | GLY  |
| 1   | I     | 940  | GLY  |
| 1   | B     | 1017 | GLU  |
| 1   | G     | 940  | GLY  |
| 1   | H     | 1054 | ARG  |
| 1   | J     | 940  | GLY  |
| 1   | F     | 940  | GLY  |
| 1   | E     | 849  | VAL  |
| 1   | I     | 849  | VAL  |
| 1   | K     | 849  | VAL  |
| 1   | B     | 941  | PRO  |
| 1   | C     | 849  | VAL  |
| 1   | L     | 941  | PRO  |
| 1   | A     | 849  | VAL  |
| 1   | D     | 941  | PRO  |
| 1   | H     | 941  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 306/370 (83%) | 291 (95%) | 15 (5%)  | 22          | 54 |
| 1   | B     | 313/370 (85%) | 292 (93%) | 21 (7%)  | 15          | 43 |
| 1   | C     | 306/370 (83%) | 291 (95%) | 15 (5%)  | 22          | 54 |
| 1   | D     | 313/370 (85%) | 292 (93%) | 21 (7%)  | 15          | 43 |
| 1   | E     | 306/370 (83%) | 292 (95%) | 14 (5%)  | 24          | 57 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | F     | 313/370 (85%)   | 292 (93%)  | 21 (7%)  | 15          | 43 |
| 1   | G     | 306/370 (83%)   | 290 (95%)  | 16 (5%)  | 21          | 52 |
| 1   | H     | 313/370 (85%)   | 290 (93%)  | 23 (7%)  | 13          | 38 |
| 1   | I     | 306/370 (83%)   | 291 (95%)  | 15 (5%)  | 22          | 54 |
| 1   | J     | 313/370 (85%)   | 292 (93%)  | 21 (7%)  | 15          | 43 |
| 1   | K     | 306/370 (83%)   | 287 (94%)  | 19 (6%)  | 16          | 46 |
| 1   | L     | 313/370 (85%)   | 293 (94%)  | 20 (6%)  | 16          | 44 |
| All | All   | 3714/4440 (84%) | 3493 (94%) | 221 (6%) | 17          | 47 |

All (221) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 670  | LEU  |
| 1   | A     | 684  | LEU  |
| 1   | A     | 686  | GLU  |
| 1   | A     | 700  | MET  |
| 1   | A     | 719  | GLN  |
| 1   | A     | 754  | THR  |
| 1   | A     | 792  | CYS  |
| 1   | A     | 828  | ARG  |
| 1   | A     | 857  | SER  |
| 1   | A     | 861  | LEU  |
| 1   | A     | 872  | LEU  |
| 1   | A     | 885  | LEU  |
| 1   | A     | 915  | ASN  |
| 1   | A     | 965  | GLU  |
| 1   | A     | 1061 | LEU  |
| 1   | B     | 670  | LEU  |
| 1   | B     | 681  | ILE  |
| 1   | B     | 692  | SER  |
| 1   | B     | 700  | MET  |
| 1   | B     | 719  | GLN  |
| 1   | B     | 739  | ARG  |
| 1   | B     | 754  | THR  |
| 1   | B     | 802  | LEU  |
| 1   | B     | 828  | ARG  |
| 1   | B     | 847  | ARG  |
| 1   | B     | 857  | SER  |
| 1   | B     | 861  | LEU  |
| 1   | B     | 872  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 885  | LEU  |
| 1   | B     | 910  | ASN  |
| 1   | B     | 933  | ILE  |
| 1   | B     | 935  | LEU  |
| 1   | B     | 947  | LEU  |
| 1   | B     | 1015 | GLU  |
| 1   | B     | 1019 | ASP  |
| 1   | B     | 1057 | ILE  |
| 1   | C     | 670  | LEU  |
| 1   | C     | 684  | LEU  |
| 1   | C     | 686  | GLU  |
| 1   | C     | 700  | MET  |
| 1   | C     | 719  | GLN  |
| 1   | C     | 754  | THR  |
| 1   | C     | 792  | CYS  |
| 1   | C     | 828  | ARG  |
| 1   | C     | 857  | SER  |
| 1   | C     | 861  | LEU  |
| 1   | C     | 872  | LEU  |
| 1   | C     | 885  | LEU  |
| 1   | C     | 915  | ASN  |
| 1   | C     | 965  | GLU  |
| 1   | C     | 1061 | LEU  |
| 1   | D     | 670  | LEU  |
| 1   | D     | 681  | ILE  |
| 1   | D     | 692  | SER  |
| 1   | D     | 700  | MET  |
| 1   | D     | 719  | GLN  |
| 1   | D     | 739  | ARG  |
| 1   | D     | 754  | THR  |
| 1   | D     | 802  | LEU  |
| 1   | D     | 828  | ARG  |
| 1   | D     | 847  | ARG  |
| 1   | D     | 857  | SER  |
| 1   | D     | 861  | LEU  |
| 1   | D     | 872  | LEU  |
| 1   | D     | 885  | LEU  |
| 1   | D     | 910  | ASN  |
| 1   | D     | 933  | ILE  |
| 1   | D     | 935  | LEU  |
| 1   | D     | 947  | LEU  |
| 1   | D     | 1015 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1020 | ASN  |
| 1   | D     | 1057 | ILE  |
| 1   | E     | 670  | LEU  |
| 1   | E     | 684  | LEU  |
| 1   | E     | 686  | GLU  |
| 1   | E     | 700  | MET  |
| 1   | E     | 719  | GLN  |
| 1   | E     | 754  | THR  |
| 1   | E     | 828  | ARG  |
| 1   | E     | 857  | SER  |
| 1   | E     | 861  | LEU  |
| 1   | E     | 872  | LEU  |
| 1   | E     | 885  | LEU  |
| 1   | E     | 915  | ASN  |
| 1   | E     | 965  | GLU  |
| 1   | E     | 1061 | LEU  |
| 1   | F     | 670  | LEU  |
| 1   | F     | 681  | ILE  |
| 1   | F     | 692  | SER  |
| 1   | F     | 700  | MET  |
| 1   | F     | 719  | GLN  |
| 1   | F     | 739  | ARG  |
| 1   | F     | 754  | THR  |
| 1   | F     | 802  | LEU  |
| 1   | F     | 828  | ARG  |
| 1   | F     | 847  | ARG  |
| 1   | F     | 857  | SER  |
| 1   | F     | 861  | LEU  |
| 1   | F     | 872  | LEU  |
| 1   | F     | 885  | LEU  |
| 1   | F     | 910  | ASN  |
| 1   | F     | 933  | ILE  |
| 1   | F     | 935  | LEU  |
| 1   | F     | 947  | LEU  |
| 1   | F     | 1015 | GLU  |
| 1   | F     | 1057 | ILE  |
| 1   | F     | 1059 | CYS  |
| 1   | G     | 670  | LEU  |
| 1   | G     | 684  | LEU  |
| 1   | G     | 686  | GLU  |
| 1   | G     | 700  | MET  |
| 1   | G     | 719  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 754  | THR  |
| 1   | G     | 792  | CYS  |
| 1   | G     | 828  | ARG  |
| 1   | G     | 857  | SER  |
| 1   | G     | 861  | LEU  |
| 1   | G     | 872  | LEU  |
| 1   | G     | 885  | LEU  |
| 1   | G     | 915  | ASN  |
| 1   | G     | 965  | GLU  |
| 1   | G     | 1000 | CYS  |
| 1   | G     | 1061 | LEU  |
| 1   | H     | 670  | LEU  |
| 1   | H     | 681  | ILE  |
| 1   | H     | 692  | SER  |
| 1   | H     | 700  | MET  |
| 1   | H     | 719  | GLN  |
| 1   | H     | 739  | ARG  |
| 1   | H     | 754  | THR  |
| 1   | H     | 776  | ASP  |
| 1   | H     | 802  | LEU  |
| 1   | H     | 828  | ARG  |
| 1   | H     | 847  | ARG  |
| 1   | H     | 857  | SER  |
| 1   | H     | 861  | LEU  |
| 1   | H     | 872  | LEU  |
| 1   | H     | 885  | LEU  |
| 1   | H     | 910  | ASN  |
| 1   | H     | 933  | ILE  |
| 1   | H     | 935  | LEU  |
| 1   | H     | 947  | LEU  |
| 1   | H     | 1015 | GLU  |
| 1   | H     | 1017 | GLU  |
| 1   | H     | 1056 | ARG  |
| 1   | H     | 1057 | ILE  |
| 1   | I     | 670  | LEU  |
| 1   | I     | 684  | LEU  |
| 1   | I     | 686  | GLU  |
| 1   | I     | 700  | MET  |
| 1   | I     | 719  | GLN  |
| 1   | I     | 754  | THR  |
| 1   | I     | 828  | ARG  |
| 1   | I     | 857  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | I     | 861  | LEU  |
| 1   | I     | 872  | LEU  |
| 1   | I     | 885  | LEU  |
| 1   | I     | 915  | ASN  |
| 1   | I     | 965  | GLU  |
| 1   | I     | 1000 | CYS  |
| 1   | I     | 1061 | LEU  |
| 1   | J     | 670  | LEU  |
| 1   | J     | 681  | ILE  |
| 1   | J     | 692  | SER  |
| 1   | J     | 700  | MET  |
| 1   | J     | 719  | GLN  |
| 1   | J     | 739  | ARG  |
| 1   | J     | 754  | THR  |
| 1   | J     | 802  | LEU  |
| 1   | J     | 828  | ARG  |
| 1   | J     | 847  | ARG  |
| 1   | J     | 857  | SER  |
| 1   | J     | 861  | LEU  |
| 1   | J     | 872  | LEU  |
| 1   | J     | 885  | LEU  |
| 1   | J     | 910  | ASN  |
| 1   | J     | 933  | ILE  |
| 1   | J     | 935  | LEU  |
| 1   | J     | 947  | LEU  |
| 1   | J     | 1015 | GLU  |
| 1   | J     | 1018 | GLU  |
| 1   | J     | 1057 | ILE  |
| 1   | K     | 670  | LEU  |
| 1   | K     | 684  | LEU  |
| 1   | K     | 686  | GLU  |
| 1   | K     | 700  | MET  |
| 1   | K     | 706  | ASP  |
| 1   | K     | 719  | GLN  |
| 1   | K     | 754  | THR  |
| 1   | K     | 762  | GLN  |
| 1   | K     | 792  | CYS  |
| 1   | K     | 828  | ARG  |
| 1   | K     | 857  | SER  |
| 1   | K     | 861  | LEU  |
| 1   | K     | 872  | LEU  |
| 1   | K     | 885  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K     | 915  | ASN  |
| 1   | K     | 965  | GLU  |
| 1   | K     | 1000 | CYS  |
| 1   | K     | 1057 | ILE  |
| 1   | K     | 1061 | LEU  |
| 1   | L     | 670  | LEU  |
| 1   | L     | 681  | ILE  |
| 1   | L     | 692  | SER  |
| 1   | L     | 700  | MET  |
| 1   | L     | 719  | GLN  |
| 1   | L     | 739  | ARG  |
| 1   | L     | 754  | THR  |
| 1   | L     | 802  | LEU  |
| 1   | L     | 828  | ARG  |
| 1   | L     | 847  | ARG  |
| 1   | L     | 857  | SER  |
| 1   | L     | 861  | LEU  |
| 1   | L     | 872  | LEU  |
| 1   | L     | 885  | LEU  |
| 1   | L     | 910  | ASN  |
| 1   | L     | 933  | ILE  |
| 1   | L     | 935  | LEU  |
| 1   | L     | 947  | LEU  |
| 1   | L     | 1015 | GLU  |
| 1   | L     | 1057 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 705 | GLN  |
| 1   | A     | 719 | GLN  |
| 1   | A     | 722 | ASN  |
| 1   | A     | 737 | HIS  |
| 1   | A     | 762 | GLN  |
| 1   | A     | 805 | ASN  |
| 1   | A     | 825 | HIS  |
| 1   | A     | 869 | ASN  |
| 1   | A     | 915 | ASN  |
| 1   | A     | 923 | ASN  |
| 1   | A     | 939 | ASN  |
| 1   | A     | 957 | ASN  |
| 1   | A     | 983 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 988  | GLN  |
| 1   | A     | 994  | HIS  |
| 1   | B     | 718  | GLN  |
| 1   | B     | 719  | GLN  |
| 1   | B     | 737  | HIS  |
| 1   | B     | 794  | ASN  |
| 1   | B     | 805  | ASN  |
| 1   | B     | 825  | HIS  |
| 1   | B     | 845  | ASN  |
| 1   | B     | 869  | ASN  |
| 1   | B     | 923  | ASN  |
| 1   | B     | 939  | ASN  |
| 1   | C     | 705  | GLN  |
| 1   | C     | 718  | GLN  |
| 1   | C     | 719  | GLN  |
| 1   | C     | 722  | ASN  |
| 1   | C     | 737  | HIS  |
| 1   | C     | 762  | GLN  |
| 1   | C     | 805  | ASN  |
| 1   | C     | 825  | HIS  |
| 1   | C     | 869  | ASN  |
| 1   | C     | 915  | ASN  |
| 1   | C     | 923  | ASN  |
| 1   | C     | 939  | ASN  |
| 1   | C     | 957  | ASN  |
| 1   | C     | 983  | GLN  |
| 1   | C     | 988  | GLN  |
| 1   | C     | 994  | HIS  |
| 1   | D     | 719  | GLN  |
| 1   | D     | 737  | HIS  |
| 1   | D     | 794  | ASN  |
| 1   | D     | 805  | ASN  |
| 1   | D     | 825  | HIS  |
| 1   | D     | 869  | ASN  |
| 1   | D     | 915  | ASN  |
| 1   | D     | 923  | ASN  |
| 1   | D     | 939  | ASN  |
| 1   | D     | 988  | GLN  |
| 1   | D     | 1020 | ASN  |
| 1   | E     | 705  | GLN  |
| 1   | E     | 718  | GLN  |
| 1   | E     | 719  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 722 | ASN  |
| 1   | E     | 737 | HIS  |
| 1   | E     | 762 | GLN  |
| 1   | E     | 805 | ASN  |
| 1   | E     | 825 | HIS  |
| 1   | E     | 869 | ASN  |
| 1   | E     | 915 | ASN  |
| 1   | E     | 923 | ASN  |
| 1   | E     | 939 | ASN  |
| 1   | E     | 957 | ASN  |
| 1   | E     | 983 | GLN  |
| 1   | E     | 988 | GLN  |
| 1   | F     | 718 | GLN  |
| 1   | F     | 719 | GLN  |
| 1   | F     | 737 | HIS  |
| 1   | F     | 781 | HIS  |
| 1   | F     | 794 | ASN  |
| 1   | F     | 805 | ASN  |
| 1   | F     | 825 | HIS  |
| 1   | F     | 869 | ASN  |
| 1   | F     | 923 | ASN  |
| 1   | F     | 939 | ASN  |
| 1   | G     | 705 | GLN  |
| 1   | G     | 718 | GLN  |
| 1   | G     | 719 | GLN  |
| 1   | G     | 722 | ASN  |
| 1   | G     | 737 | HIS  |
| 1   | G     | 762 | GLN  |
| 1   | G     | 805 | ASN  |
| 1   | G     | 825 | HIS  |
| 1   | G     | 869 | ASN  |
| 1   | G     | 913 | ASN  |
| 1   | G     | 915 | ASN  |
| 1   | G     | 923 | ASN  |
| 1   | G     | 939 | ASN  |
| 1   | G     | 957 | ASN  |
| 1   | G     | 983 | GLN  |
| 1   | G     | 988 | GLN  |
| 1   | H     | 719 | GLN  |
| 1   | H     | 737 | HIS  |
| 1   | H     | 794 | ASN  |
| 1   | H     | 805 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 825  | HIS  |
| 1   | H     | 845  | ASN  |
| 1   | H     | 869  | ASN  |
| 1   | H     | 923  | ASN  |
| 1   | H     | 939  | ASN  |
| 1   | I     | 705  | GLN  |
| 1   | I     | 718  | GLN  |
| 1   | I     | 719  | GLN  |
| 1   | I     | 722  | ASN  |
| 1   | I     | 737  | HIS  |
| 1   | I     | 762  | GLN  |
| 1   | I     | 794  | ASN  |
| 1   | I     | 805  | ASN  |
| 1   | I     | 825  | HIS  |
| 1   | I     | 869  | ASN  |
| 1   | I     | 915  | ASN  |
| 1   | I     | 923  | ASN  |
| 1   | I     | 939  | ASN  |
| 1   | I     | 957  | ASN  |
| 1   | I     | 983  | GLN  |
| 1   | I     | 988  | GLN  |
| 1   | J     | 718  | GLN  |
| 1   | J     | 719  | GLN  |
| 1   | J     | 737  | HIS  |
| 1   | J     | 794  | ASN  |
| 1   | J     | 805  | ASN  |
| 1   | J     | 825  | HIS  |
| 1   | J     | 869  | ASN  |
| 1   | J     | 923  | ASN  |
| 1   | J     | 939  | ASN  |
| 1   | J     | 1020 | ASN  |
| 1   | J     | 1063 | HIS  |
| 1   | K     | 705  | GLN  |
| 1   | K     | 718  | GLN  |
| 1   | K     | 719  | GLN  |
| 1   | K     | 722  | ASN  |
| 1   | K     | 737  | HIS  |
| 1   | K     | 762  | GLN  |
| 1   | K     | 794  | ASN  |
| 1   | K     | 805  | ASN  |
| 1   | K     | 825  | HIS  |
| 1   | K     | 869  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 913 | ASN  |
| 1   | K     | 915 | ASN  |
| 1   | K     | 923 | ASN  |
| 1   | K     | 939 | ASN  |
| 1   | K     | 957 | ASN  |
| 1   | K     | 983 | GLN  |
| 1   | K     | 988 | GLN  |
| 1   | L     | 719 | GLN  |
| 1   | L     | 737 | HIS  |
| 1   | L     | 794 | ASN  |
| 1   | L     | 805 | ASN  |
| 1   | L     | 825 | HIS  |
| 1   | L     | 845 | ASN  |
| 1   | L     | 869 | ASN  |
| 1   | L     | 915 | ASN  |
| 1   | L     | 923 | ASN  |
| 1   | L     | 939 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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 |
| 3   | IBM  | B     | 2112 | -    | 17,17,17     | 2.44 | 4 (23%)  | 19,25,25    | 1.42 | 3 (15%)  |
| 3   | IBM  | F     | 2116 | -    | 17,17,17     | 2.30 | 4 (23%)  | 19,25,25    | 1.45 | 3 (15%)  |
| 3   | IBM  | E     | 2115 | -    | 17,17,17     | 2.42 | 4 (23%)  | 19,25,25    | 1.42 | 3 (15%)  |
| 3   | IBM  | L     | 2122 | -    | 17,17,17     | 2.55 | 4 (23%)  | 19,25,25    | 1.47 | 4 (21%)  |
| 3   | IBM  | D     | 2114 | -    | 17,17,17     | 2.54 | 4 (23%)  | 19,25,25    | 1.41 | 4 (21%)  |
| 3   | IBM  | A     | 2111 | -    | 17,17,17     | 2.56 | 4 (23%)  | 19,25,25    | 1.41 | 3 (15%)  |
| 3   | IBM  | K     | 2121 | -    | 17,17,17     | 2.48 | 4 (23%)  | 19,25,25    | 1.36 | 3 (15%)  |
| 3   | IBM  | H     | 2118 | -    | 17,17,17     | 2.47 | 4 (23%)  | 19,25,25    | 1.34 | 3 (15%)  |
| 3   | IBM  | J     | 2120 | -    | 17,17,17     | 2.37 | 4 (23%)  | 19,25,25    | 1.30 | 3 (15%)  |
| 3   | IBM  | G     | 2117 | -    | 17,17,17     | 2.38 | 4 (23%)  | 19,25,25    | 1.40 | 3 (15%)  |
| 3   | IBM  | C     | 2113 | -    | 17,17,17     | 2.47 | 4 (23%)  | 19,25,25    | 1.36 | 3 (15%)  |
| 3   | IBM  | I     | 2119 | -    | 17,17,17     | 2.43 | 4 (23%)  | 19,25,25    | 1.37 | 3 (15%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 3   | IBM  | B     | 2112 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | F     | 2116 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | E     | 2115 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | L     | 2122 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | D     | 2114 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | A     | 2111 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | K     | 2121 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | H     | 2118 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | J     | 2120 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | G     | 2117 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | C     | 2113 | -    | -       | 0/4/4/4  | 0/2/2/2 |
| 3   | IBM  | I     | 2119 | -    | -       | 0/4/4/4  | 0/2/2/2 |

All (48) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | D     | 2114 | IBM  | C4-N9 | 6.64 | 1.47        | 1.36     |
| 3   | L     | 2122 | IBM  | C4-N9 | 6.58 | 1.47        | 1.36     |
| 3   | A     | 2111 | IBM  | C4-N9 | 6.56 | 1.47        | 1.36     |
| 3   | E     | 2115 | IBM  | C4-N9 | 6.48 | 1.47        | 1.36     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | H     | 2118 | IBM  | C4-N9 | 6.48  | 1.47        | 1.36     |
| 3   | A     | 2111 | IBM  | C4-N3 | 6.43  | 1.49        | 1.38     |
| 3   | B     | 2112 | IBM  | C4-N9 | 6.34  | 1.47        | 1.36     |
| 3   | I     | 2119 | IBM  | C4-N9 | 6.29  | 1.47        | 1.36     |
| 3   | K     | 2121 | IBM  | C4-N9 | 6.26  | 1.47        | 1.36     |
| 3   | F     | 2116 | IBM  | C4-N9 | 6.23  | 1.47        | 1.36     |
| 3   | G     | 2117 | IBM  | C4-N9 | 6.23  | 1.47        | 1.36     |
| 3   | C     | 2113 | IBM  | C4-N9 | 6.19  | 1.47        | 1.36     |
| 3   | K     | 2121 | IBM  | C4-N3 | 6.02  | 1.49        | 1.38     |
| 3   | J     | 2120 | IBM  | C4-N9 | 6.01  | 1.46        | 1.36     |
| 3   | L     | 2122 | IBM  | C4-N3 | 5.91  | 1.48        | 1.38     |
| 3   | E     | 2115 | IBM  | C4-N3 | 5.88  | 1.48        | 1.38     |
| 3   | C     | 2113 | IBM  | C4-N3 | 5.75  | 1.48        | 1.38     |
| 3   | D     | 2114 | IBM  | C4-N3 | 5.66  | 1.48        | 1.38     |
| 3   | G     | 2117 | IBM  | C4-N3 | 5.60  | 1.48        | 1.38     |
| 3   | B     | 2112 | IBM  | C4-N3 | 5.49  | 1.48        | 1.38     |
| 3   | I     | 2119 | IBM  | C4-N3 | 5.43  | 1.48        | 1.38     |
| 3   | H     | 2118 | IBM  | C4-N3 | 5.39  | 1.47        | 1.38     |
| 3   | J     | 2120 | IBM  | C4-N3 | 5.38  | 1.47        | 1.38     |
| 3   | F     | 2116 | IBM  | C4-N3 | 5.18  | 1.47        | 1.38     |
| 3   | H     | 2118 | IBM  | C5-N7 | 3.46  | 1.46        | 1.39     |
| 3   | C     | 2113 | IBM  | C5-N7 | 3.44  | 1.46        | 1.39     |
| 3   | L     | 2122 | IBM  | C5-N7 | 3.43  | 1.46        | 1.39     |
| 3   | D     | 2114 | IBM  | C5-N7 | 3.35  | 1.45        | 1.39     |
| 3   | I     | 2119 | IBM  | C5-N7 | 3.33  | 1.45        | 1.39     |
| 3   | C     | 2113 | IBM  | C5-C4 | -3.33 | 1.33        | 1.38     |
| 3   | A     | 2111 | IBM  | C5-C4 | -3.32 | 1.33        | 1.38     |
| 3   | J     | 2120 | IBM  | C5-N7 | 3.26  | 1.45        | 1.39     |
| 3   | K     | 2121 | IBM  | C5-N7 | 3.20  | 1.45        | 1.39     |
| 3   | G     | 2117 | IBM  | C5-N7 | 3.18  | 1.45        | 1.39     |
| 3   | J     | 2120 | IBM  | C5-C4 | -3.16 | 1.33        | 1.38     |
| 3   | B     | 2112 | IBM  | C5-N7 | 3.13  | 1.45        | 1.39     |
| 3   | B     | 2112 | IBM  | C5-C4 | -3.13 | 1.33        | 1.38     |
| 3   | I     | 2119 | IBM  | C5-C4 | -3.09 | 1.33        | 1.38     |
| 3   | E     | 2115 | IBM  | C5-N7 | 3.04  | 1.45        | 1.39     |
| 3   | K     | 2121 | IBM  | C5-C4 | -2.91 | 1.34        | 1.38     |
| 3   | F     | 2116 | IBM  | C5-C4 | -2.90 | 1.34        | 1.38     |
| 3   | H     | 2118 | IBM  | C5-C4 | -2.87 | 1.34        | 1.38     |
| 3   | A     | 2111 | IBM  | C5-N7 | 2.84  | 1.44        | 1.39     |
| 3   | D     | 2114 | IBM  | C5-C4 | -2.83 | 1.34        | 1.38     |
| 3   | L     | 2122 | IBM  | C5-C4 | -2.60 | 1.34        | 1.38     |
| 3   | F     | 2116 | IBM  | C5-N7 | 2.53  | 1.44        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | G     | 2117 | IBM  | C5-C4 | -2.53 | 1.34        | 1.38     |
| 3   | E     | 2115 | IBM  | C5-C4 | -2.30 | 1.34        | 1.38     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | F     | 2116 | IBM  | O6-C6-C5   | -3.47 | 115.66      | 124.59   |
| 3   | B     | 2112 | IBM  | O6-C6-C5   | -3.45 | 115.69      | 124.59   |
| 3   | F     | 2116 | IBM  | O6-C6-N1   | 3.42  | 126.61      | 120.36   |
| 3   | A     | 2111 | IBM  | O6-C6-C5   | -3.38 | 115.88      | 124.59   |
| 3   | B     | 2112 | IBM  | O6-C6-N1   | 3.36  | 126.50      | 120.36   |
| 3   | D     | 2114 | IBM  | O6-C6-C5   | -3.30 | 116.08      | 124.59   |
| 3   | K     | 2121 | IBM  | O6-C6-C5   | -3.27 | 116.16      | 124.59   |
| 3   | G     | 2117 | IBM  | O6-C6-N1   | 3.24  | 126.29      | 120.36   |
| 3   | I     | 2119 | IBM  | O6-C6-C5   | -3.23 | 116.25      | 124.59   |
| 3   | E     | 2115 | IBM  | O6-C6-N1   | 3.23  | 126.26      | 120.36   |
| 3   | G     | 2117 | IBM  | O6-C6-C5   | -3.20 | 116.33      | 124.59   |
| 3   | L     | 2122 | IBM  | O6-C6-C5   | -3.19 | 116.38      | 124.59   |
| 3   | E     | 2115 | IBM  | O6-C6-C5   | -3.19 | 116.38      | 124.59   |
| 3   | H     | 2118 | IBM  | O6-C6-C5   | -3.16 | 116.43      | 124.59   |
| 3   | A     | 2111 | IBM  | O6-C6-N1   | 3.16  | 126.13      | 120.36   |
| 3   | C     | 2113 | IBM  | O6-C6-C5   | -3.15 | 116.47      | 124.59   |
| 3   | I     | 2119 | IBM  | O6-C6-N1   | 3.13  | 126.08      | 120.36   |
| 3   | J     | 2120 | IBM  | O6-C6-C5   | -3.10 | 116.61      | 124.59   |
| 3   | L     | 2122 | IBM  | O6-C6-N1   | 3.02  | 125.88      | 120.36   |
| 3   | D     | 2114 | IBM  | O6-C6-N1   | 3.01  | 125.87      | 120.36   |
| 3   | J     | 2120 | IBM  | O6-C6-N1   | 3.01  | 125.86      | 120.36   |
| 3   | H     | 2118 | IBM  | O6-C6-N1   | 3.00  | 125.84      | 120.36   |
| 3   | K     | 2121 | IBM  | O6-C6-N1   | 2.91  | 125.67      | 120.36   |
| 3   | C     | 2113 | IBM  | O6-C6-N1   | 2.88  | 125.62      | 120.36   |
| 3   | E     | 2115 | IBM  | N9-C4-N3   | 2.72  | 131.75      | 127.81   |
| 3   | K     | 2121 | IBM  | N9-C4-N3   | 2.70  | 131.73      | 127.81   |
| 3   | A     | 2111 | IBM  | N9-C4-N3   | 2.47  | 131.39      | 127.81   |
| 3   | L     | 2122 | IBM  | N9-C4-N3   | 2.38  | 131.26      | 127.81   |
| 3   | L     | 2122 | IBM  | C12-C11-N3 | 2.32  | 115.75      | 112.38   |
| 3   | F     | 2116 | IBM  | N9-C4-N3   | 2.28  | 131.12      | 127.81   |
| 3   | H     | 2118 | IBM  | N9-C4-N3   | 2.27  | 131.11      | 127.81   |
| 3   | I     | 2119 | IBM  | N9-C4-N3   | 2.27  | 131.11      | 127.81   |
| 3   | C     | 2113 | IBM  | N9-C4-N3   | 2.24  | 131.06      | 127.81   |
| 3   | G     | 2117 | IBM  | N9-C4-N3   | 2.24  | 131.06      | 127.81   |
| 3   | J     | 2120 | IBM  | N9-C4-N3   | 2.23  | 131.05      | 127.81   |
| 3   | D     | 2114 | IBM  | N9-C4-N3   | 2.22  | 131.04      | 127.81   |

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| Mol | Chain | Res  | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|------|-------------|----------|
| 3   | B     | 2112 | IBM  | N9-C4-N3  | 2.21 | 131.02      | 127.81   |
| 3   | D     | 2114 | IBM  | C11-N3-C2 | 2.20 | 122.15      | 117.67   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 364/420 (86%)   | 0.29   | 24 (6%) 24 19  | 24, 42, 80, 100       | 0     |
| 1   | B     | 381/420 (90%)   | 0.50   | 33 (8%) 16 13  | 25, 50, 92, 100       | 0     |
| 1   | C     | 364/420 (86%)   | 0.24   | 25 (6%) 23 18  | 26, 43, 81, 100       | 0     |
| 1   | D     | 381/420 (90%)   | 0.50   | 36 (9%) 14 12  | 22, 47, 89, 100       | 0     |
| 1   | E     | 364/420 (86%)   | 0.21   | 26 (7%) 22 17  | 23, 42, 81, 100       | 0     |
| 1   | F     | 381/420 (90%)   | 0.52   | 37 (9%) 13 11  | 21, 45, 79, 100       | 0     |
| 1   | G     | 364/420 (86%)   | 0.27   | 30 (8%) 17 14  | 24, 44, 83, 100       | 0     |
| 1   | H     | 381/420 (90%)   | 0.65   | 40 (10%) 11 10 | 29, 52, 92, 100       | 0     |
| 1   | I     | 364/420 (86%)   | 0.16   | 21 (5%) 29 22  | 23, 42, 81, 100       | 0     |
| 1   | J     | 381/420 (90%)   | 0.53   | 42 (11%) 10 9  | 22, 46, 77, 100       | 0     |
| 1   | K     | 364/420 (86%)   | 0.96   | 50 (13%) 6 5   | 28, 51, 87, 100       | 0     |
| 1   | L     | 381/420 (90%)   | 0.94   | 56 (14%) 6 4   | 28, 54, 91, 100       | 0     |
| All | All   | 4470/5040 (88%) | 0.48   | 420 (9%) 14 12 | 21, 46, 85, 100       | 0     |

All (420) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 1016 | ALA  | 11.1 |
| 1   | D     | 1016 | ALA  | 10.7 |
| 1   | D     | 1021 | ASP  | 10.4 |
| 1   | B     | 1016 | ALA  | 10.4 |
| 1   | A     | 766  | GLY  | 10.2 |
| 1   | L     | 1016 | ALA  | 10.1 |
| 1   | E     | 1016 | ALA  | 9.0  |
| 1   | G     | 766  | GLY  | 8.7  |
| 1   | D     | 1019 | ASP  | 8.3  |
| 1   | H     | 1022 | THR  | 8.1  |
| 1   | D     | 658  | SER  | 8.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 1018 | GLU  | 8.0  |
| 1   | D     | 657  | VAL  | 7.9  |
| 1   | C     | 766  | GLY  | 7.8  |
| 1   | B     | 765  | ASN  | 7.7  |
| 1   | C     | 659  | LEU  | 7.6  |
| 1   | C     | 1016 | ALA  | 7.6  |
| 1   | D     | 1017 | GLU  | 7.5  |
| 1   | D     | 1023 | GLU  | 7.5  |
| 1   | D     | 1022 | THR  | 7.5  |
| 1   | D     | 1024 | SER  | 7.5  |
| 1   | I     | 1053 | SER  | 7.5  |
| 1   | B     | 1024 | SER  | 7.4  |
| 1   | D     | 660  | ASP  | 7.4  |
| 1   | B     | 1053 | SER  | 7.2  |
| 1   | H     | 656  | GLU  | 7.2  |
| 1   | D     | 766  | GLY  | 7.0  |
| 1   | D     | 1053 | SER  | 6.9  |
| 1   | H     | 1024 | SER  | 6.9  |
| 1   | B     | 657  | VAL  | 6.8  |
| 1   | B     | 1054 | ARG  | 6.8  |
| 1   | K     | 766  | GLY  | 6.8  |
| 1   | F     | 1024 | SER  | 6.7  |
| 1   | F     | 1019 | ASP  | 6.7  |
| 1   | B     | 1022 | THR  | 6.7  |
| 1   | F     | 656  | GLU  | 6.7  |
| 1   | K     | 660  | ASP  | 6.7  |
| 1   | D     | 1020 | ASN  | 6.6  |
| 1   | C     | 1053 | SER  | 6.6  |
| 1   | B     | 656  | GLU  | 6.5  |
| 1   | L     | 1053 | SER  | 6.5  |
| 1   | F     | 1053 | SER  | 6.5  |
| 1   | H     | 658  | SER  | 6.5  |
| 1   | B     | 766  | GLY  | 6.4  |
| 1   | L     | 766  | GLY  | 6.4  |
| 1   | A     | 1016 | ALA  | 6.4  |
| 1   | J     | 658  | SER  | 6.4  |
| 1   | J     | 656  | GLU  | 6.3  |
| 1   | H     | 1053 | SER  | 6.3  |
| 1   | F     | 658  | SER  | 6.3  |
| 1   | J     | 1053 | SER  | 6.3  |
| 1   | D     | 659  | LEU  | 6.3  |
| 1   | H     | 1018 | GLU  | 6.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 1017 | GLU  | 6.1  |
| 1   | D     | 1015 | GLU  | 6.1  |
| 1   | I     | 1054 | ARG  | 6.0  |
| 1   | I     | 1016 | ALA  | 6.0  |
| 1   | H     | 659  | LEU  | 6.0  |
| 1   | B     | 1021 | ASP  | 5.9  |
| 1   | J     | 657  | VAL  | 5.9  |
| 1   | E     | 1053 | SER  | 5.9  |
| 1   | G     | 1053 | SER  | 5.9  |
| 1   | H     | 765  | ASN  | 5.9  |
| 1   | L     | 658  | SER  | 5.9  |
| 1   | I     | 660  | ASP  | 5.9  |
| 1   | F     | 657  | VAL  | 5.8  |
| 1   | B     | 1018 | GLU  | 5.8  |
| 1   | E     | 764  | HIS  | 5.7  |
| 1   | A     | 765  | ASN  | 5.7  |
| 1   | L     | 656  | GLU  | 5.7  |
| 1   | A     | 1054 | ARG  | 5.7  |
| 1   | C     | 765  | ASN  | 5.7  |
| 1   | B     | 1023 | GLU  | 5.6  |
| 1   | L     | 1054 | ARG  | 5.6  |
| 1   | D     | 1054 | ARG  | 5.5  |
| 1   | E     | 765  | ASN  | 5.5  |
| 1   | H     | 1054 | ARG  | 5.5  |
| 1   | L     | 659  | LEU  | 5.5  |
| 1   | H     | 657  | VAL  | 5.5  |
| 1   | H     | 766  | GLY  | 5.4  |
| 1   | L     | 1024 | SER  | 5.4  |
| 1   | E     | 659  | LEU  | 5.4  |
| 1   | E     | 766  | GLY  | 5.4  |
| 1   | A     | 1053 | SER  | 5.4  |
| 1   | L     | 1022 | THR  | 5.3  |
| 1   | G     | 660  | ASP  | 5.3  |
| 1   | H     | 1019 | ASP  | 5.3  |
| 1   | A     | 1017 | GLU  | 5.3  |
| 1   | L     | 765  | ASN  | 5.2  |
| 1   | H     | 1015 | GLU  | 5.2  |
| 1   | I     | 1017 | GLU  | 5.2  |
| 1   | H     | 1020 | ASN  | 5.1  |
| 1   | F     | 659  | LEU  | 5.1  |
| 1   | K     | 783  | ARG  | 5.1  |
| 1   | B     | 1019 | ASP  | 5.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 660  | ASP  | 5.1  |
| 1   | I     | 765  | ASN  | 5.0  |
| 1   | F     | 766  | GLY  | 5.0  |
| 1   | L     | 657  | VAL  | 5.0  |
| 1   | C     | 1017 | GLU  | 4.9  |
| 1   | C     | 764  | HIS  | 4.9  |
| 1   | D     | 661  | LEU  | 4.9  |
| 1   | G     | 1054 | ARG  | 4.9  |
| 1   | D     | 765  | ASN  | 4.8  |
| 1   | B     | 1015 | GLU  | 4.8  |
| 1   | J     | 660  | ASP  | 4.8  |
| 1   | E     | 660  | ASP  | 4.8  |
| 1   | G     | 765  | ASN  | 4.8  |
| 1   | G     | 663  | LEU  | 4.7  |
| 1   | L     | 660  | ASP  | 4.7  |
| 1   | G     | 1016 | ALA  | 4.7  |
| 1   | B     | 658  | SER  | 4.7  |
| 1   | I     | 766  | GLY  | 4.6  |
| 1   | B     | 660  | ASP  | 4.6  |
| 1   | D     | 656  | GLU  | 4.6  |
| 1   | K     | 663  | LEU  | 4.5  |
| 1   | A     | 764  | HIS  | 4.5  |
| 1   | L     | 1056 | ARG  | 4.5  |
| 1   | K     | 765  | ASN  | 4.5  |
| 1   | I     | 764  | HIS  | 4.4  |
| 1   | J     | 766  | GLY  | 4.4  |
| 1   | E     | 1054 | ARG  | 4.4  |
| 1   | I     | 659  | LEU  | 4.4  |
| 1   | K     | 659  | LEU  | 4.4  |
| 1   | L     | 1023 | GLU  | 4.3  |
| 1   | F     | 1022 | THR  | 4.3  |
| 1   | H     | 1021 | ASP  | 4.2  |
| 1   | F     | 765  | ASN  | 4.2  |
| 1   | K     | 1016 | ALA  | 4.2  |
| 1   | H     | 1023 | GLU  | 4.2  |
| 1   | J     | 1022 | THR  | 4.1  |
| 1   | G     | 661  | LEU  | 4.1  |
| 1   | L     | 1018 | GLU  | 4.1  |
| 1   | B     | 1020 | ASN  | 4.1  |
| 1   | K     | 1053 | SER  | 4.1  |
| 1   | L     | 1057 | ILE  | 4.1  |
| 1   | K     | 661  | LEU  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | K     | 764  | HIS  | 4.1  |
| 1   | K     | 916  | GLY  | 4.1  |
| 1   | D     | 663  | LEU  | 4.0  |
| 1   | G     | 659  | LEU  | 4.0  |
| 1   | G     | 664  | VAL  | 4.0  |
| 1   | C     | 661  | LEU  | 4.0  |
| 1   | F     | 1021 | ASP  | 4.0  |
| 1   | A     | 662  | ILE  | 4.0  |
| 1   | I     | 946  | ASP  | 3.9  |
| 1   | H     | 1017 | GLU  | 3.9  |
| 1   | H     | 660  | ASP  | 3.9  |
| 1   | F     | 662  | ILE  | 3.9  |
| 1   | A     | 916  | GLY  | 3.8  |
| 1   | B     | 659  | LEU  | 3.8  |
| 1   | J     | 659  | LEU  | 3.8  |
| 1   | L     | 1021 | ASP  | 3.8  |
| 1   | G     | 764  | HIS  | 3.8  |
| 1   | A     | 659  | LEU  | 3.8  |
| 1   | F     | 1018 | GLU  | 3.8  |
| 1   | L     | 1017 | GLU  | 3.8  |
| 1   | C     | 662  | ILE  | 3.8  |
| 1   | L     | 663  | LEU  | 3.8  |
| 1   | J     | 765  | ASN  | 3.8  |
| 1   | K     | 664  | VAL  | 3.7  |
| 1   | J     | 763  | ILE  | 3.7  |
| 1   | F     | 660  | ASP  | 3.7  |
| 1   | L     | 1015 | GLU  | 3.7  |
| 1   | D     | 662  | ILE  | 3.7  |
| 1   | G     | 1017 | GLU  | 3.7  |
| 1   | F     | 1023 | GLU  | 3.6  |
| 1   | E     | 661  | LEU  | 3.6  |
| 1   | B     | 912  | VAL  | 3.6  |
| 1   | I     | 661  | LEU  | 3.5  |
| 1   | A     | 660  | ASP  | 3.5  |
| 1   | H     | 763  | ILE  | 3.5  |
| 1   | E     | 916  | GLY  | 3.5  |
| 1   | A     | 664  | VAL  | 3.5  |
| 1   | C     | 1015 | GLU  | 3.5  |
| 1   | J     | 1024 | SER  | 3.5  |
| 1   | I     | 662  | ILE  | 3.5  |
| 1   | J     | 912  | VAL  | 3.5  |
| 1   | I     | 663  | LEU  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | G     | 783  | ARG  | 3.5  |
| 1   | L     | 761  | GLN  | 3.4  |
| 1   | C     | 1054 | ARG  | 3.4  |
| 1   | L     | 1019 | ASP  | 3.4  |
| 1   | C     | 913  | ASN  | 3.4  |
| 1   | F     | 917  | ILE  | 3.4  |
| 1   | G     | 912  | VAL  | 3.4  |
| 1   | F     | 1020 | ASN  | 3.4  |
| 1   | F     | 686  | GLU  | 3.4  |
| 1   | K     | 1056 | ARG  | 3.4  |
| 1   | F     | 912  | VAL  | 3.3  |
| 1   | L     | 764  | HIS  | 3.3  |
| 1   | F     | 663  | LEU  | 3.3  |
| 1   | J     | 1021 | ASP  | 3.3  |
| 1   | G     | 714  | LYS  | 3.3  |
| 1   | C     | 916  | GLY  | 3.3  |
| 1   | C     | 761  | GLN  | 3.3  |
| 1   | J     | 661  | LEU  | 3.2  |
| 1   | K     | 1054 | ARG  | 3.2  |
| 1   | G     | 665  | GLU  | 3.2  |
| 1   | J     | 1019 | ASP  | 3.2  |
| 1   | K     | 784  | ILE  | 3.2  |
| 1   | A     | 661  | LEU  | 3.2  |
| 1   | J     | 1020 | ASN  | 3.2  |
| 1   | L     | 1014 | LEU  | 3.2  |
| 1   | L     | 661  | LEU  | 3.1  |
| 1   | A     | 714  | LYS  | 3.1  |
| 1   | F     | 918  | GLU  | 3.1  |
| 1   | B     | 661  | LEU  | 3.1  |
| 1   | H     | 663  | LEU  | 3.1  |
| 1   | K     | 798  | SER  | 3.1  |
| 1   | C     | 876  | HIS  | 3.1  |
| 1   | B     | 663  | LEU  | 3.1  |
| 1   | D     | 764  | HIS  | 3.1  |
| 1   | J     | 1023 | GLU  | 3.1  |
| 1   | K     | 1057 | ILE  | 3.1  |
| 1   | D     | 763  | ILE  | 3.1  |
| 1   | K     | 662  | ILE  | 3.1  |
| 1   | B     | 1017 | GLU  | 3.1  |
| 1   | K     | 1017 | GLU  | 3.0  |
| 1   | K     | 1014 | LEU  | 3.0  |
| 1   | H     | 761  | GLN  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | D     | 1014 | LEU  | 3.0  |
| 1   | K     | 912  | VAL  | 3.0  |
| 1   | J     | 1012 | GLN  | 3.0  |
| 1   | F     | 946  | ASP  | 3.0  |
| 1   | H     | 1056 | ARG  | 2.9  |
| 1   | L     | 1063 | HIS  | 2.9  |
| 1   | E     | 876  | HIS  | 2.9  |
| 1   | L     | 797  | GLU  | 2.9  |
| 1   | J     | 946  | ASP  | 2.9  |
| 1   | H     | 1063 | HIS  | 2.9  |
| 1   | C     | 663  | LEU  | 2.9  |
| 1   | H     | 1014 | LEU  | 2.9  |
| 1   | H     | 912  | VAL  | 2.9  |
| 1   | K     | 876  | HIS  | 2.9  |
| 1   | F     | 1012 | GLN  | 2.8  |
| 1   | J     | 1015 | GLU  | 2.8  |
| 1   | E     | 946  | ASP  | 2.8  |
| 1   | J     | 916  | GLY  | 2.8  |
| 1   | H     | 795  | PRO  | 2.8  |
| 1   | A     | 783  | ARG  | 2.8  |
| 1   | D     | 695  | ILE  | 2.8  |
| 1   | H     | 661  | LEU  | 2.8  |
| 1   | L     | 763  | ILE  | 2.8  |
| 1   | K     | 707  | THR  | 2.8  |
| 1   | I     | 761  | GLN  | 2.8  |
| 1   | K     | 866  | PRO  | 2.8  |
| 1   | L     | 972  | PRO  | 2.8  |
| 1   | F     | 661  | LEU  | 2.8  |
| 1   | F     | 695  | ILE  | 2.8  |
| 1   | K     | 787  | ILE  | 2.8  |
| 1   | K     | 720  | PHE  | 2.8  |
| 1   | L     | 1020 | ASN  | 2.8  |
| 1   | E     | 662  | ILE  | 2.7  |
| 1   | G     | 763  | ILE  | 2.7  |
| 1   | J     | 686  | GLU  | 2.7  |
| 1   | K     | 1015 | GLU  | 2.7  |
| 1   | F     | 913  | ASN  | 2.7  |
| 1   | A     | 1015 | GLU  | 2.7  |
| 1   | E     | 917  | ILE  | 2.7  |
| 1   | J     | 663  | LEU  | 2.7  |
| 1   | K     | 704  | PHE  | 2.7  |
| 1   | K     | 701  | TYR  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | L     | 960  | TYR  | 2.7  |
| 1   | D     | 676  | ASN  | 2.7  |
| 1   | F     | 1057 | ILE  | 2.7  |
| 1   | G     | 946  | ASP  | 2.7  |
| 1   | J     | 1014 | LEU  | 2.7  |
| 1   | K     | 785  | ALA  | 2.6  |
| 1   | L     | 1058 | PHE  | 2.6  |
| 1   | K     | 792  | CYS  | 2.6  |
| 1   | F     | 1016 | ALA  | 2.6  |
| 1   | H     | 764  | HIS  | 2.6  |
| 1   | G     | 1014 | LEU  | 2.6  |
| 1   | L     | 912  | VAL  | 2.6  |
| 1   | A     | 784  | ILE  | 2.6  |
| 1   | B     | 764  | HIS  | 2.6  |
| 1   | L     | 963  | GLY  | 2.6  |
| 1   | A     | 663  | LEU  | 2.6  |
| 1   | G     | 676  | ASN  | 2.6  |
| 1   | A     | 798  | SER  | 2.6  |
| 1   | L     | 971  | LEU  | 2.6  |
| 1   | H     | 662  | ILE  | 2.6  |
| 1   | K     | 761  | GLN  | 2.6  |
| 1   | C     | 946  | ASP  | 2.6  |
| 1   | J     | 764  | HIS  | 2.5  |
| 1   | H     | 695  | ILE  | 2.5  |
| 1   | D     | 761  | GLN  | 2.5  |
| 1   | F     | 705  | GLN  | 2.5  |
| 1   | H     | 1059 | CYS  | 2.5  |
| 1   | G     | 876  | HIS  | 2.5  |
| 1   | K     | 763  | ILE  | 2.5  |
| 1   | L     | 662  | ILE  | 2.5  |
| 1   | C     | 1012 | GLN  | 2.5  |
| 1   | J     | 968  | ASN  | 2.5  |
| 1   | A     | 946  | ASP  | 2.5  |
| 1   | K     | 803  | SER  | 2.5  |
| 1   | K     | 795  | PRO  | 2.5  |
| 1   | I     | 916  | GLY  | 2.5  |
| 1   | B     | 761  | GLN  | 2.5  |
| 1   | F     | 761  | GLN  | 2.5  |
| 1   | K     | 805  | ASN  | 2.5  |
| 1   | J     | 662  | ILE  | 2.5  |
| 1   | B     | 1073 | LYS  | 2.5  |
| 1   | H     | 913  | ASN  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 917  | ILE  | 2.4  |
| 1   | I     | 763  | ILE  | 2.4  |
| 1   | J     | 917  | ILE  | 2.4  |
| 1   | G     | 1056 | ARG  | 2.4  |
| 1   | K     | 762  | GLN  | 2.4  |
| 1   | H     | 1057 | ILE  | 2.4  |
| 1   | G     | 1067 | GLU  | 2.4  |
| 1   | B     | 1014 | LEU  | 2.4  |
| 1   | H     | 864  | SER  | 2.4  |
| 1   | K     | 709  | LEU  | 2.4  |
| 1   | E     | 1071 | ILE  | 2.4  |
| 1   | F     | 763  | ILE  | 2.4  |
| 1   | K     | 877  | VAL  | 2.4  |
| 1   | B     | 1055 | ARG  | 2.4  |
| 1   | C     | 1056 | ARG  | 2.4  |
| 1   | G     | 1055 | ARG  | 2.4  |
| 1   | J     | 1000 | CYS  | 2.4  |
| 1   | K     | 1055 | ARG  | 2.4  |
| 1   | L     | 1073 | LYS  | 2.4  |
| 1   | H     | 797  | GLU  | 2.4  |
| 1   | K     | 797  | GLU  | 2.4  |
| 1   | K     | 815  | TYR  | 2.4  |
| 1   | B     | 915  | ASN  | 2.3  |
| 1   | D     | 1056 | ARG  | 2.3  |
| 1   | H     | 676  | ASN  | 2.3  |
| 1   | L     | 1059 | CYS  | 2.3  |
| 1   | B     | 797  | GLU  | 2.3  |
| 1   | G     | 1015 | GLU  | 2.3  |
| 1   | J     | 918  | GLU  | 2.3  |
| 1   | K     | 719  | GLN  | 2.3  |
| 1   | K     | 710  | LEU  | 2.3  |
| 1   | C     | 664  | VAL  | 2.3  |
| 1   | E     | 1015 | GLU  | 2.3  |
| 1   | B     | 1057 | ILE  | 2.3  |
| 1   | J     | 695  | ILE  | 2.3  |
| 1   | A     | 761  | GLN  | 2.3  |
| 1   | J     | 761  | GLN  | 2.3  |
| 1   | D     | 917  | ILE  | 2.3  |
| 1   | A     | 913  | ASN  | 2.3  |
| 1   | C     | 676  | ASN  | 2.3  |
| 1   | I     | 1015 | GLU  | 2.3  |
| 1   | I     | 876  | HIS  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | L     | 1055 | ARG  | 2.3  |
| 1   | G     | 916  | GLY  | 2.3  |
| 1   | L     | 985  | ALA  | 2.2  |
| 1   | C     | 917  | ILE  | 2.2  |
| 1   | D     | 933  | ILE  | 2.2  |
| 1   | B     | 1066 | THR  | 2.2  |
| 1   | L     | 798  | SER  | 2.2  |
| 1   | L     | 982  | PRO  | 2.2  |
| 1   | L     | 799  | TYR  | 2.2  |
| 1   | D     | 776  | ASP  | 2.2  |
| 1   | H     | 946  | ASP  | 2.2  |
| 1   | D     | 1073 | LYS  | 2.2  |
| 1   | B     | 686  | GLU  | 2.2  |
| 1   | E     | 663  | LEU  | 2.2  |
| 1   | A     | 1056 | ARG  | 2.2  |
| 1   | E     | 783  | ARG  | 2.2  |
| 1   | K     | 806  | ILE  | 2.2  |
| 1   | B     | 916  | GLY  | 2.2  |
| 1   | L     | 969  | LEU  | 2.2  |
| 1   | F     | 681  | ILE  | 2.2  |
| 1   | E     | 676  | ASN  | 2.2  |
| 1   | D     | 912  | VAL  | 2.2  |
| 1   | J     | 776  | ASP  | 2.2  |
| 1   | L     | 946  | ASP  | 2.2  |
| 1   | J     | 980  | SER  | 2.2  |
| 1   | L     | 976  | PHE  | 2.2  |
| 1   | E     | 665  | GLU  | 2.2  |
| 1   | D     | 1057 | ILE  | 2.1  |
| 1   | J     | 1071 | ILE  | 2.1  |
| 1   | F     | 676  | ASN  | 2.1  |
| 1   | G     | 913  | ASN  | 2.1  |
| 1   | J     | 676  | ASN  | 2.1  |
| 1   | J     | 1063 | HIS  | 2.1  |
| 1   | L     | 1069 | HIS  | 2.1  |
| 1   | L     | 834  | VAL  | 2.1  |
| 1   | L     | 977  | MET  | 2.1  |
| 1   | L     | 1072 | TRP  | 2.1  |
| 1   | L     | 984  | LEU  | 2.1  |
| 1   | K     | 932  | CYS  | 2.1  |
| 1   | F     | 1054 | ARG  | 2.1  |
| 1   | J     | 1018 | GLU  | 2.1  |
| 1   | F     | 915  | ASN  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | J     | 915  | ASN  | 2.1  |
| 1   | J     | 795  | PRO  | 2.1  |
| 1   | H     | 776  | ASP  | 2.1  |
| 1   | K     | 1058 | PHE  | 2.1  |
| 1   | H     | 1055 | ARG  | 2.1  |
| 1   | K     | 723  | TYR  | 2.1  |
| 1   | G     | 762  | GLN  | 2.1  |
| 1   | E     | 913  | ASN  | 2.1  |
| 1   | I     | 912  | VAL  | 2.1  |
| 1   | K     | 872  | LEU  | 2.1  |
| 1   | E     | 1055 | ARG  | 2.1  |
| 1   | C     | 665  | GLU  | 2.1  |
| 1   | E     | 1067 | GLU  | 2.1  |
| 1   | L     | 973  | ILE  | 2.1  |
| 1   | G     | 798  | SER  | 2.1  |
| 1   | F     | 764  | HIS  | 2.1  |
| 1   | L     | 837  | ASN  | 2.1  |
| 1   | E     | 1014 | LEU  | 2.1  |
| 1   | G     | 662  | ILE  | 2.1  |
| 1   | L     | 695  | ILE  | 2.1  |
| 1   | C     | 1059 | CYS  | 2.0  |
| 1   | E     | 912  | VAL  | 2.0  |
| 1   | F     | 1071 | ILE  | 2.0  |
| 1   | J     | 681  | ILE  | 2.0  |
| 1   | J     | 978  | ASP  | 2.0  |
| 1   | K     | 917  | ILE  | 2.0  |
| 1   | I     | 705  | GLN  | 2.0  |
| 1   | L     | 1066 | THR  | 2.0  |
| 1   | D     | 918  | GLU  | 2.0  |
| 1   | I     | 665  | GLU  | 2.0  |
| 1   | L     | 776  | ASP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | IBM  | L     | 2122 | 16/16 | 0.91 | 0.17 | 68,77,78,79                 | 0     |
| 3   | IBM  | H     | 2118 | 16/16 | 0.92 | 0.18 | 72,78,79,80                 | 0     |
| 3   | IBM  | B     | 2112 | 16/16 | 0.94 | 0.13 | 54,56,59,59                 | 0     |
| 3   | IBM  | D     | 2114 | 16/16 | 0.95 | 0.10 | 35,53,56,57                 | 0     |
| 3   | IBM  | G     | 2117 | 16/16 | 0.95 | 0.10 | 44,49,50,51                 | 0     |
| 3   | IBM  | C     | 2113 | 16/16 | 0.96 | 0.09 | 36,42,48,48                 | 0     |
| 3   | IBM  | A     | 2111 | 16/16 | 0.96 | 0.09 | 36,38,42,42                 | 0     |
| 3   | IBM  | K     | 2121 | 16/16 | 0.96 | 0.10 | 54,59,60,61                 | 0     |
| 3   | IBM  | E     | 2115 | 16/16 | 0.96 | 0.10 | 28,32,35,37                 | 0     |
| 3   | IBM  | J     | 2120 | 16/16 | 0.97 | 0.09 | 31,35,40,41                 | 0     |
| 3   | IBM  | F     | 2116 | 16/16 | 0.97 | 0.07 | 28,37,40,40                 | 0     |
| 3   | IBM  | I     | 2119 | 16/16 | 0.97 | 0.08 | 35,38,39,39                 | 0     |
| 2   | MG   | H     | 2138 | 1/1   | 0.98 | 0.04 | 32,32,32,32                 | 0     |
| 2   | MG   | C     | 2128 | 1/1   | 0.99 | 0.02 | 29,29,29,29                 | 0     |
| 2   | MG   | D     | 2130 | 1/1   | 0.99 | 0.03 | 22,22,22,22                 | 0     |
| 2   | MG   | E     | 2132 | 1/1   | 0.99 | 0.03 | 29,29,29,29                 | 0     |
| 2   | MG   | B     | 2126 | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |
| 2   | MG   | K     | 2144 | 1/1   | 0.99 | 0.03 | 40,40,40,40                 | 0     |
| 2   | MG   | L     | 2146 | 1/1   | 0.99 | 0.06 | 30,30,30,30                 | 0     |
| 2   | MG   | J     | 2142 | 1/1   | 1.00 | 0.03 | 39,39,39,39                 | 0     |
| 2   | MG   | K     | 2143 | 1/1   | 1.00 | 0.02 | 20,20,20,20                 | 0     |
| 2   | MG   | A     | 2124 | 1/1   | 1.00 | 0.01 | 41,41,41,41                 | 0     |
| 2   | MG   | L     | 2145 | 1/1   | 1.00 | 0.03 | 23,23,23,23                 | 0     |
| 2   | MG   | D     | 2129 | 1/1   | 1.00 | 0.04 | 9,9,9,9                     | 0     |
| 2   | MG   | B     | 2125 | 1/1   | 1.00 | 0.01 | 4,4,4,4                     | 0     |
| 2   | MG   | E     | 2131 | 1/1   | 1.00 | 0.03 | 1,1,1,1                     | 0     |
| 2   | MG   | A     | 2123 | 1/1   | 1.00 | 0.01 | 2,2,2,2                     | 0     |
| 2   | MG   | F     | 2133 | 1/1   | 1.00 | 0.03 | 1,1,1,1                     | 0     |
| 2   | MG   | F     | 2134 | 1/1   | 1.00 | 0.03 | 19,19,19,19                 | 0     |
| 2   | MG   | G     | 2135 | 1/1   | 1.00 | 0.00 | 1,1,1,1                     | 0     |
| 2   | MG   | G     | 2136 | 1/1   | 1.00 | 0.01 | 28,28,28,28                 | 0     |
| 2   | MG   | H     | 2137 | 1/1   | 1.00 | 0.02 | 12,12,12,12                 | 0     |
| 2   | MG   | C     | 2127 | 1/1   | 1.00 | 0.02 | 5,5,5,5                     | 0     |
| 2   | MG   | I     | 2139 | 1/1   | 1.00 | 0.03 | 5,5,5,5                     | 0     |
| 2   | MG   | I     | 2140 | 1/1   | 1.00 | 0.02 | 27,27,27,27                 | 0     |
| 2   | MG   | J     | 2141 | 1/1   | 1.00 | 0.02 | 6,6,6,6                     | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.